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MULTIGROUP ONE-DIMENSIONAL SPHERICAL HARMONIC SOLUTIONS
TO THE BOLTZMANN TRANSPORT EQUATION

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MULTIGROUP ONE-DIMENSIONAL SPHERICAL HARMONIC SOLUTIONS
TO THE BOLTZMANN TRANSPORT EQUATION*

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ABSTRACT

Useful multigroup equations are derived for calculating the isotropic flux in a slab or cylindrical reactor cell. Full details are given of the reduction of the Boltzmann transport equation to spherical harmonic theory including putting the slowing down differential scattering cross section in a form suitable for calculation purposes.

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CHAPTER I

INTRODUCTION

In a nuclear reactor the majority of neutrons born from the fissioning of some fuel material such as U^{235} come out with energies somewhere between 0.1 million electron volts (Mev) and 10 Mev. For every neutron causing fission in U^{235} approximately 2.5 fast neutrons are ejected. These fast neutrons diffuse from the point of origin and are subsequently slowed down by scattering collisions with atoms of materials that are specifically provided for this purpose. During this slowing down process some of these fast neutrons are captured and some leak out of the system. Eventually after a number of scattering collisions, some neutrons will arrive at an energy where they can gain as well as lose energy from the thermal motion of the moderator atoms. The probability of fission in the fuel material is greatly increased as the neutrons approach thermal equilibrium with the atoms of the materials in the system. Thus a thermal neutron can again be captured by U^{235} and if the parasitic (non-fission) capture and leakage during slowing down and thermal diffusion are not too great, a self-sustaining chain reaction can be achieved.

In the analysis of reactor systems the fundamental variable for consideration is the angular flux function, $\phi(E, \Omega, \underline{r})$. If this quantity were known at every space point $\underline{r}$, at every energy E and in every direction Ω then other reactor physics information of interest for the time independent case could be derived. This flux function consists of

$$\phi(E, \Omega, \underline{r}) = n(E, \Omega, \underline{r})v$$

where $n(E, \Omega, r) dr d\Omega dE$ is the number of neutrons in volume element dr around r whose direction of motion is in the solid angle $d\Omega$ around Ω and with energy between E and $E + dE$. This neutron angular density function $n(E, \Omega, r)$ is multiplied by the speed, v , corresponding to the kinetic energy of the neutron where

$$E = \frac{1}{2}mv^2$$

and the mass of the neutron is m . Thus $\phi(E, \Omega, r) dE d\Omega$ is the neutrons per cm^2 per second traveling in solid angle $d\Omega$ around Ω with energies between E and $E + dE$ at position r .

The fundamental equation governing the variation of this angular flux function $\phi(E, \Omega, r)$ is the Boltzmann transport equation. This equation gives an accounting between the number of neutrons leaving and entering a given volume increment, in a given direction and in an energy range. The complete, rigorous solution of this differential-integral equation for a general three dimensional geometry presents formidable mathematical difficulties. Therefore, various mathematical and/or physical approximations are made to arrive at a solvable set of equations.

One of the most widely used approximation methods for obtaining a solvable set of equations from the Boltzmann transport equation is the method of spherical harmonics. This paper develops the basic multigroup spherical harmonic equations from the Boltzmann transport equation. Most industrial applications of one-dimensional spherical harmonics methods are centered on slab and cylindrical geometries. Only the equations for these two geometries will be developed in this paper.

Recently Honeck¹ developed a multigroup code for calculating scalar thermal neutron spectra by solving the integral transport equation

using numerical methods. This code (THERMOS) is oriented towards cylindrical cell calculations rather than a complete reactor calculation, and only isotropic neutron scattering is considered with the usual assumption that the source into the thermal group is flat across the moderator region. The source of neutrons in the thermal groups in the multigroup scheme comes from groups directly above thermal and because of the possible great differences in moderating power near thermal the flat source assumption may be a significant source of error. This code has been recently applied² to a wide variety of uranium-water lattices and considerable success has been achieved in calculating disadvantage factors. The computed disadvantage factors (ratio of average isotropic flux in moderator to that in the fuel) are about 4% higher than the measured values. A fairly limited comparison study of this code with cylindrical spherical harmonics methods showed the spherical harmonics method gave disadvantage factors about 4 to 5% lower than THERMOS². If this difference is consistent, then spherical harmonics methods with appropriate boundary conditions could be superior, in comparison to experiment, to the integral transport method.

Considerable work has been done in developing multigroup spherical harmonics methods. Frequently only two terms are retained in the expansion of the angular flux function in spherical harmonics. This gives the P-1 approximation which in general is adequate for the fast energy groups but a higher order approximation should be used in the thermal groups. This is particularly true if a study is being made of a system that has regions of widely differing nuclear properties. Bohl et al. have developed a number of multigroup codes but in every case these codes are

limited to only thermal spatial spectrum multigroup studies (SLOP-1)³, or multi-fast groups with one thermal group (PLMG,⁴ P3MG⁵). Some of the restrictive assumptions made in SLOP-1 such as isotropic slowing down into the thermal group, region-wise constant slowing down, and only one moderating material in any one problem are removed in this work. The assumption made in PLMG and P3MG of only one thermal group is also removed in this work.

Recently Marchuk⁶ used the P_3 approximation in cylindrical geometry for the calculation of thermal neutron spectra in lattice cells. Calculated spectra were found to be in fairly good agreement with measured spectra. Fifteen energy groups were considered in this work with the source only in the highest energy group. For hydrogen moderated system the slowing down source should be distributed amongst all the thermal groups.

The procedure outlined in this thesis will be for the fast groups above thermal to be treated in a standard P_1 spherical harmonics approximation. Because of the fact that the thermal absorption cross section is often quite large and variable and the thermal scattering cross section may vary considerably from region to region a higher order approximation than the P_1 is necessary in the thermal groups. Therefore, a standard P_3 approximation is made in the thermal groups for cylindrical geometry and a double P_1 (DP_1) approximation for slab geometry. The DP_1 approximation uses expansions in half-range Legendre polynomials rather than the complete range as is done in standard spherical harmonics methods. This method, first proposed by J. Yvon⁷, has been found to be considerably superior to the standard P_3 approximation with the same degree of

complexity in the basic equations. In a comparison study of methods by the author⁸ for a mono-energetic thermal group, the DP_1 computed disadvantage factor for a typical slab cell came close to that obtained by a P_{11} spherical harmonics approximation.

There is a multigroup code called ULCER⁹ which has many energy groups in both the fast and thermal energy ranges. This code is strictly multigroup diffusion theory which is not as rigorous as a standard multigroup spherical harmonics P-1 theory.

The only remaining question of importance is the limitations that will have to be placed on the number of groups, regions, and mesh points in order to have a program that will not be inordinately expensive for reactor physics analysis. It is hoped that the allowable number of groups will be sufficient such that the spectrum weighting of needed parameters will not significantly affect the results.

The proposed calculation methods described here are a compromise between the possibly more accurate and time-consuming methods of Sn^{10} and THERMOS and the less exacting methods of multigroup diffusion theory.

Difference equations are presently being derived from the equations as presented in this paper. These difference equations will be programmed and a complete computer code package for calculating the spatial spectrum in a slab or cylindrical reactor or reactor cell will be developed.

CHAPTER II

DERIVATION OF MULTIGROUP P_1 EQUATIONS

This chapter will be concerned with deriving the spherical harmonics P_1 equations from the Boltzmann transport equation. Specialization will be made to slab geometry and only slowing down transfer will be concerned. Complete details of modifying the differential scattering cross section to a form suitable for computational purposes will be given.

I. BOLTZMANN TRANSPORT EQUATION FOR FAST ENERGY RANGE

The time independent, energy dependent Boltzmann transport equation is a balance equation giving an accounting between number of particles leaving and entering a given increment of space and energy range. This equation as given by Weinberg¹¹ is

$$\begin{aligned} & \underline{\Omega} \cdot \text{grad} \phi(E, \underline{\Omega}, \underline{r}) + \Sigma_t(E, \underline{r}) \phi(E, \underline{\Omega}, \underline{r}) \\ &= \int_{\underline{\Omega}'} \int_{E'} \Sigma_s(E' \rightarrow E, \underline{\Omega}' \rightarrow \underline{\Omega}) \phi(E', \underline{\Omega}', \underline{r}) dE' d\underline{\Omega}' + S(E, \underline{\Omega}, \underline{r}). \end{aligned} \quad (\text{II.a})$$

Here $\phi(E, \underline{\Omega}, \underline{r})$ is the angular neutron flux function, E is the energy, $\underline{\Omega}$ is a unit vector giving direction of neutron velocity and $\underline{r}$ is the spatial coordinate. When each term of this equation is multiplied by an infinitesimal volume of phase space, $d\underline{r}dEd\underline{\Omega}$, physical significance can be easily associated with each term. The first term gives the leakage rate out of volume element $d\underline{r}$, in energy range E to $E + dE$ and in solid angle $d\underline{\Omega}$ around direction $\underline{\Omega}$. The second term gives the scattering and absorptions in $d\underline{r}$ that remove neutrons from energy range

E to $E + dE$ and solid angle $d\Omega$ around Ω . The first term on the right of equation (II.a) gives the rate neutrons are scattered into dr , energy range E to $E + dE$, solid angle $d\Omega$ around Ω , from higher energies E' and direction Ω' . The last term is a source into volume dr , energy range E to $E + dE$, and solid angle $d\Omega$ around the direction Ω . This includes all sources other than the elastic scattering-in source which is contained in the first term on the right of equation (II.a). This would include fission, n-2n, and inelastic slowing down sources. $\Sigma_t(E, r)$ is the total macroscopic cross section which for a mixture of isotopes is the sum of the macroscopic absorption and scattering cross sections for all elements. $\Sigma_s(E' \rightarrow E, \Omega' \rightarrow \Omega)$ is the differential scattering cross section for scattering from an energy E' , direction Ω' , to an energy E and direction Ω . Again for a mixture of scattering moderators an integral term for each isotope would have to be included on the right of equation (II.a).

II. FAST SCATTERING MECHANICS

The differential cross section for slowing down $\Sigma_s(E' \rightarrow E, \Omega' \rightarrow \Omega)$ can be written as $\Sigma_s(E \rightarrow E, \mu_0)$ where $\mu_0 = \Omega' \cdot \Omega = \cos \theta_0$ and θ_0 is laboratory angle between unit vectors Ω' and Ω . The assumption is made that the elastic scattering is only dependent on the angle through which the neutron is scattered and on energies E' and E.

