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

The optimal control of bioprocesses has attracted a lot of attention over the last fifty years. The control of fedbatch processes has been extensively studied due to the fact that 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 so 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 in [15] for single reaction systems and for a large class of growth rate functions, and more recently in [2, 4, 10, 11]. 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 in [11]. 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 [21] or [19, 25] and references herein).

Our interest in this paper is the chemostat which is an apparatus 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 [14, 17]). It presents the advantage of not being necessary to 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 [22].

Classically, the model of the chemostat is written as:

$$\left\{ \begin{array}{ll} \dot{x} & = \mu(s)x - Dx, \\ \dot{s} & = -\frac{1}{\gamma}\mu(s)x + D(s_{in} - s), \end{array} \right. \tag{1.1}$$

*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

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, $\gamma > 0$ is the biomass yield factor, 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 [9]). 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. [12, 23]). 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 partially investigated in [3]. 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 $\alpha > 0$ may be introduced in the dynamic of x and the model becomes:

$$\left\{ \begin{array}{ll} \dot{x} & = \mu(s)x - \alpha D x, \\ \dot{s} & = -\frac{1}{\gamma}\mu(s)x + D(s_{in} - s), \end{array} \right. \tag{1.2}$$

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, our aim if to address the minimal time control problem to go from one state to another for this modified chemostat model (1.2). One essential feature in (1.2) is that the recirculation parameter leads to an asymmetry between x and s (the total mass of the system is no longer conserved in batch mode i.e. when $D = 0$). We will first provide a complete study of the problem when $\alpha = 1$ extending [3] to any initial condition of the state space. In particular, we show that the optimal synthesis exhibits a switching curve whenever the total mass of the system is above s_{in} (see Theorem 3.2). In this case optimal trajectories can have three switching times before reaching the target point. In the case where $\alpha < 1$, we provide a description of optimal trajectories for Monod and Haldane kinetics under the additional assumption that the singular arc is always admissible (see [20]).

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 to derive optimality conditions. We also give properties of the *switching function* that are crucial in sections 3 and 4. In section 3, we provide an optimal feedback control for Haldane kinetics when $\alpha = 1$ (Theorems 3.1 and 3.2 are our main results), and section 4 discusses the case $\alpha < 1$. The article concludes with an appendix containing the proof of the existence of the switching curve for $\alpha = 1$ (see section 3).

2 Preliminaries

2.1 Statement of the problem

We consider the system

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

describing a chemostat model with one species, one substrate and an adimensioned yield coefficient for x (i.e. $\gamma = 1$). 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 (2.1) 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

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

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) over $[0, \infty)$ 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 $\bar{M} := \bar{x} + \bar{s}$.

Next, we consider the solutions of (2.4) backward in time starting at $(\bar{s}, \bar{M})$ at time 0. More precisely, let $z^i(\cdot) := (s^i(\cdot), M^i(\cdot))$, $i = 0, 1$, 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 $t \in [0, t_i)$ (in particular Γ_0 is a line segment). We note that $\Gamma_0 \cup \Gamma_1$ partitions F into two subsets F_α^- and F_α^+. More precisely, we take for F_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 $\text{Int}(B)$ 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 (see e.g. [13, 16]).

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 $t_f \geq 0$, $\lambda_0 \leq 0$ 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 :

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

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 [8]).
- 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 [8]). In our setting, we can show that Δ_0^α and Δ_{SA}^α are non-empty, and we can provide an explicit expression of these two sets whereas switching curves are in general more delicate to characterize by an implicit equation (in particular these 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 ϕ 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:

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

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_c such that $\frac{f_{SA}^\alpha(s(t_c),M(t_c))}{f_0^\alpha(s(t_c),M(t_c))} < 0$, resp. $\frac{f_{SA}^\alpha(s(t_c),M(t_c))}{f_0^\alpha(s(t_c),M(t_c))} > 0$.

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 :

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

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

Frame points are the points at the intersection of two frame curves. The determination of such points is 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 [5]). From the expressions of f_0 and f_{SA}, the points $E_0 := (0, \frac{s_{in}}{\alpha})$ and $E_1 := (s_{in}, s_{in})$ belong to $\Delta_0^\alpha \cap \Delta_{SA}^\alpha$ and are two steady state singular points.

Finally, recall that if a singular arc is optimal (in this case, it is also called *turnpike*, see e.g. [8]), then Legendre-Clebsch necessary optimality condition must hold true (see e.g. [20]), that is we must have

$$\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u \geq 0, \tag{2.15}$$

where $H_u := \frac{\partial H}{\partial u}$ is computed along the singular extremal trajectory. A singular extremal trajectory that is is not optimal over a time $I = [t_1, t_2]$ is called *anti-turnpike* [8].

