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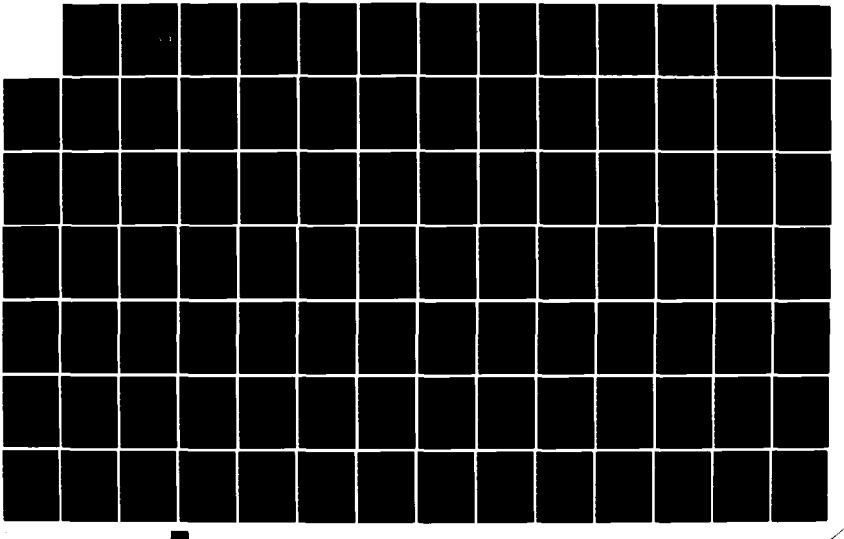

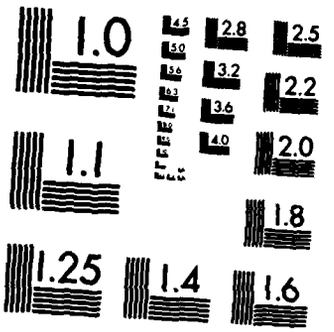

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A FINITE ELEMENT PROJECTION METHOD FOR THE SOLUTION OF PARTICLE TRANSPORT PROBLEMS WITH ANISOTROPIC SCATTERING

BY

EZE EWART WILLS

B.S., University of Maryland, 1978

M.S., Air Force Institute of Technology, 1981

DISSERTATION

Submitted in Partial Fulfillment of the
Requirements for the Degree of

Doctor of Philosophy in Engineering

The University of New Mexico
Albuquerque, New Mexico

July, 1984

AFIT/CI/NR 84-56D

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AUTHOR: Eze Ewart Wills

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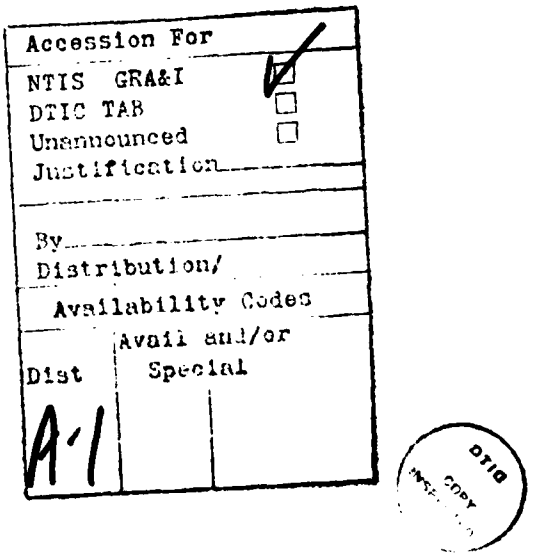

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A solution method for solving particle transport problems has been developed. This solution approach embodies a finite element projection technique and a related equivalent variational Raleigh-Ritz formalism. Particle flux in the transport equation is expressed as a linear and separable sum of odd and even components in the direction variables. Then a classical variational principle is obtained and shown to be equivalent to a Bubnov-Galerkin projected solution. A dual finite element basis of polynomial splines in space and spherical harmonics in angle is used in the Bubnov-Galerkin equations.

The general theoretical and numerical problem formalism is carried out in a 3-dimensional geometry with anisotropic scattering and with a piecewise constant energy dependence. This is a seven-dimensional problem with time dependence, three spatial and two angular or directional variables and with a multigroup treatment of the energy

dependence. The boundary conditions for most physical problems of interest are dealt with explicitly and rigorously by a classical minimization (variational) principle.

The solution method is developed as a complementary alternative to the standard solution techniques of Discrete Ordinates, Monte Carlo and the P_n method. The Galerkin projected operator and transport matrix are positive definite, symmetric and self-adjoint. This insures existence, uniqueness, and convergence of the solution. This formalism does not have the inherent properties which have produced the ray effect problem in discrete ordinates.

The computational validation of the method was obtained by a computer solution to the air-over-ground problem. This problem is of significant interest in the areas of nuclear weapons effects and radiation physics. It is modeled in cylindrical (r,z) geometry with an exponentially varying atmosphere, anisotropic scattering, anisotropic first scatter sources, and with the air-ground interface included.

Results for the air-over-ground problem are presented. These results show that this solution approach mitigates ray effects. They also show the potential of this technique to serve as a viable alternative to Discrete

Ordinates and Monte Carlo. However, further work in extending the computer implementation of the method to time and energy dependent problems, and to solving and validating this technique on a larger class of particle transport problems is required.

Transport Equation
Particle Transport
Variational Principle
Spherical Harmonics
Finite Element Projection
Raleigh-Ritz
Bubnov-Galerkin
Air-Over-Ground Problem
Anisotropic Scattering
Ray Effects

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CHAPTER I

INTRODUCTION

Particle transport occurs in many physical and engineering systems. Therefore, the solution of particle transport problems is of widespread engineering and scientific interest in many diverse areas of research, development and system applications. In the areas of plasma physics, nuclear energy (fission and fusion); radiation effects; space research and exploration, and many others, the theory, physics and modeling of particle transport processes play an important and vital role.

There are numerous solution techniques and approaches for solving particle transport problems (Sanchez and McCormick 1981). However, the most widely used solution methods are based on a particle tracking and statistical treatment of individual particle interactions and transport or on the principles of particle conservation and distribution functions. In the latter case particle conservation is usually expressed in terms of an integro-differential equation (the transport equation) and particle

number densities and distribution functions are obtained from a solution to this equation.

In general numerical solutions to particle transport problems are usually obtained by the P_n method, discrete ordinates (S_n), or Monte Carlo. The P_n and S_n techniques provide solutions to the transport equation whereas Monte Carlo is based on particle tracking and statistics. These methods provide accurate solutions for a large number of problems. However, for some problems they have severe limitations.

The Monte Carlo method, usually requires the use of many hours of expensive computer time, and for deep penetration problems it is subject to errors due to statistical inadequacies (Janni, 1979). Discrete ordinates may use fewer computer resources than Monte Carlo, however it has a computational difficulty called "ray effects" (Lathrop, 1968). Ray effects are a result of the angular discretization of the transport equation. In the S_n method this discretization constrains particles to move in specific directions. This, in turn, produces distortions in the particle flux. For problems with strong absorbers, localized sources, and high energy streaming particles, these distortions produce solutions which are inaccurate.

The P_1 method or diffusion theory is the most often used P_n method. However, unlike Monte Carlo and the S_n method, it does not allow a detailed treatment of the angular dependence of transport processes. This limitation makes diffusion theory inadequate for problems which are non-diffusive. However, higher order P_n approximations are computationally inefficient and expensive, especially in two or three space dimensions (Kaplan, et al., 1966).

The Problem and Scope

The problem is to rigorously develop a method for solving general particle transport problems. This should be a method that removes some of the limitations and inherent difficulties of Monte Carlo, discrete ordinates and the P_n method. Furthermore, this solution approach should be able to serve as a complementary alternative to the presently used techniques for solving particle transport problems.

In order to accomplish this a detailed formalism for solving the transport equation is required. Specificially, a mathematical and numerical model to solve the general transport equation with anisotropic sources and scattering and general boundary conditions will be developed. This

model is an extension of current approximate numerical techniques for solving particle transport and other engineering problems. Also, it has stable mathematical and numerical properties.

The Solution Approach

The solution approach is to first develop a mathematical formalism (model) by drawing upon the present body of knowledge and experience in solving engineering and physical problems in general and particle transport problems in particular. We begin by first examining current solution methods for solving the transport equation and then proceed by using insight and hopefully good judgment to further develop, examine and rigorously explain our mathematical and numerical models.

Our numerical model is based on the well-known techniques of finite elements, projection operators and a classical Raleigh-Ritz solution. The mathematical model is derived from a variational principle and an equivalent Bubnov-Galerkin solution of the second order forms of the transport equation. These second order equations were first introduced by Kaplan and Davis in 1967.

