Optimal Design and Control in a Class of Distributed Parameter Systems under Uncertainty—Application to Tubular Reactor with Catalyst Deactivation

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Unpredictable variations in the values of plant parameters around their nominal values are often encountered in actual operation of process plants. In order to assure that process performance meets specifications, it is preferable to design and control the process, taking into account the uncertainty in the values of the plant parameters. In this paper, a method to minimize the maximum decrease in the process performance caused by the hypothetical worst parameter variations is proposed. Necessary condition for the worst parameter variations is derived for a class of distributed parameter systems by means of the maximum principle, and then the method for obtaining the optimal design and control subject to the worst parameter variations are discussed. The method is applied to the design of a tubular reactor associated with catalyst activity decay. The reactor obtained is fairly insensitive to the variations in the process parameters while maintaining fairly good performance even at the nominal values of parameters.

The mathematical models which appear in optimal design and control problems are usually built on the basis of certain nominal values of plant parameters and/or system inputs. It is well known, however, that the actual behavior of a real system rarely agrees with that of the mathematical model because of unknown disturbances and/or the errors associated with the estimation of the parameters involved in the mathematical models. The discrepancy of the actual behavior from the predicted one often causes the undesirable performance of the system.

Recent development of the optimization theory has made it possible to study the optimal design and control problem subject to the system uncertainties. These studies may be classified into three cases according to the degree of the uncertainties of the variations in the plant parameters; 1. the statistical properties of the parameter variations are known, 2. the nominal value and the upper and lower bounds of plant parameter variations are known, and 3. only the nominal values of plant parameter are known. Works by Kittrell and Watson (*1*), Rudd and Watson (*2*), and Takamatsu and his co-workers (*3*) are intended to deal with Case 1. Those for Case 2 are works by Takamatsu and his co-workers (*3*), Rohrer and Sobral (*4*) and Tazaki (*5*). Takamatsu and his co-workers discussed the optimal design problem from the viewpoint of sensitivity analysis in which the expected values of the parameters and the region of the parameter variations are given. Rohrer and Sobral proposed a design method based on the relative sensitivity which is the minimum of the maximum deviation from optimal behavior attained by manipulating the control variable. Tazaki (*5*) introduced the performance sensitivity which is defined as the maximum decrease in the value of the objective function caused by hypothetical worst parameter variations and then proposed a design method to minimize the maximum value of the performance sensitivity by adjusting the design variable. We shall call the possible worst performance variation caused by the hypothetical worst parameter variation "the nominal performance sensitivity"; and the minimized value of the nominal performance sensitivity attained by adjusting the design and control variables "the min-max performance sensitivity." Though both Rohrer and Sobral's method and Tazaki's method employ the min-max performance sensitivity, the former method is intended to compensate the parameter variations by the control variables and not to consider the degree of freedom for design variables while the latter takes into account both the design and control variables. For Case 3 several papers based on the classical sensitivity theory have been published (*6* to *9*). Since methods described in these papers are derived on the basis of sufficiently small variations around the nominal value of plant parameter, they may not always be applied to other classes of parameter variations.

The purpose of this paper is to derive the necessary condition for the nominal performance sensitivity with a class of distributed parameter systems and to develop a method for obtaining the design and control variables which are to give the min-max performance sensitivity. The necessary condition is described in the form of the maximum principle. In order to show how this approach is significant from practical point of view, the method developed is applied to the design and control of a tubular reactor subject to catalyst deactivation.

STATEMENT OF PROBLEM

The system considered here is defined by the following set of simultaneous partial differential equations:

$$\frac{\partial x(t,z)}{\partial z} = f(x(t,z), y(t,z), u^a(t,z), p^a(t,z), d^a(t,z)), \quad 0 \leq t \leq T, \quad 0 \leq z \leq \underline{Z} \quad (1)$$

$$\frac{\partial y(t,z)}{\partial t} = h(x(t,z), y(t,z), u^a(t,z), p^a(t,z), d^a(t,z)), \quad 0 \leq t \leq T, \quad 0 \leq z \leq \underline{Z} \quad (2)$$

where x, y, u^a, p^a, and d^a which are functions of time and space are vectors

$$x(t,z) = (x_1(t,z), x_2(t,z), \ldots, x_n(t,z))^T$$

$$y(t,z) = (y_1(t,z), y_2(t,z), \ldots, y_m(t,z))^T$$

$$u^a(t,z) = (u_1{}^a(t,z), u_2{}^a(t,z), \ldots, u_r{}^a(t,z))^T$$

$$p^a(t,z) = (p_1{}^a(t,z), p_2{}^a(t,z), \ldots, p_s{}^a(t,z))^T$$

$$d^a(t,z) = (d_1{}^a(t,z), d_2{}^a(t,z), \ldots, d_v{}^a(t,z))^T$$

The boundary conditions are

$$x(t,0) = \Phi(x^b(t), u^b(t), p^b(t)) \quad (3)$$

$$y(0,z) = \Psi(y^b(z), d^b(z)) \quad (4)$$

Note that the additional controls, parameters, and design variables may be introduced at the boundary, and hence the dimensions of $u^b(t)$, $p^b(t)$, and $d^b(z)$ may not be the same as those of distributed functions, u^a, p^a, and d^a. For the sake of brevity of expression, use of the following notation

$$u = (u^{a^T}, u^{b^T})^T$$

$$p = (p^{a^T}, p^{b^T})^T$$

$$d = (d^{a^T}, d^{b^T})^T$$

will be convenient.

The following functional J is defined as a performance criterion

$$J(x, y, u, p_N, d_N) = \int_0^T G(x(t, Z), t)dt \quad (5)$$

where p_N and d_N represent the appropriate nominal values of p and d respectively. Equation (5) is fairly general and other type performance functions may be written as the same form as Equation (5) by introducing proper additional state variables.

