

Optimal control of renewable biohydrogen production: A switched system approach ^{*}

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Abstract: Biohydrogen produced from microorganisms such as cyanobacteria is a promising low cost, sustainable and environmentally friendly energy source. Recent studies have shown that high biohydrogen yield can be obtained from *Cyanothece* sp. ATCC 51142 in a fed-batch reactor. This system has been accurately described with a modified Droop model that can be used for optimization studies. Searching for the optimal operating conditions and the switching time from batch to fed-batch operation, such that the biohydrogen production is maximized, leads to a challenging singular optimal control problem. In this study, a novel reformulation based on the theory of switched systems and time-scaling transformation is proposed to address the switching of the operating modes and the optimal control structure. Solutions are found by solving an embedded optimal control problem that can be solved efficiently as a nonlinear programming problem. No mesh refinement is required to capture the switching times. Smooth optimal control profiles and clear switching structures that maximize the biohydrogen yield were found for two types of control parametrization.

Keywords: Singular optimal control, switched systems, biohydrogen production, fed-batch reactors.

1. INTRODUCTION

Hydrogen has been considered a green alternative to replace fossil fuels in diverse applications for many years as it can be used as a clean energy carrier for heat supply and transportation purposes. Hydrogen holds the potential for affordable energy supply with reduced green house gas and air pollutant emissions (Falcone et al., 2021). Recent improvements in technology and manufacturing have allowed hydrogen to play an important role in the transition towards a low-carbon economy (Staffell et al., 2019). Biological processes have gained interest for sustainable biohydrogen production from renewable energy sources (Akhlaghi and Najafpour-Darzi, 2020). In particular, biohydrogen can be obtained efficiently from different microorganisms such as cyanobacteria in a batch/fed-batch reactor (Zhang et al., 2015). Since the process performance depends on many factors such as influent substrate concentration and dilution rate, it is critical to find the optimal operating conditions that maximize the biohydrogen yield. Despite the significance, only a few efforts have been made to develop offline and online optimization studies for this specific system (del Rio-Chanona et al., 2015; del Rio-Chanona et al., 2016).

The problem of maximizing the biohydrogen yield in a fed-batch system can be cast as an optimal control (OC) problem. In fed-batch reactors, the control variable (e.g., dilution rate, influent concentration) appears linearly in the dynamic model. As a result, the problem becomes a

singular optimal control (SOC) problem leading to analytical and numerical difficulties in finding an optimal solution (Shukla and Pushpavanam, 1998). Moreover, the kinetic models (e.g., Droop model) often used in the mathematical description of these processes include highly nonlinear terms that introduce additional challenges to the solution techniques (Banga et al., 2005). Recent computational strategies have been proposed to solve SOC problems more efficiently (see Andrés-Martínez et al. (2020) and the references therein). However, those strategies usually require expensive computations, mesh refinement, parameters tuning or continuation methods, and/or derivation of an analytical expression for the singular arc. Moreover, those methods have not been tested rigorously on batch/fed-batch systems.

In this work, the SOC problem is addressed using a switched system approach. In this type of systems, the right hand side of the dynamic model consists of different modes that can be active or inactive according to a fixed or variable switching structure. In a SOC problem, the system consists of three different modes defined by each control arc. A binary function that chooses the type of arc is introduced and relaxed by applying an embedding approach. A time scaling transformation is applied to handle variable switching times. The resulting formulation is amenable to standard numerical techniques such as those based on mathematical programming. The proposed methodology is used to find an optimal control switching structure and the optimal switching time from batch to fed-batch operation such that the biohydrogen production is maximized.

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The rest of the study is structured as follows. In Section 2, the maximization of biohydrogen production is stated as a singular optimal control problem. In Section 3, an equivalent switched optimal control problem is formulated. A more tractable formulation is obtained by applying the embedding approach and time-scaling transformation. In Section 4, a solution strategy based on a direct method is explained. In Section 5, the proposed formulation is applied to maximize the biohydrogen yield. Section 6 presents conclusions and future work.

