THE CONTROL OF ABSORPTION

CROSS-SECTION FOR A NUCLEAR ROCKET

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Abstract

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The two energy and one delayed neutron group kinetics equations with approximations are employed for the nuclear rocket in this paper. The perturbation equations for kinetics are derived with the assumption that the deviation from the reference flux are small in comparison with the reference values. The temperature effect due to the change of the Fermi Age may be compensated by a feedback loop. The absorption cross-section is changed accordingly so that the system will be made independent of the effect of temperature variation.

The spatial distribution of the flux and precursor are assumed to be sinusoidal in the axial direction of the nuclear rocket. In order to obtain the maximum power in minimum time with the restriction that the reactivity or the absorption cross-section will not exceed a certain bound the first optimization requires the reference flux and precursor exponentially in time to the maximum power and remaining constant thereafter. A jump of flux occurs while the reactivity suddenly changes its value. A second optimization procedure is thus required

to round off the jump and to minimize the error for the future independent of the past disturbance or arbituary starting error.

The reduced kinetics equations are obtained from the perturbed equation by introducing exponential weighting function. The index of performance is choosen to be the integral of the square errors on perturbed neutron flux and the control effort. Maximum principle is used to derive the control laws which in turn determines the absorption cross-section, using the measured flux as feedback with a variable gain. The response of the flux and precursor having optimum control under different starting conditions are determined and plotted.

(1) Introduction

Nuclear rocket (1),(2) requires a fast start-up with relatively high reactivity. The power level may increase six decades in one minute. Lump parameter model of controlling such a system is given by previous papers (3),(4),(5) of one of the author without linear approximation. In this paper a distributed parameter model of the nuclear rocket is considered. The actual control of the reactor is due to the change of the absorption cross-section by varying the poison from the control drum in a nuclear rocket.

(2) Kinetics Equations for the Reactor in Distributed Parameters

The two energy and one delayed neutron group reactor Kinetics equations are: (6)

$$\nabla D_{\mathbf{1}} \nabla \Phi_{\mathbf{1}} - \Sigma_{\mathbf{S}} \Phi_{\mathbf{1}} + \nu (1-\beta) \Sigma_{\mathbf{f}} \Phi_{\mathbf{2}} + \lambda C = \frac{1}{V_{\mathbf{1}}} \frac{\partial \Phi_{\mathbf{1}}}{\partial t} , \qquad (1)$$

$$\nabla D_{2} \nabla \Phi_{2} - \Sigma_{a} \Phi_{2} + \Sigma_{s} \Phi_{1} = \frac{1}{V_{2}} \frac{\partial \Phi_{2}}{\partial t} , \qquad (2)$$

$$\beta \nu \Sigma_{f} \Phi_{2} - \lambda C = \frac{\partial C}{\partial t}, \tag{3}$$

where ϕ_1 , ϕ_2 = fast and thermal neutron flux, respectively,

 D_1 , D_2 = fast and thermal diffusion coefficient, respectively,

 $\Sigma_{\rm S} \ell$, $\Sigma_{\rm a}$ = removal and absorption cross-section, respectively, spatial and time dependent.

 $\Sigma_{\mathbf{f}}$ = fission cross-section, a constant

 λ = equivalent decay constant for the one delayed group case,

C = equivalent concentration of precursor for the

one delayed group case,

 β = fraction of total number of fission neutrons which are delayed

 ν = average number of fast neutrons released per fission.

In the reactor with a relatively large fuel loading density, the thermal leakage term, $\nabla D_2 \nabla \Phi_2$, is small compared to the thermal absorption rate. Also, due to the high velocity of fast neutrons the term for the rate of change of fast neutrons, i.e. $(\frac{1}{V_1}, \frac{\partial \Phi_1}{\partial t})$, can be neglected. With these approximations, Equations (1) and (2) can be written as:

$$\nabla D_{\mathbf{1}} \nabla \Phi_{\mathbf{1}} - \Sigma_{\mathbf{S}} \Phi_{\mathbf{1}} + \nu (1-\beta) \Sigma_{\mathbf{f}} \Phi_{\mathbf{2}} + \lambda C = 0, \tag{4}$$

$$\phi_1 = \frac{\Sigma_a}{\Sigma_{sl}} \phi_2 \left(1 + \frac{l \circ}{T}\right), \tag{5a}$$

where ℓ_o = infinite medium mean life time of neutron = $\frac{1}{V_2 \Sigma_a}$, where T = reactor period = $\frac{n}{\frac{dn}{dt}} = \frac{\phi_2}{\frac{d\phi_2}{dt}}$.

Since $\frac{\boldsymbol{\ell} \circ}{T} < \boldsymbol{\zeta}$ 1, Equation (5a) can be approximated as

$$\phi_1 = \frac{\Sigma_a}{\Sigma_s \ell} \phi_2 \tag{5b}$$

with the relation $\tau=\frac{D_1}{\Sigma_{\rm s}\ell}$ and neglecting $\frac{1}{2}\ln\tau$ in comparison with the term $\ln(\tau\Sigma_a\phi_2)$, Equations (4) and (5b) will give

$$\nabla^{2}(\tau \Sigma_{a} \Phi_{2}) - \Sigma_{a} \Phi_{2} + \nu(1-\beta) \Sigma_{f} \Phi_{2} + \lambda C = 0.$$
 (6)

Rewrite equation (3)

$$\nu_{\beta \Sigma_{f}} \Phi_{2} - \lambda C = \frac{\partial C}{\partial t}, \tag{7}$$

Where Equation (7) is repeated here for convenience as equations (6) and (7) form the new set of kinetics equations.

The Fermi age τ becomes

$$\tau = \tau_{R} + \tau_{m}, \qquad \tau_{R} \rangle \rangle \tau_{m} \tag{8}$$

where

 $\tau_{\rm R}$ = Fermi age at reference temperature for graphite-uranium with hydrogen as coolant.

 $\tau_{\rm T}$ = increase of Fermi age from reference temperature to a given temperature.

(3) Perturbation of Kinetics Equations

During start-up of a nuclear reactor, some disturbances or errors may introduce to cause the actual variable (flux) away from the reference (desired) variable (flux). For a nuclear rocket, it can be assumed that most of the distrubances will occur along the axial direction of the reactor. The neutron flux, for a reactor with reflector, is almost constant in the transverse direction. The actual variables can be expressed by the sum of the reference variables and their deviations. If those deviations resulted from these unexpected disturbances and errors are small in comparison with the reference values, the cross product terms of the deviations may be neglected.

Thus,

$$\begin{aligned} & \phi_{2}(z,t) \longrightarrow \phi_{R}(z,t) + \Delta \phi(z,t), & \Delta \phi(z,t) < \langle \phi_{R}(z,t), \\ & C(z,t) \longrightarrow C_{R}(z,t) + \Delta C(z,t), & \Delta C(z,t) < \langle C_{R}(z,t), \\ & \tau(z,t) \longrightarrow \tau_{R}(z,t) + \tau_{T}(z,t), & \tau_{T}(z,t) < \langle \tau_{R}, \\ & \Sigma_{a}(z,t) \longrightarrow \Sigma_{R}(z,t) + \Delta \Sigma_{a}(z,t), & \Delta \Sigma_{a}(z,t) < \langle \Sigma_{R}(z,t), \\ \end{aligned} \tag{9}$$

where the subscripts R refers to the reference variables.

