Improvement of performances of continuous biological water treatment with periodic solutions

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Abstract

We study periodic solutions of the chemostat model under an integral constraint, either on the flow rate (Pb. 1) or on the substrate concentration (Pb. 2). We give conditions on the growth kinetics for which it is possible to improve the averaged water quality (Pb. 1) or the total quantity of treated water (Pb. 2) over a given time period, compared to steady-state. When this is possible, we characterize optimal periodic solutions and show a duality between the two optimization problems. The results are illustrated on four types of growth kinetics, given by Monod, Haldane, Hill and Contois functions.

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

1 Introduction

The continuous culture of micro-organisms is of primer importance in many industrial frameworks such as biotechnology, waste water treatment... as a way to convert raw material into products of interest or to treat pollutants in contaminated waters. During the past decades, optimization of such bio-processes has been investigated either at steady state [5,14], either under periodic operation [1,11]. In production optimization, one typically looks for maximizing productivity playing with the input flow rate as a control variable. It appears that periodic operations have been proved to be better than steady-state, under precise conditions. For instance, in [1], the π-criterion has been used to characterize the best frequency of periodic controls (improving a cost function w.r.t. its value at steady-state). For water treatment, the objectives are related to water quality and are quite different:

- either minimizing the pollutant concentration at the output of the process for a given input flow rate of water to be decontaminated (objective 1) ;
- either maximizing the input flow rate of water to be treated given a threshold of pollutant concentration not be exceeded at the output (objective 2).

⋆ Preliminary results were presented at IFAC MATHMOD 2018 meeting [3]. Corresponding author: F.-Z. Tani.

Classically, such processes are well represented with the chemostat model [12,8]:

$$\begin{cases} \dot{s} \;=\; -\dfrac{1}{Y}\mu(s,x)x + D(s_{in}-s), \\ \dot{x} \;=\; \mu(s,x)x - Dx, \end{cases} \tag{1}$$

where s and x denote respectively the substrate (here the pollutant) and biomass concentrations in a tank of constant volume V. The dilution rate $D = F/V$ (where F is the input flow rate of the contaminated water) is the control variable, Y the conversion rate, s_{in} the input substrate concentration and $\mu(\cdot,\cdot)$ the specific growth rate of micro-organisms. For sake of generality, we leave open the possibility for the growth function to be density-dependent or not, i.e. μ depends on s only or also on x. Note that equilibria $(\bar{s},\bar{x})$ of (1) satisfy $\bar{x}+Y\bar{s} = s_{in}$ and $\mu(\bar{s},Y(s_{in}-\bar{s})) = \bar{D}$, that uniquely link the flow rate $\bar{D}$ to the output concentration $\bar{s}$ (when the latter equation admits more than one solution, one considers only the smallest positive one, which necessarily corresponds to a stable equilibrium, see e.g. [8]). So, given a dilution rate $\bar{D}$ in objective 1, or given a threshold $\bar{s}$ in objective 2, there is no possible improvement. However, if one considers periodic solutions of (1) with periodic controls $D(\cdot)$ over a given time period T, the total quantity of water treated during a period is $Q_T := \langle D\rangle_T T$

($\bar{Q} := \bar{D}T$ for steady-states), where

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

denotes the average of any T-periodic function $\xi(\cdot) \in L^1_{loc}$. One then looks for the two control problems:

Problem 1 *Given a quantity of water $\bar{Q}$ to be treated during a period T, does there exist a non-constant T-periodic solution such that $\langle s \rangle_T \leq \bar{s}$ and $\langle D \rangle_T \geq \bar{D}$?*

In connection with Pb. 1, we shall also investigate the optimal control problem

$$\inf_{D(\cdot)} \langle s \rangle_T \ \text{ s.t. } s(0) = s(T) \text{ and } \langle D \rangle_T \geq \bar{D}, \tag{2}$$

where $D(\cdot)$ is a measurable control taking values in $[D_-, D_+]$ with $0 \leq D_- < \bar{D} < D_+$, and $s(\cdot)$ satisfies (1).

Problem 2 *Given a threshold $\bar{s}$, does there exist a non-constant T-periodic solution such that $\langle D \rangle_T \geq \bar{D}$ and $\langle s \rangle_T \leq \bar{s}$?*

Similarly, we shall consider the optimal control problem

$$\sup_{D(\cdot)} \langle D \rangle_T \ \text{ s.t. } s(0) = s(T) \text{ and } \langle s \rangle_T \leq \bar{s}. \tag{3}$$

Typically, in waste water treatment industry, the quality of the treated water is not always measured instantaneously but averaged over a time period depending on the final destination of the treated water (housing, industry, agriculture...). In Pb. 1, the control $D(\cdot)$ satisfies an integral constraint, while in Pb. 2 there is an integral constraint over $s(\cdot)$. Hence, Pb. 2 can be seen as a kind of "dual" of Pb. 1. This is quite different from what is studied in the biochemical literature when optimizing the productivity without integral constraint on the control, as recalled previously. To our knowledge, such problems have not been yet studied in the literature. Preliminary results on these questions have been given in the conference paper [3], where Pb. 1 only is considered for a single class of growth functions, and solutions of (2) were conjectured.

