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SPACE-TIME FLUX SYNTHESIS METHODS FOR THE APPROXIMATE SOLUTION OF TIME-DEPENDENT BOLTZMANN NEUTRON TRANSPORT EQUATION

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ABSTRACT

Space-time flux synthesis methods for the approximate solution of the time-dependent Boltzmann neutron transport equation are formulated in this report. The variational and the Galerkin techniques are used. The space-dependent part of the solution is obtained with the DTF-II program – an Sn-type solution of the transport equation. Temperature feedback effects are considered in the formulation. The formulation presented here is adapted to the description of rapid transients following a large reactivity input, but the method can be easily modified to cover other reactor problems where a space-time flux description is necessary. It should be useful whenever the situation requires the transport approximation for the description of the neutron flux.

I. INTRODUCTION

Solution of the neutron migration problem in a nuclear reactor is usually obtained by straightforward finite difference approximation techniques of the equations involved. These methods are well established, and there are many codes which provide the desired solutions. There are instances, however, when the use of available computers for solving the neutron migration problem would result in prohibitive expense due to the lengthy time required to make the computations. Examples of these situations are: (1) calculation of two- or three-dimensional detailed flux shapes in complex geometries, and (2) description of the nonseparable space-time behavior of the neutron flux in several types of reactor transients. In such situations, it is convenient to have techniques available which will give a reasonably accurate description of the neutron behavior and yet cost only a fraction of the equivalent "exact" calculation.

The flux synthesis methods used here are approximate calculational techniques which satisfy these requirements. Several such methods have been developed and applied to the calculation of neutron fluxes in a reactor.[1] These "new" flux synthesis methods are improvements over the conventional or "old" flux synthesis methods from which the generic name was derived.[2] All are special cases of the mathematical technique referred to as: The Method of Weighted Residuals.[1,3] The basic assumption of the synthesis methods is that the neutron flux φ in several variables, for example, two space variables x,y and the time t, can be adequately approximated by a function, $\overline{\varphi}$, defined by

$$\varphi(x,y,t) \approx \overline{\varphi}(x,y,t) = \sum_{i=1}^{K} H_i(x,y)T_i(t) \qquad \ldots(1)$$

where $H_i(x,y)$ are given functions of some of the variables x,y, and $T_i(t)$ are unknown functions of the remaining variable, t, that have to be determined.

The method of weighted residuals is a procedure used to determine these unknown functions, consisting of the following steps. First $\overline{\varphi}(x,y,t)$ in Equation 1 is multiplied by an arbitrary weight function $W_j(x,y)$. This product is then entered into the equations for the problem in lieu of $\varphi(x,y,t)$, and integrated over the variables x and y. This process results in one differential equation in the unknown functions $T_i(t)$. Repeating the same procedure with all the members of a set of K arbitrary weight functions $W_j(j = 1, 2, \ldots, K)$, a system of K simultaneous total differential equations in the unknown functions $T_i(t)$ is obtained. The solution to this system of differential equations is the solution to the problem.

The functions $H_i(x,y)$ are usually called trial functions, whereas $T_i(t)$ are the "mixing" functions. The several weighted residual methods developed differ by the choice of weight functions used. Choice of trial functions is also arbitrary, giving place to many different variations of the method even when a particular selection of weight functions has been made. In the Galerkin synthesis method, the weight functions W_j are the same as those chosen as trial functions $W_j \equiv H_j(x,y)$. In the variational synthesis method (when applied to the neutron transport problem), a bilinear functional is set up. Its Euler equations are the neutron migration equation, and the adjoint equation which is

closely related. The solution $\varphi^*(x,y,t)$ of this adjoint equation is approximated by a function $\bar{\varphi}^*(x,y,t)$:

$$\varphi^*(x,y,t) \simeq \bar{\varphi}^*(x,y,t) = \sum_{j=1}^{K} H_j^*(x,y)T_j^*(t). \qquad \ldots(2)$$

The trial functions $H_j^*(x,y)$ used in the adjoint solution are then chosen as the weight functions for the direct problem. Similarly when solving for the adjoint function $\varphi^*(x,y,t)$, the trial functions $H_i(x,y)$ are used as weight functions for the adjoint problem. When the equation is self-adjoint, both Galerkin and variational methods are identical.

Other weighted residuals flux synthesis methods that have been developed are: the multiple spot method, the region balance method, and the least squares variational method.[1,4]

Several authors have reported successful applications of these techniques to the calculations of detailed two- or three-dimensional flux shapes and to the space-time description of the neutron flux in reactor transients.

S. Kaplan[1] applied several of these methods to the flux calculation in a two-dimensional core consisting of three regions: a rod-out core region, a rod-in core region, and a reflector. The trial functions used were one-dimensional, asymptotic space shapes for each one of the regions.[5] The results obtained for the flux shape and eigenvalue with both the Galerkin and variational syntheses were very good as compared to a PDQ (two-dimensional diffusion code) calculation of the same test case.

S. Kaplan and J. A. Bewick[6] applied the Galerkin technique to study the three-dimensional flux distribution on a model of the Shippingport Pressurized Water Reactor (PWR). They were able to reproduce very well the flux shapes predicted with the TKO code — a three-dimensional diffusion code,[7] but only after some trial and error in their choices of trial functions. This made clear how important it is to have a feeling for the kind of solutions expected when working with this type of approximating technique. In the same paper these authors developed a space-time variational technique for the diffusion equation, based on a functional proposed by Dougherty and Shen.[8] Its application in a two-energy group version to a flux tilt test case was in excellent agreement with the calculation of the same test case with Wigle[9] — a time dependent two-group slab geometry finite difference solution of the diffusion equations.

Yasinsky and Henry[10] have reported another set of test cases using the same space-time synthesis scheme. It was applied to the prediction of fluxes in a couple of bare cores in which asymmetric changes in properties induced a nonseparable transient behavior of the neutron flux. Of all the approximate methods used by them to calculate the flux (point kinetics, adiabatic, nodal, and modal methods) the flux synthesis compared best with the corresponding WIGLE calculations. In the case of a bare slab, 60 cm thick, in which a step insertion of $\$\simeq 2.5$ was followed by a ramp taking the reactivity back to zero at 0.01 sec, the calculation of the flux using three trial functions produced deviations from the "correct" value of less than 15%. The point kinetics model gave very poor

results in these tests, but as the authors point out, since feedback effects were not taken into account it is difficult to draw any quantitative conclusions from their data.

H. Fenech and V. Orphan have reported an application of the variational techniques to the study of a step insertion of reactivity with a linear temperature-dependent reactivity feedback, but without spatial dependence.[11] The temperature was included explicitly as one of the variational independent variables. The results obtained with the Galerkin method, the variational method, and the least squares method[4] are very similar in the accuracy attained. All methods predicted peak power and pulse duration with approximately 5% error.

Synthesis techniques as applied to the study of reactor burnup problems have also been reported. S. Kaplan, O. J. Marlowe, and J. Bewick[12] calculated the burnup characteristics of a three-dimensional model of the Shippingport PWR, using Galerkin synthesis. The nonlinear problem of burnup was treated as a sequence of linear problems. At each time step, the flux was synthetized. The rods were arranged in groups and withdrawn one group at a time. As a consequence, the space-time changes of the fluxes are quite complicated. The authors indicate that in order to picture these changes they had to follow an involved strategy in obtaining the several trial functions used. The results obtained for power distribution, eigenvalue, and fraction of power in the blanket region of the PWR as functions of time were excellent by comparison with a TNT-1 — three-dimensional depletion calculation.[13] Solution by the "exact" method required approximately 1 hr machine time using the Philco S-2000 for each time step. The synthesis required about one-third as much.

M. Becker and H. Fenech[14] have proposed a different treatment of the burnup problem. It is based on the least squares variational technique,[4] and a consistent account of the nonlinearity of the problem by treating the depletion equation as part of the variational principle. For a simplified one-dimensional (slab) depletion calculation, their results compare quite well with those obtained with FEVER — a one-dimensional depletion computer code.[15]

In this report, a space-time variational (or Galerkin) flux synthesis technique is developed for the time-dependent neutron transport equation. The space-angle energy description of the flux is obtained by means of DTF — an Sn-type solution of the stationary transport equations.[16] The time-dependence is synthetized. The variational principle differs from the one used previously; the form used here is the one proposed by Lewins.[16] In this formulation, the end point (final time) condition affects only the adjoint flux. The flux has to satisfy only an arbitrary initial condition.

The presence of feedback mechanisms can be included without formal complication in the Galerkin formulation. An analysis is presented of the complexities introduced in the variational formulation by feedback effects; and an approximate way of handling the problem is indicated and developed in detail in one of the appendices for a two-energy group, slab geometry synthesis in diffusion approximation.

The possible applications presented for the transport space-time synthesis scheme cover the same range of reactor problems as those reviewed in connection with the diffusion synthesis, and should be used whenever the transport approximation becomes necessary. The inclusion of feedback effects in the space-time description of neutron fluxes will make it possible to extend some of the studies previously reported to more realistic cases.[10,11]

II. VARIATIONAL METHOD

The general ideas of the variational method are well known. Here, only those features relevant to the present application will be developed directly. The time-dependent neutron transport equation can be written as follows:

$$L\varphi(\vec{r},\vec{\Omega},E,t) + \sum_{i=1}^{6} \lambda_i C_i(\vec{r},t) \frac{f_i(E)}{4\pi} = \frac{1}{v}\frac{\partial \varphi}{\partial t}, \qquad \ldots(3)$$

$$M_i\varphi(\vec{r},\vec{\Omega},E,t) - \lambda_i C_i(\vec{r},t) = \frac{\partial C_i}{\partial t}\,; \qquad \ldots(4)$$

with

$$L\varphi \equiv -\vec{\Omega}\cdot\nabla\varphi - \Sigma_T(\vec{r},E,t)\varphi + \int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega},E,\vec{\Omega}',E') + \frac{\chi(E)}{4\pi}(1-\beta)\nu\Sigma_f(\vec{r},E',t)\right]\varphi(\vec{r},\vec{\Omega}',E',t)\,d\vec{\Omega}'\,dE', \qquad \ldots(5)$$

$$M_i\varphi \equiv \beta_i \int_{\Omega}\int_{E} \nu\Sigma_f(\vec{r},E,t)\varphi(\vec{r},\vec{\Omega},E,t)\,d\vec{\Omega}\,dE\,; \qquad \ldots(6)$$

where

$\varphi(\vec{r},\vec{\Omega},E,t)$ = directional neutron flux, for point $\vec{r}$, direction $\vec{\Omega}$, energy E, at time t

$C_i(\vec{r},t)$ = i-th group delayed neutron precursor density at point $\vec{r}$ and time t

$\Sigma_T(\vec{r},E,t)$ = total neutron cross section of the reactor medium

$\Sigma_f(\vec{r},E,t)$ = fission cross section

$\Sigma_S(\vec{r},\vec{\Omega},E,\vec{\Omega}',E')$ = differential scattering cross section, for scattering from angle $\vec{\Omega}'$ and energy E' to angle $\vec{\Omega}$ and energy E

λ_i = i-th delayed neutron group decay constant

$f_i(E)$ = i-th delayed neutron group spectrum

β_i = i-th delayed neutron group fraction

$\beta = \Sigma\beta_i$

v = neutron speed

ν = neutrons produced per fission

$\chi(E)$ = fission spectrum

The flux $\varphi(\vec{r},\vec{\Omega},E,t)$ is subject to the boundary condition;

$$\varphi(\vec{R},\vec{\Omega},E,t) = 0 \qquad \text{for } \vec{\Omega}\cdot\vec{n} < 0 \qquad \ldots(7)$$

where

$\vec{R}$ = vector describing the reactor's external surface

$\vec{n}$ = outward-pointing normal to that surface

In addition, the following initial values are given:

$$\varphi(\vec{r},\vec{\Omega},E,o) = \varphi_o(\vec{r},\vec{\Omega},E) \qquad \ldots(8)$$

$$C_i(\vec{r},o) = C_{io}(\vec{r}) \qquad i = 1,2,\ldots,6, \qquad \ldots(9)$$

where φ_o and C_{io} are prescribed functions of space, angle, and energy.

