Time-optimal control of concentrations changes in the chemostat with one single species

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Time-optimal control of concentrations changes in the chemostat with one single species[*]

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Abstract

We consider 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 Pontryagin's Principle and geometric control theory for a large class of kinetics.

Keywords. Chemostat model, Optimal feedback, Pontryagin Maximum Principle, Singular control.

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 as Haldane), 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, 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 in [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 [20] or [18, 25] and references herein).

Our interest in this paper is the optimal control of 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 [21]. Classically, the model of the chemostat is written as:

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

where x and s are the micro-organisms and 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 Monod growth function), 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.* [12, 22, 11]). 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 $\alpha > 0$ can be introduced in the dynamic of x and the model becomes:

$$\begin{cases} \dot{x} & = \mu(s)x - \alpha Dx, \\ \dot{s} & = -\frac{1}{\gamma}\mu(s)x + D(s_{in} - s), \end{cases} \tag{1.2}$$

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) and for a large class of growth functions. In particular, except for some specific results obtained in section 5 in considering Haldane functions, one originality of our approach is that instead of considering models with analytical functions such as Monod or Haldane (see [14]), we establish generic results for two general classes of functions that will be said to be 'of Monod-type' or 'of Haldane-type' depending on their qualitative properties (cf. Hypotheses (H1) and (H1')). In addition, one essential feature in the model considered in the present study (*i.e.* (1.2)) is that the presence of the 'recirculation parameter α leads to an asymmetry between x and s (when $\alpha = 1$, the chemostat has a cascade structure by considering $M = x + s$ in place of x, *i.e.* the equation for M depends only on M and D). We will first provide a complete study of the problem when $\alpha = 1$ extending the preliminary results in [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 greater than s_{in} (see Theorem 4.2). 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-type functions.

The paper is organized as follows. In section 2, we state the optimal control problem, and we apply the Pontryagin Maximum Principle on the optimal control problem to derive optimality conditions. We also give properties of the *switching function* that are crucial in sections 4 and 5 to prove optimality results. Next, we characterize in section 3 the controllability set *i.e.* the set of points that can reach the target in finite horizon (see *e.g.* [23] in the fed-batch model). In section 4, we provide an optimal feedback control for Haldane-type kinetics when $\alpha = 1$ (Theorems 4.1 and 4.2 are our main results), and section 5 discusses the case $\alpha < 1$ (see Theorem 5.1 for Monod kinetics and Theorems 5.2 and 5.3 for Haldane kinetics). The article concludes with an appendix containing the proof of technical results such as the existence of a switching curve for $\alpha = 1$ and a table with the parameter values that are used in the numerical simulations.

2 Preliminaries

2.1 Statement of the problem

We consider the system

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

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 $u(\cdot)$ is the dilution rate which is the control variable. For convenience and without loss of generality, it is supposed the substrate and the biomass are in the same units. The admissible control set is defined as:

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

where u_{max} is the maximal value for the dilution rate. 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 this set.

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 section 3. 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

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

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) defined 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 from $(\bar{s}, \bar{M})$ 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 also 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 for (2.3) such that the associated trajectory steers (2.4) from (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:

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

- The pair $(\lambda_0, \lambda(\cdot))$ is non-trivial *i.e.* $(\lambda_0, \lambda(\cdot)) \neq 0$.

- The following maximization condition holds true :

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

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 the extremal is *normal*. 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

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

If we differentiate ϕ w.r.t. t, we find using (2.6) that a.e.:

$$\dot{\phi} = (M - s)[\lambda_s \mu'(s)(s_{in} - s) + (1 - \alpha)(\lambda_M + \lambda_s)\mu(s)]. \tag{2.9}$$

Now, the maximization condition (2.7) can be then expressed as follows:

$$\begin{cases} \phi(t) > 0 &\Rightarrow u(t) = +1, \\ \phi(t) < 0 &\Rightarrow u(t) = 0, \\ \phi(t) = 0 &\Rightarrow u(t) \in [0, 1]. \end{cases} \tag{2.10}$$

A *switching time* (or switching point) is a time t_0 such that the control $u(\cdot)$ is non-constant in any neighborhood of t_0. At a switching time t_0, we necessarily have $\phi(t_0) = 0$. We say that an admissible control $u(\cdot) \in \mathcal{U}$ is *bang-bang* over a time interval $[t_1, t_2]$ if $u(t) \in \{0, 1\}$ for a.e. $t \in [t_1, t_2]$. It is convenient to introduce the following notation: a Bang arc $u = 1$, resp. $u = 0$ will be denoted by B_+, resp. by B_-.

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 *collinearity 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.

- A *singular arc* (denoted by S) is a time interval $I = [t_1, t_2]$ where the switching function vanishes. In the two-dimensional setting, the corresponding trajectory necessarily belongs to the so-called *singular locus*[1] Δ_{SA}^α which is a subset of codimension 1 (see *e.g.* [19, 24] for more details on the definition).

- A *switching curve* $\mathcal{C}$ is a locus in the state space where the control u has a switching point from 1 to 0 or from 0 to 1 (the corresponding instant of switching is called *switching time*).

---

[1]If (2.4) is written $\dot{z} = f(z) + ug(z)$ with $f, g : \mathbb{R}^2 \to \mathbb{R}^2$, then Δ_{SA}^α is the set of points $z \in F$ where $g(z)$ is collinear to $[f, g](z)$, the Lie bracket of f and g, see *e.g.* [6, 7].

An important property of Δ_0^α is that any switching point of an abnormal trajectory necessarily occurs on Δ_0^α (see [7, 6]). 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:

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

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 (ordinary differential equation) satisfied by the switching function ϕ and will be crucial in the optimal synthesis of the problem (see sections 4 and 5).

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) *Let $S_+ := \left\{(s, M) \in F \; ; \frac{f_{SA}^\alpha(s,M)}{f_0^\alpha(s,M)} > 0\right\}$, resp. $S_- := \left\{(s, M) \in F \; ; \frac{f_{SA}^\alpha(s,M)}{f_0^\alpha(s,M)} < 0\right\}$. Then, if the extremal $(z(\cdot), \lambda(\cdot), u(\cdot))$ is optimal, any switching point t_c such that $(s(t_c), M(t_c)) \in S_+$, resp. $(s(t_c), M(t_c)) \in S_-$ is from $u = 1$ to $u = 0$, resp. from $u = 0$ to $u = 1$.*

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 into (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 the values of λ_M and λ_s in (2.9), 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 first that if the trajectory belongs to the set S_+ or S_-, then the control u is necessarily bang-bang from (2.10). Consider now a switching time t_c from $u = 0$ to $u = 1$ in S_+. We thus have $\phi(t_c) = 0$ and $\dot{\phi}(t_c^-) \geq 0$ (as ϕ is negative in a left neighborhood of t_c) and we obtain that $-\frac{f_{SA}^\alpha(s(t_c), M(t_c))}{f_0^\alpha(s(t_c), M(t_c))} \geq 0$ whenever $(s(t_c), M(t_c)) \notin \Delta_0^\alpha$. We thus get a contradiction as we have $(s(t_c), M(t_c)) \in S_+$. This shows that any switching point in S_+ is from $u = 1$ to $u = 0$. A similar reasoning shows the second part of (ii) in S_-. $\square$

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 [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.

Let us now turn to *Legendre-Clebsch condition* which is useful to test the optimality of a singular arc. Recall that if a singular arc is optimal (in this case, it is also called *turnpike*, see *e.g.* [7]), then Legendre-Clebsch necessary optimality condition must hold true (see *e.g.* [19]), 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 not optimal over a time interval $I = [t_1, t_2]$ is called *anti-turnpike* [7].

3 Controllability results

In this section, we characterize for each target point $(\bar{s}, \bar{M})$ the controllability set *i.e.* the set of points that can reach $(\bar{s}, \bar{M})$ in finite horizon. 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.

Proposition 3.1. *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* $E_0 \notin F_\alpha^-$, *the controllability set is* F_α^-.

