Korean J. of Chem. Eng., **12**(2), 198-206 (1995)

COMPARISON OF TWO METHODS OF OPTIMAL CONTROL SYNTHESIS: PARTIAL DIFFERENTIAL EQUATION APPROACH AND INTEGRAL EQUATION APPROACH

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(Received 23 June 1994 • accepted 9 December 1994)

Abstract—This study shows how the optimal control theory for distributed parameter systems can be implemented for a problem of tubular reactor with axial dispersion described by partial differential equations. Two methods are implemented. One is based on differential equation approach and the other is based on integral equation approach. It was found that the approach with partial differential equations is preferable to the one with integral equations for the type of problems treated in this study. Computation algorithms and programs for both cases are developed.

Key words: Distributed Parameter System, Optimal Control

INTRODUCTION

Process dynamics of many control problems are described by ordinary differential equations (ODEs) while many other problems of process control are described by partial differential equations (PDEs). The former problems are called lumped parameter systems (LPSs) and the latter are called distributed parameter systems (DPSs). The optimal control of DPSs, compared to LPSs, gives rise to many additional complexities because of the interactive nature of the variables distributed in time and space.

There are two major approaches for the optimal control synthesis for DPSs [Wang, 1985]. One approach is to use the original PDEs and apply an appropriate maximum principle derived for the PDEs. The other is to convert the PDEs to integral equations (IEs) by means of Green's function technique, and then the optimal control is obtained by applying a maximum principle developed for the IEs.

In some of the early work on optimal control of DPSs [Bansal and Chang, 1972; Wang, 1985] theory of maximum principle for specific PDE systems was developed. Some generalized necessary conditions were reported by Zone and Chang [1972], Zone [1973], and Wang [1985]. The IE method was formulated by Butkovskiy [1969] for the first time and extended by Wang [1985] for the general case.

Although a considerable amount of theory has been developed in the past, this has not been reflected sufficiently into the industrial applications. This seems to be due to the lack of real-time experience with theory and the complexity of modern chemical processes. There is, therefore, a great merit to investigate the application of optimal control theory for DPSs.

In this study, we apply the maximum principle developed by Wang [1985] to a tubular reactor problem for two different cases, a single state and a two state variable case. We developed algorithms and computer programs for the optimal control computations. In doing so, we compare two different approaches, namely, one with PDEs and the other with IEs.

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THEORY OF OPTIMAL CONTROL FOR DISTRIBUTED PARAMETER SYSTEMS

1. Problem Statement

The dynamics of the general system of nonlinear partial differential equations can be described by the following form:

$$\frac{\partial v}{\partial t} = Lv + Nv \tag{1}$$

The initial and boundary conditions can be stated as

$$\text{I.C.: } v(x, t_o) = v_o(x) \tag{2}$$

$$\text{B.C.: } A_i(\delta_l v; \partial x_i, t) = C_i(\delta_k v, u_{3i}, u_2; \partial x_i, t). \tag{3}$$

In Eq. (1), L represents a linear partial differential operator with order l and N a nonlinear operator with order $2k(k<l)$. L and N can be stated using the multi-index notation as

$$Lv = \sum_{|\beta| \le l} (-1)^{|\beta|} D^{\beta} v \tag{4}$$

$$Nv = \sum_{|\alpha| \le k} (-1)^{|\alpha|} D^{\alpha} a_{\alpha}(x, t; \delta_k v, u_1(x, t), u_2(t)). \tag{5}$$

In the above equations, $v \in R^n$ stands for the state variable vector; $t \in [t_o, t_f] \equiv T$ the time variable; $x = (x_1, x_2, \cdots, x_N)^T \in R^N$ the spatial variable vector; $\bar{l} = \max(l-1, 2k-1)$; δ_k a set of all the derivatives of orders 0, 1, $\cdots$ k; $u_1(x, t)$ the domain control, $u_2(t)$ time dependent control and $u_{3i}(\partial x_i, t)$ $(i = 1, 2, \cdots, S)$ the boundary control; ∂x_i a point on the boundary $\partial\Omega_i$ and $\partial\Omega = \cup_{i=1}^{S} \partial\Omega_i$. And, α and β are multi-indices of $\alpha = \{\alpha_1, \alpha_2, \cdots, \alpha_N\}$ and $\beta = \{\beta_1, \beta_2, \cdots, \beta_N\}$ which have the length of $|\alpha| = \left[\sum_{j=1}^{N} \alpha_j\right] \le k$, $|\beta| = \left[\sum_{j=1}^{N} \beta_j\right] \le l$.

The optimal control problem is to find controls $u_1(x, t) \in U_1$, $u_2(t) \in U_2$ and $u_{3i}(\partial x_i, t) \in U_{3i}$ which minimize the following objective function J.

$$J = \int_{t_o}^{t_f} \int_{\Omega} F(v, u_1; x, t)\, dx\, dt + \int_{\Omega} F_1(v; x, t_f)\, dx$$

$$+\sum_{i=1}^{S}\int_{t_0}^{t_f}\int_{\partial\Omega_i} F_{2i}(v,\ u_3,\ u_2,\ \partial x_i,\ t)\ d\partial x_i\ dt+\int_{t_0}^{t_f} F_3(u_2,\ t)\ dt \quad (6)$$

Here, U_1, U_2 and U_3 are admissible control sets, F, F_1, F_{2i} (i=1, 2,···, S) and F_3 are measurable scalar functions.

This general nonlinear optimal control problem can be solved using a maximum principle in the manner of following two approaches.

2. Partial Differential Equation Approach

We briefly describe the maximum principle for the nonlinear partial differential equations of two-independent variables, which are common in most chemical engineering DPSs. The state equation, Eq. (1), is expressed with two spatial variables by replacing $x=(x_1,\ x_2)=(x,\ y)$ as

$$\frac{\partial v}{\partial t}=f_1(v_{xx},\ v_{yy},\ v_{xy},\ v_x,\ v_y,\ u)+f_2(v_{xx},\ v_{yy},\ v_{xy},\ v_x,\ v_y,\ u). \quad (7)$$

For this case, the initial and boundary conditions are given by the following form:

$$\text{I.C. } v(x,\ y,\ t_0)=v_0(x,\ y) \quad (8)$$

$$\text{B.C. } v_x=g_1(v,\ u_3,\ \theta)\big|_{x=x_0} \quad (9)$$

$$v_x=\hat{g}_1(v,\ \hat{u}_3,\ \theta)\big|_{x=x_f} \quad (10)$$

$$v_y=g_2(v,\ u_3,\ \theta)\big|_{y=y_0} \quad (11)$$

$$v_y=\hat{g}_2(v,\ \hat{u}_3,\ \theta)\big|_{y=y_f}. \quad (12)$$

Here, f_1 is the linear differential function and f_2 the nonlinear differential function; $x\in[x_0,\ x_f]$ and $y\in[y_0,\ y_f]\subset\Omega$ the spatial variables, $t\in[t_0,\ t_f]\subset T$ the time variable, subscripts 0 and f indicate initial and final positions or time, respectively; $v(x,\ y,\ t)\in R^n$ the state vector, $v_x=\frac{\partial v}{\partial x}$, $v_{xx}=\frac{\partial^2 v}{\partial x^2}$ and $v_{xy}=\frac{\partial^2 v}{\partial x\partial y}$; f_1, f_2, g_1, $\hat{g}_1$, g_2, $\hat{g}_2$ function vectors; $u(x,\ y,\ t)$ the domain control, u_3 and $\hat{u}_3$ the boundary control. And, $\theta(t)$ is a spatially independent parameter governed by its own dynamics as

$$\frac{d\theta}{dt}=\varphi(\theta,\ u_2,\ t) \quad (13)$$

with the initial condition $\theta(t_0)=\theta_0$ given; $u_2(t)$ a time-dependent control; and φ vector function.