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 variable M then satisfies the ODE

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

hence (2.4) has a cascade structure. In view of (2.4) 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 $\Delta_0^1 \cap \mathrm{Int}(F) = \emptyset$, and so the only possible abnormal trajectories are the solutions of (2.4) with $u = 0$ and $u = 1$ that reach the target point $(\bar s, \bar M)$ without any switching point. 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 $\Delta^1_{SA} = \{s^\star\} \times (s^\star, +\infty)$. The *singular control* is defined as the control u_s such that $(s_{u_s}(t), M_{u_s}(t)) \in \Delta^1_{SA}$ and is given by :

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

Furthermore, $M_{u_s}(\cdot)$ satisfies the following ODE along Δ^1_{SA} :

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

We can check that Legendre optimality condition (2.15) is satisfied along the singular arc Δ^1_{SA} as a simple computation shows that

$$\frac{\partial}{\partial u} \frac{d^2}{dt^2} H_u = -\mu''(s^\star) \frac{(s_{in} - s^\star)^2}{\mu(s^\star)} \geq 0.$$

Indeed, μ is non-negative and $\mu''(s^s tar) \leq 0$ as $s^\star$ is a maximum of μ, therefore $\frac{\partial}{\partial u} \frac{d^2}{dt^2} H_u \geq 0$.

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, F_1^- can be written as:

$$F_1^- = \{(s, M) \in F \; ; \; M \leq \min(\varphi_0(s), \varphi_1(s))\}. \tag{3.4}$$

Lemma 3.1. *Suppose that $\bar{M} < s_{in}$. Then, the controllability set for (2.3) is F_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 $F \backslash F_1^-$. If the trajectory is singular, then it cannot intersect the boundary of F_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 control in* $\mathrm{Int}(F_1^-)$ *is given by :*

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

Proof. The proof follows from Proposition 2.1 (ii). Suppose that $(s_0, M_0) \in F_1^- \backslash (\Gamma_0 \cup \Gamma_1)$. 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 $(s_0, M_0) \in F_1^- \backslash (\Gamma_0 \cup \Gamma_1)$, 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 $(s_0, M_0) \in F_1^- \backslash (\Gamma_0 \cup \Gamma_1)$, then an optimal trajectory does not leave the singular arc either with $u = 0$ or $u = 1$. Therefore singular trajectories are optimal until reaching $\Gamma_0 \cup \Gamma_1$. □

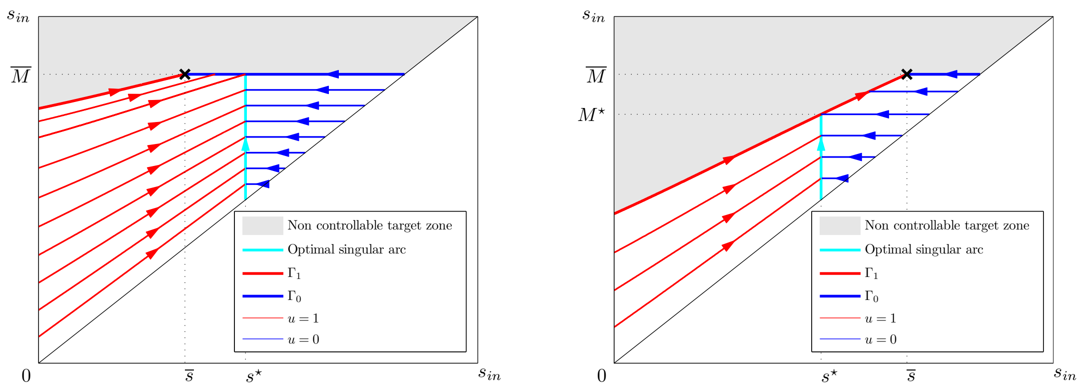

Figure 1: Optimal synthesis for $\alpha = 1$ and $\bar{M} < s_{in}$ (case I). *Picture left* : the target point is such that $\bar{s} < s^\star$ (the singular arc Δ^1_{SA} intersects Γ_0). *Picture right* : the target point is such that $\bar{s} > s^\star$ (the singular arc Δ^1_{SA} intersects Γ_1).

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 left). 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 right).*
(ii) When $s^\star > s_{in}$, the previous considerations show that for Monod kinetic function the feedback in $\mathrm{Int}(F_1^-)$

$$\left\{ \begin{array}{lll} u_m[s,M] & = 1 & \text{if } (s,M) \in F_1^- \backslash \Gamma_0, \\ u_m[s,M] & = 0 & \text{if } (s,M) \in \Gamma_0, \end{array} \right. \tag{3.6}$$

is optimal (see [9]).

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 $u = 1$) but one has $\frac{dM}{dt}_{|u=1} < 0$. The previous considerations show that the trajectory $z^1(\cdot)$ is the graph of a C^1-mapping $M \longmapsto s := \psi_1(M)$ defined over $[\bar{M}, +\infty)$ in the plane (s,M) (indeed we have $\dot{M} < 0$ along $u = 1$). Therefore, the set F_1^+ can be written:

$$F_1^+ = \{(s,M) \in F \ ; \ M \geq \bar{M} \text{ and } \max(0, \psi_1(M)) \leq s \leq s_{in}\}.$$

Lemma 3.2. *Suppose that $\bar{M} > s_{in}$. Then, the controllability set for* (2.3) *is F_1^+.*

Proof. The proof is similar to the proof of Lemma 3.1. ☐

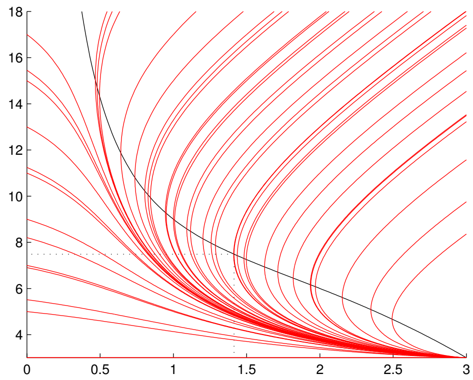

Figure 2: Solutions of (2.4) for the control $u = 1$ and different initial conditions (s_0, M_0) with $M_0 > s_{in}$ and $s_{in} = 3$. The black curve is the set of points where the tangent to this trajectory is vertical.