The paper is organized as follows. In section 2, we introduce our main assumptions on the kinetics. In Section 3, we discuss the existence of solutions of Pb. 1-2. When improvement with periodic solutions is possible, we aim at quantifying the maximal improvement as a function of the period in Sec. 4. Doing so, we apply recent results about optimal control for scalar dynamics under integral constraint on the input [4] for Pb. 1, and give an extension of these results for Pb. 2. Numerical simulations illustrate the possible gains in Section 5. Finally, some results of [4] are recalled in the Appendix.

2 Main assumptions

Since we only deal with periodic solutions of (1), we consider in the sequel the simplified dynamics for the variable $s(\cdot)$ only:

$$\dot{s} = (-\nu(s) + D(t))(s_{in} - s), \tag{4}$$

where $\nu(s) := \mu(s, s_{in} - s)$, assuming without any loss of generality $Y = 1$, and recall that $D(\cdot)$ is a measurable control with values in $[D_-, D_+]$. We shall consider the dynamics (4) on $(0, s_{in})$ and $\bar{D} \in (D_-, D_+)$ is chosen in such a way that

$$\bar{s} := \inf\{s \ ; \ \nu(s) > \bar{D}\} < s_{in}. \tag{5}$$

This choice of $\bar{D}$ avoids washout of biomass (i.e. $\bar{x} = 0$ at steady-state). Let us now introduce the following (minimal) assumption on ν.

Hypothesis 3 *The function ν is Lipschitz, non-negative, and null only at 0. The number of solutions to the equation $\nu(s) = \bar{D}$ over $(0, s_{in})$ (with $\bar{D} \in (D_-, D_+)$) is finite.*

Remark 4 *Under Hyp. 3 and (5), ν is increasing in a neighborhood of $\bar{s}$ which is then a locally stable equilibrium of (4) for the constant control $D = \bar{D}$.*

To cover a large variety of growth functions, we introduce three kinds of hypotheses.

Hypothesis 5 *The function ν is strictly convex in a neighborhood of $s = \bar{s}$.*

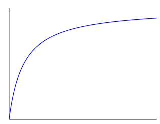
Hypothesis 6 *The function ν is strictly convex over $(0, s_{in})$.*

Hypothesis 7 *There is $\bar{\nu} \in C^0([0, s_{in}] \ ; \ \mathbb{R})$ such that*
- *$\bar{\nu} \geq \nu$ over $(0, s_{in})$ with $\bar{\nu}(\bar{s}) = \nu(\bar{s})$,*
- *$\bar{\nu}$ is concave non decreasing over $(0, s_{in})$.*

Such hypotheses are satisfied by the following kinetics (commonly found in the literature):

- Monod's kinetics [9], as an increasing function of s:

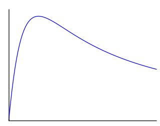
$$\mu(s) := \frac{\mu_{max} s}{K_s + s}.$$



Plot of $\mu(\cdot)$.

- Haldane's kinetics [2], which models an inhibition for large value of s:

$$\mu(s) := \frac{\mu_m s}{K_s + s + s^2/K_I}.$$

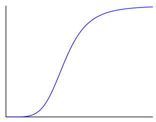


Plot of $\mu(\cdot)$.

Its maximum is reached at $\hat{s} := \sqrt{K_s K_i}$).

- Hill's kinetics [10], which exhibits a weak Allee effect for small value of s:

$$\mu(s) := \frac{\mu_{max} s^n}{K_s^n + s^n},\ (n \in \mathbb{N}^*)$$

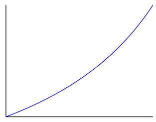


Plot of $\mu(\cdot)$.

and μ changes it concavity at $s_c =: K_s \left(\frac{n-1}{n+1}\right)^{1/n}$

- Contois's kinetics [7], which is density dependent:

$$\mu(s,x) = \frac{\mu_{max} s}{Kx + s},$$



Plot of $\nu(\cdot)$. ($K < 1$)

and ν is strictly convex for $K < 1$, concave for $K \geq 1$.

We shall next see that, depending on the kinetics, improvement of the criteria is possible or not.

3 Conditions for improvements

Our first objective is to study the existence of non-constant solutions of Pb. 1-2.

Lemma 8 *Given a pair* $(\bar{s}, \bar{D})$ *satisfying* (5)*, there are* $\varepsilon_0 > 0$ *and* $C > 0$ *such that for any* $\varepsilon \in (0, \varepsilon_0]$*, there exists a non-constant periodic solution* $s(\cdot)$ *of* (4) *such that* $\langle D \rangle_T = \bar{D}$ *or* $\langle s \rangle_T = \bar{s}$ *with* $\|s - \bar{s}\|_\infty \leq C\varepsilon$.

