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Abstract

We investigate the benefit of operating the chemostat model with periodic controls for biological water decontamination. We address a first problem of minimizing the average output concentration of pollution under a constraint of the total quantity of water treated over the period, and a second one of maximizing this quantity under a constraint on the average output concentration. We first give conditions on the growth characteristics of micro-organisms for which an improvement is possible, compared to steady-state. We then give the global optimal periodic control strategies for the first problem and show a duality between the two problems, which allows to obtain the solutions of the second problem from the first one. Results are illustrated on Monod, Haldane, Hill and Contois kinetics.

Key words: Chemostat model, periodic control, integral constraint, convexity, optimal control, duality.

1 Introduction

In the past decades, periodic operations of biological or chemical processes have been investigated to improve their performances [3,1,16,15]. Several contributions have identified situations for which a periodic solution improves an objective, such as the productivity, compared to steady state [19,1,14,10]. In the present work, we revisit this problem for the chemostat model in a waste-water treatment (WWT) context. Let us begin by recalling the equations of the model (see e.g. [11]))

$$\begin{cases} \dot{s} = -\frac{1}{Y}\mu(s,x)x + \frac{F}{V}(s_{in}-s), \\ \dot{x} = \mu(s,x)x - \frac{F}{V}x, \end{cases} \tag{1}$$

which represent the time evolution of the concentrations of substrate s and biomass b in a tank of volume V. The reactor is fed with an input flow rate F of substrate with concentration s_{in} and drawn off with the same rate (V remains then constant). Y is the conversion rate and $\mu(\cdot)$ the growth function of the micro-organisms (that depends on x or not). The removal rate $D = F/V$ is the control variable. Continuous WWT are generally operated over a large time horizon (months or years) and solutions sought among steady states. One can easily check that non-trivial equilibriums of system (1) are given by $(s,x,D) = (\bar{s}, Y(s_{in}-\bar{s}), \bar{D})$ such that

$$\bar{D} = \mu(\bar{s}, Y(s_{in}-\bar{s})). \tag{2}$$

In practice, one faces two kinds of situations:

1. A water quantity $\bar{Q}$ has to be treated on a time interval of length T. This imposes $\bar{D} = \bar{Q}/(VT)$ and thus $\bar{s}$ at steady state, from equation (2).
2. A set-point $s = \bar{s}$ is imposed. This sets $\bar{D}$ at steady-state from equation (2), and thus the treated quantity $\bar{Q} = \bar{D}VT$ during a time interval of length T.

However, the measurement of concentration s in water released in the environment is usually averaged over a certain time interval, fixed by governmental rules [1]. In this work, we study periodic solutions that can do a better job than steady state, that is to say an average s lower than $\bar{s}$ under the constraint on Q in case 1, and a treated quantity larger than $\bar{Q}$ under the constraint on s

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[1] see for instance the European 2008/105/EC Directive.

in case 2. The literature on periodic control already provides tools to answer such questions, in particular the π-criterion [6]. However, up to our knowledge, all the existing approaches consider local conditions and sinusoidal or wave controls, apart the recent work [5] which is based on the Pontryagin's Maximum Principle (PMP) and convexity. Here, we do make any restrictions on the class of controls and we moreover determine the optimal ones. For any T-periodic integrable function $\xi(\cdot)$, let us denote its average by

$$\langle \xi \rangle_T := \frac{1}{T}\int_t^{t+T} \xi(\tau)d\tau,$$

Consider the optimal control problems for the two cases

Problem 1 *Given $T > 0$ and $\bar{D} > 0$, solve*

$$\inf_{D(\cdot)} \left\{ \langle s \rangle_T ;\ s(0) = s(T), \langle D \rangle_T = \bar{D} \right\} \qquad (3)$$

Problem 2 *Given $T > 0$ and $\bar{s} > 0$, solve*

$$\sup_{D(\cdot)} \left\{ \langle D \rangle_T ;\ s(0) = s(T), \langle s \rangle_T = \bar{s} \right\}. \qquad (4)$$

where $D(\cdot)$ is sought among measurable control taking values in $[D_-, D_+]$ with $0 \leq D_- < D_+$, and $(s(\cdot), x(\cdot))$ is a periodic solution of (1). Note that the objective here is not to optimize T, differently to [19,1,14,10]. Preliminary work with a conjecture on the optimal control, verified numerically, has been presented in [4]. We show here how to apply the results from [5] on Pb. 1 and extend them for Pb. 2 to prove the global optimal solutions. Indeed, it turns out that the first problem is easier to study, and that the two problems are "dual" in the sense that the value of the constraint on $\langle D \rangle_T$ in Pb. 1 is the objective of Pb. 2 under a constraint on $\langle s \rangle_T$ whose value is the criterion of the Pb. 1. We prove a duality that allows to deduce the solutions of Pb. 2 from Pb. 1. The paper is organized as follows. After some preliminaries in Sec. 2, we investigate in Sec. 3 the existence of periodic solutions improving the steady state, depending on the characteristics of the growth function. Our results are stronger than π-criterion in the sense that we consider global solutions. Then, when an improvement is possible, we determine in Sec. 4 the optimal controls and show the duality between Pb. 1 and Pb. 2. Finally, Sec. 5 illustrates the application of the results with several growth functions of the literature.

2 Assumptions and preliminaries

Let $z = Y(s_{in} - s) - x$. One gets $\dot{z} = -Dz$ from (1). A periodic solution has thus to satisfy $z = 0$ with $s(\cdot)$ in $[0, s_{in}]$ solution of

$$\dot{s} = (D - \nu(s))(s_{in} - s) \text{ with } \nu(s) := \mu(s, Y(s_{in} - s)) \quad (5)$$

A0. The function ν is Lipschitz on $[0, s_{in}]$, non-negative and null only at 0.