Certain relations are now needed between angle θ_0 in laboratory system, and ϕ_c in center of mass system and the energy change on collision. For elastic, high energy slowing down scattering there is a unique relationship between angle of scattering and energy change. These relationships can be derived from consideration of conservation of energy

and momentum and as given in Persiani¹² are

$$\mu_o = \cos \theta_o = \frac{(A+1)}{2} \left(\frac{E}{E'} \right)^{\frac{1}{2}} - \frac{(A-1)}{2} \left(\frac{E'}{E} \right)^{\frac{1}{2}} \quad (\text{II.b})$$

$$\mu_c = \cos \phi_c = 1 - \frac{(A+1)^2}{2A} \left(1 - \frac{E}{E'} \right) \quad (\text{II.c})$$

$$\mu_o = \frac{1+A\mu_c}{(1+2A\mu_c+A^2)^{\frac{1}{2}}} \quad (\text{II.d})$$

where E' is energy before collision and E is energy after collision.

In deriving a relationship for the differential scattering cross section which is useful for calculation purposes an expansion is made in Legendre polynomials as follows:

$$\Sigma_s(E' \rightarrow E, \mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} S_{\ell}(E' \rightarrow E) P_{\ell}(\mu_o). \quad (\text{II.e})$$

The expansion coefficients are obtained in the usual manner by multiplying (II.e) by $P_m(\mu_o) d\Omega$ and integrating over Ω yielding

$$S_{\ell}(E' \rightarrow E) = 2\pi \int_{-1}^1 \Sigma_s(E' \rightarrow E, \mu_o) P_{\ell}(\mu_o) d\mu_o. \quad (\text{II.f})$$

The well-known orthogonality property of Legendre polynomials is used in this derivation. Now there is a fixed relationship between the cosine of the angle in the center of mass system and the energy change. This relationship is given in equation (II.c) and can be written as

$$E' - E = \frac{2AE'}{(A+1)^2} (1 - \mu_c). \quad (\text{II.g})$$

As Weinberg¹⁹ has done this energy-angle condition is written as a Dirac delta function in the differential cross section

$$\Sigma_s(E' \rightarrow E, \mu_o) = \Sigma_s(E', \mu_o) \delta \left[E - E' + \frac{2AE'}{(A+1)^2} (1 - \mu_c) \right]. \quad (\text{II.h})$$

It has been found that experimentally the elastic cross sections for many elements other than hydrogen are not spherically symmetric in the center of mass system for neutron energies above 100 Kev but there is a strong forward bias. Therefore, it is convenient to equate the cross section in the laboratory system, $\Sigma_s(E', \mu_o) d\mu_o$, to the cross section in the center of mass system, $\Sigma_s(E', \mu_c) d\mu_c$, and then expand the center of mass system cross section in Legendre polynomials as follows:

$$\Sigma_s(E', \mu_o) d\mu_o = \Sigma_s(E', \mu_c) d\mu_c \quad (\text{II.i})$$

$$\Sigma_s(E', \mu_c) = \Sigma_s(E') \sum_{\ell'=0}^{\infty} \frac{2\ell'+1}{4\pi} f_{\ell'}(E') P_{\ell'}(\mu_c) \quad (\text{II.j})$$

The expansion is made in this form because quite an extensive set of $f_{\ell'}(E')$ have been compiled for most moderators of interest by Joanou¹³, et al. Also, for spherically symmetric scattering in the center of mass system, $f_{\ell'}(E') = 0$ for $\ell' > 0$ and $f_0(E') = 1$ always. Here $f_1(E')$ would be the average cosine of scattering angle in center of mass system. By substituting (II.j) in (II.i) the equation for the laboratory cross section becomes

$$\Sigma_s(E', \mu_o) = \frac{d\mu_c}{d\mu_o} \Sigma_s(E') \sum_{\ell'=0}^{\infty} \frac{2\ell'+1}{4\pi} f_{\ell'}(E') P_{\ell'}(\mu_c). \quad (\text{II.k})$$

Substituting (II.k) in (II.h) and then (II.h) in (II.f) the expansion coefficients are found to be

$$S_{\ell}(E' \rightarrow E) = \sum_{\ell'=0}^{\infty} \frac{(2\ell'+1)}{2} \Sigma_S(E') f_{\ell'}(E') \int_{-1}^1 P_{\ell'}(\mu_c) P_{\ell}(\mu_o) \delta\left(E-E'+\frac{2AE'}{(A+1)^2}(1-\mu_c)\right) d\mu_c. \quad (\text{II.l})$$

By making a change of variable as is done in Persiani¹² the above integral can be evaluated. With

$$\xi = -\frac{2AE'}{(A+1)^2} (1-\mu_c) \quad (\text{II.m})$$

and

$$d\xi = \frac{2AE'}{(A+1)^2} d\mu_c \quad (\text{II.n})$$

$$S_{\ell}(E' \rightarrow E) = \sum_{\ell'=0}^{\infty} \frac{(2\ell'+1)}{2} \Sigma_S(E') f_{\ell'}(E') \frac{(A+1)^2}{2AE'} \int P_{\ell'}(\mu_c) P_{\ell}(\mu_o) \delta(E-E'-\xi) d\xi. \quad (\text{II.o})$$

From the property of Dirac delta function the expansion coefficients become

$$S_{\ell}(E' \rightarrow E) = \sum_{\ell'=0}^{\infty} \frac{(2\ell'+1)}{2} \Sigma_S(E') f_{\ell'}(E') \frac{(A+1)^2}{2AE'} P_{\ell'}(\mu_c^*) P_{\ell}(\mu_o^*) \quad (\text{II.p})$$

Here μ_c^* and μ_o^* are functions of E and E' as given in equation (II.b)

and (II.c).

Now $\alpha E'$ is the maximum energy change in collision, where

$$\alpha = \left(\frac{A-1}{A+1} \right)^2.$$

This can be seen from equation (II.c) where for a head-on collision $\mu_c = -1$ and solving for $\frac{E}{E'}$ one obtains

$$\frac{E}{E'} = 1 - \frac{4A}{(A+1)^2} = \left(\frac{A-1}{A+1} \right)^2 = \alpha. \quad (\text{II.q})$$

Thus the expansion coefficients can be written as

$$S_{\ell}(E' \rightarrow E) = \frac{\Sigma_s(E')}{(1-\alpha)E'} P_{\ell}(\mu_c^*) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*). \quad (\text{II.r})$$

Finally, when one substitutes this in equation (II.e), the following expression is obtained for the differential cross section:

$$\Sigma_s(E' \rightarrow E, \mu_o) = \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{4\pi} \frac{\Sigma_s(E') P_{\ell}(\mu_o^*) P_{\ell}(\mu_o)}{(1-\alpha)E'} \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*). \quad (\text{II.s})$$

This expression for the differential scattering cross section is then substituted in equation (II.a) to give

$$\begin{aligned} \underline{\Omega} \cdot \nabla \Phi(E, \underline{\Omega}, \underline{r}) + \Sigma_t(E, \underline{r}) \Phi(E, \underline{\Omega}, \underline{r}) &= S(E, \underline{\Omega}, \underline{r}) + \\ \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi(1-\alpha)} \int \int_{\Omega' E'} \Sigma_s(E') P_{\ell}(\mu_o^*) P_{\ell}(\mu_o) \Phi(E', \underline{\Omega}', \underline{r}) &\sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} d\Omega'. \end{aligned} \quad (\text{II.t})$$

III. BOLTZMANN TRANSPORT EQUATION IN SLAB GEOMETRY

The simplest useful spherical harmonic case is that of slab geometry in the P_1 approximation. The Boltzmann transport equation as given in equation (II.t) is now modified to the slab geometry case first by multiplying each term in the equation by $d\phi$ and integrating over the azimuthal angle ϕ where

$$\begin{aligned} \int_0^{2\pi} \phi(E, \underline{\Omega}, \underline{r}) d\phi &= 2\pi\phi(E, \underline{\Omega}, x) = \phi(E, \mu, x) \\ \int_0^{2\pi} S(E, \underline{\Omega}, \underline{r}) d\phi &= 2\pi S(E, \underline{\Omega}, x) = S(E, \mu, x). \end{aligned} \quad (\text{II.u})$$

The angular flux function in slab geometry is in this case a function of the spatial coordinate x and μ where μ is the cosine of the angle between the x axis and the direction of the neutron velocity.

The first term or leakage term in the Boltzmann transport equation²⁰ is transformed as

$$\int_0^{2\pi} \Omega \cdot \nabla \phi(E, \underline{\Omega}, \underline{r}) d\phi = \mu \frac{\partial \phi}{\partial x}(E, \mu, x). \quad (\text{II.v})$$

The addition theorem for Legendre functions¹⁴ is used to write

$$P_\ell(\mu_0) = P_\ell(\mu)P_\ell(\mu') + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_\ell^m(\mu)P_\ell^m(\mu') \cos m(\phi-\phi'). \quad (\text{II.w})$$

Using (II.u), (II.v) and (II.w) in equation (II.t) yields

$$\begin{aligned} \mu \frac{\partial \phi}{\partial x}(E, \mu, x) + \Sigma_t(E, x) \phi(E, \mu, x) &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi(1-\alpha)} \int_{\phi} \int_{\mu'} \int_{\phi'} \int_{E'} \Sigma_s(E') P_{\ell}(\mu_0^*) \cdot \\ &\left[P_{\ell}(\mu) P_{\ell}(\mu') + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} P_{\ell}^m(\mu) P_{\ell}^m(\mu') \cos m(\phi - \phi') \right] \phi(E', \underline{\Omega}', x) \cdot \\ &\sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} d\phi' d\mu' d\phi + S(E, \mu, x) \end{aligned} \quad (II.x)$$

The scattering-in term on the right of (II.x) can now be integrated over ϕ and ϕ' . The first integration drops out the sum over m because

$$\int_0^{2\pi} \cos m(\phi - \phi') d\phi = 0 \text{ for } m \text{ an integer.} \quad \text{The integration}$$

over ϕ brings in a factor of 2π and the integration over ϕ' gives

$$\int_0^{2\pi} \phi(E', \underline{\Omega}', x) d\phi' = 2\pi \phi(E, \underline{\Omega}', x) = \phi(E', \mu', x).$$

Thus the following Boltzmann transport equation for the slab geometry case results:

$$\begin{aligned} \mu \frac{\partial \phi}{\partial x}(E, \mu, x) + \Sigma_t(E, x) \phi(E, \mu, x) &= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2(1-\alpha)} \int_{\mu'} \int_{E'} \Sigma_s(E') P_{\ell}(\mu_0^*) \cdot \\ &P_{\ell}(\mu) P_{\ell}(\mu') \phi(E', \mu', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} d\mu' + S(E, \mu, x). \end{aligned} \quad (II.y)$$

IV. DERIVATION OF P_1 EQUATIONS IN SLAB GEOMETRY

The angular flux function and source function are now expanded in full range Legendre polynomials with

$$\phi(E, \mu, x) = \sum_{k=0}^{\infty} \frac{2k+1}{2} \phi_k(E, x) P_k(\mu) \quad (\text{II.z})$$

and

$$S(E, \mu, x) = \sum_{k=0}^{\infty} \frac{2k+1}{2} S_k(E, x) P_k(\mu) \quad (\text{II.a'})$$

where

$$\phi_k(E, x) = \int_{-1}^1 \phi(E, \mu, x) P_k(\mu) d\mu \quad \text{and} \quad S_k(E, x) = \int_{-1}^1 S(E, \mu, x) P_k(\mu) d\mu. \quad (\text{II.b'})$$

When (II.z) and (II.a') are substituted in (II.y) and the first term on the right integrated over μ' the result is

$$\begin{aligned} & \sum_{k=0}^{\infty} \frac{2k+1}{2} \mu P_k(\mu) \frac{\partial \phi_k(E, x)}{\partial x} + \Sigma_t(E, x) \sum_{k=0}^{\infty} \frac{2k+1}{2} \phi_k(E, x) P_k(\mu) \\ &= \sum_{k=0}^{\infty} \frac{2k+1}{2(1-\alpha)} \int_E^{\frac{E}{\alpha}} \Sigma_0(E') P_k(\mu_0^*) P_k(\mu) \phi_k(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_0^*) \frac{dE'}{E'} \\ & \quad + \sum_{k=0}^{\infty} \frac{2k+1}{2} S_k(E, x) P_k(\mu). \end{aligned} \quad (\text{II.c'})$$

Definite limits have been placed on the integral over E' . Equation (II.q) states that the maximum value of E' is $\frac{E}{\alpha}$ and for down-scattering

the minimum value of E' is E , ie., no energy loss on collision.