Several constraints must be imposed on the system in order to apply the maximum principle to the distributed parameter system. The functions f and h are assumed to be twice continuously differentiable with respect to its arguments and to satisfy the Lipshitz conditions. Controls u, parameters p, and design vectors d, are piecewise continuous and bounded functions within the convex regions U, P, and D, respectively. The control, parameter, and design vectors which satisfy these conditions are called admissible ones. The states of the system x and y are uniquely determined under their boundary conditions when control, parameter, and design vectors are given. G is the twice continuously differentiable function with respect to its arguments.

On the basis of the above definition of system, we shall consider the following problem. Find the admissible controls which maximize the performance function Equation (5) subject to the constraints of Equations (1) to (4).

With this problem we shall define the following performance sensitivity:

$$S_N \triangleq \underset{p \in P}{\text{Max}} \{J(x, y, \hat{u}, p_N, d_N) - J(x, y, \hat{u}, p, d_N)\} \quad (6)$$

where $\hat{u}$ is the solution of the problem

$$\underset{u \in U}{\text{Max}} \; J(x, y, u, p_N, d_N) \quad (7)$$

and, hence, the optimal control function obtained under the nominal values of parameters. We shall call the performance sensitivity "nominal performance sensitivity." As is seen in the definition, the nominal performance sensitivity represents the maximum decrease in the value of the performance function caused by the hypothetical worst parameter variations.

It should be noted here that the nominal performance sensitivity is a non-negative quantity. Since the first term of the right-hand side of Equation (6) is not the function of p, Equation (6) can be rewritten as

$$S_N = J(x, y, \hat{u}, p_N, d_N) - \underset{p \in P}{\text{Min}} \; J(x, y, \hat{u}, p, d_N).$$

Provided that the nominal value of the parameter is admissible one, it is obvious that

$$J(x, y, \hat{u}, p_N, d_N) \geq \underset{p \in P}{\text{Min}} \; J(x, y, \hat{u}, p, d_N)$$

from which the non-negativity of the nominal performance sensitivity follows.

NECESSARY CONDITIONS FOR THE NOMINAL PERFORMANCE SENSITIVITY

As easily seen, Equation (6) can be rewritten as the following two problems:

Problem 1. $$S_1 \triangleq \underset{u \in U}{\text{Max}} \; J(x, y, u, p_N, d_N) \quad (8)$$

Problem 2. $$S_2 \triangleq \underset{p \in P}{\text{Min}} \; J(x, y, \hat{u}, p, d_N) \quad (9)$$

Necessary Condition for the Solution to Problem 1

The necessary condition for the optimal control to Problem 1, $\hat{u}$, can be obtained by means of the maximum principle for a class of distributed parameter systems (*10* to *12*). The system equations and boundary conditions of this problem are given in the form of Equations (1) to (4) where $p = p_N$ and $d = d_N$. We shall define the following scalar function:

$$H = \langle \lambda, f \rangle + \langle \mu, h \rangle \quad (10)$$

where λ and μ are adjoint vectors defined by

$$\left.\begin{aligned}\frac{\partial\lambda(t,z)}{\partial z} &= -\frac{\partial H}{\partial x}\\ \frac{\partial\mu(t,z)}{\partial t} &= -\frac{\partial H}{\partial y}\end{aligned}\right\} \tag{11}$$

with the boundary conditions

$$\left.\begin{aligned}\lambda(t,\underline{Z}) &= \frac{\partial G}{\partial x(t,\underline{Z})}\\ \mu(T,z) &= 0\end{aligned}\right\} \tag{12}$$

Then, the necessary condition for the optimal control $\hat{u}$ is that the control is to satisfy the following maximum conditions

$$H^b[\lambda(t,0),\hat{u}^b(t)]\ (=)\ \max_{u^b\epsilon U^b} H^b[\lambda(t,0),u^b] \tag{13}$$

$$H[x,y,\lambda,\mu,\hat{u}^a(t,z)]\ (=)\ \max_{u^a\epsilon U^a} H[x,y,\lambda,\mu,u^a] \tag{14}$$

or

$$\int_0^Z H[x,y,\lambda,\mu,\hat{u}^a(t,z)]\,dz$$

$$(=)\ \max_{u^a\epsilon U^a}\int_0^Z H[x,y,\lambda,\mu,u^a]\,dz \tag{15}$$

where x, y, λ and μ are the solution of the boundary-value problem defined by Equations (1) to (4) and (11) and (12), corresponding to the admissible control u. The symbol $(=)$ indicates equality "almost everywhere" and H^b a scalar function at the boundary defined by

$$H^b = <\lambda(t,0),u^b> \tag{16}$$

Equation (15) represents the maximum condition with respect to the control u^a which is a function only of time t (10).

Necessary Condition for the Solution to Problem 2

The form of the system equation and their boundary conditions of Problem 2 is equivalent to those of Problem 1, except that control u is replaced by $\hat{u}$ and that the boundary conditions on the adjoint equations are specified as

$$\left.\begin{aligned}\lambda(t,\underline{Z}) &= -\frac{\partial G}{\partial x(t,\underline{Z})}\\ \mu(T,z) &= 0\end{aligned}\right\} \tag{17}$$

The necessary condition for the worst variation of the parameter $\hat{p}$ is that it satisfies the following maximum conditions

$$H^b[\lambda(t,0),\hat{p}^b(t)]\ (=)\ \max_{p^b\epsilon P^b} H^b[\lambda(t,0),p^b] \tag{18}$$

$$H[x,y,\lambda,\mu,\hat{p}^a(t,z)]\ (=)\ \max_{p^a\epsilon P^a} H[x,y,\lambda,\mu,p^a] \tag{19}$$

or

$$\int_0^Z H[x,y,\lambda,\mu,\hat{p}^a(t,z)]\,dz$$

$$(=)\ \max_{p^a\epsilon P^a}\int_0^Z H[x,y,\lambda,\mu,p^a]\,dz \tag{20}$$

where the scalar function at the boundary is

$$H^b = <\lambda(t,0),p^b> \tag{21}$$

MIN-MAX PERFORMANCE SENSITIVITY

It will be of particular significance in the design of system to achieve the minimum value of the nominal performance sensitivity or the min-max performance sensitivity. Though it may seem to be rather conservative, the system design based on the min-max performance sensitivity assures the system which never be worse in its actual performance than that expected.

