ON THE CONTROL OF COCURRENT TUBULAR CHEMICAL REACTORS

by

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1. Introduction

In this paper we shall consider the optimal control of a chemical reactor which consists of two concentric tubes, the inner of which contains the reactants and the space between contains the coolant. The directions of flow of the reactants and coolent will be assumed here to be parallel (the co-current model) since the rate of reaction has its maximum value at the inlet of the reactor, and so the maximum rate of heat transfer should also occur at the inlet. The controls can then be either the flow-rates of the reactant and coolant or inlet concentration and temperature.

The dynamical model of the non-adiabatic tubular reactor in the form of a set of partial differential equations is obtained by making the use of mass and energy balance and is based on the following assumptions:

(1) Heat loss to the surroundings is negligible

(2) The heat conduction takes place radially and not along the axis of the reactor.

(3) The system states (i.e. temperature, reactant concentration etc) are dependent only on the axial coordinate and are uniform throughout the cross-section of the reactor. Also, the flows are sufficiently turbulent to cause effective heat transfer.

(4) Specific heats, heat transfer coefficients, densities and rate of reaction are constant with respect to temperature and concentration variations.

(5) The metal shell is sufficiently thin and its thermal capacity is negligible so that all the heat loss from the reaction is gained by the coolant.

The equations describing a chemical reactor are well-known [1,2] and can be written in the form

$$\frac{\partial X}{\partial \tau} = -\frac{F_1}{A_1}\frac{\partial X}{\partial Z} + k(1-X) \qquad \text{(mass balance)}$$

$$\left.\begin{aligned} \frac{\partial T_1}{\partial \tau} &= -\frac{F_1}{A_1}\frac{\partial T_1}{\partial Z} - \frac{Q}{A_1 H_{c1}} + \frac{\Delta H \rho_1}{H_{c1}} k(1-X) \\ \frac{\partial T_2}{\partial \tau} &= -\frac{F_2}{A_2}\frac{\partial T_2}{\partial Z} + \frac{Q}{A_2 H_{c2}} \end{aligned}\right\} \text{(energy balance)}$$

where

X = mole fraction of product

T_1 = absolute temperature of the reactant

T_2 = absolute temperature of the coolant

F_1 = feed flow rate of reactant

F_2 = feed flow rate of coolant

k = reaction velocity per unit mole fraction of reagent

A_1, A_2 = effective cross-sectional areas of the reactant and coolant respectively

ΔH = energy per mole of produce replaced by reaction

H_{c1} = thermal capacity per unit volume of the reactant

H_{c2} = thermal capacity per unit volume of the coolant

ρ_1 = molar density of reactant

ρ_2 = molar density of coolant

and

$$k = k(t_1) = k_o e^{-b/T_1}, \quad b = E/R$$

$$Q = \frac{R_1 R_2 \pi d (F_1 F_2)^{0.8}}{R_1 F_1^{0.8} + R_2 F_2^{0.8}}$$

where E = activition energy

R = gas constant

k_o = reaction rate constant

R_1 = heat transfer coefficient from reactant to coolant

R_2 = heat transfer coefficient from coolant to reactant

To simplify the analysis, we shall assume that $F_{1s}/A_1 = F_{2s}/A_2$, and, in fact, we shall normalize F_{1s}/A_1 to 1, where the subscript s refers to the steady state. (This assumption can be removed at the expense of more notational complexity).

Putting $T_1 = \frac{\Delta H \rho_1}{H_{c1}} \theta_1$, $T_2 = \frac{\Delta H \rho_1}{H_{c1}} \theta_2$, where $H_{c1} = c_1 \rho_1$, $H_{c2} = c_2 \rho_2$, we have

$$\frac{\partial X}{\partial t} = -\frac{F_1}{A_1} \frac{\partial X}{\partial Z} + k(1-X)$$

$$\frac{\partial \theta_1}{\partial t} = -\frac{F_1}{A_1} \frac{\partial \theta_1}{\partial Z} - \frac{Q(\theta_1-\theta_2)}{A_1 H_{c1}} + k(1-X)$$

$$\frac{\partial \theta_2}{\partial t} = -\frac{F_2}{A_2} \frac{\partial \theta_2}{\partial Z} + \frac{Q(\theta_1-\theta_2)}{A_2 H_{c2}} .$$