The P_1 equations are derived from (II.c') by multiplying first by $P_0(\mu)d\mu$ and integrating each term over μ and then by $P_1(\mu)d\mu$ and again integrating over μ . Using the orthogonality property of Legendre polynomials which is

$$\int_{-1}^1 P_\ell(\mu)P_m(\mu)d\mu = \frac{2}{2\ell+1} \delta_{\ell m}$$

where δ is Kronecker's delta defined as

$$\begin{aligned} \delta_{\ell m} &= 1 & \ell &= m \\ \delta_{\ell m} &= 0 & \ell &\neq m \end{aligned}$$

and

$$\mu P_1(\mu) = \mu^2 = \frac{2}{3}P_2(\mu) + \frac{1}{3}P_0(\mu),$$

one obtains the following pair of P_1 equations in slab geometry:

$$\begin{aligned} \frac{\partial \phi_1(E, x)}{\partial x} + \Sigma_t(E, x)\phi_0(E, x) &= \frac{1}{1-\alpha} \int_E^{\frac{E}{\alpha}} \Sigma_s(E')\phi_0(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1)f_{\ell'}(E') \cdot \\ &\quad P_{\ell'}(\mu_c^*) \frac{dE'}{E'} + S_0(E, x) \end{aligned} \quad (\text{II.d'})$$

$$\begin{aligned} \frac{1}{3} \frac{\partial \phi_0(E, x)}{\partial x} + \Sigma_t(E, x)\phi_1(E, x) &= \frac{1}{1-\alpha} \int_E^{\frac{E}{\alpha}} \Sigma_s(E')\mu_c^* \phi_1(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1)f_{\ell'}(E') \cdot \\ &\quad P_{\ell'}(\mu_c^*) \frac{dE'}{E'} + S_1(E, x). \end{aligned} \quad (\text{II.e'})$$

From (II.b'), ϕ_0 is the angular flux function integrated over μ or the total isotropic flux while ϕ_1 is the net current. Normally in most studies the source, $S(E, \mu, x)$ is assumed to be isotropic. This is assumed to be the case for neutrons coming from fission, n-2n reaction and inelastic scattering. Under these assumptions

$$S_\ell(E, x) = 0 \text{ for } \ell > 0.$$

V. MULTIGROUP P_1 EQUATIONS

The total energy range is now considered to be divided up into groups with upper and lower limits such that for group j

$$E_j \leq E \leq E_{j-1}.$$

Integrating (II.d') over energy group j yields

$$\begin{aligned} \frac{\partial}{\partial x} \int_{E_j}^{E_{j-1}} \phi_1(E, x) dE + \int_{E_j}^{E_{j-1}} \Sigma_t(E, x) \phi_0(E, x) dE &= \frac{1}{1-\alpha} \int_{E_j}^{E_{j-1}} \int_E^{\frac{E}{\alpha}} \Sigma_s(E') \phi_0(E', x) dE' \\ \sum_{\ell=0}^{\infty} (2\ell+1) f_{\ell,1}(E') P_{\ell,1}(\mu_c^*) \frac{dE' dE}{E} &+ \int_{E_j}^{E_{j-1}} \frac{X(E) dE}{\lambda} \int_0^{\infty} \nu \Sigma_f(E') \phi_0(E', x) dE' + \int_{E_j}^{E_{j-1}} S_0(E, x) dE. \end{aligned}$$

(II.f')

An explicit fission source term has been introduced in this equation. The integral factor in this term over E' gives the total fast neutrons produced by fission per cc per sec. $X(E)dE$ is the fraction of those neutrons that come out from fission with energy from E to $E + dE$ and λ

is an eigenvalue introduced to arrive at a solution to the final difference equations.

Using the formulas

$$\int_{E_j}^{E^{j-1}} \phi_1(E, x) dE = \phi_1^j(x), \quad \int_{E_j}^{E^{j-1}} \Sigma_t(E, x) \phi_0(E, x) dE = \Sigma_t^j(x) \phi_0^j(x)$$

and

$$\int_{E_j}^{E^{j-1}} \frac{X(E) dE}{\lambda} \int_0^\infty \nu \Sigma_f(E') \phi_0(E', x) dE' = \frac{X^j}{\lambda} \sum_{t=1}^N \nu \Sigma_f^t \phi_0^t(x)$$

and equating the scattering-down term to a sum for $i=1$ to $i=j$ of transfer cross sections times the isotropic flux function as follows:

$$\begin{aligned} \frac{1}{1-\alpha} \int_{E_j}^{E^{j-1}} \sum_{i=1}^j \int_{E_i}^{E^{i-1}} \Sigma_s(E') \phi_0(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} dE \\ = \sum_{i=1}^j \sum_{i \rightarrow j}^0 \Sigma(x) \phi_0^i(x) \end{aligned}$$

one finds that the multigroup neutron balance equation is

$$\frac{d\phi_1^j(x)}{dx} + \Sigma_t^j(x) \phi_0^j(x) = \sum_{i=1}^j \sum_{i \rightarrow j}^0 \Sigma(x) \phi_0^i(x) + \frac{X^j}{\lambda} \sum_{t=1}^N \nu \Sigma_f^t \phi_0^t(x) + S_0^j(x). \quad (\text{II.g'})$$

In an analogous manner (II.e') is multiplied by dE and integrated over energy group j to yield

$$\frac{1}{3} \frac{d\phi_0^j(x)}{dx} + \Sigma_t^j(x) \phi_1^j(x) = \sum_{i=1}^j \sum_{i \rightarrow j}^1 \Sigma(x) \phi_1^i(x) \quad (\text{II.h'})$$

where

$$\Sigma_{i \rightarrow j}(x) = \frac{\frac{1}{1-\alpha} \int_{E_j}^{E_{j-1}} \int_{E_i}^{E_{i-1}} \Sigma_s(E') \mu_{o1}^* \phi_1(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} dE}{\int_{E_i}^{E_{i-1}} \phi_1(E', x) dE'} \quad (\text{II.i'})$$

Further details of the limits and the method of computing the group to group transfer cross sections for the fast energy groups are contained in the Appendix.

The basic P_1 multigroup equations for the fast groups in slab geometry are (II.g') and (II.h') above. If, in the sum on the right of (II.h'), all terms are omitted except the $i=j$ term, then Fick's law results for each energy group j . Fick's law states that $\underline{J} = -D \nabla \phi$ where the net current is $\underline{J}$ and the isotropic flux is ϕ . Therefore, (II.h') can be written as

$$\phi_1^j(x) = - \frac{1}{3(\Sigma_t^j - \Sigma_{j \rightarrow j}^j)} \frac{d\phi_o^j}{dx} = -D^j \nabla \phi_o^j(x). \quad (\text{II.j'})$$

When (II.j') is substituted into (II.g'), the general multigroup diffusion equation results

$$\nabla \cdot D^j \nabla \phi_o^j(x) + \Sigma_t^j(x) \phi_o^j(x) = \sum_{i=1}^j \Sigma_{i \rightarrow j}^i(x) \phi_o^i(x) + \frac{X^j}{\lambda} \sum_{t=1}^N \nu \Sigma_f^t \phi_o^t(x) + S_o^j(x). \quad (\text{II.k'})$$

Here $j = 1, 2, \dots, N$ with N as the total number of groups.

Thus the P_1 multigroup equations (II.g') and (II.h') with the sum over j retained on the right of (II.h') are better approximations to the Boltzmann transport equation than the multigroup diffusion equation, (II.k'). Only for the first group of a multigroup scheme is Fick's law valid because only the one, in-group scattering term, ($i=j$), would exist in the sum on the right of (II.h').

CHAPTER III

DERIVATION OF THE MULTIGROUP DOUBLE P_1 EQUATIONS

In the thermal energy range wide variations in the nuclear properties (scattering and absorption cross sections) between regions may be present in a reactor and then the angular flux function may not be adequately represented by a two term expansion in full range Legendre polynomials. A much improved approximation in slab geometry results if the expansion is made in half-range Legendre polynomials⁷. This type of expansion allows for a discontinuity in the angular distribution about $\mu = 0$ for a boundary between different materials in the lowest approximation. Weinberg²¹ states that this method is much to be preferred in many physical cases of interest such as a strongly absorbing fuel plate embedded in a lightly absorbing moderator.

I. BOLTZMANN TRANSPORT EQUATION FOR THERMAL ENERGY RANGE

The Boltzmann transport equation, (II.a) for the thermal groups, is now modified to include two scattering-in sources. One of these sources is from scattering collisions above some thermal cut-off energy, E_c which puts neutrons into the thermal groups. The other source is from up and down scattering collisions in the thermal range. There are not any direct fission, inelastic, or n-2n source contributions into the thermal range. However, for generality and comparison studies a fixed source will be allowed. The basic Boltzmann transport equation for the

thermal range is

$$\begin{aligned} \underline{\Omega} \cdot \nabla \phi(E, \underline{\Omega}, \underline{r}) + \Sigma_t(E, \underline{r}) \phi(E, \underline{\Omega}, \underline{r}) = & \int \int_{\underline{\Omega}' \atop E_c}^{\underline{\Omega} \atop E_c} \Sigma_s(E' \rightarrow E, \mu_o) \phi(E', \underline{\Omega}', \underline{r}) dE' d\underline{\Omega}' \\ & + \int \int_{\underline{\Omega}' \atop 0}^{E_c \atop E_c} \Sigma_s(E' \rightarrow E, \mu_o) \phi(E', \underline{\Omega}', \underline{r}) dE' d\underline{\Omega}' + S(E, \underline{\Omega}, \underline{r}). \quad (\text{III.a}) \end{aligned}$$

In the fast range above thermal with $E' \geq E_c$ the differential cross section in the first term on the right of (III.a) is again expanded in spherical harmonics exactly as was done in Chapter II. The differential cross section in the thermal range contained in the second term on right of (III.a) is also expanded in Legendre polynomials giving

$$\Sigma_s(E' \rightarrow E, \mu_o) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} S_{\ell}^{\text{th}}(E' \rightarrow E) P_{\ell}(\mu_o). \quad (\text{III.b})$$

The th superscript on S_{ℓ} is used to indicate that this expansion is made in the thermal range to differentiate from the S_{ℓ} without superscript used in Chapter II. There is no unique simple energy-angle condition such as exists for the fast range. Thus an explicit expression such as (II.r) cannot be derived for the thermal scattering expansion coefficients. However, recent developments in neutron scattering theory which take account of the thermal motions of the moderator atoms, and the binding of the atoms to each other, make it possible to calculate the expansion coefficients in the equations derived here^{15, 16, 17}.