Our intent is to propose a solution strategy that is similar to diffusion theory but has all the detailed angular or vector information of anisotropic scattering and sources. We also develop a rigorous treatment of general boundary conditions. This approach differs from discrete ordinates and the P_n method in the general formalism, solution strategy and properties and also in the treatment of boundary conditions. To accomplish this we take the view that a successful numerical solution strategy should be developed in accordance with the properties of a rigorous mathematical formulation. In fact the numerical and mathematical models to the problem should go hand in hand. Ideally we would like to have a mathematical model that complements and is compatible with the numerical approach and vice versa. In such a situation the numerical solution strategy when implemented will be best suited to highlight and use the special mathematical properties of the problem equations and thus provide a reasonable or "best" approximate solution. We therefore approached the problem by first seeking a mathematical formulation that had desirable mathematical, computational and numerical properties. These properties which are present in the P_1 or diffusion equation are desirable in that they would facilitate a numerical solution to the problem. In fact

they should allow a solution by similar and well established techniques which are being used to solve diffusion problems.

Secondly, we chose our numerical model because of our mathematical formalism and equations and the need to solve general problems of physical and engineering interest. In this numerical development we attempted to recognize and use the properties of our mathematical model. Finally we applied this solution technique to a real problem, to examine, validate and compare the results.

In summary, our mathematical development is based upon the parity and odd-even properties of spherical harmonics coupled with a Bubnov-Galerkin and classical variational approach. However, our numerical development evolves primarily upon the use of finite elements and projection operators. This use of a finite element projection technique is a logical extension of our mathematical formalism. Furthermore it provides the required flexibility needed in solving general and difficult problems.

Projection Methods and Finite Elements

Over the last two decades there has been a successful evolution of projection methods and finite elements in solving engineering problems. The use of finite elements and in particular projection methods began in the early

19th century. The finite element method is really a projection method although it is not usually recognized as such. Furthermore, many approximate methods for solving integral and differential equations are also projection methods. A detailed discussion of projection methods can be found in Atkinson (1976). Projection methods include such widely used solution techniques as Galerkin, collocation, least squares and the method of moments (Goldberg, 1978). A precise mathematical description of these methods is presented in Chapter VI.

Early 19th century mathematicians began using projection methods to solve ordinary and partial differential equations, which could not be solved in closed form (Kantorovich and Krylov, 1958). They developed techniques for expanding the solution as an infinite series of known functions with undetermined coefficients. Constraints or conditions were then applied to the approximate equations in order to "determine" the undetermined coefficients. The use of different constraints in determining the coefficients produced various projection methods whereas the use of special functions to expand the solution resulted in the finite element method.

Projection methods can be used to solve linear, non-linear and non-self-adjoint problems. These methods

are sometimes called the method of weighted residuals or error-distribution principles by engineers and applied mathematicians (Finlayson and Scriven, 1966). There are many types and classifications of projection methods depending not only upon the constraints by which the coefficients are determined but also on how the boundary conditions are treated. A somewhat unified treatment of some of these methods was developed by Crandall in 1956 and Finlayson and Scriven in 1966. However, many of these approximate solution techniques were introduced in the 1920's and 1930's. Galerkin introduced his method as early as 1915 whereas the concept of finite elements was proposed in 1924 by C. B. Biezeno. He recommended the use of special piecewise constant functions in solving stress problems. He called this projection technique the subdomain method.

However, it was in 1943 that the finite element method was formally introduced by Courant. He proposed the use of piecewise Lagrange polynomials on a triangular mesh to solve two-dimensional vibration problems. Subsequently and with the advent of computers, the finite element method has been used to solve a wide range of problems. One of the attractive features of finite elements is the inherent capability to handle difficult

problems with complicated geometries. General particle transport problems of engineering and physical interest are usually in this category.

Review of the Literature

The first use of a finite element projection technique to solve particle transport problems occurred in the early 1970's. In 1971 a number of researchers including Kaper, et al., Semenza, et al., Kang and Hansen, and Ohnishi used finite elements to solve the diffusion and steady state transport equation. In 1972 a more detailed examination of the use of finite elements to solve neutron diffusion problems was provided by Kaper, Leaf and Lindeman. They concluded that a finite element solution of the diffusion equation had advantages in terms of accuracy and convergence in comparison to the usual finite difference solution.

Other researchers including Miller, et al., Ukai, Hill, Yaun and Lewis, Seed, et al., Finkelstein and Krumbein and many others, have directly applied finite elements to solve the first order form of the transport equation. In 1974, Kaper, Leaf and Lindeman examined the application of a finite element projection of Lagrange polynomials and surface harmonics to a variational form of the second order transport equation in x-y geometry. They concluded that this approach

was inefficient and had many disadvantages in comparison to the standard solution techniques of discrete ordinates and Monte Carlo. Subsequently, Miller, et al. applied finite elements to this variational form of the transport equation and demonstrated the mitigation of ray effects. Pitkaranta and Silvennoinen also used a phase space projection of finite elements to solve eigenvalue problems in spherical geometry; whereas, Lillie and Robinson used a discrete ordinate finite element technique and a reduced functional to solve two-dimensional (x,y) transport problems.

Many other researchers have used projection methods to solve particle transport problems although most of them did not explicitly classify their approximate solution techniques as projection methods. Some of those who did were Miller and Reed (1975) who carried out a discrete ordinate to spherical harmonic conversion to mitigate ray effects and Reed (1972) who also developed a discrete ordinate-spherical harmonic solution. Others include Morel (1981) who used a collocation method with Lagrange polynomials to solve the first order form of the transport equation.

However the most widely used methods for solving particle transport problems are still the discrete ordinates (S_n) method along with Monte Carlo and the P_n method. These meth-

ods are well documented in the literature and have been used extensively to solve general problems (Bell and Glasstone, 1971). There are many S_n, Monte Carlo and diffusion production codes available in the areas of neutral and charge particle transport. Recently Fletcher (1983) has numerically developed a high order P_n projection method which uses finite elements to solve the first order transport equation. Nonetheless and despite the success and robustness of these solution techniques there is a need for alternate and complementary solution methods for solving particle transport problems. This is especially true for those problems where discrete ordinates, Monte Carlo and diffusion theory have disadvantages and limitations.

Research Objective

The purpose of this research is to develop a method for solving general particle transport problems. This method should serve as a complementary alternative to the standard solution techniques of discrete ordinates, Monte Carlo and the P_n method. The objectives of this study are grouped into three main areas. These were to first provide a theoretical and mathematical development, followed by a numerical, and then a computational treatment.

In the first area a theoretical and mathematical formulation of the problem is required. A mathematical formalism based on a variational principle and the positive definite self-adjoint second order forms of the transport equation will be provided. The boundary conditions for most physical problems of interest are dealt with by this classical minimization (variational) principle. This development which includes general boundary conditions, anisotropic sources and scattering has properties which are amenable to, and would facilitate standard numerical solution techniques.

The numerical development requires an approach which is consistent with and takes advantage of the mathematical formulation. A finite element projection technique based on spherical harmonics, piecewise polynomials, and a piecewise constant (multigroup) energy dependence, met this criteria. The general numerical treatment includes a seven dimensional time and energy dependent problem with three spatial and two angular or direction variables. The treatment of boundary conditions is based upon an equivalent classical Raleigh-Ritz solution.

In order to demonstrate the potential of this solution approach in solving particle transport problems a computer implementation of this method is required. The application to a problem which is of interest in the area of radiation

physics was chosen. In this computational treatment a validation of the method through a solution of the air-over-ground problem is provided. Specifically, this problem is modeled in cylindrical (r,z) geometry, with an exponentially varying atmosphere, anisotropic scattering, first scatter collision sources and with the air-ground interface included. In this demonstration a steady-state one group (monoenergetic) solution is achieved and examined. However, a solution of the energy and time dependent problem can be obtained from a straightforward extension of this steady-state monoenergetic solution.

Sequence of Presentation

The organization of this report covers the three main areas of research by presenting a theoretical, mathematical and numerical formulation of the general problem and by a specific computer implementation to the air-over-ground problem. In Chapters II, III and IV the mathematical model is presented and discussed along with an overview of finite elements and the second order forms of the transport equation. In Chapter V variational principles, functionals and boundary conditions are presented and discussed. We discuss projection methods and weak forms and outline the general numerical method and solution strategy in Chapters

VI and VII. An application to the air-over-ground problem which includes a computer solution and results is given in Chapter VIII. Finally, Chapter IX contains conclusions and recommendations for future extensions of this work. Here we also discuss applications to other problems of engineering and physical interest.

CHAPTER II

THE MATHEMATICAL MODEL

The usual mathematical description of particle transport is given by the transport equation (Duderstadt and Martin, 1971). This equation is an expression in a seven dimensional phase space of particle conservation in terms of particle distribution functions (number densities). The transport equation models general particle transport processes. However, it can be modified and used to model special neutral and charge particle transport problems. These modificiations occur primarily in the collision terms (Schmidt, 1979).

