

## Optimal Control of Tubular Reactors Described by Partial Differential Equations

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**ABSTRACT :** A tubular reactor model represented by partial differential equations was studied as one of nonlinear distributed parameter optimal control problems. An optimal control theory in the form of maximum principles based on nonlinear integral equations was used to develop an algorithm to solve the problem.

### INTRODUCTION

The field of distributed parameter system, which began in some 30 years ago, is concerned with the dynamic behavior of processes distributed in space as well as changing in time. The models for these systems usually are described by partial differential equations (PDE's) or integral equations (IE's). Besides the increased complexity of the model equations over ordinary differential equation systems, there are qualitative differences in system structure which give rise to new considerations in satisfying controllability, observability, and optimal conditions.

Most of chemical processes where mass transfer, heat transfer, fluidization and chemical reactions are accompanied have been modeled approximately

by using ordinary differential equations (ODE's) or some experimental methods, even though the actual processes are described by PDE's originally. In order to simulate and control these chemical processes more precisely, the PDE's should be used without any simplification or approximation. Especially, the control of the fine chemical processes requires more tight quality control than others do, this reflects the increasing trends of the needs of more accurate process models and studies based on these models.

### MATHEMATICAL MODEL AND SIMULATION

We consider the following unsteady state tubular reactor with axial dispersion, where a first order irreversible chemical reaction  $A \rightarrow B$  occurs. The system equation derived from the mass balance in the unsteady state is given in the dimensionless form (Hlavacek et. al. [3]) :

$$\frac{\partial C}{\partial t} = \frac{1}{P_e} \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z} + Da(1 - C) \exp\left[-\frac{\theta}{1 + \frac{\theta}{\gamma}}\right] \quad (1)$$

$$I. C. : C(z, 0) = h(z) \quad (2)$$

$$B. C. : z = 0 \quad P_e C(0^+, t) - \frac{\partial C}{\partial z} \Big|_{z=0^+} = 0 \quad (3)$$

$$z = 1 \quad \frac{1}{P_e} \frac{\partial C}{\partial z} \Big|_{z=1} = 0 \quad (4)$$

where  $t$  is the dimensionless time;  $h$  is a specified

function of the dimensionless space variable  $z$ ;  $C$  is the mass fraction of component B;  $\theta$  is the dimensionless temperature in the reactor;  $P_e$  is the axial Peclet number;  $D_a$  is the Damkohler number;  $\gamma$  is the dimensionless activation energy.

It is required to choose control  $\theta(z, t)$  so as to minimize the performance index

$$P = \frac{1}{2} \int_0^1 [w(C(1, t) - C_d(1, t))^2 + \int_0^1 (\theta(z, t) - \theta_d(z, t))^2 dz] dt \quad (5)$$

where  $C_d(1, t)$  and  $\theta_d(z, t)$  are the desired product concentration and the desired temperature profile in the reactor, respectively, and  $w$  is the weighting factor.

We can solve this problem by converting the partial differential equation into an equivalent integral equation and then applying the maximum principle by Wang[1].

The Green function for this two-point boundary value problem is available in Kim and Chang [4]:

$$G(z, t; \xi, \tau) = 2 \cdot \exp\left(\frac{P_e}{2} z - \frac{P_e}{4} t\right) \cdot \sum_{m=1}^{\infty} \frac{\exp\left(-\frac{\alpha_m^2}{P_e} t\right) (\alpha_m \cos \alpha_m z + \frac{P_e}{2} \sin \alpha_m z)}{\alpha_m^2 + \frac{P_e^2}{4} + P_e} \exp\left[-\frac{P_e}{2} \xi + \left(\frac{P_e}{4} + \frac{\alpha_m^2}{P_e}\right) \tau\right] \cdot (\alpha_m \cos \alpha_m \xi + \frac{P_e}{2} \sin \alpha_m \xi) \quad (6)$$

where  $\alpha_m$  is the  $m$ th positive root of

$$\tan \alpha = \frac{P_e \alpha}{\alpha^2 - \frac{P_e^2}{4}} \quad (7)$$

Then the state equation in the integral form is:

$$C(z, t) = 2 \cdot \exp\left(\frac{P_e}{2} z - \frac{P_e}{4} t\right) \cdot \sum_{m=1}^{\infty} \frac{\exp\left(-\frac{\alpha_m^2}{P_e} t\right) (\alpha_m \cos \alpha_m z + \frac{P_e}{2} \sin \alpha_m z)}{\alpha_m^2 + \frac{P_e^2}{4} + P_e} \cdot \left\{ \int_0^1 \int_0^1 \left[ \exp\left(-\frac{P_e}{2} \zeta + \left(\frac{P_e}{4} \tau + \frac{\alpha_m^2}{P_e}\right) \tau\right) \cdot (\alpha_m \cos \alpha_m \zeta + \frac{P_e}{2} \sin \alpha_m \zeta) \right] \cdot D_a (1 - C) \exp\left(\frac{\theta}{1 + \frac{\theta}{\gamma}}\right) \cdot d\zeta d\tau + \int_0^1 [h(\zeta) \exp\left(-\frac{P_e}{2} \zeta\right) \cdot (\alpha_m \cos \alpha_m \zeta + \frac{P_e}{2} \sin \alpha_m \zeta)] \cdot d\zeta \right\} \quad (8)$$

The costate equation is given by:

$$\lambda(z, t) = [C(1, t) - C_d(1, t)] - 2 \cdot \exp\left(-\frac{P_e}{2} z + \frac{P_e}{4} t\right) \cdot \sum_{m=1}^{\infty} \frac{\exp\left(-\frac{\alpha_m^2}{P_e} t\right) (\alpha_m \cos \alpha_m z + \frac{P_e}{2} \sin \alpha_m z)}{\alpha_m^2 + \frac{P_e^2}{4} + P_e} \cdot D_a \exp\left(\frac{\theta}{1 + \frac{\theta}{\gamma}}\right) \cdot \left\{ \int_{\tau=t}^1 \int_0^1 \lambda \left[ \exp\left(\frac{P_e}{2} \zeta - \frac{P_e}{4} \tau - \frac{\alpha_m^2}{P_e} \tau\right) \cdot (\alpha_m \cos \alpha_m \zeta + \frac{P_e}{2} \sin \alpha_m \zeta) \right] d\zeta d\tau \right\} \quad (9)$$

The Hamiltonian function is defined as

$$H = -\frac{1}{2} [w(C(1, t) - C_d(1, t))^2 + (\theta(z, t) - \theta_d(z, t))^2] + 2 \cdot \exp\left(-\frac{P_e}{2} z + \frac{P_e}{4} t\right) \cdot \sum_{m=1}^{\infty} \frac{\exp\left(-\frac{\alpha_m^2}{P_e} t\right) (\alpha_m \cos \alpha_m z + \frac{P_e}{2} \sin \alpha_m z)}{\alpha_m^2 + \frac{P_e^2}{4} + P_e} \cdot D_a (1 - C) \exp\left(\frac{\theta}{1 + \frac{\theta}{\gamma}}\right) \cdot$$

$$\left\{ \int_{\tau=0}^1 \int \lambda \left[ \exp \left( \frac{P_e}{2} \zeta - \frac{P_e}{4} \tau - \frac{\alpha_m^2}{P_e} \tau \right) \cdot \left( \alpha_m \cos \alpha_m \zeta + \frac{P_e}{2} \sin \alpha_m \zeta \right) \right] d\zeta d\tau \right\} \quad (10)$$

From the maximum principle [1], we have

$$H(\theta^*) \stackrel{(\equiv)}{=} \sup_{\theta \in \Theta} H(\theta) \quad (11)$$

A necessary condition for maximizing the Hamiltonian is :

$$0 = H_{\theta} = -(\theta - \theta_d) + 2 \cdot \exp \left( \frac{P_e}{2} z + \frac{P_e}{4} t \right) \cdot$$

$$\sum_{m=1}^{\infty} \frac{\exp \left( -\frac{\alpha_m^2}{P_e} t \right) \left( \alpha_m \cos \alpha_m z + \frac{P_e}{2} \sin \alpha_m z \right)}{\alpha_m^2 + \frac{P_e^2}{4} + P_e}$$

$$D_a (1 - C) \exp \left( \frac{\theta}{1 + \frac{\theta}{\gamma}} \right) \cdot \frac{1}{\left( 1 + \frac{\theta}{\gamma} \right)^2} \cdot$$

$$\left\{ \int_{\tau=0}^1 \int \lambda \left[ \exp \left( \frac{P_e}{2} \zeta - \frac{P_e}{4} \tau - \frac{\alpha_m^2}{P_e} \tau \right) \cdot \left( \alpha_m \cos \alpha_m \zeta + \frac{P_e}{2} \sin \alpha_m \zeta \right) \right] d\zeta d\tau \right\} \quad (12)$$

An algorithm based on the first gradient of Hamiltonian function :

$$\theta^{(k+1)}(z, t) = \theta^{(k)}(z, t) + \varepsilon H_{\theta}(\theta(z, t)) \quad (13)$$

where  $k$  is the iteration number and  $\varepsilon$  is a small positive number.