The objective function to be minimized is also translated as

$$\begin{aligned}J(v,\ u,\ z,\ w)=&\int_{t_0}^{t_f}\int_{x_0}^{x_f}\int_{y_0}^{y_f}F(u,\ v,\ v_x,\ v_{xx},\ v_y,\ v_{yy},\ v_{xy})\ dy\ dx\ dt\\&+\int_{x_0}^{x_f}\int_{y_0}^{y_f}F_1\{v(x,\ y,\ t_f)\}\ dy\ dx\\&+\int_{t_0}^{t_f}\int_{y_0}^{y_f}\{F_{21}(v,\ u_3,\ u_2)\big|_{x=x_0}+\hat{F}_{21}(v,\ \hat{u}_3,\ u_2)\big|_{x=x_f}\}\ dy\ dt\\&+\int_{t_0}^{t_f}\int_{x_0}^{x_f}\{F_{22}(v,\ u_3,\ u_2)\big|_{y=y_0}+\hat{F}_{22}(v,\ \hat{u}_3,\ u_2)\big|_{y=y_f}\}\ dx\ dt\\&+\int_{t_0}^{t_f}F_3(v,\ u_2)\ dt\end{aligned} \quad (14)$$

where F, F_1, F_{21}, $\hat{F}_{21}$, F_{22}, $\hat{F}_{22}$ and F_3 are scalar functions.

Let $f=f_1+f_2$, then Eq. (7) becomes

$$\frac{\partial v}{\partial t}=f(u,\ v,\ v_x,\ v_{xx},\ v_y,\ v_{yy},\ v_{xy}). \quad (15)$$

The Hamiltonians are defined by the following relations.

Domain Hamiltonian:

$$H=F+\lambda^T f \quad (16)$$

where $\lambda=(\lambda_1,\ \lambda_2,\cdots,\lambda_n)^T$ is the domain costate vector.

Time-dependent Hamiltonian:

$$\Theta=F_3+\pi^T\varphi \quad (17)$$

where $\pi=(\pi_1,\ \pi_2,\cdots,\pi_n)^T$ is the time-dependent costate vector.

Boundary Hamiltonians:

$$\text{at } x=x_0,\ h_1=F_{21}-\frac{\partial H}{\partial v_{xx}^T}g_1 \quad (18)$$

$$\text{at } x=x_f,\ \hat{h}_1=\hat{F}_{21}-\frac{\partial H}{\partial v_{xx}^T}\hat{g}_1 \quad (19)$$

$$\text{at } y=y_0,\ h_2=F_{22}-\frac{\partial H}{\partial v_{yy}^T}g_2 \quad (20)$$

$$\text{at } y=y_f,\ \hat{h}_2=\hat{F}_{22}-\frac{\partial H}{\partial v_{yy}^T}\hat{g}_2 \quad (21)$$

The costate equation is defined as

$$\frac{\partial\lambda}{\partial t}=\left(\frac{\partial H}{\partial v_{xx}}\right)_{xx}+\left(\frac{\partial H}{\partial v_{xy}}\right)_{xy}+\left(\frac{\partial H}{\partial v_{yx}}\right)_{yx}-\left(\frac{\partial H}{\partial v_x}\right)_x-\left(\frac{\partial H}{\partial v_y}\right)_y+\frac{\partial H}{\partial v}. \quad (22)$$

The transversality conditions for the costate equations are defined as

$$\text{at } x=x_0,\ \frac{\partial F_{21}}{\partial v}=\frac{\partial H}{\partial v_x}-\left(\frac{\partial H}{\partial v_{xx}}\right)_x-\left(\frac{\partial H}{\partial v_{yx}}\right)_y+\frac{\partial H}{\partial v_{xx}}\frac{\partial g_1}{\partial v} \quad (23)$$

$$\text{at } x=x_f,\ \frac{\partial\hat{F}_{21}}{\partial v}=-\frac{\partial H}{\partial v_x}+\left(\frac{\partial H}{\partial v_{xx}}\right)_x+\left(\frac{\partial H}{\partial v_{yx}}\right)_y-\frac{\partial H}{\partial v_{xx}}\frac{\partial\hat{g}_1}{\partial v} \quad (24)$$

$$\text{at } y=y_0,\ \frac{\partial F_{22}}{\partial v}=\frac{\partial H}{\partial v_y}-\left(\frac{\partial H}{\partial v_{xy}}\right)_x-\left(\frac{\partial H}{\partial v_{yy}}\right)_y+\frac{\partial H}{\partial v_{yy}}\frac{\partial g_2}{\partial v} \quad (25)$$

$$\text{at } y=y_f,\ \frac{\partial\hat{F}_{22}}{\partial v}=-\frac{\partial H}{\partial v_y}+\left(\frac{\partial H}{\partial v_{xy}}\right)_x+\left(\frac{\partial H}{\partial v_{yy}}\right)_y-\frac{\partial H}{\partial v_{yy}}\frac{\partial\hat{g}_2}{\partial v} \quad (26)$$

$$\text{at } t=t_f,\ \lambda=\frac{\partial F_1}{\partial v}. \quad (27)$$

The costate equation for π of the time-dependent Hamiltonian is

$$\begin{aligned}\frac{\partial\pi}{\partial t}=&-\frac{\partial\Theta}{\partial\theta}+\int_{y_0}^{y_f}\left(\frac{\partial g_1^T}{\partial\theta}\frac{\partial H}{\partial v_{xx}}\Big|_{x=x_0}-\frac{\partial\hat{g}_1^T}{\partial\theta}\frac{\partial H}{\partial v_{xx}}\Big|_{x=x_f}\right)dy\\&+\int_{x_0}^{x_f}\left(\frac{\partial g_2^T}{\partial\theta}\frac{\partial H}{\partial v_{yy}}\Big|_{y=y_0}-\frac{\partial\hat{g}_2^T}{\partial\theta}\frac{\partial H}{\partial v_{yy}}\Big|_{y=y_f}\right)dx.\end{aligned} \quad (28)$$

Transversality conditions for Eq. (28) are given by

$$\text{at } t=t_f,\ \pi=0 \quad (29)$$

and at all corner points, $(x_0,\ y_f,\ t)$, $(x_f,\ y_f,\ t)$, $(x_0,\ y_0,\ t)$ and $(x_f,\ y_0,\ t)$, we have

$$\frac{\partial H}{\partial v_{xy}}=0. \quad (30)$$

Necessary conditions for the optimality (Maximum principle) can be stated as follows.

