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► **To cite this version:**

Julien Schorsch, Michel Kinnaert, Radhouane Fekih-Salem, Laurent Dewasme, Cristiana Castro, et al.. Optimal control of fructo-oligosaccharide production. Proceedings of the 10th International Conference on Simulation and Modelling in the Food and Bio-Industry, (FOODSIM), Apr 2018, Ghent, Belgium. hal-02912861

HAL Id: hal-02912861

<https://hal.science/hal-02912861v1>

Submitted on 6 Aug 2020

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Optimal control of fructo-oligosaccharide production

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KEYWORDS

Pontryagin maximum principle, bang bang control, biotechnology

Abstract

The objective of this study is to determine an optimal substrate feed rate for optimizing the fructo-oligosaccharide production by *Aureobasidium pullulans* in a fed batch reactor. The feed profile is characterized by the feed start time, rate and end time. The optimization is carried out based on a simple dynamic model of the process and using Pontryagin maximum principle in the framework of singular control problems. The resulting control law is of the bang-bang type. The bioreactor is first filled-up at maximum feed rate, followed by a batch phase.

Introduction

Fructo-oligosaccharides (FOS) are dietary carbohydrates, which can be used as an alternative to sugar, offering 30% relative sweetness, and a selective increase of the probiotic bacteria development, with a preventive effect on gastrointestinal diseases, colorectal cancer and diabetes (Tomomatsu 1994). Naturally, FOS can, for instance, be harvested in significant quantities in honey, bananas and rye. However, their industrial production is delicate since several processes are required to reach acceptable degrees of purity (Nobre et al. 2015; 2016).

A convenient way to produce FOS in bioreactors arises from transfructosylation of sucrose (GF), composed of the monosaccharides glucose (G) and fructose (F), through microbial enzymes (fructosyltransferase and β -fructofuranosidase) present in microorganisms such as *Aureobasidium pullulans* (Dominguez et al. 2012) or *Aspergillus* sp. (Rocha et al. 2009). These enzymatic activities produce complex sugars, namely 1-Kestose (GF₂), Nystose (GF₃) and 1-Fructofuranosyl Nystose (GF₄) which constitute the FOS family.

Based on a simple dynamic model of the FOS production in a fed-batch reactor, the objective of this study is to maximize the FOS concentration by manipulating the substrate feed rate. The approach is based on Pontryagin maximum principle, a method that has received considerable attention in the context of bioprocess optimization and control (see e.g.

Van Impe and Bastin (1995), Smets et al. (2004)).

This paper is organized as follows. In Section 2, the dynamic model of fed-batch FOS production is presented. Section 3 deals with the optimal control problem, conclusions are drawn in Section 4.

Modeling FOS production

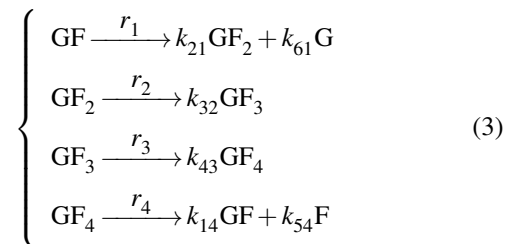
Based on a set of experimental data collected in batch and fed batch experiments, it is possible to derive the minimum number of reactions explaining the data using maximum likelihood principal component analysis (Mailier et al. 2013). A step by step parameter identification procedure can then be followed to estimate the reaction stoichiometry and kinetics. More precisely, the final model involves 8 kinetic parameters and 6 pseudo-stoichiometric coefficients and the mass balance differential equation system is as follows:

$$\begin{cases} [\dot{\text{GF}}] &= -r_1 + k_{14}r_4 + \frac{1}{V}(\text{GF}_{in} - [\text{GF}])Q \\ [\dot{\text{GF}}_2] &= -r_2 + k_{21}r_1 - \frac{[\text{GF}_2]}{V}Q \\ [\dot{\text{GF}}_3] &= -r_3 + k_{32}r_2 - \frac{[\text{GF}_3]}{V}Q \\ [\dot{\text{GF}}_4] &= -r_4 + k_{43}r_3 - \frac{[\text{GF}_4]}{V}Q \\ [\dot{\text{F}}] &= k_{54}r_4 - \frac{[\text{F}]}{V}Q \\ [\dot{\text{G}}] &= k_{61}r_1 - \frac{[\text{G}]}{V}Q \\ \dot{V} &= Q \end{cases} \quad (1)$$

where $[\alpha]$ denotes the concentration (in g.L^{-1}) of the component α . Q represents the substrate feed rate (in L.h^{-1}), which is the manipulated variable. GF_{in} is the substrate concentration (in g.L^{-1}) and V the broth volume (in L). The reaction rates (in $\text{g.L}^{-1}.\text{h}^{-1}$) are defined by Monod laws:

$$r_i = \mu_i^{\max} \frac{[\text{GF}_i]}{K_{m_i} + [\text{GF}_i]}, \quad \text{with } i = 1, 2, 3, 4, \quad (2)$$

where μ_i^{\max} denotes the maximum rate (in $\text{g.L}^{-1}.\text{h}^{-1}$) of the reaction i . K_{m_i} (in g.L^{-1}) represents the half-saturation constant associated to component i . The corresponding reaction scheme is given by:



Optimization of FOS production

The dynamic model is affine in the input Q and can be cast in the general nonlinear form

$$\frac{dX}{dt} = f(X) + g(X)Q \text{ with } t_0 \leq t \leq t_f \quad (4)$$

with the state vector $X = [GF, GF_2, GF_3, GF_4, F, G, V]$. Function f represents the reaction kinetics while g characterizes the hydrodynamics. At $t = t_0$, the process is initiated with initial concentrations and volume $X(t_0) = X_0$. The final condition is related to the maximum volume V_{\max} (in L) which should be reached at final time:

$$\Omega = V(t_f) - V_{\max} = 0. \quad (5)$$

The performance index J represents the FOS amount at final time:

$$J(t_f) = [GF_2](t_f) + [GF_3](t_f) + [GF_4](t_f) \equiv h(X), \quad (6)$$

The substrate feed rate Q is limited by the feed pump capacity. Let Q_{\max} and Q_{\min} be the upper and lower bounds respectively:

$$Q_{\min} \leq Q \leq Q_{\max}. \quad (7)$$

The objective is to find an admissible control function, $Q(t)$, which yields a system (4) trajectory satisfying (5) and (7) while maximizing the performance index J . Pontryagin maximum principle states that this problem is equivalent to the maximization of the Hamiltonian H (Bryson and Ho 1969):

$$H = \phi + \psi Q \quad (8)$$

where functions $\phi = \lambda^\top f(X)$ and $\psi = \lambda^\top g(X)$.

The costate vector λ is given by:

$$\frac{d\lambda^\top}{dt} = -\frac{\partial H}{\partial X} = -\lambda^\top \frac{\partial f}{\partial X} - \lambda^\top \frac{\partial g}{\partial X} Q. \quad (9)$$

with transversality conditions:

$$\lambda(t_f) = \frac{\partial h(X)}{\partial X} + \nu \frac{\partial \Omega(X)}{\partial X} \quad (10)$$

providing $\lambda_{GF,G,F}(t_f) = 0$, $\lambda_{GF_2,GF_3,GF_4}(t_f) = 1$ and $\lambda_\nu(t_f) = \nu$ with $\nu \in \mathbb{R}$ where λ_α is the costate associated to the state α .

The Hamiltonian (8) is affine in the control input, which is subject to the linear inequality constraints 7, and a "bang-bang" solution exists, consisting in a control sequence made of minimum and maximum input levels and singular arcs. Based on the sign of the Hamiltonian partial derivative with respect to the input Q , i.e. the value of ψ , the "bang-bang" control results from:

$$\begin{cases} \text{if } \psi < 0, \text{ then } Q = Q_{\min}, \\ \text{if } \psi = 0, \text{ then } Q = Q_s, \\ \text{if } \psi > 0, \text{ then } Q = Q_{\max}. \end{cases} \quad (11)$$

The singular control law Q_s is obtained by taking the second time derivative of ψ (see e.g. Bryson and Ho (1969)):

$$Q_s = -\frac{\lambda^\top \left(\frac{\partial q}{\partial X} f - \frac{\partial f}{\partial X} q \right)}{\lambda^\top \left(\frac{\partial q}{\partial X} g - \frac{\partial g}{\partial X} q \right)} \quad (12)$$

Table 1: Optimal control: hardware constraints and initial conditions.

Hardware constraints		Initial conditions	
GF_{in}	280 g.L ⁻¹	$[GF](t_0)$	200 g.L ⁻¹
V_{\max}	3 L	$V(t_0)$	1 L
Q_{\max}	0.5 L.h ⁻¹	$[G](t_0)$ and $[F](t_0)$	0 g.L ⁻¹
Q_{\min}	0 L.h ⁻¹	$[GF_{2,3,4}](t_0)$	0 g.L ⁻¹

under the condition that $\lambda^\top \left(\frac{\partial q}{\partial X} g - \frac{\partial g}{\partial X} q \right) \neq 0$, where q is

$$q = \frac{\partial g}{\partial X} f - \frac{\partial f}{\partial X} g. \quad (13)$$

This criteria is based on the necessary optimality conditions including

$$\frac{\partial H}{\partial Q} = \lambda^\top g = 0. \quad (14)$$

Based on this development, the following 5-step algorithm is proposed:

1. Guess t_f , ν and a substrate feed rate Q respecting the final condition (5), and integrate forward the model defined in (4).
2. Determine λ by integrating backward Equation (9).
3. Integrate forward the model defined in (4) using singular control (11).
4. Repeat Steps 2 and 3, considering $\nu = \nu + \delta\nu$, with $\delta\nu$ as small as required, until $\Omega = 0$.
5. Repeat Steps 2 to 3 with a new guess of t_f in order to maximize the performance index J (6) and nullify Hamiltonian (8).