Substituting above quantities into Equations (6) and (7) and neglecting the higher order terms, the perturbed reactor kinetics equations are:

$$\frac{\partial^{2}}{\partial z^{2}} \left[\tau_{R} \Sigma_{R} \Phi_{R} \left(\frac{\tau_{T}}{\tau_{R}} + \frac{\Delta \Sigma_{a}}{\Sigma_{R}} + \frac{\Delta \Phi}{\Phi_{R}} \right) \right] - \Sigma_{aR} \Phi_{R} \left(\frac{\Delta \Sigma_{a}}{\Sigma_{R}} + \frac{\Delta \Phi}{\Phi_{R}} \right) + \nu (1-\beta) \Sigma_{f} \Delta \Phi - \lambda \Delta C = 0,$$
(10)

$$\nu \Sigma_{f} \Delta \Phi - \lambda \Delta C = \frac{\partial}{\partial t} (\Delta C).$$
 (11)

(4) <u>Feedback Loop for Compensating Reactivity Feedback Due</u> To Temperature Effect

In the Kinetics equations the term most effected by temperature (including density) is the age, τ_T . If a feedback loop is introduced such that the change of age due to temperature, τ_T can be compensated by varying the absorption cross-section, the perturbed kinetics equations derived from Equations (10) and (11) will be independent of temperature. Thus, a much more simpler mathematics form can be obtained. This idea can be achieved by letting

$$\Delta\Sigma_{\mathbf{a}}(z,t) = \Delta\Sigma_{\mathbf{1}}(z,t) + \Delta\Sigma_{\mathbf{2}}(z,t)$$
 (12)

and

$$\frac{\partial^{2}}{\partial z^{2}} \left[\tau_{R}^{\Sigma} \Sigma_{R}^{\Phi} \left(\frac{\tau_{T}}{\tau_{R}} + \frac{\Delta \Sigma_{2}}{\Sigma_{R}} \right) \right] - \Sigma_{R}^{\Phi} \Sigma_{R}^{\Xi} = 0.$$
 (13)

Then, the perturbed kinetics equation (10) becomes

$$\frac{\partial^{2}}{\partial z^{2}} \left[\tau_{R}^{\Sigma} \Sigma_{R}^{\Phi}_{R} \left(\frac{\Delta \Sigma_{1}}{\Sigma_{R}} + \frac{\Delta \Phi}{\Phi_{R}} \right) \right] - \Sigma_{R}^{\Phi}_{R} \left(\frac{\Delta \Sigma_{1}}{\Sigma_{R}} + \frac{\Delta \Phi}{\Phi_{R}} \right) + \nu (1-\beta) \Sigma_{f}^{\Delta \Phi} + \lambda \Delta C = 0.$$

$$(14)$$

The feedback control can be obtained by solving Equation (13). The solution may be given in the form

$$\Delta\Sigma_{2}(z,t) = \frac{1}{\tau_{R}^{\Phi}_{R}(z,t)} \int_{0}^{\ell} G(z,\xi) \frac{\partial^{2}}{\partial \xi^{2}} \left[\Sigma_{R}^{\tau}\tau_{T}^{\Phi}_{R}(\xi,t)\right] d\xi, \qquad (15)$$

where $G(z,\xi)$ is the Green's function of the problem.

(5) The Reference Variables - First Optimization

Since the flux distribution in a reactor is essentially sinusoidal axially, it is reasonable to assume the reference variables as

$$\Phi_{R} = \Phi(t) \sin \frac{\pi}{\ell} z,$$

$$C_{R} = C(t) \sin \frac{\pi}{\ell} z$$
.

Substituting the above equations into Equations (6) and (7), one obtains

$$\Phi(t) = \frac{\lambda}{\Sigma_{R} \tau_{R}(\frac{\pi}{\ell})^{2} + \Sigma_{R} - \nu(1-\beta) \Sigma_{f}} C(t)$$

and

$$\frac{d}{dt} [ln C(t)] = \gamma(t), \qquad (16)$$

where

$$\gamma(t) = \frac{\lambda^{\nu \beta \Sigma}_{f}}{\Sigma_{R} \tau_{R} (\frac{\pi}{\ell})^{2} + \Sigma_{R} - \nu (1-\beta) \Sigma_{f}} - \lambda, \quad 0 \leq \gamma(t) \leq \gamma.$$

The reference absorption cross-section, Σ_R , is assumed independent of z for the reference solutions in Equations (6) and (7). The power program or Φ in nuclear rocket requires that the Φ starts at a low level Φ^a_o and reaches a high level in a minimum time. It is well known from the optimum theory that for a bounded control the optimum process requires the control variable $\gamma(t)$ operating at its extreme value, γ or zero, i.e. bang-bang type control system. Thus the following reference variable is obtained for this purpose.

$$\Phi_{R}(z,t) = \Phi_{o}^{a}e^{\gamma t} \sin \frac{\pi}{\ell} z$$

$$C_{R}(z,t) = C_{o}^{a}e^{\gamma t} \sin \frac{\pi}{\ell} z$$

$$\Phi_{R}(z,t) = \Phi_{o}^{b}e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z$$

$$C_{R}(z,t) = C_{o}^{b}e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z$$

$$C_{R}(z,t) = C_{o}^{b}e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z$$

$$T_{1} \leq t \leq T_{2}$$

where ϕ 's, C 's, γ and T_1 are constants. The reference absorption cross-section, Σ_R , is, therefore, found to be a constant at each time interval,

$$\Phi_{O}^{a} = \frac{\gamma + \lambda}{\nu_{\beta} \Sigma_{f}} C_{O}^{a}$$

$$\Sigma_{R}^{a} = \frac{\nu_{\Sigma}_{f}}{1 + \tau_{R}(\frac{\pi}{\ell})^{2}} (1 - \frac{\gamma_{\beta}}{\gamma + \lambda})$$

$$\Phi_{O}^{b} = \frac{\lambda}{\nu_{\beta} \Sigma_{f}} C_{O}^{b}$$

$$\Sigma_{R}^{b} = \frac{\nu_{\Sigma}_{f}}{1 + \tau_{R}(\frac{\pi}{\ell})^{2}}$$

$$T_{1} \langle t \langle T_{2} \rangle$$

where $C_0^a=C_0^b$ since C_R is continuous at t = T₁. It is noted that a jump of reference flux occurs at t = T₁ since $\Phi_0^a \neq \Phi_0^b$.

Equation (17) gives the solution of a time optimum problem by Equations (6) and (7) with the reactivity constraint $\rho_c . \quad \text{Thus,}$

$$k_{eff} \stackrel{\sim}{=} \frac{\frac{\nu_{\Sigma_f}}{\Sigma_a (1 + \tau_R \frac{\pi^2}{\ell^2})} = \frac{1}{1 - \frac{\gamma \beta}{\gamma + \lambda}} \stackrel{\sim}{=} 1 + \frac{\gamma \beta}{\gamma + \lambda} = 1 + \Delta k, \quad (19)$$

or $\rho = \frac{\Delta k}{\beta} = \frac{\gamma}{\gamma + \lambda} \leq \rho_c \text{ (the constraint).}$

(6) Transformation of Variables for the Perturbed Kinetics Equations

Exponential weighting functions to the variables $\Delta \Phi(z,t)$ and $\Delta C(z,t)$ in Equations (14) and (11) are introduced as

$$\Phi_{\mathbf{q}}^{\mathbf{a}}(z,t) = \frac{\Delta \Phi(z,t)}{\Phi_{\mathbf{Q}}^{\mathbf{a}} e^{\gamma t}},$$

$$\mathbf{C}_{\mathbf{q}}^{\mathbf{a}}(z,t) = \frac{\Delta \mathbf{C}(z,t)}{\mathbf{C}_{\mathbf{Q}}^{\mathbf{a}} e^{\gamma t}}.$$
(20)