Domain control:

If $u^*(x,\ y,\ t)$ yields the maximum J for given z(t) and w(t), the domain Hamiltonian must attain its absolute maximum with re-

spect to u at u* almost everywhere on $\Omega\times T$.

Boundary control:

If z*(t) yields the maximum J for given u(x, y, t) and w(t), the boundary Hamiltonian must attain its absolute maximum with respect to z at z* almost everywhere on T.

Time-dependent control:

If w*(t) yields the maximum J for given u(x, y, t) and z(t), the time-dependent Hamiltonian must attain its absolute maximum with respect to w at w* almost everywhere on T.

3. Integral Equation Approach

In this approach, the first step is to recast the system of the PDEs into that of IEs in various Sobolev spaces $W^{k,p}[\Omega\times T]$ for $1\le p\le\infty$. The conditions for this step are stated as follows:

Condition 1. The linear part of Eq. (1) subject to the homogeneous boundary conditions are expressed as:

$$\frac{\partial \nu}{\partial t}=L\nu;\ \text{B.C. } A_i(\delta_j\nu;\ \partial x_i,\ t)=0. \tag{31}$$

Green's function $G(x, t; \xi, \tau)$ exists for Eq. (31) if the conditions in Eqs. (32)-(37) in $W^{k,p}$ space, for $2\le p\le\infty$

$$\int_{t_0}^{t_f}\int_{\Omega}|D_\xi^\varphi D_\tau^\alpha G(x,\ t;\ \xi,\ \tau)|^p\ dx\ dt<\infty \tag{32}$$

$$\int_{t_0}^{t_f}\int_{\Omega}|D_\xi^\varphi D_\tau^\alpha G(x,\ t;\ \xi,\ \tau)|^p\ d\xi\ d\tau<\infty \tag{33}$$

$$\int_{t_0}^{t_f}\int_{\partial\Omega_i}|D_\xi^\varphi D_\tau^\alpha G(\partial x_i,\ t;\ \xi,\ \tau)|^p\ d\partial x_i\ dt<\infty \tag{34}$$

$$\int_{\Omega}|D_\tau^\alpha G(x,\ t;\ \xi,\ t_o)|^p\ d\xi<\infty \tag{35}$$

$$\int_{t_0}^{t_f}\int_{\partial\Omega_i}|D_\tau^\alpha G(x,\ t;\ \partial\xi_i,\ \tau)|^p\ d\partial\xi_i\ d\tau<\infty \tag{36}$$

where $|\varphi|,\ |\alpha|\le k$; and for $1\le p<2$

$$|D_\xi^\varphi D_\tau^\alpha G(x,\ t;\ \xi,\ \tau)|\le M,\ t\ne\tau\ne 0 \text{ and } M>0 \tag{37}$$

are satisfied.

Condition 2. a_α in the nonlinear function of Eq. (5) satisfies the Caratheodory conditions [9] in $W^{l,p}$ $(p\ge 1)$, which states that the derivatives of the function are measurable and continuous as well as they satisfy certain growth conditions. This is expressed simply as

$$a_\alpha\in CAR(p)\in CAR^*(p)\in CAR^{**}(p) \tag{38}$$

Condition 3. Functions in Eqs. (1)-(6) have partial derivatives with respect to argument functions and satisfy Lipschitz conditions.

Condition 4. Control functions u_1, u_2 and u_{3i} belong to admissible control sets U_1, U_2 and U_{3i}, respectively.

Once the above conditions are satisfied and the Green function is obtained, then the system of PDEs, Eqs. (1)-(5), is formulated into an integral equation as

$$\begin{aligned}\nu(x,\ t)=&\sum_{\alpha\le k}\int_{t_0}^{t_f}\int_{\Omega}a_\alpha(\xi,\ \tau;\ \delta_k\nu,\ u_1,\ u_2)D_\xi^\varphi G(x,\ t;\ \xi,\ \tau)\ d\xi\ d\tau\\&+\sum_{i=1}^{S}\int_{t_0}^{t_f}\int_{\partial\Omega_i}[\Phi_i^T D_\xi^\varphi G(x,\ t;\ \partial\xi_i,\ \tau)\ C_i(\nu,\ u_2,\ u_{3i})]\ d\partial\xi_i\ d\tau\\&+\int_{\Omega}G(x,\ t;\ \xi,\ t_o)\ \nu_o(\xi)\ d\xi\end{aligned} \tag{39}$$

where Φ_i is a vector function.

The Hamiltonians and the costate equations are evaluated as follows:

We define a function Q as

$$\begin{aligned}Q=&\int_{t_0}^{t_f}\int_{\Omega}[\lambda^T(\xi,\ \tau)\ G(\xi,\ \tau;\ x,\ t)]^T\sigma(\tau-t)d\xi\ d\tau\\&+\int_{\Omega}[\lambda_f^T(\xi)\ G(\xi,\ t_f;\ x,\ t)]^T d\xi\\&+\sum_{i=1}^{S}\int_{t_0}^{t_f}\int_{\partial\Omega_i}[\Psi_i^T(\partial\xi_i,\ \tau)\ G(\partial\xi_i,\ \tau;\ x,\ t)]^T\sigma(\tau-t)\ d\xi_i\ d\tau\end{aligned} \tag{40}$$

where

$$\begin{aligned}\Psi_i^T=&\int_{t_0}^{t_f}\int_{\Omega}[\lambda^T(\xi,\ \tau)\ g_i(\xi,\ \tau;\ \partial x_i,\ t)]^T\sigma(\tau-t)\ d\xi\ d\tau\\&+\int_{\Omega}[\lambda_f^T(\xi)\ g_i(\xi,\ t_f;\ \partial x_i,\ t)]^T d\xi\\&+\sum_{j=1}^{S}\int_{t_0}^{t_f}\int_{\partial\Omega_j}[\Psi_j^T(\partial\xi_j,\ \tau)\ g_i(\xi_j,\ \tau;\ \partial x_i,\ t)]^T\sigma(\tau-t)\ d\partial\xi_j\ d\tau\end{aligned} \tag{41}$$

and λ, λ_f, Ψ_j are costates for domain, final time and boundary, respectively.

Now, the Hamiltonians are defined as follows:

Domain Hamiltonian:

$$H(u_1,\ u_2;\ x,\ t)=F(u_1;\ x,\ t)+f^T(u_1,\ u_2;\ x,\ t)Q \tag{42}$$

Boundary Hamiltonian:

$$h_i(u_{3i},\ u_2;\ \partial x_i,\ t)=F_{2i}(u_{3i};\ \partial x_i,\ t)+C_i^T(u_{3i},\ u_2;\ \partial x_i,\ t)\Psi_i \tag{43}$$

Time-dependent Hamiltonian:

$$\Theta(u_2;\ t)=F_3(u_2)+\int_{\Omega}f^T(u_1,\ u_2)\ Q\ dx+\sum_{i=1}^{S}\int_{\partial\Omega_i}C_i^T(u_{3i},\ u_2)\Psi_i\ d\partial x_i \tag{44}$$

The costates are obtained as follows:

Domain costate equation:

$$\lambda(x,\ t)=\frac{\partial F}{\partial \nu}+\frac{\partial f^T}{\partial \nu}Q \tag{45}$$

Boundary costate equation:

$$\Psi_i(\partial x_i,\ t)=\frac{\partial F_{2i}}{\partial \nu(\partial x_i,\ t)}+\frac{\partial C_i^T}{\partial \nu(\partial x_i,t)}\Psi_i \tag{46}$$

Time-dependent costate equation:

$$\pi=-\frac{\partial\Theta}{\partial\theta}+\sum_{i=1}^{S}\int_{\partial\Omega_i}\left(\frac{\partial h_i}{\partial\theta}-\frac{\partial\hat{h}_i}{\partial\theta}\right)d\xi_i. \tag{47}$$

Maximum principles for the optimality are expressed as follows.

