OPTIMAL SPATIAL TEMPERATURE CONTROL OF A STEADY-STATE EXOTHERMIC PLUG FLOW REACTOR. PART II: SINGULAR CONTROL

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Abstract

This paper is the second in a series of two dealing with the spatial optimization of the heat exchanger temperature profiles of exothermic tubular reactors under the assumption of steady-state and plug flow characteristics. The minimum principle of Pontryagin (optimal control theory) is applied in a straightforward, analytical sense. To enable a trade-off between process performance and global heat loss a weighted cost criterion is defined. In Part I of this series, it is demonstrated that (weighted combinations of) terminal costs give rise to control inputs of bang-bang type. In this Part II, the terminal cost criterion is extended with an integral term which accounts for the global heat loss during the process. Analysis of the extremal control sequence reveals that integral cost terms generically induce control of *bang-singular-bang* type. The singular arc is carefully analyzed. Furthermore it is illustrated that a practically more feasible *bang-bang* profile exhibits near optimal performance.

1 Introduction

Although tubular reactors have been largely used in the chemical process industry for several decades, the use of partial differential equation models (PDE models) not only for numerical simulation but also for system analysis and design of estimation and control algorithms has taken an increasing importance over the last decades (see, e.g., [1], [2], [3], [5], [12], [11]) following the pioneering works of, among others, Ray (e.g., [7], [8]) and Varma and Aris [10]. This series of two papers focuses on the determination of *optimal profiles* in non-isothermal tubular reactors whose controller design is based on a PDE model of the process. Our primary choice was to consider the model of an exothermic tubular reactor in which the controlled variable is the temperature along the reactor, and the control variable is the temperature of the heat exchanger surrounding the reactor. In a first step, we assume that the axial and radial (heat and mass) dispersions are negligible. The determination of the optimal profile reduces to the study of the equations of the tubular reactor in steady-state, i.e., of differential equations where the independent variable is the spatial variable z. More precisely, we are looking for the optimal solution with respect to a defined cost function of a set of two nonlinear differential equations where the input is the heat exchanger temperature and the output is the reactor temperature. The problem results in an optimal control problem where the usual independent variable (the time t) is replaced by the spatial variable z. Different cost functions have been considered in our study. While Part I of this series of two papers focuses on terminal costs only [9], Part II takes also an integral cost term into account which reflects the global heat loss during the process.

The organization of this paper is as follows. In Section 2 the steady-state equations for a plug flow reactor are proposed. The general optimal control problem is stated and the extremal control profiles are calculated in Section 3. Afterwards the extremal profile determination is illustrated by means of an example in Section 4. In addition, the performance of a *suboptimal* but practically more feasible profile is assessed. Finally, Section 5 summarizes the main conclusions.

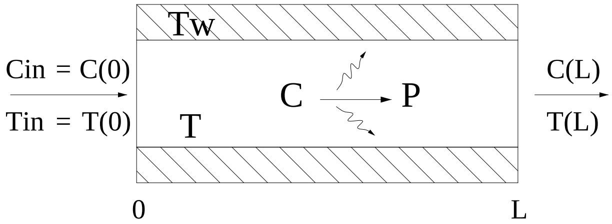

Figure 1: Non-isothermal tubular reactor with heat exchanger.

2 Plug flow steady-state reactor model

2.1 State equations for plug flow reactor

The steady-state equations for a plug flow exothermic reactor (see Figure 1) without axial and radial dispersion can be written as follows (see also [9])

$$\begin{aligned} \frac{dT}{dz} &= -\frac{\Delta H}{\rho C_p v} k_0 C e^{\frac{-E}{RT}} + \frac{4h}{\rho C_p d v}(T_w - T) \\ \frac{dC}{dz} &= -\frac{k_0}{v} C e^{\frac{-E}{RT}} \end{aligned} \tag{1}$$

with boundary conditions:

$$C(0) = C_{in} \quad \text{and} \quad T(0) = T_{in}$$

where $T(z)$ and $C(z)$ are the temperature and the reactant concentration respectively, v is the fluid superficial velocity, ΔH is the heat of reaction ($\Delta H < 0$ for an exothermic reaction), and ρ, C_p, k_0, E, R, h, d, L and T_w are the density, the specific heat, the kinetic constant, the activation energy, the ideal gas constant, the (overall) heat transfer coefficient, the reactor diameter, the reactor length and the heat exchanger temperature respectively.