The min-max performance sensitivity is defined by

$$\hat{S} \triangleq \min_{d\epsilon D}\max_{p\epsilon P}\{J(x,y,\hat{u},p_N,d) - J(x,y,\hat{u},p,d)\} \tag{22}$$

Equation (22) can be rewritten as

$$\hat{S} \triangleq \min_{d\epsilon D}\{J(x,y,\hat{u},p_N,d) - \min_{p\epsilon P} J(x,y,\hat{u},p,d)\} \tag{23}$$

$$= \min_{d\epsilon D}\{J(x,y,\hat{u},p_N,d) - J(x,y,\hat{u},\hat{p},d)\} \tag{24}$$

In Equation (24), $\hat{u}$ and $\hat{p}$ are to be obtained as the solutions of Problem 1 and Problem 2, respectively, corresponding to an appropriate given design function d. The constraint equations for this problem consist of both the constraint equations for Problem 1 and those of Problem 2, where u and p are substituted by $\hat{u}$ and $\hat{p}$, respectively. The number of the system equations are $2(n+m)$. The performance function is described as

$$J_M = J(x^1,y^1,\hat{u},p_N,d) - J(x^2,y^2,\hat{u},\hat{p},d)$$

$$= \int_0^T [G^1(x^1(t,\underline{Z}),t^1) - G^2(x^2(t,\underline{Z}),t^2)]\,dt \tag{25}$$

where the superscripts 1 and 2 stand for the functions and variables determined as the solution to Problems 1 and 2, respectively.

By means of the maximum principle of a distributed parameter system, the optimal policy is to satisfy the maximum conditions

$$H^b[\mu(0,z),\hat{d}^b(z)]\ (=)\ \max_{d^b\epsilon D^b} H^b[\mu(0,z),d^b] \tag{26}$$

$$\int_0^T H[x,y,\lambda,\mu,\hat{d}^a(t,z)]\,dt$$

$$(=)\ \max_{d^a\epsilon D^a}\int_0^T H[x,y,\lambda,\mu,d^a]\,dt \tag{27}$$

where the scalar functions H and H^b are defined as

$$H[x,y,\lambda,\mu,d^a] = H^1[x^1,y^1,\lambda^1,\mu^1,d^a]$$

$$+ H^2[x^2,y^2,\lambda^2,\mu^2,d^a] = \sum_{i=1}^{2}\{<\lambda^i,f^i> + <\mu^i,h^i>\} \tag{28}$$

$$H^b[\mu(0,z),d^b(z)] = <\mu^1(0,z),d^b(z)>$$

$$+ <\mu^2(0, z), d^b(z)> \quad (29)$$

The adjoint system is given by

$$\left.\begin{aligned} \frac{\partial \lambda^1(t,z)}{\partial z} &= -\frac{\partial H^1}{\partial x^1} \\ \frac{\partial \lambda^2(t,z)}{\partial z} &= -\frac{\partial H^2}{\partial x^2} \\ \frac{\partial \mu^1(t,z)}{\partial t} &= -\frac{\partial H^1}{\partial y^1} \\ \frac{\partial \mu^2(t,z)}{\partial t} &= -\frac{\partial H^2}{\partial y^2} \end{aligned}\right\} \quad (30)$$

$$\left.\begin{aligned} \lambda^1(t,\underline{Z}) &= -\frac{\partial G^1}{\partial x^1(t,\underline{Z})} \\ \lambda^2(t,\underline{Z}) &= \frac{\partial G^2}{\partial x^2(t,\underline{Z})} \\ \mu^1(T,z) &= \mu^2(T,z) = 0 \end{aligned}\right\} \quad (31)$$

This problem is a two-point boundary-value problem formulated by the above $2(n+m)$ system equations, associated by the adjoint Equations (30) and (31) and the maximum conditions (26) and (27). The solution to the problem will be very difficult to find if we note the high dimensionality and nonlinearity of chemical processing systems. The following gradient method in function space may be effectively used for solving this difficulty.

Step 1. Assume the initial value of $d_{(k)}$, $k = 0$, where the subscript (k) stands for the kth iteration.

Step 2. Solve Problem 1 with the value of $d_N = d_{(k)}$ and find the corresponding optimal control $\hat{u}_{(k)}$.

Step 3. Solve Problem 2 with the value of $d_N = d_{(k)}$ and $u = \hat{u}_{(k)}$ and find the worst parameter $\hat{p}_{(k)}$ which maximize the performance sensitivity.

Step 4. Using $u = \hat{u}_{(k)}$, $p = \hat{p}_{(k)}$ and $d = d_{(k)}$, integrate the $2(n+m)$-dimensional system equations forward (from $t = 0$ to $t = T$) and integrate the adjoint Equations (30) and (31) backward (from $t = T$ to $t = 0$). Then modify the design function for the $(k+1)$th iteration by

$$d^a_{(k+1)} = d^a_{(k)} + \epsilon_{(k)} \int_0^T \left(\frac{\partial H}{\partial d^a}\right)_{(k)} dt \quad (32)$$

and

$$d^b_{(k+1)} = d^b_{(k)} + \epsilon_{(k)} \left(\frac{\partial H^b}{\partial d^b}\right)_{(k)} \quad (33)$$

where ϵ is the positive step size factor.

