A Gradient-Based Extremum Seeking Control of a Substrate- and Product-Inhibited Alcoholic Fermentation Process

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Abstract: In this paper we avail of an ESC approach to maximise ethanol concentration in a fermentation process carried out in a CSTR. Ethanol is aimed to be used as a fuel, so the reactor is fed with a stream of large concentration of sugar; hence, the model considers fermentation inhibition due to large concentrations of sugar and ethanol. By considering the minimisation of substrate concentration, to indirectly maximise the ethanol concentration, we apply our recent extremum seeking control (ESC) approach. The results in this paper show that the fermentation process considered in this work is suitable for ESC techniques, and that our control strategy is capable of finding the minimum value of the substrate concentration in numerical simulations.

Keywords: Fermentation; Extremum Seeking Control; Differentiators

1. INTRODUCTION

Fermentation is a process in which a microorganism converts organic compounds into energy for its metabolism in dark, anaerobic conditions. Depending on the microorganism the product of the fermentation process range from ethanol to acetate and lactate (Müller, 2001).

In particular, the fermentation process leading to ethanol plays a key role in the production of a renewable source of fuel via microorganisms like *Saccharomyces cerevisiae* and *Zymomonas mobilis* (Zabed et al., 2017). As a source of energy, bioethanol may aid in the reduction of nonrenewable sources like oil. In addition, bioethanol may be used for disinfection purposes. There are however some drawbacks in bioethanol production as the low yield (Gray et al., 2006). In addition the low ethanol concentration in the fermentation broth makes expensive the ethanol purification (Frolkova and Raeva, 2010).

Thus, optimisation approaches are necessary to render bioethanol production economically feasible. In this light, extremum seeking control (ESC) techniques have been widely used due to their attractive properties, such as being model-free approaches and being able to adapt to time-varying, possibly unknown inputs. ESC is applicable in situations where there is a nonlinearity in the control problem, and the nonlinearity has a local minimum or maximum. The nonlinearity may be in the system as a physical nonlinearity, or it may be in the control objective, added to the system through a cost functional of an optimization problem (Ariyur and Krstic, 2003). Since robustness is key trait of ESC approaches, there are several of such approaches that rely on sliding modes (SM), given the insensitivity to matched perturbations. See, for instance, (Angulo, 2015) and (Pan et al., 2012).

Bioethanol is produced from different types of sources, which in turn classifies it in terms of "generations" (Prado-Rubio et al., 2016). This work is aimed to harness the residual sugar and yeast in a tequila factory effluent. Thus, in the following, we consider that the initial concentrations and influx to our CSTR reactor contain carbon source, yeast, and ethanol. Such medium is a hallmark of the efflux of alcoholic spirits industries, such as tequila. Thus the scenario we pose is to use the wastewaters of the alcoholic fermentation industry as raw material for the fermentation process we consider.

In this light, the objective of our control scheme is to minimise the content of the fermentation substrate in the efflux of our CSTR, thus removing as much substrate as possible and converting it to product. As a result of our fermentation process, the efflux of the reactor contains both biomass and ethanol, which may be separated by mechanical and distillation processes, respectively, before its final disposal. Although these latter processes are not considered in the scope of the current work, they are better performed when they are substrate free and, overall,

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the purification cost is benefitted with a high ethanol concentration in the fermentation broth (Walker, 2010); thus, enhancing our motivation to minimise the substrate concentration. On the other hand, since measuring sugar is easier than measuring ethanol, the substrate into the CSTR is better suited to be considered as the objective function in the framework of ESC.

In particular, the mathematical model that we consider assumes that the substrate consumption is inhibited by large concentrations of substrate. In turn, the biomass dies due to large concentrations of product (López-Caamal et al., 2021). By analysing the dilution rate to substrate concentration steady-state map, we show the applicability of ESC approaches. Thus, we control such process via our recent ESC strategy (Torres-Zúñiga et al., 2021), in order to minimise the concentration of substrate in the reactor, by means of modifying its dilution rate. We refer the interested reader to (Torres et al., 2020) for a comparison of our ESC with a traditional ESC.