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

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

Proof. In view of (2.4), we have $\dot{M}_{|u=1} > 0$, resp. $\dot{M}_{|u=1} < 0$ at a given point $(s, M) \in F$ if and only if (s, M) is below Δ_0^α, resp. above Δ_0^α. The proof of (i) and (iii) is similar by considering *the extended velocity set*

$$\left\{ \begin{pmatrix} -\mu(s)(M - s) + u(s_{in} - s) \\ u(s_{in} - s - \alpha(M - s)) \end{pmatrix} ; \ u \in [0, 1] \right\},$$

either in F_α^- (case (i)) or in F_α^+ (case (iii)), see Fig. 1. So we only prove (i).

Figure 1: Extended velocity set of (2.4) at a given point (s, M) in F_α^- (picture left) and in F_α^+ (picture right).

Consider an extremal trajectory starting in $F \backslash F_\alpha^-$. If the trajectory reaches Γ_0 at a time t_0 then there exists a left neighborhood of t_0 where the trajectory is below Δ_0^α. Moreover we can assume that t_0 is the first time where the trajectory hits Γ_0. In view of the extended velocity set in Δ_0^α (see Fig. 1) we see that the only possibility is to have $u = 0$, but this would imply that the trajectory has already reached the curve Γ_0 at a time $t < t_0$, and we thus have a contradiction with the definition of t_0. A similar reasoning shows that an extremal trajectory starting in $F \backslash F_\alpha^-$ cannot hit Γ_1. To conclude this case, we see that any initial condition in F_α^- can reach the target point by taking the control law $u = 1$ until reaching Γ_0 and then $u = 0$ until reaching the target point. This proves (i).

Let us now prove (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[2] steady-state for (2.4). As we have $s_{in} < \bar{M} < \frac{s_{in}}{\alpha}$, the trajectory necessarily intersects Γ_0 at a time $t_0 > 0$. For $t > t_0$, the control $u = 0$ steers (2.4) into the target point in finite time. This shows that the target is reachable from $F \backslash F_\alpha^-$. Let us now take an initial condition $(s_0, M_0) \in F_\alpha^-$. As $E_0 \notin F_\alpha^-$, the curve Γ_1 exits F through $s = 0$ at a value for M such that $M < \frac{s_{in}}{\alpha}$. The strategy that we now describe drives any initial condition $(s_0, M_0) \in F_\alpha^-$ to the target point. Take the control $u_{s_0} = \mu(s_0) \frac{M - s_0}{s_{in} - s_0}$ (that corresponds to $\dot{s} = 0$). From (H2) one has $\mu(s_0) \frac{M - s_0}{s_{in} - s_0} < \alpha \frac{M - s_0}{s_{in} - s_0}$, and as in this case we have $M < \bar{M} < \frac{s_{in}}{\alpha}$, we deduce that $\alpha \frac{M - s_0}{s_{in} - s_0} < 1$ using that (s, M) is below Δ_0^α. Hence the control u_{s_0} is admissible until reaching $\Gamma_0 \cup \Gamma_1$. Finally, take either $u = 0$ or $u = 1$ depending if the trajectory has reached Γ_0 or Γ_1. The corresponding trajectory reaches the target point which ends the proof. $\square$

Remark 3.1. *(i) Let γ be the graph of the unique solution of (2.4) with $u = 1$ starting from E_0. Then, case (iii) of the previous proposition occurs if and only if the target point $(\bar{s}, \bar{M})$ is above γ (in fact Γ_1 and γ cannot intersect by Cauchy-Lipschitz's Theorem).*
(ii) In the case (ii) of the previous proposition, the controllability set is the state domain F, hence any initial condition in F can reach the target point $(\bar{s}, \bar{M})$.
(iii) When $\alpha = 1$, then if $\bar{M} < s_{in}$ the controllability set for (2.3) is F_1^- whereas if $\bar{M} > s_{in}$ the controllability set for (2.3) is F_1^+.

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[2]This property is standard: as $\mu(s) < \alpha$ for all $s \in [0, s_{in}]$, one has $x(t) \to 0$ when $t \to +\infty$ which implies the result.

4 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

$$\dot{M} = u(s_{in} - M), \tag{4.1}$$

hence (2.4) has a cascade structure. In view of (4.1) we can assume that either $M < s_{in}$ or $M > s_{in}$ depending on the choice of $\bar{M}$ w.r.t. s_{in}. Indeed, for $M = s_{in}$, the optimal control problem is one-dimensional and is straightforward. We consider in this section the following hypothesis on μ:

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

Remark 4.1. (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 $\Delta_0^1 = (\{0\} \times \mathbb{R}_+^*) \cup \{(s,s) \; ; \; s \in [0, s_{in}]\} \cup ([0, s_{in}] \times \{s_{in}\})$ thus $\Delta_0^1 \cap \mathrm{Int}(F) = \emptyset$, 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

$$\dot{\phi} = \frac{(s_{in} - s)\mu'(s)}{\mu(s)} u\phi - \frac{(s_{in} - s)\mu'(s)}{\mu(s)}, \tag{4.2}$$

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 it is given by:

$$u_s(M) := \mu(s^\star)\frac{M - s^\star}{s_{in} - s^\star} \quad \text{for} \quad M > s^\star. \tag{4.3}$$

Furthermore, $M_{u_s}(\cdot)$ is solution of the ODE

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

We can check that Legendre optimality condition (2.15) is satisfied along the singular arc Δ_{SA}^1. Indeed, differentiating (4.2) w.r.t. t yields:

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

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

4.1 Study of the case $\bar{M} < s_{in}$

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 (4.1)).

- We have $\dot{s}_{|_{u=1}} > 0$. In fact, $M < s_{in}$ and (H2) imply the inequality $\mu(s) < 1 < \frac{s_{in} - s}{M - s}$. We obtain the result using (2.4).

- As $\bar{M} < s_{in}$, the singular locus becomes $\Delta_{SA}^1 = \{s^\star\} \times (s^\star, s_{in})$.

- 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_{SA}^1.

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 the controllability set F_1^- can be written as:

$$F_1^- = \{(s, M) \in F \; ; \; M \leq \min(\varphi_0(s), \varphi_1(s))\}. \tag{4.4}$$

We then have the following optimality result.

Theorem 4.1. *If* (H'1) *and* (H2) *hold true and if the target point is such that* $\bar{M} < s_{in}$, *then an optimal feedback control in* $\text{Int}(F_1^-)$ *is given by* :

$$\begin{cases} u^\star[s, M] & = 0 & \text{if } s > s^\star, \\ u^\star[s, M] & = 1 & \text{if } s < s^\star, \\ u^\star[s, M] & = u_s(M) & \text{if } s = s^\star. \end{cases} \tag{4.5}$$

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 with the control $u = 0$ or $u = 1$. Therefore singular trajectories are optimal until reaching $\Gamma_0 \cup \Gamma_1$. $\qquad\square$

The optimal synthesis provided by Theorem 4.1 is depicted on Fig 2.

Remark 4.2. *(i) If* $\bar{s} < s^\star$, *then a singular trajectory will reach* $\bar{M}$, *and then we have* $u = 0$ *until reaching the target (see Fig. 2 left). If* $\bar{s} > s^\star$, *then a singular trajectory will reach* Γ_1, *and then we have* $u = 1$ *until reaching the target (see Fig. 2 right).*
(ii) When $s^\star > s_{in}$, *the previous considerations show that for Monod-type kinetic function the feedback*

$$\begin{cases} u_m[s, M] & = 1 & \text{if } (s, M) \in F_1^- \backslash \Gamma_0, \\ u_m[s, M] & = 0 & \text{if } (s, M) \in \Gamma_0, \end{cases} \tag{4.6}$$

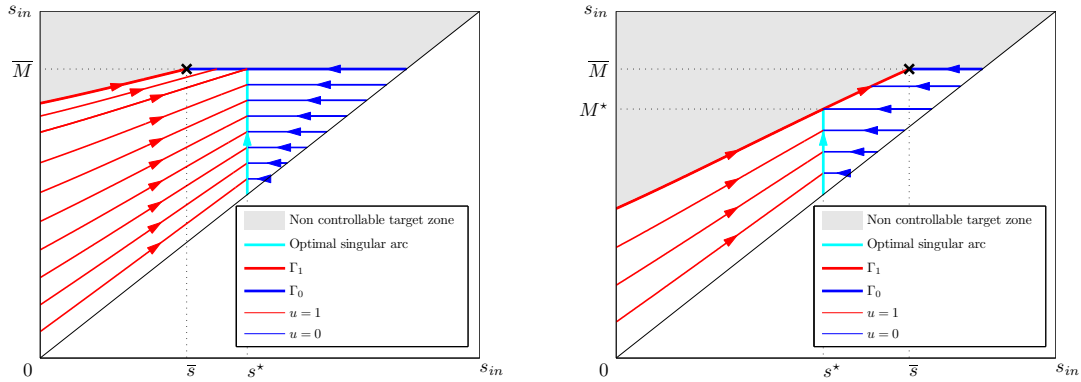*is optimal (we retrieve the results of [8]).*

Figure 2: 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_{SA}^1 intersects Γ_0). *Picture right*: the target point is such that $\bar{s} > s^\star$ (the singular arc Δ_{SA}^1 intersects Γ_1).