2. OPTIMAL CONTROL FORMULATION

This section presents the main optimal control problem addressed in this work. We show that the optimal control may contain singular arcs.

2.1 Biohydrogen maximization problem

The fixed volume fed-batch reactor dynamic model used in the present study was taken from del Rio-Chanona et al. (2015). More details of the process can also be found in Zhang et al. (2015). A modified Droop model is used to describe the biohydrogen production from the species *Cyanothece* sp. ATCC 51142 at constant temperature. The maximization of biohydrogen is formulated as the following OC problem:

$$\min_{T, N_{fed}} -H(t_f) \quad (1)$$

s.t

$$\frac{dX}{dt} = \mu_{max} X \left(1 - \frac{k_q}{q}\right) \frac{C}{K_C + C} - \mu_d X^2 \quad (2)$$

$$\frac{dC}{dt} = -Y_{C/X} \mu_{max} X \left(1 - \frac{k_q}{q}\right) \frac{C}{K_C + C} + F_{in} C_{fed} \quad (3)$$

$$\frac{dN}{dt} = -Y_{N/X} \mu_{max} X \frac{N}{K_N + N} + F_{in} N_{fed} \quad (4)$$

$$\frac{dq}{dt} = Y_{q/X} \mu_{max} \frac{N}{K_N + N} - \mu_{max} \left(1 - \frac{k_q}{q}\right) q \frac{C}{K_C + C} \quad (5)$$

$$\frac{dO}{dt} = Y_{O/X} \mu_{max} X \frac{N}{K_N + N} - Y_d \mu_d X^2 f(O) + F_{in} O_{fed} \quad (6)$$

$$\frac{dH}{dt} = Y_{H/X} X (1 - f(O)) f(N) \quad (7)$$

$$t \in [t_0, t_f] \quad (8)$$

$$f(N) = 0.5 \frac{((N - 100)^2)^{0.5} - (N - 100)}{((N - 100)^2 + 0.1)^2} \quad (9)$$

$$f(O) = \frac{O}{(O^2 + 0.1)^{0.5}} \quad (10)$$

$$F_{in} = \frac{0.1}{720 - T} \quad (11)$$

where X , C , N , q , O and H are the biomass, glycerol, nitrate, intracellular nitrogen source, oxygen and hydrogen concentrations, respectively; the functions $f(N)$ and $f(O)$ are used to regulate the start and termination of hydrogen production; F_{in} denotes the influent flow rate; C_{fed} , O_{fed} and N_{fed} are the glycerol, oxygen and nitrate concentrations in the influent, respectively; T is the time when the influent starts to be added to the reactor, i.e.,

the system switches from batch to fed-batch operation; $Y_{C/X}$, $Y_{N/X}$, $Y_{q/X}$, $Y_{O/X}$ are the yields of nutrients and products; μ_{max} is the maximum biomass specific growth rate; μ_d is the biomass specific respiration rate. The nitrate concentration N_{fed} of the influent is used as the control variable subject to the following constraints:

$$N_{fed}^L \leq N_{fed} \leq N_{fed}^U \quad (12)$$

where N_{fed}^L and N_{fed}^U are the lower and upper nitrate concentration limits, respectively. The modified Droop model used in the OC model is able to describe all the relevant growth phases of cyanobacteria, i.e., primary and secondary growth phases, stationary phase, and decay phase. Hydrogen is generated for the most part during the decay phase.

Remark The optimization of this process has been studied in del Rio-Chanona et al. (2015) and Valvassore et al. (2021) using different approaches. However, in both studies, the terms μ_{max} and μ_d are missing in equation (6). Therefore, those terms were added in the present study such that the dimensions in the model are consistent (Zhang et al., 2015; del Rio-Chanona et al., 2016).