2.2 Plug flow equations with dimensionless variables

To compensate for the large differences in order of magnitude of the model variables (possibly resulting in numerical simulation inaccuracies), the following dimensionless state variables x_1, x_2 and dimensionless control input u are introduced:

$$x_1 \triangleq \frac{T - T_{in}}{T_{in}}, \quad x_2 \triangleq \frac{C_{in} - C}{C_{in}}, \quad u \triangleq \frac{T_w - T_{in}}{T_{in}}$$

When defining the constants α, β, δ and γ as follows:

$$\alpha \triangleq k_0 e^{\frac{-E}{RT_{in}}}, \quad \beta \triangleq \frac{4h}{\rho C_p d}, \quad \delta \triangleq -\frac{\Delta H}{\rho C_p}\frac{C_{in}}{T_{in}}, \quad \gamma \triangleq \frac{E}{RT_{in}}$$

the model equations become:

$$\begin{aligned} \frac{dx_1}{dz} &= \frac{\alpha\delta}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}} + \frac{\beta}{v}(u - x_1) \qquad & x_1(0) = 0 \\ \frac{dx_2}{dz} &= \frac{\alpha}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}} & x_2(0) = 0 \end{aligned} \tag{2}$$

Simulations with constant heat exchanger temperature are shown in Part I of this series [9]. The values of the parameters and operating conditions are inspired by the values in the paper of Fjeld and Ursin [4]: $v = 0.1$ m/s, $L = 1$ m, $\delta = 0.25$ [-], $E = 11250$ cal/mole, $k_0 = 10^6$ 1/s, $4h/\rho C_p d = 0.2$ 1/s, $C_{in} = 0.02$ mole/L, $R = 1.986$ cal/mole/K, and $T_{in} = 340$ K.

3 Extremal control profile determination

3.1 Statement of the optimal control problem

The optimal control problem studied in this paper is to find an admissible control $u^*(z) \in \mathcal{U}$ which causes system (2) to follow an admissible trajectory $\mathbf{x}^* \in \mathcal{X}$ (with the process state $\mathbf{x}$ being composed of the state variables x_1 and x_2), while at the same time minimizing following performance criterion [6]:

$$\mathcal{J}[u] = \underbrace{h[\mathbf{x}(L)]}_{\text{Terminal cost}} + \underbrace{\int_0^L g[\mathbf{x}(z)]dz}_{\text{Integral cost}} \tag{3}$$

3.2 Hamiltonian and costate equations

According to the Minimum Principle of Pontryagin the *Hamiltonian* $\mathcal{H}$ for this problem is:

$$\begin{aligned} \mathcal{H} &= g[\mathbf{x}(z)] \\ &+ \lambda_1[\frac{\alpha\delta}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}} + \frac{\beta}{v}(u - x_1)] \\ &+ \lambda_2[\frac{\alpha}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}}] \\ &= \Big[g[\mathbf{x}(z)] + \lambda_1[\frac{\alpha\delta}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}} - \frac{\beta}{v}x_1] \\ &+ \lambda_2[\frac{\alpha}{v}(1 - x_2)e^{\frac{\gamma x_1}{1+x_1}}]\Big] + \Big[\lambda_1\frac{\beta}{v}\Big]u \\ &\triangleq \phi + \psi\, u \end{aligned} \tag{4}$$

with λ_1 and λ_2 the so-called costates associated to x_1 and x_2 respectively. Since the Hamiltonian does not explicitly depend on the spatial coordinate z, the Hamiltonian is *constant* when evaluated on an extremal trajectory. The costates satisfy the following dynamic equations (with $\boldsymbol{\lambda}$ the vector of $[\lambda_1 \;\; \lambda_2]^T$):

$$\frac{d\boldsymbol{\lambda}}{dz} = -\frac{\partial\mathcal{H}}{\partial\mathbf{x}} \tag{5}$$

with boundary conditions:

$$\boldsymbol{\lambda}(L) = \frac{\partial h}{\partial\mathbf{x}}\Big|_L \tag{6}$$