4.2 Study of the case $\bar{M} > s_{in}$

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 (4.1), we have $\dot{M} \leq 0$ for any control u.

- The singular control u_s is admissible provided that we have $M \in (s_{in}, M_{sat}]$ where M_{sat} is uniquely defined by $u_s(M_{sat}) = 1$, that is:

$$M_{sat} := s^\star + \frac{s_{in} - s^\star}{\mu(s^\star)}. \tag{4.7}$$

- For $M > M_{sat}$ one has $u_s(M) > 1$.

- As $\bar{M} > s_{in}$, the singular locus becomes $\Delta_{SA}^1 = \{s^\star\} \times (s_{in}, M_{sat})$.

Notice that $M_{sat} > s_{in}$ and that the unique solution of (2.4) passing through $(s^\star, M_{sat})$ is vertical at this point (see Fig. 3). Observe also that $\frac{ds}{dt}\big|_{u=1}$ is not of constant sign along $u = 1$ as in the previous case (see also Fig. 3 for the plot of the flow of (2.4) for the constant control $u = 1$), but one has $\frac{dM}{dt}\big|_{u=1} < 0$.

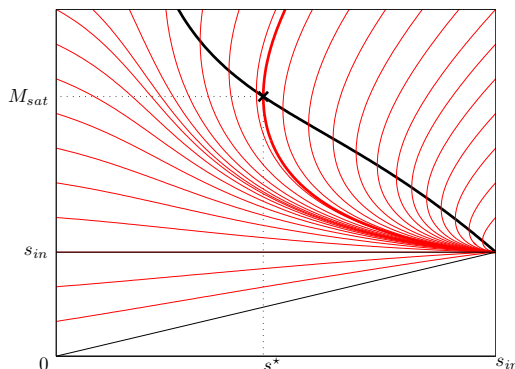

Figure 3: Flow of (2.4) with $u = 1$ ($s_{in} = 3$). The black curve is the set of points where solutions of (2.4) with $u = 1$ are vertical.

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:

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

4.2.1 Switching curve and optimal synthesis

Whereas in the case $M < s_{in}$, the singular arc is always admissible, we have now a *saturation phenomenon* for the singular control, that is the singular arc is non-admissible when $M > M_{sat}$ (see (4.7)). This will imply the existence of a switching curve $\mathcal{C}$ emanating from the singular arc. In the next lemma, we provide a description of this locus.

Lemma 4.1. *Let $\tilde{M} := \max(\bar{M}, M_{sat})$. There exists $M_e \in (\tilde{M}, +\infty]$ and a function $s_c : [\tilde{M}, M_e] \to \mathbb{R}_+$ $M \longmapsto s_c(M)$ satisfying the following properties:*

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

(2) For any $M \in (\tilde{M}, M_e)$, there exists exactly one point $s_c(M)$ such that an optimal control $u(\cdot)$ steering (2.4) to the target satisfies $u = 0$ for $s > s_c(M)$ and $u = 1$ for $s^\star < s < s_c(M)$.

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 4.3. *(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_{SA}^1, see Fig. 4 and Fig. 5*
(ii) If $\tilde{M} = \bar{M}$ i.e. if $\bar{M} > M_{sat}$, then $\mathcal{C} \cap \Delta_{SA}^1 = \emptyset$ and $\mathcal{C}$ intersect Γ_0 at the point $(s^\star, \bar{M})$, see Fig. 6.

	Subcase a: $\bar{s} < s^\star$	Subcase b: $\bar{s} > s^\star$	Optimal synthesis
Case I: $\bar{M} < s_{in}$	Fig. 2	Fig. 2	Theorem 4.1
Case II: $s_{in} < \bar{M} < M_{sat}$	Fig. 4	Fig. 5	Theorem 4.2
Case III: $\bar{M} > M_{sat}$	Fig. 6	Fig. 7	Theorem 4.2

Table 1: List of the cases illustrating Theorems 4.1 and 4.2.

We obtain the following optimality result.

Theorem 4.2. *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 :*

$$\begin{cases} u^\star[s, M] &= u_s(M) & \text{if } s = s^\star & \text{and } M < M_{sat}, \\ u^\star[s, M] &= 1 & \text{if } s < h(M) & \text{and } M > \bar{M}, \\ u^\star[s, M] &= 0 & \text{elsewhere.} \end{cases} \qquad (4.8)$$

Proof. The proof is straightforward using the previous lemma and the same arguments as in the proof of Theorem 4.1 to exclude extremal trajectories that are not optimal. $\qquad\square$

The optimal synthesis provided by Theorem 4.2 is depicted on Fig. 4, Fig. 5, Fig. 6 and 7 for different cases that are explained below.

4.2.2 Numerical simulations

We present here the numerical computation of the curve $\mathcal{C}$ defined by $M \longmapsto s_c(M)$. We consider the three-dimensional system (2.4)-(4.2) with $u = 1$ backward in time, that is:

$$\begin{cases} \frac{ds}{dt} &= \mu(s)(M - s) - s_{in} - s, \\ \frac{dM}{dt} &= -(s_{in} - M), \\ \frac{d\phi}{dt} &= -\frac{(s_{in}-s)\mu'(s)}{\mu(s)}\phi + \frac{(s_{in}-s)\mu'(s)}{\mu(s)}, \end{cases} \qquad (4.9)$$

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 necessarily satisfies $\phi(t) = 0$ (the instant t is a switching time). Hence, for a given point $(s_0, M_0) \in \Gamma_0 \cup \Delta^1_{SA}$, we integrate (4.9) from $(s_0, M_0, 0)$ at time zero 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 4.1, 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 Theorems 4.1 and 4.2, 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} (see Table 1).

Remark 4.4. *In Fig. 4, 5, 6 and 7, 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* (s_0, M_0) *for* (4.9) *on* Δ^1_{SA}, *resp. on* Γ_0.

4.2.3 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 $s_c(M_e) = s_{in}$ (see Fig. 4,5,6 picture left).