PROOF. We show first the existence of non-constant solutions of Pb. 1. Let $v(\cdot)$ be a T-periodic measurable bounded function with $\langle v \rangle_T = 0$, non null almost everywhere. Consider the control $D_\varepsilon(\cdot) := \bar{D} + \varepsilon v(\cdot)$, which takes values in $[D_-, D_+]$ for $\varepsilon > 0$ small enough (say $0 < \varepsilon \leq \varepsilon_1$), 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 (4) 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. From Rem. 4, ν has to be increasing in any sufficiently small neighborhood (s_0^-, s_0^+) of $\bar{s}$, which implies that $\theta(s_0^-, 0) > 0$, $\theta(s_0^+, 0) < 0$ and thus $\theta(s_0^-, \varepsilon) > 0$, $\theta(s_0^+, \varepsilon) < 0$ for ε sufficiently small (say $0 < \varepsilon \leq \varepsilon_2$) 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, notice that one has $s(\cdot, \bar{D}, \bar{s}) = \bar{s}$ and thus, Gronwall's Lemma implies the existence of a constant $C_1 > 0$ (depending on T and v) such that $||\tilde{s} - \bar{s}||_\infty \leq C_1\varepsilon$ for any $\varepsilon \in (0, \varepsilon_0']$ with $\varepsilon_0' := \min(\varepsilon_1, \varepsilon_2)$.

We now turn to (3). Let $y \in C^1(\mathbb{R}, \mathbb{R})$ be a T-periodic function such that $\langle y \rangle_T = 0$ (and non identically null). For ε small enough (say $0 < \varepsilon \leq \varepsilon_3$), $t \mapsto s_\varepsilon(t) := \bar{s} + \varepsilon y(t)$ is with values in $(0, s_{in})$ and satisfies $||s_\varepsilon - \bar{s}||_\infty < \|y\|_\infty \varepsilon$ as well as $\langle s_\varepsilon \rangle_T = \bar{s}$. Notice that $s_\varepsilon(\cdot)$ is a solution of (4) 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 (say $0 < \varepsilon \leq \varepsilon_4$), and thus s_ε is a non-constant periodic solution with $\langle s_\varepsilon \rangle_T = \bar{s}$ and $||s_\varepsilon - \bar{s}||_\infty < \|y\|_\infty \varepsilon$ for $0 < \varepsilon < \varepsilon_0'' := \min(\varepsilon_3, \varepsilon_4)$. This concludes the proof of the lemma taking $C := \max(C_1, \|y\|_\infty)$ and $\varepsilon_0 := \min(\varepsilon_0', \varepsilon_0'')$.

Remark 9 *Since the optimal control problems* (2) *and* (3) *involve inequality constraints, this lemma shows the existence of admissible solutions for these problems.*

In the sequel, "equality constraint" in Pb. 1, resp. Pb. 2 means that one considers solutions with $\langle D \rangle_T = \bar{D}$, resp. $\langle s \rangle_T = \bar{s}$.

Proposition 10 *If* (5) *and Hyp. 3 are verified, then:*

(i) *if Hyp. 5 is fulfilled, there exists* $T > 0$ *such that Pb. 1 and 2 admit solutions ;*

(ii) *if Hyp. 6 is fulfilled for any* $T > 0$*, any non-constant periodic solution with equality constraint gives an improvement for both problems ;*

(iii) *if Hyp. 7 is satisfied, there is no solution to Pb. 1 and 2.*

Moreover any periodic solution verifies $\langle D \rangle_T = \langle \nu(s) \rangle_T$.

PROOF. Given a non-constant T-periodic solution $s(\cdot)$ of (4) over $(0, s_{in})$, $t \mapsto \ln(s_{in} - s(t))$ is also periodic. From (4) one obtains $\langle D \rangle_T = \langle \nu(s) \rangle_T$. Recall now from Rem. 4 that ν is increasing in a neighborhood of $\bar{s}$.

Proof of (i). Under Hyp. 5, the periodic solution $s(\cdot)$ can be chosen in such a way that ν is strictly convex increasing over $s([0, T])$ (Lem. 8). 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 $Q_T/T = \langle D \rangle_T > \nu(\langle s \rangle_T) = \nu(\bar{s}) = \bar{Q}/T$ and thus the inequality $Q_T > \bar{Q}$ is fulfilled.

Proof of (ii). Under Hyp. 6, Hyp. 3 implies that ν is increasing over $(0, s_{in})$ and the former inequalities are then satisfied for any non-constant periodic solution with values in $(0, s_{in})$.

