Optimization of the concentration changes in a chemostat with one species

Terence Bayen*†, Jérôme Harmand‡†, Matthieu Sebbah§

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Abstract

Our aim in this work is to study the problem of driving in minimal time a system describing a chemostat model to a target point. This problem finds applications typically in the case where the input substrate concentration changes yielding in a new steady state. One essential feature is that the system takes into account a recirculation of biomass effect. We depict an optimal synthesis and provide an optimal feedback control of the problem by using the Pontryagin Maximum Principle and geometric control theory for both Monod and Haldane kinetics.

Keywords. Chemostat Model, Optimal feedback, Geometric control, Pontryagin Maximum Principle.

1 Introduction

INTRO A CHANGER COMPLETEMENT SAUF LE PLAN A LA FIN Dire l'intérêt du α, Dire que quand $\alpha < 1$, alors techniquement le problème est plus difficile car une dissymétrie entre s et x. Dans les références, j'ai mis principalement des articles récents sur le contrôle optimal pour un réacteur fed-batch : pour montrer la différence avec notre système (réacteur continue)

The optimal control of bioprocesses has attracted a lot of attention over the last 50 years. The control of fedbatch processes has been extensively studied due to the fact such systems are used in industries producing high value molecules for agro-food or pharmaceutical industries. In this functioning mode, the output flow rate is equal to zero such that the volume of the reactor increases over the time until its maximum working volume has been reached. The way the reactor is filled, using the input flow rate, can be seen as a control. When the growth function is monotonic, the optimal control to minimize the time necessary to reach a given substrate concentration consists in filling in the process as fast as possible until the maximum working volume is reached and then wait until the concentration of substrate has reached the target. However, when the growth rate is non-monotonic (for instance for growth functions of Haldane type), there exists a singular arc and the optimal input profile to stay on it has been proposed in a number of situations. for instance, theoretical results have been obtained by Moreno (see [14]) for single reaction systems and for a large class of growth rate functions, and more recently in [2, 3, 9, 10]. In these papers dedicated to the optimal control of wastewater treatment plants, the objective was to reach in minimal time a given target (the value of the output substrate concentration should be typically below a prescribed value). This problem has been also investigated for multi-species systems and partially solved by Gajardo et al. (see [10]). Many others papers - rather practical but not only - are available on the optimal control of fed-batch systems for the maximization of products or of the biomass (see for instance the survey by Smets and Van Impe [20] or papers like [18] or [24] and references herein).

The chemostat is an apparatus which has been introduced in the fifties to continuously cultivate microorganisms. As for a bioprocess operated in a fedbatch mode, using the input flow rate allows the user to manipulate the growth rate of microbes (see [13, 16]). It presents the advantage of not being necessary to

*Institut de Mathématiques et Modélisation de Montpellier, UMR CNRS 5149, Université Montpellier, CC 051, 34095 Montpellier cedex 5, France. tbayen@math.univ-montp2.fr

†INRA-INRIA 'MODEMIC' team, INRIA Sophia-Antipolis Méditerranée.

‡LBE-INRA, Avenue des étangs 11100 Narbonne .jerome.harmand@supagro.inra.fr

§Univ. Tecnica Federico Santa Maria, Dep. Mat., Avda Espana 1680, Valparaiso, Chile. matthieu.sebbah@usm.cl

stock the incoming flow and to treat it online. Today, it is widely used in many domains at both laboratory or industrial scales and its optimization poses a number of both practical as well as theoretical problems [21].

Classically, the model of the chemostat is written as:

$$\left\{ \begin{array}{ll} \dot{x} & = \mu(s)x - Dx, \\ \dot{s} & = -\mu(s)x + u(s_{in} - s), \end{array} \right. \tag{1.1}$$

where x and s are the micro-organisms and the substrate concentrations, respectively, μ is the growth function of the species, $s_{in} > 0$ is the input substrate concentration and D is the dilution rate.

For this system with monotonic growth function (i.e. for a growth function of Monod type), D'Ans et al. have solved the problem of going from an arbitrary initial state to another one in minimal time (see [8]). Such a problem finds application typically in the case where the input substrate concentration changes yielding in a new steady state. Converging fast towards this new equilibrium may present some practical interest. In this case, D'Ans et al. established that the control is necessary bang-bang. From their pioneering work, many authors have investigated other optimization problems such as the maximization of biogas production for anaerobic processes (see e.g. [11, 22]). The problem of minimizing the time necessary to go from an arbitrary initial point to a final one in minimal time for non-monotonic growth rates in a continuous bioreactor has been investigated in [?]. However, in modern biotechnology, any continuous reactor is equipped with a biomass retention system allowing the liquid fraction to leave the reactor while keeping an important quantity of biomass in the system through the presence of either supports for microorganisms (that may be fixed or mobile) or a separator followed by a recirculation loop for the biomass to return into the reactor medium. In such a case, the substrate (liquid fraction) and the biomass (solid fraction) are not submitted to the same dilution rate and it is said that 'the hydraulic and the solid retention times are decoupled'. To model simply such a decoupling, a term α may be introduced in the dynamic of x and the model becomes:

$$\left\{ \begin{array}{ll} \dot{x} & = \mu(s)x - \alpha ux, \\ \dot{s} & = -\mu(s)x + u(s_{in} - s), \end{array} \right. \tag{1.2}$$

where D, the actuator has been rewritten as u.

If $\alpha = 1$, the model is exactly the chemostat model while if $\alpha = 0$ no biomass is removed from the reactor. Depending on the efficiency of the separator, one has $0 \leq \alpha \leq 1$.

In this paper, we consider the problem of minimizing the time necessary to go from one state to another for this modified chemostat model.

The paper is organized as follows. In section 2, we state the optimal control problem, and we apply the Pontryagin Maximum on the optimal control problem. We also provide properties of the *switching function* that are crucial in sections 3 and 4. Section 3 provides an optimal feedback control for Haldane kinetics when $\alpha = 1$ (Proposition 3.1 and 3.2 are our main results), and section 4 discusses the case $\alpha < 1$.

2 Preliminaries

2.1 Statement of the problem

We consider the system

$$\left\{ \begin{array}{ll} \dot{x} & = \mu(s)x - \alpha ux, \\ \dot{s} & = -\mu(s)x + u(s_{in} - s), \end{array} \right. \tag{2.1}$$

describing a chemostat model with one species and one substrate. Here x, resp. s is the micro-organisms concentration, resp. substrate concentration, μ is the growth function of the species, $s_{in} > 0$ is the input substrate concentration, $\alpha \in [0, 1]$ is a coefficient for separating the biomass (or recirculation parameter), and u is the dilution rate which is the control variable. The admissible control set is defined as:

$$\mathcal{U} := \{u : [0, \infty) \to [0, u_{max}] \; ; \; u \text{ meas.}\}. \tag{2.2}$$

Given $u \in \mathcal{U}$ and an initial condition $(x_0, s_0) \in \mathbb{R}_+^* \times \mathbb{R}_+$, we denote by $(x_u(\cdot), s_u(\cdot))$ the unique solution of (2.1) defined over $[0, \infty)$ such that $x_u(0) = x_0$ and $s_u(0) = s_0$ at time 0. It is clear that the set $E := \mathbb{R}_+^* \times [0, s_{in}]$ is invariant by the dynamics (2.1), therefore we can consider initial conditions in E.