The gradient-based ESC strategy presented in (Torres-Zúñiga et al., 2021) considers a second order sliding modes algorithm to solve online optimization problems with unknown, convex, unimodal objective functions applied to single-input, single-output dynamical systems. First, a generalised Super-Twisting algorithm is used to estimate the gradient. Then, the Super-Twisting algorithm is considered as gradient-based optimization algorithm with the gradient as sliding variable.

The rest of the paper is organised as follows: In Section 2 the model for the fermentation process of interest is presented. An steady state is additionally analysed in order to determine whether the fermenter is suitable for ESC implementation. In Section 3, the ESC strategy recently propose in (Torres-Zúñiga et al., 2021) is applied to online minimise the substrate concentration in the fermentation process. In Section 4, the results of the ESC strategy applied to the fermentation process are discussed. Finally, in Section 5, conclusions about this work are stated.

2. THE MATHEMATICAL MODEL

In this section, we present a model for a fermentation process in which the biomass is inhibited by high concentrations of substrate and product, along with natural biomass death. This model was originally presented in (López-Caamal et al., 2021).

In the following, $S, X,$ and P denote the substrate, biomass, and product. Furthermore, let

$$\mathbf{c} := \begin{pmatrix} [S] \\ [X] \\ [P] \end{pmatrix}, \tag{1}$$

where $[\circ]$ denotes the concentration of its argument; we consider all concentrations in $[g/L]$. We consider constant temperature and pressure conditions in a CSTR subject to a dilution rate D $[1/hr]$, with a species concentration $\mathbf{c}_{\text{in}}$ in the influx. The interaction of species comprise the following processes:

i) **Biomass Growth**

$$S + X \xrightarrow{v_1} (1+n)X + mP, \tag{2a}$$

where $n = 1/30.303$ y $m = 7/30.303$, and v_1 follows a Haldane reaction rate (Andrews, 1968):

$$v_1 = k_{11}\frac{c_1 c_2}{c_1^2 + k_{12}c_1 + k_{13}}.$$

When considering c_2 constant, this reaction rate increases monotonically until a value c_1^*, which depends on the parameters k_{12} and k_{13}. After such a value, the reaction rate decreases asymptotically. Thus, by using such a reaction rate, we account for inhibition due to large substrate concentrations.

ii) **Product-Induced Biomass Inhibition**

$$X + P \xrightarrow{v_2} P. \tag{2b}$$

This process represents the lethal effect of the produced alcohol to the yeast that generates it. To this end, we chose a reaction rate inspired on that of Levenspiel (Levenspiel, 1980):

$$v_2 = k_{21}\left(1 - \frac{c_3}{k_{22}}\right)^{k_{23}} c_2.$$

iii) **Natural Biomass Death**

$$X \xrightarrow{v_3} 0, \tag{2c}$$

which we model via a Mass Action mechanism, hence leading to

$$v_3 = k_3 c_2.$$

Thus, in compact notation, our model is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{c}(t) = \mathbf{N}\mathbf{v}(\mathbf{c}) + D\left(\mathbf{c}_{\text{in}} - \mathbf{c}\right), \tag{3a}$$

where

$$\mathbf{N} = \begin{pmatrix} -1 & 0 & 0 \\ n & -1 & -1 \\ m & 0 & 0 \end{pmatrix}, \tag{3b}$$

and

$$\mathbf{v} = \begin{pmatrix} k_{11}\dfrac{c_1 c_2}{c_1^2 + k_{12}c_1 + k_{13}} \\ k_{21}\left(1 - \dfrac{c_3}{k_{22}}\right)^{k_{23}} c_2 \\ k_3 c_2 \end{pmatrix}. \tag{3c}$$

Finally, we account for the following parameters values

$$k_{11} = 3.8190 \times 10^3\ [g/(L\ hr)] \tag{4a}$$
$$k_{12} = 235.5119\ [g/L] \tag{4b}$$
$$k_{13} = 61.8563\ [(g/L)^2] \tag{4c}$$
$$k_{21} = 6.1786\ [1/hr] \tag{4d}$$
$$k_{22} = 116.4845\ [g/L] \tag{4e}$$
$$k_{23} = 2.6005\ [1] \tag{4f}$$
$$k_3 = 262.7081 \times 10^{-3}\ [1/hr]. \tag{4g}$$

Furthermore, we consider

$$\mathbf{c}_{\text{in}} = \begin{pmatrix} 60.518 \\ 30 \\ 10 \end{pmatrix}. \tag{5}$$

Please, be wary that such constant influx to the reactor contains all the species, since we consider that it comes from wastewaters of industries that involve fermentation processes. Along with the parameters values above and $D = 0.5$ $[1/hr]$, Figure 1 shows the species concentrations dynamics.