Step 5. Return to Step 2. Repeat the procedure until the minimum of the performance sensitivity is achieved.

Steps 2 and 3 of the above procedures may be carried out by appropriate hill climbing methods, such as the gradient method (*13*) and the conjugate gradient method (*14*).

EXAMPLE: THE DESIGN AND CONTROL OF A TUBULAR REACTOR WITH CATALYST DEACTIVATION

Several papers (*11*, *15* to *18*) have been recently published on the optimal design and control of a tubular reactor with catalyst deactivation. In these papers, the optimal design and control policies have been discussed based on the nominal values of reaction process parameters. We shall discuss here the problem in view of the min-max performance sensitivity. Great care is necessary in design and control of tubular reactors with an exothermic reaction in order to prevent formation of the so-called hot spot. Since the presence of the hot spot in the reactor may cause considerable formation of undesired products as well as a damage to the catalyst activity, formation of the hot spot will be a good measure of the well designed tubular reactor.

The reaction considered is the first-order consecutive one $A \xrightarrow{K_1} B \xrightarrow{K_2} C$ with heat generation and catalyst deactivation. The initial catalyst profile is chosen as the design variable. The control function is the shell-side coolant temperature, which is to be manipulated over a period of catalyst life time $0 \leq t \leq T$ in order to maximize the time-average yield of product B. While other types of the objective function, such as cost or profit of reactor operation, may be adopted, the time-average yield of product B is chosen here as an objective function. The inlet reactant temperature perturbation is regarded here as the uncertain plant parameter variation, since the formation of the hot spot is said to be highly dependent of the inlet reactant temperature (*20*). The rate of catalyst deactivation is considered rather slow compared to the average residence time of the reactor and, therefore, the quasi-steady state of the catalyst activity at any given time $0 \leq t \leq T$ is assumed.

Behavior of the process can be described under this assumption by a set of the equations

$$\left.\begin{aligned} \frac{\partial x_1}{\partial z} &= -K_1 x_1 y_1 \\ \frac{\partial x_2}{\partial z} &= (K_1 x_1 - K_2 x_2) y_1 \\ \frac{\partial x_3}{\partial z} &= (b_1 K_1 x_1 + b_2 K_2 x_2) y_1 + \frac{1}{\alpha}(u^a(t) - x_3) \end{aligned}\right\} \quad (34)$$

The catalyst activity change is assumed to be described by the equation (*19*)

$$\frac{\partial y_1}{\partial t} = -K_c y_1^2 \quad (35)$$

The boundary conditions are

$$\left.\begin{aligned} x_1(t,0) &= x_{10} \\ x_2(t,0) &= x_{20} \\ x_3(t,0) &= x_{30} + p^b(t) \end{aligned}\right\} \quad (36)$$

$$y_1(0,z) = d^b(z) \quad (37)$$

The performance function of the process which is to be maximized is

$$J(u^a, p^b, d^b) = \int_0^T x_2(t,\underline{Z})\, dt \quad (38)$$

The constraints imposed on the parameter and design function are

$$P^L \leq p^b(t) \leq P^U, \quad \text{for all } t \in [0, T] \quad (39)$$

$$0 \leq d^b(z) \leq 1, \quad \text{for all } z \in [0, Z] \quad (40)$$

No constraint is imposed on the domain of the control variable. The following values are used throughout this example:

$$K_1 = 0.535 \times 10^{11} \exp(-18{,}000/Rx_3),$$

$$K_2 = 0.461 \times 10^{18} \exp(-30{,}000/Rx_3),$$

$$K_c = 0.672 \times 10^{18} \exp(-28{,}000/Rx_3), \quad R = 2.0,$$

$$b_1 = 120, \quad b_2 = -50, \quad \alpha = 3.0, \quad x_{10} = 0.95,$$

$$x_{20} = 0.05, \quad x_{30} = 335°\text{K}, \quad \underline{Z} = 10, \quad T = 1.0$$

of which the values of K_1 and K_2 are taken from Bilous and Amundson (*21*).

The problem here is to find the initial catalyst activity profile (the design function) and the shell-side coolant temperature (the control function) which maximize the time-average yield of product B under the constraints Equations (34) to (37) subject to the unknown variation in the inlet reactant temperature.

The scalar function defined by Equation (10) is

$$H = [-K_1x_1y_1]\lambda_1 + [(K_1x_1 - K_2x_2)y_1]\lambda_2 + [(b_1K_1x_1 + b_2K_2x_2)y_1 + \frac{1}{\alpha}(u^a(t) - x_3)]\lambda_3 + [-K_cy_1^2]\mu_1 \quad (41)$$

The associated adjoint equation defined by Equation (11) is

$$\left.\begin{aligned}
\frac{\partial\lambda_1}{\partial z} &= K_1y_1\lambda_1 - K_1y_1\lambda_2 - b_1K_1y_1\lambda_3 \\
\frac{\partial\lambda_2}{\partial z} &= K_2y_1\lambda_2 - b_2K_2y_1\lambda_3 \\
\frac{\partial\lambda_3}{\partial z} &= \frac{E_1}{Rx_3^2}K_1x_1y_1\lambda_1 \\
&\quad - \frac{1}{Rx_3^2}(E_1K_1x_1y_1 - E_2K_2x_2y_1)\lambda_2 \\
&\quad - \frac{1}{Rx_3^2}(b_1E_1K_1x_1y_1 + b_2E_2K_2x_2y_1)\lambda_3 \\
&\quad + \frac{\lambda_3}{\alpha} + \frac{E_c}{Rx_3^2}K_cy_1^2\mu_1 \\
\frac{\partial\mu_1}{\partial t} &= K_1x_1\lambda_1 - (K_1x_1 - K_2x_2)\lambda_2 \\
&\quad - (b_1K_1x_1 + b_2K_2x_2)\lambda_3 + 2K_cy_1\mu_1
\end{aligned}\right\} \quad (42)$$