The next step in setting up a variational principle for the neutron transport problem is the definition of a functional having a stationary property about the solution of Equations 3 and 4 with conditions 7, 8, and 9. For the time-dependent neutron transport or diffusion equations, functionals with this property are bilinear and not quadratic. Definition of the functional then implies using another set of functions, φ^* and C_i^*, the adjoint flux and adjoint precursor densities. As will be seen, the stationary property for the functional will imply another set of differential equations, and another set of boundary conditions for the adjoint functions. Following the formulation of the problem given by Lewins,[16] the functional chosen here is:

$$I\left\{\varphi, C_i, \varphi^*, C_i^*\right\} \equiv \int_o^{t_f}\int_r\int_\Omega\int_E \varphi^*(\vec{r},\vec{\Omega},E,t)\left[L\varphi(\vec{r},\vec{\Omega},E,t) + \sum_{i=1}^{6}\lambda_i C_i f_i - \frac{1}{v}\frac{\partial\varphi}{\partial t}\right]d\vec{r}\,dE\,d\vec{\Omega}\,dt$$

$$+ \sum_{i=1}^{6}\int_o^{t_f}\int_r C_i^*(\vec{r},t)\left[M_i\varphi - \lambda_i C_i(\vec{r},t) - \frac{\partial C_i}{\partial t}\right]d\vec{r}\,dt$$

$$+ \int_r\int_\Omega\int_E \frac{1}{v}\varphi(\vec{r},\vec{\Omega},E,t_f)\varphi^*(\vec{r},\vec{\Omega},E,t_f)\,d\vec{r}\,d\vec{\Omega}\,dE + \sum_{i=1}^{6}\int_r C_i(\vec{r},t_f)C_i^*(\vec{r},t_f)\,d\vec{r}. \qquad \ldots(10)$$

where t_f is a fixed final time up to which the solution of the problem is considered. The integrals in $\vec{r},\vec{\Omega}$, and E extend over the entire range of these variables within the reactor system.

If the function $\varphi^*(\vec{r},\vec{\Omega},E,t)$ satisfies the following boundary condition:

$$\varphi^*(\vec{R},\vec{\Omega},E,t) = 0 \qquad \text{for } \vec{\Omega}\cdot\vec{n} > 0, \qquad \ldots(11)$$

and $\vec{R}$ and $\vec{n}$ have the same meaning as in Equation 7, the functional I given in Equation 10 can be written in the following equivalent form (Appendix I)

$$I\left\{\varphi, C_i, \varphi^*, C_i^*\right\} \equiv \int_o^{t_f}\int_r\int_\Omega\int_E \varphi(\vec{r},\vec{\Omega},E,t)\left[L^*\varphi^*(\vec{r},\vec{\Omega},E,t) + \sum_{i=1}^{6}\beta_i\nu\Sigma_f C_i^* + \frac{1}{v}\frac{\partial\varphi^*}{\partial t}\right]d\vec{r}\,d\vec{\Omega}\,dE\,dt$$

$$+ \sum_{i=1}^{6}\int_o^{t_f}\int_r C_i(\vec{r},t)\left[M_i^*\varphi^* - \lambda_i C_i^* + \frac{\partial C_i^*}{\partial t}\right]d\vec{r}\,dt$$

$$+ \int_r\int_\Omega\int_E \frac{1}{v}\varphi(\vec{r},\vec{\Omega},E,o)\varphi^*(\vec{r},\vec{\Omega},E,o)\,d\vec{r}\,d\vec{\Omega}\,dE + \sum_{i=1}^{6}\int_r C_i(\vec{r},o)C_i^*(\vec{r},o)\,d\vec{r}\,, \qquad \ldots(12)$$

where

$$L^*\varphi^* \equiv \vec{\Omega}\cdot\nabla\varphi^* - \Sigma_T\varphi^* + \int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega}',E',\Omega,E) + \frac{\chi(E')}{4\pi}(1-\beta)\nu\Sigma_f(E)\right]\varphi^*(\vec{r},\vec{\Omega}',E',t)\,d\vec{\Omega}'\,dE' \qquad \ldots(13)$$

$$M_i^*\varphi^* \equiv \lambda_i\int_\Omega\int_E f_i(E)\varphi^*(\vec{r},\vec{\Omega},E,t)\,dE\,d\vec{\Omega}\,, \qquad \ldots(14)$$

and $\varphi(\vec{r},\vec{\Omega},E,o)$, $C_i(\vec{r},o)$, $\varphi^*(\vec{r},\vec{\Omega},E,o)$, $C_i^*(\vec{r},o)$ are the values at time $t = 0$.

For I to have a stationary value, it is a necessary and sufficient condition that the first order variation vanishes identically when it is induced by a first order variation in any of the independent functions, φ, C_i, φ^*, and C_i^*.

The variation induced in I by a variation in φ^* can be easily obtained using the form in Equation 10. It is:

$$\delta I\left\{\varphi, C_i, \delta\varphi^*, C_i^*\right\} \equiv \int_o^{t_f}\int_r\int_\Omega\int_E \delta\varphi^*\left[L\varphi^* + \sum_{i=1}^{6}\lambda_i C_i f_i - \frac{1}{v}\frac{\partial\varphi}{\partial t}\right]d\vec{r}\,d\vec{\Omega}\,dE\,dt$$

$$+ \int_r\int_\Omega\int_E \frac{1}{v}\varphi(\vec{r},\vec{\Omega},E,t_f)\delta\varphi^*(\vec{r},\vec{\Omega},E,t_f)\,d\vec{r}\,d\vec{\Omega}\,dE. \qquad \ldots(15)$$

The conditions to make $\delta I \equiv 0$ are:

$$L\varphi + \sum_{i=1}^{6}\lambda_i C_i f_i - \frac{1}{v}\frac{\partial\varphi}{\partial t} = 0$$

$$\delta\varphi^*(\vec{r},\vec{\Omega},E,t_f) = 0 \qquad \ldots(16)$$

The first condition is simply Equation 3, the neutron transport equation. The second condition means that the function $\varphi^*(\vec{r},\vec{\Omega},E,t)$ will have a definite t_f with a variation identically zero by definition.

The variation induced in I by a variation in a C_i^*, obtained also from Equation 10, is:

$$\delta I\left\{\varphi, C_i, \varphi^*, \delta C_i^*\right\} \equiv \int_o^{t_f}\int_r \delta C_i^*\left[M_i\varphi - \lambda_i C_i(\vec{r},t) - \frac{\partial C_i}{\partial t}\right]d\vec{r}\ dt + \int_r C_i(\vec{r},t_f)\delta C_i^*(\vec{r},t_f)\ d\vec{r}. \qquad \ldots(17)$$

The conditions to make $\delta I = 0$ are now:

$$M_i\varphi - \lambda_i C_i(\vec{r},t) - \frac{\partial C_i}{\partial t} = 0, \qquad \ldots(4)$$

$$\delta C_i^*(\vec{r},t_f) = 0 \qquad i = 1,2,\ldots,6, \qquad \ldots(18)$$

which are the equations for the delayed neutron precursors plus the condition that the values of $C_i^*(\vec{r},t_f)$ are prescribed at the final time $t = t_f$. The next step would be to consider the variations induced in I by variations in φ and C_i^*. Before proceeding with this derivation, it is necessary at this point, to realize that the variation induced in I by variations in φ and C_i's will depend on whether or not the parameters in Equations 3 and 4 are affected by the values of functions φ and C_i^*. In other words, the variation in I will depend on feedback effects.[17] When there is no feedback, the variation in φ will produce the following variation in I, obtained from Expression 12.

$$\delta I\left\{\delta\varphi, C_i, \varphi^*, C_i^*\right\} \equiv \int_o^{t_f}\int_r\int_\Omega\int_E \delta\varphi\left[L^*\varphi^* + \sum_{i=1}^{6}\beta_i\nu\Sigma_f C_i^* + \frac{1}{v}\frac{\partial\varphi^*}{\partial t}\right]d\vec{r}\ d\vec{\Omega}\ dE\ dt$$

$$+ \int_r\int_\Omega\int_E \frac{1}{v}\,\delta\varphi(\vec{r},\vec{\Omega},E,o)\varphi^*(\vec{r},\vec{\Omega},E,o)\,d\vec{r}\ d\vec{\Omega}\ dE. \qquad \ldots(19)$$

The conditions for $\delta I = 0$ are now:

$$L^*\varphi^* + \sum_{i=1}^{6}\beta_i\nu\Sigma_f C_i^* = -\frac{1}{v}\frac{\partial\varphi^*}{\partial t}, \qquad \ldots(20)$$

$$\delta\varphi(\vec{r},\vec{\Omega},E,o) = 0. \qquad \ldots(8a)$$

Equation 20 is the adjoint equation in this case (no feedback), and the second condition expresses the fact that the initial value of the neutron flux is given. The variation produced by a δC_i is:

$$\delta I\left\{\varphi,\delta C_i,\varphi^*,C_i^*\right\} \equiv \int_o^{t_f}\int_r \delta C_i\left[M_i^*\varphi^* - \lambda_i C_i^* + \frac{\partial C_i^*}{\partial t}\right]d\vec{r}\,dt + \int_r \delta C_i(\vec{r},o)C_i^*(\vec{r},o)\,d\vec{r}\,; \qquad \ldots(21)$$

and the vanishing conditions this time are:

$$M_i^*\varphi^* - \lambda_i C_i^* + \frac{\partial C_i^*}{\partial t} = 0\,; \qquad \ldots(22)$$

$$\delta C_i(\vec{r},o) = 0 \qquad i = 1,2,\ldots,6. \qquad \ldots(9a)$$

These equations are the adjoint-delayed precursor differential equations. The other condition is an equivalent way of writing Equation 9.

Solution of the variational problem presented here is equivalent to a solution of the original differential equation problem plus the solution of the adjoint problem, as represented by Equations 20 and 22 subject to the conditions in Equations 11, 16, and 18. When the parameters in Equations 3 and 4 depend in some way on the neutron flux, the direct problem (Equations 3 and 4) becomes nonlinear. The equations for the adjoint problem in this case are no longer 20 and 22. The variation induced in Equation 12 by a variation in φ takes a different mathematical form and consequently, the stationary condition — the adjoint flux equation — also has a different form. Moreover, to calculate the time-dependent coefficients of the adjoint equation, it is necessary to know the solution to the direct problem: $\varphi(t)$. The adjoint equations remain linear, and the boundary conditions are not affected.

A detailed discussion of feedback effects on the variational formulation for a simple model is given in Appendix II.

III. THE APPROXIMATION PROCEDURE

The flux synthesis variational method is an example of the approximative technique of variational calculus referred to, usually, as the semidirect method,[18] or Kantorovich method.[19,20] It is a natural extension of the "direct" method of Rayleigh-Ritz. Here, the trial solution contains unknown functions rather than unknown scalars, as are used in the direct method.

The first step in the approximation procedure is to cast the problem into the energy multigroup formulation. This transformation can be carried out consistently in the variational approach, as has been pointed out by Selengut.[21]

It is assumed that both the flux φ and the adjoint φ^* can be expressed in the following way:

$$\varphi(\vec{r},\vec{\Omega},E,t) = \varphi_g(\vec{r},\vec{\Omega},t)\epsilon(E); \qquad E_{g-1} \le E \le E_g \qquad \ldots(23)$$

$$\varphi^*(\vec{r},\vec{\Omega},E,t) = \varphi_g^*(\vec{r},\vec{\Omega},t)\epsilon^*(E); \qquad g = 1,2,\ldots,G \qquad \ldots(24)$$

$$\int_{E_{g-1}}^{E_g} \epsilon(E)\,dE = 1; \qquad \text{where } E_g\text{'s are the energy group boundaries and G is the number of energy groups} \qquad \ldots(25)$$

$$\int_{E_{g-1}}^{E_g} \epsilon^*(E)\epsilon(E)\,dE = 1; \qquad \ldots(26)$$

which are the energy multigroup approximations of flux and adjoint. $\epsilon(E)$ and $\epsilon^*(E)$ are prescribed energy functions, the trial functions for this case. As yet, the $\varphi_g(\vec{r},\vec{\Omega},t)$ and $\varphi_g^*(\vec{r},\vec{\Omega},t)$ functions are unknown. These will be determined by requiring the functional to have a stationary value, and be subject to the same set of initial and boundary conditions specified for the variational problem.