Proof of (iii). Under Hyp. 7, Jensen's inequality applied to the concave function $\bar{\nu}$ implies that $\langle \bar{\nu}(s) \rangle_T \leq \bar{\nu}(\langle s \rangle_T)$, and since $\bar{\nu} \geq \nu$, one obtains $\langle \nu(s) \rangle_T \leq \bar{\nu}(\langle s \rangle_T)$. In Pb. 1, one has $\bar{\nu}(\bar{s}) = \nu(\bar{s}) = \bar{D} = \langle D \rangle_T = \langle \nu(s) \rangle_T$. One then obtains $\bar{\nu}(\bar{s}) \leq \bar{\nu}(\langle s \rangle_T)$ from which we deduce the inequality $\bar{s} \leq \langle s \rangle_T$, since $\bar{\nu}$ is non decreasing. In Pb. 2, one has $Q_T/T = \langle D \rangle_T = \langle \nu(s) \rangle_T$ and

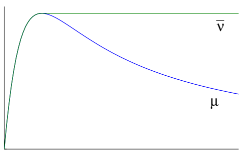
$\bar{\nu}(\langle s\rangle_T) = \bar{\nu}(\bar{s}) = \nu(\bar{s}) = \bar{Q}/T$. One then obtains $Q_T \leq \bar{Q}$ because $\langle D\rangle_T \geq \bar{D}$. In any case, no improvement is possible.

Let us now come back to the four growth functions listed above to examine how to apply Prop. 10.

• Monod's function is concave increasing and Hyp. 7 is fulfilled with $\bar{\nu} = \mu$. Thus, no improvement is possible.

• Haldane's function is neither convex neither concave. However, from (5) one has $\bar{s} \in (0, \hat{s})$ and μ is concave increasing over $[0, \hat{s}]$. Then, the function

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

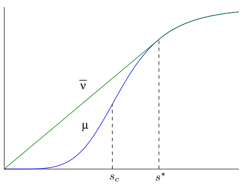


graphs of μ and $\bar{\nu}$

fulfills Hyp. 7, so, no improvement is possible.

• Hill's function also changed of concavity but is increasing. Its concave envelope on $\mathbb{R}_+$ is given by the function

$$\bar{\nu}(s) := \begin{cases} \mu'(s^*)s, & s < s^* \\ \mu(s), & s \geq s^* \end{cases}$$



graphs of μ and $\bar{\nu}$

where s^* is the unique abscissa whose tangent to the graph of μ passes through the origin: $s^* := s_c(1+n)^{\frac{1}{n}}$. If $\bar{s} < s_c$, μ is locally convex and Hyp. 5 is satisfied: improvement is possible with periodic solutions that belongs to $(0, s_c)$. If $\bar{s} \geq s^*$, $\bar{\nu}$ satisfies Hyp. 7 and no improvement is possible.

• For the Contois function, Hyp. 6 is fulfilled for $K < 1$: any non-constant periodic solution improves both criteria. For $K \geq 1$, Hyp. 7 is satisfied with $\bar{\nu} = \nu$: no improvement is possible.

4 Optimal improvements

For a given period T, we now wish to characterize periodic solutions belonging to the domain where ν is increasing and strictly convex that provide the best improvement in Pb. 1 and 2 (typically for μ of Contois or Hill type). Doing so, we are given a pair $(\bar{s}, \bar{D})$ satisfying (5), and we assume throughout this section that either Hyp. 5 or 6 is satisfied.

Lemma 11 *For any periodic solution $s(\cdot)$ of (4) such that $\langle s\rangle_T < \bar{s}$ and $\langle D\rangle_T \geq \bar{D}$, there exists $t \in [0, T]$ with $s(t) = \bar{s}$.*

PROOF. Using (4) and $\nu(\bar{s}) = \bar{D}$, we get

$$\int_0^T [\nu(s(t)) - \nu(\bar{s})] \geq 0. \quad (6)$$

Then, supposing that $s(t) < \bar{s}$ for any time $t \in [0, T]$ gives a contradiction with (6) using that ν is increasing over $s([0, T])$.

We can then consider without loss of generality solutions of (4) with $s(0) = \bar{s}$. Related to Pb. 1, we define the "value function", for $\bar{D} \in [D_-, D_+]$:

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

where $s(\cdot)$ is a solution of (4) associated with $D(\cdot)$. The usual argumentation on compactness of the set of admissible solutions and continuity of the cost function guarantees the existence of an optimal control (and thus that the infimum can be replaced by a minimum in the previous display), see e.g. [6].