The gradient method of optimization is used for obtaining the optimal control and the worst parameter variation. The control and the parameter are modified in the gradient method through the following iteration formulae:

$$u^a(t)_{(k+1)} = u^a(t)_{(k)} + \epsilon_{(k)}\int_0^{\underline{Z}}\left(\frac{\lambda_3}{\alpha}\right)_{(k)}dz, \quad \text{for all } t\epsilon[0, T] \quad (43)$$

$$p^b(t)_{(k+1)} = p^b(t)_{(k)} + \epsilon_{(k)}\lambda_3(t, 0)_{(k)}, \quad \text{for all } t\epsilon[0, T] \quad (44)$$

In order to examine the performance of the reactor designed on the basis of the nominal value of the parameter (the inlet reactant temperature) the optimal design, the optimal control, and the corresponding reactor performance are computed. We shall call the reactor nominally optimal reactor. The optimal initial profile of catalyst activity is found to be uniform, that is,

$$y_1(0, z) = d^b(z) = 1.0 \quad \text{for all } z\epsilon[0, \underline{Z}] \quad (45)$$

The boundary values of the adjoint vectors for obtaining the optimal control and the worst parameter variations are given by, respectively,

$$\left.\begin{aligned}
\lambda_1(t, \underline{Z}) &= 0 \\
\lambda_2(t, \underline{Z}) &= 1 \\
\lambda_3(t, \underline{Z}) &= 0 \\
\mu_1(T, z) &= 0
\end{aligned}\right\} \quad (46)$$

and

$$\left.\begin{aligned}
\lambda_1(t, \underline{Z}) &= 0 \\
\lambda_2(t, \underline{Z}) &= -1 \\
\lambda_3(t, \underline{Z}) &= 0 \\
\mu_1(T, z) &= 0
\end{aligned}\right\} \quad (47)$$

Computed results are shown in Figures 1 to 6. Figures 1 and 2 indicate the time variations in the optimal temperature and concentration profiles and the resulting catalyst activity profile, respectively, at the nominal value of the parameter or the inlet stream temperature, 335°K.

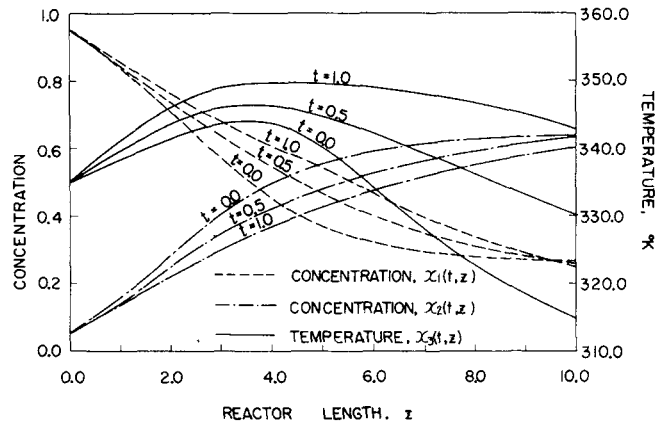

Fig. 1. Time variations of the optimal temperature and concentration profiles in the nominally optimal reactor with nominal parameter value.

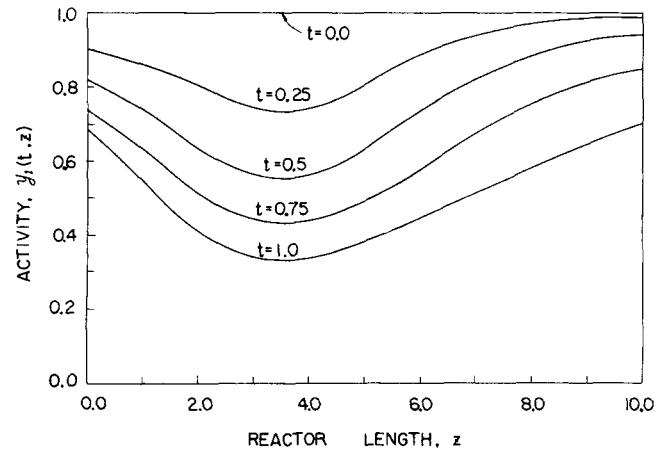

Fig. 2. Time variations of the catalyst activity profiles in the nominally optimal reactor with nominal parameter value.

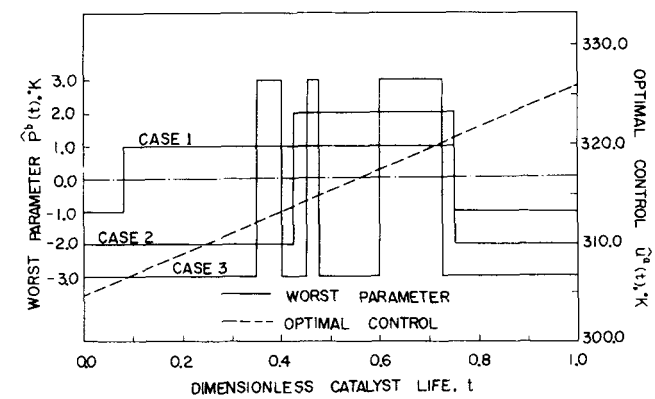

Fig. 3. Optimal control $\hat{u}^a(t)$ and the worst parameter $\hat{p}^b(t)$ for the nominally optimal reactor.