Introducing Equations 23 and 24 into Equation 10 for the functional, then integrating over the energy, takes the form: (Delayed neutron precursors are dropped for simplicity.)

$$I\{\varphi_g,\varphi_g^*\} \equiv \sum_{g=1}^{G}\left(\int_r\int_\Omega d\vec{r}\,d\vec{\Omega}\left\{\int_o^{t_f} dt\left[-\varphi_g^*(\vec{r},\vec{\Omega},t)\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega},t) - \varphi_g^*\Sigma_{Tg}(\vec{r},t)\varphi_g - \frac{1}{v_g}\varphi_g^*\frac{\partial\varphi_g}{\partial t}\right.\right.\right.$$

$$\left.\left.\left. + \sum_{g'=1}^{G}\int_{\Omega'} d\vec{\Omega}'\left\langle\Sigma_{Sgg'}(\vec{r},\vec{\Omega},\vec{\Omega}') + \frac{\chi_g}{4\pi}(1-\beta)\nu\Sigma_{fg'}(\vec{r},t)\right\rangle\varphi_g^*(\vec{r},\vec{\Omega},t)\varphi_{g'}(\vec{r},\vec{\Omega}',t)\right]\right.\right.$$

$$\left.\left. + \frac{1}{v_g}\varphi_g^*(\vec{r},\vec{\Omega},t_f)\varphi_g(\vec{r},\vec{\Omega},t_f)\right\}\right). \qquad \ldots(27)$$

This is the multigroup form of the functional, where:

$$\Sigma_{Tg}(\vec{r},t) = \int_{E_{g-1}}^{E_g} \Sigma_T(\vec{r},E,t)\epsilon^*(E)\epsilon(E)\,dE\,; \qquad \ldots(28)$$

$$\frac{1}{v_g} = \int_{E_{g-1}}^{E_g} \frac{1}{v(E)}\,\epsilon^*(E)\epsilon(E)\,dE\,; \qquad \ldots(29)$$

$$\Sigma_{Sgg'}(\vec{r},\vec{\Omega},\vec{\Omega}') = \int_{E_{g-1}}^{E_g}\int_{E_{g'-1}}^{E_{g'}} \Sigma_S(\vec{r},\vec{\Omega},E,\vec{\Omega}',E')\epsilon^*(E)\epsilon(E')\,dE\,dE'\,; \qquad \ldots(30)$$

$$\chi_g = \int_{E_{g-1}}^{E_g} \chi(E)\epsilon^*(E)\,dE\,; \qquad \ldots(31)$$

$$\Sigma_{fg'}(\vec{r},t) = \int_{E_{g'-1}}^{E_{g'}} \Sigma_f(\vec{r},E',t)\epsilon(E')\,dE'\,. \qquad \ldots(32)$$

$\varphi_g^*(\vec{r},\vec{\Omega},t_f)$, $\varphi_g(\vec{r},\vec{\Omega},t_f)$ are final values of φ_g^* and φ_g. Operating on the form of the functional in Equation 12, the following equivalent expression is obtained:

$$I\left\{\varphi_g^*,\varphi_g\right\} \equiv \sum_{g=1}^{G}\left(\int_r\int_\Omega d\vec{r}\,d\vec{\Omega}\left\{\int_o^{t_f} dt\left[\varphi_g(\vec{r},\vec{\Omega},t)\vec{\Omega}\cdot\nabla\varphi_g^*(\vec{r},\vec{\Omega},t) - \varphi_g\Sigma_{Tg}(\vec{r},t)\varphi_g^* + \frac{1}{v_g}\varphi_g\frac{\partial\varphi_g^*}{\partial t}\right.\right.\right.$$

$$\left.\left.\left. + \sum_{g'=1}^{G}\int_{\Omega'} d\Omega'\left\langle \Sigma_{Sg'g}(\vec{r},\vec{\Omega}',\vec{\Omega}) + \frac{\chi_{g'}}{4\pi}(1-\beta)\nu\Sigma_{fg}(\vec{r},t)\right\rangle\varphi_g^*(\vec{r},\vec{\Omega}',t)\varphi_g(\vec{r},\vec{\Omega},t)\right]\right.\right.$$

$$\left.\left. + \frac{1}{v_g}\varphi_g^*(\vec{r},\vec{\Omega},o)\varphi_g(\vec{r},\vec{\Omega},o)\right\}\right), \qquad \ldots(33)$$

having the same definitions for the parameters.

Imposing the stationary condition for the functional with respect to variations in the independent functions $\varphi_g(\vec{r},\vec{\Omega},t)$, or $\varphi_g^*(\vec{r},\vec{\Omega},t)$ results in a system of coupled differential equations to be satisfied by the φ_g's, and φ_g^*'s. For the φ_g's, the system is:

$$-\vec{\Omega}\cdot\nabla\varphi_g(\vec{r},\vec{\Omega},t) - \Sigma_{Tg}\varphi_g + \sum_{g'=1}^{G}\int_{\Omega'}\left[\Sigma_{Sgg'}(\vec{r},\vec{\Omega},\vec{\Omega}') + \frac{\chi_g}{4\pi}(1-\beta)\nu\Sigma_{fg'}(\vec{r},t)\right]\varphi_{g'}(\vec{r},\vec{\Omega}',t)\,d\vec{\Omega} = \frac{1}{v_g}\cdot\frac{\partial\varphi_g(\vec{r},\vec{\Omega},t)}{\partial t}$$

$$g = 1,2,\ldots,G, \qquad \ldots(34)$$

which is the multigroup form of the neutron transport equation. The only difference with the regular formulation[21] is that the group constants have been weighted with both flux and an adjoint spectrum. The usual form of the multigroup equations corresponds to a particular choice of the adjoint trial functions $\epsilon_g^*(E)$:

$$\epsilon_g^*(E) = 1 \qquad g = 1,2,\ldots,G. \qquad \ldots(35)$$

A. SPACE-TIME APPROXIMATION

The next step in the variational approximation is the assumption that each one of the functions $\varphi_g(\vec{r},\vec{\Omega},t)$ and $\varphi_g^*(\vec{r},\vec{\Omega},t)$ can be approximated as follows:

$$\varphi_g(\vec{r},\vec{\Omega},t) = \sum_{j=1}^{K_g} N_g^j(\vec{r},\vec{\Omega})T_g^j(t) \qquad g = 1,2,\ldots,G; \qquad \ldots(36)$$

$$\varphi_g^*(\vec{r},\vec{\Omega},t) = \sum_{i=1}^{K_g} N_g^{i*}(\vec{r},\vec{\Omega})T_g^{i*}(t) \qquad g = 1,2,\ldots,G. \qquad \ldots(37)$$

Trial functions $N_g^j(\vec{r},\vec{\Omega})$, and $N_g^{i*}(\vec{r},\vec{\Omega})$ are given, and the stationary property of the functional is used to determine the unknown time functions $T_g^j(t)$, and $T_g^{i*}(t)$. The choice of trial functions in Equations 36 and 37 is essentially arbitrary, both in number and type. Each choice will result, of course, in a different set of "mixing" functions T_g, T_g^*. There is no fixed procedure to select a "best" set of trial functions for a particular problem, and only experimentation can offer the answer. One successful method has been the use of N_g^j's, and N_g^{i*}'s as the stationary and asymptotic solutions of the reactor time-independent equations. When material conditions in the reactor change appreciably with time, e.g., burnup problems, temperature feedback, xenon poisoning, it may be convenient to use more than one possible asymptotic solution.

For the present general formulation, the N_g^j's, and N_g^{i*}'s are simply known functions of $\vec{r}$ and $\vec{\Omega}$. Introducing Equations 36 and 37 into 27, and then integrating over $\vec{r}$ and $\vec{\Omega}$, the functional takes the form:

$$I\left\{T_g^j, T_g^{i*}\right\} \equiv \sum_{g=1}^{G}\sum_{i=1}^{K_g}\sum_{j=1}^{K_g}\left(\int_o^{t_f}\left\{\left[-L_g^{ij} - A_g^{ij}(t)\right]T_g^{i*}(t)T_g^j(t) + \sum_{g'=1}^{G}\left[S_{gg'}^{ij}(t)T_g^{i*}T_g^i\right] - \frac{I_g^{ij}}{v_g}T_g^{i*}\frac{dT_g^j}{dt}\right\}dt + \frac{I_g^{ij}}{v_g}T_g^{i*}(t_f)T_g^j(t_f)\right), \qquad \ldots(38)$$

where

$$\int_r\int_\Omega N_g^{i*}(\vec{r},\vec{\Omega})\vec{\Omega}\cdot\nabla N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv L_g^{ij}; \qquad \ldots(39)$$

$$\int_r\int_\Omega N_g^{i*}(\vec{r},\vec{\Omega})\Sigma_{Tg}(\vec{r},t)N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv A_g^{ij}(t); \qquad \ldots(40)$$

$$\int_r\int_\Omega\int_{\Omega'} N_g^{i*}(\vec{r},\vec{\Omega})\left\langle \Sigma_{Sgg'}(\vec{r},\vec{\Omega}',\vec{\Omega}) + \frac{\chi_{g'}}{4\pi}\nu(1-\beta)\Sigma_{fg}(\vec{r},t)\right\rangle N_{g'}^j(\vec{r},\vec{\Omega}')\,d\vec{\Omega}'\,d\vec{\Omega}\,d\vec{r} \equiv S_{gg'}^{ij}(t); \qquad \ldots(41)$$

$$\int_r\int_\Omega N_g^{i*}(\vec{r},\vec{\Omega})N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv I_g^{ij}. \qquad \ldots(42)$$

An equivalent expression for the functional is obtained when Equations 36 and 37 are introduced into 33.

Imposing the stationary property on the functional, the following set of necessary and sufficient conditions is obtained:

For the $T_g(t)$ functions

$$\sum_{j=1}^{K_g}\left\{\left[-L_g^{ij} - A_g^{ij}(t)\right]T_g^j(t) + \sum_{g'=1}^{G}\left[S_{gg'}^{ij}(t)T_{g'}^j(t)\right] - \frac{I_g^{ij}}{v_g}\cdot\frac{dT_g^j}{dt}\right\} = 0; \qquad \ldots(43)$$

$$i = 1,2,\ldots,K_g$$

$$g = 1,2,\ldots,G;$$

and at time $t = 0$

$$T_g^j(o) \text{ are given (initial condition).} \qquad \ldots(44)$$

For the $T_g^{i*}(t)$ functions in the linear case

$$\sum_{i=1}^{K_g}\left\{\left[+L_g^{ij} - A_g^{ij}(t)\right]T_g^{i*}(t) + \sum_{g'=1}^{G}\left[S_{g'g}^{ij}(t)T_{g'}^{i*}\right] + \frac{I_g^{ij}}{v_g}\cdot\frac{dT_g^{i*}}{dt}\right\} = 0; \qquad \ldots(45)$$

$$j = 1,2,\ldots,K_g$$

$$g = 1,2,\ldots,G;$$

and at time $t = t_f$

$$T_g^{j*}(t_f) \text{ are given (final condition).} \qquad \ldots(46)$$

The system of ordinary differential Equations 43 and 45 with end point conditions in Equations 44 and 46 when solved for the unknown functions $T_g^j(t)$, and $T_g^{i*}(t)$, represent the solution to the variational problem and to the closely related physical problem of neutron transport. The approximate solution to the neutron flux Equation 3 can then be reconstructed using Equations 36 and 23. Similarly the adjoint can be reconstructed if necessary using Equations 37 and 24.