2.2 Singular control

The OC problem (1)-(11) can be reformulated in a more compact form as the following Mayer OC problem, where the control variable $u(t)$ appears linearly in the formulation:

$$\begin{aligned} \min_{T, u} \quad & \phi(z(t_f)) \\ \text{s.t} \quad & \dot{z}(t) = f(z(t)) + g(z(t)) u(t) \\ & u^L \leq u(t) \leq u^U \\ & z(t_0) = z_0, \quad t \in [t_0, t_f] \end{aligned} \quad (13)$$

where z is an $n \times 1$ vector of state variables and u is the control variable, which is considered piecewise continuous; $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ is a \mathcal{C}^1 function describing the terminal (or endpoint) cost; the functions $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ are of class \mathcal{C}^1 ; u^L and u^U are the lower and upper bounds on $u(t)$, respectively. Definitions of each term in (13) are provided in Appendix A. We define the Hamiltonian function for problem (13) as follows:

$$H(t) = \lambda(t)^T [f(z(t)) + g(z(t)) u(t)] \quad (14)$$

where $\lambda(t) \in \mathbb{R}^n$ are the adjoint variables. The so-called switching function can be obtained from the differentiation of $H(t)$ with respect to $u(t)$, i.e.,

$$\sigma(t) = H_u(t) = g^T(z(t)) \lambda(t) \quad (15)$$

A characterization of the solution of problem (13) can be obtained by applying the Pontryagin's minimum principle, which establishes that an optimal control $u(t)$ must minimize the Hamiltonian as follows (Ko and Steve, 1971):

$$u(t) = \begin{cases} u^L & \sigma(t) > 0, \\ u^U & \sigma(t) < 0, \\ u_s(t) & \sigma(t) = 0 \end{cases} \quad (16)$$

which means that $u(t)$ is at its lower (upper) bound when $\sigma(t) > 0$ ($\sigma(t) < 0$). These values are known as non-singular arcs. On the other hand, when $\sigma(t) = 0$, the optimal control is given by a singular arc $u_s(t) \in (u^L, u^U)$ that minimizes the Hamiltonian, i.e., $H_{u_s}(t) = 0$. However,

this expression does not contain $u_s(t)$ because $u(t)$ appears linearly in the Hamiltonian function (14). As a result, the principle does not provide enough information to derive $u_s(t)$. The points in t where the control switches between singular and non-singular arcs are called *switching times* or *switching instants*. In some particular cases, a solution to problem (13) consists only of non-singular arcs, i.e., $u(t)$ switches between u^L and u^U leading to a *bang-bang* structure. However, in general, the optimal control $u(t)$ usually consists of a concatenation of non-singular and singular arcs, e.g., *bang-singular*, *bang-singular-bang*. In order to obtain an expression for $u_s(t)$, repeated differentiation of $H_u(t)$ with respect to time must be performed until $u(t)$ appears explicitly, which is a procedure that can become quite involved. Also, there may be cases when $u(t)$ never appears. An additional complication is that the switching sequence of non-singular and singular arcs is not known *a priori*. Thus, solving the problem by applying Pontryagin's principle can become quite challenging.

Alternatively, a direct method can be applied by transforming problem (13) into a nonlinear programming problem (NLP) where $z(t)$ and $u(t)$ become decision variables at each discrete point in t . This strategy avoids the use of the switching function $\sigma(t)$ and is the approach adopted in the present study. However, the NLP becomes ill-conditioned due to the singularity leading to aggressive oscillations in the control profile (Kameswaran and Biegler, 2006). Moreover, in order to properly capture the switching sequence, a fine mesh of variable size is commonly used in the discretization of t giving rise to a very large and highly non-convex problem. To circumvent these issues, in this work we propose a reformulation of (13) such that optimal and smooth control profiles and a well-defined switching sequence are obtained at low computational effort without resorting to mesh refinement.

3. EQUIVALENT FORMULATION

This section presents a reformulation of the OC problem based on the theory of switched systems and time-scaling transformation.