Proposition 4.1. *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. Suppose that $\mathcal{C}$ stops at some point $(s_c(M_e), M_e)$ such that $\psi_1(M_e) < s_c(M_e) < s_{in}$. We then consider the unique solution of (2.4) with $u = 1$ 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 $s_c(M_e) < s_0 < s_{in}$,
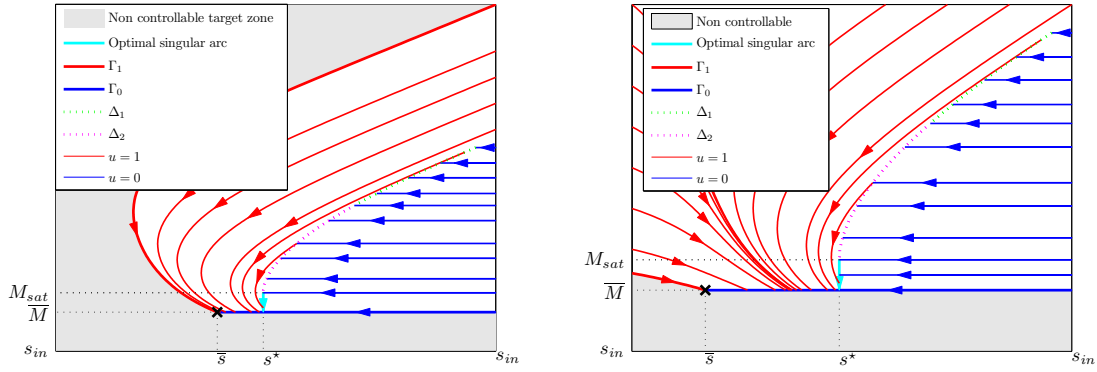
Figure 4: Case II a. Optimal synthesis for $\alpha = 1$, $s_{in} < \bar{M} < M_{sat}$ and $\bar{s} < s^\star$. The dotted line represents the switching curve $\mathcal{C}$ (in purple, resp. in green, it is obtained by integrating (4.9) backward in time from Δ_{SA}^1, resp. from Γ_0). The curve Γ_1 exits F through $s = s_{in}$ (picture left) or through $s = 0$ (picture right).
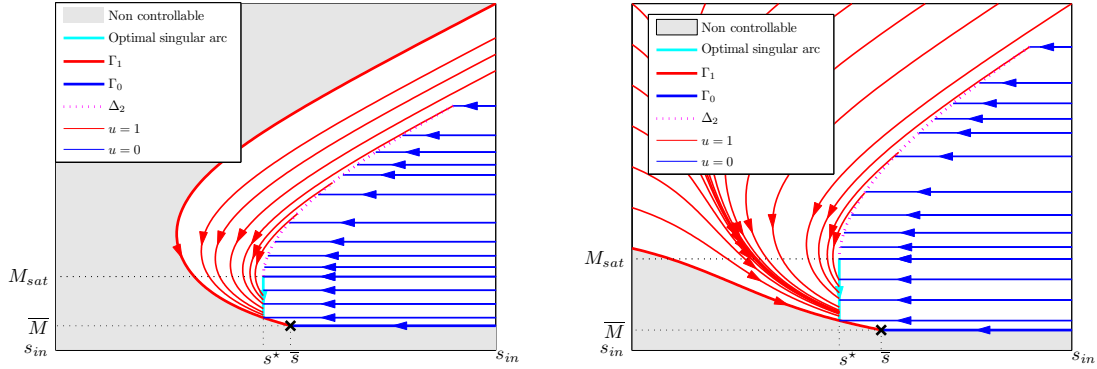

Figure 5: Case II b. Optimal synthesis for $\alpha = 1$, $s_{in} < \bar{M} < M_{sat}$ and $\bar{s} > s^\star$. The dotted line represents the switching curve $\mathcal{C}$ (in purple, resp. in green, it is obtained by integrating (4.9) backward in time from Δ_{SA}^1, resp. from Γ_0). The curve Γ_1 exits F through $s = s_{in}$ (picture left) or through $s = 0$ (picture right).

$M_0 > M_e$. 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).

Similarly, $\mathcal{C}$ cannot intersect Γ_1 before reaching $s = s_{in}$ at some point (s', M') as in that case an optimal trajectory starting from a point $(s_0, M_0) \in F_1^+$ with $s_0 > s'$, $M_0 > M'$ would necessarily satisfy $u = 1$ until reaching Γ_0 at a point $s > s^\star$. We obtain a contradiction using Proposition 2.1 (ii).

The previous arguments show that $s_c(M_e) = s_{in}$ and that $M_e \leq M_{out}$.

□

Remark 4.5. *We can prove that the curve $\mathcal{C}$ 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 4.1 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
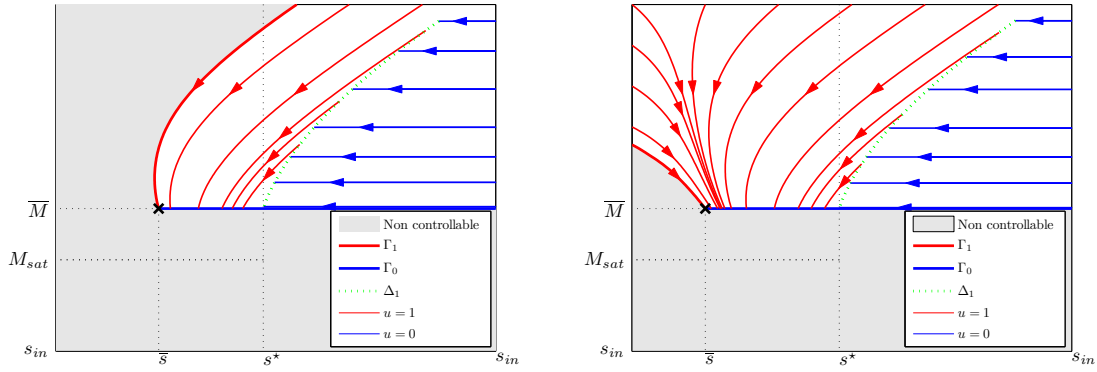
Figure 6: Case III a. Optimal synthesis for $\alpha = 1$, $M > M_{sat}$ and $\bar{s} < s^\star$. The dotted line in green represents the switching curve $\mathcal{C}$ (it is obtained by integrating (4.9) backward in time from Γ_0). The curve Γ_1 exits F through $s = s_{in}$ (picture left) or through $s = 0$ (picture right).
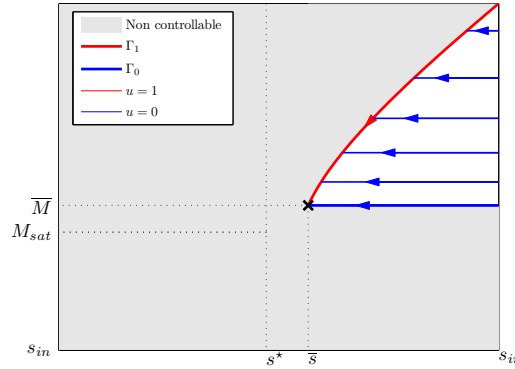

Figure 7: Case III b. Optimal synthesis for $\alpha = 1$, $M > M_{sat}$ and $\bar{s} > s^\star$. In this case, the curve Γ_1 exits F through $s = s_{in}$ only.

initial conditions such that $M \gg s_{in}$ are not interesting for a practitioner. 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 $v(x_0, s_0)$ (recall (2.3)) is the time of an arc $u = 1$ connecting $(\bar{s}, \bar{M})$ to Γ_0 or Δ_{SA}^1. Hence, if $\bar{M} \gg s_{in}$, there is no evidence that optimal trajectories will benefit from a switching time (from $u = 0$ to $u = 1$) before reaching Γ_0 or Δ_{SA}^1.

5   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_0^α is the line segment of equation:

$$\delta_0^\alpha(s) := s + \frac{s_{in} - s}{\alpha}, \ s \in [0, s_{in}].$$

Whereas in the case $\alpha = 1$ the subset of F defined by $M = s_{in}$ is invariant by (2.4) (see (4.1)), trajectories of (2.4) can cross the set Δ_0^α for $\alpha < 1$. Using (2.11), we find that the singular locus Δ_{SA}^α is the graph of the

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

where
$$\psi_{\alpha}(s) := \frac{1}{\alpha} \frac{\mu'(s)(s_{in} - s)^2}{(s_{in} - s)\mu'(s) + (1 - \alpha)\mu(s)}. \tag{5.1}$$

Note that the functions ψ_{α} and δ_{SA}^{α} 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_s^{α} as a function of s (whenever it is well defined):
$$u_s^{\alpha}(s) := \frac{\mu(s)\psi_{\alpha}(s)(1 + \psi_{\alpha}'(s))}{\alpha\psi_{\alpha}(s) + \psi_{\alpha}'(s)(s_{in} - s)}. \tag{5.2}$$

In order to verify if (2.15) holds true along a singular extremal (see section 5.1) we have the following lemma.