It is opportune at this point to note that the mathematical form of Equation 43 would be the same if, instead of using the variational flux synthesis, any of the other weighted residual techniques had been used.[1,3] Differences between the several approaches are reflected in the definition of parameters appearing in the equation. For example, in the Galerkin synthesis method, in which the weight functions are the flux functions themselves, the coefficients in Equation 43 would be:

$$\int_r\int_\Omega N_g^i(\vec{r},\vec{\Omega})\vec{\Omega}\cdot\nabla N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv L_g^{ij}\,; \qquad \ldots(39')$$

$$\int_r\int_\Omega N_g^i(\vec{r},\vec{\Omega})\Sigma_{Tg}(\vec{r},t)N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv A_g^{ij}(t)\,; \qquad \ldots(40')$$

$$\int_r\int_{\Omega'}\int_\Omega N_g^i(\vec{r},\vec{\Omega})\left\langle \Sigma_{Sgg'}(\vec{r},\vec{\Omega},\vec{\Omega}') + \frac{\chi_g}{4\pi}\nu(1-\beta)\Sigma_{fg}(\vec{r},t)\right\rangle N_{g'}^j(\vec{r},\vec{\Omega}')\,d\vec{r}\,d\vec{\Omega}\,d\vec{\Omega}' \equiv S_{gg'}^{ij}(t); \qquad \ldots(41')$$

$$\int_r\int_\Omega N_g^i(\vec{r},\vec{\Omega})N_g^j(\vec{r},\vec{\Omega})\,d\vec{r}\,d\vec{\Omega} \equiv I_g^{ij}\,. \qquad \ldots(42')$$

The form of Equation 43 that would be obtained when using the neutron diffusion equation to formulate the problem is naturally the same, as time-dependence is treated in the same way in both transport and diffusion formulations. The main change would be in the definition of the L_g^{ij} coefficients where the angular treatment is implicit. Feedback effects would result in more basic changes in Equations 43 and 45. The form of Equation 43 would not change, but the coefficients would then be functions of the flux, or temperature. In this mode, the equation would be nonlinear. In any of the weighted residual techniques, except in the variational technique, this would be the only change introduced by a temperature feedback.

In the variational flux synthesis, the presence of feedback will produce changes in the adjoint flux equations. Equations in 45 will have extra terms, and their coefficients will be determined by the solution of the direct problem. The linear character of the equations is conserved.

B. SOLUTION OF THE SYSTEM OF DIFFERENTIAL EQUATIONS

Before attempting numerical integration of the system of Equations 43 or 45, it is convenient to manipulate them into a more tractable algebraic form. Written as they are, there are K_g equations

for each energy group, and a total of

$$K_1 + K_2 + \ldots + K_g + \ldots + K_G = K \qquad \ldots(47)$$

differential equations.

Correspondingly there are K unknown functions $T_g^j(t)$. For each group the coefficients L_g^{ij}, $A_g^{ij}(t)$, and I_g^{ij} can be arranged in matrix form: $\left[L_g^{ij}\right]$, $\left[A_g^{ij}(t)\right]$, and $\left[I_g^{ij}\right]$; each a square matrix of order K_g. If the unknown functions T_g are arranged as a column vector with K components:

$$T \equiv \begin{bmatrix} T_1^1 \\ T_1^2 \\ \vdots \\ T_1^{K_1} \\ \vdots \\ T_g^1 \\ T_g^2 \\ \vdots \\ T_g^{K_g} \\ \vdots \\ T_G^1 \\ T_G^2 \\ \vdots \\ T_G^{K_G} \end{bmatrix} \qquad \ldots(48)$$

and the matrices $\left[L_g^{ij}\right]$, $\left[A_g^{ij}(t)\right]$, $\left[I_g^{ij}\right]$ are arranged in quasi-diagonal matrices of order K, $[L]$, $[A(t)]$, and $[I]$ as follows:

$$[L] \equiv \begin{bmatrix} \left[L_1^{ij}\right] & 0 \ldots 0 \\ 0 & \left[L_2^{ij}\right] \\ \vdots & \ddots \\ 0 & \ddots \left[L_G^{ij}\right] \end{bmatrix}, \qquad \ldots(49)$$

$$[A(t)] \equiv \begin{bmatrix} \left[A_1^{ij}(t)\right] & 0 \ldots 0 \\ 0 & \left[A_2^{ij}(t)\right] \\ \vdots & \ddots \\ 0 & \ddots \left[A_G^{ij}(t)\right] \end{bmatrix}, \qquad \ldots(50)$$

$$[I] \equiv \begin{bmatrix} \left[I_1^{ij}\right] & 0 \ldots 0 \\ 0 & \left[I_2^{ij}\right] \\ \vdots & \ddots \\ 0 & \cdot \left[I_G^{ij}\right] \end{bmatrix}. \qquad \ldots(51)$$

The system of Equations in 43 can be written as:

$$[I]\frac{dT}{dt} = \left\{[L] - [A(t)] + [S(t)]\right\} T, \qquad \ldots(52)$$

where S is a matrix of order K defined with the elements $S_{gg'}^{ij}$. To obtain explicit differential equations in each one of the components of T (T_g^j functions), it is necessary to obtain an explicit expression for dT/dt.

Multiplying Equation 52 by $\left[I^{-1}\right]$, the inverse of $[I]$:

$$\frac{dT}{dt} = [I]^{-1}\left\{[L] - [A(t)] + [S(t)]\right\} T, \qquad \ldots(53)$$

the desired form is obtained. The inversion of matrix I is performed only once at the start of the calculation, as it is a constant matrix and independent of feedback. Furthermore, its inversion is greatly simplified by its quasi-diagonal character. The inversion problem is not that of inverting a matrix of order K, but instead is the inversion of G submatrices of orders $K_1, K_2, \ldots, K_G$.

Numerical Integration

The system of equations in 53 is in a form suitable to integrate numerically. There are several numerical techniques available that could be used to perform the integration. An essentially stable, high order method, with a variable time step like the predictor-corrector technique in Reference 23, would be generally advisable. In practice the integration method used will depend to some extent on the characteristics of the system matrix.

In the nonlinear cases where the system matrix is a function of the unknown, it will be necessary to recalculate it as the calculation proceeds. How often this recalculation should be made and to what extent the recalculation can be expedited will depend on the particular kind of feedback considered and on the linking equations expressing it.

C. CALCULATION OF COEFFICIENT MATRIX ELEMENTS FROM DTF-II OUTPUT

Trial functions entering in the definitions of the coefficients for the variational synthesis, Equations 39 through 42, or for the Galerkin synthesis 39′ through 42′ are obtained by a DTF-II transport calculation. These $N_g^j(\vec{r},\vec{\Omega})$ and $N_g^{i*}(\vec{r},\vec{\Omega})$ functions are defined by their values on a space-angle mesh, $N_{g\ell\alpha}^j$, $N_{g\ell\alpha}^*$. (ℓ indicates the space mesh point, and α, the angular mesh point.)

It is necessary then to rewrite Equations 39 through 43 in some equivalent finite difference form, using these $N_{g\ell\alpha}^j$, $N_{g\ell\alpha}^{i*}$ values. The finite difference forms obtained are:

$$L_g^{ij} = \pi \sum_\ell \sum_\alpha \Big\langle \tfrac{1}{2} \mu_\alpha W_\alpha \left[N^{i*}_{g\ell\alpha} + N^{i*}_{g(\ell-1)\alpha}\right]\left[r_\ell + r_{\ell-1}\right]\left[N^j_{g\ell\alpha} - N^j_{g(\ell-1)\alpha}\right]$$

$$+ \eta_\alpha \Delta_\ell \left\{N^{i*}_{g\ell\alpha}\left[N^j_{g\ell\alpha^*} - N^j_{g\ell(\alpha^*-1)}\right] + N^{i*}_{g(\ell-1)\alpha}\left[N^j_{g(\ell-1)\alpha^*} - N^j_{g(\ell-1)(\alpha^*-1)}\right]\right\}\Big\rangle ; \qquad \ldots(54)$$

$$A_g^{ij}(t) = \tfrac{1}{2} \sum_\ell \left\langle \Delta\ell \Sigma_{Tg\ell}(t) \left\{ \sum_\alpha W_\alpha \left[N^{i*}_{g\ell\alpha} N^j_{g\ell\alpha} + N^{i*}_{g(\ell-1)\alpha} N^j_{g(\ell-1)\alpha}\right]\right\} \right\rangle ; \qquad \ldots(55)$$

$$S^{ij}_{gg'}(t) = \tfrac{1}{2} \sum_\ell \left\langle \Delta\ell \left\{ \sum_\alpha \sum_{\alpha'} W_\alpha W_{\alpha'} \Sigma_{S\ell g g' \alpha\alpha'} \left[N^{i*}_{g\ell\alpha} N^j_{g'\ell\alpha} + N^{i*}_{g(\ell-1)\alpha} N^j_{g(\ell-1)\alpha'}\right]\right\} \right\rangle ; \qquad \ldots(56)$$

$$I_g^{ij} = \tfrac{1}{2} \sum_\ell \left\langle \Delta\ell \left\{ \sum_\ell W_\alpha \left[N^{i*}_{g\ell\alpha} N^j_{g\ell\alpha} + N^{i*}_{g(\ell-1)\alpha} N^j_{g(\ell-1)\alpha}\right]\right\} \right\rangle . \qquad \ldots(57)$$

Details of the transformation from the continuous to the discrete expressions, and definitions of the symbols used in Formulas 54 through 57 are given in Appendix III.

D. ACCURACY OF THE METHODS

The accuracy in the results obtained with any of the weighted residual methods depends on the choice of a "good" set of trial functions. There is no "best" general recipe in selecting good trial functions for a problem. Only experience and intuition can guide the selection of trial functions for a particular problem. Serious numerical difficulties can also arise if an improper choice of trial functions is made, as described by S. Kaplan, et al.[24]

The simple expedient of increasing the number of trial functions may work, but is not a guarantee in improvement of the accuracy — not even in the variational method where it would be natural to expect this. The functional is bilinear, and as such, it is stationary around a saddle point, not an extremum.[25] Consequently, the error may simply change sign when a new set of trial functions is used, without becoming smaller. Also, as has been pointed out by Becker,[26] when the functional is not a positive definite mathematical expression, accuracy can be obtained through cancellation of errors. The flux and adjoints may then be significantly in error even when yielding the correct functional value.

The best way to gain confidence in the results obtained with the synthesis method is by comparison with results from an "exact" calculation of the same test case. This has been the regular practice in all the developments reported here, and should be done whenever possible.

APPENDIX I
EQUIVALENCE OF FORMS IN EQUATIONS 10 AND 12

The first term in Equation 10 is

$$-\int_o^{t_f}\int_r\int_\Omega\int_E \varphi^*(\vec{r},\vec{\Omega},E,t)\vec{\Omega}\cdot\vec{\nabla}\varphi(\vec{r},\vec{\Omega},E,t)\,d\vec{r}\,d\vec{\Omega}\,dE\,dt\,. \qquad \ldots(I\text{-}1)$$

Its integrand can be rewritten using the following identity

$$\vec{\nabla}\cdot(\vec{\Omega}\varphi\varphi^*) = \varphi\varphi^*\vec{\nabla}\cdot\vec{\Omega} + \vec{\Omega}\cdot\vec{\nabla}(\varphi\varphi^*) = \varphi\vec{\Omega}\cdot\vec{\nabla}\varphi^* + \varphi^*\vec{\Omega}\cdot\vec{\nabla}\varphi\,, \qquad \ldots(I\text{-}2)$$

or

$$\varphi^*\vec{\Omega}\cdot\vec{\nabla}\varphi = \vec{\nabla}\cdot(\vec{\Omega}\varphi\varphi^*) - \varphi\vec{\Omega}\cdot\vec{\nabla}\varphi^*\,. \qquad \ldots(I\text{-}3)$$

Moreover, the integral

$$\int_r \vec{\nabla}\cdot(\vec{\Omega}\varphi\varphi^*)\,d\vec{r} = \int_S (\vec{n}\cdot\vec{\Omega})\varphi(\vec{R},\vec{\Omega})\varphi^*(\vec{R},\vec{\Omega})\,ds\,, \qquad \ldots(I\text{-}4)$$

by Gauss divergence theorem; where S is the external surface of the reactor, $\vec{n}$ its normal, $\vec{R}$ a vector describing it, and ds the surface differential.