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 sake of clarity, we have postponed the proof of this lemma to the appendix. □

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

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

Remark 3.3. *(i) If $\tilde{M} = M_{sat}$ i.e. $\bar{M} \leq M_{sat}$, then the point $(s^\star, M_{sat})$ is a frame point of type $(CS)_1$ i.e. at the intersection of $\mathcal{C}$ and Δ^1_{SA}, see Fig. 3 and Fig. 4*
(ii) If $\tilde{M} = \bar{M}$ i.e. if $\bar{M} > M_{sat}$, then $\mathcal{C} \cap \Delta^1_{SA}$ and $\mathcal{C}$ intersect Γ_0 at the point $(s^\star, \bar{M})$, see Fig. 5.

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 control in $\mathrm{Int}(F_1^+)$ is given by :*

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

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. □

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 :

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

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 reaching either Δ^1_{SA} or $\Gamma_0 \backslash \{(\bar{s}, \bar{M})\}$ at a time t 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 $\Gamma_0 \cup \Delta^1_{SA}$ for which 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.

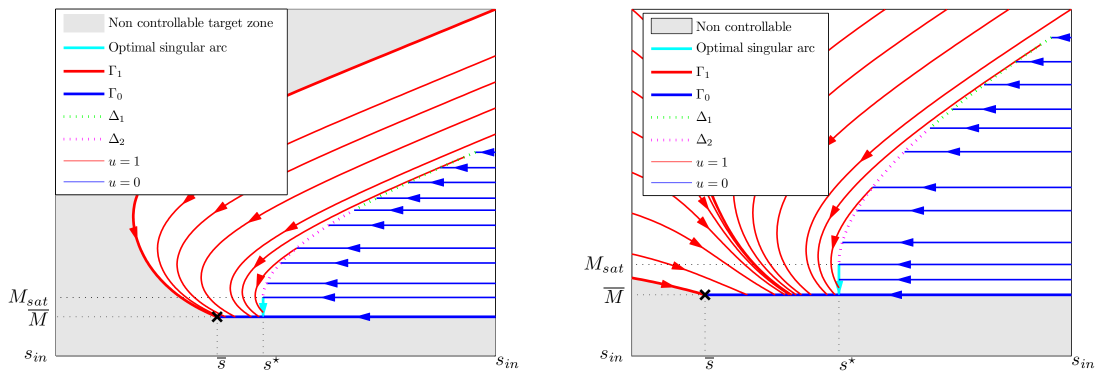

Figure 3: Case II a. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0).

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

In this section, we discuss additional properties of the switching curve $\mathcal{C}$ that are related to the curve Γ_1. First, we suppose that Γ_1 exits F through $s = s_{in}$. We can then show that $\mathcal{C}$ exits F at some point $(s_c(M_e), M_e)$ such that $s_c(M_e) = s_{in}$ as shown below.

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 $s_c(M_e) = s_{in}$.*

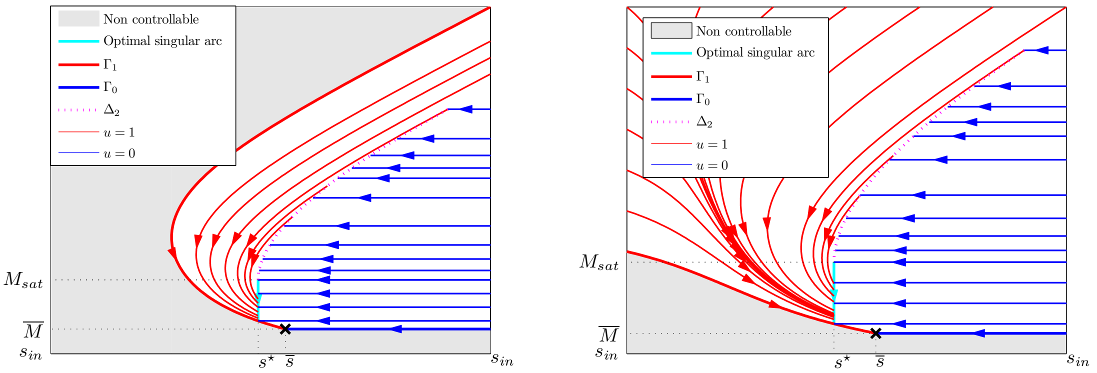

Figure 4: Case II b. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0).