Lemma 5.1. *Along a singular arc $I = [t_1, t_2]$ such that $(s_{in} - s(t))\mu'(s(t)) + (1 - \alpha)\mu(s(t))$ is non-zero over $[t_1, t_2]$, one has*

$$\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u = (1 - \alpha)(s_{in} - s(t))^2 \frac{(2 - \alpha)\mu(s(t))\mu'(s(t)) + 2(s_{in} - s(t))\mu'(s(t))^2 - (s_{in} - s(t))\mu(s(t))\mu''(s(t))}{\mu(s(t))[s_{in} - s(t) - \alpha(M(t) - s(t))][(s_{in} - s(t))\mu'(s(t)) + (1 - \alpha)\mu(s(t))]}. \tag{5.3}$$

Proof. From the expressions of f_{SA} and f_0 (see (2.11)) we obtain:
$$\frac{f_{SA}(s, M)}{f_0(s, M)} = -\frac{\alpha(M - s)((1 - \alpha)\mu(s) + \mu'(s)(s_{in} - s) - (s_{in} - s)^2\mu'(s))}{\mu(s)(s_{in} - s - \alpha(M - s))}.$$

In order to compute $\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u$, we differentiate (2.13) w.r.t. t along the singular arc $M - s = \psi_{\alpha}(s)$ keeping only the component in front of u (this computation can be also performed using Lie brackets, however we did not introduce this notation for brevity). We find that
$$\frac{d}{dt}\left(-\frac{f_{SA}(s(t), M(t))}{f_0 s, M}\right)\Big|_u = \frac{-\alpha^2(1 - \alpha)x\mu(s) + 2(s_{in} - s)(s_{in} - s - \alpha^2 x)\mu'(s) + \mu''(s)(s_{in} - s)^2(\alpha x - (s_{in} - s))}{\mu(s)(s_{in} - s - \alpha x)},$$

omitting the time dependency for brevity and writing x in place of $M - s$. By replacing x into the previous equality by $\psi_{\alpha}(s)$ using (5.1), we find (5.3). $\qquad \square$

We now discuss the optimal synthesis of the problem for Monod- and Haldane-type kinetics. In particular, we will analyze if ψ_{α} and u_s^{α} are well defined over $[0, s_{in}]$ (see (5.1) and (5.2)).

5.1 Optimal synthesis for Monod-type kinetic function

We suppose in this section that the growth rate function is given by:
$$\mu(s) := \frac{\mu_{max}s}{k + s}, \tag{5.4}$$

where $\mu_{max} > 0$ and $k > 0$. Notice that $\mu > 0$, $\mu' > 0$ and $\mu'' < 0$ over the interval $(0, s_{in}]$. Therefore ψ_{α} and δ_{SA}^{α} are well defined over $[0, s_{in}]$. From (5.1)-(5.3), 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 positive, resp. negative on the interval $(0, s_m)$, resp. (s_m, s_{in}) where $s_m \in (0, s_{in})$ is defined as 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 Δ_{SA}^{α}).

- Using (5.3) and the fact that $\mu' > 0$, $\mu'' < 0$ for Monod-type kinetics (see (5.4)), we find that Legendre-Clebsch optimality condition (2.15) is satisfied along Δ_{SA}^{α}.
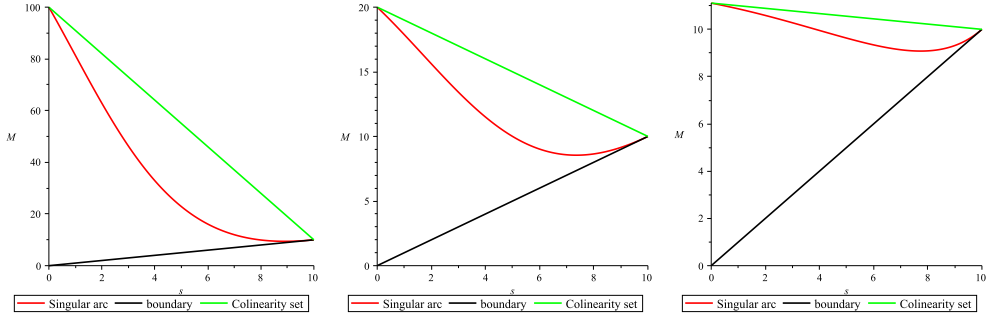
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Figure 8: Plot of Δ_0^α and Δ_{SA}^α for $\alpha = 0.1, 0.5, 0.9$ with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$.
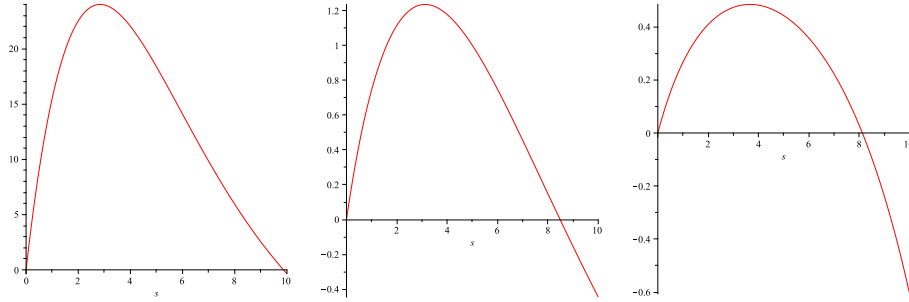

Figure 9: Plot of the singular control $s \longmapsto u_s^\alpha(s)$ given by (5.2) with $\mu(s) = \frac{s}{5+s}$ and $s_{in} = 10$ for $\alpha = 0.1, 0.5, 0.9$.

Figures 8 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 9. 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 $s \in [0, s_m)$.

Remark 5.1. *When α goes to 1, then $\psi_\alpha(s) \sim s_{in} - s$, thus we find that $u_s^\alpha(s) \sim \mu(s)$, therefore using that $\mu(s) < \alpha < 1$ for any $s \in [0, s_{in}]$ (see Hypothesis (H1)), we conclude that (H3) is satisfied when α is sufficiently close to 1.*

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 Proposition 3.1. When $E_0 \notin F_\alpha^-$, we introduce the feedback control law:

$$u_m^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \delta_{SA}^\alpha(s), \\ 0 & \text{if} \quad M > \delta_{SA}^\alpha(s) \text{ or } (M = \delta_{SA}^\alpha(s) \text{ and } s > s_m), \\ u_s^\alpha(s) & \text{if} \quad M = \delta_{SA}^\alpha(s) \text{ and } s < s_m, \end{cases} \qquad (5.5)$$

The optimal synthesis then reads as follows (see Fig. 10).

Theorem 5.1. *Suppose that μ is given by (5.4) and that (H2)-(H3) hold true. Then, one has the following optimality conditions.*

(i) If $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$, then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ is given by (5.5).

(ii) If $E_1 \in F_\alpha^-$ and $E_0 \notin F_\alpha^-$, then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ is given by (5.5) and an optimal feedback control satisfies $u = 1$ in $\mathrm{Int}(F_\alpha^+)$.

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

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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) except that there exists an abnormal extremal trajectory switching at the intersection between Γ_0 and Δ_0^α. The cost t_{abn} of this trajectory cannot be directly compared to the cost t_{min} of the trajectory corresponding to the control (5.5) as Proposition 2.1 only holds for normal trajectories. However, we can construct a sequence of normal trajectories γ_n converging to the abnormal one by considering trajectories with the control $u = 1$ until reaching Γ_0. Now, the cost t_{γ_n} of γ_n satisfies $t_{\gamma_n} \geq t_{min}$ using the previous argumentation. We then obtain the result by letting n goes to infinity.

Now, solutions of (2.4) with $u = 1$ starting above $\Gamma_0 \cup \Gamma_1$ necessarily converge to the point E_1 (see Lemma 3.1 (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 $\text{Int}(F_\alpha^+)$, we use (2.13) and similar arguments as in the proof of (i).

The proof of (iii) is similar to the proof of (ii) (by considering initial conditions above $\Gamma_0 \cup \Gamma_1$ only). $\qquad \square$

Remark 5.2. *(i) In Theorem 5.1, we point out that optimal trajectories can switch from $u = 1$ to $u = 0$ on the set $\Delta_{SA}^\alpha \cap ([0, s_m] \times [0, \bar{M}])$ that corresponds to a switching curve.*
(ii) Whenever $\alpha = 1$ and μ is of Monod-type, we know from (4.6) 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 that $\bar{M} < s_{in}$. We deduce that if α is sufficiently close to 1, then the feedback control law (5.5) coincides with (4.6). On the other hand, when $\bar{M} \geq s_{in}$, then an optimal feedback in F_α^+ is exactly the same as (4.6). This proves that the feedback control (4.6) (which does not depend on α) is optimal for any value of α sufficiently close to 1.