Thus Equations (14) and (11) become

$$\tau_{R} \frac{\partial^{2}}{\partial z^{2}} \left[\Sigma_{R}^{a} \phi_{q}^{a}(z,t) \right] + \left[\nu(1-\beta) \Sigma_{f} - \Sigma_{R}^{a} \right] \phi_{q}^{a}(z,t) + \lambda \frac{C_{o}^{a}}{\phi_{o}^{a}} C_{q}^{a}(z,t)$$

$$= \frac{\mu^{a}(z,t)}{\phi_{o}^{a}e^{\gamma t}},$$

$$\frac{\partial}{\partial t} C_{q}^{a}(z,t) = \nu_{\beta} \Sigma_{f} \frac{\phi_{o}^{a}}{C_{o}^{a}} \phi_{q}^{a}(z,t) - (\lambda + \gamma) C_{q}^{a}(z,t),$$

$$(21)$$

where

$$\mu^{a}(z,t) = -\tau_{R} \frac{\partial^{2}}{\partial z^{2}} [\phi_{R}^{a}(z,t)\Delta\Sigma_{\mathbf{1}}^{a}(z,t)] + \phi_{R}^{a}(z,t)\Delta\Sigma_{\mathbf{1}}^{a}(z,t). \quad (22)$$

By substituting the value of $\phi_R^a(z,t)$ in equation (17) into Equation (22), one obtains

$$\mu^{a}(z,t) = \Phi_{o}^{a} e^{\gamma t} \left[-\tau_{R} \frac{\partial^{2}}{\partial z^{2}} \sin \frac{\pi}{\ell} z \Delta \Sigma_{1}(z,t) + \sin \frac{\pi}{\ell} z \Delta \Sigma_{1}(z,t) \right]. \tag{23}$$

Equation (21) is further transformed by assuming the perturbed flux follows a sinusoidal distribution in the axial direction, thus

$$\phi_{q}^{a} = X_{1}^{a}(t) \sin \frac{\pi}{\ell}z,$$

$$C_{q}^{a} = X_{2}^{a}(t) \sin \frac{\pi}{\ell}z.$$
(24)

The following equations are obtained by substituting equation (18) and (24) into equation (21)

$$-A^{a}X_{1}^{a}(t) + A^{a}X_{2}^{a}(t) - u^{a}(t) = 0 ,$$

$$\frac{d}{dt}X_{2}^{a} = (\lambda + \gamma) X_{1}^{a}(t) - (\lambda + \gamma) X_{2}^{a}(t) , \qquad t \leq T_{1}$$
(25)

where

$$-A^{a} = -\tau_{R} \frac{\pi^{2}}{\ell^{2}} \Sigma_{R}^{a} - \Sigma_{R}^{a} + \nu(1-\beta)\Sigma_{f} = -\frac{\lambda \nu_{\beta}\Sigma_{f}}{\lambda + \gamma}, \qquad (26)$$

and

$$u^{a}(t) \sin \frac{\pi}{\ell} z = -\tau \frac{\partial^{2}}{R_{\partial z}^{2}} \left[\Delta \Sigma_{1}(z, t) \sin \frac{\pi}{\ell} z \right] + \Delta \Sigma_{1}(z, t) \sin \frac{\pi}{\ell} z.$$
(27)

Equation (27) admit a solution of the form

$$\Delta\Sigma_{\mathbf{1}}(z,t) \rightarrow \Delta\Sigma_{\mathbf{1}}(t) = \frac{1}{1+\tau_{R}} \frac{\pi^{2}}{\ell^{2}} \quad u^{a}(t)$$
 (28)

(7) The Control System - Second Optimization

If the system starts with the right initial condition in C_{\circ}/Φ_{\circ} in Equation (18) and the right control with a jump of Σ_R from Σ_R^a to Σ_R^b at t = T_1 , then theoretically the reactor variables will follow equation (17) with no error. However, the actual initial condition is not always the value given in equation (18). Thus the control in Σ_a will differ from Σ_R by the amount $\Delta\Sigma_a = \Delta\Sigma_1 + \Delta\Sigma_2$. Again the quantity $\Delta\Sigma_1(z,t)$ is determined from equation (28) if the control u(t) is known. The problem now is to find u(t) for any arbituary starting conditions of $X_1(t)$ and $X_2(t)$ for equation (25).

The control system should be designed such that the variables would follow as close as possible the reference variables given in equation (17). For an ideal system the variables X_1 , X_2 , and u in equation (25) should be identically

zero. With this in mind we are seeking for a minimum of a functional known as index of performance.

In the reactor start-up problem, perturbed neutron flux and the control effort are of interest. An index of performance is, therefore, chosen as

$$I = \int_{t}^{T_{1}} \left\{ [\chi_{1}^{2}(\sigma)]^{2} + \eta(\sigma) [u(\sigma)]^{2} \right\} d\sigma + \int_{T_{1}}^{T_{2}} \left\{ [\chi_{1}^{b}(\sigma)]^{2} + \eta(\sigma) [u(\sigma)]^{2} \right\} d\sigma, \qquad (29)$$

where $\eta(\sigma)$ is weighting function. The weighting function is assumed to be continuous except at the time $t = T_1$ where it may be discontinuous. It is noted that the lower limit is the present time t in equation (29). This is in consistant with the principle of Dynamic Programming(7), which is to minimize the integral from the time to go no matter where your present time is. If we can measure the perturbed flux X_1 at the present time it is possible to find a control u(t) and thus $\Delta\Sigma_1(t)$ using X_1 as feedback with a variable gain. In this manner the functional I in equation (29) will be kept at a minimum subjected to distrubance at any other time, not only to errors at the starting conditions. above viewpoint is very important in that the source or cause of disturbance is immaterial as far as the output $X_1(t)$ can be detected and readjusted by the control element producing $\Delta\Sigma_1(t)$.

We may define a new variable $X_3(\sigma)$ such that

$$X_3(\sigma)$$
 $\sigma=T_2$

thus,

$$X_{3}(\sigma) = \int_{\theta=\mathbf{t}}^{\mathbf{T}_{1}} \left\{ [X_{1}^{a}(\theta)]^{2} + \eta(\theta)[u^{a}(\theta)]^{2} \right\} d\theta$$

$$+ \int_{\theta=\mathbf{T}_{1}}^{\sigma} \left\{ [X_{1}^{b}(\theta)]^{2} + \eta(\theta)[u^{b}(\theta)]^{2} \right\} d\theta. \tag{30}$$

(8) <u>Application of Maximum Principle for a System of Algebraic</u> and Differential Equations

By rearranging equation (25) and differentiating equation (30) one obtains

$$0 = [-A^{a}X_{1}^{a}(\sigma) + A^{a}X_{2}^{a}(\sigma) - u^{a}(\sigma)] = f_{1},$$

$$\frac{d}{d\sigma}x_{2}^{a}(\sigma) = (\lambda + \gamma) X_{1}^{a}(\sigma) - (\lambda + \sigma)X_{2}^{a}(\sigma) = f_{2},$$

$$\frac{d}{d\sigma}x_{3}^{a}(\sigma) = [X_{1}^{a}(\sigma)]^{2} + \eta [u^{a}(\sigma)]^{2} = f_{3},$$
(31)

where o is the future time.

The optimum system is defined as the system for which

$$S(T_2) = \sum_{i=1}^{3} C_i X_i (\sigma = T_2),$$

 $C_1 = C_2 = 0, C_3 = 1.$ (32)

is a minimum with respect to $u(\sigma)$. The Hamiltonian is

given in Appendix A is

$$H = \sum_{i=1}^{3} p_{i} (\sigma) f_{i}, \qquad (33)$$

where p_i are the auxiliary variables.

Thus,

$$H = p_{1}(\sigma) \left[-A^{3} \chi_{1}^{a}(\sigma) + A^{a} \chi_{2}^{a}(\sigma) - u^{a}(\sigma) \right]$$

$$+ p_{2}(\sigma) \left[(\lambda + \gamma) \chi_{1}^{a}(\sigma) - (\lambda + \sigma) \chi_{2}^{a}(\sigma) \right] + p_{3}(\sigma) \left[\left[\chi_{1}^{a}(\sigma) \right]^{2} + \eta \left[u^{a}(\sigma) \right]^{2} \right].$$

$$(34)$$

A sufficient condition for a minimum of S is that the Hamiltonian H be maximized with respect to the control vector at all time. For system with unsaturated perturbed control we have from equation (Al5) in Appendix A.

$$\frac{\partial H}{\partial u_{\star}^{a}} = 0 = -p_{1}(\sigma) + p_{3}(\sigma) 2\eta u_{\star}^{a}. \tag{35}$$

or

$$u_*^a(\sigma) = \frac{p_1(\sigma)}{2^{\eta}p_3(\sigma)}, \tag{36}$$

where the asterisk denotes the optimum condition.