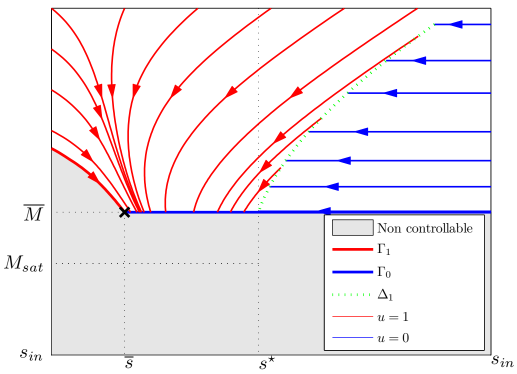

Figure 5: Case II c. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0).

Proof. Clearly, $\mathcal{C}$ cannot intersect Γ_1 before reaching $s = s_{in}$ as we would have a contradiction with the controllability set F_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 $M_e \leq M_{out}$. $\square$

Remark 3.4. *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 no longer holds. Nevertheless, we conjecture that $\mathcal{C}$ exits F at some point $M_e < +\infty$ as numerical simulations indicate. However, properties of switching curve can be in general difficult to obtain. 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

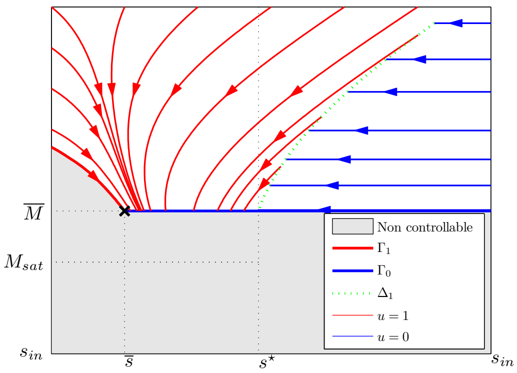

Figure 6: Case II d. Optimal synthesis for $\alpha = 1$, $M > s_{in}$. The dotted line represents the switching curve $M \longmapsto s_c(M)$ (in purple, resp. in green, it is obtained backward in time from Δ^1_{SA}, resp. from Γ_0).

infinity. When $M \to +\infty$, the dominant term in the value function $v(x_0, s_0)$ (recall (2.3)) is the time of an arc $u = 1$ connecting $(\bar{s}, \bar{M})$ to Γ_0 or Δ^1_{SA}. Hence, if $\bar{M} \gg s_{in}$, there is no evidence that optimal trajectories will benefit from a switching time until reaching Γ_0 or Δ^1_{SA}.

4 Optimal synthesis when $\alpha < 1$

In this section, we study the optimal synthesis whenever $\alpha < 1$. Unlike in the case $\alpha = 1$, the system (2.4) has not a cascade structure, and thus finding an optimal synthesis in this framework is more delicate. In this case, the set Δ^α_0 is the line segment of equation:

$$\delta^\alpha_0(s) := s + \frac{s_{in} - s}{\alpha}, \; s \in [0, s_{in}],$$

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

$$s \longmapsto M = \delta^\alpha_{SA}(s) := s + \psi_\alpha(s), \; s \in [0, s_{in}],$$

where

$$\psi_\alpha(s) := \frac{1}{\alpha} \frac{\mu'(s)(s_{in} - s)^2}{(s_{in} - s)\mu'(s) + (1-\alpha)\mu(s)}. \tag{4.1}$$

Note that the functions ψ_α and δ^α_{SA} are not well defined as $(s_{in} - s)\mu'(s) + (1-\alpha)\mu(s)$ can be zero when s is such that $\mu'(s) < 0$. By differentiating $M - s = \psi_\alpha(s)$ w.r.t. to time t supposing that the trajectory belongs to a singular arc, we find the expression of the singular control u^α_s (depending on s only):

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

In order to verify if (2.15) holds true along a singular extremal (see sections (4.1) and (4.2)), we have the following Lemma.

Lemma 4.1. *Along a singular arc $I = [t_1, t_2]$ one has*

$$\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u = -\frac{(1-\alpha)\mu(s(t)) + \mu'(s(t))(s_{in} - s(t))}{\mu(s(t))(\delta^\alpha_0(s(t)) - \delta^\alpha_{SA}(s(t)))}(\alpha\psi_\alpha(s(t)) + (s_{in} - s(t))\psi'_\alpha(s(t))), \quad t \in I. \tag{4.2}$$

Proof. Using the expressions of f_{SA} and f_0 (see (2.11)) we get

$$-\frac{f^\alpha_{SA}(s, M)}{f^\alpha_0(s, M)} = \frac{[(1-\alpha)\mu(s) + \mu'(s)(s_{in} - s)]}{\mu(s)} \frac{M - \delta^\alpha_{SA}(s)}{\delta^\alpha_0(s) - M}.$$

Then (4.2) is obtained by differentiating (2.13) w.r.t. t. □

Whereas in the case $\alpha = 1$ the subset of F defined by $M = s_{in}$ is invariant by (2.4) (see (3.1)), trajectories of (2.4) can cross the set Δ_0^α whenever $\alpha < 1$. We then consider the three following cases:

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

We have the following controllability result depending on the position of the target point $(\bar{s}, \bar{M})$ with respect to the two steady state singular points E_0 and E_1.