Throughout this paper, we are interested in the following optimal control problem. Given a target point $(\bar{x}, \bar{s}) \in E$, our aim is to steer (2.1) in minimal time from $(x_0, s_0) \in E$ to $(\bar{x}, \bar{s})$, that is:

$$v(x_0, s_0) := \inf_{u \in \mathcal{U}} t(u) \ \text{ s.t. } \ x_u(t(u)) = \bar{x} \quad \text{and} \quad s_u(t(u)) = \bar{s}, \tag{2.3}$$

where $t(u)$ is the first time such that $x_u(t(u)) = \bar{x}$ and $s_u(t(u)) = \bar{s}$. If the *value function* $v(x_0, s_0)$ is infinite, the problem has no solution, i.e. the target point is not reachable from (x_0, s_0). The determination of the *controllability set*, i.e. the set of points that can reach the target in finite horizon, is part of the analysis and will be discussed precisely in sections 3 and 4. Without any loss of generality, we suppose that $u_{max} = 1$ and we consider the following hypotheses :

(H1) The function μ satisfies $\mu(0) = 0$, is bounded, non-negative and of class C^2.

(H2) For any $s \in [0, s_{in}]$, one has $\mu(s) < \alpha$.

Remark 2.1. *Assumption (H2) amounts to saying that the washout is possible and that the dilution rate can be chosen large enough in order to compete the growth of micro-organisms.*

It will be more convenient to study (2.4) in the variables (s, M) where $M := x + s$ is the total mass of the system. By changing x into M, (2.1) can be equivalently written

$$\left\{ \begin{array}{ll} \dot{s} & = -\mu(s)(M - s) + u(s_{in} - s), \\ \dot{M} & = u(s_{in} - s - \alpha(M - s)). \end{array} \right. \tag{2.4}$$

As $x > 0$, we consider initial conditions for (2.4) in the set F defined by

$$F := \{(s, M) \in \mathbb{R}_+ \times \mathbb{R}_+ \ ; \ 0 \le s < M \text{ and } s \le s_{in}\}, \tag{2.5}$$

that is clearly invariant by (2.4). Similarly as above, we denote by $(s_u(\cdot), M_u(\cdot))$ the unique solution of (2.4) associated to a control $u \in \mathcal{U}$ such that $s_u(0) = s_0$ and $M_u(0) = x_0 + s_0$ at time 0. Moreover, we set $\bar{M} := \bar{x} + \bar{s}$.

It will be convenient to consider the solutions of (2.4) backward in time starting at $(\bar{s}, \bar{M})$ at time 0. More precisely, for $u = i$ ($i = 0$ or $i = 1$), let $z^i(\cdot) = (s^i(\cdot), M^i(\cdot))$ the unique solution of (2.4) defined over $[0, t^i)$ backward in time with $u = i$ and such that $z^i(0) = (\bar{s}, \bar{M})$. Without any loss of generality, we suppose that $t^i \in [0, \infty)$ is the first exit time of z^i of the set F, i.e. $z^i(t^i) \in \partial F$ (where ∂F is the boundary of F). We call Γ_i, $i = 0, 1$ the graph of $z_i(\cdot)$ for $t \in [0, t_i)$. We note that $\Gamma_0 \cup \Gamma_1$ partitions F into two subsets A_α and A'_α. More precisely, we take for A_α the unique component containing $\Gamma_0 \cup \Gamma_1$ and points in F below Γ_0.

Finally, if B is any given non-empty subset of $\mathbb{R}^2$, we denote by $\mathrm{Int}(B)$ its interior.

2.2 Pontryagin's Principle

In this section, we derive optimality conditions for problem (2.3) (in variables (s, M), see (2.4)). Notice that if (H1) holds true and if (x_0, s_0) is in the controllability set, then the existence of an optimal control follows by standard arguments (in fact, (2.4) is linear w.r.t. u and the admissible control set is compact). We are then in position to apply Pontryagin's Principle on (2.4) which provides necessary conditions on optimal strategies ([12, 15]).

Let $H : \mathbb{R}^2 \times \mathbb{R}^2 \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ the Hamiltonian associated to (2.4) and defined by:

$$H = H(s, M, \lambda_s, \lambda_M, \lambda_0, u) := -\lambda_s \mu(s)(M - s) + \lambda_0 + u[(\lambda_s + \lambda_M)(s_{in} - s) - \alpha\lambda_M(M - s)].$$

Let $u \in \mathcal{U}$ an optimal control of (2.3) such that the associated trajectory steers (s_0, M_0) to $(\bar{s}, \bar{M})$ in minimal time. For convenience, we write this trajectory $z(\cdot) := (s(\cdot), M(\cdot))$. According to Pontryagin's Principle, the following conditions hold true :

- There exists $t_f \ge 0$, $\lambda_0 \le 0$ and an absolutely continuous function $\lambda = (\lambda_s, \lambda_M) : [0, t_f] \to \mathbb{R}^2$ satisfying a.e. the adjoint equation $\dot{\lambda}(t) = -\frac{\partial H}{\partial z}(z(t), \lambda(t), \lambda_0, u(t))$, that is:

$$\left\{ \begin{array}{ll} \dot{\lambda}_s & = \lambda_s(\mu'(s)(M - s) - \mu(s) + u) + (1 - \alpha)\lambda_M u, \\ \dot{\lambda}_M & = \lambda_s \mu(s) + \alpha\lambda_M u. \end{array} \right. \tag{2.6}$$

- The pair $(\lambda_0, \lambda(\cdot))$ is non-trivial i.e. $(\lambda_0, \lambda(\cdot)) \neq 0$.
- The following maximization condition holds true :

$$u(t) \in \text{argmax}_{v\in[0,1]} H(s(t), M(t), \lambda_s(t), \lambda_M(t), \lambda_0, v) \ \text{ a.e. } t \in [0, t_f]. \tag{2.7}$$

We call *extremal trajectory* a triple $(z(\cdot), \lambda(\cdot), u(\cdot))$ satisfying (2.4)-(2.6)-(2.7). If $\lambda_0 = 0$, then we say that the extremal is *abnormal* whereas if $\lambda_0 < 0$, then we say that it is a *normal extremal.* In the latter, we may suppose that $\lambda_0 = -1$. Along any extremal trajectory, one has $H = 0$ (using that (2.4) is autonomous and that the terminal time is free). The *switching function* ϕ is defined by

$$\phi := (\lambda_s + \lambda_M)(s_{in} - s) - \alpha\lambda_M(M - s). \tag{2.8}$$

The maximization condition (2.7) can be then expressed as follows :

$$\begin{cases} \phi(t) > 0 & \Rightarrow u(t) = +1, \\ \phi(t) < 0 & \Rightarrow u(t) = -1, \\ \phi(t) = 0 & \Rightarrow u(t) \in [-1, 1]. \end{cases} \tag{2.9}$$

Moreover, if we differentiate ϕ w.r.t. t, a straightforward computation shows that we have :

$$\dot{\phi} = (M - s)[\lambda_s\mu'(s)(s_{in} - s) + (1 - \alpha)(\lambda_M + \lambda_s)\mu(s)]. \tag{2.10}$$

2.3 Frame curves and frame points

An important feature in the study of (2.3) is the presence of particular curves in the state space that are called *frame curves.* These curves play an important role for obtaining an optimal feedback control. In our context, they are of three types :

- The *colinearity curve* Δ_0^α is defined as the set of points where the dimension of the vector space spanned by (2.4) is equal to 1.
- The *singular locus* Δ_{SA}^α is the set of points where the switching function vanishes on a time interval (a more precise definition can be found in [7]).
- A *switching curve* $\mathcal{C}$ is a locus in the state space where the control u has a switching point i.e. the control switches from 1 to 0 or from 0 to 1 at this point (the corresponding instant of switching is called *switching time*).

