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An isoperimetric optimal control problem for a non-isothermal chemical reactor with periodic inputs

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HIGHLIGHTS

- Mathematical models of nonlinear reactions of the type "$A \to$ product" are considered.
- Periodic modulations of the inlet concentration and the temperature are applied.
- The performance maximization is treated as an isoperimetric optimal control problem.
- A theoretical estimate of the optimal number of switchings is obtained.
- Simulation results illustrate the improvement by using bang-bang controls.

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ABSTRACT

In this paper, we study the optimal control problem for a continuous stirred tank reactor (CSTR) that represents a reaction of the type "$A \to$ product". The reactor dynamics is described by a nonlinear system of ordinary differential equations controlled by two inputs: the inlet concentration and the inlet temperature. We formulate the problem of maximizing the average product of this reactor for a fixed consumption of the input component over a period of time. This kind of isoperimetric optimal control problem is analyzed by using the Pontryagin maximum principle with Lagrange multipliers. We show that the optimal controls are bang-bang and propose an upper bound for the number of switchings for the linearized problem with periodic boundary conditions. Numerical simulations confirm that our control strategy can be used to improve the reactor performance over a specified period of time in comparison to the steady-state operation.

1. Introduction

The optimization of periodic processes has been already the subject of several studies in chemical engineering and control theory (a survey of related works is presented in Section 2). The majority of publications in this area (cf. Douglas, 1967; Sinčič and Bailey, 1980; Watanabe et al., 1981) deals with smooth (or even constant) controls, so that no optimization problems with bang-bang strategies have been rigorously analyzed up to now from the mathematical viewpoint. In this paper, we will consider a chemical reaction of the type "$A \to$ product" controlled by the inlet concentration $C_{Ai}(t)$ of A and the inlet temperature $T_i(t)$ at time t.[2] An attractive goal is to maximize the conversion of A to the product over a specified period of time $t \in [0, t_f]$, which can be formulated as the minimization of the outlet concentration $C_A(t)$ provided that the mean consumption of A is fixed as $\overline{C}_{Ai}$:

$$\frac{1}{t_f}\int_0^{t_f} C_A(t)\,dt \to \min,$$

$$\frac{1}{t_f}\int_0^{t_f} C_{Ai}(t)\,dt = \overline{C}_{Ai}.$$

We assume here that the process is operated periodically, so that the inputs and the state of the reactor are periodic functions of the period t_f. To the best of our knowledge, the above isoperimetric optimal control problem has not been solved up to now for mathematical models of chemical reactions. In order to

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[2] We will introduce dimensionless variables to simplify the notations in the sequel.

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evaluate the theoretical concept studied in this work, we selected one of the most simple reactors applied in chemical reaction engineering, namely the perfectly mixed continuously operated stirred tank reactor (CSTR). Analysing this concentrated system allowed us to extract generally valid trends in the most simple way exploiting analytical solutions. The selection of the model parameters was based on exploiting available knowledge regarding the kinetics of a standard liquid phase reaction, namely the hydrolysis of acetic acid anhydride. The features of this reaction are quite typical and thus allow some generalization with respect to main trends of periodic operation.

The main contributions of this paper can be summarized as follows.

- In Section 3, we formulate the problem of maximizing the performance of a single homogeneous n-th order reaction by using a time-varying inlet concentration (Problem 1). It is shown that each control satisfying the optimality conditions is bang-bang, and the procedure for computing the control parameters is described explicitly for the case $n = 2$. A numerical example illustrates that our bang-bang control strategy ensures better performance in comparison to the sinusoidal input modulation considered in the paper (Petkovska and Seidel-Morgenstern, 2013) in terms of the nonlinear frequency response function. In contrast to the approach of Nikolić and Petkovska (2016) dealing with a truncated Fourier series for a square wave input, we analyze the optimality conditions rigorously by taking into account the periodic boundary condition $C_A(0) = C_A(t_f)$.
- The isoperimetric optimal control problem (Problem 2) is considered in Section 4 for a nonlinear system of ordinary differential equations controlled by two inputs (the inlet concentration of A and the inlet temperature). The optimality conditions are analyzed by the Pontryagin maximum principle with Lagrange multipliers (cf. Schmitendorf, 1976). In contrast to the results by Watanabe et al. (1981), we consider here a cost function which is convex, but not strictly. We show that each optimal control is bang-bang and propose an upper bound for the number of switchings N for the linearized problem with periodic boundary conditions (Proposition 1). The switching times are defined by an auxiliary system of transcendental equations. For the case of small switching times, these transcendental equations can be approximated by polynomials. Our control design scheme is based on expansions of the composition of flows corresponding to extremal inputs.
- The simulation results in Section 5 confirm that bang-bang controls with two switchings can be used to improve the reactor performance over a specified period of time t_f in comparison to the steady-state operation.