## RESULTS AND DISCUSSION

The results from computer simulation are described in figures 1 - 4. For the numerical computation, parameter values used in the literature [3] were chosen;  $P_e = 10.0$ ,  $Da = 0.07$ ,  $\gamma = 20$ . The value of  $w$  was 20.

In general, the chemical reactors are desired to be operated as closely as possible in the steady state condition, we set the desired concentration  $C_d(z)$  and the desired temperature  $\theta_d(z)$  to the steady state values as specified in the literature.

The initial concentration  $h(z)$  was set to be zero throughout the reactor. The initial guess of the temperature was chosen as a time independent function.

The improvements of the cost function with iterations is significant as shown in Fig. 4. The convergence of the algorithm was very good. The computational results show that the method developed in this work is successful in finding the optimal control in the unsteady state tubular reactor.

The state and costate equations in Eqns. (8) and (9) were solved by a numerical integration method combined with the linear algebra technique using the LEQT1F subroutine of IMSL).

## NOMENCLATURE

- C : concentration of product B
- $D_t$  : Damkohler number
- G : Green's function
- H : Hamiltonian function
- $h(z)$  : initial concentration
- P : cost function
- $P_e$  : Peclet number
- $\alpha_m$  : positive number in the Green's function
- $\gamma$  : dimensionless activation energy
- $\lambda$  : costate variable

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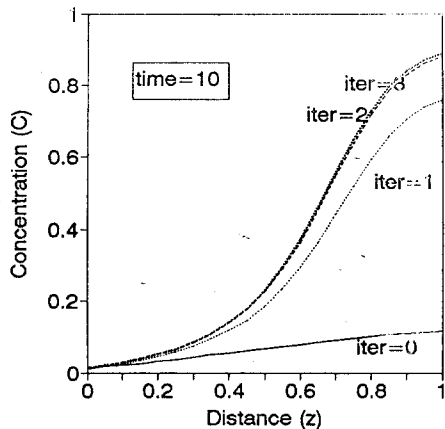


Fig. 1. Concentration profiles at time=10.

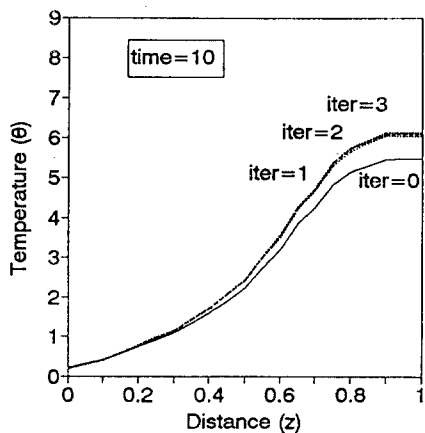


Fig. 2. Temperature profiles at time=10.

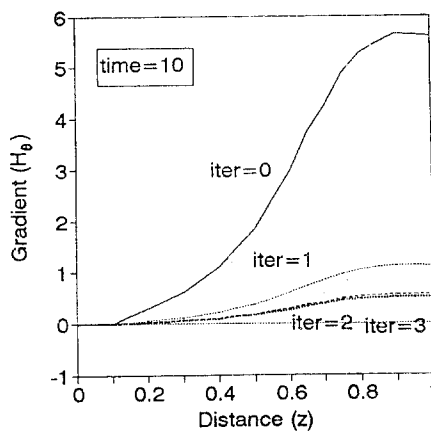


Fig. 3. Gradient profiles at time=10.

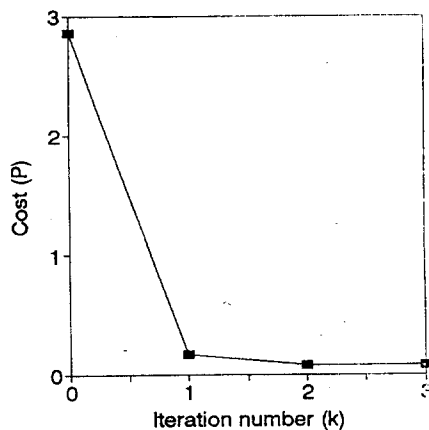


Fig. 4. Improvement of the cost function with iterations