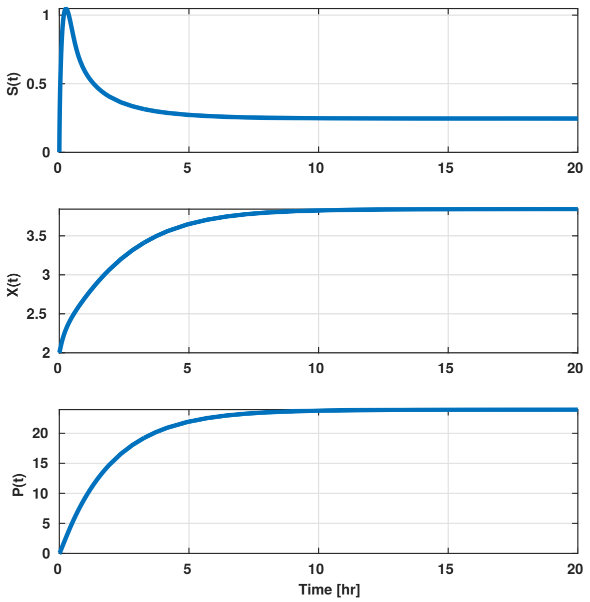

Fig. 1. Species concentrations with constant dilution rate.

2.1 *Equilibria*

Now, to determine whether the model in (3) is a candidate for applying ESC, we determine its input-output behaviour by choosing the dilution rate as the input, and substrate concentration as the output to optimise. In order to determine such map, we avail of a nonlinear optimisation routine to compute the equilibria of the model in (3), given that the nonlinearities of such model hinder an analytical treatment. The nonlinear optimisation routine that we availed of is Matlab's fminsearch, which we use to solve the following problem, for a range of values for D:

$$\bar{\mathbf{c}}(D) = \min_{\mathbf{c}} \log_{10} \left(||\mathbf{N}\mathbf{v}(\mathbf{c}) + D\left(\mathbf{c}_{\text{in}} - \mathbf{c}\right)||_1 \right), \ D \neq 0, \quad (6)$$

where $||\mathbf{r}||_1$ represents the 1-norm of the vector $\mathbf{r}$, that is to say

$$||\mathbf{r}||_1 = \sum_{i=1} |r_i| \, .$$

Thus, by minimising $||\mathbf{N}\mathbf{v}(\mathbf{c}) + D\left(\mathbf{c}_{\text{in}} - \mathbf{c}\right)||_1$ each entry of the vector is as small as possible, and thus the achieved values of $\bar{\mathbf{c}}$ are close to the equilibrium point.

By considering the parameters in (4) and the influx concentrations in (5), the results of such optmisation procedure are shown in Figure 2. The upper panel shows the value for the equilibrium for S, whereas the lower panel shows the value of the cost function. One may see that there exists a value for D such that minimises the equilibrium for S. Please notice that the lower panel of Figure 2 shows that, except for a few computations, the value of the cost function is around the computer precision.

In light of such results, the minimal value for the substrate's equilibrium is around 0.1947 $[g/L]$ and is attained with a dilution rate $D = 6 \times 10^{-5}$ $[1/hr]$. In the forthcoming section we present the ESC methodology.

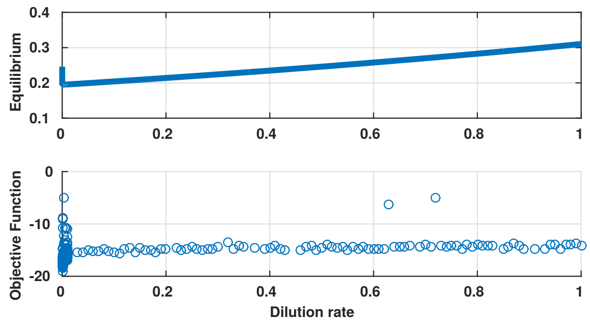

Fig. 2. Equilibria for substrate as a function of dilution rate. The upper panel shows the location of the equilibrium, while the lower one shows the value of the cost function in (6). Please notice that the objetive function is in a logarithmic scale.