We shall say that a solution $s(\cdot)$ of (5) with control $D(\cdot)$ is *admissible* for Pb. 1, resp. Pb. 2 if it is periodic and verifies $\langle D \rangle_T = \bar{D}$, resp. $\langle s \rangle_T = \bar{s}$.

A1. The pair $(\bar{s}, \bar{D})$ belongs to $(0, s_{in}) \times (D_-, D_+)$ with

$$\bar{s} := \inf\{s\ ;\ \nu(s) > \bar{D}\} \qquad (6)$$

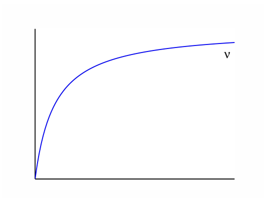
Remark 1 *If the equation $\nu(s) = \bar{D}$ admits several roots, the desired steady-state $\bar{s}$ is the lowest one as the objective of WWT is to reduce the pollution. Then ν is necessarily increasing in a neighborhood of $\bar{s}$, which implies that $\bar{s}$ is a locally stable equilibrium of (5) for $D = \bar{D}$.*

We distinguish three kinds of assumptions that cover the well known functions of the literature: Monod, Haldane, Hill functions which depend on s and the Contois one which is density dependent (i.e. depends on s and x).

A2a. ν is concave or there exists $\bar{\nu}$ concave non-decreasing such that $\bar{\nu} \geq \nu$ on $(0, s_{in})$ with $\bar{\nu}(\bar{s}) = \nu(\bar{s})$.

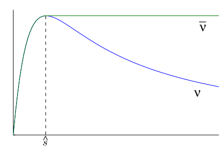
The Monod's function [12] is concave and satisfies A2a:

$$\nu(s) = \mu(s) = \frac{\mu_{max} s}{K_s + s}$$



The Haldane's function [2] is non monotonic:

$$\nu(s) = \mu(s) = \frac{\mu_m s}{K_s + s + s^2/K_I}$$
$$\hat{s} = \arg\max \nu = \sqrt{K_s K_i}$$



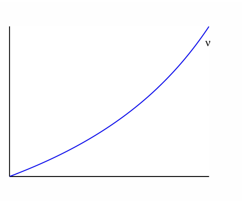
and concave only on $[0, \hat{s}]$. Under A1, one has $\bar{s} < \hat{s}$ and A2a is verified with

$$\bar{\nu}(s) = \begin{cases} \nu(s), & s < \hat{s}* \\ \nu(\hat{s}), & s \geq \hat{s} \end{cases}$$

A2b. ν is strictly convex on $(0, s_{in})$.

The Contois's function [9] depends on x and satisfies A2b when $Y > \frac{1}{K}$:

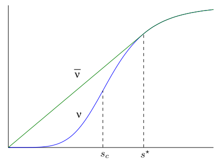
$$\nu(s) = \mu(s, Y(s_{in} - s)) = \frac{\mu_{max} s}{KY(s_{in} - s) + s}$$



A2c. ν is locally strictly convex about $\bar{s}$.

The Hill function [13] is increasing:

$$\nu(s) = \mu(s) = \frac{\mu_{max} s^n}{K_s^n + s^n} \ (n > 0)$$
$$s_c = K_s \left(\frac{n-1}{n+1}\right)^{1/n}$$



and convex for $s < s_c$. A2c is thus fulfilled for $\bar{s} < s_c$. A2a is satisfies for $\bar{s} > s^\star$, where $s^\star$ is the abscissa whose tangent to the graph of ν passes through 0, considering the function

$$\bar{\nu}(s) = \begin{cases} \mu'(s^*)s, \ s < s^* \\ \mu(s), \ s \geq s^* \end{cases} \quad \text{with } s^* = s_c(1+n)^{\frac{1}{n}}$$

Periodic solutions of (5) satisfy the following properties.

Lemma 1 *Let $s(\cdot)$ be a T-periodic solution of (5) on $(0, s_{in})$ with control $D(\cdot)$. One has the properties.*

(i) $\langle D \rangle_T = \langle \nu(s) \rangle_T$.
(ii) *If $\langle s \rangle_T \leq \bar{s}$, $\langle D \rangle_T \geq \bar{D}$ and ν is increasing on $s([0,T])$, there exists $t \in [0,T]$ such that $s(t) = \bar{s}$.*

PROOF. (i) The map $t \mapsto \ln(s_{in} - s(t))$ is T-periodic and with (5) one obtains $\langle D \rangle_T = \langle \nu(s) \rangle_T$.
(ii) Moreover (5) and $\nu(\bar{s}) = \bar{D}$ give

$$\int_0^T [\nu(s(t)) - \nu(\bar{s})] \geq 0. \tag{7}$$

Then, $s(t) < \bar{s}$ for any $t \in [0,T]$ gives a contradiction with (7) when ν is increasing over $s([0,T])$. □

3 Conditions for improvements

The first point is to show the existence of non-constant admissible solutions.

Lemma 2 *There exits non-constant admissible $s(\cdot)$ for Pb. 1 and 2. Moreover $\|s - \bar{s}\|_\infty$ can be arbitrary small.*

