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GENERAL ONE-SPACE-DIMENSIONAL MULTIGROUP

G. J. Habetler

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ABSTRACT

The numerical solution of the one-space-dimension age-diffusion equation by multigroup methods is outlined. Finite-difference equations are derived for solving the multigroup equations in a finite region where the composition is piecewise continuous. The equations contain many possible variations of multigroup problems: KAPL or ORNL multigroup; Selengut-Goertzel multigroup for hydrogenous compositions; adjoint multigroup.

GENERAL ONE-SPACE-DIMENSIONAL MULTIGROUP

G. J. Habetler

INTRODUCTION

Multigroup methods have been used successfully for some time for solving one-space-dimensional age-diffusion problems.* The age-diffusion equation is reduced to a set of coupled ordinary differential equations, called multigroup equations. For numerical computation, each group equation is usually replaced by a set of three-point finite-difference equations. These may be solved in a straightforward manner.**

In two-space-dimensional multigroup calculations, the situation is somewhat different. There is no simple method available for solving the finite-difference equations explicitly. Therefore, iterative procedures are currently being used at KAPL.

In this report we develop, for the one-space-dimensional multigroup case, three-point finite-difference equations which contain a higher degree of approximation than those used previously at KAPL.*** It is hoped that these equations will lead to a reduction of the number of mesh points necessary for a certain degree of accuracy. Since the equations are more complicated than those used previously, there may be no savings in machine calculation time for one-space-dimensional multigroup problems. However, similar equations may lead to large savings in two-space-dimensional multigroup calculations, where iteration is the time consuming factor. It is hoped that an investigation of the one-dimensional equations will inform us about the possibilities of better equations in two dimensions.

It is intended that this report be used as a layout for a general purpose one-space-dimensional multigroup setup on a high-speed digital computer. It will handle a large variety of problems. We also feel that it has great value in answering questions concerning multigroup approximations. Comparisons can be made of various schemes to determine how simplified the physical model can be and still give realistic answers.

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*Ehrlich, R. and H. Hurwitz, Jr., Nucleonics, February, 1954, p. 23. This paper contains numerous references to other articles on the subject.

**See Section G.

***Much of Section A is based on unpublished work by R. R. Coveyou, ORNL.

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In Section A, we derive three-point finite-difference equations for a differential equation of the form

$$\frac{-d}{d\zeta} D(\zeta) \frac{d}{d\zeta} \varphi(\zeta) - D(\zeta) \frac{\rho}{\zeta} \frac{d}{d\zeta} \varphi(\zeta) + A(\zeta) \varphi(\zeta) = \mathcal{S}(\zeta)$$

in a region where all the functions are continuous and possess derivatives of sufficiently high order. At interfaces between such regions $\varphi(\zeta)$ and $D(\zeta)\varphi'(\zeta)$ are continuous.

We apply the analysis of Section A to the age-diffusion equation and derive multigroup finite-difference equations in Sections B and C. KAPL and ORNL schemes for obtaining multigroup equations are included as well as inelastic-scattering and the Selengut-Goertzel approximation for hydrogeneous compositions. In Section D we derive adjoint multigroup finite-difference equations. Our results are listed in Section E.

Boundary conditions are examined in Section F.

An explicit method for solving the three-point finite-difference equations is outlined in Section G.

A. GENERAL DIFFERENCE EQUATIONS FOR ONE-DIMENSIONAL DEPENDENCY

In this section we shall derive finite-difference equations to be used for finding an approximate solution to a differential equation of the form

$$\frac{-d}{d\zeta} D(\zeta) \frac{d}{d\zeta} \varphi(\zeta) - D(\zeta) \frac{\rho}{\zeta} \frac{d}{d\zeta} \varphi(\zeta) + A(\zeta) \varphi(\zeta) = \mathcal{S}(\zeta) \tag{1}$$

where ρ is a constant which depends on the geometry of the problem ($\rho = 0$, cartesian geometry; $\rho = 1$, cylindrical geometry; $\rho = 2$, spherical geometry). The equation is to be solved in a closed region, $\zeta_I \leq \zeta \leq \zeta_{\mathcal{O}}$. With appropriate boundary conditions Equation (1) can be used to describe one-dimensional monoenergetic neutron-diffusion, where $D(\zeta)$ is the diffusion coefficient, $A(\zeta)$ is the absorption cross section, $\mathcal{S}(\zeta)$ is the neutron source and $\varphi(\zeta)$ is the neutron flux; all evaluated at the given energy. We assume that the closed region can be divided into a finite set of sub-regions, in each of which all the functions are continuous and possess derivatives of sufficiently high order. At interfaces between such sub-regions we assume that $\varphi(\zeta)$ and $D(\zeta)d\varphi/d\zeta$ are continuous.

We choose a set of points $\left\{ \zeta_n \right\}$

$$\zeta_I = \zeta_0 < \zeta_1 < \zeta_2 < \cdots\cdots < \zeta_{N-1} < \zeta_N = \zeta_{\mathcal{O}}$$

$$\Delta\zeta_n^+ \equiv \zeta_{n+1} - \zeta_n,$$

$$\Delta\zeta_n^- \equiv \zeta_n - \zeta_{n-1},$$

which will yield a suitably fine mesh for our difference equations and are such that they contain the interfaces between the subregions mentioned above as a subset. Integrating Equation (1) from

$$\zeta_n - \frac{\Delta\zeta_n^-}{2} \; (\equiv \zeta_{n-\frac{1}{2}})$$

to

$$\zeta_n + \frac{\Delta\zeta_n^+}{2} \; (\equiv \zeta_{n+\frac{1}{2}})$$

we obtain

$$-\left[D(\zeta)\frac{d}{d\zeta}\varphi(\zeta)\right]\cdot\zeta^\rho\Big|_{\zeta_{n-\frac{1}{2}}}^{\zeta_{n+\frac{1}{2}}} = \int_{\zeta_{n-\frac{1}{2}}}^{\zeta_{n+\frac{1}{2}}} [S(\zeta) - A(\zeta)\phi(\zeta)]\cdot\zeta^\rho \, d\zeta \tag{2}$$

Using Taylor's series expansion, we can express the left-hand side of Equation (2) as

$$-D(\zeta_{n+\frac{1}{2}})\,\zeta^\rho_{n+\frac{1}{2}}\,\frac{\varphi(\zeta_{n+1}) - \varphi(\zeta_n)}{\Delta\zeta_n^+} + D(\zeta_{n-\frac{1}{2}})\,\zeta^\rho_{n-\frac{1}{2}}\,\frac{\varphi(\zeta_n) - \varphi(\zeta_{n-1})}{\Delta\zeta_n^-}$$

$$+ D(\zeta_{n+\frac{1}{2}})\,\zeta^\rho_{n+\frac{1}{2}}\,\frac{1}{24}(\Delta\zeta_n^+)^2\,\varphi^{(3)}(\zeta_{n+\frac{1}{2}})$$

$$- D(\zeta_{n-\frac{1}{2}})\,\zeta^\rho_{n-\frac{1}{2}}\,\frac{1}{24}(\Delta\zeta_n^-)^2\,\varphi^{(3)}(\zeta_{n-\frac{1}{2}}) + \mathcal{O}(\Delta\zeta_n^4) \tag{3}$$

If we define

$$Q(\zeta) = S(\zeta) - A(\zeta)\,\varphi(\zeta) \tag{4}$$

we have, for the integral on the right-hand side of Equation (2),

$$\int_{\zeta_{n-\frac{1}{2}}}^{\zeta_n} Q(\zeta)\cdot\zeta^\rho\, d\zeta = \frac{Q(\zeta_n^-) + Q(\zeta_{n-1}^+)}{2}\,\frac{\zeta^{\rho+1}}{\rho+1}\Big|_{\zeta_{n-\frac{1}{2}}}^{\zeta_n}$$

$$+ \frac{Q(\zeta_n^-) - Q(\zeta_{n-1}^+)}{\Delta\zeta_n^-}\left[\frac{\zeta^{\rho+2}}{\rho+2} - \zeta_{n-\frac{1}{2}}\,\frac{\zeta^{\rho+1}}{\rho+1}\right]\Bigg|_{\zeta_{n-\frac{1}{2}}}^{\zeta_n}$$

$$-\frac{1}{24}\,\zeta^\rho_{n-\frac{1}{2}}\,(\Delta\zeta_n^-)^3\,Q^{(2)}(\zeta_{n-\frac{1}{2}}) + \mathcal{O}\left((\Delta\zeta_n^-)^4\right) , \tag{5}$$

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and
$$\int_{\zeta_n}^{\zeta_{n+\frac{1}{2}}} Q(\zeta)\cdot\zeta^\rho\, d\zeta = \frac{Q(\zeta_n+) + Q(\zeta_{n+1}-)}{2}\ \frac{\zeta^{\rho+1}}{\rho+1}\Bigg|_{\zeta_n}^{\zeta_{n+\frac{1}{2}}}$$
$$+ \frac{Q(\zeta_{n+1}^-) - Q(\zeta_n+)}{\Delta\zeta_n^+}\left[\frac{\zeta^{\rho+2}}{\rho+2} - \zeta_{n+\frac{1}{2}}\ \frac{\zeta^{\rho+1}}{\rho+1}\right]\Bigg|_{\zeta_n}^{\zeta_{n+\frac{1}{2}}}$$
$$- \frac{1}{24}\zeta^\rho_{n+\frac{1}{2}}(\Delta\zeta_n^+)^3 Q^{(2)}(\zeta_{n+\frac{1}{2}}) + \mathcal{O}\left((\Delta\zeta_n^+)^4\right) \qquad (6)$$

Using Equations (3), (5), and (6), we can write Equation (2), after multiplying through by $\Delta\zeta_n^-/\zeta_n^\rho$

$$i_n^- D(\zeta_{n-\frac{1}{2}})\left[\varphi(\zeta_n) - \varphi(\zeta_{n-1})\right] + \tau_n\, i_n^+\ D(\zeta_{n+\frac{1}{2}})\left[\varphi(\zeta_n) - \varphi(\zeta_{n+1})\right]$$
$$= \frac{\Delta\zeta_n^-}{\zeta_n{}^\rho}\left[J_n(Q) + I_{n+1}(Q)\right]$$
$$+ \frac{\Delta\zeta_n^-}{24}\Big\{ - i_n^+ D(\zeta_{n+\frac{1}{2}}) + (\Delta\zeta_n^+)^2\varphi^{(3)}(\zeta_{n+\frac{1}{2}}) - i_n^+(\Delta\zeta_n^+)^3 Q^{(2)}(\zeta_{n+\frac{1}{2}})$$
$$+ i_n^- D(\zeta_{n-\frac{1}{2}})(\Delta\zeta_n^-)^2\varphi^{(3)}(\zeta_{n-\frac{1}{2}}) - i_n^-(\Delta\zeta_n^-)^3 Q^{(2)}(\zeta_{n-\frac{1}{2}})\Big\} + \mathcal{O}(\Delta\zeta^5), \qquad (7)$$

where

$$J_n(Q) = \frac{1}{8}\ \zeta_n^\rho\,\Delta\zeta_n^-\Bigg[\left(1 - \frac{\rho\Delta\zeta_n^-}{3\zeta_n} + \frac{\rho(\rho-1)(\Delta\zeta_n^-)^2}{16\,\zeta_n{}^2}\right)Q(\zeta_{n-1}+)$$
$$+ 3\left(1 - \frac{2\rho\Delta\zeta_n^-}{9\zeta_n} + \frac{5\rho(\rho-1)(\Delta\zeta_n^-)^2}{144\,\zeta_n{}^2}\right)Q(\zeta_n^-)\Bigg] \qquad (8)$$

$$I_{n+1}(Q) = \frac{1}{8}\ \zeta_n^\rho\,\Delta\zeta_n^+\Bigg[3\left(1 + \frac{2\rho\Delta\zeta_n^+}{9\zeta_n} + \frac{5\rho(\rho-1)(\Delta\zeta_n^+)^2}{144\zeta_n{}^2}\right)Q(\zeta_n^+)$$
$$+\left(1 + \frac{\rho\Delta\zeta_n^+}{3\zeta_n} + \frac{\rho(\rho-1)(\Delta\zeta_n^+)^2}{16\,\zeta_n{}^2}\right)Q(\zeta_{n+1}-)\Bigg] \qquad (9)$$

and

$$i_n^- = \frac{\varsigma^{\rho}_{n-\frac{1}{2}}}{\varsigma^{\rho}_n} \quad ; \quad i_n^+ = \frac{\varsigma^{\rho}_{n+\frac{1}{2}}}{\varsigma^{\rho}_n} \quad ; \quad r_n = \frac{\Delta\varsigma_n^-}{\Delta\varsigma_n^+} \quad . \tag{10}$$

Thus

$$i_n^- D(\varsigma_{n-\frac{1}{2}})\left[\varphi_n - \varphi_{n-1}\right] + r_n i_n^+ D(\varsigma_{n+\frac{1}{2}})\left[\varphi_n - \varphi_{n+1}\right]$$

$$(n = 1, 2, \ldots, N-1)$$

$$= \frac{\Delta\varsigma_n^-}{\varsigma_n^{\rho}}\left[J_n(Q) + I_{n+1}(Q)\right],$$

where $Q(\varsigma_n)$ is to be interpreted as replaced by

$$Q_n = \mathcal{S}(\varsigma_n) - A(\varsigma_n)\varphi_n ,$$

is a set of possible difference equations to replace Equation (2). The solution of the difference equations is denoted by φ_n and is to be distinguished from $\varphi(\varsigma_n)$, the solution of the differential equations evaluated at ς_n. Equation (7) shows that the truncation error,

$$\epsilon(n) = \varphi(\varsigma_n) - \varphi_n$$

will be $O(\Delta\varsigma^4)$ at points where the composition is continuous and where $\Delta\varsigma_n^- = \Delta\varsigma_n^+$. At points where these conditions are not met, the truncation error will be $O(\Delta\varsigma^3)$.

We can get better difference equations if we can eliminate the bracketed quantities in Equation (7). Then our equations will be good to $O(\Delta\varsigma^5)$.

If we differentiate Equation (1) with respect to ς and solve for $D \cdot d^3\varphi/d\varsigma^3$, we find (after eliminating $d^2\varphi/d\varsigma^2$)

$$D\frac{d^3\varphi}{d\varsigma^3} = -\frac{dQ}{d\varsigma} + \frac{Q}{D}\left(\frac{\rho}{\varsigma}D + 2\frac{dD}{d\varsigma}\right)$$

$$+ \frac{d\varphi}{d\varsigma}\left[\frac{\rho(\rho+1)}{\varsigma^2}D + \frac{2\rho}{\varsigma}\frac{dD}{d\varsigma} + \frac{2}{D}\left(\frac{dD}{d\varsigma}\right)^2 - \frac{d^2D}{d\varsigma^2}\right].$$

Using this equation and the equation

$$\left.\frac{d\varphi}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}} = \frac{\varphi(\varsigma_{n+1}) - \varphi(\varsigma_n)}{\Delta\varsigma_n^+} - \frac{(\Delta\varsigma_n^+)^2}{24}\left.\frac{d^3\varphi}{d\varsigma^3}\right|_{\varsigma_{n+\frac{1}{2}}} + O\left((\Delta\varsigma_n^+)^4\right),$$

we find for an approximation for $\frac{d\varphi}{d\varsigma}$ at $\varsigma_{n+\frac{1}{2}}$

$$\left.\frac{d\varphi}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}} = \frac{1}{1+W(\varsigma_{n+\frac{1}{2}})}\left\{\frac{\varphi(\varsigma_{n+1})-\varphi(\varsigma_n)}{\Delta\varsigma_n^+} + \frac{(\Delta\varsigma_n^+)^2}{24\,D(\varsigma_{n+\frac{1}{2}})}\left.\frac{dQ}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}}\right.$$

$$\left. - \frac{(\Delta\varsigma_n^+)^2}{24}\frac{Q(\varsigma_{n+\frac{1}{2}})}{D(\varsigma_{n+\frac{1}{2}})}\left(\frac{\rho}{\varsigma_{n+\frac{1}{2}}} + \frac{2}{D(\varsigma_{n+\frac{1}{2}})}\left.\frac{dD}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}}\right)\right\} + O\left((\Delta\varsigma_n^+)^4\right)$$

where

$$W(\varsigma_{n+\frac{1}{2}}) = \frac{(\Delta\varsigma_n^+)^2}{24}\left[\frac{\rho(\rho+1)}{\varsigma^2} + \frac{2\rho}{\varsigma D(\varsigma)}\frac{dD}{d\varsigma} + \frac{2}{D^2}\left(\frac{dD}{d\varsigma}\right)^2 - \frac{1}{D}\frac{d^2D}{d\varsigma^2}\right]_{\varsigma_{n+\frac{1}{2}}}.$$

