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Optimal Control of a Tubular Reactor Using the Distributed-Parameter Method and the Numerical Method of Lines

Young-Soon Choe, Dae Ryook Yang, In-Beum Lee, Kun Soo Chang
Automation Research Center, Dept. of Chemical Engineering,
Pohang University of Science and Technology,
Pohang, Kyungbuk, KOREA

ABSTRACT: Optimal control theories based on the maximum principles have been evolved and applied to distributed parameter systems (DPSs) represented by partial differential equations (PDEs) and integral equations (IEs). This paper intends to show that an optimal control of a tubular reactor described by a one-dimensional partial differential equation was obtained using the distributed parameter control method for parabolic PDEs[1]. In developing an algorithm which implements the calculation, the method of lines (MOL) was adopted through using a package called the DSS/2[2]. For the tubular reactor system chosen for this paper, the optimal control method based on PDEs with the numerical MOL showed to be more efficient than the one based on IEs.

INTRODUCTION

Mathematical models for dynamic behavior of processes whose parameters are distributed in space and changing in time are belonged to DPSs. For about 30 years, optimal control studies for the DPSs have concentrated on developing more proper theories and searching for the applications.

Wang[1] studied a general optimal control theory based on both of parabolic PDEs and IEs including space-time domain, time domain and boundary. Wang et al.[3] presented the optimal control of nonlinear IEs and Chang and Lee[4] presented the optimal control of hyperbolic systems.

Based on the theory of [3], a tubular reactor model represented by a one-dimensional PDE had been studied as one of nonlinear distributed parameter optimal control problems[5].

In [5], the original PDE was changed into the corresponding IE by means of the Green's function method and the maximum principle for the type of IEs as derived in [1] and [3] was applied to obtain the optimal control.

In this research, the original nonlinear PDE was used without any change and the maximum principle as derived in [1] was applied to obtain the optimal control.

PROBLEM STATEMENT

One of the popular tubular reactor models with axial dispersion was chosen from the literature[5]. Since our object is to find that the optimal control theory works for nonlinear DPSs, only the mass balance was treated as the state equation and the temperature variable was chosen as the control variable.

The state equation is:

$$\frac{\partial C}{\partial t} = \frac{1}{Pe}\frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x} + Da\,(1 - C)\exp\left(\frac{T}{1 + \frac{T}{r}}\right) \qquad (1)$$

Initial Condition : $C(x, 0) = 0$ (2)

Boundary Conditions : at $x = 0$, $\frac{\partial C}{\partial x} = Pe\ C$ (3)

at $x = 1$, $\frac{\partial C}{\partial x} = 0$ (4)

The control variable T(x,t) is going to be chosen to minimize the cost function:

$$Cost = \frac{1}{2}\int_0^{t_f}\int_0^1 (T(x,t) - Td(x,t))^2\ dx\ dt \quad (5)$$

From the theory, the Hamiltonian function for this system is derived as:

$$H = -\frac{1}{2}\ (T(x,t) - Td(x,t))^2 +$$

$$R\ \{\frac{1}{Pe}\frac{\partial^2 C}{\partial x^2} - \frac{\partial C}{\partial x} + Da\ (1-C)\ exp(\frac{T}{1+\frac{T}{r}})\ \} \quad (6)$$

The costate equation is defined as:

$$R = \frac{1}{Pe}\frac{\partial^2 R}{\partial x^2} + \frac{\partial R}{\partial x} - R\ Da\ exp(\frac{T}{1+\frac{T}{r}}) \quad (7)$$

Boundary Conditions : at $x = 0$, $\frac{\partial R}{\partial x} = 0$ (8)

at $x = 1$, $\frac{\partial R}{\partial x} = -\ Pe\ R$ (9)

Final Condition : $R(x, t_f) = 0$ (10)

The derivative of the Hamiltonian becomes:

$$HT = \frac{\partial H}{\partial T}$$

$$= -\ (T - Td) + R\ Da\ (1 - C)\ \frac{1}{(1+\frac{T}{r})^2}\ exp(\frac{T}{1+\frac{T}{r}}) \quad (11)$$