PROOF. Let $v(\cdot)$ be a T-periodic measurable bounded function with $\langle v \rangle_T = 0$, non null almost everywhere. Let $D_\varepsilon(\cdot) := \bar{D} + \varepsilon v(\cdot)$, which takes values in $[D_-, D_+]$ for $\varepsilon > 0$ small enough, and verifies $\langle D_\varepsilon \rangle_T = \bar{D}$. Let $\theta(s_0, \varepsilon) := s(T, D_\varepsilon, s_0) - s_0$, where $s(t, D, s_0)$ denotes the solution of (5) at time t with $s(0) = s_0$ and control $D(\cdot)$. By continuous dependency of $s(T, D_\varepsilon, s_0)$ w.r.t. (s_0, ε), θ is continuous. As ν is increasing in any sufficiently small neighborhood (s_0^-, s_0^+) of $\bar{s}$ (Rem. 1)), one has $\theta(s_0^-, 0) > 0$, $\theta(s_0^+, 0) < 0$ and thus $\theta(s_0^-, \varepsilon) > 0$, $\theta(s_0^+, \varepsilon) < 0$ for ε sufficiently small. By the Mean value Theorem, we deduce the existence of $\tilde{s}_0 \in (s_0^-, s_0^+)$ such that $\theta(\tilde{s}_0, \varepsilon) = 0$, that is, the existence of a non-constant T-periodic solution $\tilde{s} := s(\cdot, D_\varepsilon, \tilde{s}_0)$ with $\langle D_\varepsilon \rangle_T = \bar{D}$. Finally, Gronwall's Lemma gives the existence of a constant $C > 0$ such that $||\tilde{s} - \bar{s}||_\infty \leq C\varepsilon$.
Let $y \in C^1(\mathbb{R}, \mathbb{R})$ be a non null T-periodic function such that $\langle y \rangle_T = 0$. For ε small enough, $t \mapsto s_\varepsilon(t) := \bar{s} + \varepsilon y(t)$ takes values in $(0, s_{in})$ and satisfies $||s_\varepsilon - \bar{s}||_\infty < \|y\|_\infty \varepsilon$ as well as $\langle s_\varepsilon \rangle_T = \bar{s}$. Note that $s_\varepsilon(\cdot)$ is solution of (5) for the control $D_\varepsilon(t) := \frac{\dot{s}_\varepsilon(t)}{s_{in} - s_\varepsilon(t)} + \nu(s_\varepsilon(t))$. One then has $|D_\varepsilon(t) - \bar{D}| \leq F(t, \varepsilon) := \varepsilon \left| \frac{\dot{y}(t)}{s_{in} - \bar{s} - \varepsilon y(t)} \right| + \varepsilon L |y(t)|$, where L is the Lipschitz constant of ν. As F tends to 0 when ε tends to 0, uniformly in t, we conclude that D_ε is admissible for ε small enough, and thus s_ε is a non-constant periodic solution with $\langle s_\varepsilon \rangle_T = \bar{s}$ and $||s_\varepsilon - \bar{s}||_\infty < \|y\|_\infty \varepsilon$. □

Proposition 3

(i) *Under A2a, any non-constant admissible solution for Pb. 1 or 2 verifies $\langle s \rangle_T > \bar{s}$ or $\langle D \rangle_T < \bar{D}$.*
(ii) *Under A2b, any non-constant admissible solution for Pb. 1 or 2 verifies $\langle s \rangle_T < \bar{s}$ or $\langle D \rangle_T > \bar{D}$.*
(iii) *Under A2c, there exists admissible solution for Pb. 1 or 2 that verifies $\langle s \rangle_T < \bar{s}$ or $\langle D \rangle_T > \bar{D}$, with ν strictly convex increasing on $s([0,T])$.*

PROOF. (i) Under A2a, Jensen's inequality [2] applied to the concave function $\bar{\nu}$ gives $\langle \bar{\nu}(s) \rangle_T < \bar{\nu}(\langle s \rangle_T)$ for non-constant $s(\cdot)$, and since $\bar{\nu} \geq \nu$, one obtains $\langle \nu(s) \rangle_T < \bar{\nu}(\langle s \rangle_T)$. In Pb. 1, one has $\bar{\nu}(\bar{s}) = \nu(\bar{s}) = \bar{D} = \langle D \rangle_T = \langle \nu(s) \rangle_T$ (cf Lem. 1). One then obtains $\bar{\nu}(\bar{s}) < \bar{\nu}(\langle s \rangle_T)$ from which we deduce the inequality $\bar{s} < \langle s \rangle_T$, since $\bar{\nu}$ is non decreasing. In Pb. 2, one has $\bar{\nu}(\langle s \rangle_T) = \bar{\nu}(\bar{s}) = \nu(\bar{s}) = \bar{D}$, and thus $\langle D \rangle_T = \langle \nu(s) \rangle_T < \bar{D}$.
(iii) Under A2c, a non-constant admissible $s(\cdot)$ can be chosen in such a way that ν is strictly convex increasing over $s([0,T])$ (cf Rem. 1 and Lem. 2). Jensen's inequality then gives $\langle \nu(s) \rangle_T > \nu(\langle s \rangle_T)$. In Pb. 1, one has $\nu(\bar{s}) = \bar{D} = \langle D \rangle_T > \nu(\langle s \rangle_T)$ and since ν is increasing over $s([0,T])$, we deduce that the inequality $\bar{s} > \langle s \rangle_T$ is verified. In Pb. 2, one has $\langle D \rangle_T > \nu(\langle s \rangle_T) = \nu(\bar{s}) = \bar{D}$.

[2] Let ϕ be a convex function on $\mathbb{R}$. The Jensen's inequality $\int_B \phi(\xi(\lambda)) d\lambda \geq \phi(\int_B \xi(\lambda) d\lambda)$ holds for any function ξ integrable with a measure λ on a set B. The inequality is strict if ϕ is strictly convex and ξ not constant almost everywhere.

(ii) Finally, under A2b, ν is increasing over $(0, s_{in})$ and the former inequalities are then satisfied for any non-constant periodic solution with values in $(0, s_{in})$. $\square$

Let us come back to the four growth functions given in Section 3. Prop. 3 shows that for Pb. 1 and 2 one has

(1) no improvement over steady-state for Monod or Haldane cases,
(2) a systematic improvement with non-constant solution for the Contois case when $Y > 1/K$,
(3) possible improvement over steady-state for the Hill case when $\bar{s} < s_c$, but not possible when $\bar{s} \geq s^\star$.