Since

$$Q(\varsigma_{n+\frac{1}{2}}) = \frac{Q(\varsigma_{n+1}) + Q(\varsigma_n)}{2} + O\left((\Delta\varsigma_n^+)^2\right)$$

and

$$\left.\frac{dQ}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}} = \frac{Q(\varsigma_{n+1}) - Q(\varsigma_n)}{\Delta\varsigma_n^+} + O\left((\Delta\varsigma_n^+)^2\right),$$

we have

$$\left.\frac{d\varphi}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}} = \frac{1}{1+W(\varsigma_{n+\frac{1}{2}})}\left\{\frac{\varphi(\varsigma_{n+1})-\varphi(\varsigma_n)}{\Delta\varsigma_n^+} + \frac{\Delta\varsigma_n^+}{24\,D(\varsigma_{n+\frac{1}{2}})}\left(Q(\varsigma_{n+1}) - Q(\varsigma_n)\right)\right.$$

$$\left. - \frac{(\Delta\varsigma_n^+)^2}{48}\frac{Q(\varsigma_{n+1})+Q(\varsigma_n)}{D(\varsigma_{n+\frac{1}{2}})}\left(\frac{\rho}{\varsigma_{n+\frac{1}{2}}} + \frac{2}{D(\varsigma_{n+\frac{1}{2}})}\left.\frac{dD}{d\varsigma}\right|_{\varsigma_{n+\frac{1}{2}}}\right)\right\} + O\left((\Delta\varsigma_n^+)^4\right).$$

A similar expression can be obtained for $d\varphi/d\varsigma|_{\varsigma_{n-\frac{1}{2}}}$

$$\left.\frac{d\varphi}{d\varsigma}\right|_{\varsigma_{n-\frac{1}{2}}} = \frac{1}{1+W(\varsigma_{n-\frac{1}{2}})}\left\{\frac{\varphi(\varsigma_n)-\varphi(\varsigma_{n-1})}{\Delta\varsigma_n^-} + \frac{\Delta\varsigma_n^-}{24\,D(\varsigma_{n-\frac{1}{2}})}\left(Q(\varsigma_n)-Q(\varsigma_{n-1})\right)\right.$$

$$\left. - \frac{(\Delta\varsigma_n^-)^2}{48}\,\frac{Q(\varsigma_n)+Q(\varsigma_{n-1})}{D(\varsigma_{n-\frac{1}{2}})}\left(\frac{\rho}{\varsigma_{n-\frac{1}{2}}} + \frac{2}{D(\varsigma_{n-\frac{1}{2}})}\left.\frac{dD}{d\varsigma}\right|_{\varsigma_{n-\frac{1}{2}}}\right)\right\} + O\left((\Delta\varsigma_n^-)^4\right),$$

where

$$W(\varsigma_{n-\frac{1}{2}}) = \frac{(\Delta\varsigma_n^-)^2}{24}\left[\frac{\rho(\rho+1)}{\varsigma^2} + \frac{2\rho}{\varsigma D}\frac{dD}{d\varsigma} + \frac{2}{D^2}\left(\frac{dD}{d\varsigma}\right)^2 - \frac{1}{D}\frac{d^2D}{d\varsigma^2}\right]_{\varsigma_{n-\frac{1}{2}}}.$$

If the composition is discontinuous at ς_n, we cannot find approximations for $d^2Q/d\varsigma^2|_{\varsigma_{n+\frac{1}{2}}}$ and $d^2Q/d\varsigma^2|_{\varsigma_{n-\frac{1}{2}}}$ in terms of values of $Q(\varsigma)$ at ς_{n+1}, ς_n, ς_{n-1}. Thus at points of discontinuity in composition we can substitute the above expressions for $d\varphi/d\varsigma|_{\varsigma_{n+\frac{1}{2}}}$ and $d\varphi/d\varsigma|_{\varsigma_{n-\frac{1}{2}}}$ in the left-hand side of Equation (2) but we cannot obtain a better approximation for the right-hand side than that obtained from Equations (5) and (6). Making these substitutions and dropping terms of order $O(\Delta\varsigma^3)$ we obtain, after multiplying through by $\Delta\varsigma_n^-/\varsigma_n^\rho$

$$\check{i}_n^-\,D(\varsigma_{n-\frac{1}{2}})\left[\varphi_n-\varphi_{n-1}\right] + \gamma_n\,\check{i}_n^-\,D(\varsigma_{n+\frac{1}{2}})\left[\varphi_n-\varphi_{n+1}\right]$$

$$= \frac{\Delta\varsigma_n^-}{\varsigma_n^\rho}\left[\check{J}_n(Q) + \check{I}_{n+1}(Q)\right] \qquad (11)$$

where

$$\check{i}_n^- = \frac{1}{1+W(\varsigma_{n-\frac{1}{2}})}\,i_n^-,$$

$$\check{i}_n^+ = \frac{1}{1+W(\varsigma_{n+\frac{1}{2}})}\,i_n^+,$$

$$\check{J}_n(Q) = J_n(Q) + \frac{1}{1 + W(S_{n-\frac{1}{2}})} S^{\rho}_{n-\frac{1}{2}} \frac{(\Delta S_n^-)^2}{24} \left[\frac{Q^+_{n-1} - Q^-_n}{\Delta S^-_n} + \left(\frac{\rho}{2S} + \frac{1}{D}\frac{dD}{dS} \right)_{S_{n-\frac{1}{2}}} \left(Q^+_{n-1} + Q^-_n \right) \right], \qquad (12)$$

$$\check{I}_{n+1}(Q) = I_{n+1}(Q) - \frac{1}{1 + W(S_{n+\frac{1}{2}})} S^{\rho}_{n+\frac{1}{2}} \frac{(\Delta S_n^+)^2}{24} \left[\frac{Q^+_{n} - Q^-_{n+1}}{\Delta S^+_n} + \left(\frac{\rho}{2S} + \frac{1}{D}\frac{dD}{dS} \right)_{S_{n+\frac{1}{2}}} \left(Q^+_{n} + Q^-_{n+1} \right) \right],$$

and where plus or minus signs on the Q_n 's mean evaluation from the left or right, respectively, of the nodal points S_n . Equation (11) gives truncation errors $O(\Delta S^4)$, provided D(S) and its first two derivatives are known at $S_{n\pm\frac{1}{2}}$.

At points where the composition varies continuously, the terms of $O(\Delta S^4)$ in Equation (7) can be approximated

$$-\frac{1}{24} i_n^- (\Delta S_n^-)^3 Q^{(2)}(S_{n-\frac{1}{2}}) - \frac{1}{24} i_n^+ (\Delta S_n^+)^3 Q^{(2)}(S_{n+\frac{1}{2}})$$

$$\cong -\frac{1}{12} \frac{i_n^- (\Delta S_n^-)^3 + i_n^+ (\Delta S_n^+)^3}{\Delta S_n^- + \Delta S_n^+} \left[\frac{Q_{n+1} - Q_n}{\Delta S_n^+} - \frac{Q_n - Q_{n-1}}{\Delta S_n^-} \right].$$

Using this, we obtain an equation good to $O(\Delta s^5)$

$$\hat{i}_n^- D(s_{n-\frac{1}{2}})\left[\varphi_n - \varphi_{n-1}\right] + r_n \hat{i}_n^- D(s_{n+\frac{1}{2}})\left[\varphi_n - \varphi_{n+1}\right]$$

$$= \frac{\Delta s_n^-}{s_n^\rho}\left[\hat{J}_n(Q) + \hat{I}_{n+1}(Q)\right] \qquad (13)$$

where

$$\hat{i}_n^- = \check{i}_n^-$$

$$\hat{i}_n^+ = \check{i}_n^+$$

$$\hat{J}_n(Q) = \check{J}_n(Q) + \frac{s_n^\rho}{12}\left[i_n^-(\Delta s_n^-)^3 + i_n^+(\Delta s_n^+)^3\right]\frac{Q_n^- - Q_{n-1}^+}{\Delta s_n^-(\Delta s_n^- + \Delta s_n^+)}$$

$$\hat{I}_{n+1}(Q) = \check{I}_{n+1}(Q) + \frac{s_n^\rho}{12}\left[i_n^-(\Delta s_n^-)^3 + i_n^+(\Delta s_n^+)^3\right]\frac{Q_n^+ - Q_{n+1}^-}{\Delta s_n^+(\Delta s_n^- + \Delta s_n^+)} . \qquad (14)$$

A formula (containing the degree of approximation used in the difference equations) for integrating over a region R of continuous composition extending from s_{N_1} to s_{N_2} is given by

$$\int_{s_{N_1}}^{s_{N_2}} \psi(s)\cdot s^\rho ds \cong I_{N_1+1}(\psi) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_n(\psi) + \bar{I}_{n+1}(\psi)\right) + J_{N_2}(\psi), \qquad (15)$$

where

$$\bar{J}_n(\psi) = J_n(\psi) + \frac{s_n^\rho}{12}\left[i_n^-(\Delta s_n^-)^3 + i_n^+(\Delta s_n^+)^3\right]\frac{\psi_n^- - \psi_{n-1}^+}{\Delta s_n^-(\Delta s_n^- + \Delta s_n^+)} , \qquad (16)$$

$$\bar{I}_{n+1}(\psi) = I_{n+1}(\psi) + \frac{s_n^\rho}{12}\left[i_n^-(\Delta s_n^-)^3 + i_n^+(\Delta s_n^+)^3\right]\frac{\psi_n^+ - \psi_{n+1}^-}{\Delta s_n^+(\Delta s_n^- + \Delta s_n^+)} .$$

Integrating our differential equation over the region R, we find the conservation equation

$$(\varsigma^\rho j)^-_{N_2} - (\varsigma^\rho j)^+_{N_1} = \int_{\varsigma_{N_1}}^{\varsigma_{N_2}} Q(\varsigma)\cdot \varsigma^\rho \, d\varsigma$$

where, in later sections,

$$(\varsigma^\rho j)_n = -D(\varsigma)\cdot \varsigma^\rho \left.\frac{d\varphi}{d\varsigma}\right|_{\varsigma_n}$$

will be the outward directed neutron current (multiplied by ς_n^ρ) at ς_n . Replacing the integral in our conservation equation by the approximation in Equation (15), we have

$$\begin{aligned}(\varsigma^\rho j)^-_{N_2} - (\varsigma^\rho j)^+_{N_1} &= I_{N_1+1}(Q) \\ &+ \sum_{N_1+1}^{N_2-1}\left[\bar{J}_n(Q) + \bar{I}_{n+1}(Q)\right] + J_{N_2}(Q). \qquad (17)\end{aligned}$$

In Equation (17) $j(\varsigma_n)$ is now an approximation to the neutron current at ς_n and we will redefine it in such a way that Equation (17) holds.

We would like to be able to express the current at a nodal point in terms of quantities given entirely on one or the other side of the nodal point. We therefore assume that the current can be written in either of the two forms

$$(\varsigma^\rho j)^-_n = D(\varsigma_n^-)\left[A_n Q_n^- + B_n Q_{n-1}^+ + C_n \varphi_n + E_n \varphi_{n-1}\right]$$

and

$$(\varsigma^\rho j)^+_n = D(\varsigma_n^+)\left[A'_n Q_n^+ + B'_n Q_{n+1}^- + C'_n \varphi_n + E'_n \varphi_{n+1}\right].$$

The fact that these are two-point formulas is in keeping with our using three-point difference equations.

To determine the coefficients in the defining equations for the current, we examine Equation (17). Using Equations (16), (13), and (12) we obtain

$$\sum_{N_1+1}^{N_2-1}\left[\bar{J}_n(Q)+\bar{I}_{n+1}(Q)\right]=\sum_{N_1+1}^{N_2-1}\left[\hat{J}_n(Q)+\hat{I}_{n+1}(Q)\right]$$

$$-\varsigma^{\rho}_{N_1+\frac{1}{2}}\frac{(\Delta\varsigma^{+}_{N_1})^2}{24}\left[\left(\frac{\rho}{2\varsigma_{N_1+\frac{1}{2}}}+\frac{1}{D(\varsigma_{N_1+\frac{1}{2}})}\frac{dD}{d\varsigma}\bigg|_{N_1+\frac{1}{2}}+\frac{1}{\Delta\varsigma^{-}_{N_1+1}}\right)Q^{+}_{N_1}\right.$$

$$\left.+\left(\frac{\rho}{2\varsigma_{N_1+\frac{1}{2}}}+\frac{1}{D(\varsigma_{N_1+\frac{1}{2}})}\frac{dD}{d\varsigma}\bigg|_{N_1+\frac{1}{2}}-\frac{1}{\Delta\varsigma^{-}_{N_1+1}}\right)Q^{-}_{N_1+1}\right]\frac{1}{1+W(\varsigma_{N_1+\frac{1}{2}})}$$

$$+\varsigma^{\rho}_{N_2-\frac{1}{2}}\frac{(\Delta\varsigma^{-}_{N_2})^2}{24}\left[\left(\frac{\rho}{2\varsigma_{N_2-\frac{1}{2}}}+\frac{1}{D(\varsigma_{N_2-\frac{1}{2}})}\frac{dD}{d\varsigma}\bigg|_{N_2-\frac{1}{2}}+\frac{1}{\Delta\varsigma^{+}_{N_2-1}}\right)Q^{+}_{N_2-1}\right.$$

$$\left.+\left(\frac{\rho}{2\varsigma_{N_2-\frac{1}{2}}}+\frac{1}{D(\varsigma_{N_2-\frac{1}{2}})}\frac{dD}{d\varsigma}\bigg|_{N_2-\frac{1}{2}}-\frac{1}{\Delta\varsigma^{+}_{N_2-1}}\right)Q^{-}_{N_2}\right]\frac{1}{1+W(\varsigma_{N_2-\frac{1}{2}})},$$

But, using Equation (13) and the definitions of $\hat{i}^{+}_{n}$, $\hat{i}^{-}_{n}$, we have

$$\sum_{N_1+1}^{N_2-1}\left[\hat{J}_n(Q)+\hat{I}_{n+1}(Q)\right]$$

$$=\sum_{N_1+1}^{N_2-1}\left[\frac{\varsigma^{\rho}_{n}}{\Delta\varsigma^{-}_{n}}\left\{\hat{i}^{-}_{n}D(\varsigma_{n-\frac{1}{2}})(\varphi_n-\varphi_{n-1})+r_n\hat{i}^{+}_{n}D(\varsigma_{n+\frac{1}{2}})(\varphi_n-\varphi_{n+1})\right\}\right]$$

$$=\frac{\varsigma^{\rho}_{N_1+1}}{\Delta\varsigma^{-}_{N_1+1}}\hat{i}^{-}_{N_1+1}D(\varsigma_{N_1+\frac{1}{2}})(\varphi_{N_1+1}-\varphi_{N_1})+\frac{\varsigma^{\rho}_{N_2-1}}{\Delta\varsigma^{-}_{N_2-1}}r_{N_2-1}\hat{i}^{+}_{N_2-1}D(\varsigma_{N_2-\frac{1}{2}})(\varphi_{N_2-1}-\varphi_{N_2})$$

On the basis of these results, Equation (17) becomes

$$(\zeta^\rho j)^-_{N_2} - J_{N_2}(Q) - \zeta^\rho_{N_2-\frac{1}{2}}\frac{(\Delta\zeta^-_{N_2})^2}{24}\frac{1}{1+W(\zeta_{N_2-\frac{1}{2}})}\left[\left(\frac{\rho}{2\zeta}+\frac{1}{D}\frac{dD}{d\zeta}\right)_{\zeta_{N_2-\frac{1}{2}}}(Q^+_{N_2-1}+Q^-_{N_2}) + \frac{1}{\Delta\zeta^+_{N_2-1}}(Q^+_{N_2-1}-Q^-_{N_2})\right] - \frac{\zeta^\rho_{N_2-1}}{\Delta\zeta^-_{N_2-1}} r_{N_2-1}\hat{i}^+_{N_2-1} D(\zeta_{N_2-\frac{1}{2}})\left[\varphi_{N_2-1}-\varphi_{N_2}\right]$$

$$= (\zeta^\rho j)^+_{N_2} + I_{N_1+1}(Q) - \zeta^\rho_{N_1+\frac{1}{2}}\frac{(\Delta\zeta^+_{N_1})^2}{24}\frac{1}{1+W(\zeta_{N_1+\frac{1}{2}})}\left[\left(\frac{\rho}{2\zeta}+\frac{1}{D}\frac{dD}{d\zeta}\right)_{\zeta_{N_1+\frac{1}{2}}}(Q^+_{N_1}+Q^-_{N_1+1}) + \frac{1}{\Delta\zeta^-_{N_1+1}}(Q^+_{N_1}-Q^-_{N_1+1})\right] + \frac{\zeta^\rho_{N_1+1}}{\Delta\zeta^-_{N_1+1}}\hat{i}^-_{N_1+1} D(\zeta_{N_1+\frac{1}{2}})\left[\varphi_{N_1+1}-\varphi_{N_1}\right].$$

Since ζ_{N_1} and ζ_{N_2} are arbitrary points, the two sides of the equation must equal the same constant. This constant must be taken to be zero, so that there will be zero current in the absence of neutrons. Thus we obtain the formulas

$$(\zeta^\rho j)^-_n = \check{J}_n(Q) + \frac{\zeta^\rho_{n-1}}{\Delta\zeta^-_{n-1}} r_{n-1}\hat{i}^+_{n-1} D(\zeta_{n-\frac{1}{2}})\left[\varphi_{n-1}-\varphi^-_n\right],$$

$$(\zeta^\rho j)^+_n = -\check{I}_{n+1}(Q) - \frac{\zeta^\rho_{n+1}}{\Delta\zeta^-_{n+1}}\hat{i}^-_{n+1} D(\zeta_{n+\frac{1}{2}})\left[\varphi_{n+1}-\varphi^+_n\right]. \qquad (18)$$

The fact that neutrons are conserved in passing from one region to the next is expressed by the boundary condition (at an interface ζ_n)

$$(\zeta^\rho j)^-_n = (\zeta^\rho j)^+_n. \qquad (19)$$

Substituting Formulas (18) into (19) and using

$$\varphi^-_n = \varphi^+_n$$

we obtain, after some manipulation, Equation (11) which holds at interfaces. Therefore, we have verified that Equation (11) is the proper difference equation to be used at an interface.