The addition theorem for Legendre polynomials is again used in (III.b) and (III.b) is then substituted in the second term on the right of (III.a). Equation (III.a) is then multiplied through by $d\phi$ and each term is integrated over ϕ . Again this drops out the sum over m in the

addition theorem. The integration over ϕ' in the thermal scattering-in integral is now performed finally yielding an equation analogous to (II.y) but with an additional term for the thermal up and down scattering. The final Boltzmann transport equation in the thermal energy range for slab geometry is

$$\begin{aligned} \mu \frac{\partial \phi(E, \mu, x)}{\partial x} + \Sigma_t(E, x) \phi(E, \mu, x) = & \sum_{\ell=0}^{\infty} \frac{(2\ell+1)P_{\ell}(\mu)}{2(1-\alpha)} \int_{-1}^1 \int_{E_c}^{E_c} \Sigma_0(E') P_{\ell}(\mu_c^*) P_{\ell}(\mu') \phi(E', \mu', x) \cdot \\ & \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} d\mu' + \sum_{\ell=0}^{\infty} \frac{(2\ell+1)}{2} P_{\ell}(\mu) \int_{-1}^1 \int_0^E S_{\ell}^{th}(E' \rightarrow E) P_{\ell}(\mu') \cdot \\ & \phi(E', \mu', x) d\mu' dE' + S(E, \mu, x). \end{aligned} \quad (\text{III.c})$$

II. DERIVATION OF DOUBLE P_1 EQUATIONS IN SLAB GEOMETRY

The angular flux function in (III.c) is now expanded in half range Legendre polynomials as follows:

$$\begin{aligned} \phi(E, \mu, x) = & \sum_{\ell=0}^{\infty} (2\ell+1) \psi_{\ell}(E, x) P_{\ell}(2\mu-1) \quad 0 \leq \mu \leq 1 \\ = & \sum_{\ell=0}^{\infty} (2\ell+1) \omega_{\ell}(E, x) P_{\ell}(2\mu+1) \quad -1 \leq \mu \leq 0 \end{aligned} \quad (\text{III.d})$$

For the double P_1 approximation

$$\psi_\ell(E, x) = \omega_\ell(E, x) = 0 \text{ for } \ell > 1.$$

The expansion coefficients are

$$\begin{aligned}\psi_\ell(E, x) &= \int_0^1 \Phi(E, \mu, x) P_\ell(2\mu-1) d\mu \\ \omega_\ell(E, x) &= \int_{-1}^0 \Phi(E, \mu, x) P_\ell(2\mu+1) d\mu.\end{aligned}\tag{III.e}$$

The source function is also expanded in a similar manner

$$\begin{aligned}S(E, \mu, x) &= \sum_{\ell=0}^{\infty} (2\ell+1) T_\ell(E, x) P_\ell(2\mu-1) \quad 0 \leq \mu \leq 1 \\ &= \sum_{\ell=0}^{\infty} (2\ell+1) R_\ell(E, x) P_\ell(2\mu+1) \quad -1 \leq \mu \leq 0.\end{aligned}\tag{III.f}$$

Expansions as given by (III.d) and (III.f) are now substituted in (III.c) and this equation is successively multiplied by $P_0(2\mu-1)d\mu$, $P_1(2\mu-1)d\mu$, $P_0(2\mu+1)d\mu$ and $P_1(2\mu+1)d\mu$ and integrated over the appropriate limits. That is, when the argument of the Legendre polynomial is $2\mu-1$, and $2\mu+1$, the integration is performed from zero to one, and from minus one to zero, respectively. The integrations are elementary and details for a monoenergetic thermal group are given in reference 8. The total isotropic flux and the current are defined in terms of the half range moments as

$$\phi_0(E, x) = \int_{-1}^1 \phi(E, \mu, x) P_0(\mu) d\mu = \psi_0(E, x) + \omega_0(E, x) \quad (\text{III.g})$$

$$\phi_1(E, x) = \int_{-1}^1 \phi(E, \mu, x) P_1(\mu) d\mu = \frac{1}{2} \left[\psi_0(E, x) - \omega_0(E, x) \right] + \frac{1}{2} \left[\psi_1(E, x) + \omega_1(E, x) \right]. \quad (\text{III.i})$$

This form for the current, $\phi_1(E, x)$, is obtained by breaking the integration into two parts, defining μ as

$$\mu = \frac{1}{2} P_1(2\mu+1) - \frac{1}{2} P_0(2\mu-1) \text{ for } -1 \leq \mu \leq 0$$

and

$$\mu = \frac{1}{2} P_1(2\mu-1) + \frac{1}{2} P_2(2\mu-1) \text{ for } 0 \leq \mu \leq 1$$

and then use the expansion coefficients as given in (III.e).

Using the total isotropic flux and net current definitions (III.g) and (III.i), one obtains the first double P_1 equation by multiplying (III.c) by $P_0(2\mu-1)d\mu$ and integrating between appropriate limits to yield

$$\begin{aligned} \frac{\partial \psi_0(E, x)}{\partial x} + \frac{\partial \psi_1(E, x)}{\partial x} + 2\Sigma_t(E, x)\psi_0(E, x) &= \frac{1}{1-\alpha} \int_{E_s}^{\frac{E_c}{\alpha}} \Sigma_s(E') \phi_0(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) \cdot \\ & f_{\ell', \ell}(E') P_{\ell', \ell}(\mu_c^*) \frac{dE'}{E'} + \frac{3}{2(1-\alpha)} \int_{E_s}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_1(\mu_c^*) \phi_1(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell', \ell}(E') P_{\ell', \ell}(\mu_c^*) \frac{dE'}{E'} \\ & + \int_0^{E_c} S_0^{th}(E' \rightarrow E) \phi_0(E', x) dE' + \frac{3}{2} \int_0^{E_c} S_1^{th}(E' \rightarrow E) \phi_1(E', x) dE' + 2T_0(E, x). \quad (\text{III.j}) \end{aligned}$$

Only terms for $\ell = 0$ and $\ell = 1$ for the scattering-in integrals on the right of (III.c) have been included in (III.j).

Now by defining

$$A_0(E, x) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') \phi_0(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'}$$

$$A_1(E, x) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_1(\mu_c^*) \phi_1(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'}$$

$$B_0(E, x) = \int_0^E S_0^{th}(E' \rightarrow E) \phi_0(E', x) dE'$$

$$B_1(E, x) = \int_0^E S_1^{th}(E' \rightarrow E) \phi_1(E', x) dE'$$

(III.j) can be written as

$$\begin{aligned} \frac{\partial \psi_0(E, x)}{\partial \psi} + \frac{\partial \psi_1(E, x)}{\partial \psi} + 2\Sigma_t(E, x) \psi_0(E, x) &= A_0(E, x) + B_0(E, x) \\ &+ \frac{3}{2} A_1(E, x) + \frac{3}{2} B_1(E, x) + 2T_0(E, x). \end{aligned} \quad (III.k)$$

The remaining three equations obtained by multiplying successively by $P_1(2\mu-1)d\mu$, $P_0(2\mu+1)d\mu$, $P_1(2\mu+1)d\mu$ and integrating over respective half range limits on μ are

$$\frac{1}{3} \frac{\partial \psi_0(E, x)}{\partial x} + \frac{\partial \psi_1(E, x)}{\partial x} + 2\Sigma_t(E, x) \psi_1(E, x) = \frac{1}{2} \left[A_1(E, x) + B_1(E, x) \right] + 2T_1(E, x). \quad (III.l)$$

$$\begin{aligned} \frac{\partial \omega_1(E, x)}{\partial x} - \frac{\partial \omega_0(E, x)}{\partial x} + 2\Sigma_t(E, x)\omega_0(E, x) &= A_0(E, x) + B_0(E, x) \\ &+ \frac{3}{2} \left[A_1(E, x) + B_1(E, x) \right] + 2R_0(E, x). \end{aligned} \quad (\text{III.m})$$

$$\begin{aligned} \frac{1}{3} \frac{\partial \omega_0(E, x)}{\partial x} - \frac{\partial \omega_1(E, x)}{\partial x} + 2\Sigma_t(E, x)\omega_1(E, x) &= \frac{1}{2} \left[A_1(E, x) + B_1(E, x) \right] \\ &+ 2R_1(E, x). \end{aligned} \quad (\text{III.n})$$

III. MULTIGROUP DOUBLE P_1 EQUATIONS

The multigroup double P_1 equations for energy group j are derived from (III.k) to (III.n) by multiplying each term by dE and integrating over energy range E_{j-1} to E_j .