4 Optimal improvements

Accordingly to Prop. 3, we consider here assumption A2b or A2c and look for non-constant optimal solutions on an interval where ν is strictly convex and increasing. Indeed, Pb. 1 falls into the class of scalar optimal periodic control with integral constraint on the control:

$$\begin{aligned} &\dot{x} = f(x) + ug(x), \quad x \in \mathbb{R}, \quad u(\cdot) \in [-1, 1] \\ &\inf_{u \in \mathcal{U}} \langle \ell(x) \rangle_T \text{ s.t. } x(0) = x(T) \text{ and } \langle u \rangle_T = \bar{u} \end{aligned} \tag{8}$$

for which recent results are available. In [5] it is proved that under some convexity hypotheses, optimal solutions are bang-bang and we show in the Appendix how it applies to Pb. 1. Without loss of generality, we consider solutions with $s(0) = \bar{s}$ according to Lem. 1. For $0 < t_1 < t_2 < T$, we define the *bang-bang* control:

$$\hat{D}_T(t) := \begin{cases} D_+, & 0 \leq t < t_1, \\ D_-, & t_1 \leq t < t_2, \\ D_+, & t_2 \leq t < T, \end{cases} \tag{9}$$

and posit $s_M = s(t_1)$, $s_m = s(t_2)$. The periodicity constraint $s(T) = s(0)$ can be written as

$$\int_{s_m}^{s_M} \eta(s) ds = T, \tag{10}$$

where the function $\eta : (0, s_{in}) \to \mathbb{R}$ is defined as

$$\eta(s) := \frac{1}{(D_+ - \nu(s))(s_{in} - s)} - \frac{1}{(D_- - \nu(s))(s_{in} - s)},$$

and the constraint $\langle \hat{D} \rangle_T = \bar{D}$, similarly by

$$\int_{s_m}^{s_M} \eta(s)\nu(s) ds = \bar{D}T. \tag{11}$$

The results [5] applied to Pb. 1 give the following characterization of the optimality of (9) (see Appendix).

Proposition 4 *There exists a unique pair (s_m, s_M) with $0 < s_m < \bar{s} < s_M < s_{in}$ satisfying* (10)-(11) *and the control $\hat{D}_T(\cdot)$ with $t_1 := \inf\{t > 0,\ s(t) = s_M\}$, $t_2 := \inf\{t > t_1,\ s(t) = s_m\}$ is optimal for Pb. 1*

(i) *for any $T > 0$ if ν is convex increasing on $(0, s_{in})$,*
(ii) *for $T > 0$ not too large if ν is only locally convex increasing about $\bar{s}$.*

Note that Pb. 2 is not in the form of (8). Indeed, the Hamiltonian of Pb. 2 is different from the one of Pb. 1 and the adjoint equations of the PMP have a different structure, which does not allow to easily adapt the proofs of [5] to this problem. However, we show a duality between Pb. 1 and 2. For this purpose, we introduce the *value functions* with *inequality* constraints

$$V_T(\bar{D}) := \min_{D(\cdot)} \left\{ \langle s \rangle_T \, ; \, s(0) = s(T),\ \langle D \rangle_T \geq \bar{D} \right\} \tag{12}$$

$$W_T(\bar{s}) := \max_{D(\cdot)} \left\{ \langle D \rangle_T \, ; \, s(0) = s(T),\ \langle s \rangle_T \leq \bar{s} \right\} \tag{13}$$

that we define on $\mathcal{D} := \{\bar{D} \, ; \, \exists \bar{s} \text{ s.t.} (\bar{s}, \bar{D}) \text{ fulfills A1}\}$ and $\mathcal{S} := \{\bar{s} \, ; \, \exists \bar{D} \text{ s.t.} (\bar{s}, \bar{D}) \text{ fulfills A1}\}$, respectively (standard results of the theory of optimal control [8] guarantee that optimal solutions exist for both problems).

Lemma 5 *For any $T > 0$, V_T is increasing on $\mathcal{D}$ and is the value function of Pb. 1.*

PROOF. We first show that the constraint on $\langle D \rangle_T$ is necessarily saturated. Suppose that an optimal control $D(\cdot)$ satisfies $\langle D \rangle_T > \bar{D}$, and denote by $s(\cdot)$ its associated T-periodic solution. Let $E := \{t \in [0, T] \, ; \, D(t) > \bar{D}\}$ which is necessarily such that $\text{meas}(E) > 0$. Set

$$\gamma := \min \left(\frac{\langle D \rangle_T - \bar{D}}{\text{meas}(E)}, \bar{D} - D_- \right) > 0,$$

and define a control $\tilde{D}$ on $[0, T]$ as

$$\tilde{D}(t) := \begin{cases} D(t) - \gamma & \text{if } \ t \in E, \\ D(t) & \text{if } \ t \notin E. \end{cases}$$

which takes values in $[D_-, D_+]$. In addition, one has $\bar{D} \leq \langle \tilde{D} \rangle_T < \langle D \rangle_T$. Let $\tilde{s}(\cdot, s_0)$ be the unique solution of (5) associated with $\tilde{D}(\cdot)$ and such that $\tilde{s}(0, s_0) = s_0$. One has $\tilde{s}(T, 0) > 0$ because $\tilde{s}(\cdot, 0)$ is non-negative and $\langle \tilde{D} \rangle_T > 0$ implies that $\tilde{s}(\cdot, 0)$ cannot be identically null on $[0, T]$. Moreover, one has $\tilde{D}(t) \leq D(t)$ for $t \geq 0$ and since $\text{meas}\{t \in [0, T];\ \tilde{D}(t) < D(t)\} = \text{meas}(E) > 0$, we deduce that $\tilde{s}(T, \bar{s}) < \bar{s}$ (by comparison of solutions of scalar differential equations, see e.g. [18]). Thanks to the Mean Value Theorem applied to the continuous function $s_0 \mapsto \tilde{s}(T, s_0) - s_0$, one deduces the existence of $\tilde{s}_0 \in (0, \bar{s})$ such that $\tilde{s}(T, \tilde{s}_0) = \tilde{s}_0$. The solu-