5.2 Optimality results for Haldane kinetic function

In this section, we discuss the optimal synthesis of the problem in the case where (H'1) holds true. Recall that this assumption implies $\mu'(s) > 0$ for $s \in [0, s^\star)$ and $\mu'(s) < 0$ for $s \in (s^\star, s_{in}]$. Thus, ψ_α can be not well defined if its denominator vanishes on $[0, s_{in}]$ which amounts to saying that there exist solutions of the equation

$$(s_{in} - s)\mu'(s) + (1 - \alpha)\mu(s) = 0, \tag{5.6}$$

over $[0, s_{in}]$. To simplify the study, we suppose that μ is an Haldane function, *i.e.*

$$\mu(s) := \frac{\mu_{max} s}{k_s + s + \frac{s^2}{k_i}} \quad \text{with } k_s > 0 \text{ and } k_i > 0. \tag{5.7}$$

Recall that the maximum of μ is obtained for $s^\star = \sqrt{k_i k_s} \in [0, s_{in}]$. We have the following technical lemma.

Lemma 5.2. *Suppose that μ is given by (5.7). Then the following properties hold true:*
(i) The equation (5.6) is equivalent to the cubic equation:

$$(2 - \alpha)s^3 + [(1 - \alpha)k_i - s_{in}]s^2 - \alpha k_i k_s s + k_i k_s s_{in} = 0. \tag{5.8}$$

(ii) The solutions of (5.8) satisfy one and only one of the three following properties:
- The equation (5.8) has exactly three negative solutions.
- The equation (5.8) has exactly one negative solution and two complex conjugate solutions.
- The equation (5.8) has exactly one negative solution and two positive solutions.

(iii) If α is sufficiently close to 1, then (5.6) has exactly two positive solutions over the interval $[0, s_{in}]$.

Proof. For sake of clarity, we have postponed the proof of this lemma to the appendix. $\qquad \square$
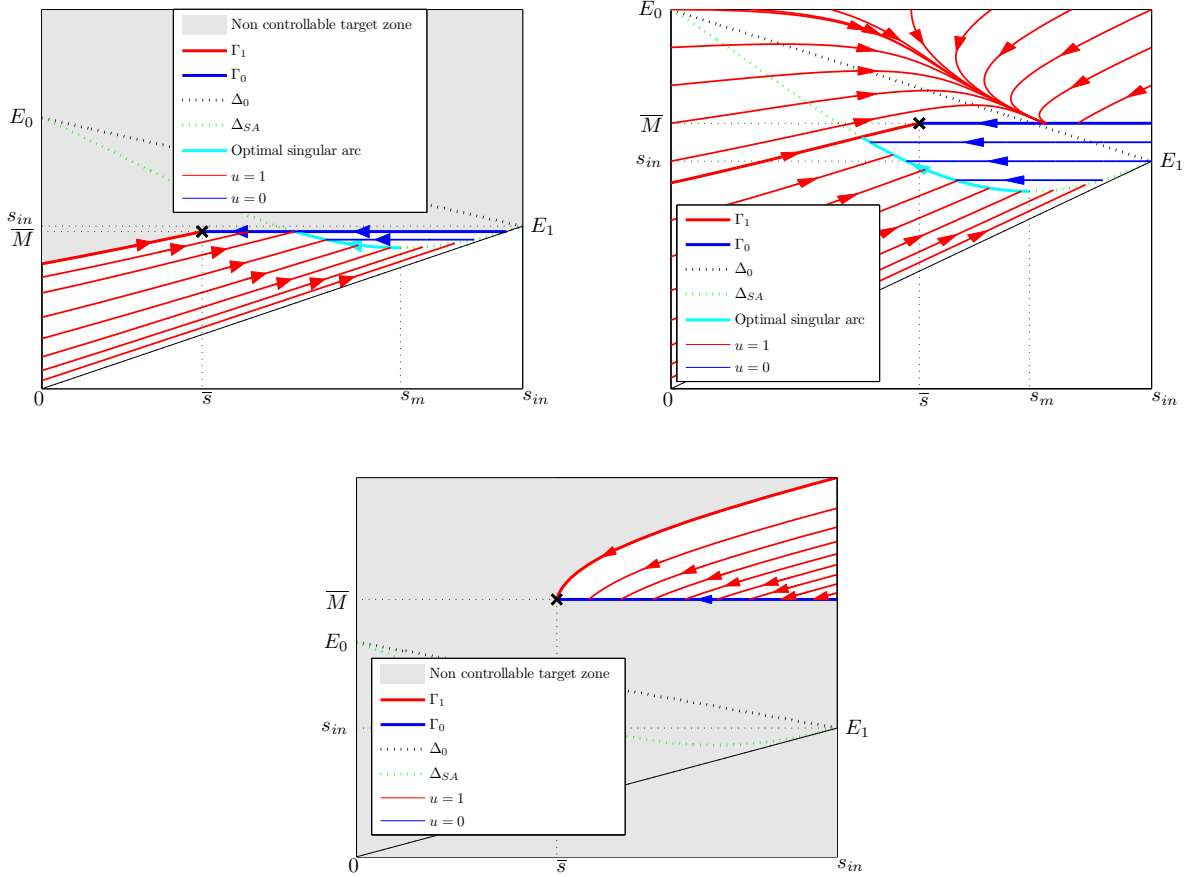
Figure 10: Optimal synthesis provided by Theorem 5.1 for $\alpha < 1$ in case (i) (above left), case (ii) (above right) and case (iii) (middle).

This result shows that only two cases occur depending on the parameter values α and s_{in}:

- The function ψ_α is well defined over $[0, s_{in}]$ i.e. (5.6) has no solution in $[0, s_{in}]$.

- The equation (5.6) has two positive solutions over $[0, s_{in}]$ and thus ψ_α has two poles on $[0, s_{in}]$.

The optimal synthesis of the problem is discussed hereafter in section 5.2.1, resp. section 5.2.2 whenever (5.6) has no solution in $[0, s_{in}]$, resp. two solutions over $[0, s_{in}]$.

5.2.1 Optimality results with one connected singular arc component

The case where (5.6) has no solution over $[0, s_{in}]$ is illustrated on Fig. 11. As for Monod-type kinetics, we observe that Δ_{SA} consists of one connected component in the set F. We introduce the following feedback control law:

$$u_h^\alpha[s, M] := \begin{cases} 1 & \text{if} \quad M < \delta_{SA}^\alpha(s), \\ 0 & \text{if} \quad M > \delta_{SA}^\alpha(s), \\ u_s^\alpha(s) & \text{if} \quad M = \delta_{SA}^\alpha(s). \end{cases} \tag{5.9}$$

We obtain the following optimality result in the line of Theorem 5.1 except that in this case the singular arc is always admissible.

Theorem 5.2. *Suppose that μ is given by (5.7), that (H2) holds true, and that the singular control is admissible in F, and that (5.6) has no solution over $[0, s_{in}]$. Then, one has the following optimality conditions.*
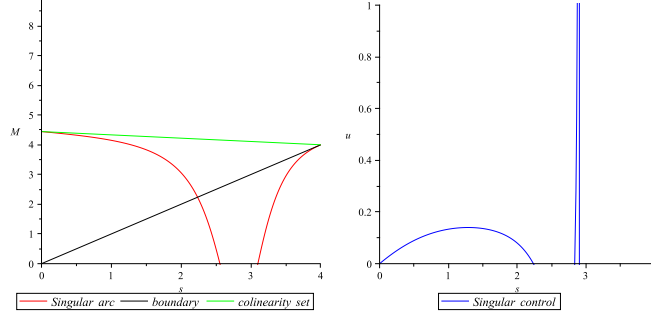
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Figure 11: *Picture Left*: Plot of the singular arc Δ_{SA}^α and of the collinearity set Δ_0^α for $\alpha = 0.9$, $s_{in} = 4$ and $\mu(s) = \frac{s}{5+s+s^2}$. *Picture Right*: plot of the corresponding singular control $s \longmapsto u_s^\alpha(s)$.