In order to complete the derivation of the optimum control law, it is necessary to develop the differential equations $^{(8)}$ for the auxiliary variables. From equations (Al3) and (Al4) in Appendix A we have

$$0 = -\frac{\partial H}{\partial X_{i}}, \qquad i = 1$$

$$\frac{dp_{i}(\sigma)}{d\sigma} = -\frac{\partial H}{\partial X_{i}}. \qquad i = 2,3. \qquad (37)$$

Applying equation (37) to equation (34) one obtains

$$0 = - [p_1(\sigma) (-A^a) + p_2(\sigma) (\lambda + \gamma) + 2p_3(\sigma) X_1^a(\sigma)],$$
 (38)

$$\frac{\mathrm{d}\mathbf{p}_{2}}{\mathrm{d}t} = -\mathbf{p}_{1}(\sigma) A^{a} + \mathbf{p}_{2}(\sigma) (\lambda + \gamma), \tag{39}$$

$$\frac{dp_3}{dt} = 0. t \leqslant \sigma \leqslant T_1 (40)$$

The free terminal conditions or natural boundary conditions are obtained from equation (A9) and (32).

i.e.
$$p_2(\sigma = T_2) = -C_2 = 0$$
. (41)

$$p_{\epsilon}(\tau = T_2) = -C_3 = -1.$$
 (42)

It is concluded from equations (40) and (42) that the quantity

$$p_3(\sigma) = -1 \text{ for all } \sigma,$$
 (43)

Substituting equation (43) into equations (38), (39) and (36) one obtains

$$-A^{a}p_{1}(\sigma) + (\lambda+\gamma) p_{2}(\sigma) - 2X_{1}^{a}(\sigma) = 0,$$

$$\frac{dp_{2}}{d\sigma} = -A^{a} p_{1}(\sigma) + (\lambda+\sigma)p_{2}(\sigma),$$

$$\mathbf{u}_{\mathbf{x}}^{a}(\sigma) = -\frac{1}{2\pi} p_{1}(\sigma).$$
(44)

Similarily, the differential equation of auxiliary variables for interval $T_1 \leqslant \sigma \leqslant T_2$ can be obtained by changing superscript a to b and γ to zero.

(9) Optimum Control Law

In order to determine the Optimum Control law, it is necessary to solve the algebraic and differential equations for the auxiliary variables and the state variables. Equations similar to Equations (25) and (44) are given here for the interval $T_1 \leqslant t \leqslant T_2$

$$-A^{b}X_{\mathbf{1}}^{b}(\sigma) + A^{b}X_{\mathbf{2}}^{b}(\sigma) - u_{\mathbf{x}}^{b}(\sigma) = 0. \tag{45}$$

$$\frac{\mathrm{d}}{\mathrm{d}\sigma} \mathbf{X}_{2}^{\mathrm{b}}(\sigma) = \lambda \mathbf{X}_{1}^{\mathrm{b}}(\sigma) - \lambda \mathbf{X}_{2}^{\mathrm{b}}(\sigma), \qquad (46)$$

$$-A^{b}p_{1}(\sigma) + \lambda p_{2}(\sigma) - 2X_{1}^{b}(\sigma) = 0, \qquad (47)$$

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathrm{p}_{2}(\sigma) = -\mathrm{A}^{\mathrm{b}}\mathrm{p}_{1}(\sigma) + \lambda\mathrm{p}_{2}(\sigma). \tag{48}$$

$$u_{x}^{b}(\sigma) = -\frac{1}{2\eta} p_{1}(\sigma). \qquad (49)$$

Eliminating p_1 from Equations (49) and (47)

$$u_{*}^{b}(\sigma) = \frac{A^{b}}{2\alpha^{b}}[-\lambda p_{2} + 2X_{1}^{b}], \qquad (50)$$

where
$$\alpha^b = \eta(A^b)^2$$
. (51)

Substituting Equation (50) into (45) gives

$$X_{2}^{b} = \frac{1}{2\alpha^{b}} \left[-\lambda p_{2} + 2(1+\alpha^{b}) X_{1}^{b} \right].$$
 (52)

The following Equation can be obtained by substituting Equation (52) into Equation (46):

$$\left[\frac{\mathrm{d}}{\mathrm{d}\sigma} + \lambda - \frac{\lambda \alpha^{\mathrm{b}}}{1 + \alpha^{\mathrm{b}}}\right] X_{\mathbf{i}}^{\mathrm{b}} - \frac{\lambda}{2[1 + \alpha^{\mathrm{b}}]} \left[\frac{\mathrm{d}}{\mathrm{d}\sigma} + \lambda\right] p_{2} = 0. \tag{53}$$

By solving p_1 from Equation (47) and substituting into Equation (48) we have

$$2X_1^b - \frac{d}{d\sigma} p_2 = 0.$$
 (54)

Solution of p_2 and X_1^b from Equation (53) and (54) are

$$p_{2}(\sigma) = F_{1}(t) \cos h \omega^{b}(\sigma-t) + F_{2}(t) \sin h \omega^{b}(\sigma-t), \quad (5)$$

$$X_{1}^{b}(\sigma) = \frac{\omega^{b}}{2} [F_{1}(t) \sin h \omega^{b}(\sigma-t) + F_{2}(t) \cos h \omega^{b}(\sigma-t)], \quad (56)$$

where

$$\omega^{b} = \lambda \sqrt{1 - \frac{\alpha^{b}}{1 + \alpha^{b}}} , \qquad (57)$$

 \cong λ for small value of α^b

the quantity t is carried as a parameter.

From Equation (52) one obtains

$$X_{2}^{b} = -\frac{1}{2\alpha^{b}} \left\{ F_{1}(t) [\lambda \cos h \omega^{b}(\sigma-t) - \omega^{b} [1+\alpha^{b}] \sin h \omega^{b}(\sigma-t)] \right\}$$

+
$$F_2(t)$$
 [$\lambda \sin h \omega^b(\sigma-t) - \omega^b[1+\alpha^b] \cos h \omega^b(\sigma-t)]$]. (58)

Using the condition that X_1^b is equal to the measured value at $\sigma = t$. Equation (56) becomes

$$X_1^b(t) = \frac{\omega^b}{2} F_2(t)$$
 (59)

Using boundary condition (41) for Equation (55) one obtains

$$F_{1}(t) = -F_{2}(t) \tan h \omega^{b}(T_{2}-t)$$

$$= -\frac{2}{\omega^{b}} \tan h \omega^{b}(T_{2}-t) X_{1}^{b}(t).$$
 (60)

The Optimum control law is obtained from Equation (50), (55) and (60)

$$u_{*}^{b}(t) = u_{*}^{b}(\sigma) \Big|_{\sigma=t} = \frac{A^{b}}{2\alpha^{b}} \left[-\lambda p_{2} \right]_{\sigma=t} + 2X_{1}^{b}(t)$$

$$= \frac{A^{b}X_{1}^{b}(t)}{\alpha^{b}} \left[\frac{\lambda}{\omega^{b}} \tanh \omega^{b}(T_{2}-t) + 1 \right]. \qquad T_{1} \leqslant t \leqslant T_{2}$$
(61)

It should be noted that there is a jump of reference X_1 at $t=T_1$ (see Figure 1). This discontinuity is due to the simplified mathematics expression by dropping the $\frac{\partial \phi_1}{\partial t}$ term in the Kinetics equation (6). However, the jump does not physically exist in the reactor if the term $\frac{\partial \phi_1}{\partial t}$ is not dropped from equation (1). In order to modify this situation, it is required that the actual flux be continuous every where. This requirement is equivalent to let the precursor and its derivatives be continuous at $t=T_1$. From this point of view, the conditions which will be used for derivation of the optimum control law in the interval $t \leqslant T_1$ are imposed as follows:

- a) The natural boundary condition given in Equation (41).
- b) The initial condition expressed as $X_{\mathbf{1}}^{a}|_{\sigma=t} = X_{\mathbf{1}}^{a}(t)$ (Measured value). (62)
- c) In order to keep precursor continuous at $t = T_1$, it is required that

$$\chi_{2}^{a(\sigma)}\Big|_{\sigma=T_{1}} = \chi_{2}^{b}(\sigma)\Big|_{\substack{\sigma=t\\t=T_{2}}}.$$
 (63)

d) The requirement for the continuity of derivative

of precursor at $t = T_1$ is mathematically expressed as (see Appendix B)

$$\frac{\partial}{\partial \sigma} X_{2}^{a}(\sigma) \Big|_{\sigma = T_{1}} = \frac{\partial}{\partial \sigma} X_{2}^{b}(\sigma) \Big|_{\substack{\sigma = t \\ t = T_{1}}} - \gamma - \gamma X_{2}^{a}(\sigma) \Big|_{\substack{\sigma = T_{1}}}.$$
 (64)

Thus, the Optimum Control law derived in Appendix C for $t < T_1$

$$u_{\star}^{a}(t) = \frac{A^{a}}{\alpha^{a}} \left[(\lambda + \gamma) \frac{\frac{1}{\omega^{a}} \left[(\gamma + \omega^{b} \Omega) G + \omega^{a} H \right] X_{1}^{a}(t) - \alpha^{a} \gamma}{\omega^{a} G + (\gamma + \omega^{b} \Omega) H} + X_{1}^{a}(t) \right], (65)$$

where

$$\alpha^{a} = \eta(A^{a})^{2},$$

$$\omega^{a} = (\lambda + \gamma) \sqrt{1 - \frac{\alpha^{a}}{1 + \alpha^{a}}},$$

 $\cong \lambda + \gamma$ for small values of α^a

$$\Omega = \frac{\lambda + \omega^{b} [1 + \alpha^{b}] \tan h \omega^{b} (T_{2} - T_{1})}{\omega^{b} [1 + \alpha^{b}] + \lambda \tan h \omega^{b} (T_{2} - T_{1})}.$$

$$G = (\lambda + \gamma) \sin h \omega^a (T_1 - t) - \omega^a [1 + \alpha^a] \cos h \omega^a (T_1 - t).$$

$$H = (\lambda + \gamma) \cos h \omega^{a} (T_{1} - t) - \omega^{a} [1 + \alpha^{a}] \sin h \omega^{a} (T_{1} - t).$$

For the homogeneous C-U²³⁵ (Hydrogen as coolant) reactor with the atom ratio about 500, using $\lambda\cong 0.1$ sec⁻¹, $\beta\cong 7.5\times 10^{-3}$, $\nu\cong 2.5$, $\Sigma_f\cong 0.09$ cm⁻¹, $\tau_R\cong 325$ cm², $\gamma\cong 0.23$ sec⁻¹ (equivalent to 69 cents reactivity), $T_2 - T_1 \geqslant 60$ sec, and $\eta\cong 2.5\times 10^4$ cm² we can approximate the following quantities as

$$A^{a} = \frac{\lambda^{\nu} \beta^{\Sigma} f}{\lambda + \nu} \approx 5.7 \times 10^{-4} \text{ cm}^{-1}, A^{b} = \nu \beta \Sigma_{f} \approx 1.875 \times 10^{-3} \text{ cm}^{-1}.$$

 $\alpha^a \cong 0.01$, $\alpha^b \cong 0.1$, $\omega^b \cong \lambda$, $\omega^a \cong \lambda + \gamma \cong \gamma + \omega^b$ and tan h $\omega^b (T_2 - T_1) \cong 1$. Substituting some approximate quantities given above into Equation (63), we have

$$\Omega \stackrel{\simeq}{=} \frac{\lambda + \omega^{D}(1+\alpha^{D})}{\omega^{D}(1+\alpha^{D}) + \lambda} = 1,$$

$$\omega^{a}G + (\gamma+\omega^{D}\Omega)H \stackrel{\simeq}{=} \omega^{a}(G+H) \stackrel{\simeq}{=} (\lambda+\gamma)\alpha^{a}e^{(\lambda+\gamma)(T_{1}-t)},$$

$$(\gamma+\omega^{D}\Omega)H + \omega^{a}G \stackrel{\simeq}{=} \omega^{a}(G+H) \stackrel{\simeq}{=} (\lambda+\gamma)\alpha^{a}e^{(\lambda+\gamma)(T_{1}-t)},$$
and
$$u_{*}^{a}(t) \stackrel{\simeq}{=} \frac{2A^{a}}{\alpha^{a}} X_{1}^{a}(t) + \frac{A^{a}\gamma}{\alpha^{a}(\lambda+\gamma)} e^{-(\lambda+\gamma)(T_{1}-t)}.$$
(66)

(10) The Response of the Flux and Precursor Having Optimum Control

The optimum flux, ϕ_* , subjected to initial errors can be obtained by solving the following differential equations which are derived from Equations (66), (61), (25) and (45),

$$\frac{\mathrm{d}}{\mathrm{d}t}X_{1*}^{a} + \frac{2(\lambda+\gamma)}{\alpha^{a}+2}X_{1*}^{a} = -\frac{2\gamma}{\alpha^{a}+2} e^{-(\lambda+\gamma)(T_{1}-t)}, \quad t \leqslant T_{1}$$
(67)

$$\frac{\mathrm{d}}{\mathrm{dt}} X_{1*}^{b} + \frac{2\lambda}{\alpha^{b} + 2} X_{1*}^{b} \stackrel{2}{=} 0 . \qquad T_{1} \leqslant t \leqslant T_{2}$$
 (68)

For the case $\alpha^b \cong 0.1$, and $\alpha^a \cong 0.01$,

i.e.
$$\alpha^{a} + 2 \stackrel{\sim}{=} 2;$$
 $\alpha^{b} + 2 \stackrel{\sim}{=} 2,$

the solution of Equations (67) and (68) are,

$$X_{\mathbf{1}*}^{a} = X_{\mathbf{1}0}^{a} e^{-(\lambda+\gamma)t} - \frac{\gamma}{\lambda+\gamma} e^{-(\lambda+\gamma)T_{\mathbf{1}}} \sin h (\lambda+\gamma)t, t \leqslant T_{\mathbf{1}}$$
 (69)

$$X_{1*}^b \cong X_{10}^b e^{-\lambda(t-T_1)}.$$
 $T_1 \leqslant t \leqslant T_2$ (70)

where

 X_{10}^{ε} = the value of X_{1}^{a} at t = 0,

 X_{10}^{b} = the value of X_{1}^{b} at t = T_{1} .