B. THE AGE-DIFFUSION EQUATION

The age-diffusion equation* is

$$-\nabla \frac{1}{3\Sigma'_{tr}(\vec{r},u)} \nabla nv(\vec{r},u) + \Sigma'_a(\vec{r},u)\, nv(\vec{r},u) = -\frac{\partial q(\vec{r},u)}{\partial u} + \chi(u)P(\vec{r}) + I(\vec{r},u) \tag{20}$$

$$-\nabla \frac{1}{3\Sigma'_{tr}(\vec{r},u_T)} \nabla nv(\vec{r},u_T) + \Sigma'_a(\vec{r},u_T)\, nv(\vec{r},u_T) = \lim_{u\to u_T}\left[q(\vec{r},u)\right] + \chi(u_T)P(\vec{r}) + I(\vec{r},u_T) \tag{21}$$

where

$q(\vec{r},u)$ is the slowing-down density

u is lethargy = $\ln E_0/E$, where E is energy, and E_o is some reference energy

$u_T = \ln E_0/E_T$ where E_T is thermal energy

$nv(\vec{r},u)$ is the neutron flux per unit u

$\Sigma'_{tr}(\vec{r},u)$ is the macroscopic transport cross section

$\Sigma'_a(\vec{r},u)$ is the macroscopic absorption cross section.

The source terms $\chi(u)P(\vec{r})$ and $I(\vec{r},u)$ represent neutrons liberated in fissions and neutrons scattered inelastically from higher energies. Thus we have

$$P(\vec{r}) = \int_{-\infty}^{u_T} \nu\Sigma'_f(\vec{r},u')\, nv(\vec{r},u')\,du' + \nu\Sigma'_f(\vec{r},u_T)\, nv(\vec{r},u_T),$$

$$I(\vec{r},u) = \int_{-\infty}^{u} \left[\sum_{(m)} \chi_{(m)}(u'\to u)\,\Sigma'_{in(m)}(\vec{r},u')\right] nv(\vec{r},u')\,du', \tag{22}$$

*For a derivation of the age-diffusion equation and a discussion of its validity in reactor problems, see Marshak, Brooks, and Hurwitz, Nucleonics, May 1949.

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where

$\chi(u)$ is the fission spectrum, normalized so that $\int_{-\infty}^{u_T} \chi(u)\, du + \chi(u_T) = 1$,

ν is the average number of neutrons emitted per fission,

$\Sigma_f(\vec{r},u)$ is the macroscopic fission cross section,

$\chi_{(m)}(u'\to u)$ is the probability that a neutron scattered inelastically, by material m, from lethargy u' reaches u, so that we have

$$\int_{u'}^{u} \chi_{(m)}(u' \to u)\, du = 1$$; and

$\Sigma_{in(m)}(\vec{r},u)$ is the macroscopic inelastic-scattering cross section of material m.

We assume a relation between the slowing-down density and the neutron flux

$$q(\vec{r},u) = S(\vec{r},u)\, nv(\vec{r},u). \tag{23}$$

At KAPL, we take

$$S(\vec{r},u) = \xi\, \Sigma_s(\vec{r},u),$$

where ξ is the average logarithmic energy-loss in moderating collisions, and $\Sigma_s(\vec{r},u)$ is the macroscopic scattering cross section. ORNL uses

$$S(\vec{r},u) = \xi\, \Sigma_t(\vec{r},u),$$

where $\Sigma_t(\vec{r},u)$ is the macroscopic total cross section.

If we restrict ourselves to the one-space-dimensional case (where we denote the space variable by ξ), our investigations in Section A give us the following finite difference representation (in space) for Equation (20):

$$\hat{i}_n^-(u)\, D(\xi_{n-1/2},u)\left[\varphi_n(u) - \varphi_{n-1}(u)\right] + \tau_n\, \hat{i}_n^+(u)\, D(\xi_{n+1/2},u)\left[\varphi_n(u) - \varphi_{n+1}(u)\right]$$

$$= \frac{\Delta \xi_n^-}{\xi_n^\rho}\left[\hat{J}_n(Q,u) + \hat{I}_{n+1}(Q,u)\right], \tag{24}$$

where the turrets are to be replaced by inverted turrets at points of discontinuity and

where

$$\begin{cases} \varphi(\varsigma, u) = nv(\varsigma, u), \\ D(\varsigma, u) = \dfrac{1}{3\Sigma'_{tr}(\varsigma, u)}, \\ Q(\varsigma, u) = -\dfrac{\partial q(\varsigma, u)}{\partial u} + \chi(u)P(\varsigma) + I(\varsigma, u) - \Sigma'_a(\varsigma, u)nv(\varsigma, u). \end{cases}$$

To derive multigroup equations from Equations (24) we restrict ourselves to a relevant energy range, E_0 to E_T, and split the corresponding lethargy range, u_0 to u_T, into increments $\Delta u_i(u_{i-1}, u_i)$, where $i = 1, 2, \ldots, T$. We average Equations (24) over a lethargy width Δu_i, obtaining

$$\overline{\hat{i}_n^- D(\varsigma_{n-1/2})\left[\varphi_n - \varphi_{n-1}\right]}_i + T_n \overline{\hat{i}_n^+ D(\varsigma_{n+1/2})\left[\varphi_n - \varphi_{n+1}\right]}_i$$

$$= \frac{\Delta\varsigma_n^-}{\varsigma_n^\rho} \overline{\left[\hat{J}_n(Q) + \hat{I}_{n+1}(Q)\right]}_i \tag{25}$$

where bars denote averages; that is,

$$\overline{\textcircled{H}(\varsigma)}_i \equiv \frac{1}{\Delta u_i}\int_{u_{i-1}}^{u_i} \textcircled{H}(\varsigma, u)\, du .$$

One approximation to Equations (25) consists of splitting the averages of products into products of averages, yielding

$$\hat{i}_{ni}^- D_i(\varsigma_{n-1/2})\left[\varphi_{ni} - \varphi_{n-1i}\right]$$

$$+ T_n \hat{i}_{ni}^+ D_i(\varsigma_{n+1/2})\left[\varphi_{ni} - \varphi_{n+1i}\right]$$

$$= \frac{\Delta\varsigma_n^-}{\varsigma_n^\rho}\left[\hat{J}_{ni}(Q_i) + \hat{I}_{n+1i}(Q_i)\right] \tag{26}$$

where

$$W_{ni} = \frac{(\Delta\varsigma_n^+)^2}{24}\left[\frac{\rho(\rho+1)}{\varsigma^2} + \frac{2\rho}{\varsigma}\frac{\overline{D'}_i}{\overline{D}_i} + 2\left(\frac{\overline{D'}_i}{\overline{D}_i}\right)^2 - \frac{\overline{D''}_i}{\overline{D}_i}\right]_{\varsigma_{n+1/2}},$$

$$\hat{i}^-_{ni} = \frac{i_n^-}{1+W_{n-1\,i}},$$

$$\hat{i}^+_{ni} = \frac{i_n^+}{1+W_{n\,i}},$$

$$\Gamma_n = \frac{\varsigma_n^\rho}{12}\;\frac{i_n^-(\Delta\varsigma_n^-)^3 + i_n^+(\Delta\varsigma_n^+)^3}{\Delta\varsigma_n^- + \Delta\varsigma_n^+},$$

$$\begin{aligned}
\hat{J}_{ni}(\chi) = &\left[\frac{\varsigma_n^\rho\Delta\varsigma_n^-}{8} - \frac{\rho\varsigma_n^{\rho-1}(\Delta\varsigma_n^-)^2}{24} + \frac{\rho(\rho-1)\varsigma_n^{\rho-2}(\Delta\varsigma_n^-)^3}{128} - \frac{\Gamma_n}{\Delta\varsigma_n^-}\right. \\
&\left. + \frac{\varsigma_{n-1/2}^\rho(\Delta\varsigma_n^-)^2}{24[1+W_{n-1\,i}]}\left(\frac{\rho}{2\varsigma} + \frac{\overline{D'}_i}{\overline{D}_i} + \frac{1}{\Delta\varsigma_n^-}\right)_{\varsigma_{n-1/2}}\right]\chi^+_{n-1} \\
&+\left[\frac{3\varsigma_n^\rho\Delta\varsigma_n^-}{8} - \frac{\rho\varsigma_n^{\rho-1}(\Delta\varsigma_n^-)^2}{12} + \frac{5\rho(\rho-1)\varsigma_n^{\rho-2}(\Delta\varsigma_n^-)^3}{384} + \frac{\Gamma_{ni}}{\Delta\varsigma_n^-}\right. \\
&\left. + \frac{\varsigma_{n-1/2}^\rho(\Delta\varsigma_n^-)^2}{24[1+W_{n-1\,i}]}\left(\frac{\rho}{2\varsigma} + \frac{\overline{D'}_i}{\overline{D}_i} - \frac{1}{\Delta\varsigma_n^-}\right)_{\varsigma_{n-1/2}}\right]\chi^-_{n},
\end{aligned} \tag{27}$$

$$\begin{aligned}
\hat{I}_{n+1\,i}(\chi) = &\left[\frac{3\varsigma_n^\rho\Delta\varsigma_n^+}{8} + \frac{\rho\varsigma_n^{\rho-1}(\Delta\varsigma_n^+)^2}{12} + \frac{5\rho(\rho-1)\varsigma_n^{\rho-2}(\Delta\varsigma_n^+)^3}{384} + \frac{\Gamma_{ni}}{\Delta\varsigma_n^+}\right. \\
&\left. - \frac{\varsigma_{n+1/2}^\rho(\Delta\varsigma_n^+)^2}{24[1+W_{ni}]}\left(\frac{\rho}{2\varsigma}\;\frac{\overline{D'}_i}{\overline{D}_i} + \frac{1}{\Delta\varsigma_n^+}\right)_{\varsigma_{n+1/2}}\right]\chi^+_{n} \\
&+\left[\frac{\varsigma_n^\rho\Delta\varsigma_n^+}{8} + \frac{\rho\varsigma_n^{\rho-1}(\Delta\varsigma_n^+)^2}{24} + \frac{\rho(\rho-1)\varsigma_n^{\rho-2}(\Delta\varsigma_n^+)^3}{128} - \frac{\Gamma_{ni}}{\Delta\varsigma_n^+}\right. \\
&\left. \frac{\varsigma_{n+1/2}^\rho(\Delta\varsigma_n^+)^2}{24[1+W_{ni}]}\left(\frac{\rho}{2\varsigma} + \frac{\overline{D'}_i}{\overline{D}_i} - \frac{1}{\Delta\varsigma_n^+}\right)_{\varsigma_{n+1/2}}\right]\chi^-_{n+1},
\end{aligned}$$

and

$$
\left.
\begin{aligned}
D_i(\xi) &= \overline{\frac{1}{3\Sigma'_t(\xi,u)_i}}\,, \\
\varphi_{ni} &= \overline{nv}_{ni}\,, \\
Q^{\pm}_{ni} &= \frac{q^{\pm}_{ni-1} - q^{\pm}_{ni}}{\Delta u_i} + \overline{\chi}^{\pm}_i P(\xi_n) + \overline{I(\xi_n)}^{\pm}_i - \overline{\Sigma'_{1a}(\xi_n)}^{\pm}_i \, \overline{nv}_{ni}
\end{aligned}
\right\} \qquad (28)
$$

with

$$
q_{ni} \equiv q_n(u_i).
$$

We can justify Equations (26) by taking a sufficient number of groups, so that cross sections are essentially constant over any group.

If we postulate the following relationship between the average and group-limit values of the slowing-down density,

$$
\overline{q}^{\pm}_{ni} = \omega^{\pm}_{1ni}\, q^{\pm}_{ni-1} + \omega^{\pm}_{2ni}\, q^{\pm}_{ni}\,, \qquad (29)
$$

and make use of an approximate equation derived from Equation (23),

$$
\overline{q}^{\pm}_{ni} = \overline{\xi(\xi_n)_i}^{\pm} \cdot \overline{nv}_{ni}\,, \qquad (30)
$$

we have

$$
Q^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1 + \frac{\omega^{\pm}_{1ni}}{\omega^{\pm}_{2ni}}\right) q^{\pm}_{ni-1} + \overline{\chi}^{\pm}_i P(\xi_n) + \overline{I(\xi_n)}_i - \left(\overline{\Sigma_{1a}(\xi_n)}^{\pm}_i + \frac{\overline{\xi(\xi_n)}^{\pm}_i}{\omega^{\pm}_{2ni}\Delta u_i}\right)\overline{nv}_{ni}
$$

Thus, if we write

$$
\left.
\begin{aligned}
A(\xi_n)_i &= \overline{\Sigma'_{1a}(\xi_n)}_i + \frac{\overline{\xi(\xi_n)}}{\omega_{2ni}\Delta u_i}\,, \\
S_{ni} &= \frac{1}{\Delta u_i}\left(1 + \frac{\omega_{1ni}}{\omega_{2ni}}\right) q_{ni-1} + \overline{\chi}_i P(\xi_n) + \overline{I(\xi_n)}_i\,,
\end{aligned}
\right\} \qquad (31)
$$

our multigroup difference equations become

$$
\begin{aligned}
&\hat{i}^-_{ni} D_i(\xi_{n-1/2})\left[\varphi_{ni} - \varphi_{n-1\,i}\right] + \tau_n \hat{i}^+_{ni} D_i(\xi_{n+1/2})\left[\varphi_{ni} - \varphi_{n+1\,i}\right] \\
&+ \frac{\Delta\xi^-_n}{\xi^p_n}\left[\hat{J}_{ni}(A_i\varphi_i) + \hat{I}_{n+1\,i}(A_i\varphi_i)\right] \\
&= \frac{\Delta\xi^-_n}{\xi^p_n}\left[\hat{J}_{ni}(S_i) + \hat{I}_{n+1\,i}(S_i)\right].
\end{aligned} \qquad (32)
$$

Equation (29) is used at KAPL with two main schemes of choosing w_{1ni} and w_{2ni}. In the first scheme we take $w_{1ni} = w_{2ni} = 1/2$. This scheme has its disadvantages. It may even lead to negative fluxes in some group, if the group widths are not small enough. In the second scheme we take $w_{1ni} = 0$ and $w_{2ni} = f_i(\varsigma_n)$, where $f_i(\varsigma_n)$ is chosen by trial and error. We may check the choice of $f_i(\varsigma_n)$ after the group equation has been solved by ascertaining whether $f_i(\varsigma_n)\, q_{ni}$ gives a reasonable estimate of $\overline{q}_{ni}$. In general, the solution does not seem very sensitive to the choice of $f_i(\varsigma_n)$, and reasonable guesses (based on previous calculations) can be made.

On the other hand, if we postulate (as does ORNL) that

$$\overline{nv}_{ni} = w_{1ni}\, nv_{ni-1} + w_{2ni}\, nv_{ni}, \tag{33}$$

and if we use Equation (30), we obtain

$$A(\varsigma_n)_i = \overline{\Sigma'_a(\varsigma_n)_i}\;\frac{S(\varsigma_n)_i}{w_{2ni}\,\Delta u_i}$$

$$\mathcal{S}_{ni} = \frac{1}{\Delta u_i}\left(1+\frac{w_{1ni}}{w_{2ni}}\,\frac{S_i(\varsigma_n)}{S_{i-1}(\varsigma_n)}\right) q_{ni-1} + \overline{\chi}_i P(\varsigma_n) + \overline{I(\varsigma_n)_i}\,. \tag{34}$$

In addition to Equations (32), another set of approximate equations which can be obtained from Equations (25) is

$$\hat{i}^-_{ni}\left[D_i^{(1)}(\varsigma_{n-1/2})\varphi_{ni} - D_i^{(2)}(\varsigma_{n-1/2})\varphi_{n-1\,i}\right] + T_n\,\hat{i}^+_{ni}\left[D_i^{(2)}(\varsigma_{n+1/2})\varphi_{ni} - D_i^{(1)}(\varsigma_{n+1/2})\varphi_{n+1\,i}\right]$$

$$+\frac{\Delta\varsigma_n^-}{\varsigma_n^p}\left[\hat{J}_{ni}(A_i\varphi_i) + \hat{I}_{n+1\,i}(A_i\varphi_i)\right]$$

$$= \frac{\Delta\varsigma_n^-}{\varsigma_n^p}\left[\hat{J}_{ni}(\mathcal{S}_i) + \hat{I}_{n+1\,i}(\mathcal{S}_i)\right] \tag{35}$$

where

$$D_i^{(1)}(\varrho_n) = \overline{\frac{1}{3\Sigma'_{1tr}(\varrho_n)S(\varrho_{n+1/2})_i}} \cdot \overline{S(\varrho_{n+1/2})_i} \, ,$$

$$D_i^{(2)}(\varrho_n) = \overline{\frac{1}{3\Sigma'_{1tr}(\varrho_n)S(\varrho_{n-1/2})_i}} \cdot \overline{S(\varrho_{n-1/2})_i} \qquad (36)$$

and where $\overline{\dfrac{\Sigma_{1a}(\varrho_n)}{S(\varrho_n)_i}} \cdot \overline{S(\varrho_n)_i}$

replaces $\overline{\Sigma_a(\varrho_n)_i}$ in A_{ni}. If we assume that $q(\varrho, u)$ changes less radically over a group width than $nv(\varrho, u)$, the use of Equations (35) rather than Equations (32) is justified. KAPL makes use of this assumption in its present calculations on the UNIVAC and the CPC.