Although the catalyst deactivation with time proceeds fairly rapidly, rise in the optimal temperature profile, particularly in the tail part of the reactor, compensates for the effects of the catalyst deactivation, and the yield of product B can be maintained fairly well at the output of the reactor. No hot spot is observed along the entire length of the reactor. With these observations, the reactor is judged to be operated fairly well at the nominal value of the inlet stream temperature. This may not be the case,

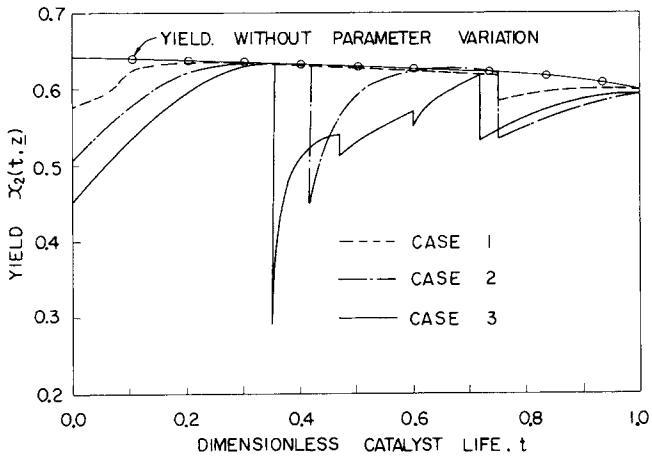

Fig. 4. Yields of product B of the nominally optimal reactor with nominal parameter value and with the worst parameter variations.

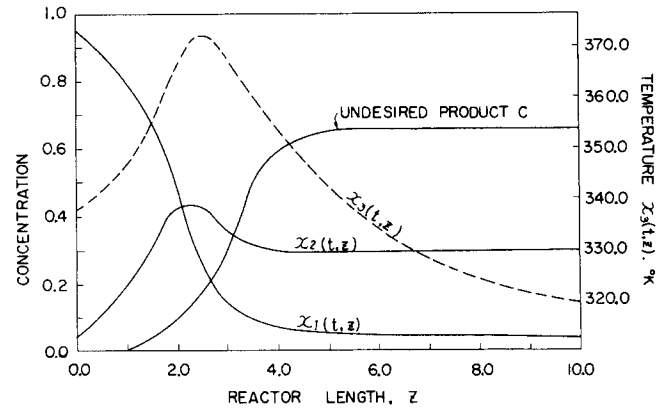

Fig. 5. Temperature and concentration profiles in the nominally optimal reactor with the worst parameter variation: $t = 0.35$, $p^L = -3$, $p^U = 3$.

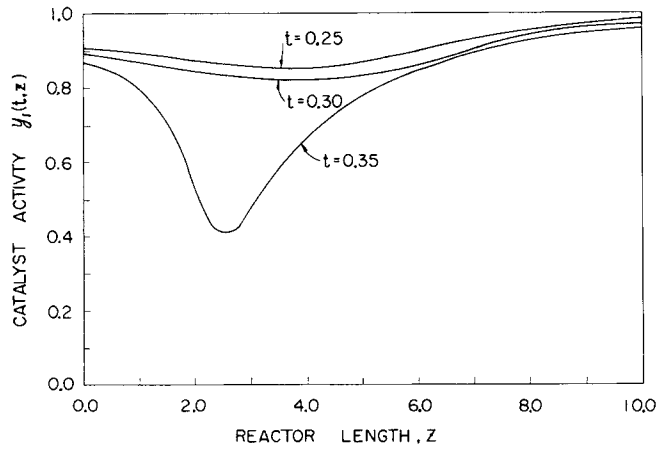

Fig. 6. Catalyst activity profiles in the min-max reactor with the worst parameter variation: $P^L = -3$, $P^U = 3$.

Table 1. Nominal Performance Sensitivities

Case	S_N ($= J(\hat{u}^a, p_N{}^b, d_N{}^b) - J(\hat{u}^a, \hat{p}^b, d_N{}^b)$)	
1	0.0107 = 0.6273	−0.6166
2	0.0355 = 0.6273	−0.5918
3	0.0703 = 0.6273	−0.5570

however, when the worst variation in the inlet stream temperature is introduced. Three admissible regions of the inlet stream temperature are considered in this example: Case 1; $P^U = 1$, $P^L = -1$, Case 2; $P^U = 2$, $P^L = -2$ and Case 3; $P^U = 3$, $P^L = -3$. The computed worst variation of the inlet stream temperature for these three regions and the corresponding optimal control are illustrated in Figure 3. The worst variations in the inlet stream temperature show so-called "bang-bang" characteristic during the period of operation. The nominal performance sensitivities and the behaviors of the yield of product B during the reactor operation are summarized in Table 1 and Figure 4, respectively. Considerable decrease in the reactor performance is observed, in Table 1, when the worst variation is introduced. As expected, the decrease in the yield of product B increases with the increase of the allowable range of the parameter variation. Moreover, very sharp decrease is observed in the instantaneous yield of product B as shown in Figure 4 which is interpreted as a formation of hot spot. Actually as shown in Figure 5 the considerable sharp rise in reaction temperature is observed along the reactor length. This results severe damage to the catalyst activity as indicated in Figure 6. The hot spot may cause not only temporary damage to the catalyst activity but also permanent damage to the catalyst structure itself.

As a whole, the nominally optimal reactor is judged to be poorly designed and operated when possible variation in the inlet stream temperature is taken into account.