Using elementary linearization techniques, we arrive at the equations

$$\frac{\partial x}{\partial t} = -\frac{1}{A_1} \left(\frac{\partial X}{\partial Z}\Big|_s\right) f_1 - \frac{F_{1s}}{A_1} \frac{\partial x}{\partial z} + (1-X_s)\left(\frac{\partial k}{\partial \theta_1}\right)\phi_1 - k_s x$$

$$\frac{\partial \phi_1}{\partial t} = -\frac{1}{A_1}\left(\frac{\partial \theta_1}{\partial Z}\Big|_s\right) f_1 - \frac{F_{1s}}{A_1} \frac{\partial \phi_1}{\partial Z} - \frac{Q_s}{A_1 H_{c1}} \phi_1 + \frac{Q_s}{A_1 H_{c1}} \phi_2$$

$$-\left(\frac{\partial Q}{\partial F_1}\right) \frac{(\theta_{1s}-\theta_{2s})}{A_1 H_{c1}} f_1 - \left(\frac{\partial Q}{\partial F_2}\right) \frac{(\theta_{1s}-\theta_{2s})}{A_1 H_{c1}} f_2$$

$$+ (1 - X_s) \left(\frac{\partial k}{\partial \theta_1}\right) \phi_1 - k_s x$$

$$\frac{\partial \phi_2}{\partial t} = -\frac{1}{A_2}\left(\frac{\partial \theta_2}{\partial Z}\bigg|_s\right) f_2 - \frac{F_{2s}}{A_2}\frac{\partial \phi_2}{\partial Z} + \left(\frac{\partial Q}{\partial F_1}\right)\frac{(\theta_{1s}-\theta_{2s})}{A_2 H_{c2}} f_1$$

$$+ \left(\frac{\partial Q}{\partial F_2}\right)\frac{(\theta_{1s}-\theta_{2s})}{A_2 H_{c2}} f_2 + \frac{Q_s}{A_2 H_{c2}}\phi_1 - \frac{Q_s}{A_2 H_{c2}}\phi_2 ,$$

where we have again denoted steady-state values with a subscript s.

Hence,

$$\begin{pmatrix} \frac{\partial x}{\partial t} \\ \frac{\partial \phi_1}{\partial t} \\ \frac{\partial \phi_2}{\partial t} \end{pmatrix} = -\begin{pmatrix} \frac{\partial x}{\partial z} \\ \frac{\partial \phi_1}{\partial Z} \\ \frac{\partial \phi_2}{\partial Z} \end{pmatrix} + \begin{pmatrix} -k_s & (1-X_s)\left(\frac{\partial k}{\partial \theta_1}\right) & 0 \\ -k_s & (1-X_s)\left(\frac{\partial k}{\partial \theta_1}\right) - \frac{Q_s}{A_1 H_{c1}} & \frac{Q_s}{A_1 H_{c1}} \\ 0 & \frac{Q_s}{A_2 H_{c2}} & -\frac{Q_s}{A_2 H_{c2}} \end{pmatrix} \begin{pmatrix} x \\ \phi_1 \\ \phi_2 \end{pmatrix}$$

$$+ \begin{pmatrix} -\frac{1}{A_1}\left(\frac{\partial X}{\partial Z}\right)\Big|_s & 0 \\ \frac{-1}{A_1}\left(\frac{\partial \theta_1}{\partial Z}\Big|_s\right) - \left(\frac{\partial Q}{\partial F_1}\right)\left(\frac{\theta_{1s}-\theta_{2s}}{A_1 H_{c1}}\right) & -\left(\frac{\partial Q}{\partial F_2}\right)\left(\frac{\theta_{1s}-\theta_{2s}}{A_1 H_{c1}}\right) \\ \left(\frac{\partial Q}{\partial F_1}\right)\left(\frac{\theta_{1s}-\theta_{2s}}{A_2 H_{c1}}\right) & -\frac{1}{A_2}\left(\frac{\partial \theta_2}{\partial Z}\Big|_s\right) + \left(\frac{\partial Q}{\partial F_2}\right)\left(\frac{\theta_{1s}-\theta_{2s}}{A_2 H_{c2}}\right) \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}$$

where $F_a = F_{1s}/A_1 = F_{2s}/A_2 = 1$ (by assumption)