tion $\tilde{s}(\cdot,\tilde{s}_0)$ (associated to $\tilde{D}(\cdot)$) is T-periodic and verifies $\tilde{s}(t,\tilde{s}_0) < s(t)$ for any $t \in [0,T]$ (by comparison of solutions). Therefore, one gets $\langle \tilde{s}(\cdot,\tilde{s}_0)\rangle_T < \langle s\rangle_T$ and we can conclude that $D(\cdot)$ is not optimal for (12) with $\langle D\rangle_T > \bar{D}$ (since $\langle \tilde{D}\rangle_T < \langle D\rangle_T$). Hence, the inequality constraint in (12) must be saturated.
Take now $\bar{D}_1, \bar{D}_2 \in \mathcal{D}$ with $\bar{D}_1 < \bar{D}_2$. Since an optimal solution of (12) necessarily saturates the inequality constraint, an optimal pair $(D_2(\cdot), s_2(\cdot))$ for $V_T(\bar{D}_2)$ is sub-optimal for $V_T(\bar{D}_1)$ (since $\langle D_2\rangle_T = \bar{D}_2 \geq \bar{D}_1$), which implies $V_T(\bar{D}_2) = \langle s_2\rangle_T \geq V_T(\bar{D}_1)$. □

Proposition 6 *For any $\bar{s} \in \mathcal{S}$ and $T > 0$ that satisfy conditions of Prop. 4, one has the duality*

$$W_T(\bar{s}) = \max\{\bar{D} \in \mathcal{D};\ V_T(\bar{D}) = \bar{s}\} = V_T^{-1}(\bar{s}) \quad (14)$$

and W_T is the value function of Pb. 2.

PROOF. Assume first that ν is convex increasing on $(0, s_{in})$ and let us show that V_T is continuous on $\mathcal{D}$ for any $T > 0$. According to Prop. 4, for any $\bar{D} \in \mathcal{D}$, there exists a unique pair $(s_m, s_M) \in (0, s_{in})^2$ satisfying (10)-(11), that is,

$$F(s_m, s_M, \bar{D}) := \begin{bmatrix} \int_{s_m}^{s_M} \eta(s)ds - T \\ \int_{s_m}^{s_M} \eta(s)\nu(s)ds - \bar{D}T \end{bmatrix} = 0$$

Moreover, the Jacobian matrix of F w.r.t. (s_m, s_M)

$$\begin{bmatrix} -\eta(s_m) & \eta(s_M) \\ -\eta(s_m)\nu(s_m) & \eta(s_M)\nu(s_M) \end{bmatrix}$$

is non singular. By the Implicit Function Theorem, s_m and s_M are C^1 functions of $\bar{D}$, and $\hat{D}_T(\cdot)$ is then continuous in L^1 w.r.t. $\bar{D}$. Recall that the map $D(\cdot) \mapsto s(\cdot, D)$ is continuous from L^1 into C^0 (see e.g. Th. 4.2 in [7]), so that $\bar{D} \mapsto s(\cdot, \hat{D}_T)$ is continuous, and thus V_T as well. Since ν is increasing, $\mathcal{S}$ is an interval, invariant by dynamics (5). Let $[\bar{s}_-, \bar{s}_+] = \text{clo}\,\mathcal{S}$ and $\bar{D}_\pm = \nu(\bar{s}_\pm)$. Since V_T is continuous and increasing (Lem. 5), Prop. 4 gives $\lim_{\bar{D}\in\mathcal{D},\bar{D}\to\bar{D}_\pm} V_T(\bar{D}) = \bar{s}_\pm$. V_T is thus invertible on $\mathcal{S}$ with $V_T^{-1}(I) = \mathcal{D}$. Take $\bar{s} \in \mathcal{S}$ and $D^\dagger := V_T^{-1}(\bar{s})$. Let $D(\cdot)$ be an optimal control for Pb. 1 with $\langle D\rangle_T = D^\dagger$, which generates a solution $s(\cdot)$ with $s(T) = s(0)$ and $\langle s\rangle_T = \bar{s}$. The control $D(\cdot)$ is then sub-optimal for Pb. 2, i.e. $W_T(\bar{s}) \geq \langle D\rangle_T = D^\dagger$. Suppose now that there exists an optimal control $\tilde{D}(\cdot)$ for Pb. 2 with $\langle \tilde{D}\rangle_T > D^\dagger$, and let $\tilde{s}(\cdot)$ be the associated solution satisfying the constraint $\langle \tilde{s}\rangle_T \leq \bar{s}$. Since V_T is increasing, one gets $V_T(\langle \tilde{D}\rangle_T) > V_T(D^\dagger)$. However, by definition of V_T, one has $V_T(\langle \tilde{D}\rangle_T) \leq \langle \tilde{s}\rangle_T \leq \bar{s}$, leading to a contradiction. We conclude that one has necessarily $W_T(\bar{s}) = D^\dagger$. As V_T is increasing, an optimal solution for (4) has to saturate the constraint $\langle s\rangle_T \leq \bar{s}$, and thus W_T is the value function for Pb. 2.
If ν is convex increasing only over a sub-interval $I \subset (0, s_{in})$ with $\bar{s} \in I$, consider any increasing convex function $\bar{\nu}$ which coincides with ν on I. Denote by $\bar{V}_T$, $\bar{W}_T$ the corresponding value functions. One then has

$$\bar{W}_T(\bar{s}) = \max\{\bar{D}\,;\ \bar{V}_T(\bar{D}) = \bar{s}\} = \bar{V}_T^{-1}(\bar{s}).$$

For T small enough, V_T and $\bar{V}_T$ coincide in a neighborhood of $\bar{s}$, and W_T, $\bar{W}_T$ as well in a neighborhood of $\bar{D} = \nu(\bar{s})$. Thus, $V_T^{-1}(\bar{s})$ is non empty and as V_T is increasing, $V_T^{-1}(\bar{s})$ is unique, equal to $\bar{V}_T^{-1}(\bar{s})$ and one has also $\max\{\bar{D}\,;\ V_T(\bar{D}) = \bar{s}\} = V_T^{-1}(\bar{s})$. Finally, (14) is fulfilled for T not too large. □

Finally, the constraint $\langle s\rangle_T = \bar{s}$ can be expressed for the controls (9) similarly as done in (11) with

$$\int_{s_m}^{s_M} s\ \eta(s)ds = \bar{s}\,T. \quad (15)$$

The duality given in Prop. 6 gives then an optimality result for Pb. 2 from Prop. 4.