The transport equation along with the relevant boundary and interface conditions is mathematically a boundary value problem. This equation which is the starting point of our solution strategy is outlined and examined in the following sections. We also briefly mention the main solution methods for solving particle transport problems. Except for the Monte Carlo method these solution techniques are based primarily upon the standard and usual solution approaches for solving initial and boundary value problems.

The Transport Equation

A derivation of the general transport equation, by imposing particle conservation and balance on an elemental volume in phase space can be found in Duderstadt and Martin (1979). This model which includes external macroscopic forces and long-range collisions can be written as

$$\frac{\partial n}{\partial t}(\hat{r},\hat{v},t) + \hat{v}\cdot\nabla n(\hat{r},\hat{v},t) + \frac{\hat{F}}{m}(\hat{r},t)\cdot\nabla_v n(\hat{r},\hat{v},t) = \left.\frac{\partial n}{\partial t}\right)_{coll} + q(\hat{r},\hat{v},t) \tag{1}$$

where

$\hat{r}$ = the spatial position vector

$\hat{v}$ = the particle velocity vector

t = the time variable with respect to some initial or starting time

$n(\hat{r},\hat{v},t)$ = unnormalized particle phase space density or probability distribution function

∇ = spatial gradient operator

∇_v = velocity gradient operator

$\frac{\hat{F}}{m}(\hat{r},t) = \frac{e}{m}[\hat{E}(\hat{r},t) + \hat{v} \times \hat{B}(\hat{r},t)]$ = particle acceleration

$\hat{E}(\hat{r},t)$ = electric field

$\hat{B}(\hat{r},t)$ = magnetic field

$\left.\frac{\partial n}{\partial t}\right)_{coll}$ = rate of change of particle distribution as a result of collisions. This term is usually called the collision operator

$q(\hat{r},\hat{v},t)$ = external particle source and intrinsic particle sources due to fissions, (n,2n) reactions, etc.

Equation (1) can also be derived from the BBGKY heirarchy of equations (Krall and Trivelpiece, 1973). The BBGKY hierarchy is a system of equations whereby the distribution function of a many body system is expressed in terms of functionals of single particle density distributions. A density expansion to first order when carried out produces the transport equation.

If we consider a solution to Eq (1) at long times and/or at large distances from sources or boundaries the problem can be formulated as an initial value problem (Duderstadt and Martin, 1979). In such instances details of the initial and/or boundary conditions can be ignored and the time relaxation or slowing down to an equilibrium or quasi-equilibrium state is usually described and studied as an initial value problem. However, if we are interested in particle distributions in the vicinity of sources and boundaries we must construct our solution in terms of a boundary value problem. Here we seek and develop a solution to Eq (1) as a boundary value problem.

To further develop the transport equation and the precise model which will be used we seek simplifications to Eq (1). First we limit the collisional processes to those which are uncorrelated, and instantaneous or localized in space. In a sense we are limited to collision events which are well separated in terms of mean free paths, i.e., the particle mean free path must be larger than the range of interaction forces. Then we can write the collision operator as

$$\left.\frac{\partial n}{\partial t}\right)_{coll} = \int d^3\hat{v}' |\hat{v}'| \sigma_s(\hat{r},\hat{v}'\rightarrow\hat{v}) n(\hat{r},\hat{v}',t) - |\hat{v}| \sigma_t(\hat{r},\hat{v}) n(\hat{r},\hat{v},t) \tag{2}$$

where $d^3\hat{v}$ is an elemental volume in velocity space and

$\sigma_t(\hat{r},\hat{v})$ = probability per unit distance travelled that a particle at position $\hat{r}$ and with velocity $\hat{v}$ will have an interaction, and

$\sigma_s(\hat{r},\hat{v}'\rightarrow\hat{v})$ = probability per unit distance travelled that at position $\hat{r}$ a particle with velocity $\hat{v}'$ will undergo a collision and produce a particle with velocity $\hat{v}$; and

$|\hat{v}|$ = particle speed (a scalar)

At this point we can ignore all collective effects and if electric and magnetic fields along with the initial and

boundary conditions are given we can now attempt to solve Eq (1) directly. However, this is still a formidable task and we usually make further simplifications. If we cannot ignore collective effects and make these simplifications, as is the case in a dense plasma with a small debye length, then we must attempt to solve Eq (1) and determine the electric and magnetic fields self-consistently using Maxwell's equations.

To obtain the usual neutral particle (Boltzmann) transport equation, we further ignore all macroscopic forces and delete the force term $\frac{F}{m}\cdot\nabla_v n(\hat{r},\hat{v},t)$. This is a reasonable approximation if there is no external electromagnetic field or charge particles present, or if the external magnetic field is weak and the particle distribution function is isotropic in velocity space. With these assumptions we can now write the reduced transport equation (Tran and Ligou, 1981) as

$$\frac{\partial n}{\partial t}(\hat{r},\hat{v},t) + \hat{v}\cdot\nabla n(\hat{r},\hat{v},t) + |v|\sigma_t(\hat{r},\hat{v})n(\hat{r},\hat{v},t) = \int d^3\hat{v}'\,|v'|\sigma_s(\hat{r},\hat{v}'\to v)n(\hat{r},\hat{v}',t) + q(\hat{r},\hat{v},t) \quad (3)$$

The integral term in Eq (3) represents a source of scattered particles from all other velocities into the velocity space $\hat{v}$. This term is usually called the scattering kernel.

We are now in a position to make a change of variables which is required in the usual multigroup formalism, and also to write Eq (3) in terms of the angular or phase space flux. To do this we must first write the angular or phase space flux as

$$\phi(\hat{r},\hat{v},t) = |\hat{v}|n(\hat{r},\hat{v},t) \tag{4}$$

and the velocity vector as

$$\hat{v} = |\hat{v}|\hat{\Omega} \tag{5}$$

where $\hat{\Omega}$ is the direction of particle travel and the particle speed $|\hat{v}|$ can be written in terms of its energy as

$$|\hat{v}| = \left(\frac{2E}{m}\right)^{\frac{1}{2}} \tag{6}$$

Making the change of variable from $\hat{v}$ to E and $\hat{\Omega}$ we can now write the transport equation in terms of the angular flux $\phi(\hat{r},E,\hat{\Omega},t)$ as

$$\frac{1}{|\hat{v}|}\frac{\partial\phi}{\partial t}(\hat{r},E,\hat{\Omega},t) + \hat{\Omega}\cdot\nabla\phi(\hat{r},E,\hat{\Omega},t) + \sigma_t(\hat{r},E)\phi(\hat{r},E,\hat{\Omega},t)$$
$$= \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \, \sigma_s(\hat{r},E',\hat{\Omega}'\rightarrow E,\hat{\Omega})\phi(\hat{r},E',\hat{\Omega}',t) + q(\hat{r},E,\hat{\Omega},t) \tag{7}$$

Eq (7) is the standard time dependent transport equation, which, with associated initial and boundary conditions is primarily a description of neutral particle transport. However, depending upon the treatment of the scattering kernel it can also be used to describe and solve certain charged particle transport problems (Przbylski and Ligou, 1981).

It is important to note that Eq (7) is an integral-differential equation with seven independent variables, where we have rewritten the angular or phase space flux from a function of $(\hat{r},\hat{v},t) = (x,y,z,v_x,v_y,v_z,t)$ to one where $(\hat{r},\hat{v},t) = (\hat{r},E,\hat{\Omega},t) = (x,y,z,E,\theta,\chi,t)$, and $\hat{r}$ is in a rectangular spatial geometry. The source term $q(\hat{r},E,\hat{\Omega},t)$ contains sources due to fissions and other absorption processes which depend on the angular flux. Furthermore, and although this is not usually true, Eq (7) could be non-linear if the scattering cross-section (σ_s) is expressed as a function of the angular flux.

The Boundary, Continuity and Interface Conditions

In order to complete our description of the problem and formulate a numerical solution we must first specify initial and boundary conditions. The initial condition is simply given by

$$\phi(\hat{r},E,\hat{\Omega},t_o) = \phi_o(\hat{r},E,\hat{\Omega}) \text{ for all } \hat{r}, E \text{ and } \hat{\Omega} \qquad (8)$$

where t_o is some initial time.