(Note that, in the above linearization, we have written

$$X = x + X_s,\ \theta_i = \phi_i + \theta_{is},\ F_i = f_i + F_{is},\ i = 1,2)$$

These equations are now in the standard control form

$$\dot{x} = Ax + Bu,$$

although the data x is now an element of a Banach space. This will be discussed further in the next section.

We first mention some existing literature on the control of chemical reactors. First, Fjeld and Ursin[3] investigated a plug-flow, empty tubular reactor with a low-order state-variable model approximation, by dividing the cooling jacket of the reactor into a finite number of sections and assuming that the heat transfer coefficient of each segment can be varied independently of one another. The flow rates were chosen as control variables. Oh and Schmitz[4] studied a plug-flow recycle reactor using a conventional PID controller to stabilize the reactor.

Georgakis, Aris and Ammundson[5,6,7] studied the control problem of an empty rubular reactor with uniform wall temperature. A state-variable model was derived by means of orthogonal collocation in space and a Luenberger observer was used to estimate the unavailable concentration measurements. Recently Boniun et al[8] have considered the dynamic behaviour of an autothermal tubular reactor with internal countercurrent heat exchanger. The system of partial differential equations governing the problem was again discretized by the method of orthogonal collocation.

In this paper we shall avoid the use of such discretizations by considering the reactor equations as ordinary differential equations in an infinite dimensional space. This will also obviate the difficulty encountered in frequency-domain methods when the coefficients of the spatial derivatives depend on the spatial coordinates.

2. Notation and Terminology

In this paper we shall consider the system dynamics to be defined by an ordinary differential equation

$$\frac{dx}{dt} = Ax + Bu \ , \ x(o) = x_o \qquad (2.1)$$

whose state x(t) belongs to a Banach space for each t. The operator B is bounded, but the operator A will be unbounded and so the operator exp(At) may not be defined by the usual series representation. Instead it is possible to define a semigroup T(t) of bounded operators which has similar properties to the exponential, namely

$$T(o) = I \text{ (identity operator)}$$

$$T(t_1+t_2) = T(t_1)T(t_2) \quad (t_1, t_2 \geq o)$$

$$\lim_{t \to o^+} T(t)x = x \text{ , for all } x \in X$$

and

$$Ax = \lim_{t \to o^+} \frac{1}{t}(T(t)-I)x, \quad x \in D(a) \text{ (the domain of A).}$$

T(t) is said to be generated by A and the solution of (2.1) is given by the variation of constants formula

$$x(t) = T(t)x_o + \int_o^t T(t-s)Bu(s)ds \text{ , } x_o \in D(A). \qquad (2.2)$$

Note that (2.2) is well-defined even when $x_o \in X \setminus D(A)$ and so any solution of (2.2) with $x_o \in X$ may be regarded as a generalized solution of (2.1) called a mild solution.

The state of our system will be represented by a triplet $\psi = (x, \phi_1, \phi_2)$ of functions each of which is an element of the Hilbert space $L^2(\Omega)$, where Ω is the spacial domain on which the system is defined. The space of all such ψ will be denoted by $L^2(\Omega; R^3)$ which has the inner product

$$< \psi_1, \psi_2 > = \int_\Omega \psi_1^T(z)\psi_2(z)dz \quad , \quad \psi_1, \psi_2 \quad L^2(\Omega;R^3)$$