In each of the multigroup equations so far considered, it is to be noticed that a contribution from the i-1st group enters into the source for the ith group. Therefore, in solving the multigroup equations, we must proceed down from the top group (lowest lethargy, where $q_{n0} = 0$). The thermal equation, when taken over into difference form, can be taken as the last of the multigroup equations if we set $\Delta u_T = 1$ and $\frac{1}{w_{2nT}} = 0$.

The fission source term, $P(\varrho_n)$, in the finite-difference multigroup equations can be expressed as

$$P(\varrho_n) = \sum_{j=1}^{T-1} \overline{\nu\Sigma'_{1f}(\varrho_n)_j} \cdot \overline{nv_{nj}} \cdot \Delta u_j + \nu\Sigma'_{1f}(\varrho_n, u_T) \cdot nv_n(u_T),$$

while the inelastic-scattering source term is given by

$$\overline{I(\varrho_n)_i} = \sum_{j=1}^{i-1} \left[\sum_{(m)} \overline{\chi}_{ji(m)} \overline{\Sigma_{in(m)}(\varrho_n)_j} \right] \cdot \overline{nv_{nj}} \cdot \Delta u_j, \quad (i \geq 2),$$

where

$$\overline{\chi}_{ji(m)} = \frac{1}{\Delta u_i \Delta u_j} \int_{u \in \Delta u_i} \int_{u' \in \Delta u_j} \chi_{(m)}(u' \to u)\, du'\, du.$$

To provide a scheme of calculation for the multigroup equations, an initial fission source distribution is assumed, the multigroup equations are solved for the $\overline{n v}_{ni}$ with this assumed source distribution, and a new fission source distribution is calculated from the $\overline{n v}_{ni}$. Normalized in some fashion, this is to be used as input for the next calculation through the groups; and this procedure is continued until suitable convergence is reached. Experience at KAPL (with a one-dimensional setup on UNIVAC) has shown that only a few source iterations are necessary. Thus the source terms in our finite-difference multigroup equations can be written as

$$\overline{\chi}_i P(\varsigma_n) + \sum_{j=1}^{i-1} \left[\sum_{(m)} \overline{\chi}_{ji(m)} \overline{\Sigma_{fin(m)}(\varsigma_n)}_j \right] \overline{n v}_{nj} \Delta u_j \,, \tag{37}$$

where $P(\varsigma_n)$ is a curve determined previous to this particular multigroup calculation.

A numerical check on the multigroup calculation is the neutron balance,

$$D_i^R + A_i^R + E_i^R = \overline{\chi}_i \Delta u_i P^R + E_i^{R-1} + D_{i-1}^R + I_i^R \,, \tag{38}$$

which accounts for the conservation of neutrons in a region R in the ith group, where $\overline{\chi}_i \Delta u_i P^R$ is the fission source in that region and group, A_i^R is the absorption in that region and group, E_i^R is the neutron escape from the Rth region into the (R+1)st, D_i^R is the neutron degradation out of the ith group in the Rth region, and I_i^R is the source of neutrons in the ith group and Rth region as a result of inelastic scattering.

Taking these quantities to be normalized such that

$$\frac{\int_0^{\varsigma_N} P(\varsigma)\varsigma^\rho d\varsigma}{\int_0^{\varsigma_N} C(\varsigma)\varsigma^\rho d\varsigma} = 1 \,,$$

where

$$C(\varsigma) = \begin{cases} 1 \text{ if } \varsigma \text{ is in a region having fission,} \\ 0 \text{ elsewhere ,} \end{cases}$$

we have the following formulas (where we have assumed that the Rth region, extending from ς_{N_1} to ς_{N_2}, is a region of continuous variation in composition):

$$P^R = \frac{1}{V}\left[I_{N_1+1}(P) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_n(P) + \bar{I}_{n+1}(P)\right) + J_{N_2}(P)\right], \tag{39}$$

$$A_i^R = \frac{\Delta u_i}{V}\Big[I_{N_1+1}(\bar{\Sigma}_{ai}\,\overline{nv}_i) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_n(\bar{\Sigma}_{ai}\,\overline{nv}_i) + \bar{I}_{n+1}(\bar{\Sigma}_{ai}\,\overline{nv}_i)\right) \tag{40}$$

$$+ J_{N_2}(\bar{\Sigma}_{ai}\,\overline{nv}_i)\Big],$$

$$E_i^R = \frac{\Delta u_i}{V}\Big[\frac{\varsigma_{N_2-1}^{\rho}}{\Delta\bar{\varsigma}_{N_2}}\tau_{N_2-1}\,\hat{i}^{+}_{N_2-1\,i}\left(D_i^{(2)}(\varsigma_{N_2-\frac{1}{2}})\,\overline{nv}_{N_2-1\,i} - D_i^{(1)}(\varsigma_{N_2-\frac{1}{2}})\,\overline{nv}_{N_2 i}\right)$$

$$+ \check{J}_{N_2 i}(Q_i)\Big], \tag{41}$$

$$D_i^R = \frac{1}{V}\left[I_{N_1+1}(q_i) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_n(q_i) + \bar{I}_{n+1}(q_i)\right) + J_{N_2}(q_i)\right], \tag{42}$$

and

$$I_i^R = \frac{\Delta u_i}{V}\left[I_{N_1+1}(\bar{I}_i) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_n(\bar{I}_i) + \bar{I}_{n+1}(\bar{I}_i)\right) + J_{N_2}(\bar{I}_i)\right], \tag{43}$$

where

$$\bar{I}^{\pm}_{n i} = \sum_{j=1}^{i-1}\left[\sum_{(m)} \bar{\chi}_{ji(m)}\,\overline{\Sigma_{in(m)}(\varsigma_n)}_j\right]\overline{nv}_{nj}\,\Delta u_j, \qquad (i \geq 2) \tag{44}$$

and

$$V = \int_0^{\varsigma_N} c(\varsigma)\,\varsigma^{\rho}\,d\varsigma .$$

C. THE SELENGUT-GOERTZEL METHOD

Following Selengut and Goertzel, we have a simple age-diffusion approximation for hydrogenous compositions (when the other materials present scatter only elastically)

$$-\nabla \frac{1}{3\Sigma'_{1tr}(\vec{r},u)} \nabla nv(\vec{r},u) + \left(\Sigma'_{1sH}(\vec{r},u) + \Sigma'_{1a}(\vec{r},u)\right) nv(\vec{r},u) = -\frac{\partial q(\vec{r},u)}{\partial u} + \chi(u)P(\vec{r}) + \eta(\vec{r},u) \, ,$$

$$-\nabla \frac{1}{3\Sigma'_{1tr}(\vec{r},u_T)} \nabla nv(\vec{r},u_T) + \Sigma'_{1a}(\vec{r},u_T)\, nv(\vec{r},u_T) = \lim_{u \to u_T}\left[q(\vec{r},u) + \eta(\vec{r},u)\right] + \chi(u_T)P(\vec{r}),$$

where $\eta(\vec{r},u)$ satisfies the subsidiary equation

$$\frac{\partial \eta(\vec{r},u)}{\partial u} + \eta(\vec{r},u) = \Sigma'_{1sH}(\vec{r},u)\, nv(\vec{r},u) \, . \tag{45}$$

Here $\Sigma'_{1sH}(\vec{r},u)$ is the macroscopic scattering cross section for hyrogen, $\Sigma'_{1tr}(\vec{r},u)$ and $\Sigma'_{1a}(\vec{r},u)$ are the macroscopic transport cross section and macroscopic absorption cross section, respectively, of the entire composition, and $S(\vec{r},u)$ involves all materials other then hydrogen.

On solving Equation (45), we find

$$\eta(\vec{r},u) = \eta(\vec{r})_{i-1}\, e^{-(u-u_{i-1})} + e^{-u}\int_{u_{i-1}}^{u} e^{u'}\Sigma'_{1sH}(\vec{r},u')\, nv(\vec{r},u')\, du' \, .$$

Hence if Σ'_{1sH} and nv are essentially constant over the ith group

$$\overline{\eta(\vec{r})}_i = \eta(\vec{r})_{i-1}\,\frac{1-e^{-\Delta u_i}}{\Delta u_i} + \frac{\overline{nv(\vec{r})}_i \cdot \overline{\Sigma'_{1sH}(\vec{r})}_i}{\Delta u_i}\left[\Delta u_i - 1 + e^{-\Delta u_i}\right] . \tag{46}$$

The finite-difference equations obtained from Equation (44) in the one-dimensional case will differ from the difference equations obtained in Section B only in the extra terms added to the absorption and the source

$$\begin{cases} A_{(S.G.)}{}^{\pm}_{ni} = A^{\pm}_{ni} + \dfrac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma'}_{1sH}{}^{\pm}_{ni} \, , & (i = 1, 2, \ldots, T-1) \\[2ex] \mathcal{S}_{(S.G.)}{}^{\pm}_{ni} = \mathcal{S}^{\pm}_{ni} + \dfrac{1-e^{-\Delta u_i}}{\Delta u_i}\,\eta^{\pm}_{n\,i-1} \, , & \end{cases}$$

$$\begin{cases} A_{(S.G.)}{}^{\pm}_{nT} = A^{\pm}_{nT} \, , \\[1ex] \mathcal{S}_{(S.G.)}{}^{\pm}_{nT} = \mathcal{S}^{\pm}_{nT} + \eta^{\pm}_{n\,T-1} \, , \end{cases} \tag{47}$$

and the fact that they are accompanied by the subsidiary difference equations

$$\eta^{\pm}_{ni} = \eta^{\pm}_{ni-1} + \left(e^{-\Delta u_i} - 1\right)\left(\eta^{\pm}_{ni-1} - \overline{nv_{ni}\Sigma'_{1SH}{}^{\pm}_{n}}_{\,i}\right). \qquad (i=1,2,\ldots,T-1) \qquad (48)$$

If we make use of the assumption that $\eta(\varsigma,u)$ changes less radically over the group than does $nv(\varsigma,u)$, we must replace $\overline{\Sigma'_{1SH}}{}^{\pm}_{ni}$ in Equations (47) and (48) by

$$\overline{\left(\frac{\Sigma_{1SH}{}^{\pm}_{n}}{S^{\pm}_{n}}\right)_i} \cdot \overline{S}^{\pm}_{ni} \,.$$

In computing the group-by-group balance for this method, it is necessary to compute the extra sum

$$H_i^R = \frac{1}{V}\left[I_{N_1+1}(\eta_i) + \sum_{N_1+1}^{N_2-1}\left(\bar{J}_m(\eta_i) + \bar{I}_{m+1}(\eta_i)\right) + \bar{J}_{N_2}(\eta_i)\right]. \qquad (49)$$

This enters into the balance equations as

$$D_i^R + A_i^R + E_i^R + H_i^R = \bar{\chi}_i^R \Delta u_i P^R + E_i^{R-1} + D_{i-1}^R + H_{i-1}^R + I_i^R \qquad (50)$$

It is to be noted that the Selengut-Goertzel approximation can be considered as a special case of inelastic scattering by one material. When $\eta(\vec{r},u)$ is written in the form

$$\eta(\vec{r},u) = \int_{-\infty}^{u} e^{-u+u'}\,\Sigma'_{1SH}(\vec{r},u')\,nv(\vec{r},u')\,du', \qquad (51)$$

and compared with $I(\vec{r},u)$ in Equation (22), we see that the two are the same if we take

$$\chi_{(H)}(u' \to u) = e^{-u+u'} \qquad (52)$$

and $\Sigma'_{1SH}(\vec{r},u)$ to be the inelastic scattering cross section for hydrogen.

D. ADJOINT EQUATIONS

In this section, we determine the multigroup adjoint equations. We do this by finding the adjoint equations for the age-diffusion problem, and then forming multigroup difference equations from them.

The age-diffusion equation, with no inelastic scattering, can be written in the operational form

$$M \cdot \Phi = 0, \qquad (53)$$

where

$$\Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix} = \begin{pmatrix} nv(\vec{r},u)_{u<u_T} \\ nv(\vec{r},u_T) \end{pmatrix},$$

and the operator M is given by

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix},$$

where

$$\left.\begin{aligned} M_{11} &= -\nabla \frac{1}{3\Sigma'_{1tr}(\vec{r},u)} \nabla\cdot + \Sigma'_{1a}(\vec{r},u) + \frac{\partial}{\partial u}\cdot S\cdot - \chi(u)\nu \int_0^{u_T} du\, \Sigma'_{1f}(\vec{r},u)\cdot \\ M_{12} &= -\chi(u)\nu\Sigma'_{1f}(u_T)\cdot \\ M_{21} &= -\chi(u_T)\nu \int_0^{u_T} du \cdot \Sigma'_{1f}(\vec{r},u)\cdot \\ M_{22} &= -\nabla \frac{1}{3\Sigma'_{1tr}(\vec{r},u_T)} \nabla\cdot + \Sigma'_{1a}(\vec{r},u_T) - S(\vec{r},u_T) - \chi(u_T)\nu\Sigma'_{1f}(\vec{r},u_T)\,. \end{aligned}\right\} \qquad (54)$$

The adjoint operator M* can be determined from the relationship

$$(\Psi, M\cdot\Phi) = (M^*\cdot\Psi, \Phi), \qquad (55)$$

where Φ and Ψ are any two functions that satisfy the boundary conditions of the problem, and (Ψ, Φ) is the "inner product" defined by

$$(\Psi, \Phi) = \int_V \int_0^{u_T} \Psi(\vec{r},u)\cdot\Phi(\vec{r},u)\,du\,dV + \int_V \psi(\vec{r},u_T)\cdot\Phi(\vec{r},u_T)\,dV\,. \qquad (56)$$

The adjoint equation is then

$$M^*\cdot\Psi = 0\,. \qquad (57)$$

We split the operator M into four terms:

$$M = M^{(1)} + M^{(2)} + M^{(3)} + M^{(4)},$$

where

$$M^{(1)} = \begin{pmatrix} -\nabla \frac{1}{3\Sigma_{1tr}'(\vec{r},u)} \nabla & 0 \\ 0 & -\nabla \frac{1}{3\Sigma_{1tr}'(\vec{r},u_T)} \nabla \end{pmatrix},$$

$$M^{(2)} = \begin{pmatrix} \Sigma_{1a}'(\vec{r},u) & 0 \\ 0 & \Sigma_{1a}'(\vec{r},u_T) \end{pmatrix},$$

$$M^{(3)} = \begin{pmatrix} \frac{\partial}{\partial u} S(\vec{r},u) & 0 \\ 0 & -S(\vec{r},u_T) \end{pmatrix},$$

and

$$M^{(4)} = \begin{pmatrix} -\chi(u)\nu \int_0^{u_T} du\, \Sigma_{1f}'(\vec{r},u)\cdot & -\chi(u)\nu\Sigma_{1f}'(\vec{r},u_T) \\ -\chi(u_T)\nu \int_0^{u_T} du\, \Sigma_{1f}'(\vec{r},u)\cdot & -\chi(u_T)\nu\Sigma_{1f}'(\vec{r},u_T) \end{pmatrix}.$$

We will examine each term separately to determine its adjoint. We take Φ and Ψ to vanish on the outside of the reactor and at u = 0. Across discontinuities in composition, we will take

$$\Phi, \quad \Psi, \quad \frac{1}{3\Sigma_{1tr}'} \nabla \Phi \Big|_n$$

and $\frac{1}{3\Sigma_{1tr}'} \nabla \Psi \Big|_n$ to be continuous.

Using Green's Theorem and Equation (56) we see that

$$\left(\Psi, -\nabla \frac{1}{3\Sigma_{1tr}'} \nabla \Phi\right) = \left(\frac{1}{3\Sigma_{1tr}'} \nabla \Psi, \nabla \Phi\right) = \left(-\nabla \frac{1}{3\Sigma_{1tr}'} \nabla \Psi, \Phi\right), \tag{58}$$

that is, the first term in M is self-adjoint. This is also true for the second term, since

$$(\Psi, \Sigma_{1a}' \cdot \Phi) = (\Sigma_{1a}' \Psi, \Phi) \tag{59}$$

For the third term we have

$$(\Psi, M^{(3)}\Phi) = \int_V \int_0^{u_T} \Psi_1 \frac{\partial}{\partial u}(S\Phi_1)\, du\, dV - \int_V \Psi_2(\vec{r},u_T) S(\vec{r},u_T) \Phi_2(\vec{r},u_T)\, dV$$

$$= \int_V \Big[\Psi_1(\vec{r},u) S(\vec{r},u) \Phi_1(\vec{r},u)\Big]_0^{u_T} - \int_V \int_0^{u_T} S(\vec{r},u) \frac{\partial \Psi_1(\vec{r},u)}{\partial u} \Phi_1(\vec{r},u)\, du\, dV$$

$$- \int_V \Psi_2(\vec{r},u_T) S(\vec{r},u_T) \Phi_2(\vec{r},u_T)\, dV = -\int_V \int_0^{u_T} S(\vec{r},u) \frac{\partial \Psi_1(\vec{r},u)}{\partial u} \Phi_1(\vec{r},u)\, du\, dV,$$

since $\Phi_1(\vec{r},u_T) = \Phi_2(\vec{r},u_T)$, $\Psi_1(\vec{r},u_T) = \Psi_2(\vec{r},u_T)$ and $\Phi_1(\vec{r},0) = 0$.