3.1 Switched optimal control problem

Let $i \in \mathcal{I} = \{1, \dots, 3\}$ indicate the kind of control arc $u_i(t)$. Without loss of generality, we let $u_1(t)$, $u_2(t)$, $u_3(t)$ represent u^L , u^U , $u_s(t)$, respectively. Thus, the dynamic constraints in problem (13) can be written as a switched system as follows:

$$\dot{z}(t) = \sum_{i=1}^3 \alpha_i(t) [f(z(t)) + g(z(t)) u_i(t)], \quad z(t_0) = z_0 \quad (17)$$

for $u_i(t) \in \Omega$ where $\Omega \subset \mathcal{R}$ is a compact and convex set; $\alpha_i(t) \in \{0, 1\}$ is a binary function that selects only one arc u_i to become active at time t , i.e.,

$$\sum_{i=1}^3 \alpha_i(t) = 1 \quad (18)$$

Since the functions $f(\cdot)$ and $g(\cdot)$ do not depend on u_i , and constraint (18) must be satisfied, we can rewrite equation (17) as follows:

$$\dot{z}(t) = f(z(t)) + g(z(t)) w(t), \quad z(t_0) = z_0 \quad (19)$$

where:

$$w(t) = \sum_{i=1}^3 \alpha_i(t) u_i(t) \quad (20)$$

Therefore, depending on the values of $\alpha_i(t)$, $w(t)$ becomes u^L , u^U or $u_s(t)$. The initial and final states are assumed to satisfy $(t_0, z(t_0)) \in \mathcal{T}_0 \times \mathcal{B}_0$ and $(t_f, z(t_f)) \in \mathcal{T}_f \times \mathcal{B}_f$ for a compact set $\mathcal{B} = \mathcal{T}_0 \times \mathcal{B}_0 \times \mathcal{T}_f \times \mathcal{B}_f \subset \mathcal{R}^{2n+2}$. Since the fixed values u^L and u^U appear explicitly in the switched formulation, the only continuous control variable is $u_s(t)$. Thus, a switched SOC problem is defined as follows:

$$\min_{T, \alpha_i, u_s \in \Omega, i \in \mathcal{I}} \phi(z(t_f)) \quad (21)$$

subject to constraints (18), (19) and boundary conditions $(t_0, z(t_0), t_f, z(t_f)) \in \mathcal{B}$. Problem (21) can be solved as a mixed-integer OC problem, which may be computationally expensive and requires special algorithms, e.g., outer approximations and branch and bound.

3.2 Embedding approach

We embed the system (17) into a larger family by relaxing the condition $\alpha_i(t) \in \{0, 1\}$ to $\alpha_{Ei}(t) \in [0, 1]$ for $i \in \mathcal{I}$ such that binary variables are avoided. Thus, the embedded system takes the following form:

$$\dot{z}_E(t) = f(z_E(t)) + g(z_E(t)) w_E(t), \quad z_E(t_0) = z_0 \quad (22)$$

where:

$$w_E(t) = \sum_{i=1}^3 \alpha_{Ei}(t) u_{Ei}(t) \quad (23)$$

such that

$$\sum_{i=1}^3 \alpha_{Ei}(t) = 1 \quad (24)$$

We can define an embedded SOC as follows:

$$\min_{T, \alpha_{Ei}, u_{Es} \in \Omega, i \in \mathcal{I}} \phi(z_E(t_f)) \quad (25)$$

subject to constraints (22), (24) and boundary conditions $(t_0, z_E(t_0), t_f, z_E(t_f)) \in \mathcal{B}$. We assume that the set of admissible pairs (z_E, u_E) is nonempty and that there is a compact set which includes all the points $(t, z_E(t))$ for $t \in [t_0, t_f]$. An important result from switched systems theory is that the set of trajectories of the switched system (17) is dense in the set of trajectories of the embedded system (22) (Bengea and DeCarlo, 2005). Therefore, a solution of the embedded OC (25) is either binary (one of the α_i is 1, whereas the others are 0) or a trajectory of the embedded system can be approximated by trajectories of the switched system to an arbitrary precision. As a result, it is possible to generate optimal solutions for the switched OC (21) by solving the embedded version (25).