Domain control:

If $u_1^*(x, t)$ minimizes J for given u_2 and u_{3i}, then H must attain its absolute maximum with respect to $u_1(x, t)$ at $u_1^*(x, t)$, almost everywhere on $\Omega\times T$.

Boundary controls:

If $u_{3i}^*(\partial x_i, t)$ minimizes J for given $u_1(x, t)$, $u_2(t)$ and $u_{3j}(\partial x_j, t)$, $j\ne i$, then h_i must attain its absolute maximum with respect to u_{3i} at u_{3i}^* on $\partial\Omega_i\times T$.

Time-dependent control:

If the time dependent control $u_2^*(t)$ minimizes J for given u_1 and u_{3i}, then Θ must attain its absolute maximum with respect to $u_2(t)$ at $u_2^*(t)$ almost everywhere on T.

Table 1. Single state variable case with $J=\frac{1}{2}\int_0^{\tau_f}\int_0^1 w[x_d(\xi,\tau)-(\xi,\tau)]^2+[\theta_d(\xi,\tau)-\theta(\xi,\tau)]^2\ d\xi\ d\tau$

	PDE	IE
State equation	$\frac{\partial x}{\partial \tau}=L_x x+N[\theta(\xi,\tau)](1-x)$	$x(\xi,\tau)=\int_0^{\tau}\int_0^1 G_1(\xi,\tau,z,t)N[\theta(z,t)][1-x(z,t)]\,dz\,dt$
Costate equation	$\frac{\partial \lambda_1}{\partial \tau}=L_{x1}\lambda_1-N[\theta(\xi,\tau)]\lambda_1+w[x_d-x]$	$\lambda_1(\xi,\tau)=w[x_d-x]-\int_0^{\tau}\int_0^1 G_1(\xi,\tau,z,t)N[\theta(\xi,\tau)]\lambda_1(z,t)\,dz\,dt$
Hamiltonian function	$H(\xi,\tau)=-\frac{1}{2}\{w(x_d-x)^2+(\theta_d-\theta)^2\}+\lambda_1\{L_x x+N[\theta(\xi,\tau)](1-x)\}$	$H(\xi,\tau)=-\frac{1}{2}\{w(x_d-x)^2+(\theta_d-\theta)^2\}-\int_0^{\tau}\int_0^1\lambda_1(z,t)\,G_1(\xi,\tau,z,t)N[\theta(z,t)][1-x(z,t)]dz\,dt$
Optimal condition	$\theta_d-\theta^*=-\frac{\lambda_1}{\left(1+\frac{\theta^*}{\gamma}\right)^2}(1-x)N(\theta^*)$	$\theta_d-\theta^*=-\int_0^{\tau}\int_0^1\frac{\lambda_1(z,t)\,G_1(\xi,\tau,z,t)\,N[\theta^*(z,t)][1-x(z,t)]}{\left[1-\frac{\theta^*(\xi,\tau)}{\gamma}\right]^2}dz\,dt$

OPTIMAL CONTROL FOR TUBULAR REACTORS

Now, we calculate the optimal control for the tubular reactor problems using the theory stated above. We consider two cases; single state variable and two state variable cases. The nonlinear optimal control is obtained for the former and the linear optimal control for the latter.

1. Problem Statement

We consider a tubular reactor of a non-isothermal axially-dispersed one-dimensional model with a first-order irreversible exothermic reaction. The model in a dimensionless form is commonly represented by

Mass balance:

$$\frac{\partial x}{\partial \tau}=\frac{1}{Pe_x}\frac{\partial^2 x}{\partial \xi^2}-\frac{\partial x}{\partial \xi}+Da(1-x)\exp\left[\frac{\theta}{1+\frac{\theta}{\gamma}}\right] \tag{48}$$

Energy balance:

$$\frac{\partial \theta}{\partial \tau}=\frac{1}{Pe_\theta}\frac{\partial^2 \theta}{\partial \xi^2}-\frac{\partial \theta}{\partial \xi}+DaB(1-x)\exp\left[\frac{\theta}{1+\frac{\theta}{\gamma}}\right]-b(\theta-\theta_w) \tag{49}$$

Initial conditions: $[x]_{\tau=0}=0$; $[\theta]_{\tau=0}=0$ (50), (51)

Boundary conditions: $\left[\frac{\partial x}{\partial \xi}=Pe_x x\right]_{\xi=0}$; $\left[\frac{\partial \theta}{\partial \xi}=Pe_\theta\theta\right]_{\xi=0}$ (52), (53)

$\left[\frac{\partial x}{\partial \xi}=0\right]_{\xi=1}$; $\left[\frac{\partial \theta}{\partial \xi}=0\right]_{\xi=1}$ (54), (55)

where x is the conversion in the reaction; θ the temperature; τ the time; ξ the axial position; Pe_x the Peclet number of the mass flow; Pe_θ the Peclet number of the energy flow; Da the Damköhler number; γ the activation energy. B and b are the coefficients related to the heat of reaction and the heat transfer, respectively, and θ_w indicates the temperature of the reactor wall.

For the single state variable case, we consider only the mass balance as the state equation. The reactor temperature is considered as the control variable which is involved nonlinearly as shown in Eq. (48). The following objective function is chosen for this case.

$$J=\frac{1}{2}\int_0^{\tau_f}\int_0^1[w\{x_d(\xi,\tau)-x(\xi,\tau)\}^2+\{\theta_d(\xi,\tau)-\theta(\xi,\tau)\}^2]\ d\xi\ d\tau \tag{56}$$

For the two state variable case, the mass and energy balances are both considered. The reactor wall temperature is chosen to be the control variable. Now, the control variable is involved linearly as shown in Eq. (49). The following objective function is minimized for the two state variable case.

$$J=\frac{1}{2}\int_0^1 w[(x_d-x)_{\tau=\tau_f}]^2\ d\xi+\frac{1}{2}\int_0^{\tau_f}\int_0^1[\theta_d(\xi,\tau)]^2\ d\xi\ d\tau \tag{57}$$

In Eqs. (56) and (57), w is a weighting, $x_d(\xi,\tau)$ and $\theta_d(\xi,\tau)$ indicate the desired values.

We now show how PDE and IE approaches apply to each control problem.