Thus we have

$$M^{*(3)} = \begin{pmatrix} -S(\vec{r},u)\frac{\partial}{\partial u} & 0 \\ 0 & 0 \end{pmatrix}. \tag{60}$$

For the last term we have

$$-\int_V\int_0^{u_T}\Psi_1(\vec{r},u)\,\chi(u)\,\nu\left[\int_0^{u_T}\Sigma_f(\vec{r},u')\,\Phi_1(\vec{r},u')\,du' + \Sigma_{1f}(\vec{r},u_T)\,\Phi_2(\vec{r},u_T)\right]du\,dV\ -$$

$$-\int_V\Psi_2(\vec{r},u_T)\,\chi(u_T)\,\nu\left[\int_0^{u_T}\Sigma_{1f}(\vec{r},u')\,\Phi_1(\vec{r},u')\,du' + \Sigma_{1f}(\vec{r},u_T)\,\Phi_2(\vec{r},u_T)\right]dV$$

$$= -\int_V\int_0^{u_T}\Phi_1(\vec{r},u)\,\Sigma_{1f}(\vec{r},u)\,\nu\left[\int_0^{u_T}\chi(u')\,\Psi_1(\vec{r},u')\,du' + \chi(u_T)\,\Psi_2(\vec{r},u_T)\right]du\,dV$$

$$-\int_V\Phi_2(\vec{r},u_T)\,\Sigma_{1f}(\vec{r},u_T)\,\nu\left[\int_0^{u_T}\chi(u')\,\Psi_1(\vec{r},u')\,du' + \chi(u_T)\,\Psi_2(\vec{r},u_T)\right]dV,$$

and hence

$$M^{*(4)} = \begin{pmatrix} -\Sigma_{1f}(\vec{r},u)\,\nu\int_0^{u_T}du\,\chi(u) & -\Sigma_{1f}(\vec{r},u)\,\nu\,\chi(u_T) \\ -\Sigma_{1f}(\vec{r},u_T)\,\nu\int_0^{u_T}du\,\chi(u) & -\Sigma_{1f}(\vec{r},u_T)\,\nu\,\chi(u_T) \end{pmatrix}. \tag{61}$$

Thus we see that our adjoint equations are

$$-\nabla\frac{1}{3\Sigma_{tr}(\vec{r},u)}\nabla\psi(\vec{r},u) + \Sigma_{1a}(\vec{r},u)\,\psi(\vec{r},u) = S(\vec{r},u)\frac{\partial\psi(\vec{r},u)}{\partial u} + \Sigma_{1f}(\vec{r},u)\,\nu\left[\int_0^{u_T}\chi(u')\,\psi(\vec{r},u')\,du' + \chi(u_T)\,\psi(\vec{r},u_T)\right]$$

$$-\nabla\frac{1}{3\Sigma_{tr}(\vec{r},u_T)}\nabla\psi(\vec{r},u_T) + \Sigma_{1a}(\vec{r},u_T)\,\psi(\vec{r},u_T) = \Sigma_{1f}(\vec{r},u)\,\nu\left[\int_0^{u_T}\chi(u')\,\psi(\vec{r},u')\,du' + \chi(u_T)\,\psi(\vec{r},u_T)\right], \tag{62}$$

with ψ satisfying the same boundary conditions as φ.

The next step is to derive multigroup equations from Equations (62) for the one-space-dimensional case. At points of continuous variation in composition there are two sets of difference equations which can be obtained from Equation (62). If we assume that the $\psi_n(u)$ are fairly constant over the group widths assumed, we have the approximate equations

$$\hat{i}^{-}_{ni}\, D_i(\varsigma_{n-\frac{1}{2}})\left[\overline{\psi}_{ni} - \overline{\psi}_{n-1\,i}\right] + r_n\, \hat{i}^{+}_{ni}\, D_i(\varsigma_{n+\frac{1}{2}})\left[\overline{\psi}_{ni} - \overline{\psi}_{n+1\,i}\right]$$

$$= \frac{\Delta \varsigma_n^-}{\varsigma_n^{\rho}}\left[\hat{J}_{ni}(Q_i) + \hat{I}_{n+1\,i}(Q_i)\right], \tag{63}$$

where

$$Q^{\pm}_{ni} = \frac{1}{\Delta u_i}\overline{S}^{\pm}_{ni}\left(\psi_{ni} - \psi_{ni-1}\right) + \overline{\Sigma}^{\pm}_{f\,ni}\,\nu\left[\int_0^{u_T}\chi(u')\psi(\varsigma_n,u')\,du' + \chi(u_T)\psi(\varsigma_n,u_T)\right] - \overline{\Sigma}^{\pm}_{a\,ni}\,\overline{\psi}_{ni}\,.$$

If we assume that the $S_n(u)\psi_n(u)$ change less rapidly over the group widths than do the $\psi_n(u)$, a set of somewhat more reasonable equations are

$$\hat{i}^{-}_{ni}\left[D_i^{(1)}(\varsigma_{n-\frac{1}{2}})\,\overline{\psi}_{ni} - D_i^{(2)}(\varsigma_{n-\frac{1}{2}})\,\overline{\psi}_{n-1\,i}\right]$$

$$+ r_n\,\hat{i}^{+}_{ni}\left[D_i^{(1)}(\varsigma_{n+\frac{1}{2}})\,\overline{\psi}_{ni} - D_i^{(2)}(\varsigma_{n+\frac{1}{2}})\,\overline{\psi}_{n+1\,i}\right]$$

$$= \frac{\Delta \varsigma_n^-}{\varsigma_n^{\rho}}\left[\hat{J}_{ni}(Q_i) + \hat{I}_{n+1\,i}(Q_i)\right], \tag{64}$$

where the D's are those defined in Section B, and where

$$Q^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(S^{\pm}_{ni}\psi_{ni} - S^{\pm}_{ni-1}\psi_{ni-1}\right) + \Sigma^{\pm}_{1f\,ni}\,\nu\left[\int_0^{u_T}\chi(u')\psi(\varsigma_n,u')\,du' + \chi(u_T)\psi(\varsigma_n,u_T)\right] - \left(\frac{\overline{\Sigma^{\pm}_{a\,n}}}{S^{\pm}_{n\,i}}\cdot\overline{S}^{\pm}_{ni} + \overline{S}^{\pm}_n\,\frac{\ln S^{\pm}_{ni}/S^{\pm}_{ni-1}}{\Delta u_i}\right)\overline{\psi}_{ni}.$$

We see that the adjoint multigroup equations are very similar to the usual multigroup equations. Instead of an initial guess at the usual source, we guess at the adjoint source

$$P^*(\varsigma) = \nu\left[\int_0^{u_T}\chi(u')\psi(\varsigma,u')\,du' + \chi(u_T)\psi(\varsigma,u_T)\right].$$

It is seen from the form of the equation at thermal energy that we might start our calculations at thermal energy. To proceed further, we again introduce one of the two conditions, either

$$\overline{\psi}_{ni} = \gamma_{1ni}\,\psi_{ni} + \gamma_{2ni}\,\psi_{ni-1}$$

or

$$\overline{S}^{\pm}_{ni}\,\overline{\psi}_{ni} = \gamma^{\pm}_{1ni}\,S^{\pm}_{ni}\,\psi_{ni} + \gamma^{\pm}_{2ni}\,S^{\pm}_{ni-1}\,\psi_{ni-1}\,.$$

Then, except for the thermal group, Equations (63) become

$$\begin{aligned}
&\hat{i}^{-}_{ni}\,D_i(\varsigma_{n-\frac{1}{2}})\left[\overline{\psi}_{ni} - \overline{\psi}_{n-1i}\right] + r_n\,\hat{i}^{+}_{ni}\,D_i(\varsigma_{n+\frac{1}{2}})\left[\overline{\psi}_{ni} - \overline{\psi}_{n+1i}\right] \\
&\quad + \frac{\Delta\varsigma_n^-}{\varsigma_n^\ell}\left[\hat{J}_{ni}(A_i\overline{\psi}_i) + \hat{I}_{n+1i}(A_i\overline{\psi}_i)\right] \\
&\quad = \frac{\Delta\varsigma_n^-}{\varsigma_n^\ell}\left[\hat{J}_{ni}(\mathcal{S}_i) + \hat{I}_{n+1i}(\mathcal{S}_i)\right],
\end{aligned} \tag{65}$$

with either of the two possibilities

$$\text{a)}\begin{cases}
A^{\pm}_{ni} = \overline{\Sigma}^{\pm}_{a\,ni} + \dfrac{\overline{S}^{\pm}_{ni}}{\gamma_{2ni}\,\Delta u_i} \\[2ex]
\mathcal{S}^{\pm}_{ni} = \dfrac{1}{\Delta u_i}\left(1 + \dfrac{\gamma_{1ni}}{\gamma_{2ni}}\right)\overline{S}^{\pm}_{ni}\,\psi_{ni} + \overline{\Sigma}^{\pm}_{f\,ni}\,P^*_n\,,
\end{cases}$$

$$\text{b)}\begin{cases}
A^{\pm}_{ni} = \overline{\Sigma}^{\pm}_{a\,ni} + \dfrac{\overline{S}^{\pm}_{ni}}{\gamma^{\pm}_{2ni}\,\Delta u_i}\,\dfrac{\overline{S}^{\pm}_{ni}}{S^{\pm}_{ni-1}} \\[2ex]
\mathcal{S}^{\pm}_{ni} = \dfrac{1}{\Delta u_i}\left(1 + \dfrac{\gamma^{\pm}_{1ni}}{\gamma^{\pm}_{2ni}}\,\dfrac{S^{\pm}_{ni}}{S^{\pm}_{ni-1}}\right)\overline{S}^{\pm}_{ni}\,\psi_{ni} + \overline{\Sigma}^{\pm}_{f\,ni}\cdot P^*_n\,.
\end{cases} \tag{66}$$

Equations (64) become

$$
\begin{aligned}
&\hat{i}^{-}_{ni}\left[D_i^{(1)}(\varsigma_{n-\frac{1}{2}})\,\bar{\psi}_{ni} - D_i^{(2)}(\varsigma_{n-\frac{1}{2}})\,\bar{\psi}_{n-1\,i}\right] \\
&\quad + r_n\,\hat{i}^{+}_{ni}\left[D_i^{(1)}(\varsigma_{n+\frac{1}{2}})\,\bar{\psi}_{ni} - D_i^{(2)}(\varsigma_{n+\frac{1}{2}})\,\bar{\psi}_{n+1\,i}\right] \\
&\quad + \frac{\Delta\varsigma_n^{-}}{\varsigma_n^{\rho}}\left[\hat{J}_{ni}(A_i\bar{\psi}_i) + \hat{I}_{n+1\,i}(A_i\bar{\psi}_i)\right] \\
&\quad = \frac{\Delta\varsigma_n^{-}}{\varsigma_n^{\rho}}\left[\hat{J}_{ni}(\mathcal{S}_i) + \hat{I}_{n+1\,i}(\mathcal{S}_i)\right],
\end{aligned}
\tag{67}
$$

with the two possibilities

$$
\text{a)}\;\begin{cases}
A^{\pm}_{ni} = \dfrac{\overline{\Sigma'^{\pm}_{1an}}}{S^{\pm}_{n\,i}}\cdot \bar{S}^{\pm}_{ni} + \dfrac{\bar{S}^{\pm}_{ni}}{\Delta u_i}\ln\dfrac{S^{\pm}_{ni}}{S^{\pm}_{n\,i-1}} + \dfrac{S^{\pm}_{n\,i-1}}{\gamma_{2ni}\,\Delta u_i} \\[2ex]
\mathcal{S}^{\pm}_{ni} = \dfrac{1}{\Delta u_i}\left(1+\dfrac{\gamma_{1ni}}{\gamma_{2ni}}\,\dfrac{S^{\pm}_{n\,i-1}}{S^{\pm}_{n\,i}}\right)S^{\pm}_{ni}\psi_{ni} + \bar{\Sigma}^{\pm}_{1f\,n\,i}\cdot P_n^{*},
\end{cases}
\tag{68}
$$

$$
\text{b)}\;\begin{cases}
A^{\pm}_{ni} = \dfrac{\overline{\Sigma'^{\pm}_{1an}}}{S^{\pm}_{n\,i}}\cdot \bar{S}^{\pm}_{ni} + \dfrac{\bar{S}^{\pm}_{ni}}{\Delta u_i}\ln\dfrac{S^{\pm}_{ni}}{S^{\pm}_{n\,i-1}} + \dfrac{\bar{S}^{\pm}_{ni}}{\gamma^{\pm}_{2ni}\,\Delta u_i} \\[2ex]
\mathcal{S}^{\pm}_{ni} = \dfrac{1}{\Delta u_i}\left(1+\dfrac{\gamma^{\pm}_{1ni}}{\gamma^{\pm}_{2ni}}\right)S^{\pm}_{ni}\psi_{ni} + \bar{\Sigma}^{\pm}_{1f\,ni}\,P_n^{*}.
\end{cases}
$$

We again include the thermal equation in the multigroup equations by taking it as the last i group.

These equations are quite similar to Equations (32) and (35). For the adjoint calculations, we proceed from the last group (thermal energy) to the first.

If inelastic scattering is present, our operator M has the additional term

$$
M^{(5)} = \begin{pmatrix}
-\displaystyle\int_0^u du'\,\Sigma_{in}(u'\to u) & 0 \\[2ex]
-\displaystyle\int_0^u du'\cdot\Sigma_{in}(u'\to u_T) & 0
\end{pmatrix}
\tag{69}
$$

35

where

$$\Sigma_{in}(u'\to u) = \sum_{(m)}{}' \chi_{(m)}(u'\to u)\,\Sigma'_{in}(u').$$

To find its adjoint, we consider

$$(\Psi, M^{(5)}\Phi) = -\int_V\int_0^{u_T}\Psi_1(u)\int_0^{u}\Sigma'_{in}(u'\to u)\,\Phi_1(u')\,du'\,du\,dV - \int_V\Psi_2(u_T)\int_0^{u_T}\Sigma'_{in}(u'\to u_T)\,\Phi_1(u')\,du'\,dV.$$

Changing the order of integration in the first integral, we have

$$(\Psi, M^{(5)}\Phi) = -\int_V\int_0^{u_T}\Phi_1(u)\int_u^{u_T}\Sigma'_{in}(u\to u')\,\Psi_1(u')\,du'\,du\,dV - \int_V\int_0^{u_T}\Phi_1(u)\,\Sigma'_{in}(u'\to u_T)\,\Psi_2(u_T)\,du\,dV.$$

Hence we have

$$M^{*(5)} = \begin{pmatrix} -\int_u^{u_T} du'\cdot\Sigma'_{in}(u\to u')\cdot & -\Sigma'_{in}(u\to u_T) \\ 0 & 0 \end{pmatrix}, \tag{70}$$

and our adjoint equations become

$$-\nabla\frac{1}{3\Sigma'_{tr}(\vec r,u)}\nabla\psi(\vec r,u) + \Sigma'_a(\vec r,u)\,\psi(\vec r,u) = S(\vec r,u)\frac{\partial\psi}{\partial u} + \Sigma'_f(\vec r,u)\,P^*(\vec r) + \left[\int_u^{u_T}\Sigma_{in}(u\to u')\,\psi(u')\,du' + \Sigma_{in}(u\to u_T)\,\psi(u_T)\right]$$

$$-\nabla\frac{1}{3\Sigma'_{tr}(\vec r,u_T)}\nabla\psi(\vec r,u_T) + \Sigma'_a(\vec r,u_T)\,\psi(\vec r,u_T) = \Sigma'_f(\vec r,u_T)\,P^*(\vec r). \tag{71}$$

The effect of inelastic scattering, therefore, is to add another term to $\mathcal{S}_{ni}$ in Equations (66) and (68), that is,

$$\mathcal{S}^{\pm}_{ni\,(inelastic)} = \mathcal{S}^{\pm}_{ni} + \sum_{j=i+1}^{T}{}' \left[\sum_{(m)}{}' \bar\chi_{(m)ij}\,\bar\Sigma_{in(m)ni}\cdot\bar\Psi_{nj}\cdot\Delta u_j\right]. \tag{72}$$

For the Selengut-Goertzel method, our operator M has the additional term

$$M^{(6)} = \begin{pmatrix} e^{-u}\int_0^{u} du\cdot e^{u}\,\Sigma_{1SH}(u)\cdot - \Sigma_{1SH}(u) & 0 \\ e^{-u_T}\int_0^{u_T} du\cdot e^{u}\,\Sigma_{1SH}(u) & 0 \end{pmatrix} \tag{73}$$

This is easily seen when we write $\eta(\vec{r},u)$ as

$$\eta(\vec{r},u) = e^{-u}\int_0^u e^{u'}\Sigma'_{sH}(\vec{r},u')\varphi(\vec{r},u')du' . \tag{74}$$