By using the definition of X_1^a and X_1^b in equation (24) and (20) one obtains

$$\Delta \phi^{a}(z,t) = \left\{ \Delta \phi^{a}_{o} e^{-\lambda t} - \frac{\gamma}{\lambda + \gamma} \phi^{a}_{o} e^{-(\lambda + \gamma)T_{1} + \gamma t} \sin h (\lambda + \gamma)t \right\} \sin \frac{\pi}{\ell} z.$$

$$t \leqslant T_{1} \qquad (71)$$

$$\Delta \phi^{b}(z,t) \cong \left\{ \Delta \phi^{b}_{o} e^{-\lambda(t-T_{1})} \right\} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z, \quad T_{1} \leqslant t \langle T_{2} \rangle$$
 (72)

where

 $\frac{\gamma}{\lambda + \gamma} \phi_o^a = \phi_o^a - \phi_o^b$ from equation (18).

$$\Delta \phi_{\circ}^{b} e^{\boldsymbol{\gamma} T_{1}} = (\phi_{\circ}^{a} - \phi_{\circ}^{b}) e^{\boldsymbol{\gamma} T_{1}} - \Delta \phi^{a} \Big|_{t=T_{1}} \cong \frac{\phi_{\circ}^{a} - \phi_{\circ}^{b}}{2} e^{\boldsymbol{\gamma} T_{1}}.$$
(see Figure 1) (73)

Then

$$\Phi_{\star}^{a} = \Phi_{R}^{a} + \Delta \Phi,$$

$$\Phi_{\star}^{a} = \left\{ \Phi_{\circ}^{a} e^{\gamma t} + \Phi_{\circ}^{a} e^{-\lambda t} - (\Phi_{\circ}^{a} - \Phi_{\circ}^{b}) e^{-(\lambda + \gamma)T_{1} + \gamma t} \sin h (\lambda + \gamma) t \right\} \sin \frac{\pi}{\ell} z, \quad t \in T_{1} (74)$$

$$\Phi_{\star}^{b} \cong \left\{ \frac{\Phi_{\circ}^{a} - \Phi_{\circ}^{b}}{2} e^{\gamma T_{1} - \lambda (t - T_{1})} + \Phi_{\circ}^{b} e^{\gamma T_{1}} \right\} \sin \frac{\pi}{\ell} z. \quad T_{1} \in t \subset T_{2} (75)$$

$$A = \lambda T_{1} = \lambda t \quad \text{a.s.} \quad t \in T_{1} (74)$$

When t = T₁, it is known that $\phi_0^a e^{-\lambda T_1} \cong 0$ and $\phi_*^a \Big|_{t=T_1} \cong \phi_*^b \Big|_{t=T_1}$.

Therefore the derivatives of ϕ_*^a at t = T₁ is discontinuous.

Substituting Equation (74) and (75) into Equation (7), the Optimum precursor are obtained:

$$C_{\star}^{a} = \left\{ \begin{array}{l} C_{\circ}^{a} e^{\gamma t} + \left[(\lambda + \gamma)t + 1 \right] e^{-\lambda t} \Delta C_{\circ}^{a} + \frac{\gamma}{2} e^{-(\lambda + \gamma)T_{1}} \left[t e^{-\lambda t} \right] \\ - \frac{e^{\gamma t}}{\lambda + \gamma} \sin h \left(\lambda + \gamma \right) t \right] \right\} \sin \frac{\pi}{\ell} z, \qquad t \leq T_{1}$$

$$C_{\star}^{b} \cong C_{\star}^{a} \Big|_{t=T_{1}} e^{-\lambda \left(t - T_{1} \right)} + C_{\circ}^{a} e^{\gamma T_{1}} + \frac{C_{\circ}^{a} \gamma}{2} e^{\gamma T_{1}} t e^{-\lambda \left(t - T_{1} \right)}.$$

$$T_{1} \leq t \leq T_{2}$$

$$(76)$$

It can be proved that at t = T_1 both C_* and $\frac{\partial}{\partial t}C_*$ are continuous.

The response of ϕ_* and C_* are calculated for the typical nuclear powered rocket start-up, i.e. $\gamma \cong 0.23~{\rm sec}^{-1}~\lambda \cong 0.1~{\rm sec}^{-1}$, by using equations (72), (73), (74) and (75) with initial errors of 100% and -50%. The reference initial power is 10KW and final power is 10^6 KW. The rate of rise of power is one decade per ten seconds, corresponding to 69 cents of reactivity. Two curves for

$$\frac{\Phi_*}{\Phi_o^a}$$
 and $\frac{C_*}{C_o^a}$ vs time are plotted in fingure 1 and 2, respectively.

The actual response shown in figure 1 is very close to the desired response even subjected to an initial error as high as 100%.

(11) Conclusion

Attempts are made to control the absorption cross-section of the nuclear rocket with distributed parameter kinetics. Two optimization procedure are taken; one with bang-bang control for the reference flux and precursor, another to eliminate the jump by maximum principle. Closed form solutions for the control laws are obtained.

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References

- (1) Mohler, R.R. "Optimal Control of Nuclear-Reactor Systems" ANS Transactions Vol 7. No. 1. June 1964
- (2) Mohler, R.R. "Optimal Control of Nuclear-Reactor Processes" LAMS 3068, March 1964
- (3) Shen, C.N. and Haag F.G. "Adaptive Control for Nuclear Reactor Start-up and Regulation". Transaction of the American Nuclear Society, Vol. 6, No. 1, P 109, 1963
- (4) Shen, C.N. and Haag, F.G. "Application of Optimum Control to Nuclear Reactor Start-up" Institute of Electrical and Electronics Engineers, Transaction of Nuclear Science, NS-11, No. 2, p. 1, March 1964.
- (5) Shen, C.N. and Haag, F.G. "Optimum Nuclear Rocket Start-up to Develop Full Power at Exact Time with Consideration of Noise" Presented at the Sixth International Instruments and Measurements Conference, Special Section on Automatic Control, Stockholm, Sweden, September 1964.
- (6) Meghreblian, R. V. and Holmes, D. K., "Reactor Analysis" McGraw Hill 1960.
- (7) Bellman, R. "Dynamic Programming" Princeton University Press, 1957.
- (8) Pontigagin, L.D. Boltyanskii, V.G. Gamkrelisze, R.V. and Mischenko, E.F. "The Mathematical Theory of Optimal Processes", Interscience Publishers, John Wiley, N.Y. 1962.

APPENDIX A

Maximum Principle for a System of Algebraic and Differential Equations

The system is described by the following set of algebraic and differential equations:

$$0 = f_{1} (X_{1} . . X_{m}, X_{m+1} . . X_{n}, X_{n+1}, u_{1} . . u_{k}, . . u_{r}) i=1, . . m,$$
(A1)

$$\frac{dx_{\mathbf{i}}(\sigma)}{d\sigma} = f_{\mathbf{i}}(X_{\mathbf{i}} ... X_{\mathbf{m}}, X_{\mathbf{m+1}} ... X_{\mathbf{n}}, X_{\mathbf{n+1}}, u_{\mathbf{i}}, ... u_{\mathbf{k}} ... u_{\mathbf{r}})$$

$$i=m+1, ... n+1 \quad (A2)$$

$$X_i(\sigma=t)=X_i(t)$$
 i = 1, . . m, m+1, . . . n+1 (A3) where $X_i(\sigma)$ are state variables and u_k are control variables.

The problem is to minimize

$$S(T_2) = \sum_{i=1}^{n+1} C_i X_i (\sigma = T_2)$$

$$= \int_t^{T_2} \sum_{i=1}^{n+1} C_i X_i d\sigma + \sum_{i=1}^{n+1} C_i X_i (\sigma = t) (A4)$$

The method of calculus of variation may be applied to derive the maximum principle for the case of unbounded control variables for fixed time. The quantity $S(T_2)$ in Equation (A4) remains the same by introducing Lagrange multipliers $p_1(\sigma)$ to adjoin the contraints imposed by equations (A1) and (A2)

$$S(T_{2}) = \int_{t}^{T_{2}} \sum_{i=1}^{n+1} C_{i} \dot{X}_{i} d\sigma + \sum_{i=1}^{n+1} C_{i} X_{i} (\sigma=t)$$

$$+ \int_{t}^{T_{2}} \left\{ \sum_{i=1}^{m} p_{i} (O-f_{i}) + \sum_{i=m+1}^{n+1} p_{i} (\dot{X}_{i}-f_{i}) \right\} d\sigma \qquad (A5)$$

First order variation are taken for the state and control variables about a stationary path as

$$X_{\underline{i}} = \overline{X}_{\underline{i}} + \varepsilon \xi_{\underline{i}}(t)$$

$$X_{\underline{i}} = \overline{X}_{\underline{i}} + \varepsilon \xi_{\underline{i}}(t)$$

$$u_{\underline{k}} = \overline{u}_{\underline{k}} + \varepsilon \zeta_{\underline{k}}(t)$$
(A6)