An important property of Δ_0^α is that any switching point of an abnormal trajectory necessarily occurs on Δ_0^α (see [7]). In our setting, we can compute easily Δ_0^α and Δ_{SA}^α as follows whereas switching curves are in general more delicate to characterize by an implicit equation (in particular such curves are usually target dependent). If $f_0^\alpha : \mathbb{R}^2 \to \mathbb{R}$ and $f_{SA}^\alpha : \mathbb{R}^2 \to \mathbb{R}$ are the functions defined by :

$$\begin{array}{ll} f_0^\alpha(s, M) & := -\mu(s)(M - s)(s_{in} - s - \alpha(M - s)), \\ f_{SA}^\alpha(s, M) & := (M - s)[\alpha(M - s)((1 - \alpha)\mu(s) + \mu'(s)(s_{in} - s)) - (s_{in} - s)^2\mu'(s)], \end{array} \tag{2.11}$$

then, a straightforward computation shows that:

$$\Delta_0^\alpha = \{(s, M) \in F \ ; \ f_0^\alpha(s, M) = 0\} \ \text{ and } \ \Delta_{SA}^\alpha = \{(s, M) \in F \ ; \ f_{SA}^\alpha(s, M) = 0\}. \tag{2.12}$$

The next proposition provides a linear ODE satisfied by the switching function and will be crucial in the optimal synthesis of the problem (see sections 3 and 4).

Proposition 2.1. *Let $(z(\cdot), \lambda(\cdot), u(\cdot))$ a normal extremal trajectory. Then, the following properties hold true.*

(i) There exists a function $g_\alpha : \mathbb{R} \times (F\backslash\Delta_0^\alpha) \to \mathbb{R}$, $(u, s, M) \longmapsto g_\alpha(u, s, M)$ such that one has:

$$\dot{\phi}(t) = g_\alpha(u(t), s(t), M(t))\phi(t) - \frac{f_{SA}^\alpha(s(t), M(t))}{f_0^\alpha(s(t), M(t))} \ \text{ a.e. } t \in [0, T], \tag{2.13}$$

provided that $(s(t), M(t)) \notin \Delta_0^\alpha$.

(ii) If $(z(\cdot), \lambda(\cdot), u(\cdot))$ is optimal, then it cannot have a switching point from $u = 1$ to $u = 0$, resp. from $u = 0$ to $u = 1$ at a time t such that $\frac{f_{SA}^{\alpha}(s(t),M(t))}{f_0^{\alpha}(s(t),M(t))} > 0$, resp. $\frac{f_{SA}^{\alpha}(s(t),M(t))}{f_0^{\alpha}(s(t),M(t))} < 0$.

Proof. To prove (i), notice that $\lambda_s = \frac{u\phi - 1}{\mu(s)(M-s)}$ using that $H = 0$. From the expression of ϕ, we get:

$$\lambda_M = \frac{\phi - \lambda_s(s_{in} - s)}{s_{in} - s - \alpha(M - s)}. \tag{2.14}$$

If we replace λ_s in (2.14), we obtain $\lambda_M = \frac{\mu(s)(M-s)\phi - (u\phi-1)(s_{in}-s)}{\mu(s)(M-s)(s_{in}-s-\alpha(M-s))}$. Now, if we substitute in (2.10) this expression of λ_M and the one for λ_s, we obtain (2.13) with :

$$g_\alpha(u, s, M) := \frac{\mu'(s)(s_{in} - s)}{\mu(s)} u + (1 - \alpha)(M - s) \frac{\mu(s) - \alpha u}{s_{in} - s - \alpha(M - s)}$$

To prove (ii), notice that at a switching time t from $u = +1$ to $u = -1$, we necessarily have $\phi(t) = 0$ and $\dot{\phi}(t) \leq 0$. Hence, we obtain that $\frac{f_{SA}^{\alpha}(s(t),M(t))}{f_0^{\alpha}(s(t),M(t))} \leq 0$ whenever $(s(t), M(t)) \notin \Delta_0^{\alpha}$. At a switching time t from $u = 0$ to $u = 1$, a similar reasoning shows the second part of (ii). □

Frame points are the points at the intersection of two frame curves. The determination of such points is also crucial for the optimal synthesis. A frame point of type (C, S) is by definition a point at the intersection of a switching curve and the singular locus. More precisely, (C, S) points are of two types : either the singular arc emanates from such a point (in that case it is a $(C, S)_1$ point), or the singular arc stops to be optimal at this point (in that case it is a $(C, S)_2$ point). A *steady state singular point* is a frame point at the intersection of Δ_0^{α} and Δ_{SA}^{α} (see [4]).

3 Optimal synthesis when $\alpha = 1$

In this section, we study (2.3) in the particular case where $\alpha = 1$ which corresponds to the case where no biomass filtration is considered in the chemostat model (2.1). The quantity M then satisfies the ODE

$$\dot{M} = u(s_{in} - M). \tag{3.1}$$

Therefore, we can assume that either $M < s_{in}$ (case I) or $M > s_{in}$ (case II) depending on the choice of the $\bar{M}$ w.r.t. s_{in}. Indeed, for $M = s_{in}$, the optimal control problem is one-dimensional and is straightforward.

We suppose in this section that μ satisfies the following assumption :

(H'1) The function μ satisfies $\mu(0) = 0$, is bounded, non-negative, of class C^2 and has a unique maximum $s^\star \in (0, s_{in})$.

Remark 3.1. (H′1) *is verified in the case of Haldane kinetic function $\mu(s) = \frac{\mu_{max} s}{k_s + s + \frac{s^2}{k_i}}$ with $k_i > 0$, $k_s > 0$.*

It is straightforward to check that $\Delta_0^1 \cap F = \emptyset$, and so the only possible abnormal trajectories are the solutions of (2.4) with $u = 0$ and $u = 1$ that reach the target point $(\bar{s}, \bar{M})$. Hence, we can assume that $\lambda_0 = -1$, so (2.13) becomes

$$\dot{\phi} = \frac{(s_{in} - s)\mu'(s)}{\mu(s)} u\phi - \frac{(s_{in} - s)\mu'(s)}{\mu(s)}, \tag{3.2}$$

which in particular implies that the singular locus is the line $\Delta_{SA}^1 = \{s^\star\} \times (s^\star, +\infty)$. The *singular control* is defined as the control u_s such that $(s_{u_s}(t), M_{u_s}(t)) \in \Delta_{SA}^1$ and is given by :

$$u_s(M) := \mu(s^\star) \frac{M - s^\star}{s_{in} - s^\star}. \tag{3.3}$$

Furthermore, M satisfies the following ODE along Δ_{SA}^1 :

$$\dot{M}_{|u=u_s(M)} = \mu(s^\star) \frac{(M - s^\star)(s_{in} - M)}{s_{in} - s^\star}.$$