Lemma 4.2. *If* (H1) *and* (H2) *hold true and* $(\bar{s}, \bar{M}) \in F$ *is a given target point, then:*

(i) If $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case I), then the controllability set is F_α^-.

(ii) If $E_1 \in F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case II), then the controllability set is F.

(iii) If $E_1 \in F_\alpha^-$ and $E_0 \in F_\alpha^-$ (case III), then the controllability set is F_α^+

Proof. The proof of (i) and (iii) is the same as in Lemma 3.1 and 3.2. For proving (ii), consider a solution of (2.4) with $u = 1$ starting in $F \backslash F_\alpha^-$. From (H2), this trajectory converges to the point (s_{in}, s_{in}) which is a globally asymptotically stable steady-state for (2.4). In case II, we have $s_{in} < \bar{M} < \frac{s_{in}}{\alpha}$, hence the trajectory necessarily intersects Γ_0 at a time $t_0 > 0$. For $t > t_0$, the control $u = 0$ steers the (2.4) into the target point in finite time. □

Remark 4.1. *In the case II above, the controllability set is the state domain F, hence any initial condition in F can reach the target point $(\bar{s}, \bar{M})$.*

4.1 Optimal synthesis for Monod kinetic function

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

$$\mu(s) := \frac{\mu_m s}{k + s}, \tag{4.3}$$

where $\mu_m > 0$ and $k > 0$. Notice that $\mu > 0$ and $\mu' > 0$ over $(0, s_{in}]$. Therefore ψ_α and δ_{SA}^α are well defined over $[0, s_{in}]$. From (4.1)-(4.2), we can make the following observations:

- We have $\Delta_0^\alpha \cap \Delta_{SA}^\alpha := \{E_0, E_1\}$. Moreover, for any $s \in (0, s_{in})$ one has $\delta_{SA}^\alpha(s) < \delta_0^\alpha(s)$.
- The singular control $s \longmapsto u_s^\alpha(s)$ is negative on the interval (s_m, s_{in}) where $s_m \in (0, s_{in})$ is the unique point such that $(\delta_{SA}^\alpha)'(s_m) = 0$.
- The steady state singular point E_0, resp. E_1 is attractive, resp. repulsive for the dynamical system (2.4) with the feedback control $u = u_s^\alpha(s)$ (indeed one has $\dot{M} = \alpha u_s^\alpha(s)(\delta_0^\alpha(s) - \delta_{SA}^\alpha(s))$ along the singular arc).
- Using (4.2), Legendre-Clebsch optimality condition (2.15) is satisfied along Δ_{SA}^α.

Figures 7 depicts the singular locus Δ_{SA}^α and the collinearity set Δ_0^α 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^α can be larger than 1 which corresponds to the maximal admissible value for the control. To simplify the study, we consider the following assumption on the admissibility of the singular arc:

(H3) The singular control satisfies $u_s^\alpha(s) \leq 1$ 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 as in Lemma 4.2. When $E_0 \notin F_\alpha^-$, we introduce the feedback control law :

$$u_m^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \delta_{SA}^\alpha(s), \\ 0 & \text{if} \quad M > \delta_{SA}^\alpha(s) \text{ or } (M = \delta_{SA}^\alpha(s) \text{ and } s > s_m), \\ u_s^\alpha(s) & \text{if} \quad M = \delta_{SA}^\alpha(s) \text{ and } s < s_m, \end{cases} \tag{4.4}$$

The optimal synthesis then reads as follows (see also Fig. 8).

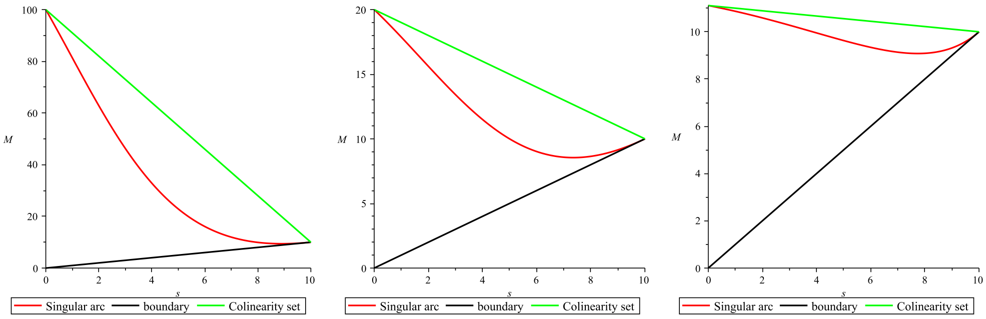

Figure 7: Plot of Δ_0^α and Δ_{SA}^α for $\alpha = 0.1, 0.5, 0.9$ with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$.

