Computers and Chemical Engineering 95 (2016) 71–74

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

Short communication

On the various local solutions to a two-input dynamic optimization problem

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ARTICLE INFO

Article history:
Received 2 March 2016
Received in revised form 2 September 2016
Accepted 4 September 2016
Available online 6 September 2016

Keywords:
Process optimization
Batch processes
Numerical methods
Analytical methods
Constrained optimization
Sensitivity

ABSTRACT

Solving a multi-input dynamic optimization of a batch processes is a complex problem involving interactions between input variables and constraints over time. The problem gets more difficult due to the presence of local solutions that have almost the same cost but widely varying structures. This paper studies various local optimal solutions for a non-isothermal semi-batch reactor with the feed rate and temperature as inputs and a heat removal constraint. Three solution patterns were studied, all consisting in meeting the heat removal constraint for the first part and seeking the compromise between the main and side reactions in the later part. A sensitivity analysis shows that the best solution pattern among those studied does not change with variations in parameters or initial conditions.

1. Introduction

The solutions to multi-input dynamic optimization problems can be fairly intricate because of the interactions between the inputs and the constraints over time. There are many examples of this in the literature, most of which are problems with 2–7 inputs and 20–50 differential equations (Cervantes and Biegler, 1998; Schlegel and Marquardt, 2006). These problems are typically solved numerically (Kadam et al., 2007; Skogestad, 2000; Würth et al., 2011) and, as a result, there is no physical interpretation of the solution in terms of the types and sequence of arcs.

In contrast, Srinivasan et al. (2003) used an analytical approach to solve a simple two-input problem. The inputs are either constrained or sensitivity-seeking arcs. The solution presented in that paper corresponds to a local optimum with only three arcs. It illustrates well the analytical method and the interaction between the two inputs and the constraints. However, in recent years, the authors have been confronted with alternative numerical solutions that are "supposed to be better" than the one proposed in that paper. Some of the solutions are indeed better, while others give a better cost because they slightly violate the path constraints due to numerical inaccuracies.

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http://dx.doi.org/10.1016/j.compchemeng.2016.09.003

This note compares these alternative optimal solutions by computing them *analytically*. The analytical approach has the advantage of not violating the constraints. Furthermore, a sensitivity analysis is presented to show whether the solution could easily change from one form to another when parameters change.

2. Problem formulation

The two-input optimization problem considered in Srinivasan et al. (2003) is briefly recalled. It consists of a non-isothermal semi-batch reactor with the series reactions $A + B \rightarrow C \rightarrow D$ and a heat-removal constraint. The reactor temperature and the feed rate of B are considered as manipulated variables. The system is described by the following equations:

$$\dot{c}_A = -k_1 c_A c_B - \frac{u}{V} c_A \quad (1)$$

$$\dot{c}_B = -k_1 c_A c_B + \frac{u}{V} (c_{Bin} - c_B) \quad (2)$$

$$\dot{c}_C = k_1 c_A c_B - k_2 c_C - \frac{u}{V} c_C \quad (3)$$

$$\dot{V} = u \quad (4)$$

where c_X is the concentration of the species X, c_{Bin} the concentration of B in the feed, k_i the kinetic parameter for the i^{th} reaction,

u the feed rate of B, and V the volume of the reactor. The kinetic parameters follow Arrhenius law:

$$k_i = k_{i0} \exp\left(-\frac{E_i}{RT}\right)$$

where k_{i0} is the pre-exponential factor, E_i the activation energy, R the gas constant, and T the temperature.

The optimization problem maximizes the production of the desired product C:

$$\begin{aligned}
&\max_{u,T} J = c_C(t_f)V(t_f) \\
&s.t. Equation 1-4 \\
&T_{min} \le T(t) \le T_{max} \\
&u_{min} \le u(t) \le u_{max} \\
&V(t) \le V_{max} \\
&(-\Delta H_1)k_1 c_A(t) c_B(t) V(t) + (-\Delta H_2) k_2 c_C(t) V(t) \le q_{rx,max}
\end{aligned} \tag{5}$$

Numerical values are given in Table 1.

The only possible options for the feed-rate input are $u_{\min}$, $u_{\max}$, and $u_{\text{path}}(t)$, that is, the feed rate is either at its bounds or determined by the heat-removal constraint. The analytical expression for $u_{\text{path}}(t)$ is provided in the original article:

$$u_{path} = V \frac{\Delta H_1 k_1^2 c_A c_B (c_A + c_B) + \Delta H_2 k_2 \left(k_1^2 c_A c_B - k_2 c_C\right)}{\Delta H_1 k_1 c_A (c_{Bin} - c_B)} - \frac{\dot{T} V}{RT} \frac{\Delta H_1 E_1 k_1 c_A c_B + \Delta H_2 E_2 k_2 c_C}{\Delta H_1 k_1 c_A (c_{Bin} - c_B)}$$

The possible options for the temperature input are $T_{\min}$, $T_{\max}$, $T_{\text{path}}(t)$, and $T_{\text{sens}}(t)$. This means that the temperature is either at its

Table 1
Parameters, bounds and initial conditions.