The boundary conditions depend on the problem of interest. In this study we will consider a set of the most common boundary conditions. These are:

a. Vacuum boundary. This is a boundary condition where particles are allowed to leave the surface but are not allowed to reenter it. This imposes the condition that all incoming flux is zero at the surface. In effect this boundary condition says that the flux is zero for all incoming directions and it is usually written as

$$\phi(\hat{r}_s,E,\hat{\Omega},t) = 0 \quad \text{for all } \hat{\Omega} \text{ such that } \hat{\Omega}\cdot\hat{n} < 0 \qquad (9)$$

where $\hat{r}_s$ denotes the boundary and $\hat{n}$ is a unit outward normal to the surface.

b. Incident source. In this case particles are allowed to enter and leave the system. The entering particles represent an incident source of particles on the boundary. This boundary condition can be written as

$$\phi(\hat{r}_s,E,\hat{\Omega},t) = q_s(\hat{r}_s,E,\hat{\Omega},t) \quad \text{for all } \hat{\Omega} \text{ such that } \hat{\Omega}\cdot\hat{n} < 0 \qquad (10)$$

where q_s is known.

c. Dirichlet boundary condition. The angular flux can be completely specified at the boundary as

$$\phi(\hat{r}_s,E,\hat{\Omega},t) = \phi_s(\hat{r}_s,E,\hat{\Omega},t) \tag{11}$$

where $\phi_s(\hat{r}_s,E,\hat{\Omega},t)$ is given and could be a known seven dimensional function specified at the boundary, or a constant in some or all of the independent variables $(\hat{r},E,\hat{\Omega},t)$.

d. Albedo or reflecting boundary. For this boundary condition we assume that some of the particles leaving the system are reflected back into the system. This condition can be represented as (Duderstadt and Hamilton, 1976)

$$\phi(\hat{r}_s,E,-\hat{\Omega},t) = \alpha(\hat{r}_s)\phi(\hat{r}_s,E,\hat{\Omega},t) \tag{12}$$

where $\alpha(\hat{r}_s)$ is the local albedo or fraction of particles which are reflected. If $\alpha(\hat{r}_s) = 1$, then this is the usual condition of total reflection where all the particles are reflected back across the surface. It is important to note that the albedo could be a function of $\hat{r}_s,\hat{\Omega},E$ and t (Chilton et al., 1984). However, in order to simplify the notation we have chosen to write it as a function of $\hat{r}_s$ only.

The interface and continuity conditions are just expressions of continuity of the angular flux in space and

time (Bell and Glasstone, 1970). They can be written as

$$\lim_{s\to o} \phi(\hat{r} + s\hat{\Omega},\hat{\Omega},E,t + s/v) = \lim_{s\to o} \phi(\hat{r} - s\hat{\Omega},\hat{\Omega},E,t - s/v) \qquad (13)$$

where s represents a distance of particle travel along $\hat{\Omega}$ and $\hat{r}$ could be any point within the problem domain to include an interface. This condition requires the continuity of particle flux in space and time for a given energy and direction. Note that the flux can be discontinuous in velocity (direction and energy), and it usually is especially at vacuum boundaries and at interfaces (Bell and Glasstone, 1970).

Summary

Now we have a complete and general mathematical description of neutral particle transport processes and conservation, as it is represented by the first order form of the time dependent transport equation. Further descriptions and simplifications can be made with respect to the time, energy, angular and space dependences, and also with respect to scattering and sources. However, with or without these additional simplifications, the main solution techniques for solving the transport equation with associated

boundary and continuity conditions are the P_n method or diffusion theory, discrete ordinates, and Monte Carlo. These methods are well documented and a complete and detailed description of them can be found in the literature. See Bell and Glasstone (1970), Greenspan, et al. (1968) and Duderstadt and Hamilton (1976). These descriptions will not be repeated here. Instead, we will now present an alternate finite element method for solving the second order forms of Eq (7) with the boundary and continuity conditions of Eqs (9) through (13).

CHAPTER III

THE FINITE ELEMENT METHOD

The finite element method is a projection method where the problem solution is expanded in a finite sum of piecewise functions. The basic projection procedure is to divide the problem space into a finite number of discrete subdomains called elements and to define the solution in terms of locally defined functions with unknown coefficients. This trial space of piecewise functions, which are locally defined on individual elements of the problem space, forms a local basis where the unknown and to be determined coefficients are usually called generalized coordinates (Desai and Abel, 1972). Thus the fundamental concept of the finite element method is that the solution can be approximated by a local basis and some projection or approximation technique.

Widespread use of the finite element method began in the 1950's, with its use in solving structural problems in the design of aircraft. Since then the method has been applied to problems in such diverse areas as solid and fluid mechanics, heat transfer, and particle transport. Its versatility and advantages in solving problems with

differing material properties, complex and irregular geometries, and with a variety of boundary conditions have contributed to the success of this solution approach in solving general problems of physical and engineering interest. Its relation to a classical Raleigh-Ritz solution and the method of projections, coupled with a theoretical foundation in approximation theory, has assured convergence for many problems (Whiteman, 1975). Also, the usual practice of using a local basis of piecewise polynomials and standard element types and shapes, facilitates the numerical treatment and computer implementation of the method. These factors coupled with the availability of large computers have made the finite element method successful. We will discuss some of these factors in the following sections.

Discretization of the Problem Domain

When applying the finite element method the problem space must be divided into subregions or elements (Hinton and Owen, 1979). The numerical analyst or engineer must decide as to the number, type and shape of elements to be used. He must also decide upon the number of nodes (interpolation points) within each element, the type of nodal variables, and the type of interpolation functions.

Usually for one-dimensional problems with one independent variable the element is a straight line with two nodes and a linear Lagrange polynomial basis. However, if a local basis of higher order Lagrange polynomials is used then the number of nodes must correspond to the order of the polynomials.

In two and three dimensions there is a wider choice of elements available. The most common two-dimensional elements are the triangle, rectangle, and general quadrilateral. Again, the number and types of nodes and nodal variables depend on the element type and the order of the interpolating polynomials. For problems in three dimensions with axial symmetry we can construct axisymmetric ring elements. These elements which are defined by two independent variables are usually useful in cylindrical geometry. They are really based on two dimensional elements, which then allow us to construct axisymmetric triangles, rectangles or quadrilateral ring elements. Other three-dimensional elements are the tetrahedron, parallelepiped or right prism, and the general hexahedron (Tong and Rossettos, 1977).

In addition there are a large number and variety of element types and shapes other than the most commonly used ones. It is also possible to construct elements with curved

sides. These elements are very useful for modeling problems with curved boundaries. They are usually constructed in a local element coordinate system called natural coordinates. In these coordinates they are straight-edged elements, however, when they are transformed back into the problem or global frame they produce elements with curved sides (Whiteman, 1976). Figure 1 shows some two and three-dimensional elements.

Polynomial Basis and Generalized Coordinates

The most widely used and accepted trial functions are polynomials. These functions are used to represent the behavior of the solution within each element. They also determine the number of nodes within each element and the type of nodal variables. Depending on the approximating or shape functions, we can have elements with interior and exterior nodes (Oden and Reddy, 1976). Exterior nodes are those nodes which are on the surface or boundaries of the element. Interior nodes are located within the element boundaries. Furthermore, interior nodes usually lead to a computational procedure called condensation whereby the overall size of the problem matrices and equations is reduced.

The unknown coefficients of the interpolating polynomials are called generalized coordinates. They are not

local coordinate global coordinate

a. 3-node triangle

local coordinate global coordinate

b. 6-node triangle

local coordinate global coordinate

c. 8-node quadrilateral

local coordinate global coordinate

d. 10-node tetrahedron

Figure 1. Isoparametric Element Shapes

associated with actual nodal values of the solution and therefore they do not have any direct physical meaning. However, the usual practice in the finite element procedure is to express these element shape functions in terms of nodal or point values of the solution. These are the unknown coefficients which are to be determined from the approximating procedure of the finite element method. They now represent the solution at specified points (nodes) within the problem domain (Zienkiewicz, 1971). This expression of the unknown polynomial coefficients in terms of nodal values gives a direct physical interpretation to the solution and also insures inter-element continuity.

The most common and widely used polynomial basis is the Lagrange polynomial. However, Hermite and higher order spline bases have also been used. We can derive the Lagrange polynomials in terms of the solution values at the nodes; whereas, Hermite polynomials allow this derivation in terms of the solution and its first derivative. In a Hermite or higher order spline basis the unknown coefficients usually represent not only solution values at the nodes but also solution derivatives (Prenter, 1975).

The interpolating Lagrange polynomial can be written as (Atkinson, 1978)

$$L_k(x) = \Pi \left(\frac{x - x_m}{x_k - x_m} \right), \quad m = 0,1...k-1,k+1...n \tag{14}$$

where $L_k(x)$ is a product of n terms and represents the k^{th} piecewise polynomial of degree n. At $x = x_k$ the polynomial $L_k(x)$ is equal to one and at $x = x_m$ with $m \neq k$ it is equal to zero. Therefore each polynomial has n zeros.

For a one dimensional element with n points (nodes) we can usually approximate our solution $\phi(x)$ by

$$\phi(x) \cong \sum_{i=0}^{n} \phi_i L_i(x) \tag{15}$$

where $\phi_i = \phi(x_i)$ and represents the solution values at the nodes. $L_i(x)$ then represents our shape or trial functions.

An alternate shape function can be written for this element in terms of a monomial basis and generalized coordinates as follows

$$\phi(x) = \sum_{i=0}^{n} \alpha_i x^i \tag{16}$$

where α_i represents the generalized coordinates or unknown coefficients. A direct procedure for deriving the Lagrange

basis Eq (15) from Eq (16) can be found in Heubner, 1975. Derivations and expressions of Hermite and general spline bases can be found in the literature and will not be repeated here. Interpolation polynomials in two and three dimensions and for various element types and shapes can also be found in most books on the finite element method. It is not our purpose to present them here. However, we will now briefly discuss the concept of natural coordinates and parametric elements.