It is clear from this definition of the inner product that $L^2(\Omega;R^3)$ is naturally isomorphic to $\bigoplus_{i=1}^{3} L^2(\Omega;R)$ (i.e. the direct sum of three identical copies of $L^2(\Omega;R)$ and so a basis of $L^2(\Omega;R^3)$ may be represented in the form

$$\begin{pmatrix} e_1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ e_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ e_1 \end{pmatrix}, \begin{pmatrix} e_2 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ e_2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ e_2 \end{pmatrix}, \ldots, \tag{2.3}$$

where $\{e_i\}_{i\geq 1}$ is a basis of $L^2(\Omega;R)$. The basis in (2.3) will be denoted in the sequel by $\{\bar{e}_i\}_{i\geq 1}$ for a fixed basis $\{e_i\}$.

Finally, if B is a bounded operator on $L^2(\Omega;R^3)$, then B^* will denote the adjoint operator of B defined by

$$\langle B^* h_1, h_2 \rangle = \langle h_1, B h_2 \rangle \quad , \quad h_1, h_2 \in L^2(\Omega;R^3).$$

For a more complete discussion of the above, see Yosida[9], Curtain, Pritchard[10].

3. The Linearized System

As we have seen, the linearized model of the reactor may be written in the form

$$\frac{\partial x}{\partial t} = -\frac{\partial x}{\partial z} + a_{11}x + a_{12}\phi_1 + b_{11}f_1$$

$$\frac{\partial \phi_1}{\partial t} = -\frac{\partial \phi_1}{\partial z} + a_{21}x + a_{22}\phi_1 + a_{23}\phi_2 + b_{21}f_1 + b_{22}f_2$$

$$\frac{\partial \phi_2}{\partial t} = -\frac{\partial \phi_2}{\partial z} + a_{32}\phi_1 + a_{33}\phi_2 + b_{31}f_1 + b_{32}f_2$$

where the coefficients are defined in the introduction. These equations may be expressed in the compact form

$$\frac{\partial \psi}{\partial t} = -\frac{\partial \psi}{\partial z} + A\psi + B u, \tag{3.1}$$

where $\psi = (x, \phi_1, \phi_2)^T$, $u = (f_1, f_2)^T$ and the A and B matrices (which depend on z) are, of course

$$A = (a_{ij})_{1\leq i,j\leq 3} \quad (a_{13} = a_{31} = 0)$$

$$B = (b_{ij})_{1\leq i\leq 3,\, 1\leq j\leq 2} \quad (b_{12} = 0)$$

We shall suppose that equation (3.1) is defined on the interval $\Omega = [0,L]$, in the spacial z-domain. On the boundary, ψ is given by some fixed value $\bar{\psi} \in R^3$, and so we introduce the operator P defined by

$$P\psi = -\frac{d\psi}{dz} \tag{3.2}$$

where P is defined on the subspace D(P) of $L^2(\Omega;R^3)$ given by

$D(P) = \{\psi \in L^2(\Omega;R^3) : d\psi/dz \in L^2(\Omega;R^3), \psi(o) = \bar{\psi}\}$. Of course, in (3.2), the derivative is defined in the generalized sense; also D(P) is (isomorphic to) $H_o'(\Omega;R^3)$. (Lions, Magenes[11], Adams[12]).

It is well known Yosida[9] that P generates a semigroup defined by

$$(T_t\psi)(z) = \psi(-t + z) \tag{3.3}$$

for any $\psi \in L^2(]-\infty,L];R^3)$. Now, regarding A as an operator on $L^2(]-\infty,L];R^3)$ it is clear that A is bounded and so the operator