This becomes:

$$
\begin{aligned}
\frac{d\lambda_1}{dz} &= -\frac{\partial g[\mathbf{x}(z)]}{\partial x_1} \\
&\quad -\lambda_1[\frac{\alpha\delta}{v}(1-x_2)e^{\frac{\gamma x_1}{1+x_1}}\frac{\gamma}{(1+x_1)^2}-\frac{\beta}{v}] \\
&\quad -\lambda_2[\frac{\alpha}{v}(1-x_2)e^{\frac{\gamma x_1}{1+x_1}}\frac{\gamma}{(1+x_1)^2}] \\
\frac{d\lambda_2}{dz} &= -\frac{\partial g[\mathbf{x}(z)]}{\partial x_2}+\lambda_1[\frac{\alpha\delta}{v}e^{\frac{\gamma x_1}{1+x_1}}]+\lambda_2[\frac{\alpha}{v}e^{\frac{\gamma x_1}{1+x_1}}]
\end{aligned} \tag{7}
$$

3.3 Extremal control determination

Clearly, if the integral cost part is no explicit function of u, the control variable u appears linearly in the Hamiltonian $\mathcal{H}$. As a result, the extremal control $u^*(z)$ depends on the value of ψ, as follows:

if $\psi > 0$, then $u^*(z) = u_{MIN}$

if $\psi = 0$ for $z \in [z_i, z_{i+1}]$, then $u^*(z) = u_{sing}(z)$

if $\psi < 0$, then $u^*(z) = u_{MAX}$

which is a control of the *bang-singular-bang* type. u_{MIN} and u_{MAX} represent the lower and upper bound on the control input respectively.

3.4 Singular arc analysis

On a singular interval $[z_i,z_{i+1}]$, we have that $\psi = 0$. The singular control $u_{sing}(z)$ is then obtained by repeatedly differentiating ψ with respect to z until u appears explicitly. After two successive differentiations following expression for u_{sing} is obtained:

$$
\begin{aligned}
u_{sing} &= x_1 - \frac{\alpha\delta}{\beta}(1-x_2)e^{\frac{\gamma x_1}{1+x_1}} \\
&\quad + \frac{v}{\beta}\Bigg[\frac{\dfrac{\partial g[\mathbf{x}(z)]}{\partial x_2} - \dfrac{\partial^2 g[\mathbf{x}(z)]}{\partial x_1 \partial x_2}\dfrac{dx_2}{dz}}{\dfrac{\partial^2 g[\mathbf{x}(z)]}{\partial x_1^2} - \dfrac{\partial g[\mathbf{x}(z)]}{\partial x_1}\Big(\dfrac{\gamma}{(1+x_1)^2} - \dfrac{2}{1+x_1}\Big)}\Bigg]
\end{aligned} \tag{8}
$$

At this point the following remarks can be formulated.
Remark 1. The singular control is not explicitly dependent on the costates λ_1 and λ_2.
Remark 2. In a generic case the denominator of the singular control (8) is different from zero along the singular arc. Since two successive differentiations are needed to compute $u_{sing}(z)$, this problem is a singular control problem of order 2.
Remark 3. In the limiting case that $g[\mathbf{x}(\mathbf{z})]$ is not explicitly dependent on the state x_1, $\lambda_1(z)$ as well as $\lambda_2(z)$ are equal to zero along the singular arc which makes a singular arc not possible. The extremal control reduces then to a *bang-bang* control sequence (see also [9]).

Remark 4. The singular control (8) consists of two parts. The first part (i.e., the first two terms) is *independent* of cost function (3), while the second part (i.e., the last term) is largely influenced by the selection of the integrand $g[\mathbf{x}(\mathbf{z})]$ in cost function (3).
Remark 5. When substituting singular control (8) in the first state equation (2), we obtain

$$
\frac{dx_1}{dz} = \Bigg[\frac{\dfrac{\partial g[\mathbf{x}(z)]}{\partial x_2} - \dfrac{\partial^2 g[\mathbf{x}(z)]}{\partial x_1 \partial x_2}\dfrac{dx_2}{dz}}{\dfrac{\partial^2 g[\mathbf{x}(z)]}{\partial x_1^2} - \dfrac{\partial g[\mathbf{x}(z)]}{\partial x_1}\Big(\dfrac{\gamma}{(1+x_1)^2} - \dfrac{2}{1+x_1}\Big)}\Bigg]
$$

From this the following result is obtained.

RESULT 1
A sufficient condition for the reactor temperature to be constant along the singular arc is that the integrand $g[\mathbf{x}(\mathbf{z})]$ does not depend explicitly on the second state $x_2(z)$. ■

4 Case study: Optimal control with integral and terminal cost

The determination of the optimal heat exchanger temperature profile for cost 3 will be illustrated with an example.