Proposition The embedded SOC problem (25) satisfies sufficient conditions for existence of a solution.

Proof. In addition to the assumptions previously made on the pairs (z_E, u_E) , $(t, z_E(t))$ and on the sets \mathcal{B} and Ω , it is required that the function $f(z_E(t)) + g(z_E(t))$ is affine in each control u_{Ei} (Bengea and DeCarlo, 2005) to guarantee the existence of a solution to problem (25). This property is fulfilled given that the singularity comes from the fact that $u(t)$ occurs linearly in the original formulation.

Note that problem (25) contains only continuous variables; hence, it can be solved using standard numerical methods, such as indirect or direct approaches. However, the presence of singular arcs u_{E_s} and the unknown switching sequence of arcs requires a special treatment. This is discussed next.

3.3 Time-scaling transformation

We divide the time interval into M subintervals $k = 1, \dots, M$, with $0 = \tau_0 < \tau_1 < \dots < \tau_M = t_f$, where τ_k for $k = 1, \dots, M - 1$ are the switching instants at which the control switches from one arc to another. These instants can be treated as decision variables such that they are optimally located. Thus, we apply a time-scaling transformation that maps the variable switching instants to equally spaced points on a new time domain s (Teo et al., 1999). This new domain is evenly divided into M subintervals with fixed points $0 = s_0 < s_1 < \dots < s_M = M$, where s_j for $j = 1, \dots, M - 1$ are now fixed switching instants. The relation between t and s is given by:

$$\dot{t}(s) = \sum_{k=1}^M v_k \chi_k(s), \quad t(s_0) = 0, \quad t(s_M) = t_f \quad (26)$$

where $v_k = \tau_k - \tau_{k-1} \geq 0$ is the duration of subinterval k , and $\chi_k(s)$ is the indicator function. When (26) is integrated, we obtain:

$$t(s) = \sum_{k=1}^{j-1} v_k + v_j (s - s_j + 1), \quad s \in (s_{j-1}, s_j] \quad (27)$$

$$j \in \mathcal{J} = \{1, \dots, M\}$$

hence, for each $k = 1, \dots, M$, we can recover the switching instant τ_k as follows:

$$t(k) = \sum_{j=1}^k v_j = \sum_{j=1}^k (\tau_j - \tau_{j-1}) = \tau_k \quad (28)$$

We denote the value of α_{E_i} on $(s_{j-1}, s_j]$ as $\alpha_{E_{ij}}$ for $j \in \mathcal{J}$. Thus, the dynamic system can be rewritten in the new time domain s as follows:

$$\dot{\hat{z}}_E(s) = \sum_{j=1}^M v_j [f(\hat{z}_E(s)) + g(\hat{z}_E(s)) \hat{w}_E(s)] \chi_j(s) \quad (29)$$

where

$$\hat{w}_E(s) = \sum_{i=1}^3 \hat{\alpha}_{E_{ij}} \hat{u}_{E_i}(s) \quad (30)$$

such that

$$\sum_{i=1}^3 \hat{\alpha}_{E_{ij}} = 1, \quad j = 1, \dots, M \quad (31)$$

Since the process begins in batch operation and then switches to fed-batch, the variable T becomes the first switching instant τ_1 . Accordingly, an embedded SOC problem in the new time domain s can be defined as follows:

$$\min_{\substack{\hat{\alpha}_{E_{ij}}, v_j, \hat{u}_{E_s} \in \Omega, \\ i \in \mathcal{I}, j \in \mathcal{J}}} \phi(\hat{z}_E(s_M)) \quad (32)$$

subject to constraints (26), (29), (31) and boundary conditions $(t_0, \hat{z}_E(t_0), t_f, \hat{z}_E(t_f)) \in \mathcal{B}$. Therefore, for a given number M of subintervals in s , the optimal values of $\hat{\alpha}_{E_{ij}}$ select the type of arc i for each subinterval j . Furthermore, the values of v_j define the duration of each subinterval and

hence the switching instants in the original time domain t .