The necessary condition for maximizing the Hamiltonian is

$$\frac{\partial H}{\partial T} = 0. \quad (12)$$

NUMERICAL METHOD

An algorithm to find optimal T(x,t) which satisfies (12) is as follows:

1. At k = 0, guess T(x,t) for $0 \le t \le t_f$ and $0 \le x \le 1$.
2. For $0 \le t \le t_f$:
   a) get C(x,t) by solving equations (1) - (4) numerically
   b) guess R(x,0)
   c) get R(x,t) by solving equations (7) - (9) numerically.
   d) Check if the calculated $R(x, t_f)$ satisfies the final condition (10):
      if $R(x, t_f) = 0$, go to 3;
      if $R(x, t_f) \neq 0$, $R^{new}(x,0) = .1 * R^{old}(x,0)$
      and go to c).
3. Get HT(x,t) from (11) with known C(x,t), R(x,t) and T(x,t).
   Calculate the Cost using the equation (5).
4. Check if the necessary condition (12) satisfies:
   if $HT = 0$ go to 5.
   if $HT \neq 0$, $T^{k+1}(x,t) = T^{*}(x,t) + eps * HT(x,t)$
   and go to 2.
5. Optimal T(x,t) is obtained. Print the results and stop.

For the step (2), we used Schiesser's DSS/2 package[2] which was developed using the MOL. It was found to be easy in implementing the system using the available numerical software.

RESULTS AND DISCUSSION

Figs 1 - 5 summarize the results visually. These results show that the optimal control theory, for the nonlinear parabolic PDEs is quite useful as well as the theory for the nonlinear IEs in the previous studies[1],[3],[5].

Fig. 1 shows that we could get the minimal cost in only one iteration with an appropriate iteration weighting (eps). The value of eps seems not to be greater than 1 because Fig. 2 shows that HT could be oscillatory with too much weightings. With a small eps, the convergence was slower than the large one as expected. In this study, without using various values of eps at each iteration or time and steps, an excellent convergence was possible. The appropriate value of eps may be dependent upon systems.

Figs 3 - 5 illustrate the dynamic behaviors of the state variable, the control variable and the costate variable, respectively . We could find the final value problem of the costate equation described with the equations (7) - (10) could be solved with reasonable guesses in the numerical step 2-b.

From this particular experience we could find that the optimal control solution for PDEs of DPSs is much easier to obtain than the one for IEs for some systems. Also using PDEs directly has some advantage over using IEs. First, it is not always easy to convert the PDEs to the IEs by means of the Green's method. Second, programming with PDEs is much simpler and easy to understand, especially if a differential equation simulator is available. Third, in general the IEs consume larger computing time due to the matrix inversion and the eigenvalues involved.

We found also that the MOL could be useful for the optimal control of DPSs, especially with a infinite boundary condition at the reactor outlet.

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NOMENCLATURE

C : conversion of reactant A

Da : Damkohler number

eps : weighting on HT in iteration

H : Hamiltonian

HT : derivative of the H, $\frac{\partial H}{\partial T}$

k : iteration counter

Pe : axial Peclet number

r : dimensionless activation energy

R : costate variable

t : dimensionless time variable

t_f : final time

T : temperature (control)

Td : desired temperature

x : dimensionless space variable

REFERENCES

[1] Wang, F.Y., *Optimal Control Theory for Distributed Parameter Processes Based on Integral Equation Representations*, Ph. D. Thesis, University of Waterloo, Waterloo, Ont., Canada (1985)

[2] Schiesser, W.E., *Micro-DSS/2: Differential Systems Simulator Version 2*, Lehigh University (1985)

[3] Wang, F.Y., I.B. Lee and K.S. Chang, "Necessary Conditions in the Optimal Control of Nonlinear Integral Equations," Proc. '89 KACC vol.2, pp947-951 (1989)

[4] Chang, K.S. and I.B. Lee, "Necessary Optimality Conditions in the Small for Degenerate Hyperbolic Distributed Parameter Control Systems," Proc.'90 KACC vol.2, pp1043-1048 (1990)