Natural Coordinates

A local coordinate system which depends on the element type and shape, and has values which range between one and minus one is called a natural coordinate system. These coordinates are defined with respect to element geometry and with a linear variation between nodes. Each coordinate in a n-dimensional system has unit value at one node and zero value at all other nodes. Also, the coordinate functions are usually normalized to one, so that a sum of these functions at any point within the element equals one.

Natural coordinates provides the flexibility of constructing elements of different types, shapes, nodes, nodal variables and interpolation functions. They are very useful in the development of close form integration formulas for evaluating the integrals of the problem equations. Also

they are essential to the construction of elements with curved sides.

The development of natural coordinates for a large number of elements can be readily found in the literature (Tong and Rossettos, 1977). In one, two and three dimensions this development and the concept of natural coordinates is usually synonymous with length, area and volume coordinates respectively. Furthermore, a simple and straightforward prescription for defining a natural coordinate system is based upon the use of Lagrange polynomials. For a three dimensional element we can write the element coordinates as

$$x = \sum_{i=1}^{m} x_i L_i(\varepsilon) \tag{17}$$

$$y = \sum_{i=1}^{m} y_i L_i(\eta) \tag{18}$$

$$z = \sum_{i=1}^{m} z_i L_i(\beta) \tag{19}$$

where ε, η and β range between one and minus one, and x_i, y_i, and z_i represent nodal values of the element in the global or problem coordinates; m is the number of element nodes and L_i represents the usual Lagrange interpolant of

Eq (14). Then we can write the element approximation or shape functions as

$$\phi(\varepsilon,\eta,\beta) = \sum_{i=1}^{m} \phi_i N_i(\varepsilon,\eta,\beta) \tag{20}$$

where $\phi_i = \phi_i(\varepsilon,\eta,\beta)$ and represents the solution values at the nodes. Also

$$N_i(\varepsilon,\eta,\beta) = L_i(\varepsilon)L_i(\eta)L_i(\beta) \tag{21}$$

There are many other ways of deriving a natural coordinate representation of the element trial space. A similar representation to Eq (21) for one and two dimensional elements can also be obtained using Lagrange polynomials. However, in general, this approach is limited, especially in the construction of high order cubic and quintic elements (Huebner, 1975). For these elements, other approaches are used, which reduce the number of interior nodes. An example of this is the family of high-order rectangular elements developed by Ergatoudis, et al., (1968). These elements have only exterior nodes, but they also allow the parametric representation of natural coordinates.

For problems with complex geometries and curved boundaries an accurate physical description can be achieved in the finite element representation by the use of parametric elements. These are curved-sided elements in the global or problem coordinates. The idea is to map or transform straight-sided elements in the natural coordinates to curved-sided elements in global coordinates. Then, to evaluate the problem equations and solve the problem in this global problem space. Unlike a solution in the natural coordinate space where we can use closed form integration formulas we must now use numerical integration techniques. Numerical integration is usually required because of the complexity of the integrals in the global problem space (Segerlind, 1976).

In transforming from the natural or local coordinates to the global coordinates we usually assume that this transformation (Jacobian) exists and is unique. However, there are prescriptions and checks to ensure that this is indeed the case (Aziz, 1972). Furthermore, in an isoparametric representation which satisfies certain completeness criteria, existence and uniqueness is guaranteed (Huebner, 1975).

There are three basic categories of parametric elements depending upon the number of element nodes and the interpola-

tion polynomial. The underlying concept is that the interpolating polynomial which determines and maps the element shape can be different than those of the solution or trial space. For an isoparametric representation (or element) these polynomials are the same. However for a subparametric element its shape is defined by a lower order polynomial than those of the trial space whereas a superparametric element is defined by higher order polynomials. As an example, an isoparametric element could be represented by Eqs (17) to (19) where the L_i's are the same as those of Eq (21).

Application to Transport Problems

The application of finite elements to transport problems began in the 1970's with a finite element solution of the diffusion equation (Kaper, et al., 1972). For the one speed diffusion equation the Galerkin projection approach produces a self-adjoint system which is equivalent to a classical Raleigh-Ritz solution (Strang and Fix, 1973). Because of this equivalence the finite element method gained widespread acceptance as a viable approach to solving particle diffusion problems. Questions of existence, uniqueness and convergence of the solution could be dealt with

in the framework of a variational principle and the minimization of a functional, or in terms of the related energy methods of Miklin (1966).

The finite element method has also been applied to the transport equation. Kaper, et al., (1974), Ohnishi (1971), Ukai (1972), Reed (1973), Fletcher (1983) and others have used finite elements to solve the first order forms of the transport equation. Phase-space finite elements in both the space and angle variables have been used. Also, applications of the discrete ordinate method in angle and the finite element method in space have produced the Onetran (Hill, 1975) and Trident (Seed et al., 1977) computer codes. Other finite element applications based on the second order forms of the transport equation, have also been conducted (Sanchez and McCormick, 1982). Specific examples of these applications will be presented in the next chapter.

CHAPTER IV

FINITE ELEMENTS AND SECOND ORDER FORMS

The finite element method is usually a mathematical and numerical technique for obtaining an approximate solution to a large class of problems. Initially it was developed and used to solve problems in stress analysis (Heubner, 1975). Later, as the mathematical foundation of the method was established it gained widespread acceptance and use in solving a larger class of problems.

Finite elements are based on projection procedures, however, they can also be used in the Raleigh-Ritz technique of first recasting the problem in an equivalent variational form and then seeking a solution on the basis of an energy minimization principle (Strang and Fix, 1973). Nonetheless, the original Raleigh-Ritz procedure did not include this finite element approach. Instead the solution was expanded in the form of a linearly independent set of global trial functions. Unlike the finite element method, these global functions were neither piecewise polynomials nor were they equal to zero on parts of the problem domain.

Using this expansion of global trial functions, the Raleigh-Ritz procedure was to find an extremum (minimum or maximum) of the variational principle (functional). If this linear combination of globally defined functions did not extremize the functional, then the class (or space) of functions was expanded by the addition of more functions. This expansion of the trial space continues until a linear combination of functions which is an extremum of the functional is obtained (Miklin, 1964).

In the finite element approach the problem domain is divided into smaller regions or elements, and the trial functions are piecewise polynomials which are zero on parts of the solution domain (a local basis). Also, the trial space (number of trial functions) is expanded by using more elements and not by the addition of a new class of functions. Because of these differences the finite element method is more adaptable towards a numerical (computer) solution than the original Raleigh-Ritz procedure.

For some problems the classical Raleigh-Ritz procedure is really a Galerkin projection method. For these problems it can be shown (Finlayson and Scriven, 1966) that the Galerkin method is equivalent to Raleigh-Ritz. An identical set of matrix equations and therefore the same solution is achieved by either method. Therefore, for many

problems the use of finite elements in a classical Raleigh-Ritz solution can be considered to be a finite element projection method. These concepts will be described in some detail in Chapter VI of this report.

Projection methods however, do not usually include the use of a variational principle or the calculus of variations. In some problems a variational principle has not been developed or may not exist, and therefore, the Raleigh-Ritz approach cannot be used. Nonetheless, in such cases, projection methods can be used to solve the problem. Therefore projection methods can be extended to a wider class of problems than Raleigh-Ritz.

The equivalence between Raleigh-Ritz and the Galerkin method usually exists for problems which are self-adjoint. This equivalence is useful when considering questions of existence, uniqueness, convergence, error bounds and the treatment of boundary conditions (Miklin, 1964). Therefore, a mathematical formalism which is self-adjoint and equivalent to a classical Raleigh-Ritz solution is desirable. Unfortunately however, the first order form of the transport equation is non-self-adjoint (Duderstadt and Martin, 1979). This is due to the scattering kernel, and streaming operator or gradient term of Eq (7), which are non-self-adjoint.

In contrast, the diffusion equation (Duderstadt and Hamilton, 1976) which is similar to a Sturm-Liouville problem is self-adjoint with an equivalent classical Raleigh-Ritz solution (Hardin, 1977). However, the diffusion equation does not have the detailed angular information which is required in the solution of most problems of general engineering and physical interest. For these problems a mathematical model which is self-adjoint and retains the detailed angular information of Eq (7) is required. This model is the second order form of the transport equation which in the limit of diffusion theory reduces to the diffusion equation.

The Even and Odd Parity Equations

In order to obtain a mathematical model which is self-adjoint and would permit a rigorous treatment of general boundary conditions, the even and odd parity forms of the transport equation will be developed. The starting point of this development will be a simplified form of Eq (7) and the associated boundary conditions of Chapter II. These simplifications will result in the steady state and energy independent or one group transport equation. We will begin our development with a brief discussion of the usual numerical strategies for solving

time and energy dependent problems. This is the general problem, presented in Chapter II, which we would like to solve. Therefore, our intent is to explain that the following monoenergetic steady state treatment can be easily extended to time and energy dependent problems. A complete and general treatment of particle transport requires this time and energy dependent solution.