We shall, therefore, try to avoid this poor performance of the reactor by adjusting the initial catalyst activity profile in the sense of the min-max performance sensitivity. We shall call the reactor designed in view of the min-max performance sensitivity min-max reactor. When the initial cumulative catalyst activity $D_t = \int_0^{\underline{Z}} d^b(z)\, dz$ is not imposed as a constraint, there exists a trivial solution $d^b(z) = 0$ for all $z \epsilon [0, \underline{Z}]$ as expected from the system equations and their boundary conditions. Since this solution is meaningless for the objective of the process, the following equality constraint should be imposed:

$$\int_0^{\underline{Z}} d^b(z)\, dz - D_t = 0 \tag{48}$$

The adjoint equations and their boundary conditions for the optimal design problem are formulated according to Equations (28) to (31), although its details are not described here. The algorithm which is used to obtain the optimal catalyst activity profile is based on the following iterative modification of the nominal catalyst activity profile:

$$d^b(z)_{(k+1)} = d^b(z)_{(k)} + \epsilon_{(k)} \left[\left(\mu_1{}^1(0,z) + \mu_1{}^2(0,z) \right)_{(k)} + \eta \right], \quad \text{for all } z \epsilon [0, \underline{Z}] \tag{49}$$

where η is the Lagrange multiplier for equality (48). The initial cumulative catalyst activity $D_t = 8.5$ is chosen and

the admissible region of the parameter variation is that of Case 3.

Computed results for the optimal initial catalyst activity profile are shown in Figures 7 to 10. The optimal design of catalyst activity profile shows "bang-bang" characteristic along the reactor length, as shown in Figure 7. The time variations in the optimal temperature and concentration profiles at the nominal value of the inlet stream temperature are shown in Figure 8. When compared with the case of the uniform initial catalyst activity profile, the optimal profile shifts the main reaction zone to downstream at all time of operation. The computed worst variation of the inlet stream temperature and the corresponding optimal control are shown in Figure 9. The parameter variation reaches to its upper bound only at the final period of reactor operation. As is seen in Figure 10, the substantially smaller variation than that in the uniform initial catalyst activity case is observed in the instantaneous yield of product B during the reactor operation. Moreover, the formation of hot spot is considerably reduced.

The min-max performance sensitivity of the reactor is computed as

$$\hat{S} = J(\hat{u}^a, p_N{}^b, \hat{d}^b) - J(\hat{u}^a, \hat{p}^b, \hat{d}^b)$$

$$= 0.6018 - 0.5913 = 0.0105 \quad (50)$$

This is considerably smaller than the nominal performance sensitivity $S_N = J(\hat{u}^a, p_N{}^b, d_N{}^b) - J(\hat{u}^a, \hat{p}^b, d_N{}^b) = 0.0703$ of the nominally optimal reactor.

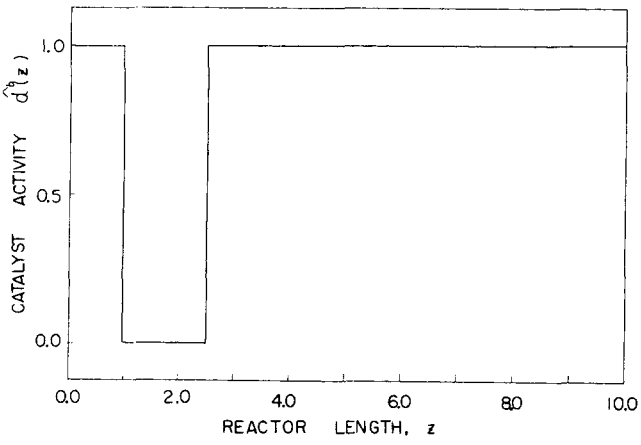

Fig. 7. Optimal design function $\hat{d}^b(z)$ for the min-max reactor.

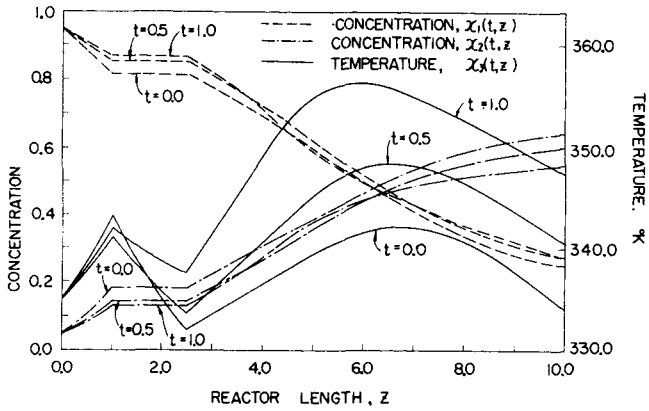

Fig. 8. Time variations of the optimal temperature and concentration profiles in the min-max reactor with nominal parameter value.

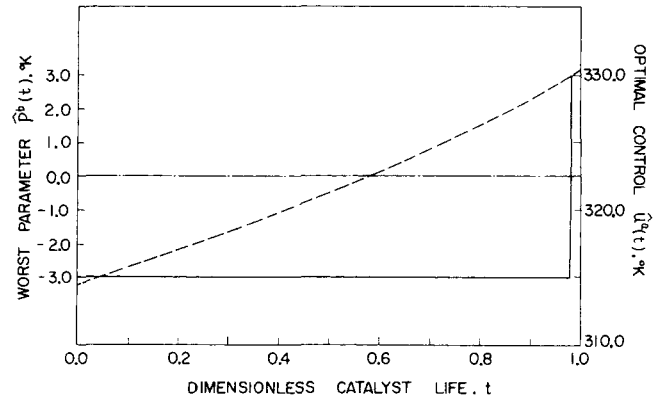

Fig. 9. Optimal control $\hat{u}^a(t)$ and the worst parameter $\hat{p}^b(t)$ for the min-max reactor.