2. Partial Differential Equation Approach

Since the original PDEs are directly used, this approach is straightforward to implement. Following the theory stated above, we constructed Table 1 for the single variable case and Table 2 for the two variable case. These Tables provide state equations, costate equations, Hamiltonian function and optimal control equation for each case as Eqs. (63)-(66) in Table 1 and Eqs. (71)-(76) in Table 2.

For the PDE approach, we solve two sets of PDEs which are for the state and the costate variables as Eqs. (63) and (64) in Table 1, and Eqs. (71)-(74) in Table 2. The initial and boundary conditions are given for the state equations as Eqs. (50)-(55). For the costate equations, so-called the transversality conditions are provided in Appendix according to Eqs. (23)-(27).

The optimal control equation of the single variable case, Eq. (66) in Table 1, is from the necessary condition for the optimality, $\left(\frac{\partial H}{\partial \theta}\right)_{\theta=\theta^*}=0$; and that of the two variable case, Eq. (76) in Table 2, is from $\left(\frac{\partial H}{\partial \theta_w}\right)_{\theta_w=\theta_w^*}=0$. The optimal control equation for the single variable case is nonlinear in terms of the control variable, θ^*. The solution is obtained by the optimization technique. For this calculation, most frequently used is the first-variation steepest-descent method [Chang, 1978]:

$$\theta^{k+1}(\xi,\tau)=\theta^k(\xi,\tau)+\varepsilon\left(\frac{\partial H}{\partial \theta}\right) \tag{58}$$

Table 2. Two state variable case with $J=\frac{1}{2}\int_0^1 w[(x_d-x)_{\tau=\tau_f}]^2\ d\xi+\frac{1}{2}\int_0^{\tau_f}\int_0^1[\theta_u(\xi,\tau)]^2\ d\xi\ d\tau$

	PDE	IE
State equation	$\frac{\partial x}{\partial \tau}=L_x x+N(\theta)(1-x)$	$x(\xi,\tau)=\int_0^{\tau_f}\int_0^1 G_1(\xi,\tau,z,t)N[\theta(z,t)][1-x(z,t)]\ dz\ dt$
	$\frac{\partial \theta}{\partial \tau}=L_\theta\theta+B\ N(\theta)(1-x)-b(\theta-\theta_u)$	$\theta(\xi,\tau)=\int_0^{\tau_f}\int_0^1 G_2(\xi,\tau,z,t)\{N[\theta(z,t)][1-x(z,t)]-b(\theta-\theta_u)\}\ dz\ dt$
Costate equation	$\frac{\partial \lambda_1}{\partial \tau}=L_{x1}\lambda_1-N(\theta)(\lambda_1+B\ \lambda_2)$	$\lambda_1(\xi,\tau)=\int_0^{\tau_f}\int_0^1 N(\theta)(G_1\lambda_1+B\ G_2\lambda_2)\ dz\ dt$
	$\frac{\partial \lambda_2}{\partial \tau}=L_{x2}\lambda_2-N(\theta)(1-x)\frac{(\lambda_1+B\lambda_2)}{\left(1+\frac{\theta}{\gamma}\right)^2}-b\lambda_2$	$\lambda_2(\xi,\tau)=\int_0^{\tau_f}\int_0^1\left\{N(\theta)\frac{G_1\lambda_1+BG_2\lambda_2}{\left(1+\frac{\theta}{\gamma}\right)^2}-b\ G_2\lambda_2\right\}\ dz\ dt$
Hamiltonian function	$H(\xi,\tau)=-\frac{1}{2}\theta_u^2+\lambda_1[L_x x+N[\theta(\xi,\tau)](1-x)]$ $+\lambda_2\{L_\theta\theta+B\ N(\theta)(1-x)-b(\theta-\theta_u)\}$	$H(\xi,\tau)=-\frac{1}{2}\theta_u^2+\int_0^{\tau_f}\int_0^1\{\lambda_1 G_1 N(\theta)(1-x)$ $+\lambda_2[G_2N(\theta)(1-x)-b(\theta-\theta_u)]\}\ dz\ dt$
Optimal condition	$\theta_u^*=b\ \lambda_2$	$\theta_u^*=\int_0^{\tau_f}\int_0^1 b\ \lambda_2\ G_2\ dz\ dt$

where k is the iteration number and ε is a weighting for the Hamiltonian gradient.

With the PDE approach, we end up with a two-point boundary-value problem (TPBVP); the initial value PDE for the state plus the final value PDE for the costate. The solution technique for the PDEs is the numerical method of lines [Schiesser, 1991] by means of DSS/2 [Schiesser, 1985]. The algorithm developed for the computation is summarized as follows.

Single Variable Case:

(1) At k=0, set $\theta^k(\xi,\tau)$ for $0\le\tau\le\tau_f$ and $0\le\xi\le1$.
(2) For $0\le\tau\le\tau_f$, solve the TPBVP* to obtain $x(\xi,\tau)$ and $\lambda_1(\xi,\tau)$.
(3) Find the optimal control $\theta^*(\xi,\tau)$ by Eq. (66);
if $\theta^k(\xi,\tau)$ is not equal to $\theta^*(\xi,\tau)$, repeat the whole steps from Step 2
with k=k+1 and Eq. (58).

TPBVP*

(i) solve the state PDE,
(ii) guess $\lambda_1(\xi,0)$,
(iii) solve the costate PDE and obtain $\lambda_1^{calc}(\xi,\tau_f)$
(iv) check that $\lambda_1^{calc}(\xi,\tau_f)$ satisfies the transversality condition Eq. (A-10), if satisfies, go to Step 3,
if not, repeat Steps (iii) and (iv) by substituting $\lambda_1(\xi,0)=\lambda_1^{calc}(\xi,\tau_f)$.

Two Variable Case:

1. At k=0, guess $\theta_u^k(\xi,\tau)$ for $0\le\tau\le\tau_f$ and $0\le\xi\le1$.
2. For $0\le\tau\le\tau_f$, solve the TPBVP**.
3. Find the optimal control $\theta_u^*(\xi,\tau)$ by Eq. (76);
if $\theta_u^*(\xi,\tau)=\theta_u^k(\xi,\tau)$; the optimal control is obtained;
if not, repeat from Step 2 by replacing k=k+1 and $\theta_u^k(\xi,\tau)=\theta_u^*(\xi,\tau)$.

TPBVP**

(i) solve the state PDEs,
(ii) guess $\lambda_1(\xi,0)$ and $\lambda_2(\xi,0)$,
(iii) solve the costate PDEs and obtain $\lambda_1^{calc}(\xi,\tau_f)$ and $\lambda_2^{calc}(\xi,\tau_f)$,
(iv) check that $\lambda_1^{calc}(\xi,\tau_f)$ and $\lambda_2^{calc}(\xi,\tau_f)$ satisfy the transversality conditions;
if satisfies, go to Step 3,
if not, repeat Steps (iii) and (iv) by substituting $\lambda_1(\xi,0)=w(x_d-x)_{\tau=\tau_f}$ and $\lambda_2(\xi,0)=\lambda_2^{calc}(\xi,\tau_f)$.