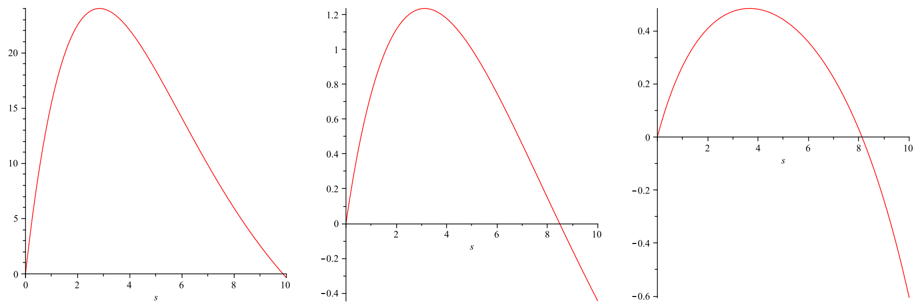

Figure 8: Plot of the singular control with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$ for $\alpha = 0.1, 0.5, 0.9$.

Theorem 4.1. *Suppose that μ is given by* (4.3) *and that (H2)-(H3) hold true. Then, an optimal synthesis reads as follows.*

(i) If $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case I), then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ *is given by* (4.4).

(ii) If $E_1 \in F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case II), then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ *is given by* (4.4) *and an optimal feedback control satisfies $u = 1$ in* $\mathrm{Int}(F_\alpha^+)$.

(iii) If $E_1 \in F_\alpha^-$ and $E_0 \in F_\alpha^-$ (case III), then an optimal feedback control satisfies $u = 1$ in $\mathrm{Int}(F_\alpha^+)$.

Proof. Let us prove (i). 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 $F_\alpha^- \backslash (\Gamma_0 \cup \Gamma_1)$ such that $M < \delta_{SA}^\alpha(s)$, resp. $M > \delta_{SA}^\alpha(s)$. Hence, optimal trajectories can only switch on the singular locus Δ_{SA}^α. It follows that an optimal control satisfies $u = 1$ when $M < \delta_{SA}^\alpha(s)$ and $u = 0$ when $M > \delta_{SA}^\alpha(s)$. Moreover, we deduce that at some point $(s, M) \in \Delta_{SA}^\alpha$ 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 F_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 (see Lemma 4.2 (ii)). Hence, trajectories with $u = 1$ starting in F_α^+ necessarily intersect Γ_0 (as $E_1 \in F_\alpha^-$). To prove that an optimal control satisfies $u = 1$ in $\mathrm{Int}(F_\alpha^+)$, 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 $\mathrm{Int}(F_1^-)$ as solutions of (2.4) with $u = 1$ satisfy $\frac{dM}{dt} = 0$ on Δ_0^α. □

Remark 4.2. *(i) In Theorem 4.1, we point out that optimal trajectories switch from $u = 1$ to $u = 0$ on the singular locus restricted to (s_m, s_{in}) which corresponds to a switching curve.*
(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_{SA}^α.*

(iii) It is interesting to observe that when $\alpha \to 1$, then one has $\delta_0^\alpha(s) \to s_{in}$ and $\delta_{SA}^\alpha(s) \to s_{in}$. Suppose $\bar{M} < s_{in}$. Thus we deduce that if α is sufficiently close to 1, then (4.4) *coincides with* (3.6)