Proposition 7 *There exists a unique pair (s_m, s_M) with $0 < s_m < \bar{s} < s_M < s_{in}$ satisfying (10)-(15), and $\hat{D}_T(\cdot)$ with $t_1 := \inf\{t > 0,\ s(t) = s_M\}$, $t_2 := \inf\{t > t_1,\ s(t) = s_m\}$ is an optimal control for Pb. 2*

(i) for any $T > 0$ if ν is convex increasing on $(0, s_{in})$,

(i) for $T > 0$ not too large, if ν is only locally convex increasing about $\bar{s}$.

Finally, Prop. 4 and 7 show that the optimal controls are piecewise constant and not smooth signals. In practice, this means that if one chooses $D_- = 0$, the bioprocess has to operated as a succession of batch and chemostat modes. Moreover, the optimal switching can be obtained as feedback (and not as open loop), by solving the system (10)-(11) or (10)-(15). In the next section, we show how to compute it on concrete examples.

5 Numerical illustrations

We have already proved in Sec. 3 that no improvement is possible with Monod and Haldane functions: steady state $s = \bar{s}$ with $D = \bar{D}$ is thus optimal for Pb. 1 and 2. We focus now on Contois and Hill cases. Let us show how we have proceeded to determine numerically the optimal synthesis. For Pb. 1, the constraint $\langle D\rangle_T = \bar{D}$ applied to the bang-bang control (9) imposes a relation between the switching times t_1, t_2

$$t_2 = t_2(t_1) := t_1 + T\frac{D_+ - \bar{D}}{D_+ - D_-}. \quad (16)$$

As we know from Prop. 4 that t_1 is unique for satisfying the periodicity constraint $s(T) = s(0)$ (and that one can impose $s(0) = \bar{s}$ without loss of generality), it can be determined as the unique zero of the map $t_1 \mapsto s_{t_1,t_2(t_1)}(T) - \bar{s}$ on $(0, T)$, where $s_{t_1,t_2}(\cdot)$ is solution of (5) with $\hat{D}_T(\cdot)$ and $s(0) = \bar{s}$. We have used a dichotomy method, which gives a better accuracy than using general optimal control solver such as Bocop. For Pb. 2, the constraint $\langle s \rangle_T = \bar{s}$ cannot be written as easily as (16). We have then used the duality result (Prop. 6) by inverting the function V_T to determine the optimal value $\langle D \rangle_T$ and then the optimal synthesis. Indeed, for a given value $\bar{s}$, as we know that optimal $\langle D \rangle_T > \bar{D} = \nu(\bar{s})$, we look for value D such that $V_T(D) = \bar{s}$ only for $D > \nu(\bar{s})$.

For the Contois's case, we have used the parameters

μ_{max}	K	Y	s_{in}	D_-	D_+
$2\,h^{-1}$	5	1	$8\,mg/l$	$0.02\,h^{-1}$	$1.95\,h^{-1}$

Fig. 1 depicts an optimal solution and Fig. 2 the optimal cost which is decreasing w.r.t. T, as it is indeed proved in ref [5]. We have also computed the values functions

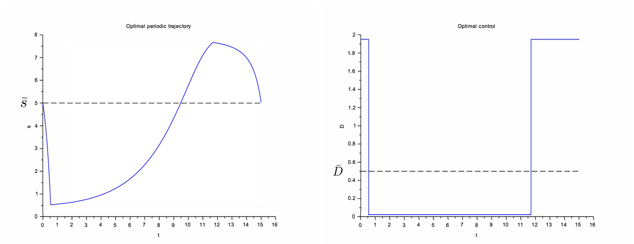


Fig. 1. Optimal solution of Pb. 1 with $\bar{D} = 0.5\,h^{-1}$ and $T = 15\,h$ (steady-state solution in dashed line)

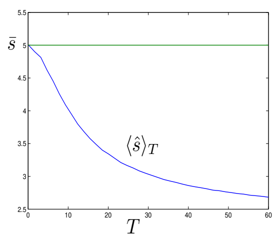


Fig. 2. Optimal cost of Pb. 1 with $\bar{D} = 0.5\,h^{-1}$ function of T

(12), (13) for Pb. 1 and 2 for two different T (Fig. 3). Note that we have represented the graphs of the functions ν and ν^{-1} which represent the values of the criterions at steady-state solution. Finally, we have computed the relative gains compared to the steady-state solution $(\bar{s} - V_T(\bar{D}))/\bar{s}$, $(W_T(\bar{s}) - \bar{D})/\bar{D}$ for each problem (Fig. 4). Such diagrams can help the practitioners to decide, depending on the characteristics of the application (nominal flow rate, maximal period on which average water quality can be considered), if a periodic operation is worth the be operated.