3.1 Study of case I : $\bar{M} < s_{in}$

In that case, we can consider initial conditions $(s, M) \in F$ satisfying $M < s_{in}$. The system under consideration satisfies the following properties :

- We have $\dot{M} \geq 0$ for any control u (see (3.1)).
- We have $\dot{s}_{|u=1} > 0$ (in fact, $M < s_{in}$ and (H2) imply the inequality $\mu(s) < 1 < \frac{s_{in}-s}{M-s}$).
- The singular locus Δ^1_{SA} is such that $\Delta^1_{SA} = \{s^\star\} \times (s^\star, s_{in})$.
- The singular control u_s is admissible, i.e. $u_s(M) \in [0,1]$ for any $M \in (s^\star, s_{in})$ and $\dot{M} > 0$ along Δ^1_{SA}.

The previous considerations show that for $i = 0, 1$ the trajectory $z^i(\cdot)$ is the graph of a C^1-mapping $s \longmapsto M := \varphi_i(s)$ in the plane (s, M). Therefore, A_1 can be written as:

$$A_1 := \{(s, M) \in F \ ; \ M \leq \min(\varphi_0(s), \varphi_1(s))\}. \tag{3.4}$$

Lemma 3.1. *Suppose that $\bar{M} < s_{in}$. Then, the controllability set for* (2.3) *is* A_1.

Proof. According to Pontryagin's Principle, an extremal trajectory contains three types of arcs : $u = 1$, $u = 0$ or $u = u_s$ (singular arc). Let us consider an extremal trajectory starting in $F \backslash A_1$. If the trajectory is singular, then it cannot intersect the boundary of A_1 as we have $\dot{M} > 0$ along the singular arc Δ^1_{SA}. Notice also that an arc $u = 1$ cannot intersect Γ_1 (by Cauchy-Lipschitz Theorem) nor Γ_0 as $M_{|u=1}(\cdot)$ is increasing. Similarly an arc $u = 0$ cannot intersect Γ_0 (by Cauchy-Lipschitz Theorem) nor Γ_1 (as we have $\dot{s} < 0$ along $u = 0$). The result follows. □

We deduce the following optimality result.

Theorem 3.1. *If* (H′1) *and* (H2) *hold true and $\bar{M} < s_{in}$, an optimal feedback policy in* $\mathrm{Int}(A_1)$ *is given by :*

$$\begin{cases} u^\star[s, M] & = 0 & \text{if } s > s^\star, \\ u^\star[s, M] & = 1 & \text{if } s < s^\star, \\ u^\star[s, M] & = u_s(M) & \text{if } s = s^\star. \end{cases} \tag{3.5}$$

Proof. The proof follows from Proposition 2.1 (ii). Suppose that $(s_0, M_0) \in A_1 \backslash (\Gamma_0 \cup \Gamma_1)$. Then, if $s_0 < s^\star$, we must have $u = 1$ until reaching either $s = s^\star$ or Γ_0. Otherwise, we would have $u = 0$ by Pontryagin's Principle, and the trajectory would necessarily have a switching point at a time $t_0 > 0$ (if not, then it cannot reach the target). At this time t_0, we have $\dot{\phi}(t_0) \geq 0$ in contradiction with $\dot{\phi}(t_0) = -\frac{(s_{in}-s(t_0))\mu'(s(t_0))}{\mu(s(t_0))} < 0$. Hence, we have $u = 1$ until reaching either the singular arc or Γ_0. Similar arguments show that if s_0 is such that $s_0 > s^\star$, then we have $u = 0$ until reaching either $s = s^\star$ or Γ_1. We deduce that for any point $(s_0, M_0) \in A_1 \backslash (\Gamma_0 \cup \Gamma_1)$, the optimal control satisfies $u = 1$ if $s_0 < s^\star$ and $u = 0$ if $s_0 > s^\star$. Finally, the previous argumentation shows also that if $s_0 = s^\star$ and $(s_0, M_0) \in A_1 \backslash (\Gamma_0 \cup \Gamma_1)$, then an optimal trajectory does not leave the singular arc either with $u = 0$ or $u = 1$. Therefore singular trajectories are optimal until reaching $\Gamma_0 \cup \Gamma_1$. □

The optimal synthesis provided by Theorem 3.1 is depicted on Fig 1.

Remark 3.2. *(i) If $\bar{s} < s^\star$, then a singular trajectory will reach $\bar{M}$, and then will satisfy $u = 0$ until reaching the target (see Fig. 1). If $\bar{s} > s^\star$, then a singular trajectory will reach Γ_1, and then will satisfy $u = 1$ until reaching the target (see Fig. 1).*
(ii) When $s^\star > s_{in}$, the previous considerations show that for Monod kinetic function the feedback in $\mathrm{Int}(A_1)$

$$\begin{cases} u_m[s, M] & = 1 & \text{if } (s, M) \in A_1 \backslash \Gamma_0, \\ u_m[s, M] & = 0 & \text{if } (s, M) \in \Gamma_0, \end{cases} \tag{3.6}$$

is optimal (see [8]).

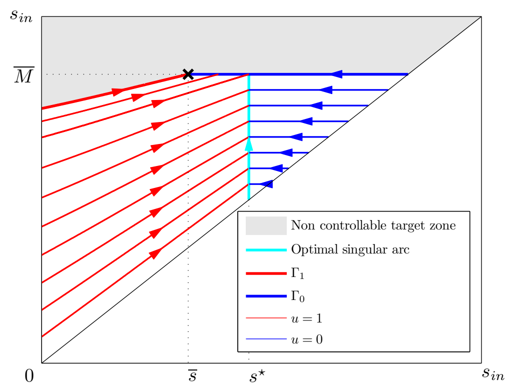

Figure 1: Optimal synthesis for $\alpha = 1$ and $\bar{M} < s_{in}$ (case I). *Picture left* : the target point is such that $\bar{s} < s^{\star}$ (the singular arc Δ^1_{SA} intersects Γ_0). *Picture right* : the target point is such that $\bar{s} > s^{\star}$ (the singular arc Δ^1_{SA} intersects Γ_1.

3.2 Study of case II : $\bar{M} > s_{in}$

In that case, we can consider initial conditions $(s, M) \in F$ such that $M > s_{in}$. The system under consideration satisfies the following properties :

- From (3.1), we have $\dot{M} \leq 0$ for any control u.
- The singular control u_s is admissible provided that $M \in (s_{in}, M_{sat}]$ where $u_s(M_{sat}) = 1$, that is :

$$M_{sat} := s_{in} + (s_{in} - s^{\star}) \left[\frac{1}{\mu(s^{\star})} - 1 \right]. \tag{3.7}$$

- The singular locus Δ^1_{SA} then becomes $\Delta^1_{SA} = \{s^{\star}\} \times (s_{in}, M_{sat})$.