Proposition 12 *The mapping V_T is the value function of (2) and it is increasing.*

PROOF. Suppose that an optimal control $D(\cdot)$ (non-constant) satisfies $\langle D\rangle_T > \bar{D}$. Denote by $s(\cdot)$ its associated T-periodic solution and 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

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

The control $\tilde{D}$ is with values in $[D_-, D_+]$ and so, it is admissible. 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 (4) 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. [13]). 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 solution $\tilde{s}(\cdot, \tilde{s}_0)$ (associated to $\tilde{D}$) 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 is not optimal for (2) with $\langle D\rangle_T > \bar{D}$ (since $\langle \tilde{D}\rangle_T < \langle D\rangle_T$). Hence, the inequality constraint in (2) must be saturated.
Let now $\bar{D}_1, \bar{D}_2 \in [D_-, D_+]$ be such that $0 < \bar{D}_1 < \bar{D}_2$. Since an optimal solution of (2) necessarily saturates the inequality constraint, $V_T(\bar{D}_1)$ is the value function associated with (2) which means that

$$V_T(\bar{D}_1) := \min_{D(\cdot)} \left\{ \langle s\rangle_T \, ; \, s(0) = s(T) = \bar{s}, \; \langle D\rangle_T \geq \bar{D}_1 \right\}.$$

If follows that an optimal pair $(D_2(\cdot), s_2(\cdot))$ for $V_T(\bar{D}_2)$ is admissible for $V_T(\bar{D}_1)$ (since $\langle D_2\rangle_T = \bar{D}_2 \geq \bar{D}_1$) which implies that $\langle s_2\rangle_T \geq V_T(\bar{D}_1)$ and thus the result.

Remark 13 *For Pb. 1, if $T > 0$ and $\bar{D} \in (D_-, D_+)$ are such that an improvement exists, then one has $V_T(\bar{D}) < \bar{s}$ where $\bar{s}$ is defined in* (5).

Let I be a sub-interval of $[0, s_{in}]$ containing $\bar{s}$ defined by (5), that is invariant by (4) for any control $D(\cdot) \in [D_-, D_+]$. We consider bang-bang controls:

$$\hat{D}_T(t) := \begin{cases} D_+, & 0 \leq t < t_1, \\ D_-, & t_1 \leq t < t_2, \\ D_+, & t_2 \leq t < T, \end{cases} \tag{7}$$

(where $0 < t_1 < t_2 < T$) and posit $s_M = s(t_1)$, $s_m = s(t_2)$, which belong to I. One can check that a solution $s(\cdot)$ of (4) with $s(0) = \bar{s}$ and control $\hat{D}_T(\cdot)$ is T-periodic if and only if one has

$$\int_{s_m}^{s_M} \eta(s)ds = T, \tag{8}$$

where the function $\eta : I \to \mathbb{R}$ is defined as

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

In the same way, $\hat{D}(\cdot)$ satisfies $\langle \hat{D}\rangle_T = \bar{D}$ if and only if

$$\int_{s_m}^{s_M} \eta(s)\nu(s)ds = \bar{D}T. \tag{9}$$

To conclude about the optimality of a control of type (7), we shall apply recent results [4] on periodic optimal control problems governed by a scalar dynamics under an L^1-norm constraint on the control (see Appendix).

Proposition 14 *For any $\bar{D} \in (D_-, D_+)$, there exists a unique pair $(s_m, s_M) \in (0, s_{in})^2$ satisfying* (8)-(9) *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. 1*

(i) *for any $T > 0$ if ν is convex increasing on I,*

(ii) *for $T > 0$ not too large if ν is locally convex increasing near $\bar{s}$.*

PROOF. Posit $u := aD + b \in [-1, 1]$ with

$$a := \frac{2}{D_+ - D_-}, \; b := -\frac{D_+ + D_-}{D_+ - D_-}$$

and define for $s \in I$:

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

so that (4) rewrites $\dot{s} = f(s) + ug(s)$. One can also check that we are exactly in the conditions of Th. A2 and Th. A4 given in Appendix. Therefore $\hat{D}_T(\cdot)$ is optimal.

We now turn to Pb. 2 which involves an integral constraint on the state and not on the control. Therefore, the results recalled in Appendix do not apply. Indeed, an integral constraint on the state is more difficult to grasp than for the control, as it cannot be formulated regardless of the dynamics, and extending the results in [4] is not straightforward. Nevertheless, we show that there exists a form of *duality* between Pb. 1 and 2. Doing so, we define the "dual" value function, for $\bar{s} \in I$:

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

Similarly to V_T, the above supremum can be replaced by a maximum (see [6]).

Proposition 15 *For any $\bar{s} \in I$ and T that satisfy conditions of Prop. 14, one has*

$$W_T(\bar{s}) = \max\{\bar{D} \in [D_-, D_+]; \; V_T(\bar{D}) = \bar{s}\} = V_T^{-1}(\bar{s}), \tag{10}$$

and W_T is the value function of (3).