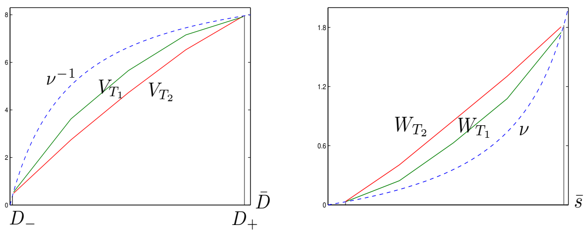


Fig. 3. Value functions for Pb. 1 (left) and Pb. 2 (right) with $T_1 = 15\,h$ and $T_2 = 50\,h$

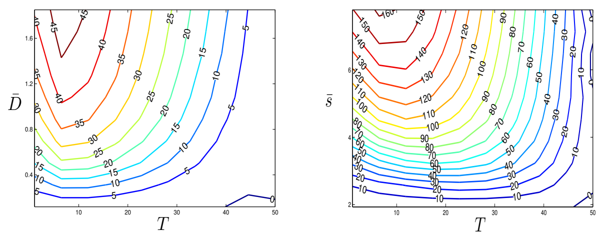


Fig. 4. Iso-value of the relative gains for Pb. 1 (left) and Pb. 2 (right)

For the Hill's case, we have used the parameters

μ_{max}	K_s	n	Y	s_{in}	D_-	D_+
$5\,h^{-1}$	$3\,mg/l$	3	1	$6\,mg/l$	$0.05\,h^{-1}$	$4.5\,h^{-1}$

and conducted similar computations of optimal solutions as long as T is such that the bang-bang solution belongs to the domain where ν is convex (see Fig. 5). For larger

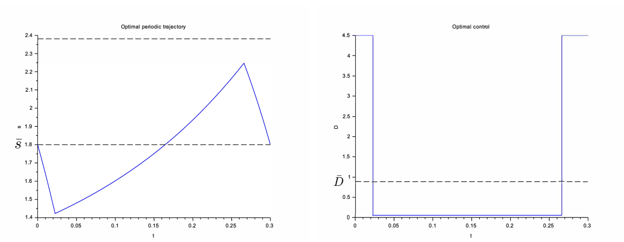


Fig. 5. Optimal solution of Pb. 1 with $\bar{D} = 0.89\,h^{-1}$ and $T = 0.3\,h$. The upper dashed line on the left delimits the domain where ν is convex

values of T, Prop. 4(ii) and Prop. 7(ii) cannot guarantee the optimality of the control $\hat{D}_T(\cdot)$. Nevertheless, we observe on Fig. 6-left that its cost, denoted $\hat{J}_T$, keeps improving with T up to $\bar{T}$, the minimum of $T \mapsto \hat{J}_T$. For $T > \bar{T}$, we propose a bang-bang strategy with $2k$ or $2(k+1)$ switches, where $k := E[T/\bar{T}] > 1$, as follows

$$\tilde{D}_T(t) := \begin{cases} \hat{D}_{\bar{T}}(t - i\bar{T}), \ t \in [i\bar{T}, (i+1)\bar{T}), \ i = \overline{0, k-1}, \\ \hat{D}_\tau(t - k\bar{T}), \ t \in [k\bar{T}, T) \text{ if } \tau = T - k\bar{T} > 0, \end{cases}$$

whose cost is equal to

$$\tilde{J}_T := \frac{k\bar{T}\,\hat{J}_{\bar{T}} + \tau\,\hat{J}_\tau}{T} \quad \text{(where } \tau = T - k\bar{T}\text{).}$$

(see Fig. 6-left). It is clear that $\tilde{J}_T = \hat{J}_{\bar{T}}$ when $T = k\bar{T}$ (which is thus better than steady-state). Moreover, one has $\hat{J}_\tau < \bar{s}$ (as $\tau < \bar{T}$ and $\hat{J}_T < \bar{s}$ for $T \in (0, \bar{T}]$). We conclude that $\tilde{J}_T < \bar{s}$ for any $T > 0$ (since it is a convex combination of $\hat{J}_{\bar{T}}$ and $\hat{J}_\tau$). Fig. 6-right gives the relative gain of this strategy, the "zigzaging" effect being due to the non-monotonicity of $\hat{J}_T$ for $T > \bar{T}$. Finally, similarly to Fig. 3, we plot on Fig. 7 the graphs

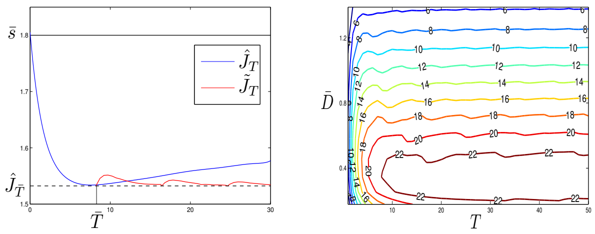


Fig. 6. Costs $\hat{J}_T$, $\tilde{J}_T$ for $\bar{D} = 0.89\,h^{-1}$ (left) and iso-value of the relative gain for the $\tilde{D}(\cdot)$ strategy (right)

of the function $\tilde{V}_T : \bar{D} \mapsto \tilde{J}_T$ and its "dual" function $\tilde{W}_T : \bar{s} \mapsto \max\{\bar{D}\,;\tilde{V}(\bar{D}) = \bar{s}\}$.

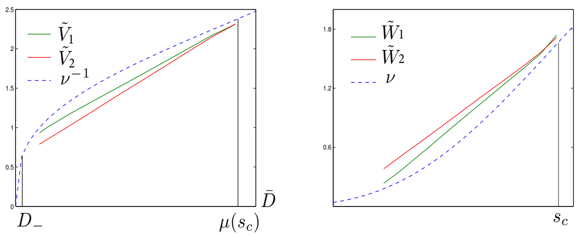


Fig. 7. Graphs of $\tilde{V}_T$ (left) and $\tilde{W}_T$ (right) with $T_1 = 2\,h$ and $T_2 = 50\,h$

6 Conclusion

This work reveals the role played by the convexity of the growth function to obtain improvements with non-constant periodic controls, which allows to distinguish three possibilities: impossibility of improvement (Monod's or Haldane's kinetics), conditional improvement (Hill's kinetics) or systematic improvement (Contois's kinetics with $KY > 1$). Thanks to a duality, we show that for both problems: minimizing the average output concentration under integral constraint on the control, or maximizing the integral of the control under constraint on the average output concentration, bang-bang controls are optimal among all periodic solutions, and we characterize the two optimal switching times. This approach provides to practitioners the maximal improvement that can be expected when playing with periodic operations. Note also that measuring the performances of periodic controls can be a way to discriminate between several growth models, as proposed in the conference paper [17]. Further extensions of this work could consider multiple species (species coexistence in the chemostat being generically not possible at steady-state) or biogas production as an additional criterion.