Clearly if $\varphi(\vec{R},\vec{\Omega})$ and $\varphi^*(\vec{R},\vec{\Omega})$ satisfy conditions in Equations 7 and 11, the integral in Equation I-4 is zero for any direction $\vec{\Omega}$. Equation I-1 is then transformed into

$$\int_o^{t_f}\int_r\int_\Omega\int_E \varphi(\vec{r},\vec{\Omega},E,t)\vec{\Omega}\cdot\vec{\nabla}\varphi^*(\vec{r},\vec{\Omega},E,t)\,d\vec{r}\,d\vec{\Omega}\,dE\,dt\,. \qquad \ldots(I\text{-}5)$$

The second term in Equation 10 is not transformed; it keeps its form.

$$-\int_o^{t_f}\int_r\int_\Omega\int_E \varphi(\vec{r},\vec{\Omega},E,t)\Sigma_T(\vec{r},E,t)\varphi^*(\vec{r},\vec{\Omega},E,t)\,d\vec{r}\,d\vec{\Omega}\,dE\,dt\,. \qquad \ldots(I\text{-}6)$$

The third term in Equation 10 is

$$\int_o^{t_f}\int_r\int_\Omega\int_E \varphi^*(\vec{r},\vec{\Omega},E,t)\left\{\int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega},E,\Omega',E') + \frac{\chi(E)}{4\pi}(1-\beta)\nu\Sigma_f(\vec{r},E',t)\right]\varphi(\vec{r},\vec{\Omega}',E',t)\,d\vec{\Omega}'\,dE'\right\}d\vec{r}\,d\vec{\Omega}\,dE\,dt. \qquad \ldots(I\text{-}7)$$

In the definite integral

$$\int_{\Omega}\int_{E}\int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega},E,\vec{\Omega}',E') + \frac{\chi(E)}{4\pi}(1-\beta)\nu\Sigma_f(\vec{r},E',t)\right]\varphi(\vec{r},\vec{\Omega}',E',t)\varphi^*(\vec{r},\vec{\Omega},E,t)\,d\vec{\Omega}\,dE\,d\vec{\Omega}'\,dE'; \quad \ldots(I\text{-}8)$$

the name of the mute variables can be interchanged without altering the value of the integral, so it is equal to

$$\int_{\Omega}\int_{E}\int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega}',E',\vec{\Omega},E) + \frac{\chi(E')}{4\pi}(1-\beta)\nu\Sigma_f(\vec{r},E,t)\right]\varphi(\vec{r},\vec{\Omega},E,t)\varphi^*(\vec{r},\vec{\Omega}',E',t)\,d\vec{\Omega}\,dE\,d\vec{\Omega}'\,dE', \quad \ldots(I\text{-}9)$$

and the transformed Equation I-7 is

$$\int_{o}^{t_f}\int_{r}\int_{\Omega}\int_{E}\varphi(\vec{r},\vec{\Omega},E,t)\left\{\int_{\Omega'}\int_{E'}\left[\Sigma_S(\vec{r},\vec{\Omega}',E',\vec{\Omega},E) + \frac{\chi(E')}{4\pi}(1-\beta)\nu\Sigma_f(\vec{r},E,t)\right]\varphi^*(\vec{r},\vec{\Omega}',E',t)\,d\vec{\Omega}'\,dE'\right\}d\vec{r}\,d\vec{\Omega}\,dE\,dt. \quad \ldots(I\text{-}10)$$

The fourth terms are

$$\sum_{i=1}^{6}\int_{o}^{t_f}\int_{r}\int_{\Omega}\int_{E}\varphi^*(\vec{r},\vec{\Omega},E,t)\lambda_i f_i C_i(\vec{r},t)\,d\vec{r}\,d\vec{\Omega}\,dE\,dt. \quad \ldots(I\text{-}11)$$

Writing them as

$$\sum_{i=1}^{6}\int_{o}^{t_f}\int_{r}C_i(\vec{r},t)\left[\lambda_i\int_{\Omega}\int_{E}f_i(E)\varphi^*(\vec{r},\vec{\Omega},E,t)\,d\vec{\Omega}\,dE\right]d\vec{r}\,dt = \sum_{i=1}^{6}\int_{o}^{t_f}\int_{r}C_i(\vec{r},t)M_i^*\varphi^*\,d\vec{r}\,dt \quad \ldots(I\text{-}11')$$

gives the transformed expression.

The fifth term is

$$-\int_{o}^{t_f}\int_{r}\int_{\Omega}\int_{E}\varphi^*(\vec{r},\vec{\Omega},E,t)\frac{1}{v}\frac{\partial\varphi}{\partial t}\,d\vec{r}\,d\vec{\Omega}\,dE\,dt. \quad \ldots(I\text{-}12)$$

Doing the time integral by parts, gives

$$\int_{o}^{t_f}\int_{r}\int_{\Omega}\int_{E}\varphi(\vec{r},\vec{\Omega},E,t)\frac{1}{v}\frac{\partial\varphi^*}{\partial t}\,d\vec{r}\,d\vec{\Omega}\,dE\,dt - \int_{r}\int_{\Omega}\int_{E}\frac{1}{v}\varphi(\vec{r},\vec{\Omega},E,t_f)\varphi^*(\vec{r},\vec{\Omega},E,t_f)\,d\vec{r}\,d\vec{\Omega}\,dE$$

$$+\int_{r}\int_{\Omega}\int_{E}\frac{1}{v}\varphi(\vec{r},\vec{\Omega},E,o)\varphi^*(\vec{r},\vec{\Omega},E,o)\,d\vec{r}\,d\vec{\Omega}\,dE. \quad \ldots(I\text{-}12')$$

The sixth terms

$$\sum_{i=1}^{6} \int_{o}^{t_f} \int_{r} C_i^*(\vec{r},t) M_i \varphi \, d\vec{r} \, dt \qquad \ldots(I\text{-}13)$$

are rewritten as

$$\int_{o}^{t_f} \int_{r} \int_{\Omega} \int_{E} \varphi(\vec{r},\vec{\Omega},E,t) \left[\sum_{i=1}^{6} \beta_i \nu \Sigma_f(\vec{r},E,t) C_i^*(\vec{r},t) \right] d\vec{r} \, d\vec{\Omega} \, dE \, dt \, , \qquad \ldots(I\text{-}13')$$

using the definitions found in Equation 6.

The seventh terms are simply rewritten as

$$- \sum_{i=1}^{6} \int_{o}^{t_f} \int_{r} C_i(\vec{r},t) \lambda_i C_i^*(\vec{r},t) \, d\vec{r} \, dt \, . \qquad \ldots(I\text{-}14)$$

The eighth terms finally are integrated by parts in time, giving

$$\sum_{i=1}^{6} \left\{ \int_{o}^{t_f} \int_{r} C_i(\vec{r},t) \frac{\partial C_i^*}{\partial t} - \int_{r} C_i(\vec{r},t_f) C_i^*(\vec{r},t_f) \, d\vec{r} + \int_{r} C_i(\vec{r},o) C_i^*(\vec{r},o) \, d\vec{r} \right\} . \qquad \ldots(I\text{-}15)$$

The sum of Equations I-5, -6, -10, -11′, -12′, -13′, -14, and -15 gives Equation 12

$$I\{\varphi, C_i, \varphi^*, C_i^*\} \equiv \int_{o}^{t_f} \int_{r} \int_{\Omega} \int_{E} \varphi(\vec{r},\vec{\Omega},E,t) \left[L^* \varphi^*(\vec{r},\vec{\Omega},E,t) + \sum_{i=1}^{6} \beta_i \nu \Sigma_f C_i^* + \frac{1}{v} \frac{\partial \varphi^*}{\partial t} \right] d\vec{r} \, d\vec{\Omega} \, dE \, dt$$

$$+ \sum_{i=1}^{6} \int_{o}^{t_f} \int_{r} C_i(\vec{r},t) \left[M_i^* \varphi^* - \lambda_i C_i^* + \frac{\partial C_i}{\partial t} \right] d\vec{r} \, dt$$

$$+ \int_{r} \int_{\Omega} \int_{E} \frac{1}{v} \varphi(\vec{r},\vec{\Omega},E,o) \varphi^*(\vec{r},\vec{\Omega},E,o) \, d\vec{r} \, d\vec{\Omega} \, dE + \sum_{i=1}^{6} \int_{r} C_i(\vec{r},o) C_i^*(\vec{r},o) \, d\vec{r} \, . \qquad \ldots(12)$$

APPENDIX II

VARIATIONAL FLUX SYNTHESIS IN A TWO-ENERGY GROUP, SLAB-GEOMETRY DIFFUSION MODEL WITH TEMPERATURE FEEDBACK

The flux synthesis variational method will be applied here to solve the following.

A. THE PROBLEM

Calculate the space-time behavior of the two-energy group description of the neutron flux in a multiregion slab reactor with temperature feedback for a large insertion of reactivity.

The equations for the problem are:

$$\frac{\partial}{\partial x}\left(D_1 \frac{\partial \varphi_1}{\partial x}\right) - \Sigma_1 \varphi_1 + \chi_1 \nu (1-\beta)(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) = \frac{1}{v_1}\frac{\partial \varphi_1}{\partial t}, \qquad \ldots(II\text{-}1)$$

$$\frac{\partial}{\partial x}\left(D_2 \frac{\partial \varphi_2}{\partial x}\right) - \Sigma_2 \varphi_2 + \chi_2 \nu (1-\beta)(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) + \Sigma_r \varphi_1 = \frac{1}{v_2}\frac{\partial \varphi_2}{\partial t}, \qquad \ldots(II\text{-}2)$$

$$\frac{K}{\rho C_p}(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) = \frac{\partial T}{\partial t}, \qquad \ldots(II\text{-}3)$$

where the subscripts 1 and 2 indicate fast and slow energy group parameters; Σ_1 and Σ_2 are total cross sections; Σ_{f1} and Σ_{f2} are fission cross sections, and Σ_r is the removal cross section. K is a conversion factor from fissions to some unit of energy, ρ is the density of the reactor material, and C_p is its specific heat. Delayed neutrons are not taken into account. The temperature equation does not have a conduction term, the assumption being that the transient is too fast for any temperature equalization to take place. These omissions are not essential.

The parameters Σ_1, Σ_2, Σ_{f1}, Σ_{f2}, ρ and C_p will be specified functions of the temperature T.

If the left and right boundaries of the slab are $x = a$ and $x = b$, and there are x_ℓ ($\ell = 1, \ldots, 2$) interval boundaries where the reactor properties are discontinuous, the following boundary conditions have to be satisfied.

$$\varphi_1(a) = \varphi_1(b) = \varphi_2(a) = \varphi_2(b) = 0; \qquad \ldots(II\text{-}4)$$

$$\left.\begin{aligned} \varphi_1(x_{\ell-}) &= \varphi_1(x_{\ell+}) \\ \varphi_2(x_{\ell-}) &= \varphi_2(x_{\ell+}) \end{aligned}\right\}; \qquad \ldots(II\text{-}5)$$

$$\left.\begin{aligned} D_1(x_{\ell-},t)\frac{\partial \varphi_1(x_{\ell-})}{\partial x} &= D_1(x_{\ell+},t)\frac{\partial \varphi_1(x_{\ell+})}{\partial x} \\ D_2(x_{\ell-},t)\frac{\partial \varphi_2(x_{\ell-})}{\partial x} &= D_2(x_{\ell+},t)\frac{\partial \varphi_2(x_{\ell+})}{\partial x} \end{aligned}\right\}; \qquad \ldots(II\text{-}6)$$

$\ell = 1, 2, \ldots N$, for all times

where

$f(x_{\ell-})$ = value of function $f(x)$ at the point x_ℓ, when approaching it from the left

$f(x_{\ell+})$ = value of function $f(x)$ at the point x_ℓ, when approaching it from the right.

At time $t = 0$ and every $a \le x \le b$

$$\left.\begin{aligned} \varphi_1(x,o) &= \varphi_{10} \\ \varphi_2(x,o) &= \varphi_{20} \\ T(x,o) &= T_o \end{aligned}\right\} , \qquad \ldots(II\text{-}7)$$

where $\varphi_{10}, \varphi_{20}, T_o$ are given functions of x.

The functional chosen is

$$I\{\varphi_1,\varphi_2,T,\varphi_1^*,\varphi_2^*,T^*\} \equiv \int_o^{t_f}\int_a^b \left\{ \frac{\partial\varphi_1^*}{\partial x} D_1 \frac{\partial\varphi}{\partial x} + \varphi_1^*\left[-\Sigma_1\varphi_1 + \chi_1\nu(1-\beta)(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) - \frac{1}{v_1}\frac{\partial\varphi_1}{\partial t}\right]\right.$$

$$+ \frac{\partial\varphi_2^*}{\partial x} D_2 \frac{\partial\varphi_2}{\partial x} + \varphi_2^*\left[-\Sigma_2\varphi_2 + \chi_2\nu(1-\beta)(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) + \Sigma_f\varphi_1 - \frac{1}{v_2}\frac{\partial\varphi_2}{\partial t}\right]$$

$$\left. + T^*\left[\frac{K}{\rho C_p}(\Sigma_{f1}\varphi_1 + \Sigma_{f2}\varphi_2) - \frac{\partial T}{\partial t}\right]\right\} dx\,dt + \int_a^b \left[\frac{\varphi_1^*(t_f)\varphi_1(t_f)}{v_1} + \frac{\varphi_2^*(t_f)\varphi_2(t_f)}{v_2} + T^*(t_f)T(t_f)\right] dx; \qquad \ldots(II\text{-}8)$$

and $\varphi_1^*, \varphi_2^*, T^*$ are adjoint functions, to be defined shortly

t_f = final time (time up to which the solution is to be carried out).