[5] Choe, Y.S., I.B. Lee and K.S. Chang, "Optimal Control of Tubular Reactors Described by Partial Differential Equations," Proc. '92 KACC vol.2, pp436-439 (1992)

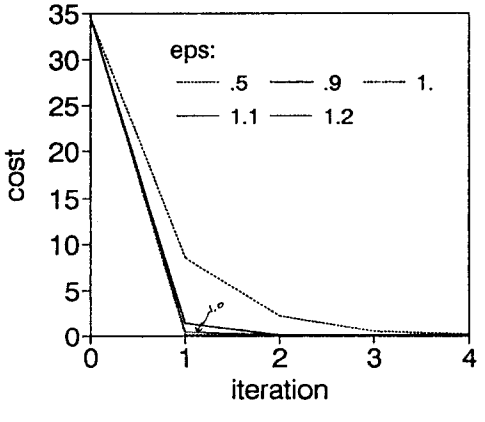

Fig. 1 Cost reductions to the iterations with different weightings (eps)

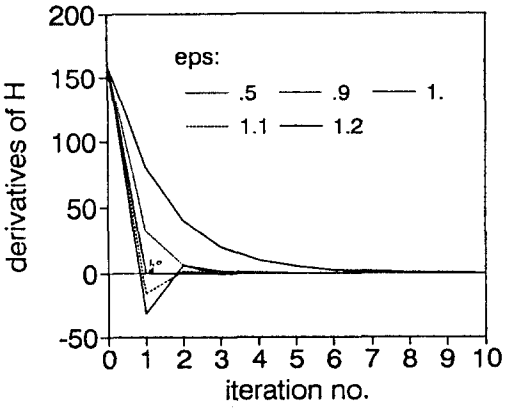

Fig. 2 Behaviors of the derivatives of the Hamiltonian to the iterations with different weightings (eps)

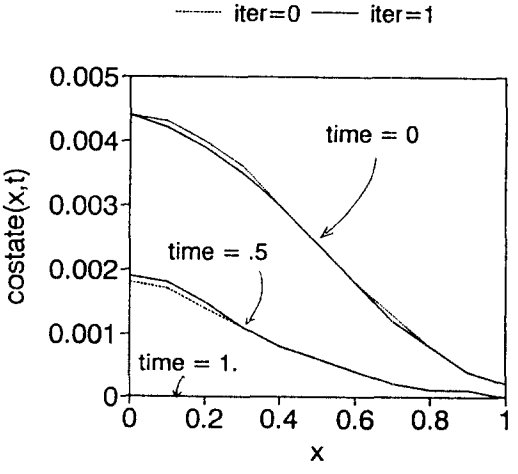

Fig. 5 Costate profiles

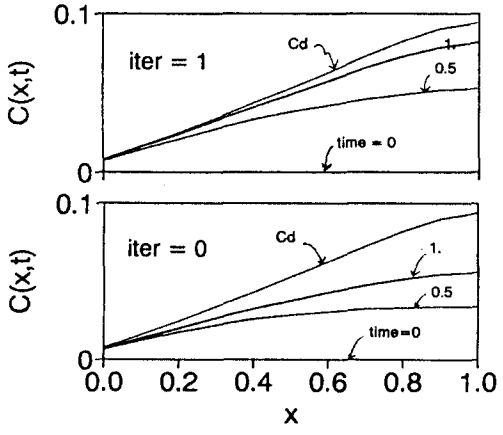

Fig. 3 Concentration profiles

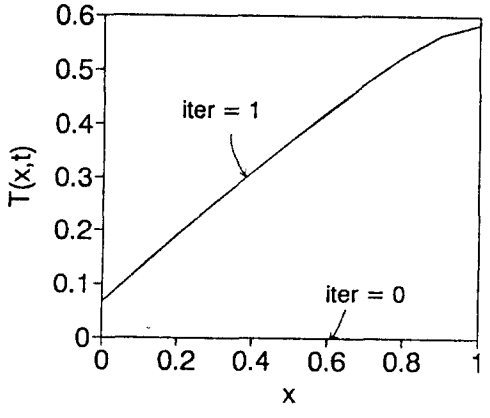

Fig. 4 Temperature profiles