$$\mathcal{A} = P + A$$

generates a semigroup S_t (see Kato[13]) given by the integral equation

$$S_t\psi_o = T_t\psi_o + \int_o^t T_{t-s} A S_t u_o ds.$$

The solution of this equation is given by the series

$$S_t\psi_o = \sum_{n=o}^{\infty} u_n(t) \tag{3.4}$$

where

$$u_o(t) = T_t\psi_o$$

$$u_n(t) = \int_o^t T_{t-s} A u_{n-1}(s) ds \quad , n \geq 1.$$

Writing u_n explicitly in terms of the spacial coordinate z, we have

$$u_n(t,z) = \int_o^t A(z-t+s)\, u_{n-1}(s,z-t+s)\,ds$$

By induction, it follows that

$$u_n(t,z) = \int_o^t \int_o^{s_1} \cdots \int_o^{s_{n-1}} A(z-t+s_1)\ldots A(z-t+s_n)\, u_o(s_n,z-t+s_n)\,ds_n\ldots ds_1$$

or

$$u_n(t,z) = \int_o^t \int_o^{s_1} \cdots \int_o^{s_{n-1}} \Big(\prod_{i=1}^{n} A(z-t+s_i)\Big)(T_{s_n}\psi_o)(z-t+s_n)\,ds_n\ldots ds_1$$

$$= \int_o^t \int_o^{s_1} \cdots \int_o^{s_{n-1}} \Big(\prod_{i=1}^{n} A(z-t+s_i)\,ds_n\ldots ds_1\Big)\,\psi_o(z-t).$$

Writing

$$\alpha(t,z) = 1 + \sum_{n=1}^{\infty} \int_o^t \int_o^{s_1} \cdots \int_o^{s_{n-1}} \Big(\prod_{i=1}^{n} A(z-t+s_i)\Big)\,ds_n\ldots ds_1,$$

it follows that

$$(S_t\,\psi_o)(z) = \alpha(t,z)\,\psi_o(z-t),$$

where we can regard S_t as being defined on $L^2(\Omega,R^3)$, by defining, for $\psi_o' \in L^2(\Omega;R^3)$

$$\psi_o(z) = \begin{cases} \psi_o'(z) & \text{if } z \geq o \\ \bar{\psi} & \text{if } z < o \end{cases}$$

We therefore have a well-defined solution of (3.1) given by

$$\psi(t,z) = (S_t\psi_o)(z) + \int_o^t (S_{t-s}B\,u)(z)\,ds, \text{for } \psi_o \in L^2(\Omega;R^3)$$

In the next section we shall define an appropriate quadratic cost functional for this problem and see that a Riccati equation for the optimal control may be derived.

4. The Optimal Control Problem

Having obtained the general solution to the linearized equation, the only remaining point is to define the cost functional for the control problem. Since a linearization has been made about the equilibrium solution for x, ϕ_1, it seems reasonable to choose the functional

$$J = \langle \psi(T) - \psi', M(\psi(T) - \psi') \rangle_{L^2(\Omega)}$$
$$+ \int_0^T \{ \langle \psi(t) - \psi', M(\psi(t) - \psi') \rangle_{L^2(\Omega)} + u^T R\, u \}\, dt ,$$

where M is the operator defined on $L^2(\Omega;R^3)$ by

$$M\psi = (x, \phi_1, o)^T$$

for $\psi = (x, \phi_1, \phi_2)^T \in L^2(\Omega;R^3)$, and R is a positive self-adjoint matrix in R^4.

We therefore have a tracking problem defined on $L^2(\Omega;R^3)$, the solution of which can be found in Curtain and Pritchard[10]. In fact, the optimal control is given by

$$u_\infty(t) = - R^{-1}B^* Q(t)\ \psi(t) - R^{-1}B^* s_\infty(t) ,$$

where

$$s_\infty(t) = - U^*(T,t)M\psi' - \int_t^T U^*(p,t)M\psi'\, dp$$

with Q(t) satisfying the inner product Riccati equation

$$\frac{d}{dt} \langle Q(t)h,k \rangle + \langle Q(t)h, Ak \rangle + \langle Ah, Q(t)k \rangle + \langle Mh,k \rangle$$
$$= \langle Q(t)BR^{-1}B^* Q(t)h,k \rangle \qquad (4.1)$$

on the interval $[0,T]$ with the final condition

$$Q(T) = M \tag{4.2}$$

and $U(t,s)$ satisfying the equation

$$U(t,s)h = S_{t-s}h - \int_s^t S_{t-\alpha} B R^{-1} B^* Q(\alpha) U(\alpha,s) h d\alpha \tag{4.3}$$

for any $h,k \in L^2(\Omega;R^3)$.