Integrating by parts in time and rearranging terms, it is easy to see that

$$I\{\varphi_1,\varphi_2,T,\varphi_1^*,\varphi_2^*,T^*\}$$

$$\equiv \int_o^{t_f}\int_a^b \left\{ \frac{\partial\varphi_1^*}{\partial x} D_1 \frac{\partial\varphi_1}{\partial x} + \varphi_1\left[-\Sigma_1\varphi_1^* + (1-\beta)\nu\Sigma_{f1}(\chi_1\varphi_1^* + \chi_2\varphi_2^*) + \Sigma_r\varphi_2^*) + \frac{K}{\rho C_p}\Sigma_{f1}T^* + \frac{1}{v_1}\frac{\partial\varphi_1^*}{\partial t}\right]\right.$$

$$\left. + \frac{\partial\varphi_2^*}{\partial x} D_2 \frac{\partial\varphi_2}{\partial x} + \varphi_2\left[-\Sigma_2\varphi_2^* + (1-\beta)\nu\Sigma_{f2}(\chi_1\varphi_1^* + \chi_2\varphi_2^*) + \frac{K}{\rho C_p}\Sigma_{f2}T^* + \frac{1}{v_2}\frac{\partial\varphi_2^*}{\partial t}\right] + T\frac{\partial T^*}{\partial t}\right\} dx\,dt$$

$$+ \int_a^b \left[\frac{\varphi_1^*(o)\varphi_1(o)}{v_1} + \frac{\varphi_2^*(o)\varphi_2(o)}{v_2} + T^*(o)T(o)\right] dx \qquad \ldots(II\text{-}9)$$

is an equivalent form of the functional. If no temperature feedback is present, the stationary conditions for the functional are:

1) the set of Equations II-1, -2, and -3;

2) $\delta\omega_1(a,t) = \delta\omega_1(b,t) = \delta\varphi_2(a,t) = \delta\varphi_2(b,t) = 0 \qquad 0 \le t \le t_f$,

$\delta\omega_1(x,o) = \delta\omega_2(x,o) = \delta T(x,o) = 0 \qquad a \le x \le b$

equivalent to the set of conditions in Equations II-4 and -7;

3) conditions expressed in Equation II-6;

4) the following set of equations for the adjoint functions:

$$\frac{\partial}{\partial x}\left(D_1 \frac{\partial \omega_1^*}{\partial x}\right) - \Sigma_1 \varphi_1^* + (1-\beta)\nu\Sigma_{f1}(\chi_1\varphi_2^* + \chi_2\varphi_2^*) + \Sigma_r\varphi_2^* + \frac{K}{\rho C_p}\Sigma_{f1}T^* = -\frac{1}{v_1}\frac{\partial \varphi_1^*}{\partial t} , \qquad \ldots(II-10)$$

$$\frac{\partial}{\partial x}\left(D_2 \frac{\partial \omega_2^*}{\partial x}\right) - \Sigma_2 \varphi_2^* + (1-\beta)\nu\Sigma_{f2}(\chi_1^*\varphi_1^* + \chi_2\varphi_2^*) + \frac{K}{\rho C_p}\Sigma_{f2}T^* = -\frac{1}{v_2}\frac{\partial \varphi_2^*}{\partial t} , \qquad \ldots(II-11)$$

$$0 = \frac{\partial T^*}{\partial t} ; \qquad \ldots(II-12)$$

5) $\delta\omega_1^*(a,t) = \delta\omega_1^*(b,t) = \delta\omega_2^*(a,t) = \delta\omega_2^*(b,t) = 0 \qquad 0 \le t \le t_f$, $\qquad \ldots(II-13')$

or, equivalent, though less general

$$\omega_1^*(a,t) = \omega_1^*(b,t) = \omega_2^*(a,t) = \omega_2^*(b,t) = 0 \qquad 0 \le t \le t_f , \qquad \ldots(II-13)$$

and

$$\delta\omega_1^*(x,t_f) = \delta\omega_2^*(x,t_f) = \delta T^*(x,t_f) = 0 \qquad a \le x \le b , \qquad \ldots(II-14')$$

or its equivalent

$$\left.\begin{aligned} \omega_1^*(x,t_f) &= \omega_{1f}^* \\ \omega_2^*(x,t_f) &= \omega_{2f}^* \\ T^*(x,t_f) &= T_f^* \end{aligned}\right\} \qquad a \le x \le b \qquad \text{given functions of } x ; \qquad \ldots(II-14)$$

6) the equivalent of condition in Equation II-6

$$\left.\begin{aligned} D_1(x_{\ell-},t)\frac{\partial \omega_1^*(x_{\ell-})}{\partial x} &= D_1(x_{\ell+},t)\frac{\partial \omega_1^*(x_{\ell+})}{\partial x} \\ D_2(x_{\ell-},t)\frac{\partial \omega_2^*(x_{\ell-})}{\partial x} &= D_2(x_{\ell+},t)\frac{\partial \omega_2^*(x_{\ell+})}{\partial x} \end{aligned}\right\} . \qquad \ldots(II-15)$$

The solution of Equation II-12 is

$$T^*(x,t) = const = T_f^* , \qquad \ldots(II-16)$$

and taking

$$T_f^* = 0 , \qquad \ldots(II-16')$$

the function $T^*(x,t) = 0$ at all points and times in the system. Clearly T^* plays no role in the calculation, and the whole process can be carried out without explicit reference to the temperature or its

adjoint. If there is a temperature feedback, all the conditions remain the same, except those in Equation II-12.

The variation of Equation II-9, with respect to T when the parameters depend on T, has to take into account the variation with T of terms of the form $\Sigma(T)\varphi\varphi^*$, which will be

$$\delta\left[\Sigma(T)\varphi\varphi^*\right] = \frac{\partial\Sigma}{\partial T}\varphi\varphi^*\delta T$$

to first order approximation.

Taking this into account, Equation II-12 takes the form:

$$\varphi_1\varphi_1^*\frac{\partial\Sigma_1}{\partial T} + \varphi_2\varphi_2^*\frac{\partial\Sigma_2}{\partial T} + (1-\beta)\nu\left[\varphi_1\frac{\partial\Sigma_{f1}}{\partial T} + \varphi_2\frac{\partial\Sigma_{f2}}{\partial T}\right]\left[\chi_1\varphi_1^* + \chi_2\varphi_2^*\right] + T^*\left[\varphi_1\frac{\partial\left(\frac{K\Sigma_{f2}}{\rho C_p}\right)}{\partial T} + \varphi_2\frac{\partial\left(\frac{K\Sigma_{f2}}{\rho C_p}\right)}{\partial T}\right] = -\frac{\partial T^*}{\partial t}. \quad \ldots(II-17)$$

The changes introduced by the presence of feedback are then:

1) The Equations II-1, -2, and -3, and conditions for fluxes and temperature are the same in form but nonlinear in character.

2) The Equations II-10, -11, and -17 for the adjoints are linear but with several new terms. The coefficients are explicit functions of time.

3) To calculate the coefficients in the adjoint system as such, it is necessary to know the solution of the direct problem.

The boundary and final conditions for the adjoints do not change.

B. THE APPROXIMATION PROCEDURE

It is assumed that the functions $\varphi_1, \varphi_2, T, \varphi_1^*, \varphi_2^*$, and T^* can be expressed in the following forms:

$$\left.\begin{aligned}\varphi_1(x,t) &= \sum_{i=1}^{K_1}\Phi_1^i(x)F_1^i(t)\\ \varphi_2(x,t) &= \sum_{i=1}^{K_2}\Phi_2^i(x)F_2^i(t)\\ T(x,t) &= \sum_{i=1}^{K_3}\mathcal{T}^i(x)\theta^i(t)\end{aligned}\right\} \quad \ldots(II-18$$

$$\left.\begin{aligned} \varphi_1^*(x,t) &= \sum_{j=1}^{K_1} \Phi_1^{j*}(x) F_1^{j*}(t) \\ \varphi_2^*(x,t) &= \sum_{j=1}^{K_2} \Phi_2^{j*}(x) F_2^{j*}(t) \\ T^*(x,t) &= \sum_{j=1}^{K_3} \mathcal{T}^{j*}(x) \theta^{j*}(t) \end{aligned}\right\} \qquad \ldots(II\text{-}19)$$

The functions Φ_1^i, Φ_2^i, $\mathcal{T}^i$ are space-dependent approximate solutions of Equations II-1, -2, and -3 at different times during the transient.

The functions Φ_1^{j*}, Φ_2^{j*}, $\mathcal{T}^{j*}$ are space-dependent approximate solutions of the system of Equations II-10, -11, and -12 in the linear case, or of Equations II-10, -11, and -17 when there is temperature feedback.

Introducing these expressions into the functional (Formulas II-8 and -9), integrating over the space dimension, and then imposing the stationary conditions for arbitrary variations in the functions $F_1^i(t)$, $F_2^i(t)$, $\theta^i(t)$, $F_1^{j*}(t)$, $F_2^{j*}(t)$, and $\theta^{j*}(t)$, a system of first order time differential equations will be obtained for these functions.

After introducing Expressions II-18 and -19 into Equations II-8 and -9, and integrating over the space dimension, the functional takes two equivalent forms:

$$\begin{aligned} I\left\{F_1^i, F_2^i, \theta^i; F_1^{j*}, F_2^{j*}, \theta^{j*}\right\} \equiv \int_o^{t_f} \Bigg\langle & \sum_{j=1}^{K_1} \sum_{i=1}^{K_1} \left\{ F_1^{j*} F_1^i \left[L_1^{ij} + A_{11}^{ij}(t,T) \right] - F_1^{j*} \frac{dF_1^i}{dt} I_1^{ij} \right\} \\ & + \sum_{j=1}^{K_1} \sum_{i=1}^{K_2} F_1^{j*} F_2^i A_{12}^{ij}(t,T) + \sum_{j=1}^{K_2} \sum_{i=1}^{K_2} \left\{ F_2^{j*} F_2^i \left[L_2^{ij} + A_{22}^{ij}(t,T) \right] - F_2^{j*} \frac{dF_2^i}{dt} I_2^{ij} \right\} \\ & + \sum_{j=1}^{K_2} \sum_{i=1}^{K_1} F_2^{j*} F_1^i A_{21}^{ij}(t,T) + \sum_{j=1}^{K_3} \sum_{i=1}^{K_1} \theta^{j*} F_1^i Q_1^{ij}(t,T) + \sum_{j=1}^{K_3} \sum_{i=1}^{K_2} \theta^{j*} F_2^i Q_2^{ij}(t,T) \\ & - \sum_{j=1}^{K_3} \sum_{i=1}^{K_3} \theta^{j*} \frac{d\theta^i}{dt} I_3^{ij} \Bigg\rangle dt + \sum_{j=1}^{K_1} \sum_{i=1}^{K_1} F_1^{j*}(t_f) F_1^i(t_f) I_1^{ij} \\ & + \sum_{j=1}^{K_2} \sum_{i=1}^{K_2} F_2^{j*}(t_f) F_2^i(t_f) I_2^{ij} + \sum_{j=1}^{K_3} \sum_{i=1}^{K_3} \theta^{j*}(t_f) \theta^i(t_f) I_3^{ij} \ , \end{aligned} \qquad \ldots(II\text{-}20)$$

and

$$I\left\{F_1^i, F_2^i, \theta^i; F_1^{j*}, F_2^{j*}, \theta^{j*}\right\} \equiv \int_o^{t_f} \Bigg\langle \sum_{j=1}^{K_1}\sum_{i=1}^{K_1}\left\{F_1^i F_1^{j*}\left[L_1^{ij} + A_{11}^{ij}(t,T)\right] + F_1^i \frac{dF_1^{j*}}{dt} I_1^{ij}\right\} + \sum_{j=1}^{K_2}\sum_{i=1}^{K_1} F_1^i F_2^{j*} A_{21}^{ij}(t,T)$$