Solving TPBVPs usually takes most computing efforts for the PDE approach. For this study, a reasonable convergence was achieved by the back-substitution method as described with the algorithms. The most important and difficult part of the computation, as far as we have experienced with the problem in this study, is to provide a proper guess for the initial value of the costate variables. The convergence is very sensitive to the initial guess.

3. Integral Equation Approach

The first step in this method is to convert Eqs. (48)-(55) to integral equations using Green's function technique. Since the system satisfies the four conditions described previously with Eqs. (32)-(38), the Green's function for the problem exists. By means of Eqs. (39)-(47), we derive the equations for states, costates, Hamiltonian and optimal control as shown in Tables 1 and 2.

The overall procedure for the IE approach can be divided into the construction of equation part and the calculation part. The former part leads to Eqs. (67)-(69) and (77)-(81). And the latter part focuses on obtaining the optimal control by solving Eqs. (70) and (82), which satisfy the necessary condition for optimality. Here, the calculation is easier than that of the PDE case. If the equation is linear, it is solved algebraically as described in the following example of Fredholm's second type integral equations in Eqs. (59)-(62).

Integral Equation:

$$y(x,t)=\int_0^t\int_0^1 G(x,t,\xi,\tau)\ [1-y(\xi,\tau)]\ d\xi\ d\tau$$
$$=\int_0^t\int_0^1 G(x,t,\xi,\tau)\ d\xi\ d\tau-\int_0^t\int_0^1 G(x,t,\xi,\tau)\ y(\xi,\tau)\ d\xi\ d\tau \tag{59}$$

Using the trapezoidal rule, we get

$$\int_0^t G(x,t,\xi,\tau)\ y(\xi,\tau)\ d\xi$$
$$=\Delta\xi\sum_{i=2}^{m-1} G_i(x,t,\tau)y_i(\tau)+\frac{\Delta\xi}{2}[G_1(x,t,\tau)y_1(\tau)+G_m(x,t,\tau)y_m(\tau)] \tag{60}$$

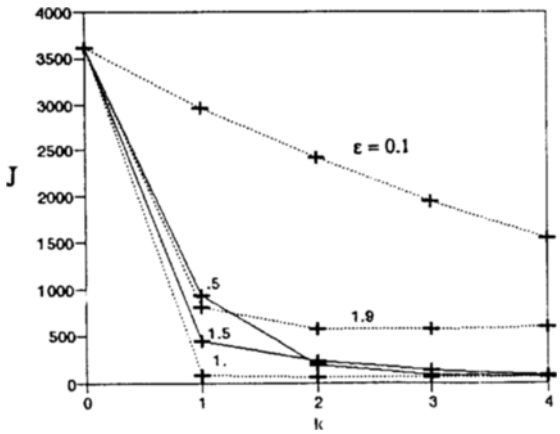

Fig. 1. Influence of ε on the behavior of convergence of the objective function with iterations.

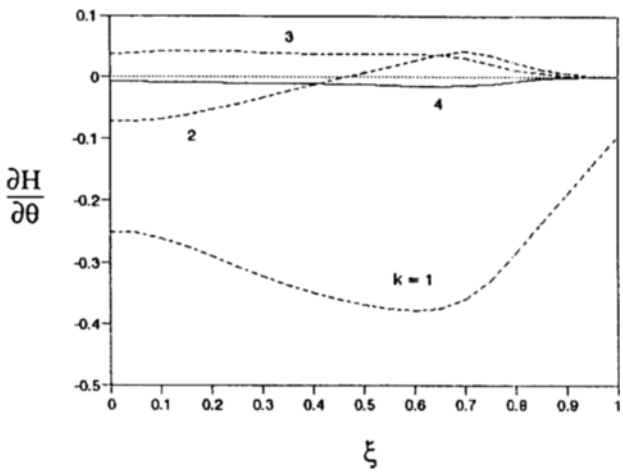

Fig. 2. Profile of Hamiltonian gradient with iterations.

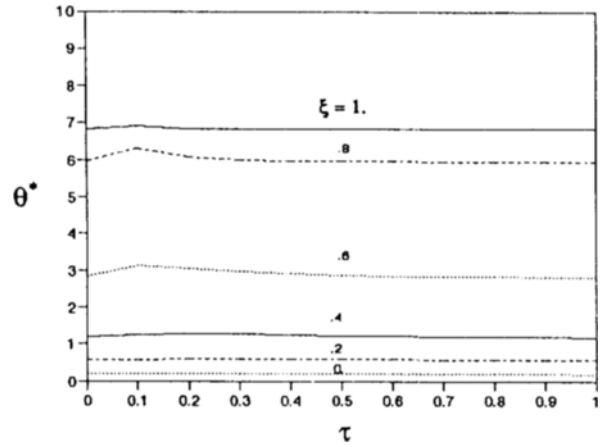

Fig. 3. Optimal control at different reactor locations.

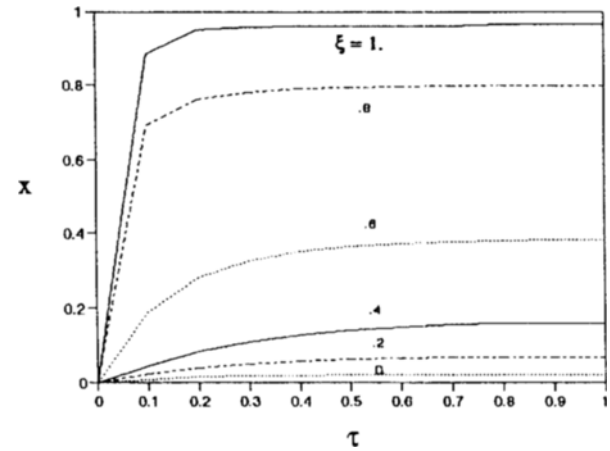

Fig. 4. Transient trajectories of the state variable by the optimal control at different reactor positions.

Therefore, we have

$$\int_0^t\int_0^1 G(x,\ t,\ \xi,\ \tau)\ y(\xi,\ \tau)\ d\xi\ d\tau$$
$$= \Delta\tau \sum_{j=2}^{nj-1}\left[\Delta\xi \sum_{i=2}^{ni-1} G_{ij}(x,\ t)y_{ij} + \frac{\Delta\xi}{2}\{G_{1j}(x,\ t)y_{1j} + G_{ni,j}(x,\ t)y_{ni,j}\}\right]$$
$$+ \frac{\Delta\tau}{2}\left[\Delta\xi \sum_{i=2}^{ni-1} G_{i1}(x,\ t)y_{i1} + \frac{\Delta\xi}{2}\{G_{11}(x,\ t)y_{11} + G_{ni,1}(x,\ t)y_{ni,1}\}\right.$$
$$\left. + \Delta\xi \sum_{i=2}^{ni-1} G_{i,nj}(x,\ t)y_{i,nj} + \frac{\Delta\xi}{2}\{G_{i,nj}(x,\ t)y_{i,nj} + G_{ni,nj}(x,\ t)y_{ni,nj}\}\right] \quad (61)$$

where ni is the number of integral grids in space and nj is the number of integral grids in time.