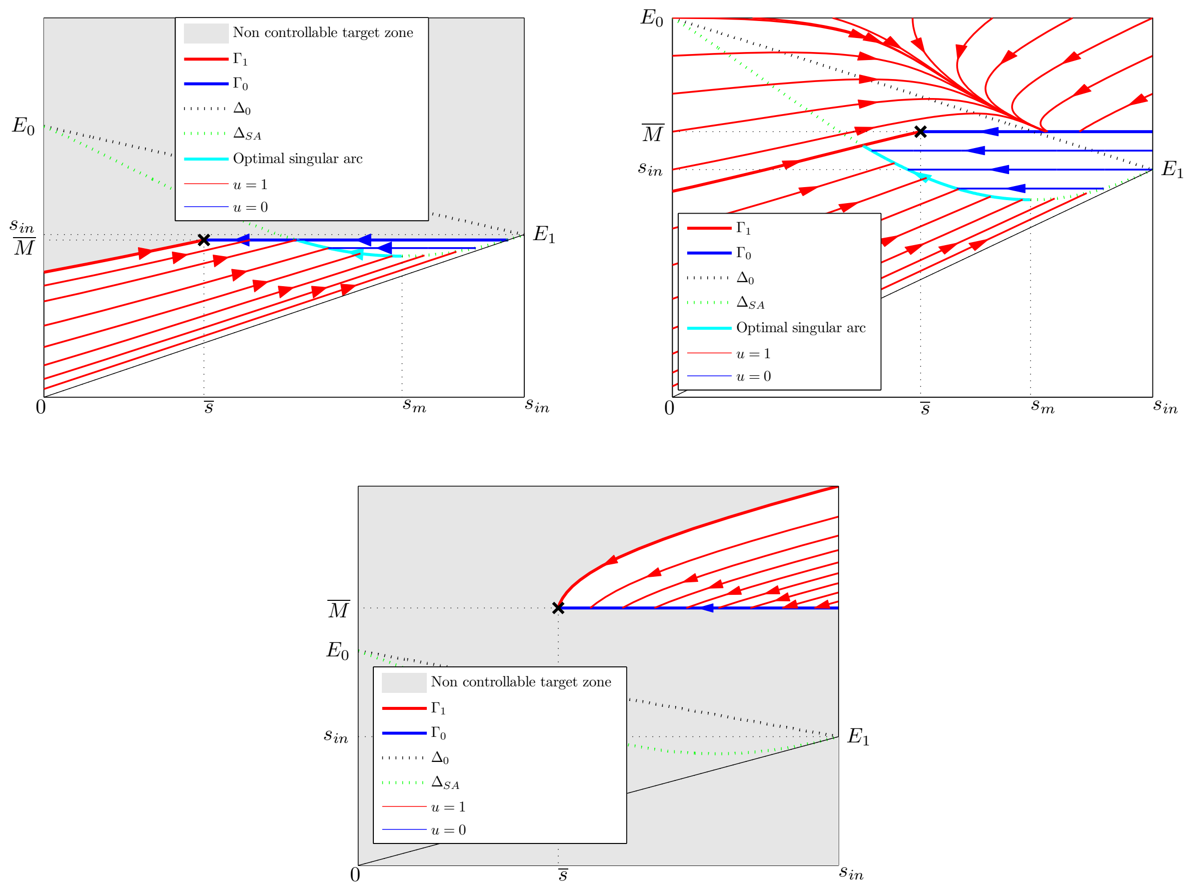

Figure 9: Optimal synthesis provided by Theorem 4.1 in case I (above left), case II (above right) and case III (middle).

4.2 Discussion for Haldane kinetic function

In this section, we discuss the optimal synthesis of the problem for Haldane kinetics (i.e. we suppose that (H′1) holds true). Recall that $\mu'(s) > 0$ for $s \in [0, s^\star]$ and $\mu'(s) < 0$ for $s \in [s^\star, s_{in}]$. The singular locus Δ_{SA}^α and the collinearity set Δ_0^α are represented for different values of the parameter α on Fig. 10. From (4.1)-(4.2), we can make the following observations:

- There exists $0 < s_1^\alpha < s_2^\alpha < s_{in}$ such that $s \longmapsto s + \psi_\alpha(s)$ is well-defined over $[0, s_1^\alpha) \cup (s_1^\alpha, s_2^\alpha) \cup (s_2^\alpha, s_{in}]$. Moreover, $\lim_{s \to s_1^\alpha, s > s_1^\alpha} \delta_{SA}^\alpha(s) = \lim_{s \to s_2^\alpha, s < s_2^\alpha} \delta_{SA}^\alpha(s) = +\infty$.
- For $s \in [0, s_1)$, one has $\delta_{SA}^\alpha(s) < \delta_0^\alpha(s)$ and for $s \in (s_1^\alpha, s_2^\alpha)$ one has $\delta_{SA}^\alpha(s) > \delta_0^\alpha(s)$. For $s \in (s_2^\alpha, s_{in}]$, $\delta_{SA}^\alpha(s) \notin F$.
- By definition of Δ_0^α we have $\dot{M} > 0$ if and only if $M < \delta_0^\alpha(s)$. Along the singular arc Δ_{SA}^α, we then have $\dot{M} > 0$, resp. $\dot{M} < 0$ for $s \in [0, s_1)$, resp. $s \in (s_1, s_2)$.
- There exists a point $s_c \in (s_1^\alpha, s_2^\alpha)$ such that Legendre-Clebsch optimality condition (2.15) is satisfied only for $s \in [0, s_1^\alpha) \cup (s_1^\alpha, s_c]$. Hence the singular locus restricted to $[s_c, s_2^\alpha)$ is not optimal (i.e. it is an anti-turnpike).

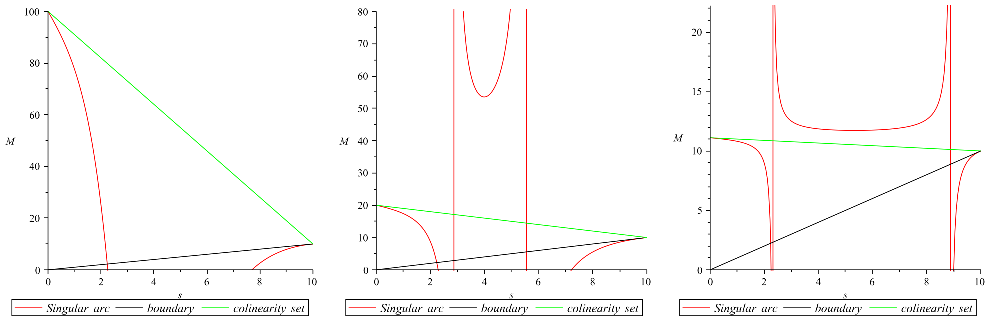

Figure 10: Plot of Δ_0^α (in green) and Δ_{SA}^α (in red) for $\alpha = 0.1$ (picture left), $\alpha = 0.5$ (picture in the middle), $\alpha = 0.9$ (picture right) with $\mu(s) = \frac{s}{5+s+s^2}$ and $s_{in} = 10$.

To simplify the study, we consider the following assumption on the admissibility of the singular arc:

(H'3) The singular control satisfies $u_s^\alpha(s) \in [0,1]$ for any $s \in [0, s_c]$ such that $(s, \delta_{SA}^\alpha(s)) \in F$.