3. GRADIENT-BASED ESC

In the previous section, we showed that the steady state map from dilution rate to the steady state of $[S]$ is convex and thus suitable for ESC. By minimising the steady state of the substrate, we ensure that the CSTR's efflux contains as little substrate concentration as possible.

Let us consider the compact state space model

$$\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{c}, \boldsymbol{c}_{in}, u); \ \boldsymbol{c}(0) = \boldsymbol{c}_0 \quad (7a)$$

$$y(t) = J(\boldsymbol{c}) \, , \quad (7b)$$

where $\boldsymbol{c} \in \mathcal{M} \subseteq \mathbb{R}^3$, $u = D \in \mathcal{N} \subseteq \mathbb{R}$, $\boldsymbol{c}_{in} \in \mathcal{M}$, and $y \in \mathbb{R}$ is the performance output. Besides, the functions $\boldsymbol{f} : \mathcal{M} \times \mathcal{N} \to \mathbb{R}^n$ and $J : \mathcal{M} \to \mathbb{R}$ are sufficiently smooth on $\mathcal{M}$.

The performance output is the aspect of the fermenter behavior that we desire to bring to the minimum value. In our case, $J(\boldsymbol{c}) = [S]$, and it is considered to be available throughout measurements. Please notice that by minimising $[S]$, one indirectly maximises product concentration. First, let us consider the following assumptions:

Assumption 1. There exists a smooth function $\boldsymbol{l} : \mathcal{N} \to \mathcal{M}$ such that $\boldsymbol{f}(\boldsymbol{c}^*, u) = 0$ if and only if $\boldsymbol{c}^* = \boldsymbol{l}(u)$.

Assumption 2. The equilibrium point $\boldsymbol{c}^* = \boldsymbol{l}(u)$ of the system (7) is locally asymptotically stable for each u in the operating region $\mathcal{N}$. Indeed, as it was shown in Figure 1, $\boldsymbol{c}^*$ is locally asymptotically stable.

Assumption 3. The input-output map in steady state

$$y = J(l(u)) = J(u) \quad (8)$$

is convex and unimodal in the operating region $\mathcal{N}$. Indeed, as it was shown in Figure 2, $J(u)$ is convex and unimodal for $u \in (0, 1]$.

Assumption 4. There exists $u^* \in \mathcal{N}$ such that:

$$(J \circ l)'(u^*) = 0,$$

$$(J \circ l)''(u^*) > 0.$$

Indeed, as it was shown in Figure 2, there exists such a point $u^* \in (0, 1]$.

Using these assumptions, we reduce the dynamic minimisation of the performance function (7b) to the problem of minimising (8) in the steady state. In addition, we assure that $J(u)$ has a unique minimiser u^* in $\mathcal{N}$.

In this light, we choose the following minimisation problem

$$\begin{aligned}&\min_{u\in\mathcal{N}} J(u)\\&\text{such that:}\\&\frac{\mathrm{d}\boldsymbol{c}}{\mathrm{d}t} = \boldsymbol{f}(\boldsymbol{c},\boldsymbol{c}_{in},u);\ \boldsymbol{c}(0)=\boldsymbol{c}_0\\&y(t)=J(\boldsymbol{c})\,.\end{aligned} \tag{9}$$

In order to solve such a minimisation problem, we make use of our gradient-based ESC strategy (Torres-Zúñiga et al., 2021). Such an approach hinges on the estimation of the input-output gradient, which we achieve via an online parametric differentiation; that is to say, given that

$$\frac{\partial y}{\partial u} = \frac{\frac{\mathrm{d}}{\mathrm{d}t}y}{\frac{\mathrm{d}}{\mathrm{d}t}u},\ \frac{\mathrm{d}}{\mathrm{d}t}u \neq 0,$$

one can estimate $\dfrac{\partial y}{\partial u}$ via the online differentiation of $y(t)$ and $u(t)$. To this end we avail of the differentiator presented in (López-Caamal and Moreno, 2019). Let

$$\boldsymbol{\theta} := \begin{pmatrix} y\\ u\end{pmatrix}, \tag{10}$$

whose first time-derivative is

$$\boldsymbol{\omega} := \begin{pmatrix} \dot{y}\\ \dot{u}\end{pmatrix}, \tag{11}$$