Consider a cost criterion of the following type:

$$
\mathcal{J}[u] = (1-A)\underbrace{(1-x_2(L))}_{\mathcal{J}_1[u]} + \frac{A}{K_2}\int_0^L \underbrace{x_1^2(z)dz}_{\mathcal{J}_3[u]} \tag{9}
$$

with A the trade-off coefficient between terminal and integral cost and K_2 a user defined weighting factor to bring the two costs in the same order of magnitude.

The terminal cost part is a measure for the process efficiency while the integral cost part accounts for the total heat loss.

4.1 Singular arc analysis

Since the integral cost is no function of the second state $x_2(z)$ expression (8) reduces to

$$
u_{sing} = x_1 - \frac{\alpha\delta}{\beta}(1-x_2)e^{\frac{\gamma x_1}{1+x_1}} \tag{10}
$$

As mentioned before, this control keeps the temperature in the reactor constant along the singular arc.
This is summarized in the following result:

RESULT 2
If the performance index is a sum of terminal and integral costs as in (9), then the optimal heat exchanger temperature profile $u^*(z)$ is of the bang-singular-bang type inducing a constant reactor temperature $T(z)$ during the singular arc. ■

The above analysis has shown that the control will be of the *bang-singular-bang* type. This is translated in a heat exchanger temperature profile moving from its maximum value (400 K) towards its minimum value (280 K) via a singular arc. In other words, the profile starts at $u(z) = u_{MAX}$ for $0 \leq z \leq z_1$, then switches to the singular control, i.e., $u(z) = u_{SING}$ for $z_1 \leq z \leq z_2$ and ends with $u(z) = u_{MIN}$ for $z_2 \leq z \leq L$. This will cause the temperature in the reactor to increase from the fixed inlet temperature T_{in} (i.e., 340 K) towards the value T^* at z_1 which will be kept constant until z_2 is reached and will decrease afterwards. A qualitative view of this heat exchanger temperature profile is presented in Figure 2.

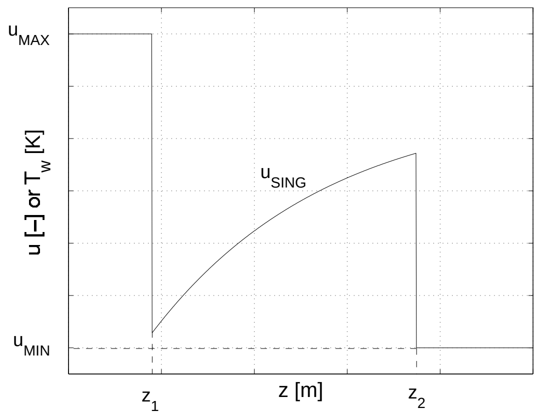

Figure 2: Maximum-singular-minimum profile.

4.2 Maximum-singular-minimum profile

This profile induces two degrees of freedom, namely z_1 or, equivalently T^* (i.e., the value at which the temperature is kept constant along the singular arc), and z_2. Hence, a hierarchic optimization is performed: given a value for T^* (with a fixed value for A and K_2), the z_2 switching position is optimized in such a way that performance index (9) reaches a minimum.

Figure 3 illustrates the behavior of the terminal cost $J_1[T_w]$ (dotted line) and integral cost $J_3[T_w]$ (full line) as a function of the selected temperature setpoint T^*. Observe that – in order to improve the interpretability of the results – in all forthcoming Figures the costs are shown using the original variables instead of the dimensionless variables (see also the Figure captions). Following observations can be made. First of all, a high T^* value induces a high conversion of the chemical. Secondly, the optimum T^* value for the integral cost is, rather evidently, equal to T_{in}, i.e., 340 K.