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Appendix

Ref. [5] deals with general problems of the form (8) on an invariant interval $I = (a, b)$ such that
H1. g is positive on I, $f(a) - g(a) = 0$ and $f(b) + g(b) = 0$
H2. $f - g < 0$ and $f + g > 0$ on I
Under the following hypotheses
$\overline{\mathbf{H}}$. There exists $\bar{x} \in I$ such that $\psi(\bar{x}) = \bar{u}$ where the function $\psi := -f/g$, with $(\psi(x) - \psi(\bar{x})(x - \bar{x}) > 0$ for any $x \in I \setminus \{\bar{x}\}$.
H3. ℓ is increasing on I and $\gamma := \psi \circ \ell^{-1}$ is strictly convex increasing on $\ell(I)$.
it is proved that for any $T > 0$ the optimal solutions of (8) are bang-bang with exactly two commutations at points $x_m < \bar{x} < x_M$ that are uniquely defined (Prop. 3.2 and Th. 3.6).

For our Pb. 1, we take for I the largest open interval containing $\bar{s}$ that is invariant for (5) with controls in $[D_-, D_+]$ and posit $u := \alpha D + \beta \in [-1, 1]$ with

$$\alpha := \frac{2}{D_+ - D_-},\ \beta := -\frac{D_+ + D_-}{D_+ - D_-}$$

We define for $s \in I$:

$$f(s) := (-\nu(s) - \beta/\alpha)(s_{in} - s)\ ;\ g(s) := (s_{in} - s)/\alpha,$$
$$\ell(s) := s\ ;\ \psi(s) := \alpha\nu(s) - \beta,$$

Clearly, H1 and H2 are satisfied. Under A2b, ψ is increasing convex and $\overline{\text{H}}$, H3 are thus fulfilled. We then obtain the optimality of the bang-bang control (9) which has exactly two commutations, and its uniqueness, as stated in Prop. 4 (i). Ref. [5] also relaxes hypotheses $\overline{\text{H}}$, H3 and states that if it is fulfilled only locally about $\bar{x}$, then the same conclusions hold provide that $T > 0$ is not too large (Th. 4.1). This gives the result (ii) of Prop. 4.

References

[1] E. Abulesz and G. Lyberatos. Periodic optimization of continuous microbial growth processes. *Biotechnology and Bioengineering*, 29:1059–1065, 1987.

[2] J.F. Andrews. A mathematical model for the continuous culture of microorganisms utilizing inhibitory substrates. *Biotechnology and Bioengineering*, 10(6):707–723, 1968.

[3] J.E. Bailey. Periodic operation of chemical reactors: a review. *Chemical Engineering Communications*, 1(3):111–124, 1974.

[4] T. Bayen, A. Rapaport, and F.-Z. Tani. Optimal periodic control of the chemostat with Contois growth function. *IFAC-PapersOnLine (9th Vienna International Conference on Mathematical Modelling)*, 51(2):730–734, 2018.

[5] T. Bayen, A. Rapaport, and F.-Z. Tani. Optimal periodic control for scalar dynamics under integral constraint on the input. *Mathematial Control & Related Fields*, 2019 (on line).

[6] S. Bittanti, G. Fronza, and G. Guardabassi. Periodic control: A frequency domain approach. *IEEE Transactions on Automatic Control*, 18:33–38, 1973.

[7] A. Bressan and B. Piccoli. *Introduction to the mathematical theory of control*. American Institute of Mathematical Sciences, Springfield, 2007.

[8] L. Cesari. *Optimization – Theory and Applications. Problems with ordinary differential equations*. Springer, 1983.

[9] D.E. Contois. Kinetics of Bacterial Growth: Relationship between Population Density and Specific Growth Rate of Continuous Cultures. *Journal of General Microbiology*, 21:40–50, 1959.

[10] G. D'Avino, S. Crescitelli, P.L. Maffettone, and M. Grosso. On the choice of the optimal periodic operation for a continuous fermentation process. *Biotechnology Progress*, 26:1580–1589, 2010.

[11] J. Harmand, C. Lobry, A. Rapaport, and T. Sari. *The Chemostat: mathematical theory of microorganisms cultures*. ISTE Wiley, 2017.

[12] J. Monod. La technique de culture continue: Théorie et applications. *Annales de l'Institut Pasteur*, 79:390–410, 1950.

[13] H. Moser. The dynamics of bacterial populations maintained in the chemostat. *Carnegie Institution of Washington Publication*, 1958.

[14] S. Parulekar. Analysis of forced periodic operations of continuous bioprocesses: single input variations. *Chemical Engineering Science*, 3(55):2481–2502, 1998.

[15] L. Ruan and X.D. Chen. Comparison of several periodic operations of a continuous fermentation process. *Biotechnology Progress*, 12(2):286–288, 1996.

[16] P.L. Silveston and R.R. Hudgins. *Periodic Operation of Chemical Reactors*. Butterworth-Heinemann, 2013.

[17] F. Tani, A. Rapaport, and T. Bayen. Periodic controls for discriminating density dependent growth in the chemostat. In *IEEE 58th Conference on Decision and Control (CDC)*, pages 4735–4740, Nice, France, 2019.

[18] W. Walter. *Ordinary Differential Equations*. Springer, 1998.

[19] N. Watanabe, K. Onogi, and M. Matsubara. Periodic control of continuous stirred tank reactors-I: The pi criterion and its applications to isothermal cases. *Chemical Engineering Science*, 36(5):809–818, 1981.