(i) *If $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$, then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ is given by (5.9).*

(ii) *If $E_1 \in F_\alpha^-$ and $E_0 \notin F_\alpha^-$, then an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ is given by (5.9) ; an optimal control in F_α^+ satisfies $u = 1$ until reaching Γ_0.*

(iii) *If $E_1 \in F_\alpha^-$ and $E_0 \in F_\alpha^-$, then an optimal control in F_α^+ satisfies $u = 1$ until reaching Γ_0.*

Proof. The proof is similar to the proof of Theorem 5.1 apart from the fact that the singular arc is supposed to be always admissible in the set F *i.e.* $u_s(s) \in [0, 1]$ for any $s \in [0, s_{in}]$. □

Remark 5.3. *As in Theorem 4.1, the optimal strategy in F_α^- is a most rapid approach to a singular arc.*

5.2.2 Optimality results in the case of two connected singular arc components

In this case, we suppose that (5.6) has two positive solutions over $[0, s_{in}]$. The optimal synthesis is more intricate as in section 5.2.1 as the singular arc will consist of two connected components in the set F:

$$\Delta_{SA}^\alpha = \hat{\Delta}_{SA}^\alpha \cup \check{\Delta}_{SA}^\alpha,$$

with $\check{\Delta}_{SA}^\alpha$, resp. $\hat{\Delta}_{SA}^\alpha$ below, resp. above Δ_0^α. The singular locus Δ_{SA}^α and the collinearity set Δ_0^α are represented for different values of the parameter α on Fig. 12. From (5.1)-(5.3), we can make the following observations:

- There exists $0 < s_1^\alpha < s^\star < s_2^\alpha < s_{in}$ such that $s \longmapsto \delta_{SA}(s) = s + \psi_\alpha(s)$ 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 any $s \in [0, s_1^\alpha)$, 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 $\dot{M} > 0$ at some point $(s, M) \in F$ 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 $s \in [0, s_1^\alpha)$, resp. $s \in (s_1^\alpha, s_2^\alpha)$.

- Using (5.3), we can show that there exists a point $s_c \in (s_1^\alpha, s_2^\alpha)$ such that Legendre-Clebsch optimality condition (2.15) $\frac{\partial}{\partial u}\frac{d^2}{dt^2}H_u > 0$ is satisfied only over the interval $[0, s_c)$. Hence the restriction to the interval $[s_c, s_2^\alpha)$ of the singular arc $s \longmapsto \delta_{SA}^\alpha(s)$ is not optimal (*i.e.* it is an anti-turnpike).

To simplify the study, we consider the following assumption on the admissibility of the singular arc $\check{\Delta}_{SA}^\alpha$.

(H'3) The singular control satisfies $u_s^\alpha(s) \in [0, 1]$ for any $s \in [0, s_1^\alpha)$ such that $(s, \delta_{SA}^\alpha(s)) \in F$.

Numerical simulations indicate that this assumption is verified if α is sufficiently close to 1 (see Fig. 13). However even for α close to 1, the singular control always exceeds the maximal admissible value in the interval (s_1^α, s_2^α) as the denominator of (5.2) vanishes. We obtain the following optimality result.
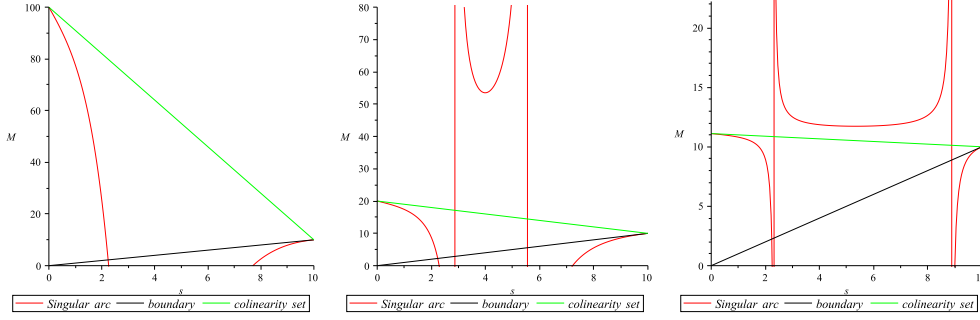
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Figure 12: Plot of Δ_0^α (in green) and Δ_{SA}^α (in red) for $\alpha = 0.1$ (picture left), $\alpha = 0.5$ (picture in the middle), $\alpha = 0.9$ (picture right) with $\mu(s) = \frac{s}{5+s+s^2}$ and $s_{in} = 10$.
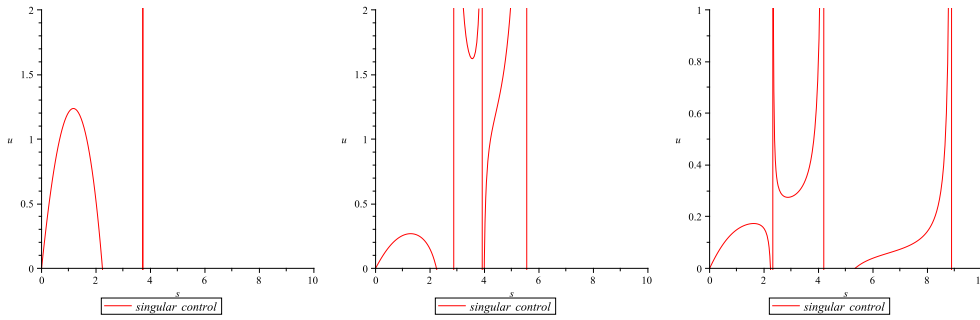

Figure 13: Plot of the singular control for $\alpha = 0.1$ (picture left), $\alpha = 0.5$ (picture in the middle), $\alpha = 0.9$ (picture right) with $\mu(s) = \frac{s}{5+s+s^2}$ and $s_{in} = 10$.

Theorem 5.3. *Suppose that μ is given by (5.7) and that (H2)-(H'3) hold true. Then, if $E_1 \notin F_\alpha^-$ and $E_0 \notin F_\alpha^-$, an optimal feedback control in $\mathrm{Int}(F_\alpha^-)$ is given by (5.9).*

Proof. The proof utilizes similar arguments as the proof of Theorem 5.1 except that in this case the singular arc is always admissible in the set F *i.e.* $u_s(s) \in [0,1]$ for any $s \in [0, s_{in}]$ (see (H'3)). $\qquad\square$

The previous Theorem is illustrated on Fig. 14.

Remark 5.4. *Notice that the feedback (5.9) corresponds to a most rapid approach to the singular arc $\check{\Delta}_{SA}^\alpha$ as in Theorem 4.1. 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 (5.9) obtained in Theorem 5.3 converges to (4.8) when α goes to 1 (see Fig. 14).*

When dealing with cases (ii) and (iii) of Proposition 3.1, several difficulties may appear. On the one hand there is a saturation phenomenon of the singular control as when $\alpha = 1$ (typically when M becomes large); on the other hand, Legendre-Clebsch optimality condition will fail to hold for certain choices of the target point (in particular if $(\bar{s}, \bar{M})$ is located between the two components of the singular locus). To simplify the study, we have considered only the case where the target point is such that $\Gamma_0 \cap \check{\Delta}_{SA}$ is non-empty. More precisely, we have the following optimality result in the same spirit as Theorem 4.2.