4. SOLUTION STRATEGY

4.1 Direct method

Problem (32) can be solved with a direct method, i.e., it is fully discretized and solved as an NLP. For a given number of M subintervals, we apply orthogonal collocation on each subinterval j (Finlayson, 1980). In order to reduce the ill conditioning of the NLP caused by the singular arc $\hat{u}_{E_s}(s)$, we use the values of $\hat{u}_{E_s}(s)$ at certain discrete points in each subinterval to parameterize the singular arc. For fed-batch reactors, the control is usually parameterized as a piecewise constant function. In the present work, we also use a cubic spline interpolation as it can adopt different shapes (e.g., straight lines, monotonic and non-monotonic curves) and avoid harsh oscillations (Andrés-Martínez et al., 2020). Thus, within each subinterval, the control variable is continuous but it is allowed to jump from one subinterval to another. Therefore, mesh refinement procedures are not needed to capture the switching instants as they are fixed *a priori* in the new domain s . An educated initial guess can be obtained by solving problem (13) as an NLP after full discretization. This coarse solution provides insights into the maximum number of control arcs.

4.2 Properties of the solution

When solving problem (32), two types of solutions can be obtained: $\hat{\alpha}_{E_{ij}}$ takes binary values for each subinterval j , or $\hat{\alpha}_{E_{ij}}$ takes nonbinary values for some subintervals. The former means that a solution to the switched SOC problem (21) has been found, whereas a binary solution can be constructed in the latter case (Bengea and DeCarlo, 2005). However, a nonbinary solution of $\hat{\alpha}_{E_{ij}}$ implies that the optimal control $\hat{w}_E(s)$ given by the expression (30) consists of a combination of u^L , u^U and $\hat{u}_{E_s}(s)$. Thus, $\hat{w}_E(s)$ can take values within the interval (u^L, u^U) , i.e., it is also a singular arc. Consequently, unless the singular arc is required to be given uniquely by $\hat{u}_{E_s}(s)$, it is not necessary to construct binary solutions and we can let the singular and non-singular arcs be given by $\hat{w}_E(s)$.

5. NUMERICAL STUDY

In this section, the proposed formulation (32) is applied to solve the OC problem (1)-(11). The parameter values and the operating conditions were taken from del Rio-Chanona et al. (2015) and are listed in Table 1 and Table 2, respectively. The value of K_C is found in the same reference as $K_C = 0$. Thus, the term $C/(K_C + C)$ is reduced to 1. Influent nitrate concentration limits were set to $N_{fed}^L = 0.0$ mg L⁻¹ and $N_{fed}^U = 4000$ mg L⁻¹. The total number of subintervals was fixed to $M = 8$ based on a coarse solution obtained by direct transcription of problem (13). Six Radau points were used for collocation. The following constraints were explicitly added in the formulation to prevent these variables from taking negative values: $C \geq 0$, $N \geq 0$, $O \geq 0$, $H \geq 0$. Solutions were obtained in Julia (1.6.2)/JuMP (0.21.9)

(Bezanson et al., 2017; Dunning et al., 2017). The NLP problems were solved with Ipopt (3.13.4) (Wächter and Biegler, 2006).