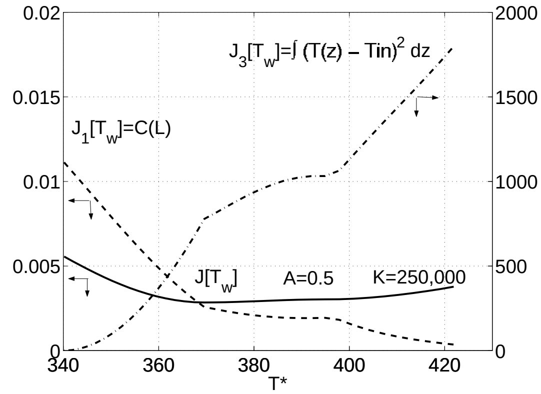

Figure 3: Maximum-singular-minimum profile. Cost criteria as function of setpoint temperature T^*. $J_1[T_w] = C(L)$, $J_3[T_w] = \int_0^L (T(z) - T_{in})^2 dz$ and $J[T_w] = (1 - A)J_1[T_w] + A/K_2\ J_3[T_w]$ with A = 0.5 and K_2 = 250,000.

4.3 Comparison of maximum-singular-minimum profile with maximum-minimum profile

The *bang-bang* type solution -which is the *true* optimal control in case of a terminal cost only [9]- computed in Part I of this series of two papers is proposed here in the context of *parametric* optimization of a limited number of degrees of freedom within a given control profile structure. Although optimality in the sense of the minimum principle cannot be guaranteed, the profile of Part I has attractive properties with respect to practical implementation. The heat exchanger should consist of two parts (the one at $T_w = T_{w,MAX}$ and the other at $T_w = T_{w,MIN}$) of appropriate lengths determined by z_1.

We consider a step profile which starts at $T_w(z) = T_{w,MAX}$ for $0 \leq z \leq z_1$ and then switches to $T_w(z) = T_{w,MIN}$ for $z_1 \leq z \leq L$. Observe that there is one degree of freedom, namely, the position z_1 at which the switch occurs.

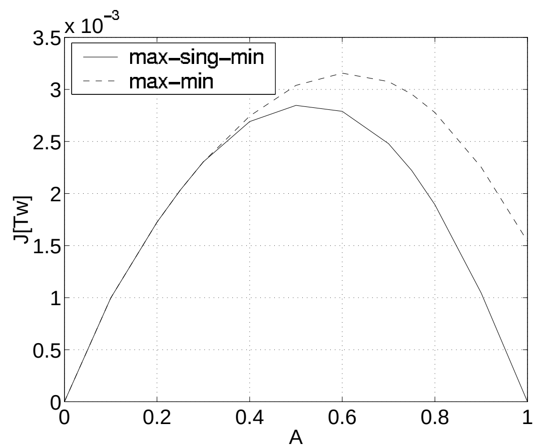

Figure 4: Comparison of *maximum-singular-minimum* profile (–) with *maximum-minimum* profile (--) for $J[T_w] = (1 - A)J_1[T_w] + A/K_2\ J_3[T_w]$ with K_2 = 250,000.

Figure 4 illustrates the behavior of the minima of cost (9) evaluated for different A values for the *maximum-singular-minimum* profile (full line) as well as for the *maximum-minimum* profile (dotted line). Corresponding optimal profiles are plotted in Figure 5 for A equal to 0.3 (left plots) and 0.7 (right plots) respectively. Clearly, the performance of the suboptimal *maximum-minimum* profile is comparable with that of the optimal profile. More specifically, if A is small (e.g., equal to 0.3), i.e., more emphasis on the conversion efficiency, the cost values for the different profiles practically coincide and the *maximum-singular-minimum* profile reduces to the *maximum-minimum* profile. If A is large (e.g., equal to 0.7), i.e., more emphasis on the minimization of global heat loss, the overall cost of the truly optimal *bang-singular-bang* profile is significantly smaller although the chemicals conversion with an optimized *maximum-minimum* profile is slightly better. Remark that for large values of A the *maximum-singular-minimum* profile reduces to a *maximum-singular* profile.

These observations are summarized in following result.

RESULT 3
From a practical point of view, the near optimal bang-bang profile is an excellent alternative for the theoretically optimal bang-singular-bang profile. ■

5 Conclusions

In this work optimal control theory is applied to a steady-state plug flow reactor, in which a chemical is converted into a desired product In contrast with time varying processes the independent variable is now the space coordinate z. The traditional trade-off between process performance and energy consumption is translated into a cost criterion with terminal and integral parts in this Part II (of a series of two papers). It is generically demonstrated that the optimal heat exchanger temperature profile for this combined cost criterion is of *bang-singular-bang* type. If the integral cost part is no function of the chemicals concentration the singular control keeps the reactor temperature constant. Furthermore, it is illustrated that a *maximum-minimum* profile (which is more feasible from a practical implementation point of view) has near optimal performance.