2. Related work

The paper by Douglas (1967) was among the first theoretical studies, where the effects of time-varying inputs were estimated for nonlinear reaction models. A second-order isothermal reaction was considered there under the assumption that the feed composition is modulated by the sine function, and the method of small parameter was used to approximate the output behavior with correction terms of different orders of magnitude. It was shown that the frequency response of the system under consideration contains higher order harmonic terms in additional to the fundamental component. It follows from the analysis of the frequency response function that the average output value is close to the corresponding steady-state value for very low and very high frequency inputs. The case of simultaneous modulation of the feed composition and the flow rate with sinusoidal functions was considered in the paper (Douglas, 1967) as well. It was pointed out that the maximum improvement in the conversion is obtained when both amplitudes are large, and the phase shift is close to 180°. The optimum design problem is addressed in the book (Douglas, 1988) in the sense of steady-state operations, when the goal is to find the values of the design variables maximizing the profitability of the process (e.g., the capital charge factor).

In the paper (Horn and Lin, 1967), a CSTR model whose dynamical behavior is governed by a system of two nonlinear ordinary differential equations with one control variable is considered. For the optimal control problem with periodic boundary conditions, the first variation of the cost function is evaluated with the use of the adjoint system of equations. If this first variation is nonzero for a given periodic process, then the performance can be improved by using "the hill climbing method in function space", described in the paper. Some simulation results, based on this method, are presented to illustrate the possibility of improving an initial steady-state control.

A single non-isothermal reaction is considered in the paper (Hicks and Ray, 1971) by assuming that the coolant flow-rate is controlled within given bounds. The problem of minimizing a quadratic cost functional is formulated without periodic boundary conditions, and the candidates for optimal controls are chosen as polynomials or bang-bang controls with unknown switching times. Then an iterative scheme for computing the control parameters is presented based on numerical integration of the state equations and Rosenbrock's method for unconstrained optimization.

The paper (Sinčič and Bailey, 1980) exploits the second variation of the cost function in the frequency domain for examples of chemical reactions involving at most two control signals. To simplify the formula for the second variation, the authors assumed that the control variations are sinusoidal functions with one principal frequency. The process response has been also simulated for bang-bang controls with the use of a numerical hill-climbing method, however, no results concerning the computation of switching times have been presented.

The question whether the performance of an isothermal CSTR may be improved by using periodic perturbations of a given steady-state control is studied in the paper (Watanabe et al., 1981). If a steady-state input is in the interior of the set of control values, and if certain conditions on the transfer function of the linearized system hold, then the above steady-state control is not optimal. In this case, sinusoidal perturbations of the input with large frequencies can be used to improve the reactor performance in comparison to its steady-state operation. It is shown that, for the reaction of order $n > 1$, the reactor performance can be improved by fluctuating the feed concentration only.

In the papers (Gottlieb et al., 1983; Hoffmann and Schädlich, 1986; Schädlich et al., 1983), an isothermal reaction scheme of the type "$\nu_1 A_1 + \nu_2 A_2 \rightarrow product$" with the power law rate $r = kC_1^{n_1} C_2^{n_2}$ is considered under the assumption that the sum of the inlet concentrations of A_1 and A_2 is constant. By applying Hölder's inequality to the integral of the product concentration, a priori estimates of the degree of conversion are obtained for different values of n_1 and n_2 in Gottlieb et al. (1983). In particular, the conversion cannot be improved with respect to the steady-state operation if $0 < n_1 < 1, 0 < n_2 < 1$, and $n_1 + n_2 \leqslant 1$. This property is also established in the paper (Grabmüller et al., 1985) for an isothermal plug-flow tube reactor model by exploiting the convexity of the function that generates the solutions in the method of characteristics. The Legendre-Clebsch condition is used in Schädlich et al. (1983) to check the optimality of steady state operations of a CSTR. In particular, it is shown that the steady-state operation is not optimal if $\nu_1 > 1$ for homogeneous systems. If the inlet concentrations are bang-bang controls with a given period