Stationary values of $S(T_2)$ in Equation (A5) are determined by taking the partial derative of $S(T_2)$ with respect to ϵ and setting result to zero.

$$\frac{\partial S}{\partial \boldsymbol{\varepsilon}} = \int_{t}^{T_{2}} \left\{ \sum_{i=1}^{n+1} C_{i} \dot{\boldsymbol{\xi}}_{i} + \sum_{i=m+1}^{n+1} p_{i} \dot{\boldsymbol{\xi}}_{i} - \sum_{i=1}^{n+1} p_{i} \frac{\partial \tilde{f}_{i}}{\partial X_{j}} \boldsymbol{\xi}_{j} \right\} d\sigma$$

$$- \int_{t}^{T_{2}} \left\{ \sum_{i=1}^{n+1} \sum_{k=1}^{r} p_{i} \frac{\partial \tilde{f}_{i}}{\partial u_{k}} \boldsymbol{\zeta}_{k} \right\} d\sigma = 0$$
(A7)

The first two tems of the right-hand side of the above equation may be integrated by parts to obtain the following

$$\sum_{i=1}^{m} C_{i} \boldsymbol{\xi}_{i} \begin{vmatrix} T_{2} & n+1 \\ t & + \sum_{i=m+1}^{m} (C_{i} + p_{i}) \boldsymbol{\xi}_{i} \end{vmatrix}_{t}^{T_{2}}$$

$$= \int_{t}^{T_{2}} \left\{ \sum_{i=m+1}^{m+1} \dot{p}_{i} + \sum_{i=1}^{m+1} p_{j} \frac{\partial \bar{f}_{j}}{\partial x_{i}} \right\} \boldsymbol{\xi}_{i} d\sigma$$

$$+ \int_{t}^{T_{2}} \sum_{i=1}^{m+1} \sum_{k=1}^{r} p_{i} \frac{\partial \bar{f}_{i}}{\partial u_{k}} \zeta_{k} d\sigma \qquad (A8)$$

Since Equation (A8) must be satisfied for arbitrary ξ_i and ζ_k the coefficients of these terms must be zero, i.e.

$$C_{1} = 0$$
 $i = 1, ... m$ $C_{1} = -p_{1}(T_{2})$ $i = m+1, ... n+1$ (A9)

$$0 = -\sum_{j=1}^{n+1} p_j \frac{\partial \overline{f}_i}{\partial X_i} \quad i = 1, \dots m$$

$$\dot{p}_i = -\sum_{j=1}^{n+1} p_j \frac{\partial \overline{f}_j}{\partial X_i}, \quad i = m+1, \dots n+1$$
(Alo)

$$\sum_{i=1}^{n+1} p_i \frac{\partial \bar{f}_i}{\partial u_k} = 0, \quad k = 1, \dots, r.$$
(All)

If the Hamiltonian is defined as

$$H = \sum_{i=1}^{n+1} p_i \bar{f}_i \qquad (A12)$$

then

$$0 = -\frac{\partial H}{\partial X_1} \qquad i=1, \dots m \qquad (A13)$$

$$\frac{\mathrm{d}p_{i}}{\mathrm{d}\sigma} = -\frac{\partial H}{\partial X_{i}} \qquad i=m+1, \dots, n+1$$
 (A14)

$$\frac{\partial H}{\partial u_k} = 0 \qquad k=1, \dots r \qquad (A15)$$

Appendix B

Condition for the Derivative of Precursor to be Continuous at

$$t = T_1$$

By definition of equations (20), (24), and (17)

$$X_{2}^{a}(\sigma) = \frac{C_{q}^{a}(\sigma,z)}{\sin\frac{\pi}{\ell}z} = \frac{\Delta C^{a}(\sigma,z)}{C_{o}^{a}e^{\gamma\sigma}\sin\frac{\pi}{\ell}z} = \frac{C^{a}-C_{R}^{a}}{C_{o}^{a}e^{\gamma\sigma}\sin\frac{\pi}{\ell}z} = \frac{C^{a}-C_{R}^{a}}{C_{o}^{a}e^{\gamma\sigma}\sin\frac{\pi}{\ell}z} - 1$$

$$X_{2}^{b}(\sigma) = \frac{C_{q}^{b}(\sigma,z)}{\sin\frac{\pi}{\ell}z} = \frac{\Delta C^{b}(z)}{C_{o}^{a}e^{\gamma T_{1}}\sin\frac{\pi}{\ell}z} = \frac{C^{b}-C_{R}^{b}}{C_{o}^{a}e^{\gamma T_{1}}\sin\frac{\pi}{\ell}z} = \frac{C^{b}-C_{R}^{b}}{C_{o}^{a}e^{\gamma T_{1}}\sin\frac{\pi}{\ell}z} = \frac{C^{b}-C_{R}^{b}}{C_{o}^{a}e^{\gamma T_{1}}\sin\frac{\pi}{\ell}z} - 1$$

$$(B-2)$$

Thus

$$\frac{\partial}{\partial \sigma} X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}} - \frac{\partial}{\partial \sigma} X_{2}^{b}(\sigma) \Big|_{t=T_{1}} = \frac{\partial}{\partial \sigma} \frac{c^{a}}{c_{o}^{a} e^{\gamma \sigma_{\sin} \frac{\pi}{\ell} z}} \Big|_{\sigma=T_{1}}$$

$$- \frac{\partial}{\partial \sigma} \frac{c^{b}}{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{t=T_{1}} = \frac{\frac{\partial c^{a}}{\partial \sigma}}{c_{o}^{a} e^{\gamma \sigma_{\sin} \frac{\pi}{\ell} z}} \Big|_{\sigma=T_{1}} - \frac{\gamma c^{a}}{c_{o}^{a} e^{\gamma \sigma_{\sin} \frac{\pi}{\ell} z}} \Big|_{\sigma=T_{1}}$$

$$- \frac{\partial c^{b}}{\partial \sigma} \Big|_{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{t=T_{1}} = t$$

$$\frac{\partial c^{b}}{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{t=T_{1}} = t$$

$$\frac{\partial c^{b}}{\partial \sigma} \Big|_{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{t=T_{1}} = t$$

$$\frac{\partial c^{b}}{\partial \sigma} \Big|_{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{t=T_{1}} = t$$

$$\frac{\partial c^{b}}{\partial \sigma} \Big|_{c_{o}^{a} e^{\gamma T_{1}} \sin \frac{\pi}{\ell} z} \Big|_{c_{o}^{a} e^{\gamma T_$$

For continuous slope of precursor at $\sigma = T_1$ i.e.

$$\frac{\partial c^{a}(\sigma)}{\partial \sigma} \Big|_{\sigma=T_{1}} = \frac{\partial c^{b}(\sigma)}{\partial \sigma} \Big|_{\substack{\sigma=t\\t=T_{1}}},$$

one obtains

$$\frac{\partial}{\partial \sigma} X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}} - \frac{\partial}{\partial \sigma} X_{2}^{b}(\sigma) \Big|_{\substack{\sigma=t \\ t=T_{1}}} = -\frac{\gamma C^{a}(\sigma,z)}{C_{o}^{a} e^{\gamma \sigma} \sin \frac{\pi}{\ell} z} \Big|_{\sigma=T_{1}}$$

$$-\gamma \frac{C_{R}^{a} + \Delta C^{a}}{C_{o}^{a} e^{\gamma \sigma} \sin \frac{\pi}{\ell} z} \Big|_{\sigma=T_{1}} = -\gamma - \gamma X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}}$$

$$(B-4)$$

Appendix C: Optimum Control Law

Optimum control law for the time interval $t \leq T_1$ can be derived by solving equation (25) and (44). The solutions are similar to that of interval $T_1 \leq t \leq T_2$ except superscript b changed to a and arbitrary constants F to E