Applying Eq. (61) to Eq. (59), we finally write the following equation:

$$(\bar{I} - \bar{G})\bar{y} = \bar{G};\ \ \bar{y} = (\bar{I} - \bar{G})^{-1}\bar{G} \quad (62)$$

where $\bar{I}$ is the identity matrix; $\bar{y}$; and $\bar{G}$ the (ni×nj) by (ni×nj) matrix.

Eq. (62) contains the matrix inversion, which sometimes makes the computation difficult.

The algorithm for this approach for the single variable case can be developed:

(1) At k=0, set $\theta^k(\xi,\ \tau)$ for $0\le\tau\le\tau_f$ and $0\le\xi\le1$.

(2) For $0\le\tau\le\tau_f$, solve the IEs to obtain $x(\xi,\ \tau)$ and $\lambda_i(\xi,\ \tau)$:

(3) Find the optimal control $\theta^*(\xi,\ \tau)$ by Eq. (70);
if $\theta^k(\xi,\ \tau)$ is not equal to $\theta^*(\xi,\ \tau)$, repeat the whole steps from Step 2
with k=k+1 and Eq. (58).

RESULTS AND DISCUSSION

Figs. 1-4 shows results from the single variable case based on PDE and IE approaches. We see that two methods lead to identical solutions. Fig. 1 shows the influence of ε in Eq. (58) on the behavior of convergence of the objective function with iterations. For this problem, with too small ε, e.g., ε=0.1 in the figure, the convergence becomes very slow, and with too large ε, e.g., ε=1.9, the computation diverges. The best choice of ε for this problem seems to be ε=1. The optimal ε also depends on w in the objective function. Since there is no set rule to determine ε optimally, we determined the value empirically after some computational experience.

Fig. 2 shows that the profile of Hamiltonian gradient in the reactor approaches zero indicating that the optimal control is achieved. This numerical computation verifies the theory of optimal control for DPSs. Fig. 3 shows the time-responses of the

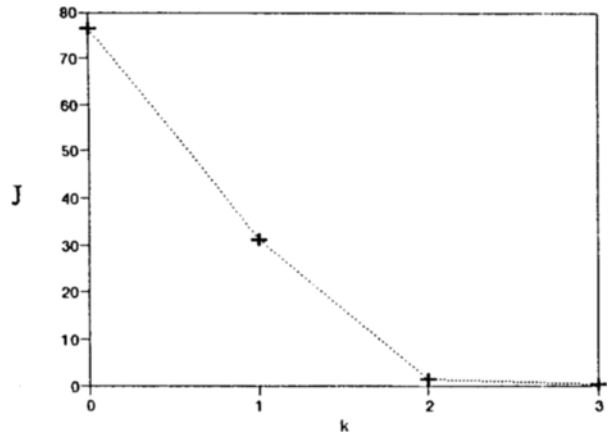

Fig. 5. Decrease in the objective function with iterations.

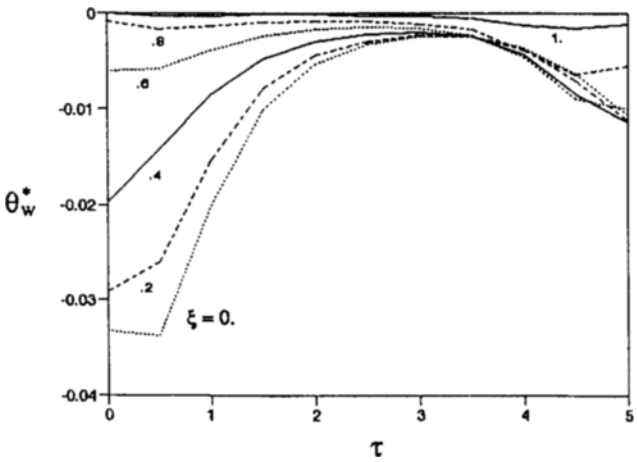

Fig. 6. Optimal control profile change at different time.

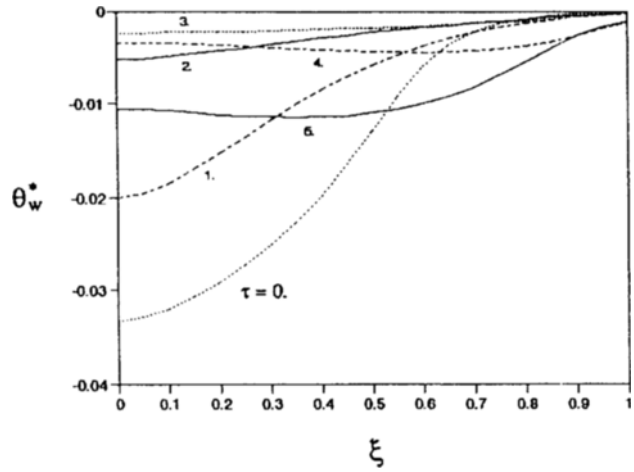

Fig. 7. Change of optimal control profile with position.

Table 3. Comparison of IE and PDE methods for a tubular reactor problem

	IE	PDE
Solution approach	analytical	approximated
Equations involved	algebraic equations	differential equations
Pre-calculation	conversion needed (PDEs→IEs)	direct treatment (as PDEs)
Time-consuming steps	calculation of positive roots, matrix inversion	two-point boundary value problem
Programming	requires detailed programming	adaptable to available programs
Computing time	>15 min	<3 min

optimal control at different reactor locations. The control changes gradually with time. This optimal control also causes the slow state response as shown in Fig. 4.

The results from the two variable case based on PDE approach are shown in Figs. 5-7. The figures show the optimal coolant temperature profiles minimizing the objective function in Eq. (57). The time τ runs from 0 to 5.

Fig. 5 shows the decrease in the objective function with iterations. Fortunately, the simple back-substitution used for the two-point boundary value problem converged well. Fig. 6 shows the change of optimal control profile with position and Fig 7 shows the optimal control profiles at several reactor positions plotted against time. From these figures, we see that there are significant differences in optimal controls at initial and final time depending on positions. The control changes more rapidly near the reactor entrance than near the exit.

Although the results from both PDE and IE approaches are identical, as observed in the single variable case, the computational features are different. This is summarized in Table 3.

The IE approach provides the exact solution, while the PDE approach leads to an approximate solution. In IE approach, the initial and boundary conditions of partial differential equations can be absorbed into one integral equation, which is finally treated like an algebraic equation given in Eq. (62). Except for the matrix inversion, the computation is simple for linear integral equations. For nonlinear integral equations, however, this is not the case.

One of the time-consuming steps of the IE approach is in the determination of a sufficient number of positive roots of the characteristic equation with sufficient accuracy. The value of m, which indicates the number of the roots, heavily depends on Peclet number. With less than 100 positive roots, e.g., $m<100$, the results of the open-loop simulation are not satisfactory for $Pe=10$. For larger values of Pe, e.g., $Pe>100$, the numerical calculation becomes excessive since it requires too many positive roots. On the other hand, this is avoided with the PDE approach. The two-point boundary value problem, however, can be a burden for the PDE approach. Thus the IE approach may be useful for the reactor of small Pe numbers.