PROOF. Assume first that ν is convex increasing on I and let us show that V_T is continuous on (D_-, D_+) for any $T > 0$. For any $\bar{D} \in (D_-, D_+)$, there exists a unique pair $(s_m, s_M) \in (0, s_{in}^2$ satisfying (8)-(9), that is,

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

and 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 [6]), so that $\bar{D} \mapsto s(\cdot, \hat{D}_T)$ is continuous, and thus V_T as well. Write $I = [s_-, s_+]$. As I is invariant and ν increasing, one has necessarily $V_T(D_-) = s_-$, $V_T(D_+) = s_+$. Since V_T is continuous and increasing (Prop. 12), it is thus invertible on I with $V_T^{-1}(I) = [D_-, D_+]$. Take $\bar{s} \in I$ and let $D^\dagger := V_T^{-1}(\bar{s})$. Let $D(\cdot)$ be an optimal control for Pb. 1 (i.e. such that $\langle D \rangle_T = D^\dagger$), 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 (3) has to saturate the constraint $\langle s \rangle_T \leq \bar{s}$, and thus W_T is value function.
If ν is convex increasing only over a sub-interval $J \subset I$ with $\bar{s} \in J$, consider any increasing convex function $\bar{\nu}$ which coincides with ν on J. Denote by $\bar{V}_T$, $\bar{W}_T$ the corresponding 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, (10) is fulfilled for T not too large.

For the the bang-bang controls (7), the constraint $\langle s \rangle_T = \bar{s}$ can be written, similarly as done before, with

$$\int_{s_m}^{s_M} s\,\eta(s)ds = \bar{s}\,T. \qquad (11)$$

Prop. 14 and 15 lead then to the following characterization of optimal solutions for Pb. 2.

Proposition 16 *There exists a unique pair* $(s_m, s_M) \in (0, s_{in}^2$ *satisfying* (8)-(11), *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 I,

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

Remark 17 *If an improvement exists for some $T > 0$ and $\bar{s} \in I$ in Pb. 2, then one has $W_T(\bar{s}) > \bar{D}$ where $\bar{D}$ is defined in* (5).

5 Numerical illustrations

Let us first examine how the optimal switching times t_1, t_2 of $\hat{D}_T$ can be computed. For Pb. 1, the constraint $\langle D \rangle_T = \bar{D} = \nu(\bar{s})$ applied to the bang-bang control (7) imposes a relation between t_1, t_2 that we write as follows.

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

From Prop. 14, t_1 is unique and can be then 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 the unique solution of (4) associated with $\hat{D}_T$ such that $s(0) = \bar{s}$. We present below numerical simulations of optimal solutions of Pb. 1 and Pb. 2 for Contois's kinetics, and then for Hill's kinetics.

For Contois's kinetics with $K > 1$ (which is convex increasing), for any $\bar{D} \in (D_-, D_+)$ and $T > 0$ one has $V_T(\bar{D}) < \bar{s} = \nu^{-1}(\bar{D})$ since the improvement is systematic. We depict on Fig. 1-left the inverse of ν and the optimal cost V_T (for $T = 15$ and $T = 50$) as functions of $\bar{D}$. We depict on Fig. 2-left the optimal cost as a function of T (for a given $\bar{D}$) which is decreasing accordingly to Lem. A3. We also compute the relative gain

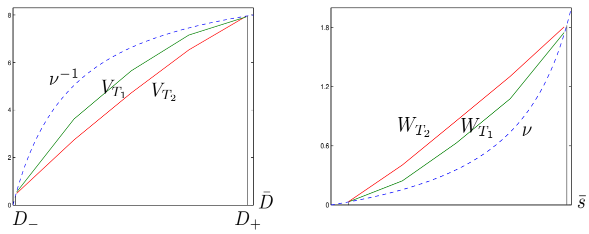


Fig. 1. Left: V_{T_1}, V_{T_2}, ν^{-1} w.r.t. $\bar{D}$. Right: W_{T_1}, W_{T_2}, ν w.r.t. $\bar{s}$ (for the Contois kinetics with $T_1 = 15$, $T_2 = 50$, $s_{in} = 8$, $m = 2$, $K = 5$, $D_+ = 1.95$, $D_- = 0.02$)

(for Pb. 1) given by $G_1(T, \bar{D}) := (\bar{s} - V_T(\bar{D}))/\bar{s}$ using periodic control versus constant control and we depict the corresponding iso-values on Fig. 2-right. Such a diagram 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 operated one.
For Pb. 2, the constraint $\langle s \rangle_T = \bar{s}$ (on the state variable) is more delicate to handle. However, according to the duality given by Prop. 15, one can solve Pb. 1 for any $\bar{D} \in (D_-, D_+)$ and inverse the function V_T. Notice that the improvement condition implies that one has $W_T(\bar{s}) > \nu(\bar{s})$ in I. Therefore, in order to compute $W_T(\bar{s})$ for a given value $\bar{s} \in I$, one can look for $\bar{D}$ satisfying $V_T(\bar{D}) = \bar{s}$ only for values $\bar{D}$ above $\nu(\bar{s})$. We plot ν and the optimal cost W_T (for $T = 15$ and $T = 50$) as functions of $\bar{s}$ on Fig. 1-right. Similarly to Pb. 1, we compute the relative gain $G_2(T, \bar{D}) := (W_T(\bar{s}) - \bar{D})/\bar{D}$ and plot its iso-values on Fig. 3

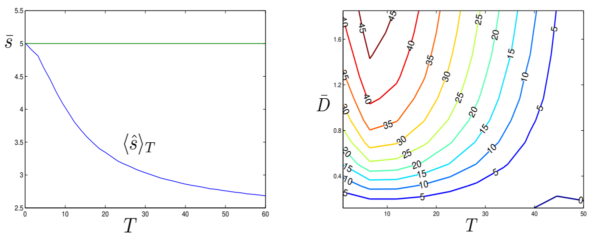


Fig. 2. Left: optimal cost w.r.t. T for the Contois law with $s_{in} = 8$, $m = 2$, $K = 5$, $D_+ = 1.95$, $D_- = 0.02$, $\bar{D} = 0.5$. Right: Iso-values of G_1 (for the Contois function) in %.