The scattering integrals on the right side of each equation are replaced by sums of transfer cross section from group to group multiplied by appropriate expansion coefficients and the final equations are

$$\begin{aligned} \frac{d\psi_0^j(x)}{dx} + \frac{d\psi_1^j(x)}{dx} + 2\Sigma_t^j(x)\psi_0^j(x) &= \sum_{i=1}^{N_{th}-1} \Sigma_0^i(x) \phi_0^i(x) + \frac{3}{2} \sum_{i=1}^{N_{th}-1} \Sigma_1^i(x) \phi_1^i(x) \\ &+ \sum_{i=N_{th}}^N \Sigma_0^i(x) \phi_0^i(x) + \frac{3}{2} \sum_{i=N_{th}}^N \Sigma_1^i(x) \phi_1^i(x) + 2T_0^j(x). \end{aligned} \quad (\text{III.o})$$

$$\begin{aligned} \frac{1}{3} \frac{d\psi_0^j(x)}{dx} + \frac{d\psi_1^j(x)}{dx} + 2\Sigma_t^j(x)\psi_1^j(x) &= \frac{1}{2} \sum_{i=1}^{N_{th}-1} \Sigma_1^i(x) \phi_1^i(x) \\ &+ \frac{1}{2} \sum_{i=N_{th}}^N \Sigma_1^i(x) \phi_1^i(x) + 2T_1^j(x). \end{aligned} \quad \text{III.p)}$$

$$\begin{aligned}
\frac{d\omega_1^j(x)}{dx} - \frac{d\omega_0^j(x)}{dx} + 2\Sigma_t^j(x)\omega_0^j(x) &= \sum_{i=1}^{N_{th}-1} \Sigma_0(x)\phi_0^i(x) - \frac{3}{2} \sum_{i=1}^{N_{th}-1} \Sigma_1(x)\phi_1^i(x) \\
&+ \sum_{i=N_{th}}^N \Sigma_0^*(x)\phi_0^i(x) - \frac{3}{2} \sum_{i=N_{th}}^N \Sigma_1^*(x)\phi_1^i(x) + 2R_0^j(x) \quad (III.q)
\end{aligned}$$

$$\begin{aligned}
\frac{1}{3} \frac{d\omega_0^j(x)}{dx} - \frac{d\omega_1^j(x)}{dx} + 2\Sigma_t^j(x)\omega_1^j(x) &= \frac{1}{2} \sum_{i=1}^{N_{th}-1} \Sigma_1(x)\phi_1^i(x) + \frac{1}{2} \sum_{i=N_{th}}^N \Sigma_1^*(x)\phi_1^i(x) \\
&+ 2R_1^j(x). \quad (III.r)
\end{aligned}$$

The group to group transfer cross section are

$$\Sigma_{i \rightarrow j}^{\ell}(x) = \frac{\frac{1}{1-\alpha} \int_{E_j}^{E_{j-1}} \int_{E_i}^{E_{i-1}} \Sigma_s(E') P_{\ell}(\mu_0^*) \phi_{\ell}(E', x) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} dE}{\int_{E_i}^{E_{i-1}} \phi_{\ell}(E', x) dE'} \quad (III.s)$$

$$\Sigma_{i \rightarrow j}^{\ell*}(x) = \frac{\int_{E_j}^{E_{j-1}} \int_{E_i}^{E_{i-1}} S_{\ell}^{th}(E \rightarrow E') \phi_{\ell}(E', x) dE' dE}{\int_{E_i}^{E_{i-1}} \phi_{\ell}(E', x) dE'} \quad (III.t)$$

The double P_1 approximations to the full range moments ϕ_2 and ϕ_3 are needed to put the four equations above into a set of standard P_3 spherical harmonics equations with modified coefficients. Complete details of

relating ϕ_2 and ϕ_3 to the half-range moments are given in reference 8.

The final results are

$$\phi_2^*(E, x) = \frac{3}{4} \left[\psi_1(E, x) - \omega_1(E, x) \right]$$

and

$$\phi_3^*(E, x) = \frac{1}{8} \left[\omega_0(E, x) - \psi_0(E, x) \right] + \frac{3}{8} \left[\omega_1(E, x) + \psi_1(E, x) \right]. \quad (\text{III.u})$$

An asterisk is placed on ϕ_2 and ϕ_3 to indicate that these are only approximations to the full range moments. The exact full range moments ϕ_2 and ϕ_3 contain terms in $\psi_\ell(E, x)$ and $\omega_\ell(E, x)$ with $\ell > 1$ but these terms are set equal to zero for the double P_1 approximation.

If important, higher order terms than the $\ell = 1$ can be retained in the integrals on the right of (III.c). The fixed source term, $S(E, \underline{Q}, \underline{r})$, is normally assumed as constant and isotropic in a region.

Retaining terms of order $\ell = 2$ and $\ell = 3$ in addition to the $\ell = 0$ and $\ell = 1$ terms, setting the fixed source equal to $\frac{S_0}{2}$ and using (III.u) one obtains the following equations:

$$\begin{aligned} \frac{d\psi_0^j(x)}{dx} + \frac{d\omega_1^j(x)}{dx} + 2\Sigma_t^j(x)\psi_0^j(x) &= \sum_{i=1}^{N_{th}-1} \left[\Sigma_{i \rightarrow j}^0(x) + \frac{3}{2} \Sigma_{i \rightarrow j}^1(x) \phi_1^i \right. \\ &- \frac{7}{8} \Sigma_{i \rightarrow j}^3(x) \phi_3^{i*} \left. \right] + \sum_{i=N_{th}}^N \left[\Sigma_{i \rightarrow j}^{0*}(x) \phi_0^i(x) + \frac{3}{2} \Sigma_{i \rightarrow j}^{1*}(x) \phi_1^i(x) \right. \\ &- \frac{7}{8} \Sigma_{i \rightarrow j}^{3*}(x) \phi_3^{i*}(x) \left. \right] + S_0 \end{aligned} \quad (\text{III.v})$$

$$\begin{aligned}
\frac{1}{3} \frac{d\psi_o^j(x)}{dx} + \frac{d\psi_1^j(x)}{dx} + 2\Sigma_t^j(x)\psi_1^j(x) &= \sum_{i=1}^{N_{th}-1} \left[\frac{1}{2} \Sigma(x) \phi_1^i(x) + \frac{5}{4} \Sigma(x) \phi_2^{i*}(x) \right. \\
&\left. + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right] + \sum_{i=N_{th}}^N \left[\frac{1}{2} \Sigma(x) \phi_1^{i*}(x) + \frac{5}{4} \Sigma(x) \phi_2^{i*}(x) + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right]
\end{aligned}
\tag{III.w}$$

$$\begin{aligned}
\frac{d\omega_1^j(x)}{dx} - \frac{d\omega_o^j(x)}{dx} + 2\Sigma_t^j(x)\omega_o^j(x) &= \sum_{i=1}^{N_{th}-1} \left[\Sigma(x) \phi_o^i(x) - \frac{3}{2} \Sigma(x) \phi_1^i(x) \right. \\
&\left. + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right] + \sum_{i=N_{th}}^N \left[\Sigma(x) \phi_o^{i*}(x) - \frac{3}{2} \Sigma(x) \phi_1^{i*}(x) + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right] \\
&+ S_o.
\end{aligned}
\tag{III.x}$$

$$\begin{aligned}
\frac{1}{3} \frac{d\omega_o^j(x)}{dx} - \frac{d\omega_1^j(x)}{dx} + 2\Sigma_t^j(x)\omega_1^j(x) &= \sum_{i=1}^{N_{th}-1} \left[\frac{1}{2} \Sigma(x) \phi_1^i(x) - \frac{5}{4} \Sigma(x) \phi_2^{i*}(x) \right. \\
&\left. + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right] + \sum_{i=N_{th}}^N \left[\frac{1}{2} \Sigma(x) \phi_1^{i*}(x) - \frac{5}{4} \Sigma(x) \phi_2^{i*}(x) + \frac{7}{8} \Sigma(x) \phi_3^{i*}(x) \right].
\end{aligned}
\tag{III.y}$$

The procedure for slab geometry, as stated in the introduction, is to use a standard P_1 solution in the fast range with a double P_1 approximation in the thermal range. Therefore, the scattering down source terms from $i = 1$ to $i = N_{th}-1$, such as $\Sigma_{i \rightarrow j}^2 \phi_2^{i*}(x)$ and $\Sigma_{i \rightarrow j}^3 \phi_3^{i*}(x)$, would not be available. The first fast group is group 1 and the first thermal group is group N_{th} .

As was done in reference 8 various combinations of equations (III.v) through (III.y) can be taken to yield

$$\frac{d\phi_1^j(x)}{dx} + \left[\Sigma_t^j(x) - \Sigma_{j \rightarrow j}^{0*}(x) \right] \phi_0^j(x) = \sum_{i=1}^{N_{th}-1} \Sigma_{i \rightarrow j}^0(x) + \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{0*}(x) \phi_0^i(x) + 2S_0. \quad (III.z)$$

$$\begin{aligned} \frac{d\phi_0^j(x)}{dx} + 2 \frac{d\phi_2^{j*}(x)}{dx} + 3 \left[\Sigma_t^j(x) - \Sigma_{j \rightarrow j}^{1*}(x) \right] \phi_1^j(x) &= 3 \sum_{i=1}^{N_{th}-1} \Sigma_{i \rightarrow j}^1(x) \phi_1^i(x) \\ &+ 3 \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{1*}(x) \phi_1^i(x). \end{aligned} \quad (III.a')$$

$$\begin{aligned} \frac{d\phi_1^j(x)}{3dx} + 4 \frac{d\phi_3^{j*}(x)}{dx} + \left[8 \Sigma_t^j(x) - \frac{15}{2} \Sigma_{j \rightarrow j}^{2*}(x) \right] \phi_2^{j*}(x) \\ = \frac{15}{2} \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{2*}(x) \phi_2^{i*}(x). \end{aligned} \quad (III.b')$$

$$\frac{d\phi_2^{j*}(x)}{dx} + \left[6 \Sigma_t^j(x) - \frac{21}{8} \Sigma_{j \rightarrow j}^{3*}(x) \right] \phi_3^{j*}(x) = \frac{21}{8} \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{3*}(x) \phi_3^{i*}(x). \quad (III.c')$$

Equation (III.z) is obtained by adding (III.v) and (III.x) and transferring the term for $i = j$ from the right side of the equation to the left side to combine with $\Sigma_t^j(x)$. The other equations are obtained in a similar manner. Also above thermal scattering terms involving expansion

coefficients of ϕ_2^{i*} and ϕ_3^{i*} have not been included. The basic set of double P_1 equations are (III.z), (III.a'), (III b') and (III.c').

CHAPTER IV

DERIVATION OF MULTIGROUP P_3 EQUATIONS

This chapter will not consider separately, as was done previously in slab geometry, the complete details of the derivation of both the fast P_1 equations and the thermal P_3 equations. In this standard spherical harmonic method for cylindrical geometry the angular flux function for any order P_n is expanded in full range associated Legendre polynomials. Therefore, the fast range P_1 equations can be obtained from the thermal range P_3 equations, first by deleting the thermal source term for up and down scattering collisions in the thermal range, second by omitting all terms with expansion coefficients higher than one, and third by adding a fission source term. Quite complete details of the derivation of the P_3 equations in the thermal energy range will now be shown.

I. BOLTZMANN TRANSPORT EQUATION IN CYLINDRICAL GEOMETRY

If (II.t) is modified to include a source term for thermal scattering the Boltzmann transport equation is

$$\Omega \cdot \nabla \phi(E, \underline{\Omega}, \underline{r}) + \Sigma_t(E, \underline{r}) \phi(E, \underline{\Omega}, \underline{r}) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi(1-\alpha)} \int_{\underline{\Omega}'} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_{\ell}(\mu_{\Omega}^*) P_{\ell}(\mu_{\Omega}) \cdot$$

$$\phi(E', \underline{\Omega}', \underline{r}) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_{\Omega}^*) \frac{dE'}{E'} d\underline{\Omega}' + \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \int_{\underline{\Omega}'} \int_0^{E_c} S_{\ell}^{th}(E' \rightarrow E) \cdot$$

$$P_{\ell}(\mu_{\Omega}) \phi(E', \underline{\Omega}', \underline{r}) dE' d\underline{\Omega}' + S(E, \underline{\Omega}, \underline{r}). \quad (\text{IV.a})$$

In cylindrical geometry, infinite in the z direction, the angular flux function has four variables. These variables are the energy E , the distance r which is perpendicular to z axis, and the angles θ , and ϕ which specify the direction $\underline{\Omega}$. The angle between the z axis and $\underline{\Omega}$ is θ and the angle between the projection of $\underline{\Omega}$ on the xy plane and direction r is ϕ . The relationship of these angles to the coordinate axis is shown in Figure 1.