The usual multigroup treatment of the energy dependence in particle transport problems is well-established (Bell and Glasstone, 1970). This multigroup formalism involves approximating the energy variable by piecewise constant functions on fixed energy intervals called energy groups. This produces a discontinuous approximation in energy and a set of coupled one group or monoenergetic problems. The multigroup formalism is a straightforward extension of the monoenergetic development to include multigroup fluxes, scattering, sources and a set of coupled one group problems. Therefore, a one group development is directly applicable and can be easily extended to an energy dependent treatment of particle transport.

In the time dependent case there are a number of approaches available. These approaches include the well-known point kinetics model of reactor physics, and an exponential time dependence (Bell and Glasstone, 1970). For

diffusion theory, the assumption of an exponential time dependence produces a non-linear problem and involves an eigenvalue search for the largest time eigenvalue (Wachpress, 1966). However, the usual discrete model is to represent the time derivative of Eq (7) by an explicit forward or weighted difference (Duderstadt and Martin, 1979). This finite difference approximation in contrast to the multigroup energy formalism retains the basic steady state treatment. It involves a set of implicitly coupled steady state (time independent) problems whereas the multigroup formalism produces a set of implicitly coupled one group problems. Therefore, energy and time dependent problems can be solved by a straightforward extension of our steady state monoenergetic treatment.

To be precise, we can discretize the time and energy dependence of Eq (7) and write it as

$$\frac{\phi_b^{\ell+1} - \phi_b^{\ell}}{v_b \Delta t_\ell} + L\, \phi_b{}^{\ell+1}(\hat{r},\hat{\Omega}) = Q_b{}^{\ell+1} \qquad (22)$$

and then rewrite it as

$$\tilde{L}\, \phi_b^{\ell+1}(\hat{r},\hat{\Omega}) = \tilde{Q}_b{}^{\ell+1} \qquad (23)$$

where the operator,

$$L\circ = \hat{\Omega}\cdot\nabla\circ + \sigma_{tb}\circ - \int_{4\pi} d\hat{\Omega}'\,\sigma_{sb\to b}(\hat{r},\hat{\Omega}'\to\hat{\Omega})\circ \tag{24}$$

and

$$\tilde{L} = L + \frac{1}{v_b \Delta t_\ell} \tag{25}$$

and

$$\tilde{Q}_b^{\ell+1} = Q_b^{\ell+1} + \frac{\phi_b^\ell}{v_b \Delta t_\ell} \tag{26}$$

Also $\Delta t_\ell = t_{\ell+1} - t_\ell$, where ℓ and b represent the time and energy indices respectively, and ϕ_b, $\phi_b^{\ell+1}$, σ_{tb}, $\sigma_{sb\to b}$ and $Q_b^{\ell+1}$ are the usual multigroup defined quantities (Bell and Glasstone, 1970). Therefore, Eq (23) is a set of one group, steady state equations with modified and redefined sources, fluxes and cross-sections. In fact, these equa-

tions represent the one group steady-state form of Eq (7) with modified sources as in Eq (26) and with a modified total cross-section $\tilde{\sigma}_t$ defined as

$$\tilde{\sigma}_t = \sigma_{tb} + \frac{1}{v_b \Delta t_\ell} \tag{27}$$

The significance of Eq (23) is that we have reduced the problem to a set of coupled algebraic equations in time and energy. Starting with some initial condition we can solve for the time dependence by a simple marching scheme. At each step we must then solve implicitly a set of coupled one group equations for the group angular flux. This is the usual procedure for obtaining a complete seven-dimensional solution to the transport equation (Dupree, et al., 1971 and Hill, 1976). This fully implicit scheme is unconditionally stable (Clark and Hansen, 1964).

Since we have reduced the problem to a series of steady-state one group problems we will now drop the explicit time and energy dependence and proceed with our development. However, it is important to bear in mind this obvious extension to general time dependent and multigroup problems. Following the derivation of Kaplan

and Davis (1967), Wheaton (1978), and Wills (1981) we can write the monoenergetic steady-state form of Eqs (7) or (23) in terms of the $-\hat{\Omega}$ vector, where $-\hat{\Omega}$ represents the direction opposite to $\hat{\Omega}$. This gives

$$-\hat{\Omega}\cdot\nabla\phi(\hat{r},-\hat{\Omega}) + \sigma_t(\hat{r})\Phi(\hat{r},-\hat{\Omega}) - \int_{4\pi} d\hat{\Omega}'\,\sigma_s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\phi(\hat{r},\hat{\Omega}') = Q(\hat{r},-\hat{\Omega}) \tag{28}$$

where in the case of Eq (23) the source Q and the total cross-section $\sigma_t(\hat{r})$ are defined in accordance with Eqs (26) and (27), and we have dropped the explicit time and energy dependent notation.

The even and odd parity terms will now be defined as

$$\Psi^g(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{\phi(\hat{r},\hat{\Omega}) + \phi(\hat{r},-\hat{\Omega})\right\} \tag{29}$$

$$\Psi^u(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{\phi(\hat{r},\hat{\Omega}) - \phi(\hat{r},-\hat{\Omega})\right\} \tag{30}$$

$$Q^g(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{Q(\hat{r},\hat{\Omega}) + Q(\hat{r},-\hat{\Omega})\right\} \tag{31}$$

$$Q^u(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{Q(\hat{r},\hat{\Omega}) - Q(\hat{r},-\hat{\Omega})\right\} \tag{32}$$

$$\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \tfrac{1}{2}\left\{\sigma_s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') + \sigma_s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\right\} \tag{33}$$

$$\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = \tfrac{1}{2}\left\{\sigma_s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') - \sigma_s(\hat{r},-\hat{\Omega}\cdot\hat{\Omega}')\right\} \tag{34}$$

where

$\psi^g(\hat{r},\hat{\Omega})$ = even parity flux

$\psi^u(\hat{r},\hat{\Omega})$ = odd parity flux

$Q^g(\hat{r},\hat{\Omega})$ = even parity source

$Q^u(\hat{r},\hat{\Omega})$ = odd parity source

$\sigma_s^g(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ = even parity scattering cross-section

$\sigma_s^u(\hat{r},\hat{\Omega}\cdot\hat{\Omega}')$ = odd parity scattering cross-section

We can now proceed as in Wills (1981), to derive the even and odd parity second order forms of the transport equation which are

$$-\hat{\Omega}\cdot\nabla K^u(\hat{r})\hat{\Omega}\cdot\nabla\psi^g(\hat{r},\hat{\Omega}) + G^g(\hat{r})\psi^g(\hat{r},\hat{\Omega}) = Q^g(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla K^u(\hat{r})Q^u(\hat{r},\hat{\Omega}) \tag{35}$$

and

$$-\hat{\Omega}\cdot\nabla K^{g}(\hat{r})\hat{\Omega}\cdot\nabla\Psi^{u}(\hat{r},\hat{\Omega}) + G^{u}(\hat{r})\Psi^{u}(\hat{r},\hat{\Omega}) = Q^{u}(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla K^{g}(\hat{r})Q^{g}(\hat{r},\hat{\Omega}) \tag{36}$$

We can express the odd parity flux in terms of the even parity flux as

$$\Psi^{u}(\hat{r},\hat{\Omega}) = K^{u}(\hat{r})\left\{Q^{u}(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi^{g}(\hat{r},\hat{\Omega})\right\} \tag{37}$$

and the odd parity flux as,

$$\Psi^{g}(\hat{r},\hat{\Omega}) = K^{g}(\hat{r})\left\{Q^{g}(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi^{u}(\hat{r},\hat{\Omega})\right\} \tag{38}$$

and the operators G^{g}, G^{u}, K^{u} and K^{g} are defined as (Wills, 1981),

$$G^{g}(\hat{r})_{\circ} = \sigma_{t}(\hat{r})_{\circ} - \sum_{\ell=0}^{L}\sum_{m=-\ell}^{+\ell}\sigma_{\ell}^{g}(\hat{r})Y_{\ell,m}(\hat{\Omega})\int_{4\pi}d\hat{\Omega}'Y_{\ell,m}^{*}(\hat{\Omega}')_{\circ} \tag{39}$$

$$G^u(\hat{r})_\circ = \sigma_t(\hat{r})_\circ - \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \sigma_\ell^u(\hat{r}) Y_{\ell,m}(\hat{\Omega}) \int_{4\pi} d\hat{\Omega}' Y^*_{\ell,m}(\hat{\Omega}')_\circ \quad (40)$$

$$K^g(\hat{r}) = \left[G^g(\hat{r})\right]^{-1}$$

$$= \sigma_t^{-1}(\hat{r}) \left[1_\bullet + \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \frac{\sigma_\ell^g(\hat{r})}{\sigma_\ell(\hat{r}) - \sigma_\ell^g(\hat{r})} Y_{\ell,m}(\hat{\Omega}) \int_{4\pi} d\hat{\Omega}' Y^*_{\ell,m}(\hat{\Omega}')_\bullet \right] \quad (41)$$

$$K^u(\hat{r}) = \left[G^u(\hat{r})\right]^{-1}$$

$$= \sigma_t^{-1}(\hat{r}) \left[1_\bullet + \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} \frac{\sigma_\ell^u(\hat{r})}{\sigma_t(\hat{r}) - \sigma_\ell^u(\hat{r})} Y_{\ell,m}(\hat{\Omega}) \int_{4\pi} d\hat{\Omega}' Y^*_{\ell,m}(\hat{\Omega}')_\bullet \right] \quad (42)$$