Notice that $\frac{ds}{dt}_{|u=1}$ is not of constant sign along $u = 1$ as in case I (see Fig. 2 for the plot of solutions of (2.4) with $u = 1$). The previous considerations show that the trajectory $z^1(\cdot)$ is the graph of a C^1-mapping

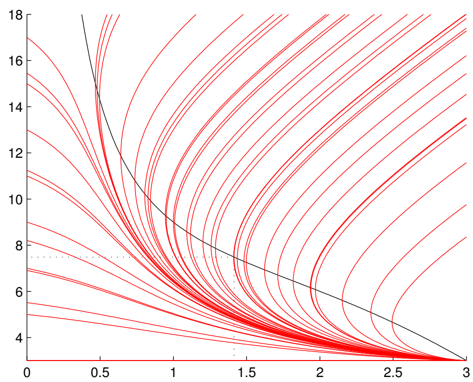

Figure 2: Solutions of (2.4) for the control $u = 1$ and different initial conditions (s_0, M_0) with $M_0 > s_{in}$. The black curve is the set of points where the tangent to this trajectory is vertical.

$M \longmapsto s := \psi_1(M)$ defined over $[\bar{M}, +\infty)$ in the plane (s, M) (indeed we have $\dot{M} < 0$ along $u = 1$). Therefore, the set A'_1 can be written:

$$A'_1 := \{(s, M) \in F \ ; \ M \geq \bar{M} \text{ and } \max(0, \psi_1(M)) \leq s \leq s_{in}\}.$$

Lemma 3.2. *Suppose that $\bar{M} > s_{in}$. Then, the controllability set for* (2.3) *is A_1'.*

Proof. The proof is similar to the proof of Lemma 3.1. $\square$

3.2.1 Switching curve and optimal synthesis

Whereas in the case $M < s_{in}$, the singular arc is always admissible, we have now a *saturation phenomena* for the singular control, that is the singular arc is non-admissible when $M > M_{sat}$ (see (3.7)). This will imply the existence of a switching curve $\mathcal{C}$. We now provide a description of this locus.

Lemma 3.3. *Let $\tilde{M} := \max(\bar{M}, M_{sat})$. Then, there exists $M_e \in (\tilde{M}, +\infty]$ and a function $s_c : [\tilde{M}, M_e] \rightarrow \mathbb{R}_+$ $M \longmapsto s_c(M)$ satisfying the following properties :*

(1) If $M_e < +\infty$, then one has $s_c(M_e) = s_{in}$. Moreover, one has $s_c(\tilde{M}) = s^\star$ and $s_c(M) \in (s^\star, s_{in})$ for any $M \in (\tilde{M}, M_e)$.

(2) For any $M \in (\tilde{M}, M_e)$, there exists exactly one point $s_c(M)$ such that an optimal control u satisfies $u = 0$ for $s > s_c(M)$ and $u = 1$ for $s^\star < s < s_c(M)$.

Proof. For brevity, we have postponed the proof of this lemma in the appendix. $\square$

The switching curve $\mathcal{C}$ is then defined as

$$\mathcal{C} := \{(s_c(M), M) \ ; \ M \in [M^\star, M_e]\}.$$

We obtain the following optimality result.

Theorem 3.2. *Suppose that* (H′1) *and* (H2) *hold true, that $\bar{M} > s_{in}$, and let $h(M) := \max(s^\star, s_c(M))$ for $M \in [\bar{M}, M_e]$. Then, an optimal feedback policy in* $\mathrm{Int}(A_1')$ *is given by :*

$$\left\{ \begin{array}{lll} u^\star[s, M] & = u_s(M) & \text{if } s = s^\star \text{ and } M < M_{sat}, \\ u^\star[s, M] & = 1 & \text{if } s < h(M) \text{ and } M > \bar{M}, \\ u^\star[s, M] & = 0 & \text{elsewhere} \end{array} \right. \tag{3.8}$$

Proof. The proof is straightforward using the previous lemma and following the proof of Theorem 3.1 to exclude extremal trajectories that are not optimal. $\square$

The optimal synthesis provided by Theorem 3.2 is depicted on Fig. 3, Fig. 4 and Fig. 5 in different cases explained below.

3.2.2 Numerical simulations

First, we summarize the numerical compution of the curve $\mathcal{C}$ defined by $M \longmapsto s_c(M)$. We consider the system (2.4)-(3.2) with $u = 1$ backward in time :

$$\left\{ \begin{array}{lll} \frac{ds}{dt} & = & \mu(s)(M - s) - s_{in} - s, \\ \frac{dM}{dt} & = & -(s_{in} - M), \\ \frac{d\phi}{dt} & = & -\frac{(s_{in}-s)\mu'(s)}{\mu(s)}\phi - \frac{(s_{in}-s)\mu'(s)}{\mu(s)}, \end{array} \right. \tag{3.9}$$

with initial conditions $(s_0, M_0, 0)$ such that $(s_0, M_0) \in \Gamma_0 \cup \Delta^1_{SA}$. We know that an optimal trajectory that reaches at time t either Δ_{SA} or $\Gamma_0 \backslash \{(\bar{s}, \bar{M})\}$ is such that $\phi(t) = 0$. Hence, for a given point $(s_0, M_0) \in \Gamma_0 \cup \Delta^1_{SA}$, we integrate (3.9) from $(s_0, M_0, 0)$ at $t = 0$ until the first time $t_c > 0$ such that $\phi(t_c) = 0$ and $(s(t_c), M(t_c)) \in F$. Thanks to Lemma 3.3, we know that there exist points of $\Gamma_0 \cup \Delta^1_{SA}$ such that such a switching time t_c exists. We repeat this procedure for points $(s_0, M_0) \in \Gamma_0 \cup \Delta^1_{SA}$ until finding completely $M \longmapsto s_c(M)$.

To highlight Theorem 3.2, we have considered the following cases depending on the choice of the target point $(\bar{s}, \bar{M})$ w.r.t. the singular arc and the value of M_{sat}.

- **Case II a** (see Fig. 3) : $\bar{M} < M_{sat}$ and $\bar{s} < s^\star$. The two figures correspond to the case where $z_1(\cdot)$ leaves F either through $s = 0$ or $s = s_{in}$.

- **Case II b** (see Fig. 4) : $\bar{M} < M_{sat}$ and $\bar{s} > s^{\star}$. The two figures correspond to the case where $z_1(\cdot)$ leaves F either through $s = 0$ or $s = s_{in}$.
- **Case II c** (see Fig. 5) : $\bar{M} > M_{sat}$ and $\bar{s} < s^{\star}$. The two figures correspond to the case where $z_1(\cdot)$ leaves F either through $s = 0$ or $s = s_{in}$.
- **Case II d** (see Fig. 6) : $\bar{M} > M_{sat}$ and $\bar{s} > s^{\star}$. The two figures correspond to the case where $z_1(\cdot)$ leaves F either through $s = 0$ or $s = s_{in}$.

In Fig. 3, 4, 5 and 6, the switching curve $\mathcal{C}$ can be decomposed as $\mathcal{C} = \Delta_1 \cup \Delta_2$. The curve Δ_1 (in purple), resp. Δ_2 (in green) corresponds to initial conditions for system (3.9) on Δ^1_{SA}, resp. on Γ_0.