Given that $\dot{\boldsymbol{\omega}}$ is elementwise bounded, a fixed-time estimate of $\boldsymbol{\omega}(t)$ may be obtained via

$$\begin{aligned}\dot{\hat{\boldsymbol{\theta}}}(t) &= -k_1\boldsymbol{\phi}^1\left(\hat{\boldsymbol{\theta}}-\boldsymbol{\theta}\right)+\hat{\boldsymbol{\omega}}(t)\\ \dot{\hat{\boldsymbol{\omega}}}(t) &= -k_2\boldsymbol{\phi}^2\left(\hat{\boldsymbol{\theta}}-\boldsymbol{\theta}\right),\end{aligned} \tag{12}$$

where $\hat{\boldsymbol{\theta}}$ ($\hat{\boldsymbol{\omega}}$, resp.) denotes the estimation of $\boldsymbol{\theta}$ ($\boldsymbol{\omega}$, resp.), and

$$\begin{aligned}\boldsymbol{\phi}^1(\mathbf{x}) &= \left(\eta\,||\mathbf{x}||_2^{-p}+\beta+\gamma\,||\mathbf{x}||_2^{q}\right)\mathbf{x},\quad \boldsymbol{\phi}^1(\mathbf{0}) := \mathbf{0},\\ \boldsymbol{\phi}^2(\mathbf{x}) &= \left(\eta(1-p)\,||\mathbf{x}||_2^{-p}+\beta+\gamma(1+q)\,||\mathbf{x}||_2^{q}\right)\boldsymbol{\phi}^1(\mathbf{x})\,.\end{aligned} \tag{13}$$

Furthermore $\eta,\beta,\gamma>0$, $\dfrac{1}{2}\geq p>0$, and $q>0$; and k_1 and k_2 are such that the matrix

$$\mathbf{A} = \begin{pmatrix} -k_1 & 1\\ -k_2 & 0\end{pmatrix} \tag{14}$$

is Hurwitz.

Thus, the estimate of the input-output gradient can be computed as

$$\frac{\partial y}{\partial u} = \frac{\hat{\omega}_1}{\hat{\omega}_2}. \tag{15}$$

Upon such computation, the ESC proposed in (Torres-Zúñiga et al., 2021) states that for the sliding variable $\sigma = \dfrac{\partial y}{\partial u}$, the control input $u(t)$ computed as

$$\begin{aligned}u(t) &= -\lambda|\sigma|^{1/2}\mathrm{sign}(\sigma)+u_1(t)\,,\\ \dot{u}_1(t) &= -\alpha\,\mathrm{sign}(\sigma)\,,\end{aligned} \tag{16}$$

where $\lambda>0$ and $\alpha>0$, brings the output $y(t)$, the concentration of the substrate in the fermenter $[S]$, to its minimum value in the steady state.

To avail of such control law, we keep constant the input $u(t)$ for a time period, until the output $y(t)$ reaches its steady state. Once achieved, we update the input $u(t)$ with the new estimation of the gradient, to steer $y(t)$ to a new steady state. Thus, by repeatedly following this process, the output $y(t)$ oscillates around its minimal value. In the following section, we present the numerical results of applying this strategy to the model in (3).

4. RESULTS

In this section, we apply the ESC (16) to the model in (3), accounting for the numerical value of the parameters in (4) and the species' influx concentration in (5). We consider an optimisation period of 168 units of time; that is to say, every 168 units of time we update the dilution rate according our ESC law. The parameters for both, the differentiator in (12) and the Super-Twisting controller (16) are shown in Table 1.

Parameter	Value
η	0.001
β	0.01
γ	0.005
p	0.3
q	0.1
k_1	1
k_2	1
α	0.0008
λ	0.0005

Table 1. Parameters of the ESC.

Furthermore, we consider the following initial conditions

$$\begin{aligned}c_1(0)&=0\\c_2(0)&=2\\c_3(0)&=0\\D(0)&=0.5\end{aligned}$$

With such parameters, Figure 3 and Figure 4 show the substrate concentration and the dilution rate as a function of time, respectively.