Remark 4.3. *In case II and III of section 4, the state domain is unbounded, hence Hypothesis* (H′3) *amounts to saying that M cannot take arbitrarily large values.*

Using the same arguments as in the proof of Theorem 4.1, we have the following optimality result.

Theorem 4.2. *Suppose that* (H′1), (H2) *and* (H′3) *hold true. Then an optimal control satisfies the following properties:*

(i) If $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case I), then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ *is given by*

$$u_h^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \delta_{SA}^\alpha(s) \\ 0 & \text{if} \quad M > \delta_{SA}^\alpha(s) \\ u_s^\alpha(s) & \text{if} \quad M = \delta_{SA}^\alpha(s) \quad \text{and } s \in [0, s_1^\alpha);\ (s, \delta_{SA}^\alpha(s)) \in F. \end{cases} \tag{4.5}$$

(ii) If $E_1 \in F_\alpha^-$ and $E_0 \notin F_\alpha^-$ (case II), then for any initial condition in F_α^+, an optimal control satisfies $u = 0$ and $u = 1$ until reaching Γ_0. Moreover, for any initial condition in F_α^-, an optimal control is given by (4.5).

(iii) If $E_1 \in F_\alpha^-$ and $E_0 \in F_\alpha^-$ (case III), then an optimal feedback control in F_α^+ is given by

$$u_h^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \delta_{SA}^\alpha(s) \\ 0 & \text{if} \quad M > \delta_{SA}^\alpha(s) \\ u_s^\alpha(s) & \text{if} \quad M = \delta_{SA}^\alpha(s) \quad \text{and } s \in (s_1^\alpha, s_c) \end{cases} \tag{4.6}$$

Remark 4.4. *(i) In the previous Theorem, Case I and Case III corresponds to a most rapid approach to the singular arc Δ_{SA}^α as in Theorem 3.1.*
(ii) When α goes to 1, we have $f_{SA}^\alpha(s, M) \to f_{SA}^1(s, M) = (M - s)(s_{in} - s)(M - s_{in})\mu'(s)$ and we have seen that Δ_{SA}^1 is the line segment $\{s^\star\} \times (s^\star, s_{in})$. Thus, the feedback control (4.5) *obtained in Theorem 4.2 converges to* (3.8) *when α goes to 1.*

Whenever $s_{in} < \bar{M} < \frac{s_{in}}{\alpha}$ (as in case II of section 4.1), then we can show that the
then there is a saturation phenomenon for the singular arc and the existence of a switching curve. Hence similar results can be expected . However, we have not detailed this for brevity.

5 Conclusion, Discussion, Perspectives

In this paper, we have provided an optimal synthesis of a two-dimensional system describing a chemostat model including recirculation. The analysis has revealed the importance of turnpike singular arcs in the optimal synthesis. We has shown that optimal trajectories are based on a most rapid approach to a turnpike (in absence of saturation phenomenon) depending on the kinetics. When the singular control saturates the maximal admissible value, then the optimal synthesis exhibits a switching curve and the existence of frame points.

From a practical point of view, the analysis has raised the following points:

- Whereas singular arcs usually appear for Haldane kinetics (see e.g. [2, 15]), our results show that a singular arc appears for Monod kinetics. This is due to the presence of the recirculation parameter α.
- We have pointed out that the optimal synthesis depends on the position of the target point w.r.t. characteristic elements of the system (such as steady state singular points). This information can be useful for a practitioner to drive optimally the system to a target point.
- Whenever $\alpha < 1$, there exist target points that can be reached by any initial condition in the state space. The analysis of the problem has also revealed that for $\alpha = 1$, this cannot happen (this is due to the existence of an invariant manifold by the system). Thus, a practitioner can take advantage of a chemostat with a recirculation loop to pilot the system to a desired target from any initial condition in the state space.
- The optimal feedback (4.4) is robust in the sense that if α is close to one, then it coincides with the optimal one for $\alpha = 1$ (see (3.6)).
- The optimal synthesis highly depends on the parameter α, nevertheless we can observe that when α goes to 1, the optimal synthesis slightly differs from the case $\alpha = 1$. However, we are not aware of general results concerning the behavior of optimal syntheses or feedback controls w.r.t. parameters.

In general uncertainties can affect the system, hence our optimal feedback strategies can be used to drive the system optimally to a neighborhood of the target point and then a feedback control is designed to stabilize the system at the desired target. The combination of these two approaches could be the basis of future works.

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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. Hence, we have two cases depending if the trajectory has a switching point from $u = 0$ to $u = 1$ or not. 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 $s = s_{in}$ in the case where $\tilde{M}$ is such that $\tilde{M} = \bar{M}$.

Finally, take an initial condition (s_0, M_0) such that $\tilde{M} < M_0 < M_{out}$ and $s_0 > s^\dagger(M_0)$. Suppose that we have $u = 1$ at time 0. Then, as $s_0 > s^\dagger(M_0)$, the trajectory necessarily satisfies $u = 1$ until reaching Γ_0 (using claim 6.1), and we obtain again a contradiction. Thus, there exists a unique 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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