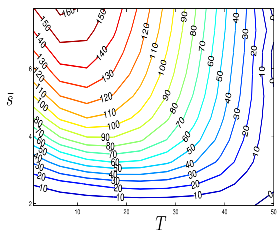


Fig. 3. Iso-values of G_2 (for the Contois function) in %.

For Hill's kinetics, we fix $\bar{D}$ in $(D_-, \mu(s_c))$ where the function is convex and chose $D_+ > \mu(s_c)$. Note that ν is increasing on $\mathbb{R}_+$, therefore, from Th. A2, there exists a unique $(s_m, s_M) \in I^2$ satisfying (8)-(9) for any $T > 0$. We can then compute the cost $\langle s \rangle_T$ obtained with the control $\hat{D}_T$ (since it is defined by the pair (s_m, s_M)) that we denote $\hat{J}_T$ (see Fig. 4-left). It is proved in [4] that the optimal cost is a decreasing function of T as long as periodic solutions belong to a domain where ν is convex (see Lem. A3). Numerical simulations give in our case a period $T_{max} \simeq 0.4$ for which the conditions of Th. A4 are verified for any $T \leq T_{max}$. For $T > T_{max}$, we have no guarantee that bang-bang controls stay optimal and we ignore about the monotonicity of $T \mapsto \hat{J}_T$. Nevertheless, we observe on Fig. 4 that $T \mapsto \hat{J}_T$ still decreases on $(T_{max}, \bar{T})$, where $\bar{T}$ denotes the minimum of $T \mapsto \hat{J}_T$. We propose, for $T > \bar{T}$, a control function $\tilde{D}_T$ with $2k$ or $2(k+1)$ switches, where $k := E[T/\bar{T}] > 1$, as

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

whose cost is given by

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

It is clear that $\tilde{J}_T = \hat{J}_{\bar{T}}$ when $T = k\bar{T}$ and is then below $\bar{s}$. 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 $\tilde{J}_T < \bar{s}$ when $\tau \neq 0$ (since it is a convex combination of $\hat{J}_{\bar{T}}$ and $\hat{J}_\tau$), see Fig. 4-left. We also plot the relative gain of control $\tilde{D}_T$ versus constant control, given by $\tilde{G}_1(T, \bar{D}) := (\bar{s} - \tilde{J}_T)/\bar{s}$ with $\bar{D} \in (D_-, \mu(s_c))$ (see Fig. 4-right). Finally, we present in Fig. 5 the value functions of Pb. 1 and Pb. 2, i.e., the maps $\bar{D} \mapsto \tilde{V}_T(\bar{D})$, $\bar{s} \mapsto \tilde{W}_T(\bar{s})$, where $\tilde{V}_T(\bar{D})$ is the cost $\tilde{J}_T$ obtained for $\bar{D}$ and $\tilde{W}_T(\bar{s}) := \max\{\bar{D}\,;\, \tilde{V}_T(\bar{D})\}$.

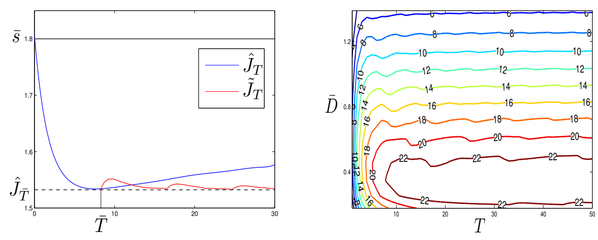


Fig. 4. Left: costs $\hat{J}_T$, $\tilde{J}_T$ for the Hill law with $s_{in} = 6$, $m = 5$, $K = 3$, $n = 3$, $D_+ = 4.5$, $D_- = 0.05$, $\bar{s} = 1.8$, where $\bar{T} \simeq 8.21$. Right: Iso-values of $\tilde{G}_1$ (for the Hill function) in %.