Numerical results

The dynamic model (1), as well as another candidate model proposed in (Jung et al. 1989) and identified so as to match the available experimental data, are used in the optimization procedure. Initial conditions and constraints are listed in Table 1.

The two optimization problems (based on the two candidate models) lead to similar input trajectories (i.e., the feed rate represented in subplot A of Fig. 1): a fed-batch phase of approximately 4 hours at maximum flow rate $Q_{\max} = 0.5 \text{ L.h}^{-1}$ until the bioreactor is completely filled, followed by a batch phase ($Q_{\min} = 0 \text{ L.h}^{-1}$). This profile maximizes the productivity of GF_2 , direct by-product of the inlet substrate GF.

Model (1) suggests a reaction rate r_1 which always remains below the maximum value μ_1^{\max} , and a global reaction rate, defined by $f_{GF_2} + f_{GF_3} + f_{GF_4}$, increasing even after the fed-batch phase and reaching a maximum within 10 hours (see subplot C in Fig. 1). The model of (Jung et al. 1989) behaves slightly differently with r_1 first at its maximum, thus implying a maximal global reaction rate (subplot C in Fig. 1) during the fed-batch phase followed by a decrease when the bioreactor is no longer fed. Consequently, the predicted productivity and yield (given by Equations (15)) are 2.75

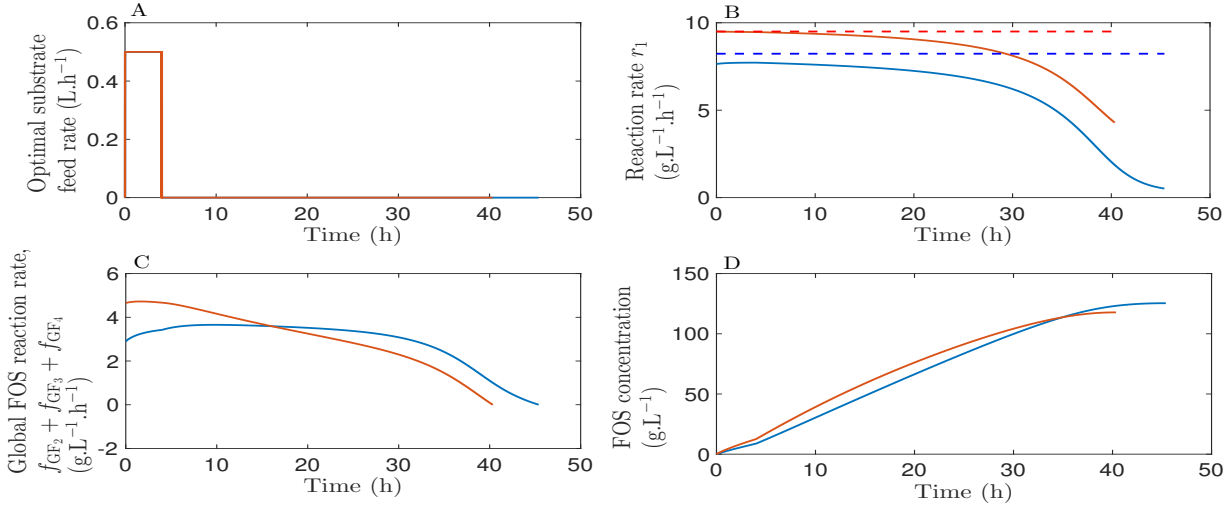


Figure 1: Subplot A shows the optimal substrate feed rate. Subplot B shows the reaction rates (continuous lines) and the associated maximum rates (dotted line). The global FOS production rate is displayed in subplot C. Subplot D shows the evolution of the FOS concentrations. The blue and red colors correspond respectively to model (1) and the model from (Jung et al. 1989).

$\text{g.L}^{-1}.\text{h}^{-1}$ and 49.3% with model (1). These numbers have to be compared to the prediction based on the model of (Jung et al. 1989), which is a slightly higher productivity of $2.92 \text{ g.L}^{-1}.\text{h}^{-1}$ and lower yield of 46.5%. Indeed, in the first case, 125 g.L^{-1} of FOS are obtained after 45.4 hours while in the second case, 118 g.L^{-1} are obtained after 40.3 hours.

$$\begin{cases} \mathcal{P}(t_f) = \frac{[\text{GF}_2](t_f) + [\text{GF}_3](t_f) + [\text{GF}_4](t_f)}{V(t_f)}, \\ \mathcal{Y}(t_f) = V_{\max} \frac{[\text{GF}_2](t_f) + [\text{GF}_3](t_f) + [\text{GF}_4](t_f)}{[\text{GF}](t_0)V(t_0) + \text{GF}_{\text{in}}(V_{\max} - V(t_0))}. \end{cases} \quad (15)$$

Conclusion

A bang-bang control strategy is proposed for the optimization of the FOS production, which consists in a fed-batch phase at maximum flow rate followed by a batch phase.

Acknowledgements

The authors gratefully acknowledge the financial support from the F.R.S.-FNRS, the Belgium National Fund for the Scientific Research, (PDR: T.0196.13).

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