To solve the Riccati equation (4.1), introduce an orthonormal basis $\{\bar{e}_h\}_{h\geq 1} \subseteq D(A)$ of $L^2(\Omega;R^3)$ as in section 2. Then,

$$< \dot{Q}(t)\bar{e}_i, \bar{e}_j > + < Q(t)\bar{e}_i, \mathcal{A}\bar{e}_j > + < \mathcal{A}\bar{e}_i, Q(t)\bar{e}_j > + < M\bar{e}_i, \bar{e}_j >$$

$$= < Q(t) B R^{-1} B^* Q(t)\bar{e}_i, \bar{e}_j >$$

or,

$$\dot{q}_{ij} + \sum_{k=1}^{\infty} q_{ij} a_{jk} + \sum_{k=1}^{\infty} a_{ij} q_{jk} = \sum_{\ell=1}^{\infty} \sum_{k=1}^{\infty} q_{ik} \underline{b}_\ell^T R^{-1} \underline{b}_k q_{\ell j} - m_{ij} \tag{4.4}$$

where,

$$Q(t)\bar{e}_i = \sum_{j=1}^{\infty} q_{ij}(t)\bar{e}_j$$

$$\mathcal{A}\bar{e}_i = \sum_{j=1}^{\infty} a_{ij}\bar{e}_j$$

$$M\bar{e}_i = \sum_{j=1}^{\infty} m_{ij}\bar{e}_j$$

and

$$B^*\bar{e}_i = \underline{b}_i \in R^2$$

The final condition for equation (4.4) is $Q(T) = M$ or

$$q_{ij}(T) = m_{ij} \tag{4.5}$$

Equations (4.4) and (4.5) define an infinite dimensional nonlinear system of ordinary differential equations which are difficult to solve numerically. To alleviate this problem, replace the operator M by the operator $P_L M$, where P_L is the projection onto the subspace of $L^2(\Omega;R^3)$ generated by the basis elements $\bar{e}_1, \ldots, \bar{e}_L$. In terms of the cost functional, this means that we are requiring only the first L Fourier coefficients of the error $\psi(t) - \psi'$ to be minimized. Provided L is sufficiently large, this should be satisfactory.

The equation (4.4), which as a unique solution, can therefore be seen to reduce to the system

$$\left.\begin{aligned} \dot{q}_{ij} + \sum_{k=1}^{L} q_{ij}a_{jk} + \sum_{k=1}^{L} a_{ik}q_{jk} &= \sum_{\ell=1}^{L}\sum_{k=1}^{L} q_{ij}\underline{b}_\ell^T R^{-1}\underline{b}_k\, q_{\ell j} - m_{ij} \\ q_{ij}(T) &= m_{ij} \end{aligned}\right\} 1\leq i,j\leq L \qquad (4.6)$$

This equation can be solved numerically for Q, which can then be used in (4.3) to determine U(t,s). In fact, let

$$U(t,s)\bar{e}_i = \sum_{i=1}^{\infty} u_{ij}(t,s)\bar{e}_j \ ;$$

then, putting $h = \bar{e}_i$ in (4.3), we obtain

$$\sum_{j=1}^{\infty} u_{ij}(t,s)\bar{e}_j(z) = \alpha(t-s,z)\bar{e}_i(z-t+s) - \int_s^t S_{t-\beta}BR^{-1}B^*Q(\beta)\sum_{i=1}^{\infty} u_{ij}(\alpha,s)\bar{e}_j(z)\,d\beta$$

$$= \alpha(t-s,z)\bar{e}_i(z-t+s) - \int_s^t S_{t-\beta}\sum_{\ell=1}^{\infty}\sum_{j=1}^{L}\sum_{k=1}^{L} u_{ij}(\beta,s)q_{jk}(\beta)\underline{b}_\ell^T R^{-1}\underline{b}_k\bar{e}_\ell(z)\,d\beta$$