5.1 Results

The optimal influent nitrate concentration profiles are shown in Figure 1 for piecewise constant ($w_c(t)$) and cubic spline expressions ($w_{sp}(t)$) for $\hat{u}_{Es}(s)$. At the beginning of the fed-batch operation, both control profiles take a singular arc that promotes a rapid increase of biomass (Figure 2), which is slightly greater for $w_{sp}(t)$ as the singular arc is touching u^U almost the entire subinterval. This increase delays the hydrogen production at the beginning of the operation (Figure 3) as the nitrogenase activity is inhibited during this phase. At around 100 hours, the biomass concentration exhibits a short stationary phase followed by a decay phase. After approximately 155 hours, the nitrogenase activity is stimulated; hence, there is a substantial increase in hydrogen. During this subinterval both control profiles follow a singular arc for a long period such that the hydrogen production keeps increasing. The difference in the shape of each singular arc during this phase (Figure 1) leads to evident but small differences in the biomass concentration and hydrogen production profiles, as shown in Figures 2 and 3, respectively. After the second singular arc, $w_c(t)$ switches to the lower bound u^L and then to another singular arc very close to u^L . This structure is not observed for $w_{sp}(t)$ which switches from the second singular arc to another singular arc directly. Then, both control profiles remain at u^L until t_f is reached, which suggests that the influent nitrate is completely suppressed for the remaining operation time.

The optimal control profile when $\hat{u}_{Es}(s)$ is represented by a constant function in each subinterval is as follows:

$$w_c(t) = \begin{cases} u_s(t) & t \in [19.836, 137.745] \\ u_s(t) & t \in [137.745, 429.310] \\ u_L & t \in [429.310, 468.274] \\ u_s(t) & t \in [468.274, 600.442] \\ u_L & t \in [600.442, 720] \end{cases} \quad (33)$$

The corresponding objective function value is $H(t_f) = 537.484$ mL/L. The optimal switching time from batch to fed-batch operation is $T = 19.836$. The problem was solved in 0.701 CPU seconds.

The optimal control profile when $\hat{u}_{Es}(s)$ is represented by a cubic spline interpolation in each subinterval is as follows:

$$w_{sp}(t) = \begin{cases} u_s(t) & t \in [20.271, 117.276] \\ u_s(t) & t \in [117.276, 479.450] \\ u_s(t) & t \in [429.310, 603.195] \\ u_L & t \in [603.195, 720] \end{cases} \quad (34)$$

The corresponding objective function value is $H(t_f) = 540.964$ mL/L. The optimal switching time from batch to fed-batch operation is $T = 20.271$. The problem was solved in 0.587 CPU seconds.

Note that even though the problem was solved with eight subintervals, the control profiles consist of five and four arcs for $u_c(t)$ and $u_{sp}(t)$, respectively. The hydrogen production is only 0.65% higher when $\hat{u}_E(s)$ is represented by

Table 1. Parameter values.

parameter	value	parameter	value
μ_{max} [h^{-1}]	0.04765	$Y_{N/X}$ [mg g^{-1}]	244.6
k_q	0.6281	$Y_{q/X}$	1.723
μ_d [$\text{L g}^{-1} \text{h}^{-1}$]	0.008559	Y_d [L g^{-1}]	26.22
K_N [mg L^{-1}]	50.0	$Y_{C/X}$ [mmol g^{-1}]	20.83
$Y_{H/X}$ [mL g^{-1}]	2.34	$Y_{O/X}$ [$\text{L g}^{-1} \text{h}^{-1}$]	14.60

Table 2. Operating conditions.

$X(t_0)$	0.2 g L ⁻¹	$H(t_0)$	0.0 mL
$C(t_0)$	50 mmol L ⁻¹	O_{fed}	20%
$N(t_0)$	150 mg L ⁻¹	C_{fed}	50 mmol L ⁻¹
$q(t_0)$	1.0	t_f	720 h
$O(t_0)$	20%		

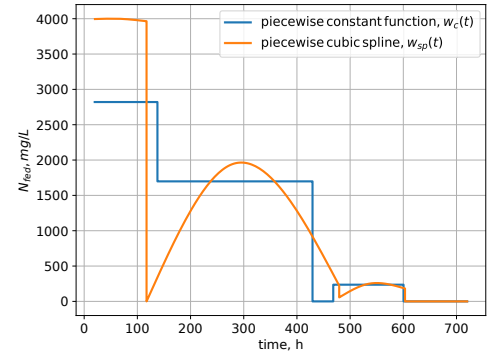


Fig. 1. Optimal control profiles.