Figure 1. A Set of Cylindrical Coordinates.

The leakage term in (IV.a) above in this coordinate system is transformed²¹ as

$$\underline{\Omega} \cdot \nabla \phi(E, \underline{\Omega}, r) = \sin \theta \left[\cos \phi \frac{\partial \phi(E, \theta, \phi, r)}{\partial r} - \frac{\sin \phi}{r} \frac{\partial \phi(E, \theta, \phi, r)}{\partial \phi} \right] \quad (\text{IV.b})$$

The angular flux function in this section will use the symbol Φ in order to avoid confusion with the independent variable azimuthal angle ϕ . The spherical harmonics expansion for the angular flux function in this

geometry will be the same as that used by Marchuk⁶ as follows:

$$\Phi(E, \theta, \phi, r) = \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{2n+1}{2} F_{n0}(E, r) P_n(\mu) + \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n (2n+1) \frac{(n-m)!}{(n+m)!} \cdot$$

$$F_{nm}(E, r) P_n^m(\mu) \cos m\phi. \quad (\text{IV.c})$$

Here $\mu = \cos \theta$ and $P_n^m(\mu)$ are the associated Legendre polynomials.

The above series, (IV.c) along with the addition theorem expression (II.w) can now be substituted in the scattering integrals on the right of (IV.a) and the integration performed over $\underline{\Omega}'$. The summation index of m used in the addition theorem, (II.w) will now be changed to t to avoid confusion with the sum over m used in (IV.c). The integration over $\underline{\Omega}'$ in both the first and second term on the right of (IV.a) will be identical. Therefore, only the details for the second term will now be shown. Substituting expansion (IV.c) for Φ and using the addition theorem, (II.w) one obtains

$$\sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \int_0^{E_c} S_{th}(E' \rightarrow E) \int_0^{2\pi} \int_{-1}^1 \left[P_{\ell}(\mu) P_{\ell}(\mu') + 2 \sum_{t=1}^{\ell} \frac{(\ell-t)!}{(\ell+t)!} P_{\ell}^t(\mu) P_{\ell}^t(\mu') \right] \cdot$$

$$\cos t(\phi - \phi') \left[\frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{2n+1}{2} F_{n0}(E', r) P_n(\mu') + \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n (2n+1) \frac{(n-m)!}{(n+m)!} \cdot \right.$$

$$\left. F_{nm}(E', r) P_n^m(\mu') \cos m\phi' \right] d\mu' d\phi' dE'. \quad (\text{IV.d})$$

The expression (IV.d) can now be reduced considerably by first integrating over ϕ' using the fact that

$$\int_0^{2\pi} \cos t(\phi - \phi') d\phi' = \int_0^{2\pi} \cos m\phi' d\phi' = 0 \text{ for } m \text{ and } t \text{ integers,}$$

and

$$\int_0^{2\pi} \cos t(\phi - \phi') \cos m\phi' d\phi' = \pi \cos m\phi \text{ for } t = m, \quad (\text{IV.e})$$

otherwise this integral is zero.

The integration of (IV.e) can be effected by using trigonometric identities

$$\cos t(\phi - \phi') \cos m\phi' = \cos t\phi \cos t\phi' \cos m\phi' + \sin t\phi \sin t\phi' \cos m\phi' \quad (\text{IV.f})$$

$$\cos t\phi' \cos m\phi' = \frac{1}{2} \left[\cos(t+m)\phi' + \cos(t-m)\phi' \right] \quad (\text{IV.g})$$

$$\sin t\phi' \cos m\phi' = \frac{1}{2} \left[\sin(t-m)\phi' + \sin(t+m)\phi' \right] \quad (\text{IV.h})$$

When (IV.g) and (IV.h) are substituted in (IV.f), the following expression to be integrated over ϕ' results

$$\int_0^{2\pi} \frac{1}{2} \left\{ \cos t\phi \left[\cos(t+m)\phi' + \cos(t-m)\phi' \right] + \sin t\phi \left[\sin(t-m)\phi' + \sin(t+m)\phi' \right] \right\} d\phi'. \quad (\text{IV.i})$$

Thus for t and m positive integers all terms integrate to zero in (IV.i) except the second term in the integrand which integrates to

$$\int_0^{2\pi} \frac{1}{2} \cos t\phi \cos(t-m)\phi' d\phi' = \pi \cos m\phi \text{ for } t = m \text{ only.}$$

Combining these results into (IV.d) and using the fact that t must equal m to omit the sum over t yields

$$\sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \int_0^{E_c} S_{\ell}^{th}(E' \rightarrow E) \int_{-1}^1 \left[P_{\ell}(\mu) P_{\ell}(\mu') \sum_{n=0}^{\infty} \frac{2n+1}{2} F_{n0}(E', r) P_n(\mu') \right. \\ \left. + \sum_{n=\ell}^{\infty} \sum_{m=1}^n \frac{(\ell-m)!}{(\ell+m)!} \frac{(2n+1)(n-m)!}{(n+m)!} P_{\ell}^m(\mu) P_{\ell}^m(\mu') F_{nm}(E', r) F_n^m(\mu') \cos m\phi \right] d\mu' dE'. \quad (IV.j)$$

The integration in (IV.j) over μ' can now be performed using the orthogonality property of Legendre and associated Legendre polynomials. The associated Legendre polynomial orthogonality property is

$$\int_{-1}^1 P_{\alpha}^m(\mu) P_n^m(\mu) d\mu = \frac{2(n+m)!}{(2n+1)(n-m)!} \delta_n^{\alpha}. \quad (IV.k)$$

Again δ_n^{α} is the Kronecker delta which is zero if $n \neq \alpha$ and unity if $n = \alpha$. This orthogonality property can be easily derived from the spherical harmonic orthogonality property as given in Meghreblan and Holmes¹⁸. Thus in the second term in (IV.j) n must equal ℓ and the integration over μ' is performed in both terms to yield

$$\sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \int_0^{E_c} S_{\ell}^{th}(E' \rightarrow E) \left[P_{\ell}(\mu) F_{\ell 0}(E', r) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} F_{\ell m}(E', r) \cdot \right. \\ \left. P_{\ell}^m(\mu) \cos m\phi \right] dE'. \quad (IV.l)$$

The complete Boltzmann transport equation, (IV.a) can now be written in cylindrical geometry using (IV.b) to transform the leakage term and (IV.1) in the scattering integrals to give

$$\begin{aligned}
 \sin \theta \left(\cos \phi \frac{\partial \Phi}{\partial r} - \frac{\sin \phi}{r} \frac{\partial \Phi}{\partial \phi} \right) + \Sigma_t(E, r) \Phi = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi(1-\alpha)} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_{\ell}(\mu_o^*) \left[P_{\ell}(\mu) \cdot \right. \\
 \left. F_{\ell 0}(E', r) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} F_{\ell m}(E', r) P_{\ell}^m(\mu) \cos m\phi \right] \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} \\
 + \sum_{\ell=0}^{\infty} \frac{2\ell+1}{4\pi} \int_0^{E_c} S_{\ell}^{th}(E' \rightarrow E) \left[P_{\ell}(\mu) F_{\ell 0}(E', r) + 2 \sum_{m=1}^{\ell} \frac{(\ell-m)!}{(\ell+m)!} F_{\ell m}(E', r) P_{\ell}^m(\mu) \cos m\phi \right] dE' \\
 + S(E, \theta, \phi, r). \tag{IV.m}
 \end{aligned}$$

II. DERIVATION OF P_3 EQUATIONS

The expansion (IV.c) is now substituted into the terms on the left in (IV.m) and a similar expansion is used for the source function, $S(E, \theta, \phi, r)$. The angular flux function for a cylinder of infinite height must be symmetric with respect to reflection for planes perpendicular to the axis²². This would require that

$$\Phi(E, \theta, \phi, r) = \Phi(E, \pi - \theta, \phi, r). \tag{IV.n}$$

In this development the angle θ enters through the associated Legendre

polynomials, $P_n^m(\mu)$ and because of (IV.n), this must be an even function in μ , ie., $P_n^m(-\mu) = P_n^m(\mu)$. This is true providing $n + m$ is an even number. Thus the following sets of value for $F_{\ell m}(E, r)$ are allowed in the P_3 approximation:

$$\begin{array}{lll}
 (1) \quad \begin{array}{l} \ell=0 \\ m=0 \end{array} & (3) \quad \begin{array}{l} \ell=2 \\ m=0 \end{array} & (5) \quad \begin{array}{l} \ell=3 \\ m=1 \end{array} \\
 (2) \quad \begin{array}{l} \ell=1 \\ m=1 \end{array} & (4) \quad \begin{array}{l} \ell=2 \\ m=2 \end{array} & (6) \quad \begin{array}{l} \ell=3 \\ m=3 \end{array}
 \end{array} \quad (IV.o)$$

After substitution of the appropriate expansions in (IV.c) the equation is then multiplied by $P_r^t(\mu) \cos t\phi d\Omega$ and each term is integrated over all Ω . The integrations are elementary except for the leakage terms on the left of (IV.m). Giving attention only to the leakage term and making the substitutions and multiplications as stated above one obtains the expansion

$$\begin{aligned}
 & \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{(2n+1)}{2} \frac{\partial F_{n0}(E, r)}{\partial r} \int_{-1}^1 \int_0^{2\pi} \sin \theta \cos \phi P_n(\mu) P_r^t(\mu) \cos t\phi d\phi d\mu \\
 & + \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n (2n+1) \frac{(n-m)!}{(n+m)!} \frac{\partial F_{nm}(E, r)}{\partial r} \int_{-1}^1 \int_0^{2\pi} \sin \theta \cos \phi P_n^m(\mu) \cos m\phi \cdot
 \end{aligned}$$

$$P_r^t(\mu) \cos t\phi d\phi d\mu + \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n (2n+1) \frac{(n-m)!}{(n+m)!} \frac{m}{r} F_{nm}(E, r) \cdot$$

$$\int_{-1}^1 \int_0^{2\pi} \sin \theta \sin \phi P_n^m(\mu) \sin m\phi P_r^t(\mu) \cos t\phi d\phi d\mu. \quad (IV.p)$$