Here we have followed the usual practice of expanding the scattering cross-section in spherical harmonics ($Y_{\ell m}$), and the $*$ superscript means the complex conjugate function. Also, the even and odd parity scattering cross-section coefficients are defined (Wills, 1981) as

$$\sigma_\ell^g(\hat{r}) = \begin{cases} \sigma_\ell(\hat{r}) & \text{for } \ell \text{ - even} \\ 0 & \text{for } \ell \text{ - odd} \end{cases} \quad (43)$$

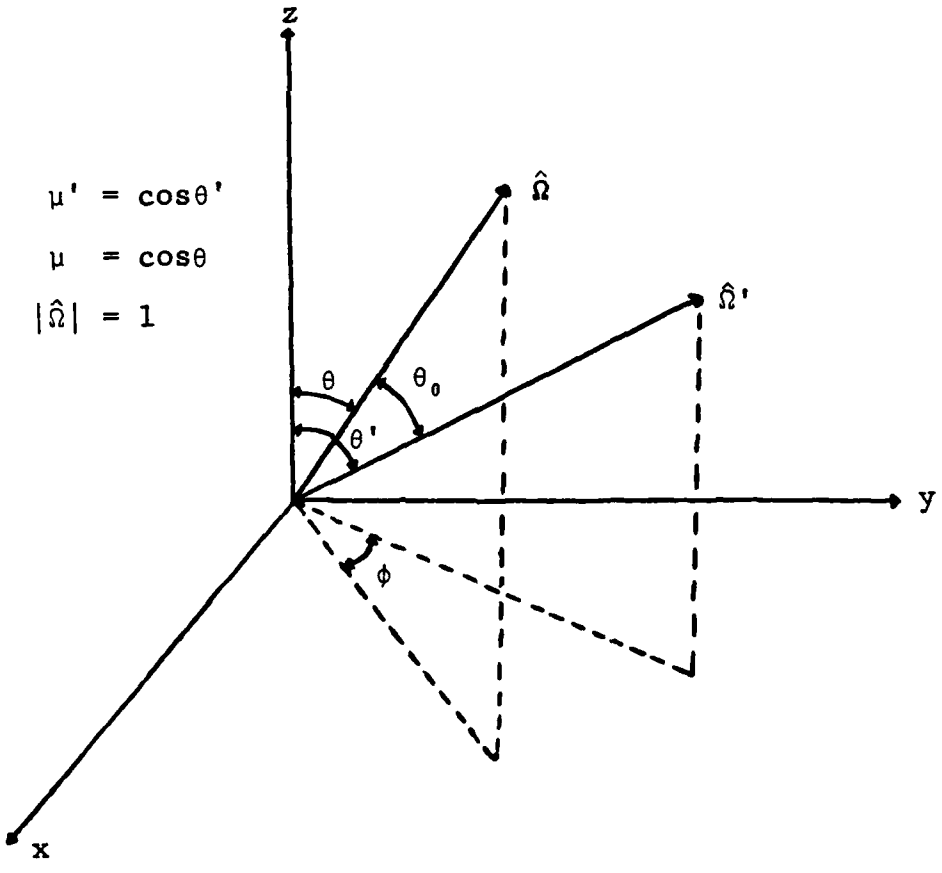
$$\sigma_\ell^u(\hat{r}) = \begin{cases} \sigma_\ell(\hat{r}) & \text{for } \ell \text{ - odd} \\ 0 & \text{for } \ell \text{ - even} \end{cases} \tag{44}$$

where $\sigma_\ell(\hat{r})$ is the Legendre scattering cross-section expansion coefficients. These coefficients originate from the usual expansion or fit of the cross-section data with Legendre polynomials. This expansion can be written as

$$\sigma_s(u_o) = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} \sigma_\ell P_\ell(u_o) \tag{45}$$

where u_o is the angle of scatter (See Figure 2) and it is normally assumed that scattering depends only on the angle of scatter and not on the azimuthal angle or the incident direction (Duderstadt and Hamilton, 1976). The cross-section expansion of Eq (45) can now be transformed or expressed in terms of the problem coordinates by use of the addition theorem (Bell and Glasstone, 1970).

In order to complete our development of the second order forms of the transport equation, we will now discuss the associated boundary conditions. These boundary conditions which were presented in Chapter II must now be re-



$\mu_0 = \cos\theta_0 = \hat{\Omega}\cdot\hat{\Omega}'$ = cosine of the angle of scatter

$= \mu\mu' + \sqrt{(1 - \mu^2)(1 - \mu'^2)} \cos\phi$

ϕ = azimuthal angle

Figure 2. Scattering Angle

written in terms of the even and odd parity flux. So as to reduce the algebra we will now write them as

$$\psi^g(\hat{r}_s,\hat{\Omega}) + \psi^u(\hat{r}_s,\hat{\Omega}) = \alpha(\hat{r}_s)\left[\psi^g(\hat{r}_s,\hat{\Omega}) - \psi^u(\hat{r}_s,\hat{\Omega})\right] + bq_s(\hat{r}_s,\hat{\Omega}) \quad \text{for } \hat{\Omega}\cdot\hat{n} < 0 \qquad (46)$$

where the adjoint boundary condition is

$$\psi^g(\hat{r}_s,\hat{\Omega}) + \psi^u(\hat{r}_s,\hat{\Omega}) = \alpha(\hat{r}_s)\left[\psi^g(\hat{r}_s,\hat{\Omega}) + \psi^u(\hat{r}_s,\hat{\Omega})\right] + bq_s(\hat{r}_s,\hat{\Omega}) \quad \text{for } \hat{\Omega}\cdot\hat{n} > 0 \qquad (47)$$

and $o \leq \alpha(\hat{r}_s) \leq 1$, and b is equal to zero or one.

For the,

1. Vacuum boundary

   $\alpha(\hat{r}_s) = b = 0$

and,

2. Incident source

   $\alpha(\hat{r}_s) = 0$; $b = 1$

and,

3. Albedo condition

$o < \alpha(\hat{r}_s) \leq 1 \; ; \; b = 0$

and,

4. Mixed condition

$o < \alpha(\hat{r}_s) \leq 1 \; ; \; b = 1$

also for the,

5. Dirichlet condition

$$\psi^g(\hat{r}_s,\hat{\Omega}) + \psi^u(\hat{r}_s,\hat{\Omega}) = \phi_s(\hat{r}_s,\hat{\Omega}) \qquad (48)$$

and ψ^g and ψ^u can also be found from Eqs (29) and (30). Finally, the interface and continuity conditions require that the odd and even parity flux be continuous in space and time for a given energy and direction.

We have now presented the second order forms of the transport equation. In this derivation the angular flux is expressed in terms of even and odd components on the unit sphere. These components are the even and odd parity fluxes which are just the sum and difference of the forward and adjoint angular flux (Bell and Glasstone, 1970).

It is imporatnt to note that unlike the first order transport equation, this second order formalism is positive definite and self-adjoint. This is because the operators of Eqs (35) and (36) are positive definite and self-adjoint. (Kaplan and Davis, 1967).

The Application of Finite Element Projections to Second Order Forms

The application of a finite element projection method to solve particle transport problems is not a new concept. Kaplan, in 1961, proposed a projection technique for solving three-dimensional reactor problems. This technique, which he called flux synthesis, was based upon a variational Galerkin type solution of the diffusion equation. Later, Kaplan, et al., (1967) extended this idea to solve the transport equation. They based their solution on a variational principle whose Euler-Lagrange equations are the second order forms of the transport equation. They also used special ellipsoid trial functions and a space-angle synthesis approach to solve steady-state Milne problems with isotropic scattering.

The concept of space-angle synthesis is really a projection technique for modeling the angular dependence of the transport equation. The angular flux is represented by a

linear combination of known functions and mixing coefficients, which are required to satisfy the problem equations in an approximate sense (Natelson, 1968). In contrast discrete ordinates or the S_n method restricts particles to move in certain fixed directions and allows only a finite number of degrees of freedom in angle.