$$+ \sum_{j=1}^{K_2}\sum_{i=1}^{K_2}\left\{F_2^i F_2^{j*}\left[L_2^{ij} + A_{22}^{ij}(t,T)\right] + F_2^i \frac{dF_2^{j*}}{dt} I_2^{ij}\right\} + \sum_{j=1}^{K_1}\sum_{i=1}^{K_2} F_2^i F_1^{j*} A_{12}^{ij}(t,T)$$

$$+ \sum_{j=1}^{K_3}\sum_{i=1}^{K_1} F_1^i \theta^{j*} Q_1^{ij}(t,T) + \sum_{j=1}^{K_3}\sum_{i=1}^{K_2} F_2^i \theta^{j*} Q_2^{ij}(t,T) + \sum_{j=1}^{K_3}\sum_{i=1}^{K_3} \theta^i \frac{d\theta^{j*}}{dt} I_3^{ij} \Bigg\rangle dt$$

$$+ \sum_{j=1}^{K_1}\sum_{i=1}^{K_1} F_1^i(o) F_1^{j*}(o) + \sum_{j=1}^{K_2}\sum_{i=1}^{K_2} F_2^i(o) F_2^{j*}(o) + \sum_{j=1}^{K_3}\sum_{i=1}^{K_3} \theta^i(o)\theta^{j*}(o) \; ; \qquad \ldots(II\text{-}21)$$

with the following set of definitions

$$L_1^{ij} = \int_a^b \frac{\partial \Phi_1^{j*}}{\partial x} D_1 \frac{\partial \Phi_1^i}{\partial x} dx \; , \qquad \ldots(II\text{-}22)$$

$$L_2^{ij} = \int_a^b \frac{\partial \Phi_2^{j*}}{\partial x} D_2 \frac{\partial \Phi_2^i}{\partial x} dx \; , \qquad \ldots(II\text{-}23)$$

$$A_{11}^{ij}(t,T) = \int_a^b \left[-\Sigma_1(x,t,T) + \chi_1 \nu(1-\beta)\Sigma_{f1}(x,t,T)\right] \Phi_1^{j*} \Phi_1^i \, dx \; , \qquad \ldots(II\text{-}24)$$

$$A_{22}^{ij}(t,T) = \int_a^b \left[-\Sigma_2(x,t,T) + \chi_2 \nu(1-\beta)\Sigma_{f2}(x,t,T)\right] \Phi_2^{j*} \Phi_2^i \, dx \; , \qquad \ldots(II\text{-}25)$$

$$A_{12}^{ij}(t,T) = \int_a^b \chi_1 \nu(1-\beta)\Sigma_{f2}(x,t,T) \Phi_1^{j*} \Phi_2^i \, dx \; , \qquad \ldots(II\text{-}26)$$

$$A_{21}^{ij}(t,T) = \int_a^b \chi_2 \nu(1-\beta)\Sigma_{f1}(x,t,T) \Phi_2^{j*} \Phi_1^i \, dx \; , \qquad \ldots(II\text{-}27)$$

$$I_1^{ij} = \int_a^b \frac{\Phi_1^{j*} \Phi_1^i}{v_1} dx \; , \qquad \ldots(II\text{-}28)$$

$$I_2^{ij} = \int_a^b \frac{\Phi_2^{j*}\Phi_2^i}{v_2}\,dx\,, \qquad \ldots(II\text{-}29)$$

$$I_3^{ij} = \int_a^b \mathcal{J}^{j*}\,\mathcal{J}^i\,dx\,, \qquad \ldots(II\text{-}30)$$

$$Q_1^{ij}(t,T) = \int_a^b \frac{K\Sigma_{f1}(x,t,T)}{\rho(x,t,T)C_p(x,t,T)}\,\mathcal{J}^{j*}\Phi_1^i\,dx\,, \qquad \ldots(II\text{-}31)$$

$$Q_2^{ij}(t,T) = \int_a^b \frac{K\Sigma_{f2}(x,t,T)}{\rho(x,t,T)C_p(x,t,T)}\,\mathcal{J}^{j*}\Phi_2^i\,dx\,. \qquad \ldots(II\text{-}32)$$

The stationary conditions of the functional for arbitrary variations in the functions F_1, F_2, θ, F_1^{j*}, F_2^{j*}, and θ^{j*} are (feedback effects included):

$$\sum_{i=1}^{K_1}\left\{\left[L_1^{ij} + A_{11}^{ij}(t,T)\right]F_1^i(t) - I_1^{ij}\frac{dF_1^i}{dt}\right\} + \sum_{i=1}^{K_2} F_2^i A_{12}^{ij}(t,T) = 0 \quad j = 1,2,\ldots,K_1\,; \qquad \ldots(II\text{-}33)$$

$$\sum_{i=1}^{K_2}\left\{\left[L_2^{ij} + A_{22}^{ij}(t,T)\right]F_2^i(t) - I_2^{ij}\frac{dF_2^{ij}}{dt}\right\} + \sum_{i=1}^{K_1} F_1^i A_{21}^{ij}(t,T) = 0 \quad j = 1,2,\ldots,K_2\,; \qquad \ldots(II\text{-}34)$$

$$\sum_{i=1}^{K_1} Q_1^{ij}(t,T)F_1^i + \sum_{i=1}^{K_2} Q_2^{ij}F_2^i - \sum_{i=1}^{K_3} I_3^{ij}\frac{d\theta^i}{dt} = 0 \qquad j = 1,2,\ldots,K_3\,; \qquad \ldots(II\text{-}35)$$

with conditions

$$\left.\begin{aligned} F_1^i(o) &= F_{10}^i \quad i = 1,2,\ldots,K_1 \\ F_2^i(o) &= F_{20}^i \quad i = 1,2,\ldots,K_2 \\ \theta^i(o) &= \theta_o^i \quad i = 1,2,\ldots,K_3 \end{aligned}\right\} \text{ fixed initial values }, \qquad \ldots(II\text{-}36)$$

and

$$\sum_{j=1}^{K_1}\left\{\left[L_1^{ij} + A_{11}^{ij}(t,T)\right]F_1^{*j} + I_1^{ij}\frac{dF_1^{*j}}{dt}\right\} + \sum_{j=1}^{K_2} A_{21}^{ij}(t,T)F_2^{*j} + \sum_{j=1}^{K_3} Q_1^{ij}(t,T)\theta^{j*} = 0 \quad i = 1,2,\ldots,K_1\,; \ldots(II\text{-}37)$$

$$\sum_{j=1}^{K_2}\left\{\left[L_2^{ij} + A_{22}^{ij}(t,T)\right]F_2^{j*} + I_2^{ij}\frac{dF_2^{j*}}{dt}\right\} + \sum_{j=1}^{K_1} A_{12}^{ij}(t,T)F_1^{j*} + \sum_{j=1}^{K_3} Q_2^{ij}(t,T)\theta^{j*} = 0 \qquad i = 1,2,\ldots,K_2 ; \quad \ldots(II\text{-}38)$$

$$\left[\sum_{\ell=1}^{K_1}\sum_{k=1}^{K_1}\frac{\partial A_{11}^{k\ell}}{\partial T}F_1^k F_1^{\ell*} + \sum_{\ell=1}^{K_2}\sum_{k=1}^{K_2}\frac{\partial A_{22}^{k\ell}}{\partial T}F_2^k F_2^{\ell*} + \sum_{\ell=1}^{K_2}\sum_{k=1}^{K_1}\frac{\partial A_{21}^{k\ell}}{\partial T}F_1^k F_2^{\ell*} + \sum_{\ell=1}^{K_1}\sum_{k=1}^{K_2}\frac{\partial A_{12}^{k\ell}}{\partial T}F_2^k F_1^{\ell*}\right.$$

$$\left. + \sum_{\ell=1}^{K_3}\sum_{k=1}^{K_1}\frac{\partial Q_1^{k\ell}}{\partial T}F_1^k\theta^{\ell*} + \sum_{\ell=1}^{K_3}\sum_{k=1}^{K_2}\frac{\partial Q_2^{k\ell}}{\partial T}F_2^k\theta^{\ell*}\right]\mathcal{T}^i + \sum_{j=1}^{K_3} I_3^{ij}\frac{d\theta^{j*}}{dt} = 0$$

$$i = 1,2,\ldots,K_3 ; \quad \ldots(II\text{-}39)$$

with conditions

$$\left.\begin{aligned} F_1^{j*}(t_f) &= F_{1f}^{j*} \qquad j = 1,2,\ldots,K_1 \\ F_2^{j*}(t_f) &= F_{2f}^{j*} \qquad j = 1,2,\ldots,K_2 \\ \theta^{j*}(t_f) &= \theta_f^{j*} \qquad j = 1,2,\ldots,K_3 \end{aligned}\right\} \quad \text{fixed final values .} \qquad \ldots(II\text{-}40)$$

The system of Equations II-33, -34, and -35 with conditions found in -36 is nonlinear, and its solution does not depend on the solution for the adjoint flux and adjoint temperature mixing functions — Equations II-37, -38, -39 with conditions of Equation -40.

On the other hand, the system in Equations II-37, -38, and -39 is linear and its time-dependent coefficients depend on the solution of the direct problem. To calculate these coefficients, it is necessary to know $F_1^i(t)$, $F_2^i(t)$, and $T(t)$, which is the solution for the system of Equations II-33, -34, and -35.

In this approximate formulation the solution to the direct problem is not completely independent from the solution of the adjoint problem. The coefficients in Equations II-33, -34, and -35 (definitions II-22 through -32) depend on the functions, $\Phi_1^{j*}(x)$, $\Phi_2^{j*}(x)$, and $\mathcal{T}^{j*}(x)$, which are approximate solutions of the adjoint problem, as expressed in Equations II-10, -11, and -17. Getting approximate solutions for Equations II-10, -11, and -17, and then using them in the coefficient definitions does not seem practical. A more direct (perhaps, less accurate) method is obtained if the space-dependent approximate solutions of Equations II-10, -11, and -12, with assumption in Equation II-16 , are taken as the approximate solutions to Equations II-10, -11, and -17 which are introduced in the coefficient definitions. Then the system of Equations II-33, -34, and -35 is solved. If this is considered a good approximation to the solution of the problem, the procedure stops there and Equations II-37, -38, and -39 are not to be considered.

If there is reason to believe that the approximation obtained is poor and further investigation desired on the effect of improved adjoint trial functions, it is suggested that the following iteration process be used.

The first order solution to the direct problem is employed to calculate the coefficients in the adjoint system of Equations II-37, -38, and -39. This gives a set of functions, $F_1^{j*}(t)$, $F_2^{j*}(t)$, and $\theta^{j*}(t)$. Using Equation II-19 the adjoint magnitudes are reconstructed. A new set of approximate space-dependent functions, $\Phi_1^{j*}(x)$, $\Phi_2^{j*}(x)$, and $\mathcal{T}^{j*}(x)$, is now defined as approximations to the space-time functions just obtained. This new set of adjoint trial functions is then used to generate a new set of coefficients for Equations II-33, -34, and -35, etc.

For the type of application developed here, in which the flux shapes are desired and not the value of the functional, it will hardly be necessary or practical to refine the calculation through the iteration process. In fact, the use of the Galerkin method, without any reference to adjoints, has proved to be a good approximation in several instances.