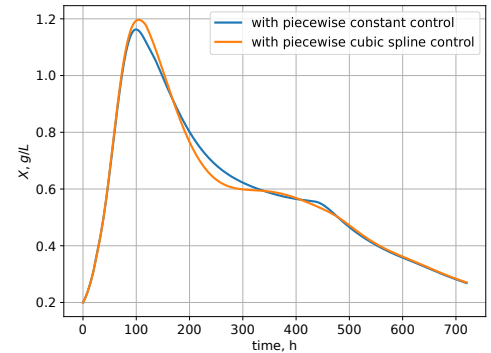


Fig. 2. Optimal biomass concentration.

a cubic spline interpolation in each subinterval as the control variable has more degrees of freedom. Moreover, two different control representations lead to similar biomass and hydrogen profiles. This is a common feature of SOC problems as some uniqueness properties are lost.

The results obtained in the present study are significantly different from those reported in the literature due to the differences in the model (see Remark in Section 2). Nevertheless, clear advantages can be identified in terms of computational complexity. del Rio-Chanona et al. (2015) report 152 seconds to solve the optimization problem with an initial guess obtained after 9 hours, whereas Valvassore et al. (2021) report 30 minutes to obtain their best solution. Therefore, the present formulation is attractive to address singular optimal control problems for challenging batch/fed-batch systems.

6. CONCLUSION

In the current study, the optimal control of a batch/fed-batch reactor to maximize the hydrogen production from *Cyanotheca* sp. ATCC 51142 described with a modified Droop model has been studied. A novel switched system formulation was developed to capture the singular control structure and the switching between batch and fed-batch operation. The resulting optimal control problem was solved efficiently as a nonlinear programming problem. Rigorous numerical treatments, such as mesh refinement and continuation methods, are avoided. Smooth optimal control profiles and clear switching structures were found such that the hydrogen production is maximized. Future work aims at implementing the proposed reformulation to a broader class of singular control systems.

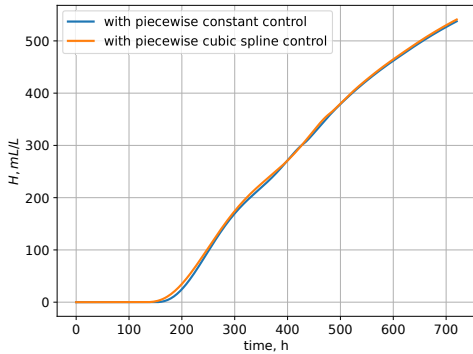


Fig. 3. Optimal hydrogen production.

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Appendix A. FUNCTIONS IN PROBLEM (13)

$$f(z(t)) \equiv \begin{bmatrix} \mu_{max}X \left(1 - \frac{k_q}{q}\right) \frac{C}{K_C + C} - \mu_d X^2 \\ -Y_{C/X} \mu_{max}X \left(1 - \frac{k_q}{q}\right) \frac{C}{K_C + C} + F_{in} C_{fed} \\ -Y_{N/X} \mu_{max}X \frac{N}{K_N + N} \\ Y_{q/X} \mu_{max} \frac{N}{K_N + N} - \mu_{max} \left(1 - \frac{k_q}{q}\right) q \frac{C}{K_C + C} \\ Y_{O/X} \mu_{max}X \frac{N}{K_N + N} - Y_d \mu_d X^2 f(O) + F_{in} O_{fed} \\ Y_{H/X} X (1 - f(O)) f(N) \end{bmatrix} \quad (A.1)$$

$$g(z(t)) \equiv [0 \ 0 \ F_{in} \ 0 \ 0 \ 0]^T \quad (A.2)$$

$$\phi(z(t_f)) \equiv -H(t_f) \quad (A.3)$$

$$z(t) \equiv [X \ C \ N \ q \ O \ H]^T \quad (A.4)$$

$$u(t) \equiv N_{fed} \quad (A.5)$$