Proposition 5.1. *Suppose that μ is given by (5.7), that (H2) holds true, and that $E_0 \in F_\alpha^-$, $E_1 \in F_\alpha^-$. Moreover, we suppose that the target point is such that $\bar{M} > \delta_{SA}^\alpha(s_c)$. Then, an optimal control u steering (2.4) from an initial condition $(s_0, M_0) \in F_\alpha^+$ such that $M_0 > \delta_{SA}^\alpha(s_0)$ is of type $B_- B_+ S$ (with at most two switching points) until reaching Γ_0 or Γ_1.*

Proof. As $E_0 \in F_\alpha^-$ and $E_1 \in F_\alpha^-$, the controllability set F_α^+ is above the set Δ_0^α. We deduce that $-\frac{f_{SA}^\alpha(s,M)}{f_0^\alpha(s,M)} < 0$, resp. $-\frac{f_{SA}^\alpha(s,M)}{f_0^\alpha(s,M)} > 0$ if (s, M) is below $\hat{\Delta}_{SA}^\alpha$, resp. above $\hat{\Delta}_{SA}^\alpha$. Now, Proposition 2.1 (ii) implies that an
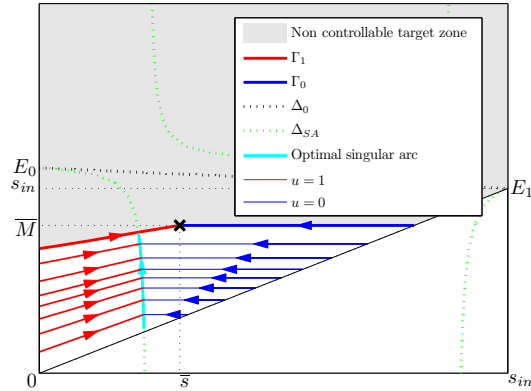
Figure 14: Optimal synthesis in F_α^- for Haldane kinetics, see Proposition 5.3 case (i).

optimal bang-bang control can switch only from $u = 0$ to $u = 1$ above $\hat{\Delta}_{SA}^\alpha$. Moreover, an optimal control cannot switch from $u = 1$ to $u = 0$ below $\hat{\Delta}_{SA}^\alpha$ and before reaching Γ_0. Otherwise, the trajectory would necessary switch from $u = 0$ to $u = 1$ below $\hat{\Delta}_{SA}^\alpha$ implying a contradiction with Proposition 2.1 (ii). Now, as $\bar{M} > \delta_{SA}^\alpha(s_c)$ any admissible singular arc (*i.e.* such that $u_s^\alpha(s) \in [0,1]$) is optimal until reaching Γ_0 or Γ_1. Thus an optimal control is of type $B_- B_+ S$ until reaching $\Gamma_0 \cup \Gamma_1$. $\qquad\square$

Remark 5.5. *As mentioned above, this case in not complete as certain target points below Δ_{SA}^α may not satisfy the assumptions of Proposition 5.1. However, this assumption can be verified by choosing α sufficiently close to 1.*

6 Conclusion, Discussion, Perspectives

In this paper, we have provided an optimal synthesis of a two-dimensional system describing a chemostat model including a retention system. The analysis has revealed the importance of turnpike singular arcs in the optimal synthesis. We have shown that optimal trajectories are based on a most rapid approach to a turnpike (in absence of saturation phenomenon) depending on the kinetics. For $\alpha = 1$ and a growth function of Haldane-type, the singular strategy consists in maintaining the substrate concentration in the chemostat model equal to $s^\star$ which corresponds to the point where μ is maximal. When the singular control saturates (it attains the maximal admissible value), then the optimal synthesis exhibits a switching curve and frame points exist. Optimal controls have at most three switching points (in the latter case an optimal control is of type $B_- S B_+ B_-$). When $\alpha < 1$, we also observe a splitting of the singular arc Δ_{SA}^1 into two components in the case of Haldane kinetics.

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

- 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.

- The optimal feedback control laws that we have obtained are quite simple and may be implemented easily (see *e.g.* [4, 15] for a practical implementation of a singular strategy in biotechnology).

- Whereas singular arcs usually appear for Haldane-type kinetics (see *e.g.* [2, 15]), our results show that a singular arc appears for Monod-type kinetics as long as $\alpha \neq 1$.

- Whenever $\alpha < 1$, there exist target points that can be reached from 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 for the system). Thus, a practitioner can take advantage of this

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remark to pilot adequately a chemostat with a recirculation loop to a desired starting from any initial condition in the state space. In some engineering systems, the value of α can be chosen as a control parameter when using reactors in recirculation mode.

- The optimal feedback control laws that we have obtained are robust in the following sense. For Monod-type kinetics, the optimal feedback (5.5) coincides with (4.6) if α is close to 1, and so it does not depend on α (see remark 5.2 (iii)). Hence, it drives optimally (2.4) to the target point for any value of α sufficiently close to 1.

- As shown in section 5.2, the optimal synthesis depends on the parameter α, nevertheless we can observe that when α goes to 1, the optimal synthesis slightly differs from the case $\alpha = 1$ (see *e.g.* Remark 5.4). However, we are not aware of general results concerning the behavior of optimal syntheses or optimal feedback control laws 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. Extensions include the synthesis of optimal control for more complex systems including biological schemes described by cascade of reactions or where different substrates are consumed at different rates by several groups of microorganisms.

Acknowledgments

7   Appendix

Proof of Lemma 4.1. The following claim is crucial and follows from (4.2) and Proposition 2.1 (ii).

Claim 7.1. *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. $s(t) < s^\star$.*

Step 1. Let us first 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 $(s(\cdot), M(\cdot))$ starting from this point. Suppose that we have $u = 0$ until reaching $s = s^\star$ 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 switching point from $u = 0$ to $u = 1$ at a time t_0 such that $s^\star < s(t_0) < s_0$ (the uniqueness follows from Claim 7.1).

Let us 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 7.1), but we have again a contradiction on Γ_0 using claim 7.1. 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 4.1 (1)-(2).* First, we have $s_c(M) \to s^\star$ when $M \downarrow \tilde{M}$. Otherwise, we would have a contradiction by using Claim 7.1 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 trajectory and such that $s_0 > s_c(M_e)$ and $M_0 > M_e$. We then have $u = 1$ until reaching $M = M_e$ at a substrate concentration greater than $s^\star$. We necessarily have a contradiction by Claim 7.1 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 part (1) of Lemma 4.1. The proof of (2) is a direct consequence of Claim 7.1. □

Proof of Lemma 5.2. The proof of (i) follows by a direct computation replacing the expression of μ given by (5.7) into (5.6). To prove (ii), observe that if (5.8) has three solutions (s_1, s_2, s_3) in $\mathbb{R}$, then $s_1 s_2 s_3 = -\frac{s_{in} k_i k_s}{2-\alpha} < 0$ and $s_1 + s_2 + s_3 = -\frac{(1-\alpha)k_i - s_{in}}{2-\alpha} < s_{in}$. In this case, we obtain that either (5.8) has three negative solutions or it has exactly one negative solution and two positive ones. Suppose now that (5.8) has only one real solution $s_1 \in \mathbb{R}$. Then, there exist $\alpha \in \mathbb{R}$ and $\beta > 0$ such that (5.8) is equivalent to $(s - s_1)(s^2 + \alpha s + \beta) = 0$. It follows that $-s_1 \beta = \frac{k_i k_s s_{in}}{2-\alpha}$. Thus, we have $s_1 < 0$ which ends the proof of (ii). To prove (iii), observe that if α goes to one, then the implicit function Theorem implies that (5.6) has a positive solution in a neighborhood of $s^\star$. We deduce from (ii) that there exist exactly two positive solutions of (5.6) for $\alpha \in [0, 1)$ close to 1. Moreover, if we substitute $s = s_{in}$ into $\rho(s) := (s_{in} - s)\mu'(s) + (1-\alpha)\mu(s)$ and into $\rho'(s) = (s_{in} - s)\mu''(s) - \alpha\mu'(s)$, we obtain positive quantities. Thus, the positive solutions of (5.6) are in the interval $[0, s_{in}]$. □

The table below provides the parameter values used for the simulations of optimal trajectories (recall (5.4) and (5.7)).

Figure	Case	Growth function	α	μ_{max}	k_s	k_i	s_{in}	$\overline{s}$	$\overline{M}$
2 left	I	Haldane	1	1	2	1	3	1	2.5
2 right	I	Haldane	1	1	2	1	3	2	2.5
4 left	II a	Haldane	1	1	2	1	3	1.1	6
4 right	II a	Haldane	1	1	2	1	3	0.5	6
5 left	II b	Haldane	1	1	2	1	3	1.6	4.5
5 right	II b	Haldane	1	1	2	1	3	1.7	4
6 left	III a	Haldane	1	1	2	1	3	0.7	10
6 right	III a	Haldane	1	1	2	1	3	0.5	10
7	III b	Haldane	1	1	2	1	3	1.7	8.5
10 left	(i)	Monod	0.6	1	2	-	3	1	2.9
10 right	(ii)	Monod	0.6	1	2	-	3	1.55	3.5
10 bottom	(iii)	Monod	0.6	1	2	-	3	1.25	6
14	-	Haldane	0.9	1	5	1	10	3	8

Figure 15: Parameter values used for the simulations of Fig. 2, 4, 5, 6, 7, 10, and 14.

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