The orthogonality property of the spherical function series used in (IV.c) is

$$\int_{-1}^1 \int_0^{2\pi} P_n^m(\mu) \cos m\phi P_r^t(\mu) \cos t\phi d\phi d\mu = \frac{2\pi(n+m)!}{(2n+1)(n-m)!} \delta_m^t \delta_n^r$$

$$= \frac{4\pi}{2n+1} \text{ if } m=t=0. \quad (\text{IV.q})$$

To perform the integrations over $\underline{\Omega}$ in (IV.p) by using the orthogonality property (IV.q), the following recursion relations¹⁷ and trigonometric identities are needed:

$$\sin \theta P_n^m(\mu) = \frac{P_{n+1}^{m+1}(\mu) - P_{n-1}^{m+1}(\mu)}{2n+1}. \quad (\text{IV.r})$$

$$\sin \theta P_n^m(\mu) = \frac{(n+2-m)(m-1-n)P_{n+1}^{m-1}(\mu) + (n+m-1)(m+n)P_{n-1}^{m-1}(\mu)}{2n+1} \quad (\text{IV.s})$$

$$\cos m\phi \cos \phi = \frac{1}{2} \left[\cos (m+1)\phi + \cos (m-1)\phi \right] \quad (\text{IV.t})$$

$$\sin m\phi \sin \phi = \frac{1}{2} \left[\cos (m-1)\phi - \cos (m+1)\phi \right]. \quad (\text{IV.u})$$

Rewriting (IV.p), using (IV.r) to (IV.u) one obtains

$$\frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{1}{2} \frac{\partial F_{n0}(E, r)}{\partial r} \int_{-1}^1 \int_0^{2\pi} \left[P_{n+1}^1(\mu) - P_{n-1}^1(\mu) \right] \cos \phi P_r^t(\mu) \cos t\phi d\phi d\mu$$

$$+ \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{(n-m)!}{2(n+m)!} \frac{\partial F_{nm}(E, r)}{\partial r} \int_{-1}^1 \int_0^{2\pi} \left[P_{n+1}^{m+1}(\mu) - P_{n-1}^{m+1}(\mu) \right] \cos (m+1)\phi P_r^t(\mu) \cos t\phi d\phi d\mu$$

$$+ \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{(n-m)!}{2(n+m)!} \frac{\partial F_{nm}(E, r)}{\partial r} \int_{-1}^1 \int_0^{2\pi} \left[(n+2-m)(m-1-n) P_{n+1}^{m-1}(\mu) + (n+m-1)(m+n) P_{n-1}^{m-1}(\mu) \right] \cdot$$

$$\cos(m-1)\phi P_r^t(\mu) \cos t\phi d\phi d\mu - \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{(n-m)!}{2(n+m)!} \frac{m}{r} F_{nm}(E, r) \cdot$$

$$\int_{-1}^1 \int_0^{2\pi} \left[P_{n+1}^{m+1}(\mu) - P_{n-1}^{m+1}(\mu) \right] \cos(m+1)\phi P_r^t(\mu) \cos t\phi d\phi d\mu + \frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{m=1}^n \frac{(n-m)!}{2(n+m)!} \cdot$$

$$\frac{m}{r} F_{nm}(E, r) \int_{-1}^1 \int_0^{2\pi} \left[(n+2-m)(m-1-n) P_{n+1}^{m-1}(\mu) + (n+m-1)(m+n) P_{n-1}^{m-1}(\mu) \right] \cos(m-1)\phi \cdot$$

$$P_r^t(\mu) \cos t\phi d\phi d\mu. \quad (IV.v)$$

With full use being made of the orthogonality property, (IV.q), the integration over $\underline{\Omega}$ is performed both on the leakage expression (IV.v) for successive pairs of (r, t) as indicated in (IV.o) and on the other terms in (IV.m) to finally yield the following six equations:

$$\frac{\partial F_{11}}{\partial r}(E, r) + \frac{F_{11}}{r}(E, r) + \Sigma_t(E, r) F_{00}(E, r) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') F_{00}(E', r) \sum_{\ell'=0}^{\infty} (2\ell'+1) \cdot$$

$$f_{\ell,}(E') P_{\ell,}(\mu_c^*) \frac{dE'}{E'} + \int_0^{E_c} S_o^{th}(E \rightarrow E') F_{00}(E', r) dE' + S_{00}(E, r) \quad (IV.w)$$

$$\frac{1}{3} \frac{\partial F_{00}}{\partial r}(E, r) - \frac{1}{3} \frac{\partial F_{20}}{\partial r} + \frac{1}{6} \frac{\partial F_{22}}{\partial r} + \frac{F_{22}}{3r}(E, r) + \Sigma_t(E, r) F_{11}(E, r)$$

$$\begin{aligned}
&= \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_1(\mu_o^*) F_{11}(E', r) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell', (E')} P_{\ell', (\mu_c^*)} \frac{dE'}{E'} \\
&\quad + \int_0^{\frac{E_c}{\alpha}} S_1^{th}(E \rightarrow E) F_{11}(E', r) dE' + S_{11}(E, r). \quad (IV.x)
\end{aligned}$$

$$- \frac{1}{5} \frac{\partial F_{11}(E, r)}{\partial r} + \frac{1}{5} \frac{\partial F_{31}(E, r)}{\partial r} - \frac{F_{11}(E, r)}{5r} + \frac{F_{31}(E, r)}{5r} + \Sigma_t(E, r) F_{20}(E, r)$$

$$\begin{aligned}
&= \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_2(\mu_o^*) F_{20}(E, r) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell', (E')} P_{\ell', (\mu_c^*)} \frac{dE'}{E'} \\
&\quad + \int_0^{\frac{E_c}{\alpha}} S_2^{th}(E \rightarrow E) F_{20}(E', r) dE' + S_{20}(E, r). \quad (IV.y)
\end{aligned}$$

$$- \frac{1}{5} \frac{\partial F_{31}(E, r)}{\partial r} + \frac{6}{5} \frac{\partial F_{11}(E, r)}{\partial r} + \frac{1}{10} \frac{\partial F_{33}(E, r)}{\partial r} - \frac{6}{5} \frac{F_{11}(E, r)}{r} + \frac{F_{31}(E, r)}{5r}$$

$$+ \frac{3F_{33}(E, r)}{10r} + \Sigma_t(E, r) F_{22}(E, r) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_2(\mu_o^*) \cdot$$

$$F_{22}(E', r) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell', (E')} P_{\ell', (\mu_c^*)} \frac{dE'}{E'} + \int_0^{\frac{E_c}{\alpha}} S_2^{th}(E \rightarrow E) F_{22}(E', r) dE'$$

$$+ S_{22}(E, r). \quad (IV.z)$$

$$\frac{6}{7} \frac{\partial F_{20}(E, r)}{\partial r} - \frac{1}{14} \frac{\partial F_{22}(E, r)}{\partial r} - \frac{F_{22}(E, r)}{7r} + \Sigma_t(E, r) F_{31}(E, r) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_3(\mu_o^*) \cdot$$

$$F_{31}(E', r) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} + \int_0^{E_c} S_3^{th}(E' \rightarrow E) F_{31}(E', r) dE' \\ + S_{31}(E, r). \quad (IV.a')$$

$$\frac{15}{7} \frac{\partial F_{22}(E, r)}{\partial r} - \frac{30}{7} \frac{F_{22}(E, r)}{r} + \Sigma_t(E, r) F_{33}(E, r) = \frac{1}{1-\alpha} \int_{E_c}^{\frac{E_c}{\alpha}} \Sigma_s(E') P_3(\mu_0^*) dE'.$$

$$F_{33}(E', r) \sum_{\ell'=0}^{\infty} (2\ell'+1) f_{\ell'}(E') P_{\ell'}(\mu_c^*) \frac{dE'}{E'} + \int_0^{E_c} S_3^{th}(E' \rightarrow E) F_{33}(E', r) dE' \\ + S_{33}(E, r). \quad (IV.b')$$

III. MULTIGROUP P_3 EQUATIONS IN CYLINDRICAL GEOMETRY

Each equation from (IV.w) to (IV.b) is now integrated over energy group j as was done previously for the P_1 and double P_1 equations. The integrals are replaced by products of scattering transfer cross sections and appropriate angular flux components to yield

$$\frac{dF_{11}^j(r)}{dr} + \frac{F_{11}^j(r)}{r} + \Sigma_t^j(r) F_{00}^j(r) = \sum_{i=1}^j \Sigma_{i \rightarrow j}^0(r) F_{00}^i(r) + \sum_{i=N_{th}}^N \Sigma_{i \rightarrow j}^{0*}(r) F_{00}^i(r) \\ + S_{00}^j(r) \quad (IV.c')$$

$$\frac{dF_{00}^j(r)}{dr} - \frac{dF_{20}^j(r)}{dr} + \frac{1}{2} \frac{dF_{22}^j(r)}{dr} + \frac{F_{22}^j(r)}{r} + 3\Sigma_t^j(r) F_{11}^j(r)$$

$$= 3 \sum_{i=1}^j \sum_{i \rightarrow j}^1 (r) F_{11}^i(r) + 3 \sum_{i=N_{th}}^N \sum_{i \rightarrow j}^{1*} (r) F_{11}^i(r) + 3S_{11}^j(r) \quad (\text{IV.d'})$$

$$\frac{dF_{31}^j(r)}{dr} - \frac{dF_{11}^j(r)}{dr} + \frac{F_{31}^j(r)}{r} - \frac{F_{11}^j(r)}{r} + 5\Sigma_t^j(r)F_{20}^j(r) = 5 \sum_{i=1}^j \sum_{i \rightarrow j}^2 (r) F_{20}^i(r)$$

$$+ 5 \sum_{i=N_{th}}^N \sum_{i \rightarrow j}^{2*} (r) F_{20}^i(r) + 5 S_{20}^j(r). \quad (\text{IV.e'})$$

$$\frac{12dF_{11}^j(r)}{dr} + \frac{dF_{33}^j(r)}{dr} - \frac{2dF_{31}^j(r)}{dr} - \frac{12F_{11}^j(r)}{r} + \frac{2F_{31}^j(r)}{r} + \frac{3F_{33}^j(r)}{r} + 10\Sigma_t^j(r)F_{22}^j(r)$$

$$= 10 \sum_{i=1}^j \sum_{i \rightarrow j}^2 (r) F_{22}^i(r) + 10 \sum_{i=N_{th}}^N \sum_{i \rightarrow j}^{2*} (r) F_{22}^i(r) + 10S_{22}^j(r) \quad (\text{IV.f'})$$

$$\frac{12dF_{20}^j(r)}{dr} - \frac{dF_{22}^j(r)}{dr} + \frac{2F_{22}^j(r)}{r} + 14\Sigma_t^j(r)F_{31}^j(r) = 14 \sum_{i=1}^j \sum_{i \rightarrow j}^3 (r) F_{31}^i(r)$$

$$+ 14 \sum_{i=N_{th}}^N \sum_{i \rightarrow j}^{3*} (r) F_{31}^i(r) + 14S_{31}^j(r). \quad (\text{IV.g'})$$

$$\frac{15dF_{22}^j(r)}{dr} - \frac{30F_{22}^j(r)}{r} + 7\Sigma_t^j(r)F_{33}^j(r) = 7 \sum_{i=1}^j \sum_{i \rightarrow j}^3 (r) F_{33}^i(r)$$

$$+ 7 \sum_{i=N_{th}}^N \sum_{i \rightarrow j}^{3*} (r) F_{33}^i(r) + 7S_{33}^j(r). \quad (\text{IV.h'})$$

In the thermal groups with $N_{th} \leq j < N$, the upper limit for the first sum on the right in each of the above equations is $(N_{th}-1)$. The asterisk is again placed on the thermal group transfer cross sections.