Using Equation (73), we see that

$$(\Psi, M^{(6)}\Phi) = \int_V\int_0^{u_T}\Psi_1(u)\left[e^{-u}\int_0^u e^{u'}\Sigma'_{sH}(u')\Phi_1(u')du' - \Sigma'_{sH}(u)\Phi_1(u)\right]du\,dV$$

$$+\int_V \Psi_2(u_T)\,e^{-u_T}\int_0^{u_T} e^{u'}\Sigma'_{sH}(u')\Phi_1(u')\,du'\,dV$$

$$=\int_V\int_0^{u_T}\Phi_1(u)\left\{e^{u}\Sigma'_{sH}(u)\left[\int_u^{u_T}\Psi_1(u')e^{-u'}du' + \Psi_2(u_T)e^{-u_T}\right]\right.$$

$$\left. - \Sigma'_{sH}(u)\;\Psi_1(u)\right\}du\,dV.$$

Hence we have

$$M^{*(6)} = \begin{pmatrix} e^{u}\Sigma'_{sH}(u)\int_u^{u_T} du\cdot e^{-u}\cdot - \Sigma'_{sH}(u)\cdot & e^{u}\Sigma'_{sH}(u)e^{-u_T} \\ 0 & 0 \end{pmatrix} \tag{75}$$

If we let

$$\lambda(\vec{r},u) = e^{u}\int_u^{u_T} e^{-u'}\psi(\vec{r},u')\,du' + e^{u-u_T}\,\psi(\vec{r},u_T)\,, \tag{76}$$

the adjoint equation to the Selengut-Goertzel equation is given by

$$-\nabla\frac{1}{3\Sigma_{tr}(\vec{r},u)}\nabla\psi(\vec{r},u) + \left(\Sigma'_a(\vec{r},u)+\Sigma'_{sH}(\vec{r},u)\right)\psi(\vec{r},u) = S(\vec{r},u)\frac{\partial\psi}{\partial u} + \Sigma'_f(\vec{r},u)\,P^*(\vec{r}) + \lambda(\vec{r},u)\Sigma'_{sH}(\vec{r},u)$$

$$-\nabla\frac{1}{3\Sigma_{tr}(\vec{r},u_T)}\nabla\psi(\vec{r},u_T) + \Sigma'_a(\vec{r},u_T)\psi(\vec{r},u_T) = \Sigma'_f(\vec{r},u_T)\,P^*(\vec{r})\,, \tag{77}$$

where $\lambda(\vec{r}, u)$ satisfies

$$\frac{\partial \lambda}{\partial u} = \lambda - \psi . \tag{78}$$

The one-space-dimensional finite-difference multigroup equations corresponding to Equation (77) will again be either Equations (65) or (67) with the following changes in Equations (66) and (68):

$$\left.\begin{aligned}
A_{(S.G.*)}{}^{\pm}_{ni} &= A^{\pm}_{ni} + \frac{1-e^{-\Delta u_i}}{\Delta u_i} \overline{\Sigma}_{1SH}{}^{\pm}_{ni} , \\
\mathcal{S}_{(S.G.*)}{}^{\pm}_{ni} &= \mathcal{S}^{\pm}_{ni} + \frac{1-e^{-\Delta u_i}}{\Delta u_i} \lambda_{ni} \overline{\Sigma}_{1SH}{}^{\pm}_{ni} , \qquad (i = 1, 2, \ldots, T-1) \\
A_{(S.G.*)}{}^{\pm}_{nT} &= A^{\pm}_{nT} , \\
\mathcal{S}_{(S.G.*)}{}^{\pm}_{nT} &= \mathcal{S}^{\pm}_{ni} .
\end{aligned}\right\} \tag{79}$$

The multigroup difference equations will be accompanied by the subsidiary difference equations

$$\lambda_{n\,i-1} = \lambda_{ni} + (e^{-\Delta u_i} - 1)(\lambda_{ni} - \Psi_{ni}) , \qquad (i = 1, 2, \cdots, T) \tag{80}$$

$$\lambda_{nT} = \Psi_{nT} . \tag{81}$$

E. FORMULAS: MULTIGROUP DIFFERENCE EQUATIONS

In this section we gather the multigroup equations together in the form

$$\begin{aligned}
&\hat{i}^{-}_{ni} \left[D_i^{(1)}(\varsigma_{n-\frac{1}{2}}) \varphi_{ni} - D_i^{(2)}(\varsigma_{n-\frac{1}{2}}) \varphi_{n-1\,i} \right] + r_n \hat{i}^{+}_{ni} \left[D_i^{(2)}(\varsigma_{n+\frac{1}{2}}) \varphi_{ni} - D_i^{(1)}(\varsigma_{n+\frac{1}{2}}) \varphi_{n+1\,i} \right] \\
&\qquad + \frac{\Delta \varsigma_n^-}{\varsigma_n^\rho} \left[\hat{J}_{ni}(A_i \varphi_i) + \hat{I}_{n+1\,i}(A_i \varphi_i) \right] \\
&\qquad = \frac{\Delta \varsigma_n^-}{\varsigma_n^\rho} \left[\hat{J}_{ni}(\mathcal{S}_i) + \hat{I}_{n+1\,i}(\mathcal{S}_i) \right] ,
\end{aligned} \tag{82}$$

where the $\hat{i}^{-}_{mi}$, $\hat{i}^{+}_{mi}$ are given by

$$\hat{i}^{-}_{mi} = \frac{\varsigma^{p}_{m-\frac{1}{2}}/\varsigma^{p}_{m}}{1 + W_{m-1\,i}} ,$$

$$\hat{i}^{+}_{mi} = \frac{\varsigma^{p}_{m+\frac{1}{2}}/\varsigma^{p}_{m}}{1 + W_{m\,i}} , \tag{83}$$

$$W_{mi} = \frac{(\Delta\varsigma^{+}_{m})^{2}}{24}\left[\frac{p(p+1)}{\varsigma^{2}} + \frac{2p}{\varsigma}\frac{\bar{D}'_{i}}{\bar{D}_{i}} + 2\left(\frac{\bar{D}'_{i}}{\bar{D}_{i}}\right)^{2} - \frac{\bar{D}''_{i}}{\bar{D}_{i}}\right]_{\varsigma_{m+\frac{1}{2}}} ,$$

while the linear forms $\hat{J}_{mi}$ and $\hat{I}_{m+1\,i}$ are given by

$$\hat{J}_{mi}(Q) = \left[\frac{\varsigma^{p}_{m}\Delta\varsigma^{-}_{m}}{8} - \frac{p\varsigma^{p-1}_{m}(\Delta\varsigma^{-}_{m})^{2}}{24} + \frac{p(p-1)\varsigma^{p-2}_{m}(\Delta\varsigma^{-}_{m})^{3}}{128} + \frac{\varsigma^{p}_{m-\frac{1}{2}}(\Delta\varsigma^{-}_{m})^{2}}{24[1+W_{m-1i}]}\left(\frac{p}{2\varsigma} + \frac{\bar{D}'_{i}}{\bar{D}_{i}} + \frac{1}{\Delta\varsigma^{-}_{m}}\right)_{\varsigma_{m-\frac{1}{2}}} - \frac{\Gamma_{m}}{\Delta\varsigma^{-}_{m}}\right]Q(\varsigma^{+}_{m-1})$$

$$+ \left[\frac{3\varsigma^{p}_{m}\Delta\varsigma^{-}_{m}}{8} - \frac{p\varsigma^{p-1}_{m}(\Delta\varsigma^{-}_{m})^{2}}{12} + \frac{5p(p-1)\varsigma^{p-2}_{m}(\Delta\varsigma^{-}_{m})^{3}}{384} + \frac{\varsigma^{p}_{m-\frac{1}{2}}(\Delta\varsigma^{-}_{m})^{2}}{24[1+W_{m-1i}]}\left(\frac{p}{2\varsigma} + \frac{\bar{D}'_{i}}{\bar{D}_{i}} - \frac{1}{\Delta\varsigma^{-}_{m}}\right)_{\varsigma_{m-\frac{1}{2}}} + \frac{\Gamma_{m}}{\Delta\varsigma^{-}_{m}}\right]Q(\varsigma^{-}_{m})$$

$$\hat{I}_{m+1i}(Q) = \left[\frac{3\varsigma^{p}_{m}\Delta\varsigma^{+}_{m}}{8} + \frac{p\varsigma^{p-1}_{m}(\Delta\varsigma^{+}_{m})^{2}}{12} + \frac{5p(p-1)\varsigma^{p-2}_{m}(\Delta\varsigma^{+}_{m})^{3}}{384} - \frac{\varsigma^{p}_{m+\frac{1}{2}}(\Delta\varsigma^{+}_{m})^{2}}{24[1+W_{mi}]}\left(\frac{p}{2\varsigma} + \frac{\bar{D}'_{i}}{\bar{D}_{i}} + \frac{1}{\Delta\varsigma^{+}_{m}}\right)_{\varsigma_{m+\frac{1}{2}}} + \frac{\Gamma_{m}}{\Delta\varsigma^{+}_{m}}\right]Q(\varsigma^{+}_{m}) \tag{84}$$

$$+ \left[\frac{\varsigma^{p}_{m}\Delta\varsigma^{+}_{m}}{8} + \frac{p\varsigma^{p-1}_{m}(\Delta\varsigma^{+}_{m})^{2}}{24} + \frac{p(p-1)\varsigma^{p-2}_{m}(\Delta\varsigma^{+}_{m})^{3}}{128} - \frac{\varsigma^{p}_{m+\frac{1}{2}}(\Delta\varsigma^{+}_{m})^{2}}{24[1+W_{mi}]}\left(\frac{p}{2\varsigma} + \frac{\bar{D}'_{i}}{\bar{D}_{i}} - \frac{1}{\Delta\varsigma^{+}_{m}}\right)_{\varsigma_{m+\frac{1}{2}}} - \frac{\Gamma_{m}}{\Delta\varsigma^{+}_{m}}\right]Q(\varsigma^{-}_{m+1})$$

in which

$$\Gamma_{m} = \begin{cases} \dfrac{\varsigma^{p}_{m}}{12}\,\dfrac{i^{-}_{m}(\Delta\varsigma^{-}_{m})^{3} + i^{+}_{m}(\Delta\varsigma^{+}_{m})^{3}}{\Delta\varsigma^{-}_{m} + \Delta\varsigma^{+}_{m}} , & \text{if } \varsigma_{m} \text{ is not an interface} \\[2ex] 0 , & \text{if } \varsigma_{m} \text{ is an interface} \end{cases} \tag{85}$$

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We allow for the two possible cases

$$(a) \qquad D_i^{(1)}(\varsigma_m) = D_i^{(2)}(\varsigma_m) = \overline{\frac{1}{3\Sigma_{tr}(\varsigma_m)}}_i$$

$$(b) \quad \begin{cases} D_i^{(1)}(\varsigma_m) = \overline{\frac{1}{3\Sigma_{tr}(\varsigma_m)\, S(\varsigma_{m+\frac{1}{2}})}}_i \cdot \overline{S(\varsigma_{m+\frac{1}{2}})}_i \\ D_i^{(2)}(\varsigma_m) = \overline{\frac{1}{3\Sigma_{tr}(\varsigma_m)\, S(\varsigma_{m-\frac{1}{2}})}}_i \cdot \overline{S(\varsigma_{m-\frac{1}{2}})}_i \end{cases} \tag{86}$$

The types of multigroup equations which we have encountered can be listed as:

(1-a) "KAPL multigroup" where $\bar{q}^{\pm}_{mi} = \omega_{1m i}^{\pm} q^{\pm}_{m\,i-1} + \omega_{2m i}^{\pm} q^{\pm}_{mi}$ and Equation (86a) applies

$$\begin{aligned} A(\varsigma_m^{\pm})_i &= \overline{\Sigma_a(\varsigma_m^{\pm})}_i + \frac{\overline{S(\varsigma_m^{\pm})}_i}{\omega_{2mi}^{\pm}\,\Delta u_i}, \qquad (i = 1, 2, \cdots, T) \\ \mathcal{S}^{\pm}_{mi} &= \frac{1}{\Delta u_i}\left(1 + \frac{\omega_{1mi}^{\pm}}{\omega_{2mi}^{\pm}}\right) q^{\pm}_{m\,i-1} + \bar{\chi}_i P(\varsigma_m^{\pm}) + \sum_{j=1}^{i-1}\left[\sum_{(m)} \bar{\chi}_{ji(m)}\, \overline{\Sigma_{in(m)}(\varsigma_m^{\pm})}_j\right] \overline{n v}_{nj}\, \Delta u_j, \\ \frac{1}{\omega_{2mT}^{\pm}} &= 0, \quad \Delta u_T = 1, \\ q^{\pm}_{m0} &= 0; \end{aligned} \tag{87}$$

(1-b) "KAPL multigroup" where $\bar{q}^{\pm}_{mi} = \omega_{1mi}^{\pm} q^{\pm}_{m\,i-1} + \omega_{2mi}^{\pm} q^{\pm}_{mi}$ and Equation (86b) applies

$$\begin{aligned} A(\varsigma_m^{\pm})_i &= \left(\frac{\Sigma_a(\varsigma_m^{\pm})}{S(\varsigma_m^{\pm})}\right)_i \cdot \overline{S(\varsigma_m^{\pm})}_i + \frac{\overline{S(\varsigma_m^{\pm})}_i}{\omega_{2mi}^{\pm}\,\Delta u_i}, \qquad (i = 1, 2, \cdots, T) \\ \mathcal{S}^{\pm}_{mi} &= \frac{1}{\Delta u_i}\left(1 + \frac{\omega_{1mi}^{\pm}}{\omega_{2mi}^{\pm}}\right) q^{\pm}_{m\,i-1} + \bar{\chi}_i P(\varsigma_m^{\pm}) + \sum_{j=1}^{i-1}\left[\sum_{(m)} \bar{\chi}_{ji(m)} \overline{\left(\frac{\Sigma_{in(m)}(\varsigma_m^{\pm})}{S(\varsigma_m^{\pm})}\right)}_j \cdot \overline{S(\varsigma_m^{\pm})}_j\right] \cdot \overline{n v}_{nj}\, \Delta u_j, \\ \frac{1}{\omega_{2mT}^{\pm}} &= 0, \quad \Delta u_T = 1, \\ q^{\pm}_{m0} &= 0; \end{aligned} \tag{88}$$

(2-a) "ORNL multigroup" where $\overline{n v}_{m i} = \omega_{1mi}\, n v_{m\,i-1} + \omega_{2mi}\, n v_{m\,i}$ and Equation (86a) applies

$$A(\varsigma_m^{\pm})_i = \overline{\Sigma_{1a}(\varsigma_m^{\pm})}_i + \frac{S(\varsigma_m^{\pm})_i}{\omega_{2mi}\,\Delta u_i},$$

$$\mathcal{S}_{m\,i}^{\pm} = \frac{1}{\Delta u_i}\left(1 + \frac{\omega_{1mi}}{\omega_{2mi}}\,\frac{S(\varsigma_m^{\pm})_i}{S(\varsigma_m^{\pm})_{i-1}}\right) q_{m\,i-1}^{\pm} + \overline{\chi}_i\, P(\varsigma_m^{\pm}) \qquad (i = 1, 2, \cdots, T)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ji(m)}\, \overline{\Sigma_{1in(m)}(\varsigma_m^{\pm})}_j\right] \overline{n v}_{mj}\, \Delta u_j, \qquad (89)$$

$$\frac{1}{\omega_{2mT}} = 0, \quad \Delta u_T = 1,$$

$$q_{m\,0}^{\pm} = 0;$$

(2-b) "ORNL multigroup" where $\overline{n v}_{m i} = \omega_{1mi}\, n v_{m\,i-1} + \omega_{2mi}\, n v_{m\,i}$ and Equation (86b) applies

$$A(\varsigma_m^{\pm})_i = \left(\overline{\frac{\Sigma_{1a}(\varsigma_m^{\pm})}{S(\varsigma_m^{\pm})}}\right)_i \cdot \overline{S(\varsigma_m^{\pm})}_i + \frac{S(\varsigma_m^{\pm})_i}{\omega_{2mi}\,\Delta u_i},$$

$$\mathcal{S}_{m\,i}^{\pm} = \frac{1}{\Delta u_i}\left(1 + \frac{\omega_{1mi}}{\omega_{2mi}}\,\frac{S(\varsigma_m^{\pm})_i}{S(\varsigma_m^{\pm})_{i-1}}\right) q_{m\,i-1}^{\pm} + \overline{\chi}_i\, P(\varsigma_m^{\pm}) \qquad (i = 1, 2, \ldots, T)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ji(m)} \left(\overline{\frac{\Sigma_{1in(m)}(\varsigma_m^{\pm})}{S(\varsigma_m^{\pm})}}\right)_j \cdot \overline{S(\varsigma_m^{\pm})}_j\right] \overline{n v}_{mj}\, \Delta u_j, \qquad (90)$$

$$\frac{1}{\omega_{2mT}} = 0, \quad \Delta u_T = 1,$$

$$q_{m\,0}^{\pm} = 0;$$

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(3-a) Selengut-Goertzel multigroup, where $\bar{q}^{\pm}_{ni} = \omega_{1ni}^{\pm} q^{\pm}_{n\,i-1} + \omega_{2ni}^{\pm} q^{\pm}_{ni}$ and Equation (86a) applies