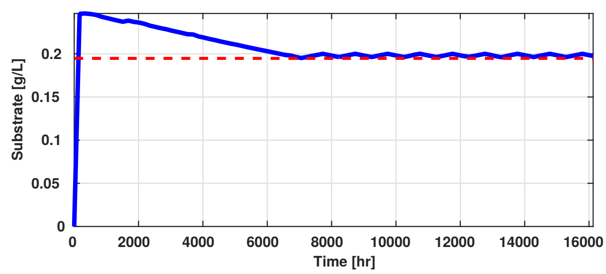

Fig. 3. Substrate concentration in the CSTR subject to the dilution rate depicted in Figure 4. The red, discontinuous line shows the location of the minimal value for the substrate. In turn, the blue, solid line shows the substrate concentration.

Now, Figure 5 shows the gradient estimation with which the ESC is computed. Please notice that after time 8000, the gradient oscillates around zero, thus indicating that the extremum value has been achieved. Please notice in Figure 3 that the achieved substrate concentration is slightly above the smallest steady state for substrate.

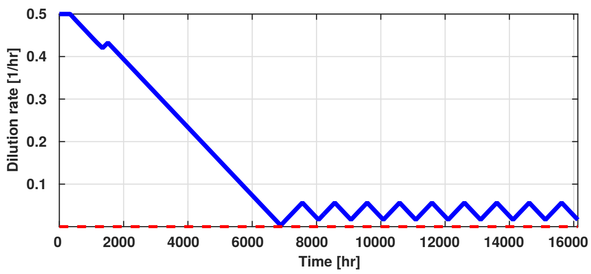

Fig. 4. Dilution rate as computed with (16). The red, discontinuous line represents the dilution rate that yield the smallest substrate concentration.

This might be due to the numerical errors during the computation of steady state, the gradient, and the solution of the ESC law.

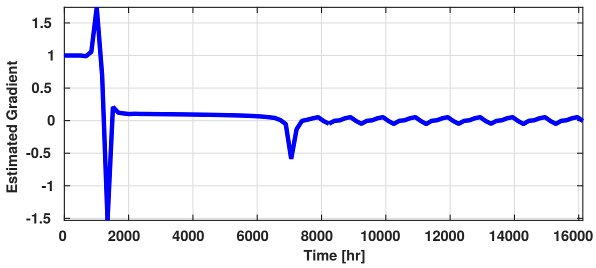

Fig. 5. Estimated input-iutput gradient.

Finally, Figures 6 and 7 show the time response for biomass and ethanol, respectively. As it can be observed in Figure 7, the concentration of the ethanol produced in the CSTR was increased to its maximum value, indicating that the substrate was mainly converted to product.

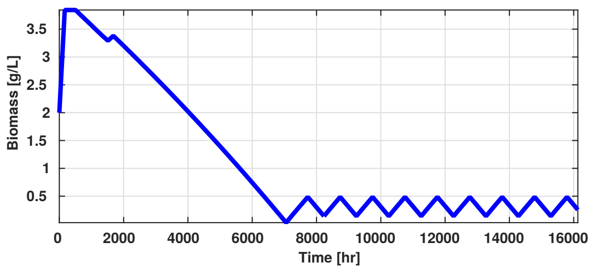

Fig. 6. Biomass concentration as a function of time.

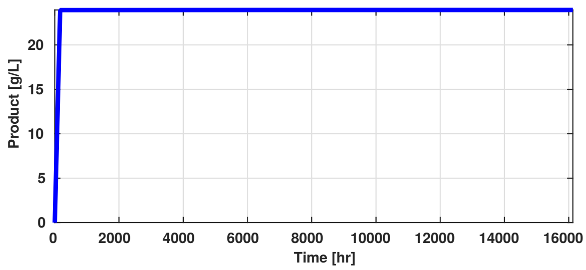

Fig. 7. Ethanol concentration as a function of time.

5. CONCLUSION

In this paper we analysed whether our alcoholic fermentation model is suitable to be controlled via an extremum seeking strategy, by considering the minimisation of substrate in the reactor. Once determined the feasibility, we applied our recent gradient-based ESC strategy. Although the optimisation is possible, our numerical results suggest large convergence time to the minimal substrate concentration in the reactor. On the other hand, the simulations demonstrated that by minimising the substrate concentration, the ethanol concentration was indirectly maximised.

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