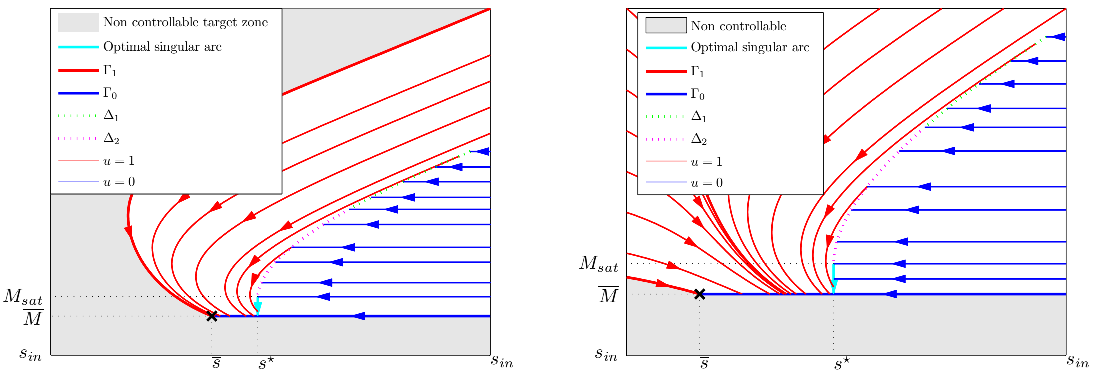

Figure 3: Case II a. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0.

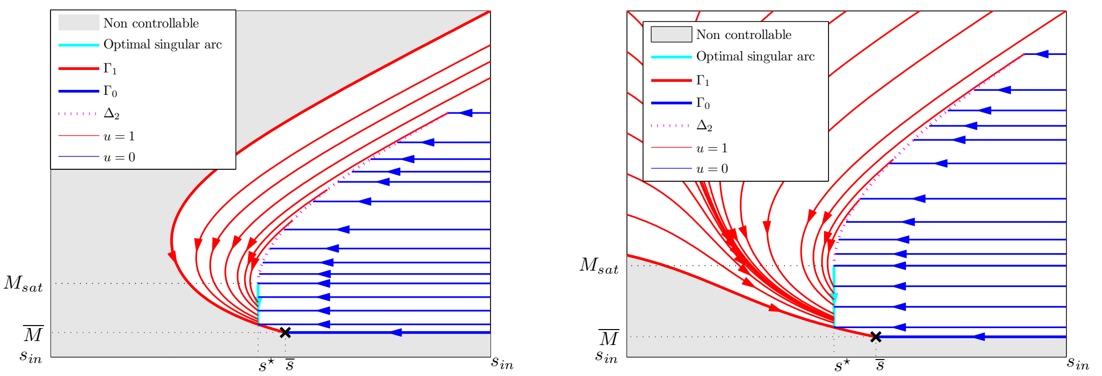

Figure 4: Case II b. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0.

3.2.3 Additional properties of the switching curve $\mathcal{C}$

The aim of this section is to provide additional properties on the switching curve $\mathcal{C}$ depending on the behavior of the curve Γ_1. First, we analyze the case where Γ_1 exits F through $s = s_{in}$. We can then show that $\mathcal{C}$ leaves F at a value $(s_c(M_e), M_e)$ such that $s_c(M_e) = s_{in}$ as shown in the next proposition.

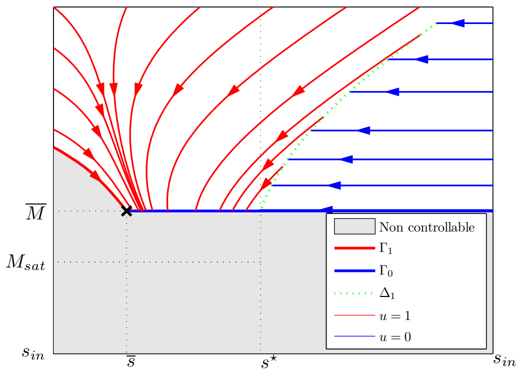

Figure 5: Case II c. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0.

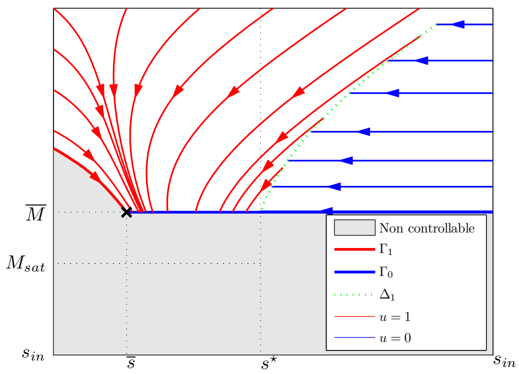

Figure 6: Case II d. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0).

Proposition 3.1. *Suppose that Γ_1 intersects the boundary of F at some point (s_{in}, M_{out}) with $M_{out} > \tilde{M}$. Then, we have $M_e \leq M_{out}$ and $s_c(M_e) = s_{in}$.*

Proof. Clearly, $\mathcal{C}$ cannot intersect Γ_1 before reaching $s = s_{in}$ as we would have a contradiction with the controllability set A'_1. Suppose now that $\mathcal{C}$ stops at some point $(s_c(M_e), M_e)$ such that $\psi_1(M_e) < s_c(M_e) < s_{in}$. Then, we consider the unique solution of (2.4) backward in time from $(s_c(M_e), M_e)$, and we call $\tilde{\Gamma}$ the restriction of its graph in F. Now, take an initial condition $(s_0, M_0) \in F$ below $\tilde{\Gamma}$ and such that $s_c(M_e) < s_0 < s_{in}$, $M_0 > M_e$. Then, if we have $u = 1$ at time $t = 0$, we obtain a contradiction as the corresponding trajectory reaches Γ_0 at a point $s > s^\star$ (see Proposition 2.1 (ii)). Thus, we must have $u = 0$ until reaching $s = s^\star$ as no switching point occurs. We have again a contradiction by Proposition 2.1 (ii). This shows that $s_c(M_e) = s_{in}$ and that $M_e \leq M_{out}$. □

Remark 3.3. *We can prove that $\mathcal{C}$ is continuous by showing first the continuity of t_c w.r.t. initial conditions (this point follows by considering t_c as the first entry time into the target $\phi \geq 0$ and using regularity properties of the value function [1]). The continuity of $\mathcal{C}$ then follows from the continuity of solutions of an ODE w.r.t. initial conditions. For brevity, we have not detailed this point.*

When Γ_1 exits F through $s = 0$, the controllability set A_2 is unbounded, therefore the proof of Proposition 3.1 cannot be applied in this case. Nevertheless, we believe that $\mathcal{C}$ exits F at some point $M_e < +\infty$ as in the previous case. Notice that initial conditions such that $M \gg s_{in}$ are not interesting for a practionner. Observe also that the time of an arc $u = 0$ connecting s_{in} to $s^\star$ is equal to $\int_{s^\star}^{s_{in}} \frac{d\sigma}{\mu(\sigma)(M-\sigma)}$. Clearly, this integral goes to zero if M goes to infinity. When $M \to \infty$, the dominant term in the value function $v(x_0, s_0)$ of (2.3) is therefore the time spent by an arc $u = 1$ connecting M_0 to Γ_0 or Δ^1_{SA}.