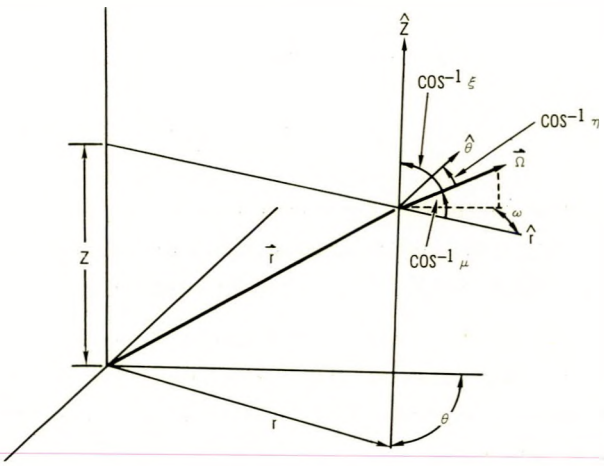

Figure 1.
Description of Position Vector $\vec{r}$ and Direction Vector $\vec{\Omega}$ in Cylindrical Geometry

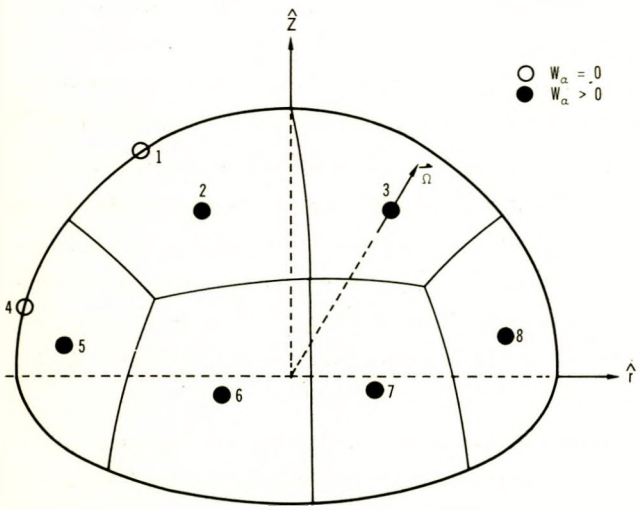

Figure 2.
Discrete Directions for S_4 for Cylinders

APPENDIX III

CALCULATION OF THE COEFFICIENTS IN EQUATIONS 43 AND 45 FROM DTF-II OUTPUT

The basic functions $N_g^i(\vec{r},\vec{\Omega})$ and $N_g^{i*}(\vec{r},\vec{\Omega})$ appearing in the definition of the coefficients of Equations 43 and 45 depend on the radius vector $\vec{r}$ and on the direction vector $\vec{\Omega}$. The coordinate system to be used in the description of these functions is depicted in Figure 1. Cylindrical coordinates r, z, θ are used to specify the position vectors. The unit direction vector $\vec{\Omega}$ is determined by the angle ω and a direction cosine ξ.

The angular coordinates are related by

$$\mu = \sqrt{1-\xi^2}\cos\omega \qquad -\pi \le \omega \le \pi ,$$
$$\eta = \sqrt{1-\xi^2}\sin\omega \qquad -1 \le \xi \le 1 . \qquad \ldots(III\text{-}1)$$

The solid angle differential is simply:

$$d\vec{\Omega} = d\xi\, d\mu . \qquad \ldots(III\text{-}2)$$

The results of a DTF-II calculation using this coordinate system will be sets of numbers $N_{g\ell\alpha}$, representing the values of the functions $N_g(\vec{r},\vec{\Omega})$ at the points of a space-angle mesh. The space mesh is the normal reticulate corresponding to cylindrical coordinates. The angular mesh is that corresponding to an Sn integration of the transport equation. $n(n+2)/4$ directions are chosen in a quadrant of the unit sphere in velocity space ($n = 2, 4, \ldots$). These directions are divided into $n/2$ levels, i.e., different values of ξ. In cylindrical geometry all $n(n+2)/4$ directions are significant (Figure 2). Each direction α is given a weight W_α corresponding to the area associated with that direction on the unit sphere. For these directions the discrete angular fluxes $N_{g\ell\alpha}$ represent the average value of the angular flux, at space point ℓ and energy group g, over the area of the unit sphere represented by W_α, i.e.,

$$\int_\Omega N(\vec{r},E,\vec{\Omega})\, d\vec{\Omega} = \sum_\alpha W_\alpha N_{g\ell\alpha} . \qquad \ldots(III\text{-}3)$$

Each direction α is given an average value of the direction cosine μ, such that

$$\int_{\Delta\Omega_\alpha} \mu\, d\vec{\Omega} = \mu_\alpha W_\alpha , \qquad \ldots(III\text{-}4)$$

where $\Delta\vec{\Omega}_\alpha$ is the unit sphere area corresponding to the direction α.

In addition, a number $n(n+2)/4$ of α^* directions — corresponding to the edges of the angular zones — are defined. The values $N_{g\ell\alpha^*}$ represent the angular fluxes going in those directions only. For these directions $W_{\alpha^*} = 0$. The direction α^* with $\omega = \pi$ is a startup direction.

Assuming that a linear angular dependence of the flux within the angular zones is chosen, it is possible to calculate the edge fluxes $N_{g\ell\alpha^*}$'s as functions of the $N_{g\ell\alpha}$'s and the fluxes in the corresponding startup direction by:

$$N_{\alpha^*} = 2N_{\alpha} - N_{\alpha^*-1} \cdot \qquad \ldots(III\text{-}5)$$

The detailed specification of the coefficients as defined in Equations 39 through 42 in terms of the magnitudes $N_{g\ell\alpha}$ and $N_{g\ell\alpha^*}$ will be carried out here for a particular case: The flux and adjoint are functions only of r, ξ, and ω since there is no z or θ dependence. In this case, the subindex indicates the radial dependence.

Finite difference expressions for Equations 40 and 42 are

$$A_g^{ij}(t) = \int_r \int_{\Omega} N_g^{i*}(\vec{r},\vec{\Omega})\Sigma_{Tg}(\vec{r},t)N_g^j(\vec{r},\vec{\Omega})\, d\vec{r}\, d\vec{\Omega}$$

$$= \frac{1}{2}\sum_{\ell}\left\langle \Delta\ell\Sigma_{Tg\ell}(t)\left\{\sum_{\alpha} W_{\alpha}\left[N_{g\ell\alpha}^{i*}N_{g\ell\alpha}^{j} + N_{g(\ell-1)\alpha}^{i*}N_{g(\ell-1)\alpha}^{j}\right]\right\}\right\rangle, \qquad \ldots(III\text{-}6)$$

$$I_g^{ij} = \int_r \int_{\Omega} N_g^{i*}(\vec{r},\vec{\Omega})N_g^j(\vec{r},\Omega)\, d\vec{r}\, d\vec{\Omega} = \frac{1}{2}\sum_{\ell}\left\langle \Delta\ell\left\{\sum_{\alpha} W_{\alpha}\left[N_{g\ell\alpha}^{i*}N_{g\ell\alpha}^{j} + N_{g(\ell-1)\alpha}^{i*}N_{g(\ell-1)\alpha}^{j}\right]\right\}\right\rangle, \qquad \ldots(III\text{-}7)$$

where

$\Sigma_{Tg\ell}$ = total cross section for group g at mesh point (radius) ℓ

$2\pi r_{\ell}\Delta r = \Delta\ell$ = volume element at mesh point ℓ

$N_{g\ell\alpha}^{i*}$ = value of i-th adjoint flux trial for group g, at mesh point ℓ and direction α

$N_{g\ell\alpha}^{j}$ = value of j-th flux trial for group g at mesh point ℓ and direction α

Definition for $\Sigma_{Sgg'}$ in Equation 30 has to be extended to

$$W_{\alpha}W_{\alpha'}\Sigma_{Sgg'\alpha\alpha'}(\vec{r},t) = \int_{\Delta\ell_{\alpha}}\int_{\Delta\ell_{\alpha'}}\left[\Sigma_{Sgg'}(\vec{r},\vec{\Omega}',\vec{\Omega}) + \frac{\chi_{g'}}{4\pi}\nu(1-\beta)\Sigma_{fg}(\vec{r},t)\right]d\vec{\Omega}\, d\vec{\Omega}'. \qquad \ldots(III\text{-}8)$$

In order to write the finite difference form of Equation 41

$$S_{gg'}^{ij}(t) = \int_r\int_{\ell}\int_{\ell'} N_g^{i*}(\vec{r},\vec{\Omega})\left[\Sigma_{Sgg'}(\vec{r},\vec{\Omega},\vec{\Omega}') + \frac{\chi_{g'}}{4\pi}\nu(1-\beta)\Sigma_{fg}(\vec{r},t)\right]N_{g'}^j(\vec{r},\Omega')\, d\vec{\Omega}'\, d\vec{\Omega}\, d\vec{r}$$

$$\cong \frac{1}{2}\sum_{\ell}\left\langle \Delta\ell\left\{\sum_{\alpha}\sum_{\alpha'} W_{\alpha}W_{\alpha'}\Sigma_{S\ell gg'\alpha\alpha'}\left[N_{g\ell\alpha}^{i*}N_{g'\ell\alpha'}^{j} + N_{g(\ell-1)\alpha}^{i*}N_{g'(\ell-1)\alpha'}^{i}\right]\right\}\right\rangle, \qquad \ldots(III\text{-}9)$$

where $\Sigma_{S\ell gg'\alpha\alpha'}$ are the values of $\Sigma_{Sgg'\alpha\alpha'}(\vec{r})$ at mesh point r_ℓ. The first step in obtaining a finite difference approximation for Equation 39 is to write the form of $\vec{\Omega} \cdot \vec{\nabla} N$ explicitly for the particular case considered. Therefore

$$N^*(r,\xi,\omega)\vec{\Omega} \cdot \vec{\nabla} N(r,\xi,\omega) = N^* \mu \frac{\partial N}{\partial r} - \frac{1}{r} N^* \eta \frac{\partial N}{\partial r}. \qquad \ldots(III-10)$$

The integral in Equation 39 then takes the form

$$\int_r \int_\xi \int_\omega \left[N_g^{i*} \mu \frac{\partial N_g^j}{\partial r} - \frac{1}{r} N_g^{i*} \eta \frac{\partial N_g^j}{\partial \omega} \right] 2\pi r \, dr \, d\omega \, d\xi \ . \qquad \ldots(III-11)$$

Integration of the first term in Equation III-11 over an element of volume and angle gives

$$2\pi \int_{\Delta\Omega_\alpha} d\xi \, d\omega \, \mu(\xi,\omega) \int_{r_{\ell-1}}^{r_\ell} N_g^{i*}(r,\xi,\omega) \frac{\partial N_g^j}{\partial r} \, r \, dr$$

$$= \frac{\pi}{2} \mu_\alpha W_\alpha \left[N_{g\ell\alpha}^{i*} + N_{g(\ell-1)\alpha}^{i*} \right] \left[r_\ell + r_{\ell-1} \right] \left[N_{g\ell\alpha}^{j} - N_{g(\ell-1)\alpha}^{j} \right]. \qquad \ldots(III-12)$$

Integration of the second term in Equation III-11 over the element of volume and angle gives

$$2\pi \int_{r_{\ell-1}}^{r_\ell} dr \int_{\Delta\Omega_\alpha} d\xi \, d\omega \, \eta(\xi,\omega) N_g^{i*}(r,\xi,\omega) \frac{\partial N_g^j}{\partial \omega}$$

$$= \pi \bar{\eta}_\alpha \Delta\ell \left\{ N_{g\ell\alpha}^{i*} \left[N_{g\ell\alpha^*}^{j} - N_{g\ell(\alpha^*-1)}^{j} \right] + N_{g(\ell-1)\alpha}^{i*} \left[N_{g(\ell-1)\alpha^*}^{j} - N_{g(\ell-1)(\alpha^*-1)}^{j} \right] \right\}, \qquad \ldots(III-13)$$

where $\bar{\eta}_\alpha$ is the average value of $\eta(\xi,\omega)$ over the area $\Delta\Omega_\alpha$. This value can be calculated by integration or with some approximate definition.

Summing Equations III-12 and -13 over all mesh points and angles and then adding the results gives:

$$L_g^{ij} = \int_r \int_\Omega N_g^{i*}(\vec{r},\vec{\Omega})\vec{\Omega} \cdot \vec{\nabla} N_g^j(\vec{r},\vec{\Omega}) \, d\vec{r} \, d\vec{\Omega}$$

$$= \pi \sum_\ell \sum_\alpha \Bigg\langle \frac{1}{2} \mu_\alpha W_\alpha \left[N_{g\ell\alpha}^{i*} + N_{g(\ell-1)\alpha}^{i*} \right] \left[r_\ell + r_{\ell-1} \right] \left[N_{g\ell\alpha}^{j} - N_{g(\ell-1)\alpha}^{j} \right]$$

$$+ \bar{\eta}_\alpha \Delta\ell \left\{ N_{g\ell\alpha}^{i*} \left[N_{g\ell\alpha^*}^{j} - N_{g\ell(\alpha^*-1)}^{j} \right] + N_{g(\ell-1)\alpha}^{i*} \left[N_{g(\ell-1)\alpha^*}^{j} - N_{g(\ell-1)(\alpha^*-1)}^{i} \right] \right\} \Bigg\rangle. \qquad \ldots(III-14)$$

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