The term for $i=j$ on the right in (IV.c') and (IV.d') is now transformed to the left, an isotropic fission source term is introduced for the fast groups and all components for m and/or n greater than one are deleted for the P_1 fast group equations to yield

$$\begin{aligned} \frac{dF_{11}^j(r)}{dr} + \frac{F_{11}^j(r)}{r} + \left[\Sigma_t^j(r) - \sum_{j \rightarrow j}^o \right] F_{oo}^j(r) = \sum_{i=1}^{j-1} \sum_{i \rightarrow j}^o \Sigma^o(r) F_{oo}^i(r) \\ + \frac{X^j(r)}{\lambda} \sum_{i=1}^N \nu \Sigma_f^i F_{oo}^i(r) + S_{oo}(E, r). \end{aligned} \quad (IV.i')$$

$$\frac{1}{3} \frac{dF_{oo}^j(r)}{dr} + \left[\Sigma_t^j(r) - \sum_{j \rightarrow j}^1 \right] F_{11}^j(r) = \sum_{i=1}^{j-1} \sum_{i \rightarrow j}^1 \Sigma^1(r) F_{11}^i(r). \quad (IV.j')$$

The P_3 thermal group equations are derived from (IV.c') to (IV.h') by transforming the in-group scattering terms to the left and deleting all in-group source terms from the fast groups for ℓ and/or m greater than one. The following equations result:

$$\begin{aligned} \frac{dF_{11}^j(r)}{dr} + \frac{F_{11}^j(r)}{r} + \left[\Sigma_t^j(r) - \sum_{j \rightarrow j}^{o*} \right] F_{oo}^j(r) = \sum_{i=1}^{N_{th}-1} \sum_{i \rightarrow j}^o \Sigma^o(r) F_{oo}^i(r) \\ + \sum_{\substack{i=N_{th} \\ i \neq j}}^N \sum_{i \rightarrow j}^{o*} \Sigma^o(r) F_{oo}^i(r) + S_{oo}^j(r) \end{aligned} \quad (IV.k')$$

$$\begin{aligned}
& \frac{dF_{00}^j}{dr}(r) - \frac{dF_{20}^j}{dr}(r) + \frac{1}{2} \frac{dF_{22}^j}{dr}(r) + \frac{F_{22}^j(r)}{r} + 3 \left[\Sigma_t^j(r) - \Sigma_{j \rightarrow j}^{1*}(r) \right] F_{11}^j(r) \\
& = 3 \sum_{i=1}^{N_{th}-1} \Sigma_{i \rightarrow j}^1(r) F_{11}^i(r) + 3 \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{1*}(r) F_{11}^i(r).
\end{aligned} \tag{IV.1'}$$

$$\begin{aligned}
& \frac{dF_{31}^j}{dr}(r) - \frac{dF_{11}^j}{dr}(r) + \frac{F_{31}^j(r)}{r} - \frac{F_{11}^j(r)}{r} + 5 \left[\Sigma_t^j(r) - \Sigma_{j \rightarrow j}^{2*}(r) \right] F_{20}^j(r) \\
& = 5 \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{2*}(r) F_{20}^i(r).
\end{aligned} \tag{IV.m'}$$

$$\begin{aligned}
& \frac{12dF_{11}^j}{dr}(r) + \frac{dF_{33}^j}{dr}(r) - \frac{2dF_{31}^j}{dr}(r) - \frac{12F_{11}^j(r)}{r} + \frac{2F_{31}^j(r)}{r} + \frac{3F_{33}^j(r)}{r} \\
& + 10 \left[\Sigma_t^j(r) - \Sigma_{j \rightarrow j}^{2*}(r) \right] F_{22}^j(r) = 10 \sum_{\substack{i=1 \\ i \neq j}}^{N_{th}} \Sigma_{i \rightarrow j}^{2*}(r) F_{22}^i(r).
\end{aligned} \tag{IV.n'}$$

$$\begin{aligned}
& \frac{12dF_{20}^j}{dr}(r) - \frac{dF_{22}^j}{dr}(r) - \frac{2F_{22}^j(r)}{r} + 14 \left[\Sigma_t^j(r) - \Sigma_{j \rightarrow j}^{3*}(r) \right] F_{31}^j(r) \\
& = 14 \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{3*}(r) F_{31}^i(r).
\end{aligned} \tag{IV.o'}$$

$$\begin{aligned}
& \frac{15dF_{22}^j}{dr}(r) - \frac{30F_{22}^j(r)}{r} + 7 \left[\Sigma_t^j(r) - \Sigma_{j \rightarrow j}^{3*}(r) \right] F_{33}^j(r) = 7 \sum_{\substack{i=N_{th} \\ i \neq j}}^N \Sigma_{i \rightarrow j}^{3*}(r) F_{33}^i(r).
\end{aligned} \tag{IV.p'}$$

This set of P_3 equations are identical to those derived by Marchuk⁶ except that in this development the group to group transfer sources have been fully displayed. Also the coupling between the P_1 fast group equations and the P_3 thermal group equations has been considered. The above equations (IV.k') to (IV.p') can be written in matrix form and difference equations derived as Marchuk⁶ has done.

CHAPTER V

SUMMARY

From the general Boltzmann transport equation, the multigroup spherical harmonic equations have been derived for the P_1 and double P_1 approximations in slab geometry and for the P_1 and P_3 approximations in cylindrical geometry. The source integrals for down-scattering have been reduced to transfer cross sections which are fully defined and in a form convenient for calculation. The coupling between the fast and thermal energy groups is retained giving a consistent formulation of the reduction of the energy dependent Boltzmann transport equation to multigroup spherical harmonic theory.

Difference equations can be derived from the spherical harmonic equations as given here. These difference equations along with appropriate boundary conditions will be programmed to yield a computer solution to the angular flux function. Of major interest is the total isotropic flux spectra as a function of position in the reactor or reactor cell. From this flux spectra other important reactor physics information can consistently be obtained such as thermal utilization, thermal and epithermal disadvantage factors and few group reactor constants.

Calculated flux spectra and disadvantage factors will be compared to experimental values to determine the accuracy of the approximations made in this work.

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APPENDIX: COMPUTATION OF SCATTERING TRANSFER CROSS SECTIONS

A computer program has been written to calculate the group to group down-scattering transfer cross sections for any isotope k . The following integrals are evaluated by numerical integration methods:

$$\sigma_{i \rightarrow j}^{\beta} = \frac{\int_c^d \int_a^b \frac{\sigma_k(E')(2\ell+1)}{(1-\alpha_k)} P_{\ell}(\mu_{ok}^*) \phi(E') \sum_{\ell'=0}^6 (2\ell'+1) f_{\ell',k}(E') P_{\ell'}(\mu_{ok}^*) \frac{dE'}{E'} dE}{\int_{E_i}^{E_{i-1}} \phi(E) dE}$$

The variation of $\phi(E)$ in the present program is taken as $\frac{1}{E}$ for all groups. Some investigation has been made into using a fission spectrum variation of $\phi(E)$ in the fast range and a $\frac{1}{E}$ variation in the epithermal range. The quantities μ_o^* and μ_c^* are defined by (II.b) and (II.c) in Section II. For a particular isotope k , α_k is defined as $\alpha_k = \frac{(A_k-1)}{(A_k+1)}$ where A_k is mass number of isotope k .

The maximum value of ℓ' on the sum is six. This order Legendre expansion is adequate to represent the anisotropic scattering in the center of mass system for present experimental data. A $(2\ell+1)$ factor is included in the definition of the scattering transfer cross section. This factor must be divided out to obtain transfer cross sections consistent with the equations derived in this work.

The limits on the integral are set by various tests as follows:

1. Integral is zero if $E_i \geq \frac{E_{j-1}}{\alpha}$

$$2. \quad E_i \geq \frac{E_j}{\alpha}, \quad \frac{E_{j-1}}{\alpha} > E_i, \quad \frac{E_{j-1}}{\alpha} < E_{i-1}$$

$$\begin{aligned} a &= E_i & c &= \alpha E_i \\ b &= \frac{E_j}{\alpha} & d &= E_{j-1} \end{aligned} \quad \text{Integration first with respect to } dE'.$$

$$3. \quad \frac{E_j}{\alpha} > E_i, \quad \frac{E_{j-1}}{\alpha} < E_{i-1}$$

$$\begin{aligned} a &= E_i & c &= E_j \\ b &= \frac{E_j}{\alpha} & d &= E_{j-1} \end{aligned} \quad \text{Integration order same as 2 above.}$$

$$4. \quad \frac{E_j}{\alpha} < E_i, \quad \frac{E_{j-1}}{\alpha} \geq E_{i-1}$$

$$\begin{aligned} a &= \alpha E' & c &= E_i \\ b &= E_{j-1} & d &= E_{i-1} \end{aligned} \quad \text{Integrate first with respect to } dE.$$

$$5. \quad \frac{E_j}{\alpha} > E_i, \quad \frac{E_{j-1}}{\alpha} > E_{i-1}$$

The integral for this case will consist of the sum of two integrals with limits as follows:

$$\begin{aligned} a_1 &= E_i & c_1 &= E_j & a_2 &= E_i & c_2 &= \alpha E_{i-1} \\ b_1 &= \frac{E_j}{\alpha} & d_1 &= \alpha E_{i-1} & b_2 &= E_{i-1} & d_2 &= E_{j-1} \end{aligned}$$

In both cases the integration is first with respect to dE'

$$6. \quad \frac{E_j}{\alpha} \geq E_{i-1},$$

$$a = E_i \quad c = E_j$$

$$b = E_{i-1} \quad d = E_{j-1}$$

Integrate first with respect to dE'

The limits on the integral and the test for within-group scattering are

$$1. \quad E_j \geq \alpha E_{j-1}$$

$$a = E \quad c = E_j$$

$$b = E_{j-1} \quad d = E_{j-1}$$

For within-group scattering $E_i = E_j$ and $E_{i-1} = E_{j-1}$.

$$2. \quad E_j < \alpha E_{j-1}$$

Again this total integral is the sum of two integrals with limits as follows:

$$a_1 = E \quad c_1 = E_j$$

$$b_1 = \frac{E}{\alpha} \quad d_1 = \alpha E_{j-1}$$

$$a_2 = E \quad c_2 = \alpha E_{j-1}$$

$$b_2 = E_{j-1} \quad d_2 = E_{j-1}$$

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