Parameter	Value	Units
k_{10}	4	L/(mol h)
k_{20}	800	1/h
E_1	6e3	J/mol
E_2	20e3	J/mol
R	8.31	J/(mol K)
ΔH_1	−30e3	J/mol
ΔH_2	−10e3	J/mol
u_{min}	0	L/h
u_{max}	1	L/h
T_{min}	20	°C
T_{max}	50	°C
V_{max}	1.1	L
$q_{rx,max}$	1.5e5	W
c_{A0}	10	mol/L
c_{B0}	1.1685	mol/L
c_{C0}	0	mol/L
V_0	1	L
c_{Bin}	20	mol/L
t_f	0.5	h

Table 2
Types and sequence of arcs for the three considered solutions.

Solution	Inputs	t_0 to t_1	t_1 to t_2	t_2 to t_3	t_3 to t_4	t_4 to t_f
Solution 1	u	u_{path}	u_{path}	$u_{\min}$	–	
3 arcs, $T_{\max}$	T	$T_{\max}$	T_{sens}	T_{sens}		
Solution 2	u	u_{path}	u_{path}	$u_{\min}$	$u_{\min}$	$u_{\min}$
5 arcs, $T_{\max}$	T	$T_{\max}$	T_{sens}	T_{path}	$T_{\max}$	T_{sens}
Solution 3	u	$\mu_{\max}$	u_{path}	$u_{\min}$	$u_{\min}$	$u_{\min}$
5 arcs, u_{max}	T		$T_{\min}$	T_{path}	$T_{\max}$	T_{sens}

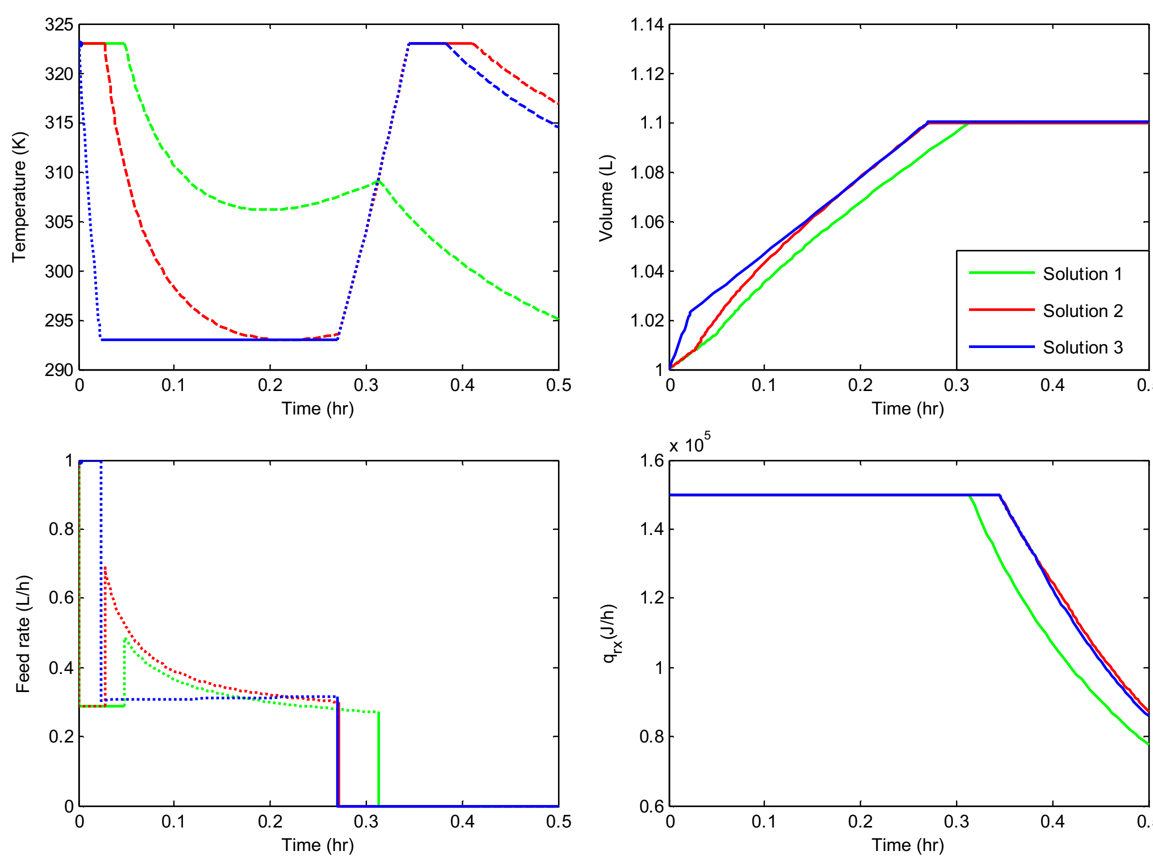

Fig. 1. Temperature, feed-rate, volume, and heat-removal profiles for the nominal case.