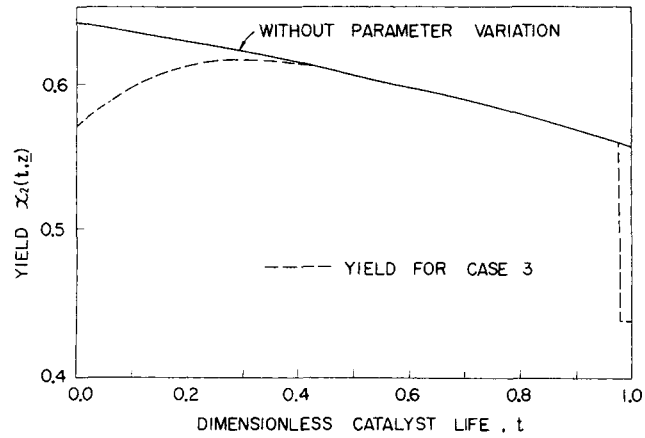

Fig. 10. Yields of product B in the min-max reactor with nominal parameter value and with the worst parameter variation.

It should be noted here that, although in principle the design based on the min-max performance sensitivity is considered quite conservative, the actual loss in the reactor performance is not at all substantial in this example. This is seen in the values of the performance function; $J(\hat{u}^a, p_N{}^b, d_N{}^b) = 0.6273$, $J(\hat{u}^a, \hat{p}^b, d_N{}^b) = 0.5570$, $J(\hat{u}^a, p_N{}^b, \hat{d}^b) = 0.6018$ and $J(\hat{u}^a, \hat{p}^b, \hat{d}^b) = 0.5913$. With the nominal value of the parameter, the min-max reactor shows only 4.0% or $J(\hat{u}^a, p_N{}^b, d_N{}^b) - J(\hat{u}^a, p_N{}^b, \hat{d}^b) = 0.0255$ decrease in the value of the performance function. Moreover, the min-max reactor gives the value of performance function of $J(\hat{u}^a, \hat{p}^b, \hat{d}^b) = 0.5913$ for the worst parameter variation which is smaller by only 5.7% than that ($J(\hat{u}^a, p_N{}^b, d_N{}^b) = 0.6273$) of the nominally optimal reactor with the nominal parameter value.

We can summarize the computed results by saying that the min-max reactor gives much better performance than the nominally optimal reactor for the worst parameter variation while keeping fairly good performance with the nominal parameter value.

CONCLUSION

The proposed method of design and control for a process subject to the unknown parameter variations, which is to minimize the maximum decrease in the values of the ob-

jective function due to the hypothetical worst parameter variations, provides an effective mean to assure the process to meet specifications imposed on the process performance. Although it seems to be a very conservative design and control method, fairly good performance of the process even with the nominal values of the parameters is observed in an illustrative example.

The minimum of the maximum (min-max) performance sensitivity will provide a good measure for the reasonable design margin of a process subject to the uncertainty in its parameter values. Application to the marginal design problem to meet specifications will be a future extension of the min-max performance sensitivity.

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NOTATION

A = chemical component
B = chemical component
$b_1, b_2 = (-\Delta H_1)/C_p \cdot \rho, (-\Delta H_2)/C_p \cdot \rho$
C = chemical component
C_p = specific heat
D, D^a, D^b = admissible sets of design functions d, d^a, d^b
D_t = initial cumulative catalyst activity defined by

$$\int_0^{\underline{Z}} d^b(z)\, dz$$

d, d^a, d^b = design functions
E_1, E_2 = activation energies for main reaction
E_c = activation energy for catalyst deactivation
f = vector-valued function
G = integrand of functional J
h = vector-valued function
H, H^b = scalar functions
$\Delta H_1, \Delta H_2$ = heat of reactions
J, J_M = performance functions
K_1, K_2 = rate constants for main reaction,

$$K_{i0} \exp\left(-\frac{E_i}{Rx_3}\right), \quad i = 1, 2$$

K_c = rate constant for catalyst deactivation,

$$K_{c0} \exp\left(-\frac{E_c}{Rx_3}\right)$$

K_{10}, K_{20}, K_{c0} = pre-exponential factors
m = dimension of state function $y(t, z)$
n = dimension of state function $x(t, z)$
P, P^a, P^b = admissible sets of parameter functions p, p^a, p^b
p, p^a, p^b = parameter functions
P^U, P^L = upper and lower bounds of parameter function
R = gas constant
r = dimension of distributed control function $u^a(t, z)$
S_N = nominal performance sensitivity defined by Equation (6)
$\hat{S}$ = min-max performance sensitivity defined by Equation (22)
s = dimension of distributed parameter function $p^a(t, z)$
T = final time
t = time variable
U, U^a, U^b = admissible sets of control functions u, u^a, u^b
u, u^a, u^b = control functions
v = dimension of distributed design function $d^a(t, z)$
x = state function
x_{10}, x_{20}, x_{30} = constants defined by Equation (36)
y = state function
$\underline{Z}$ = length
z = distance variable

Greek Letters

α = heat exchange parameter
ϵ = step size factor
η = Lagrange Multiplier
λ, μ = adjoint functions
ρ = density
Φ = function of boundary condition defined by Equation (3)
Ψ = function of boundary condition defined by Equation (4)

Superscripts

a = distributed
b = boundary
$\wedge$ = optimal or worst

Subscripts

(k) = kth iteration
N = nominal

Symbols

$<, >$ = inner product of two vectors
$( )^T$ = transpose
$\triangleq$ = stands for equal by definition

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