We found that the programming of PDEs with the numerical method of lines is easier and more flexible than that of IEs with the trapezoidal rule. Since the numerical method of lines does the computation with one less dimension than other conventional PDE solving methods, we can handle the problem using a smaller memory size. Even a PC/486 compatible can handle the computation without difficulty.

The overall computing time with the PDE approach is much less than with the IE approach. Therefore, it can be concluded that the PDE approach for the optimal control of distributed parameter systems is preferable to the IE approach at least for the type of reactor problems studied here.

CONCLUSIONS

The optimal controls of a tubular reactor were obtained using maximum principles for the parabolic nonlinear partial differential equations and the integral equations. The maximum principles were used in the numerical computation to find the optimal control for the cases of one state and two state variables. Computation algorithms and Fortran codes for both approaches were developed. The method using the partial differential equation approach seems to be more preferable for the present type of tubular reactor problems.

ACKNOWLEDGMENTS

We would like to acknowledge the financial support of Korea Science and Engineering Foundation through the Automation Research Center at Pohang University of Science and Technology (POSTECH).

NOMENCLATURE

b : dimensionless parameter for the heat exchange
B : dimensionless parameter for the heat of reaction
Da : Damköhler number
CAR(p) : class of functions satisfying Caratheodory property
$D^u u$: derivatives of function u
F, F_1, F_2, F_3 : measurable functions in the objective function
f, f_1, f_2 : measurable functions in the state equation
G, G_1, G_2 : Green's functions
H : domain Hamiltonian
h : boundary Hamiltonian
J : objective function
L : linear differential operator
M : positive number
N : nonlinear differential operator
p : positive number used for Sobolev spaces
Pe_c : Peclet number of the mass flow
Pe_θ : Peclet number of the energy flow
S : positive integer
t : time variable
u : domain control
U : admissible control region
v : state variable
$W^{k,p}$: Sobolev spaces
w : a weighting value in the objective function
w : time-dependent control
x : spatial variable, reaction conversion
x_d : desired reaction conversion
z : boundary control, dummy variable

Greek Letters

α : multi-index, $\{\alpha_1, \alpha_2, \cdots, \alpha_n\}$, eigenvalue for the mass balance
$|\alpha|$: length of the multi-index α, $\sum_{i=1}^{N} \alpha_i$
β : multi-index, eigenvalue for the energy balance
γ : dimensionless activation energy
ε : weighting for the Hamiltonian gradient
θ : spatially independent parameter, dimensionless temperature
θ_d : desired temperature profile in the reactor, dimensionless
θ_w : exterior temperature of the reactor wall, dimensionless
Θ : time-dependent Hamiltonian function
λ : costate variable vector
λ_1, λ_2 : costate variables
ξ : dimensionless length, axial location in the reactor
ζ : spatial dummy variable vector
τ : dimensionless time
τ_f : final time, dimensionless
π : costate variable
Ω : domain in R^n
$\partial\Omega$: boundary of domain

Superscripts

k : iteration counter
calc : calculated value
* : optimal
N : number of spatial variables
n : number of state variables
T : transpose

Subscripts

d : desired property
f : final property
m, n : eigenvalue counter
o : starting position
1 : related with the first state variable
2 : related with the second state variable

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APPENDIX

Supplements for Tables 1 and 2:

$$L_x=\frac{1}{Pe_x}\frac{\partial^2}{\partial\xi^2}-\frac{\partial}{\partial\xi} \tag{A-1}$$

$$L_\theta=\frac{1}{Pe_\theta}\frac{\partial^2}{\partial\xi^2}-\frac{\partial}{\partial\xi} \tag{A-2}$$

$$L_{\lambda 1}=\frac{1}{Pe_x}\frac{\partial^2}{\partial\xi^2}+\frac{\partial}{\partial\xi} \tag{A-3}$$

$$L_{\lambda 2}=\frac{1}{Pe_\theta}\frac{\partial^2}{\partial\xi^2}+\frac{\partial}{\partial\xi} \tag{A-4}$$

$$N[\theta(\xi,\tau)]=Da\ \exp\left[\frac{\theta(\xi,\tau)}{1+\frac{\theta(\xi,\tau)}{\gamma}}\right] \tag{A-5}$$

$$G_1=2\ \exp\left[\frac{Pe_x}{2}(\xi-z)-\frac{Pe_x}{4}(\tau-t)\right]\left[\sum_{m=1}^{\infty}\frac{\exp\left[\frac{\alpha_m^2}{Pe_x}(t-\tau)\right]}{\alpha_m^2+\frac{Pe_x^2}{4}+Pe_x}\cdot\left\{\alpha_m^2\cos\alpha_m\xi+\frac{Pe_x}{2}\sin\alpha_m\xi\right\}\left\{\alpha_m^2\cos\alpha_m z+\frac{Pe_x}{2}\sin\alpha_m z\right\}\right] \tag{A-6}$$

$$G_2=2\ \exp\left[\frac{Pe_\theta}{2}(\xi-z)-\frac{Pe_\theta}{4}(\tau-t)\right]\left[\sum_{n=1}^{\infty}\frac{\exp\left[\frac{\beta_n^2}{Pe_\theta}(t-\tau)\right]}{\beta_n^2+\frac{Pe_\theta^2}{4}+Pe_\theta}\cdot\left\{\beta_n^2\cos\beta_n\xi+\frac{Pe_\theta}{2}\sin\beta_n\xi\right\}\left\{\beta_n^2\cos\beta_n z+\frac{Pe_\theta}{2}\sin\beta_n z\right\}\right] \tag{A-7}$$

α_m: m^{th} positive root of

$$\left(\alpha^2-\frac{Pe_x^2}{4}\right)(\tan\alpha)-Pe_x\,\alpha=0 \tag{A-8}$$

β_n: n^{th} positive root of

$$\left(\beta^2-\frac{Pe_\theta^2}{4}\right)(\tan\beta)-Pe_\theta\,\theta=0 \tag{A-9}$$

Transversality Conditions:

1. Single State Variable Case

$$(\lambda_1)_{\tau=\tau_f}=0 \tag{A-10}$$

$$\left(\frac{\partial\lambda_1}{\partial\xi}=0\right)_{\xi=0} \tag{A-11}$$

$$\left(\frac{\partial\lambda_1}{\partial\xi}=-Pe_x\lambda_1\right)_{\xi=1} \tag{A-12}$$

2. Two State Variable Case

$$(\lambda_1)_{\tau=\tau_f}=w(x_d-x)_{\tau=\tau_f} \tag{A-13}$$

$$\left(\frac{\partial\lambda_1}{\partial\xi}=0\right)_{\xi=0} \tag{A-14}$$

$$\left(\frac{\partial\lambda_1}{\partial\xi}=-Pe_x\lambda_1\right)_{\xi=1} \tag{A-15}$$

$$(\lambda_2)_{\tau=\tau_f}=0 \tag{A-16}$$

$$\left(\frac{\partial\lambda_2}{\partial\xi}=0\right)_{\xi=0} \tag{A-17}$$

$$\left(\frac{\partial\lambda_2}{\partial\xi}=-Pe_\theta\lambda_2\right)_{\xi=1} \tag{A-18}$$