4 Optimal synthesis when $\alpha < 1$

In this section, we study the optimal synthesis whenever $\alpha < 1$. The set Δ_0^α is the line segment of equation:

$$\xi_\alpha(s) := s + \frac{s_{in} - s}{\alpha},\ s \in [0, s_{in}],$$

and the singular locus Δ^α_{SA} is the graph of the curve :

$$s \longmapsto M = \zeta_\alpha(s) := s + \psi_\alpha(s),\ s \in [0, s_{in}],$$

where

$$\psi_\alpha(s) := \frac{1}{\alpha} \frac{\mu'(s)(s_{in} - s)^2}{(s_{in} - s)\mu'(s) + (1 - \alpha)\mu(s)}.$$

The function ψ_α and ζ_α may be undefined at some points of $[0, s_{in}]$ if $\mu' < 0$. By differentiating $M - s = \psi_\alpha(s)$ w.r.t. to the time along a singular arc, one finds the expression of the singular control:

$$u_s(s) = \mu(s)\psi_\alpha(s)\frac{1 + \psi_\alpha'(s)}{\alpha\psi_\alpha(s) + \psi_\alpha'(s)(s_{in} - s)}.$$

4.1 Optimal synthesis for Monod kinetic function

We suppose in this section that the growth rate function is given by :

$$\mu(s) := \frac{\mu_m s}{k + s}, \tag{4.1}$$

where $\mu_m > 0$ and $k > 0$. Notice that μ, resp. μ' is positive over $(0, s_{in}]$, resp. over $[0, s_{in}]$. Therefore ψ_α and ζ_α are well defined over $[0, s_{in}]$. Moreover, we can make the following observations :

- If $E_0 := (0, \frac{s_{in}}{\alpha})$ and $E_1 := (s_{in}, s_{in})$, then we have $\Delta_0^\alpha \cap \Delta^\alpha_{SA} := \{E_0, E_1\}$.
- The steady state singular point E_0, resp. E_1 is attractive, resp. repulsive for the dynamical system (2.4) with the feedback control $u = u_s(s)$.
- The singular control $s \longmapsto u_s(s)$ is negative on the interval (s_m, s_{in}) where $s_m \in (0, s_{in})$ is the unique point such that $\zeta'(s_m) = 0$.

Figures 7 depicts the singular locus Δ^α_{SA} and the collinearity set Δ^α_0 for different values of α. The corresponding singular control is plotted on Figure 8. We observe that if α is small, then the singular control u_s can be larger than 1 which corresponds to the maximal admissible value for the control. To simplify the study, we consider the following assumption :

(H3) The singular control satisfies $u_s(M) \leq 1$ for any $s \in [0, s_m]$.

If Hypothesis (H3) is satisfied, then the singular arc is admissible on $[0, s_m]$. The optimal synthesis will depend on the position of the target point $(\bar{s}, \bar{M})$ w.r.t. the points E_0 and E_1. More precisely, we consider the three following cases:

- Case I : $E_1 \notin A_\alpha$ and $E_0 \notin A_\alpha$
- Case II : $E_1 \in A_\alpha$ and $E_0 \notin A_\alpha$
- Case III : $E_1 \in A_\alpha$ and $E_0 \in A_\alpha$

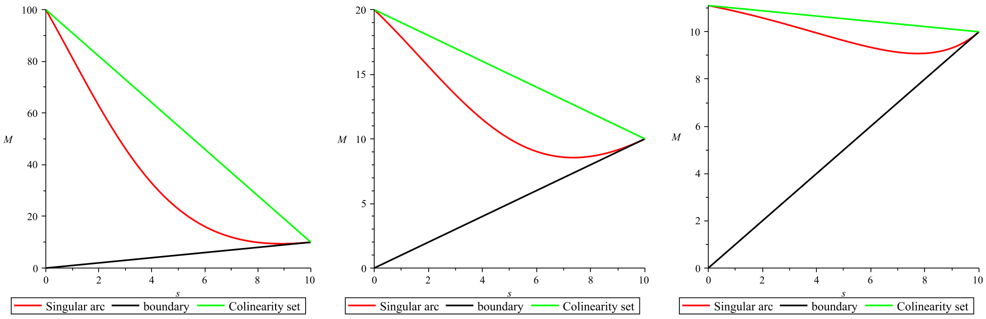

Figure 7: Plot of Δ_0^α and Δ_{SA}^α for $\alpha = 0.1, 0.5, 0.9$ with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$.

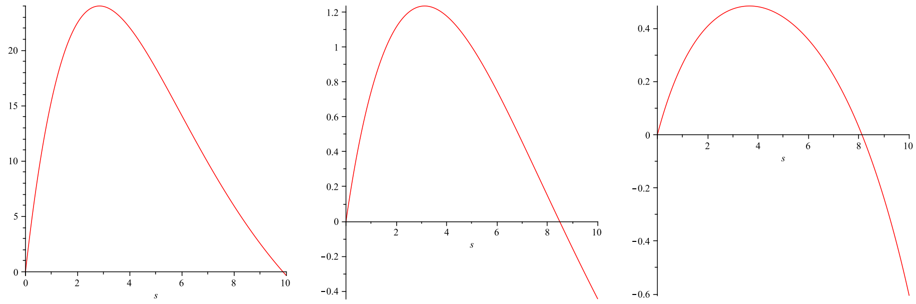

Figure 8: Plot of the singular control with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$ for $\alpha = 0.1, 0.5, 0.9$.

Note that if $E_1 \in A_\alpha$, then E_0 is in A'_α, hence the case $E_1 \notin A_\alpha$ and $E_0 \in A_\alpha$ is not possible. When $E_0 \notin A_\alpha$, we introduce the feedback control law :

$$u_m^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \zeta_\alpha(s), \\ 0 & \text{if} \quad M > \zeta_\alpha(s) \text{ or } (M = \zeta_\alpha(s) \text{ and } s > s_m), \\ u_s(M) & \text{if} \quad M = \zeta_\alpha(s) \text{ and } s < s_m, \end{cases} \tag{4.2}$$

The optimal synthesis then reads as follows.

Theorem 4.1. *Suppose that μ is given by (4.1) and that (H2)-(H3) hold true. Then, an optimal synthesis reads as follows.*

(i) If $E_1 \notin A_\alpha$ and $E_0 \notin A_\alpha$ (case I), then the controllability set is A_α and an optimal feedback policy in $\mathrm{Int}(A_\alpha)$ is given by (4.2).

(ii) If $E_1 \in A_\alpha$ and $E_0 \notin A_\alpha$ (case II), then the controllability set is F. Moreover, an optimal feedback policy in $\mathrm{Int}(A_\alpha)$ is given by (4.2), and an optimal control satisfies $u = 1$ in $\mathrm{Int}(A'_\alpha)$.

(iii) If $E_1 \in A_\alpha$ and $E_0 \in A_\alpha$ (case III), then the controllability set is A'_1 and an optimal control satisfies $u = 1$ in $\mathrm{Int}(A'_\alpha)$.