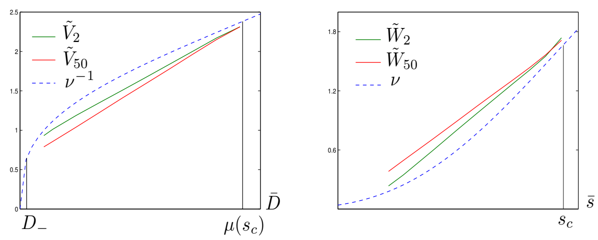


Fig. 5. Left: $\tilde{V}_{T_1}$, $\tilde{V}_{T_2}$, ν^{-1} w.r.t. $\bar{D}$. Right: $\tilde{W}_{T_1}$, $\tilde{W}_{T_2}$, ν w.r.t. $\bar{s}$ (for Hill kinetics with $T_1 = 2$, $T_2 = 50$, $s_{in} = 6$, $m = 5$, $K = 3$, $n = 3$ $D_+ = 4.5$, $D_- = 0.05$)

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 $K < 1$). Thanks to a duality argumentation, 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 periodic solutions, and we characterize the two optimal switching times. This approach provides to practitioners the maximal improvement that can be expected playing with periodic operations. Further extensions of this work could consider multiple species (species coexistence in the chemostat being generically possible only for non-constant controls) or biogas production as an additional criterion.

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Appendix

In this section, we recall the main results of [4] (written with x in place of s). Consider a one-dimensional controlled dynamics

$$\dot{x} = f(x) + ug(x), \quad x \in \mathbb{R}, \quad u(\cdot) \in [-1, 1] \tag{12}$$

and the optimal control problem

$$\inf_{u \in \mathcal{U}} \frac{1}{T} \int_0^T \ell(x(t))dt \text{ s.t. } x(0) = x(T) \text{ and } \langle u \rangle_T = \bar{u}$$

where $\mathcal{U}$ denotes the set of admissible controls. Functions f, g, ℓ are supposed to be of class C^1. In [4], it is assumed that there is an interval $I := (a, b)$ with $a < b$ such that $g > 0$, $f - g < 0$ and $f + g > 0$ over I, with $f(a) - g(a) = 0$ and $f(b) + g(b) = 0$ (this amounts to require that I is invariant and that (12) is controllable).

Hypothesis A1 *The function $\psi := -f/g$ verifies*

(i) *There is a unique $\bar{x} \in I$ such that $\psi(\bar{x}) = \bar{u}$ and $(\psi(x) - \psi(\bar{x})(x - \bar{x}) > 0$ for any $x \in I \setminus \{\bar{x}\}$.*

(ii) *ℓ is increasing over I and $\gamma := \psi \circ \ell^{-1}$ is strictly convex increasing over $\ell(I)$.*

Next, define the function

$$\eta(x) := \frac{1}{f(x) + g(x)} - \frac{1}{f(x) - g(x)}, \quad x \in I,$$

and for x_m, x_M such that $a < x_m < \bar{x} < \bar{x}_M < b$ and $x(0) = \bar{x}$, consider the bang-bang control

$$\hat{u}_T(t) := \begin{cases} +1, \ 0 \le t < t_1 := \inf\{t > 0, \ x(t) = x_M\}, \\ -1, \ t_1 \le t < t_2 := \inf\{t > t_1, \ x(t) = x_m\}, \\ +1, \ t_2 \le t < T. \end{cases}$$

The following results are proved in [4] (Th. 3.6 and 4.1).

Theorem A2 *Under Hyp. A1*(i)*, for any $T > 0$, there exists a unique pair $(x_m, x_M) \in I^2$ such that*

$$\int_{x_m}^{x_M} \eta(x)dx = T \text{ and } \int_{x_m}^{x_M} \psi(x)\eta(x)dx = T\bar{u}. \tag{13}$$

Moreover, if Hyp. A1(ii) *is fulfilled then the control $\hat{u}_T(\cdot)$ defined by (x_m, x_M) satisfying* (13) *is optimal for the initial condition $x(0) = \bar{x}$.*

One has also the following property.

Lemma A3 *Under conditions of Th. A2, the optimal cost (which corresponds to $\hat{u}_T$) is decreasing w.r.t. T.*

Hyp. A1 can be relaxed considering the interval $[x_T^-, x_T^+]$ with $x_T^- = x(t^+, u^+)$, $x_T^+ = x(t^-, u^-)$, where $x(\cdot, u^\pm)$ are the solutions of (12) for the one switch controls

$$u^-(t) = \left| \begin{array}{l} -1, \ t \in [0, t^-), \\ \ \ 1, \ t \in [t^-, T], \end{array} \right. ; \ u^+(t) = \left| \begin{array}{l} \ \ 1, \ t \in [0, t^+), \\ -1, \ t \in [t^+, T], \end{array} \right.$$

with $x(0, u^\pm) = \bar{x}$ and t^-, t^+ are such that $x(T, u^\pm) = \bar{x}$.

Theorem A4 *For any $T > 0$ such that Hyp. A1*(i) *is fulfilled on $[x_T^-, x_T^+]$ instead of I, there exists a unique pair $(x_m, x_M) \in I^2$ satisfying* (13)*. If moreover Hyp. A1*(ii) *is fulfilled on $[x_m, x_M]$, then the control $\hat{u}_T(\cdot)$ is optimal.*

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