$$= \alpha(t-s,z)\bar{e}_i(z-t+s) - \int_s^t \alpha(t-\beta,z)\sum_{\ell=1}^{\infty}\sum_{j=1}^{L}\sum_{k=1}^{L} u_{ij}(\beta,s)q_{jk}(\beta)\underline{b}_\ell^T R^{-1}\underline{b}_k\bar{e}_\ell(z-t+\beta)\,d\beta$$

and so

$$u_{ij}(t,s) = E(i,j,t-s) - \sum_{m=1}^{L}\sum_{k=1}^{L}\int_s^t q_{mk}(\beta)\{\sum_{\ell=1}^{\infty}\underline{b}_\ell^T R^{-1}\underline{b}_k\, E(\ell,j,t-\beta)\}u_{ij}(\beta,s)\,d\beta \qquad (4.7)$$

where $E(i,j,t) = \langle \alpha(t,z)\bar{e}_i(z-t), \bar{e}_j(z) \rangle$. Let $\underline{u}_i(t,s)$ be the column vector consisting of $u_{ij}(t,s)$ for $1 \leq j \leq L$. Then (4.7) is clearly an integral equation for $\underline{u}_i(t,s)$ (for each $i \geq 1$) which can be solved by standard methods. Then, S_∞ is given by

$$s_\infty(t) = - \sum_{i=1}^{\infty} \sum_{j=1}^{L} u_{ij} \bar{e}_i \langle \psi', \bar{e}_j \rangle - \int_t^T \sum_{i=1}^{\infty} \sum_{j=1}^{L} u_{ij}(p,t) \bar{e}_i \langle \psi', \bar{e}_j \rangle dp$$

$$= - \sum_{i=1}^{\infty} \sum_{j=1}^{L} \{u_{ij}(T,t) + \int_t^T u_{ij}(p,t)dp\} \bar{e}_i \langle \psi', \bar{e}_j \rangle$$

and the optimal control is

$$u_\infty(t) = - \sum_{j=1}^{L} \sum_{i=1}^{L} \langle \psi(t), \bar{e}_i \rangle q_{ij}(t) R^{-1} \underline{b}_j$$

$$- \sum_{i=1}^{\infty} \sum_{j=1}^{L} \{u_{ij}(T,t) + \int_t^T u_{ij}(p,t)dp\} R^{-1} \underline{b}_i \langle \psi', \bar{e}_j \rangle \quad . \qquad (4.8)$$

It is therefore seen that the only on-line computation which has to be done is the evaluation of the Fourier coefficients of the state $\psi(t)$ and the summations involved in the expression for $u_\infty(t)$. Of course, this assumes that a measure of the state $\psi(t)$ throughout the reactor is available. If $\psi(t)$ cannot be measured everywhere then the application of an optimal filter to give an estimte $\psi^*(t)$ must be considered. ψ^* would then be used in the expression (4.8) instead of the (unknown) true state $\psi(t)$. The evaluation of ψ^* will be considered in a future paper.

5. Conclusions

A theoretical study of the optimal control of a chemical reactor has been considered from the viewpoint of distributed parameter theory. It has been shown that the optimal control may be derived from an infinite-dimensional Riccati equation without the need to take Laplace transforms in t and z, which has been applied in previous studies of

this problem. The latter approach, of course, is only applicable when the coefficients in the differential equation are independent of the spacial variable z. In the general situation, however, this is not the case and approximations must be made to apply the transform integral. The infinite-dimensional approach does not require such approximations and thus is more general than the transformation theory.

The cost functional chosen in this paper is the mean squared error of the actual and equilibrium states. Since the dynamic equations are obtained as a linearization of the true nonlinear dynamics about the equilibrium states, this would seem to be a good functional to choose, since large excursions from the equilibrium state would mean that the linearized equations are no longer valid.

As stated earlier, the problem of optimal estimates of the actual states and the implementation of the control will be considered in a future paper.

6. References

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