Proof. Let us prove (i). Using section 3.1 and the equivalence $\frac{dM}{ds}_{|u=1} > 0 \iff M < s + \frac{1}{\alpha}(s_{in} - s)$, one can easily show that the controllability set is A_α. Moreover, from (2.13), we obtain that an optimal control cannot switch from $u = 0$ to $u = 1$, resp. from $u = 1$ to $u = 0$ at some point in $A_\alpha \backslash (\Gamma_0 \cup \Gamma_1)$ such that $M < \zeta(s)$, resp. $M > \zeta(s)$. Hence, optimal trajectories can only switch on the singular locus Δ_{SA}^α. It follows that an optimal control satisfies $u = 1$ when $M < \zeta(s)$ and $u = 0$ when $M > \zeta(s)$. Moreover, we deduce that at some point (s, M)
$inDelta_{SA}^\alpha$ either we have $s \leq s_m$ and $u = u_s$ (from (2.13), optimal trajectories cannot leave the singular arc before reaching $\Gamma_0 \cup \Gamma_1$) or $s > s_m$ and then an optimal control necessarily satisfies $u = 0$.

To prove (ii), notice that the optimality result in A_α is similar to (i). Now, solutions of (2.4) with $u = 1$ starting above $\Gamma_0 \cup \Gamma_1$ necessarily converge to the point E_1 (recall (H2)). Hence, trajectories with $u = 1$ starting in A'_α necessarily intersect Γ_0 (as $E_1 \in A_\alpha$). To prove that an optimal control satisfies $u = 1$ in $\mathrm{Int}(A'_\alpha)$, we use (2.13) and similar arguments as in the proof of (i).

The proof of (iii) is similar to the proof of (ii) except that the target point cannot be reached by points in $\mathrm{Int}(A_1)$. □

Remark 4.1. *(i) We point out that optimal trajectories can switch from $u = 1$ to $u = 0$ on the part of the singular locus defined for $s \in (s_m, s_{in})$.*
(ii) Whenever $\alpha = 1$ and μ is of Monod type, we know from (3.6) *that no singular arc occurs. We see that when $\alpha < 1$, then optimal strategies can take advantage of a singular arc depending on the position of the target point w.r.t. Δ^α_{SA}.*
(iii) It is interesting to observe that when $\alpha \to 1$, then one has $\xi_\alpha(s) \to s_{in}$ and $\zeta_\alpha(s) \to s_{sin}$. Hence, if $\bar{M} < s_{in}$, then the optimal control policy (4.2) *converges to the feedback* (3.6) *as expected.*

4.2 Discussion for Haldane kinetic function

TODO? Or just give the idea of the synthesis?

5 Conclusion, Discussion, Perspectives

- Dans le cas Monod, lorsque $\alpha \to 1$ on retrouve la même synthèse que lorsque $\alpha = 1$, ouf.
- Message : dans le cas Monod, lorsque $\alpha \neq 1$ il y a un arc singulier (pas d'arc singulier pour Monod quand $\alpha = 1$. De plus, l'ensemble de contrôlabilité peut être plus grand. La synthèse dépend de la position de la cible par rapport à la courbe Δ_α.
- Perspectives? Inclure la mortalité ($\alpha > 1$) : mais bon les équations sont les mêmes donc il suffirait de regarder ce cas aussi qui ne doit pas être très différent...
- Perspectives? Etudier le système en dimension 4 de digestion anaérobie proposé par Olivier Bernard sans mortalité et sans α (cf mail Jérôme) : quel système?

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6 Appendix

Proof of Lemma 3.3. The following claim is crucial and follows from 3.2 and Proposition 2.1 (ii).

Claim 6.1. *Any extremal trajectory cannot switch from $u = 1$ to $u = 0$, resp. from $u = 0$ to $u = 1$ at a point $(s(t), M(t))$ such that $s(t) > s^\star$, resp. $s(t) < s^\star$ (t).*

Step 1. Let us prove the existence of the switching curve $s_c : [\tilde{M}, M_e] \to [s^\star, s_{in}]$.

Consider an initial condition (s_0, M_0) such that $s_0 > s^\star$, $M_0 > \tilde{M}$ and an optimal trajectory starting from this point. Suppose that we have $u = 0$ until reaching $s^\star$ at a time t_0. We then have $u = 0$ for any time $t > t_0$, and the trajectory cannot reach the target. Therefore, either we have $u = 1$ at time 0 until reaching $s = s^\star$ with $M < M_{sat}$ or $M = \bar{M}$, or there exists a unique point switching point to $u = 1$ at a time t_0 such that $s^\star < s^\dagger(t_0) < s_0$ (the uniqueness follows from Claim 6.1).

Let us now denote by $M \longmapsto s^\dagger(M)$ the unique solution of (2.4) with $u = 1$ backward in time from $(s^\star, \tilde{M})$ satisfying the Cauchy problem:

$$\frac{d\sigma}{dM} = -\frac{\mu(\sigma)(M-s) + s_{in} - \sigma}{s_{in} - M}, \quad \sigma(\tilde{M}) = s^\star.$$

When $\tilde{M} = M_{sat}$ we know that this curve is tangent to the singular arc at $(s^\star, M^\star)$. Therefore, it leaves F through $s = s_{in}$ i.e. there exists a unique point M_{out} such that $s^\dagger(M_{out}) = s_{in}$. By a monotonicity argument, we argue that it also leaves F through $s = s_{in}$ whenever $\tilde{M} = \bar{M}$.

Finally, take an initial condition (s_0, M_0) such that $\tilde{M} < M_0 < M_{out}$ and $s_0 > s^\dagger(M_0)$. Claim 6.1 then implies the existence and uniqueness of a switching point from $u = 0$ to $u = 1$ at a time t_0 such that $s(t_0) > s^\star$. Hence, we have proved that for any $M \in [\tilde{M}, M_{out}]$, there exists exactly one switching point that we denote $s_c(M)$. We then define $M_e \in [M_{out}, +\infty]$ as :

$$M_e := \sup\{M > M_{out} \ ; \ s_c(\cdot) \text{ is defined over } [M_{out}, M]\}.$$

Step 2. *Proof of Lemma 3.3 (1)-(2).* First, we have $s_c(M)$ goes to $s^\star$ when $M \downarrow \tilde{M}$. Otherwise, we would have a contradiction by using Claim 6.1 and $s^\dagger(\cdot)$. Now, If $M_e < +\infty$, we necessarily have $s_c(M_e) = s_{in}$. Otherwise, we would have $s_c(M_e) \in (s^\star, s_{in})$. In that case, we consider the unique solution of (2.4) with $u = 1$ backward in time from $(s_c(M_e), M_e)$. Then, consider an initial condition (s_0, M_0) below this curve and such that $s_0 > s_c(M_e)$ and $M_0 > M_e$. We then have $u = 1$ until reaching $M = M_e$. We necessarily have a contradiction by Claim 6.1 as the trajectory cannot switch to $u = 0$ at a time t_0 such that $s(t_0) > s^\star$. Therefore, we have $s_c(M_e) = s_{in}$. Finally, we have seen by construction of s_c that we have $s_c(M) \in (s^\star, s_{in})$ for any point $M \in (M^\star, M_e)$. This proves Lemma 3.3 (1). The proof of (2) is a direct consequence of Claim 6.1.

□

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