$$A(\varsigma^{\pm}_{n})_i = \overline{\Sigma'_{1a}(\varsigma^{\pm}_{n})}_i + \frac{\overline{S(\varsigma^{\pm}_{n})}_i}{\omega^{\pm}_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}_i \,,$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1+\frac{\omega^{\pm}_{1ni}}{\omega^{\pm}_{2ni}}\right) q^{\pm}_{n\,i-1} + \overline{\chi}_i\, P(\varsigma^{\pm}_{n}) + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\eta^{\pm}_{n\,i-1} \qquad (i=1,2,\ldots,T)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)}{}' \,\overline{\chi}_{ji(m)}\,\overline{\Sigma_{in(m)}(\varsigma^{\pm}_{n})}_j\right] \overline{nv}_{nj}\,\Delta u_j \,, \qquad (91)$$

$$\eta^{\pm}_{ni} = \eta^{\pm}_{n\,i-1} + (e^{-\Delta u_i}-1)\left(\eta^{\pm}_{n\,i-1} - \overline{nv}_{ni}\,\overline{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}_i\right),$$

$$\frac{1}{\omega^{\pm}_{2nT}} = 0 \,,\quad \Delta u_T = 1 \,,\quad e^{-\Delta u_T} = 0 \,,\quad \overline{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}_T = 0 \,,$$

$$q^{\pm}_{n0} = 0 \,,\quad \eta^{\pm}_{n0} = 0 \,;$$

(3-b) Selengut-Goertzel multigroup, where $\bar{q}^{\pm}_{ni} = \omega_{1ni}^{\pm} q^{\pm}_{n\,i-1} + \omega_{2ni}^{\pm} q^{\pm}_{ni}$ and Equation (86b) applies

$$A(\varsigma^{\pm}_{n})_i = \overline{\left(\frac{\Sigma'_{1a}(\varsigma^{\pm}_{n})}{S(\varsigma^{\pm}_{n})}\right)}_i \cdot \overline{S(\varsigma^{\pm}_{n})}_i + \frac{\overline{S(\varsigma^{\pm}_{n})}_i}{\omega^{\pm}_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\left(\frac{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}{S(\varsigma^{\pm}_{n})}\right)}_i \cdot \overline{S(\varsigma^{\pm}_{n})}_i \,,$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1+\frac{\omega^{\pm}_{1ni}}{\omega^{\pm}_{2ni}}\right) q^{\pm}_{n\,i-1} + \overline{\chi}_i\, P(\varsigma^{\pm}_{n}) + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\eta^{\pm}_{n\,i-1} \qquad (i=1,2,\ldots,T)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)}{}' \,\overline{\chi}_{ji(m)}\,\overline{\left(\frac{\Sigma_{in(m)}(\varsigma^{\pm}_{n})}{S(\varsigma^{\pm}_{n})}\right)}_j \cdot \overline{S(\varsigma^{\pm}_{n})}_j\right] \overline{nv}_{nj}\,\Delta u_j \,, \qquad (92)$$

$$\eta^{\pm}_{ni} = \eta^{\pm}_{n\,i-1} + (e^{-\Delta u_i}-1)\left(\eta^{\pm}_{n\,i-1} - \overline{nv}_{ni}\,\overline{\left(\frac{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}{S(\varsigma^{\pm}_{n})}\right)}_i \cdot \overline{S(\varsigma^{\pm}_{n})}_i\right),$$

$$\frac{1}{\omega^{\pm}_{2nT}} = 0 \,,\quad \Delta u_T = 1 \,,\quad e^{-\Delta u_T} = 0 \,,\quad \overline{\Sigma'_{1SH}(\varsigma^{\pm}_{n})}_T = 0 \,,$$

$$q^{\pm}_{n0} = 0 \,,\quad \eta^{\pm}_{n0} = 0 \,;$$

(3-c) Selengut-Goertzel multigroup, where $\overline{nv_{ni}} = \omega_{1ni}\, nv_{ni-1} + \omega_{2ni}\, nv_{ni}$ and (86a) applies

$$A(\varsigma_n^\pm)_i = \overline{\Sigma_{1a}(\varsigma_n^\pm)_i} + \frac{S(\varsigma_n^\pm)_i}{\omega_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma_{1SH}'(\varsigma_n^\pm)_i},$$

$$\mathcal{S}_{ni}^\pm = \frac{1}{\Delta u_i}\left(1+\frac{\omega_{1ni}}{\omega_{2ni}}\frac{S(\varsigma_n^\pm)_i}{S(\varsigma_n^\pm)_{i-1}}\right) q_{ni-1}^\pm + \overline{\chi}_i\,P(\varsigma_n^\pm) \qquad (i=1,2,\ldots,T)$$

$$+\frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\eta_{ni-1}^\pm + \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ji(m)}\,\overline{\Sigma_{1in(m)}'(\varsigma_n^\pm)_j}\right]\overline{nv_{nj}}\cdot\Delta u_j, \tag{93}$$

$$\eta_{ni}^\pm = \eta_{ni-1}^\pm + \left(e^{-\Delta u_i}-1\right)\left(\eta_{ni-1}^\pm - \overline{nv_{ni}}\,\overline{\Sigma_{1SH}'(\varsigma_n^\pm)_i}\right),$$

$$\frac{1}{\omega_{2nT}} = 0,\quad \Delta u_T = 1,\quad e^{-\Delta u_T} = 0,\quad \overline{\Sigma_{1SH}'(\varsigma_n^\pm)_T} = 0,$$

$$q_{n0}^\pm = 0,\quad \eta_{n0}^\pm = 0;$$

(3-d) Selengut-Goertzel multigroup, where $\overline{nv_{ni}} = \omega_{1ni}\, nv_{ni-1} + \omega_{2ni}\, nv_{ni}$ and Equation (86b) applies

$$A(\varsigma_n^\pm)_i = \overline{\left(\frac{\Sigma_{1a}'(\varsigma_n^\pm)}{S(\varsigma_n^\pm)}\right)_i}\cdot\overline{S(\varsigma_n^\pm)_i} + \frac{S(\varsigma_n^\pm)_i}{\omega_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\overline{\left(\frac{\Sigma_{1SH}'(\varsigma_n^\pm)}{S(\varsigma_n^\pm)}\right)_i}\cdot\overline{S(\varsigma_n^\pm)_i},$$

$$\mathcal{S}_{ni}^\pm = \frac{1}{\Delta u_i}\left(1+\frac{\omega_{1ni}}{\omega_{2ni}}\frac{S(\varsigma_n^\pm)_i}{S(\varsigma_n^\pm)_{i-1}}\right) q_{ni-1}^\pm + \overline{\chi}_i\,P(\varsigma_n^\pm) \qquad (i=1,2,\ldots,T)$$

$$+\frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\eta_{ni-1}^\pm + \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ji(m)}\overline{\left(\frac{\Sigma_{1in(m)}'(\varsigma_n^\pm)}{S(\varsigma_n^\pm)}\right)_j}\cdot\overline{S(\varsigma_n^\pm)_j}\right]\overline{nv_{nj}}\,\Delta u_j, \tag{94}$$

$$\eta_{ni}^\pm = \eta_{ni-1}^\pm + \left(e^{-\Delta u_i}-1\right)\left(\eta_{ni-1}^\pm - \overline{nv_{ni}}\,\overline{\left(\frac{\Sigma_{1SH}'(\varsigma_n^\pm)}{S(\varsigma_n^\pm)}\right)_i}\,\overline{S(\varsigma_n^\pm)_i}\right),$$

$$\frac{1}{\omega_{2nT}} = 0,\quad \Delta u_T = 1,\quad e^{-\Delta u_T} = 0,\quad \overline{\Sigma_{1SH}'(\varsigma_n^\pm)_T} = 0,$$

$$q_{n0}^\pm = 0,\quad \eta_{n0}^\pm = 0;$$

(4-a) Adjoint to 1-a, where $\overline{S(\varsigma_m^\pm)_i}\,\overline{m}_{ni} = \gamma_{1\,m\,i}^{\,\pm} S(\varsigma_m^\pm)_{i-1} m_{ni-1} + \gamma_{2\,m\,i}^{\,\pm} S(\varsigma_m^\pm)_i m_{ni}$

$$A(\varsigma_m^\pm)_i = \overline{\Sigma_a(\varsigma_m^\pm)_i} + \frac{\overline{S(\varsigma_m^\pm)_i}}{\gamma_{2\,m\,i}^{\,\pm}\,\Delta u_i}\,\frac{\overline{S(\varsigma_m^\pm)_i}}{S(\varsigma_m^\pm)_i},$$

$$(i = 1, 2, \ldots, T)$$

$$\mathscr{S}_{mi}^{\pm} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma_{1\,m\,i}^{\,\pm}}{\gamma_{2\,m\,i}^{\,\pm}}\,\frac{S(\varsigma_m^\pm)_{i-1}}{S(\varsigma_m^\pm)_i} - \delta_{1i}\right)\overline{S(\varsigma_m^\pm)_i}\,m_{n\,i-1} + \overline{\Sigma_f(\varsigma_m^\pm)_i}\cdot P^*(\varsigma_m^\pm)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ij(m)}\,\overline{\Sigma_{in(m)}(\varsigma_m^\pm)_i}\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (95)$$

$$\frac{1}{\gamma_{2m1}} = 0\,, \quad \Delta u_1 = 1\,, \quad m_{n0} = 0\,,$$

$$\delta_{1i} = \begin{cases} 1 & i = 1 \\ 0 & i \neq 1 \end{cases};$$

(We have relabeled the groups for the adjoint cases, so that the thermal group is i = 1.)

(4-b) Adjoint to 1-b, where $\overline{S(\varsigma_m^\pm)_i}\,\overline{m}_{ni} = \gamma_{1\,m\,i}^{\,\pm} S(\varsigma_m^\pm)_{i-1} m_{ni-1} + \gamma_{2\,m\,i}^{\,\pm} S(\varsigma_m^\pm)_i m_{ni}$

$$A(\varsigma_m^\pm)_i = \overline{\left(\frac{\Sigma_a(\varsigma_m^\pm)}{S(\varsigma_m^\pm)}\right)_i}\cdot\overline{S(\varsigma_m^\pm)_i} + \frac{\overline{S(\varsigma_m^\pm)_i}}{\gamma_{2\,m\,i}^{\,\pm}\,\Delta u_i} + \frac{\overline{S(\varsigma_m^\pm)_i}}{\Delta u_i}\ln\frac{S(\varsigma_m^\pm)_{i-1}}{S(\varsigma_m^\pm)_i},$$

$$\mathscr{S}_{mi}^{\pm} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma_{1\,m\,i}^{\,\pm}}{\gamma_{2\,m\,i}^{\,\pm}} - \delta_{1i}\right)S(\varsigma_m^\pm)_{i-1}\,m_{n\,i-1} + \overline{\Sigma_f(\varsigma_m^\pm)_i}\,P^*(\varsigma_m^\pm) \qquad (i = 1, 2, \ldots, T)$$

$$+ \sum_{j=1}^{i-1}\left[\sum_{(m)} \overline{\chi}_{ij(m)}\,\overline{\left(\frac{\Sigma_{in(m)}(\varsigma_m^\pm)}{S(\varsigma_m^\pm)}\right)_i}\cdot\overline{S(\varsigma_m^\pm)_i}\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (96)$$

$$\frac{1}{\gamma_{2m1}} = 0\,, \quad \Delta u_1 = 1\,, \quad m_{n0} = 0\,;$$

(5-a) Adjoint to 2-a, where $\overline{m}_{ni} = \gamma_{1ni}\, m_{ni-1} + \gamma_{2ni}\, m_{ni}$

$$A(\varsigma_n^{\pm})_i = \overline{\Sigma'_{1a}(\varsigma_n^{\pm})}_i + \frac{\overline{S(\varsigma_n^{\pm})}_i}{\gamma_{2ni}\,\Delta u_i}\,, \qquad (i = 1, 2, \ldots, T)$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma_{1ni}}{\gamma_{2ni}} - \delta_{1i}\right)\overline{S(\varsigma_n^{\pm})}_i\, m_{ni-1} + \overline{\Sigma'_{1f}(\varsigma_n^{\pm})}_i\; P^*(\varsigma_n^{\pm}) + \sum_{j=1}^{i-1}{}'\left[\sum_{(m)}{}'\,\overline{\chi}_{ij(m)}\,\overline{\Sigma'_{1in(m)}(\varsigma_n^{\pm})}_i\right] m_{nj}\,\Delta u_j\,, \tag{97}$$

$$\frac{1}{\gamma_{2n1}} = 0\,, \quad \Delta u_1 = 1\,, \quad m_{n0} = 0\,;$$

(5-b) Adjoint to 2-b, where $\overline{m}_{ni} = \gamma_{1ni}\, m_{ni-1} + \gamma_{2ni}\, m_{ni}$

$$A(\varsigma_n^{\pm})_i = \left(\overline{\frac{\Sigma'_{1a}(\varsigma_n^{\pm})}{S(\varsigma_n^{\pm})}}\right)_i \cdot \overline{S(\varsigma_n^{\pm})}_i + \frac{S(\varsigma_n^{\pm})_i}{\gamma_{2ni}\,\Delta u_i} + \frac{\overline{S(\varsigma_n^{\pm})}_i}{\Delta u_i}\ln\frac{S(\varsigma_n^{\pm})_{i-1}}{S(\varsigma_n^{\pm})_i} \qquad (i = 1, 2, \ldots, T)$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma_{1ni}}{\gamma_{2ni}}\,\frac{S(\varsigma_n^{\pm})_i}{S(\varsigma_n^{\pm})_{i-1}} - \delta_{1i}\right) S(\varsigma_n^{\pm})_{i-1}\, m_{ni-1} + \overline{\Sigma'_{1f}(\varsigma_n^{\pm})}_i\; P^*(\varsigma_n^{\pm}) + \sum_{j=1}^{i-1}{}'\left[\sum_{(m)}{}'\,\overline{\chi}_{ij(m)}\left(\overline{\frac{\Sigma'_{1in(m)}(\varsigma_n^{\pm})}{S(\varsigma_n^{\pm})}}\right)_i \cdot \overline{S(\varsigma_n^{\pm})}_i\right] m_{nj}\,\Delta u_j\,, \tag{98}$$

$$\frac{1}{\gamma_{2n1}} = 0\,, \quad \Delta u_1 = 1\,, \quad m_{n0} = 0\,;$$

(6-a) Adjoint to 3-a, where $\overline{S(\zeta_m^\pm)}_i\,\overline{m}_{ni} = \gamma_{1mi}^{\pm} S(\zeta_m^\pm)_{i-1} m_{ni-1} + \gamma_{2mi}^{\pm} S(\zeta_m^\pm)_i\, m_{ni}$

$$A(\zeta_m^\pm)_i = \overline{\Sigma_{1a}(\zeta_m^\pm)}_i + \frac{\overline{S(\zeta_m^\pm)}_i}{\gamma_{2mi}^\pm\,\Delta u_i}\,\frac{\overline{S(\zeta_m^\pm)}_i}{S(\zeta_m^\pm)_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma_{1sH}(\zeta_m^\pm)}_i\,, \qquad (i=1,2,\ldots,T)$$

$$\mathcal{S}_{ni}^\pm = \frac{1}{\Delta u_i}\left(1+\frac{\gamma_{1mi}^\pm}{\gamma_{2mi}^\pm}\,\frac{S(\zeta_m^\pm)_{i-1}}{S(\zeta_m^\pm)_i}-\delta_{1i}\right)\overline{S(\zeta_m^\pm)}_i\, m_{ni-1} + \overline{\Sigma_{1f}(\zeta_m^\pm)}_i \cdot P^*(\zeta_m^\pm)$$

$$+\frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma_{1sH}(\zeta_m^\pm)}_i\,\lambda_{ni-1} + \sum_{j=1}^{i-1}\left[\sum_{(m)}\bar{\chi}_{ij(m)}\,\overline{\Sigma_{1in(m)}(\zeta_m^\pm)}_i\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (99)$$

$$\lambda_{ni} = \lambda_{ni-1} + (e^{-\Delta u_i}-1)(\lambda_{ni-1} - \overline{m}_{ni}),$$

$$\frac{1}{\gamma_{2n1}} = 0\,,\quad \Delta u_1 = 1\,,\quad \overline{\Sigma_{1sH}(\zeta_m^\pm)}_1 = 0\,,\quad e^{-\Delta u_1} = 0\,,$$

$$m_{n0} = 0\,,\quad \lambda_{n0} = 0\;;$$

(6-b) Adjoint to 3-b, where $\overline{S(\zeta_m^\pm)}_i\,\overline{m}_{ni} = \gamma_{1mi}^{\pm} S(\zeta_m^\pm)_{i-1} m_{ni-1} + \gamma_{2mi}^{\pm} S(\zeta_m^\pm)_i\, m_{ni}$

$$A(\zeta_m^\pm)_i = \left(\frac{\overline{\Sigma_{1a}(\zeta_m^\pm)}}{S(\zeta_m^\pm)}\right)_i \overline{S(\zeta_m^\pm)}_i + \frac{\overline{S(\zeta_m^\pm)}_i}{\Delta u_i}\ln\frac{S(\zeta_m^\pm)_{i-1}}{S(\zeta_m^\pm)_i} + \frac{\overline{S(\zeta_m^\pm)}_i}{\gamma_{2mi}^\pm\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\left(\frac{\overline{\Sigma_{1sH}(\zeta_m^\pm)}}{S(\zeta_m^\pm)}\right)_i \overline{S(\zeta_m^\pm)}_i\,, \qquad (i=1,2,\ldots,T)$$