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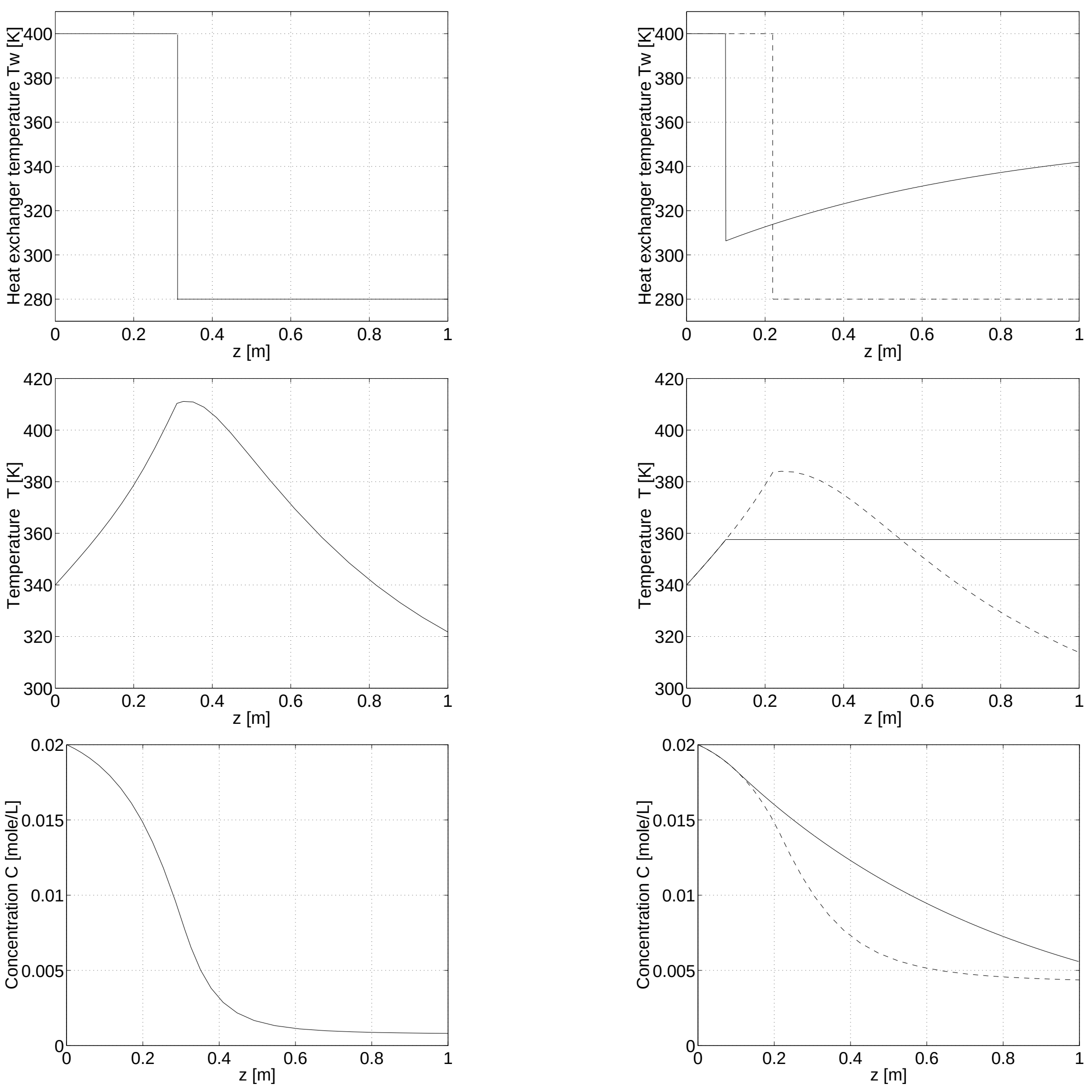

Figure 5: Comparison of *maximum-singular-minimum* profile (–) with *maximum-minimum* profile (- -) for $J[T_w] = (1-A)J_1[T_w] + A/K_2\ J_2[T_w]$ with K_2 = 250,000 and A = 0.3 (left plots) or A = 0.7 (right plots). Upper: heat exchanger temperature profiles. Middle: reactor temperature profiles. Bottom: reactant concentration profiles.