$$u_{*}^{a}(\sigma) = \frac{A^{a}}{2\alpha^{a}} \left\{ -(\lambda + \gamma)p_{2} + 2X_{1}^{a} \right\}, \qquad (C-1)$$

$$p_{2}(\sigma) = E_{1}(t) \cos h \, \omega^{a}(\sigma - t) + E_{2}(t) \sin h \, \omega^{a}(\sigma - t) \quad (C-2)$$

$$X_{1}^{a} = \frac{\omega^{a}}{2} \left\{ E_{1}(t) \sin h \, \omega^{a}(\sigma - t) + E_{2}(t) \cos h \, \omega^{a}(\sigma - t) \right\} \quad (C-3)$$

$$X_{2}^{a} = -\frac{1}{2\alpha^{a}} \left\{ E_{1}(t) \left[(\lambda + \gamma) \cos h \, \omega^{a}(\sigma - t) - \omega^{a}(1 + \alpha^{a}) \sin h \, \omega^{a}(\sigma - t) \right] + E_{2}(t) \left[(\lambda + \gamma) \sin h \, \omega^{a}(\sigma - t) - \omega^{a}(1 + \alpha^{a}) \cos h \, \omega^{a}(\sigma - t) \right] \right\} \quad (C-4)$$

where

$$ω^{a} = (λ+γ)\sqrt{1 - \frac{α^{a}}{1+α^{a}}},$$

$$\stackrel{\sim}{=} λ+γ \text{ for small values of } α^{a},$$

and the quantity t here is carried as a parameter.

Arbitrary constants can be determined by using the imposed conditions in equations (63) and (64)

Substituting equation (58) into equations (63) and (64) one obtains the following equations, respectively:

$$X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}} = \frac{-1}{2\alpha^{b}} \left[\lambda F_{1}(T_{1}) - \omega^{b}(1+\alpha^{b}) F_{2}(T_{1}) \right] \qquad (C-5)$$

$$\frac{\partial}{\partial \sigma} X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}} + \gamma X_{2}^{a}(\sigma) \Big|_{\sigma=T_{1}} + \gamma = \frac{-\omega^{b}}{2\alpha^{b}} \left[-\omega^{b}(1+\alpha^{b}) F_{1}(T_{1}) + \lambda F_{2}(T_{1}) \right] \qquad (C-6)$$

Let
$$t = T_1$$
 in equation (60), we have
$$F_1(T_1) = -F_2(T_1) \tan h \omega^b (T_2 - T_1)$$
 (C-7)

Eliminating $F_1(T_1)$ and $F_2(T_1)$ among above three equations leads to

$$\frac{\partial}{\partial \sigma} X_{2}^{a}(\sigma) \Big|_{\sigma = T_{1}} + (\gamma + \omega^{b} \Omega) X_{2}^{a}(\sigma) \Big|_{\sigma = T_{1}} + \gamma = 0$$
 (C-8)

where

$$\Omega = \frac{\lambda + \omega^{b} (1 + \alpha^{b}) \tan h \omega^{b} (T_{2} - T_{1})}{\omega^{b} (1 + \alpha^{b}) + \lambda \tan h \omega^{b} (T_{2} - T_{1})}$$
 (C-9)

Substituting Equation (C-4) into Equation (C-8), we have $E_1(t) \left[\omega^a G + (\gamma + \omega^b \Omega) H \right] + E_2(t) \left[(\gamma + \omega^b \Omega) G + \omega^a H \right] - 2\alpha^a \gamma = 0$ (C-10) where

$$G = (\lambda + \gamma) \sin h \omega^{a}(T_{1} - t) - \omega^{a}(1 + \alpha^{\alpha}) \cos h \omega^{a}(T_{1} - t)$$

$$H = (\lambda + \gamma) \cos h \omega^{a}(T_{1} - t) - \omega^{a}(1 + \alpha^{a}) \sin h \omega^{a}(T_{1} - t)$$

Using the Equation (C3), the following equation is obtained

$$X_1^a(t) = \frac{\omega^a}{2} E_2(t)$$
 (C-11)

Combining with equation (C-10) gives

$$E_{1}(t) = -\frac{\frac{2}{\omega^{a}} \left[(\gamma + \omega^{b} \Omega)G + \omega^{a} H \right] X_{1}^{a}(t) - 2\alpha^{a} \gamma}{\omega^{a}G + (\gamma + \omega^{b}\Omega) H}$$
(C-12)

The optimum Control law is obtained from equation (C-1)

$$u_{\star}^{a}(t) = u_{\star}^{a}(\sigma) \int_{\sigma=t}^{a} \frac{A^{a}}{2\alpha^{a}} \left[-(\lambda+\gamma)E_{1}(t) + 2X_{1}^{a}(t) \right]$$

$$= \frac{A^{a}}{\alpha^{a}} \left\{ (\lambda+\gamma) \frac{\frac{1}{\omega^{a}} \left[(\gamma+\omega^{b}\Omega)G + \omega^{a}H \right] X_{1}^{a}(t) - \alpha^{a}\gamma}{\omega^{a}G + (\gamma+\omega^{b}\Omega)H} + X_{1}^{a}(t) \right\} t < T_{1}$$
(C-13)

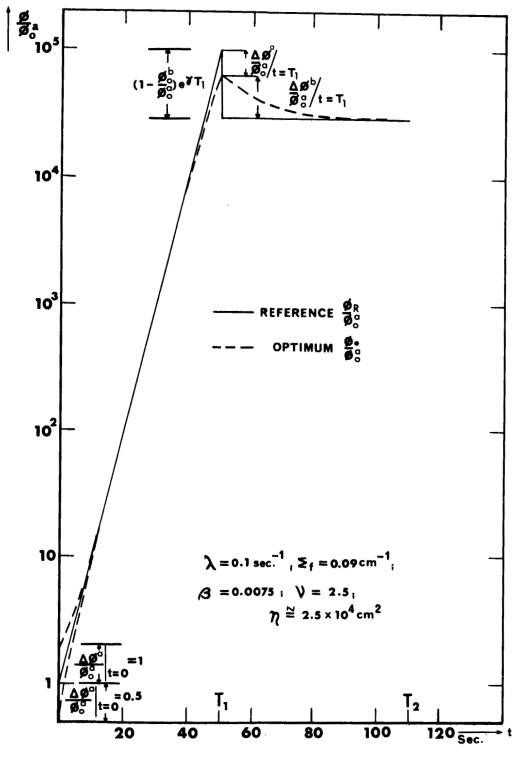


FIG.1 RESPONSE OF FLUX

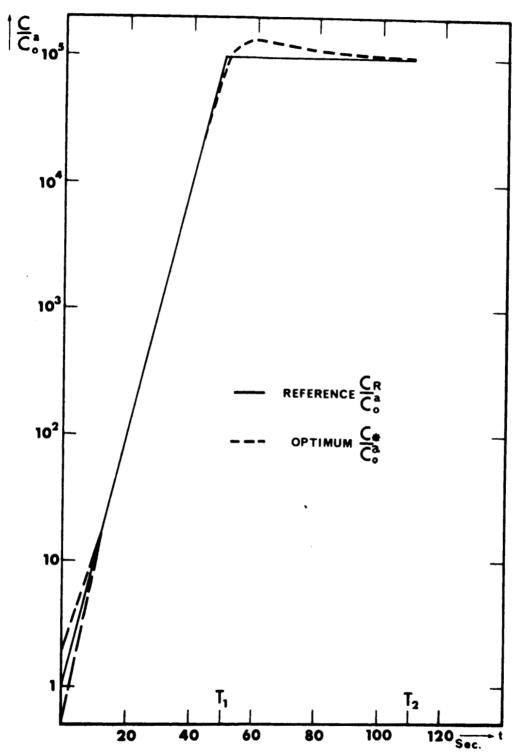


FIG. 2 RESPONSE OF PRECURSORS