$$\mathcal{S}_{mi}^\pm = \frac{1}{\Delta u_i}\left(1+\frac{\gamma_{1mi}^\pm}{\gamma_{2mi}^\pm}-\delta_{1i}\right)S(\zeta_m^\pm)_{i-1}\, m_{ni-1} + \overline{\Sigma_{1f}(\zeta_m^\pm)}_i \cdot P^*(\zeta_m^\pm)$$

$$+\frac{1-e^{-\Delta u_i}}{\Delta u_i}\left(\frac{\overline{\Sigma_{1sH}(\zeta_m^\pm)}}{S(\zeta_m^\pm)}\right)_i \overline{S(\zeta_m^\pm)}_i\,\lambda_{ni-1} + \sum_{j=1}^{i-1}\left[\sum_{(m)}\bar{\chi}_{ij(m)}\left(\frac{\overline{\Sigma_{1in(m)}(\zeta_m^\pm)}}{S(\zeta_m^\pm)}\right)_i \cdot \overline{S(\zeta_m^\pm)}_i\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (100)$$

$$\lambda_{ni} = \lambda_{ni-1} + (e^{-\Delta u_i}-1)(\lambda_{ni-1} - \overline{m}_{ni}),$$

$$\frac{1}{\gamma_{2n1}} = 0\,,\quad \Delta u_1 = 1\,,\quad \overline{\Sigma_{1sH}(\zeta_m^\pm)}_1 = 0\,,\quad e^{-\Delta u_1} = 0\,,$$

$$m_{n0} = 0\,,\quad \lambda_{n0} = 0\;;$$

(6-c) Adjoint to 3-c, where $\overline{m}_{ni} = \gamma_{1ni}\, m_{ni-1} + \gamma_{2ni}\, m_{ni}$

$$A(\varsigma_m^{\pm})_i = \overline{\Sigma_{1a}(\varsigma_m^{\pm})}_i + \frac{\overline{S(\varsigma_m^{\pm})}_i}{\gamma_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma_{1SH}(\varsigma_m^{\pm})}_i\,, \qquad (i=1,2,\cdots,T)$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma^{\pm}_{1mi}}{\gamma^{\pm}_{2mi}} - \delta_{1i}\right)\overline{S(\varsigma_m^{\pm})}_{i-1}\, m_{ni-1} + \overline{\Sigma_{1f}(\varsigma_m^{\pm})}_i\; P^*(\varsigma_m^{\pm})$$

$$+ \frac{1-e^{-\Delta u_i}}{\Delta u_i}\,\overline{\Sigma_{1SH}(\varsigma_m^{\pm})}_i\,\lambda_{ni-1} + \sum_{j=1}^{i-1}\left[\sum_{(m)} \bar{\chi}_{ij(m)}\,\overline{\Sigma_{1in(m)}(\varsigma_m^{\pm})}_i\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (101)$$

$$\lambda_{ni} = \lambda_{ni-1} + (e^{-\Delta u_i} - 1)(\lambda_{ni-1} - \overline{m}_{ni})\,,$$

$$\frac{1}{\gamma_{2n1}} = 0\,,\quad \Delta u_1 = 1\,,\quad e^{-\Delta u_1} = 0\,,\quad \overline{\Sigma_{1SH}(\varsigma_n^{\pm})}_1 = 0\,,$$

$$m_{n0} = 0\,,\quad \lambda_{n0} = 0\,;$$

(6-d) Adjoint to 3-d, where $\overline{m}_{ni} = \gamma_{1ni}\, m_{ni-1} + \gamma_{2ni}\, m_{ni}$

$$A(\varsigma_m^{\pm})_i = \left(\frac{\overline{\Sigma_{1a}(\varsigma_m^{\pm})}}{S(\varsigma_m^{\pm})}\right)_i \overline{S(\varsigma_m^{\pm})}_i + \frac{\overline{S(\varsigma_m^{\pm})}_i}{\Delta u_i}\ln\frac{S(\varsigma_m^{\pm})_{i-1}}{S(\varsigma_m^{\pm})_i}$$

$$+ \frac{S(\varsigma_m^{\pm})_i}{\gamma_{2ni}\,\Delta u_i} + \frac{1-e^{-\Delta u_i}}{\Delta u_i}\left(\frac{\overline{\Sigma_{1SH}(\varsigma_m^{\pm})}}{S(\varsigma_m^{\pm})}\right)_i \overline{S(\varsigma_m^{\pm})}_i\,, \qquad (i=1,2,\cdots,T)$$

$$\mathcal{S}^{\pm}_{ni} = \frac{1}{\Delta u_i}\left(1 + \frac{\gamma_{1ni}}{\gamma_{2ni}}\,\frac{S(\varsigma_m^{\pm})_i}{S(\varsigma_m^{\pm})_{i-1}} - \delta_{1i}\right)S(\varsigma_m^{\pm})_{i-1}\, m_{ni-1} + \overline{\Sigma_{1f}(\varsigma_m^{\pm})}_i\; P^*(\varsigma_n^{\pm})$$

$$+ \frac{1-e^{-\Delta u_i}}{\Delta u_i}\left(\frac{\overline{\Sigma_{1SH}(\varsigma_m^{\pm})}}{S(\varsigma_m^{\pm})}\right)_i \overline{S(\varsigma_m^{\pm})}_i + \sum_{j=1}^{i-1}\left[\sum_{(m)} \bar{\chi}_{ij(m)}\left(\frac{\overline{\Sigma_{1in(m)}(\varsigma_m^{\pm})}}{S(\varsigma_m^{\pm})}\right)_i \overline{S(\varsigma_m^{\pm})}_i\right]\overline{m}_{nj}\,\Delta u_j\,, \qquad (102)$$

$$\lambda_{ni} = \lambda_{ni-1} + (e^{-\Delta u_i} - 1)(\lambda_{ni-1} - \overline{m}_{ni})\,,$$

$$\frac{1}{\gamma_{2n1}} = 0\,,\quad \Delta u_1 = 1\,,\quad e^{-\Delta u_1} = 0\,,\quad \overline{\Sigma_{1SH}(\varsigma_m^{\pm})}_1 = 0\,,$$

$$m_{n0} = 0\,,\quad \lambda_{n0} = 0\,.$$

F. BOUNDARY CONDITIONS

The three types of boundary conditions which we may have are:

1. Flux zero at an extrapolated endpoint. Here we assume that for an extreme point in our nodal system, the flux is zero, that is,

$$\varphi_B = 0 . \tag{103}$$

This is the simplest of the three conditions.

2. The assumption of an infinite homogeneous outer region, where no degradation is allowed, yielding a radiation-condition at the boundary

$$\frac{(\xi^\rho j)_B}{\xi_B^\rho \varphi_B} = \operatorname{sign}(j_B)\left[\sqrt{AD} + \frac{\rho D}{2\xi_B} + D\sqrt{\frac{D}{A}}\,\frac{\rho}{4}\left(\frac{\rho}{2}-1\right)\frac{1}{\xi_B^2} + O\left(\frac{1}{\xi_B^3}\right)\right]_{\text{OUTER REG. COMP.}} \tag{104}$$

where the left-hand side of the equation is to be evaluated from the inside of the boundary. In the cartesian case, this reduces to the simpler equation

$$\frac{(\xi^\rho j)_B}{\xi_B^\rho \varphi_B} = \operatorname{sign}(j_B)\sqrt{A\,D}\,\Big|_{\text{OUTER REG. COMP.}} \tag{105}$$

which may be used at the origin (the $1/\xi_B$ terms vanishing). In the cylindrical and spherical cases, Equation (104) will be used, if at all, at an outer boundary, where φ is small and ξ_B is large. Hence it may be expeditious to use Equation (105) in place of Equation (104), making the use of Equation (104) uniform.

3. At a boundary of symmetry, we have a variation of Equation (104), that is,

$$\frac{(\xi^\rho j)_B}{\xi_B^\rho \varphi_B} = 0 . \tag{106}$$

Equations (105) and (104) may be combined in the general equation

$$\frac{(\xi^\rho j)_B}{\xi_B^\rho \varphi_B} = \alpha_B . \tag{107}$$

At an exterior boundary, ξ_N , boundary condition (107) leads to the finite difference equation

$$\check{J}_{Ni}(Q_i) + \frac{\xi_{N-1}^\rho}{\Delta\xi_{N-1}^-}\,\tau_{N-1}\,\hat{i}^+_{N-1}\left[D_i^{(2)}(\xi_{N-\frac{1}{2}})\varphi_{N-1\,i} - D_i^{(1)}(\xi_{N-\frac{1}{2}})\varphi_{Ni}\right] = \xi_N^\rho \varphi_{Ni}\,\alpha_{Ni} . \tag{108}$$

If Equation (107) were to be applied at the origin, the finite difference equation at the origin would be

$$\check{I}_{1i}(Q_i) + \frac{\varsigma_1^{\rho}}{\Delta\varsigma_1^{-}}\,\hat{i}_{1}\left[D_i^{(1)}(\varsigma_{\frac{1}{2}})\varphi_{1i} - D_i^{(2)}(\varsigma_{\frac{1}{2}})\varphi_{oi}\right]$$
$$= -\alpha_{oi}\,\varphi_{oi}\,\delta_{o\rho}\,. \qquad (109)$$

Equation (109) can be expanded to

$$\frac{1}{\Delta\varsigma_o(1+W_{oi})}\left[D_i^{(1)}(\varsigma_{\frac{1}{2}})\varphi_{1i} - D_i^{(2)}(\varsigma_{\frac{1}{2}})\varphi_{oi}\right]$$
$$+ Q_i(\varsigma_o)\left\{\frac{\Delta\varsigma_o}{4(\rho+1)}\left[1+\frac{1}{\rho+2}\right] - \frac{\Delta\varsigma_o^{\,2}}{24(1+W_{oi})}\left(\frac{\rho}{\Delta\varsigma_o} + \left(\frac{D'}{D}\right)_{\varsigma_{\frac{1}{2}}} + \frac{1}{\Delta\varsigma_o}\right)\right\}$$
$$+ Q_i(\varsigma_1)\left\{\frac{\Delta\varsigma_o}{4(\rho+1)}\left[1-\frac{1}{\rho+2}\right] - \frac{\Delta\varsigma_o^{\,2}}{24(1+W_{oi})}\left(\frac{\rho}{\Delta\varsigma_o} + \left(\frac{D'}{D}\right)_{\varsigma_{\frac{1}{2}}} - \frac{1}{\Delta\varsigma_o}\right)\right\}$$
$$= -\alpha_{oi}\,\varphi_{oi}\,\delta_{o\rho}\left(\frac{2}{\Delta\varsigma_o}\right)^{\rho}. \qquad (110)$$

It can be shown that Equation (110) is the finite difference equation obtained when we integrate the differential equation

$$-\frac{d}{d\varsigma}D(\varsigma)\frac{d}{d\varsigma}\varphi(\varsigma) - D(\varsigma)\frac{\rho}{\varsigma}\frac{d}{d\varsigma}\varphi(\varsigma) + A(\varsigma)\varphi(\varsigma) = \mathcal{S}(\varsigma)$$

over the region extending from 0 to $\Delta\varsigma_o/2$, use the boundary condition

$$-D_i\left.\frac{d\varphi_i}{d\varsigma}\right|_{\varsigma=0} = \alpha_{oi}\,\varphi_{oi},$$

and proceed as in Section A.

G. THE THREE-TERM LINEAR SYSTEM

For each group, i, we have to solve a simultaneous system of equations of the form

$$a_{ni}\,\varphi_{n+1\,i} - b_{ni}\,\varphi_{ni} + c_{ni}\,\varphi_{n-1\,i} + d_{ni} = 0 \qquad (n = 0, 1, \ldots, N) \tag{111}$$

for the fluxes φ_{ni} in the group. As we have seen previously, the general equations for interior points are

$$\begin{aligned}
a_{ni} &= r_n\left[\hat{\imath}^{+}_{ni}\,D^{(1)}_{ni} - z^{+}_{ni}\,A^{-}_{n+1\,i}\right],\\
b_{ni} &= \hat{\imath}^{-}_{ni}\,D^{(1)}_{n-1\,i} + x^{-}_{ni}\,A^{-}_{ni} + r_n\left[\hat{\imath}^{+}_{ni}\,D^{(2)}_{ni} + x^{+}_{ni}\,A^{+}_{ni}\right],\\
c_{ni} &= \hat{\imath}^{-}_{ni}\,D^{(2)}_{n-1\,i} - z^{-}_{ni}\,A^{+}_{n-1\,i},\\
d_{ni} &= r_n\left[z^{+}_{ni}\,\mathcal{S}^{-}_{n+1\,i} + x^{+}_{ni}\,\mathcal{S}^{+}_{ni}\right] + x^{-}_{ni}\,\mathcal{S}^{-}_{ni} + z^{-}_{ni}\,\mathcal{S}^{+}_{n-1\,i},
\end{aligned} \tag{112}$$

where we have written

$$\begin{aligned}
\frac{\Delta\varsigma^{-}_{n}}{\varsigma^{\rho}_{n}}\,\hat{J}_{ni}(\Theta_i) &= z^{-}_{ni}\,\Theta^{+}_{n-1\,i} + x^{-}_{ni}\,\Theta^{-}_{ni},\\
\frac{\Delta\varsigma^{-}_{n}}{\varsigma^{\rho}_{n}}\,\hat{I}_{n+1\,i}(\Theta_i) &= r_n\left[x^{+}_{ni}\,\Theta^{+}_{ni} + z^{+}_{ni}\,\Theta^{-}_{n+1\,i}\right].
\end{aligned} \tag{113}$$

For the origin, n = 0, we can include Equation (110) by

$$\begin{aligned}
a_{0i} &= \left[(\varsigma^{\rho}_{n}\,\hat{\imath}^{+}_{ni})_{n=0}\,D^{(1)}_{0i} - (\varsigma^{\rho}_{n}\,z^{+}_{ni})_{n=0}\,A^{-}_{1i}\right],\\
b_{0i} &= \left[(\varsigma^{\rho}_{n}\,\hat{\imath}^{+}_{ni})_{n=0}\,D^{(2)}_{0i} + (\varsigma^{\rho}_{n}\,x^{+}_{ni})_{n=0}\,A^{+}_{0i}\right] - \alpha_{0i}\,\delta_{0\rho}\,\Delta\varsigma_0,\\
c_{0i} &= 0,\\
d_{0i} &= \left[(\varsigma^{\rho}_{n}\,z^{-}_{ni})_{n=0}\,\mathcal{S}^{-}_{1i} + (\varsigma^{\rho}_{n}\,x^{+}_{ni})_{n=0}\,\mathcal{S}^{+}_{0i}\right].
\end{aligned} \tag{114}$$

To use condition (103) at the origin, we would have to take

$$a_{oi} = 0,$$

$$c_{oi} = 0,$$

$$d_{oi} = 0.$$

For n = N, we must have either Equation (107) or Equation (108) holding. For the first we have

$$
\begin{aligned}
b_{Ni} &= \hat{\imath}^{-}_{Ni} D^{(1)}_{N-1\,i} + x^{-}_{Ni} A^{-}_{Ni} + \Delta\varsigma^{-}_{N} \alpha_{Ni}, \\
c_{Ni} &= \hat{\imath}^{-}_{Ni} D^{(2)}_{N-1\,i} - z^{-}_{Ni} A^{+}_{N-1\,i}, \\
d_{Ni} &= x^{-}_{Ni} \mathcal{A}^{-}_{Ni} + z^{-}_{Ni} \mathcal{A}^{+}_{N-1\,i}, \\
\varphi_{N+1\,i} &= 0, \\
a_{Ni} &= 1,
\end{aligned}
\qquad (115)
$$

while for the second we have

$$
\begin{aligned}
b_{Ni} &= 1, \\
a_{Ni} &= 1, \\
d_{Ni} &= 0, \\
c_{Ni} &= 0, \\
\varphi_{N+1\,i} &= 0.
\end{aligned}
\qquad (116)
$$

The method used for solving Equations (111) has been explained in detail elsewhere. First, proceeding outward from n = 0, where

$$X_{oi} = \frac{a_{oi}}{b_{oi}},$$

$$Z_{oi} = \frac{d_{oi}}{b_{oi}},$$

we calculate the two sets of quantities

$$X_{ni} = \frac{a_{ni}}{b_{ni} - c_{ni} X_{n-1\,i}}\,, \qquad (n = 1, 2, \ldots, N) \tag{117}$$

$$Z_{ni} = \frac{X_{ni}(c_{ni} Z_{n-1\,i} + d_{ni})}{a_{ni}}\,.$$

Then, as is easily shown, we can work back in calculating the φ_{ni} by

$$\varphi_{ni} = Z_{ni} + X_{ni}\,\varphi_{n+1\,i}\,. \tag{118}$$

With all the algebraic manipulation involved in using Equations (117) and (118), it would be wise to have some sort of check on the solution of our equations. Let us suppose that Equations (117) and (118) yield a set of $\varphi_{n\,i}$. Do they satisfy Equations (111)? As we proceed in calculating the $\varphi_{n\,i}$ we might also calculate

$$\epsilon_{ni} = a_{ni}\varphi_{n+1\,i} - b_{ni}\varphi_{ni} + c_{ni}\varphi_{n-1\,i} + d_{ni}\,, \tag{119}$$

Then we could have an estimate of the error involved in the solution of the system by machine. One estimate might be

$$\epsilon_i^2 = \sum_{n=0}^{N-1} \beta_n\, \epsilon_{n\,i}^2\,, \tag{120}$$

where the β_n are properly chosen weighting factors.