In 1973, this space-angle synthesis projection technique was used by Miller, et al. to solve a one dimensional neutron transport problem. Later, in 1973, they extended this solution method to two-dimensional problems in x-y geometry with isotropic scattering and sources. A four-dimensional tensor product of linear and bilinear polynomials on a finite element grid, was used in the minimization of a functional for the even parity transport equation. Their approach involved the use of both rectangular and triangular elements and the imposition of vacuum and reflective boundary conditions. The vacuum boundary conditions were treated as natural conditions whereas reflection was an essential boundary condition to be imposed on the trial space. As a result of these calculations they concluded that this finite element solution mitigated the ray effect problem which is present in discrete ordinates (Lathrop, 1968).

Other researchers including Kaper, et al., (1974), Briggs, et al. (1975), Ackroyd (1979), and Blomquist and Lewis (1980), have used finite elements to solve the second order transport equation. Kaper, et al. (1974), applied finite elements based on a variational formulation to the two-dimensional multigroup transport equation. They used high order cubic finite elements, surface harmonic tensors, and linear Lagrange polynomials over the angular domain. This was coupled with a product of piecewise and global Lagrange polynomials in space. Their conclusion was that high order finite elements were not a viable alternative to discrete ordinates.

Subsequently, Briggs, et al., in 1975, applied finite elements to the variational problem of the second order one group two-dimensional neutron transport equation in x-y geometry. They examined the potential of this solution approach to mitigate ray effects and concluded that ray effect mitigation was due to the elliptic operators of the finite element formalism whereas the discrete ordinate equation was hyperbolic. The elliptic nature of the finite element equations allowed the coupling or averaging of the particle streaming along different paths (directions). They argued that this elliptic coupling which is also present in the diffusion equation, but absent in the S_n method, is essential for ray effect mitigation.

CHAPTER V

VARIATIONAL PRINCIPLES

Variational methods have played an important role in many areas of mathematical physics. Many physical problems, especially in the areas of thermodynamics and classical and quantum mechanics, are connected with the calculus of variations. Variational calculus and in particular Hamilton's principle, have played a vital role in describing the dynamics of particle motion (Lanczos, 1949). Unlike Newton's laws of motion, which are based upon the vector quantities of momentum and force, Hamilton's (variational) principle provides an alternate mathematical description in terms of energy, which is a scalar.

In this variational model the basic concept is that the motion of a mechanical system can be described by finding the minimum (or maximum) of a definite integral (functional). This minimization or variational problem is dealt with by the calculus of variations (Courant and Hilbert, 1953). Using a variational calculus approach, it is possible to show the equivalence between a variational problem and the usual description in terms of a

differential equation. In the case of Hamilton's principle, which describes a mechanical system, the functional is defined in terms of the kinetic and potential energy of the system. However, upon taking the first variation of this functional, we can derive the Euler-Lagrange equation; which, for this problem is just Newton's equation of motion.

This alternate and equivalent formulation of a problem, in terms of a differential equation; or as a variational problem, leads directly to classical approximation techniques for solving a large number of problems. We have already mentioned the classical Raleigh-Ritz solution for diffusion problems, and its equivalence to the Galerkin method. The energy methods of Miklin are also in this category where there is a direct relation between projection methods and Raleigh-Ritz. In fact, this relationship can be easily established for problems which are self-adjoint (Strang and Fix, 1973).

An important consideration in problem solving besides the usual analytical questions of existence, uniqueness, convergence and stability is the treatment of boundary conditions. For problems where a variational approach is available these issues can usually be dealt with in a simple and straightforward manner. As an example of this,

we can normally recast a linear self-adjoint problem in terms of a variational principle and a quadratic functional. We can then consider these issues within the variational context.

In the following sections of this chapter we will briefly discuss linear self-adjoint variational problems. We will examine the treatment of boundary conditions, the classical Raleigh-Ritz solution strategy and applications to the parity equations. Our primary intent in this development is to later establish an equivalence to the Galerkin method. In doing so, we will then be able to treat the analytical issues and boundary conditions within this variational framework.

The Model Problem

It is well-known that some boundary value problems can be written as a variational problem (functional); whose minimum is a function which also satisfies the boundary value problem. Therefore, instead of seeking a solution to the boundary value problem directly, we can seek to find the minimum of a functional. This is usually accomplished by selecting linear combinations of functions on some function space (admissible class of functions). In practice, for linear problems with quadratic functionals, this minimization procedure produces a set of coupled

linear algebraic equations which are not difficult to solve. However, for general non-linear problems this minimization process can produce serious computational difficulties.

A functional is basically the integral of a function, whose arguments or independent variables are themselves functions, and which assigns a real number to each independent variable (function). Therefore, a functional is an expression which converts a function into a scalar. As an example of this, and to make these ideas more precise, we will now present a linear problem and an associated quadratic functional. Our goal is to discuss in a simple setting a linear boundary value problem and the related variational problem. Later, we will extend these concepts to the transport problem.

We begin by writing the classical three-dimensional Sturm-Liouville problem in operator notation as

$$Lu(\hat{r}) = f(\hat{r}) \tag{50}$$

where the self-adjoint operator (Miklin, 1964)

$$L\circ = -\nabla\cdot(p(\hat{r})\nabla\circ) + q(\hat{r})\circ \tag{51}$$

and ∇ represents the usual gradient operator. The associated boundary condition can be written as

$$a(\hat{r}_s)\nabla u(\hat{r}_s)\cdot\hat{n} + b(\hat{r}_s)u(\hat{r}_s) + c(\hat{r}_s) = 0 \tag{52}$$

Eq (52) is the general mixed boundary condition. Setting a, b or c equal to zero, we can obtain the Neumann and Dirichlet homogenous and non-homogenous boundary conditions.

The quadratic functional corresponding to the above problem, Eq (50), can be written as (Mitchell and Wait, 1977)

$$I(u) = \int_V \left[p(\hat{r})\nabla u\cdot\nabla u + q(\hat{r})u^2 - 2f(\hat{r})u(\hat{r})\right]d\hat{r} + \oint_S \left[b(\hat{r}_s)u^2 + 2c(\hat{r}_s)u\right] d\hat{s} \tag{53}$$

where the first integral in Eq (53) is over the entire problem domain (volume) and the second is a surface integral on the problem boundaries.

Eq (53) represents a variational problem which has been studied extensively. It can be shown (Wouk, 1979) that a linear problem of the form of Eq (50), has a solution which is the minimum of the quadratic functional, Eq (53). Furthermore the Euler-Lagrange equation of this functional is the Sturm-Liouville equation. The usual mathematical issues of existence, uniqueness and convergence are also dealt with by Wouk and Miklin. They have shown that for the classical Raleigh-Ritz minimization of Eq (53) existence, uniqueness and convergence are assured.

Therefore, a numerical solution to the Sturm-Liouville problem can be obtained by solving the equivalent variational problem. This solution exists, and can be readily obtained, because the Raleigh-Ritz minimization process produces an operator which is positive definite symmetric. Based on this positive definite operator, we can then prove and answer the questions of existence, uniqueness and convergence. Furthermore, and because of the self-adjoint nature of Eq (50), we can show that a direct solution by the Galerkin method also produces a positive definite operator. By either the variational or Galerkin approach

we end up with an identical algebraic problem (Miklin, 1964). The algebraic problem is positive definite symmetric, which insures that a numerical solution exists.

These concepts for the model Sturm-Liouville problem are well-known. They have the usual mathematical definitions and meanings; these will not be repeated here. However, theorems, proofs, definitions and a detailed analysis of the Galerkin method and variational problem can be found in Wouk (1979). The Galerkin method is also presented and discussed in Chapter VI. Presently we will continue to introduce these concepts for the model problem.

The Boundary Conditions. An important consideration in the formulation of a variational problem is the treatment of boundary conditions. It is the usual practice to include in the functional representation of a problem some or all of the boundary conditions. For most problems this is a difficult undertaking. There are no standard or straightforward procedures for converting a boundary value problem into an equivalent variational problem. However, for linear self-adjoint problems there are some guidelines. These guidelines are based upon the relation between the variational problem and a projected Galerkin solution. (See the energy methods of Miklin, 1964). Nonetheless,

the questions of boundary conditions is often a separate and difficult issue.

The usual approach is to use experience, knowledge and insight to define a functional which treats many of the boundary conditions as "natural" conditions. Natural boundary conditions are those conditions which are automatically satisfied by a solution of the variational problem. For a minimum problem the combination of functions that minimizes the functional will also satisfy the natural boundary conditions. These conditions are a priori eliminated from consideration in the solution of the variational problem. Instead, we must consider those conditions which are not satisfied by the minimizing function. These are usually called essential or principal boundary conditions.

The essential boundary conditions are imposed by requiring that the functions which minimize the functional also explicitly satisfy these conditions. We are only allowed to choose linear combinations of functions in the minimizing sequence that satisfy all the essential boundary conditions. However, we still must determine which conditions are natural or essential. Although there are some guidelines in this regard (Miklin, 1964), the usual practice is to examine the minimum or stationary point of

the functional. This involves the calculus of variations and the concept of a variation which we will now introduce.

Let us suppose that $u(\hat{r})$ is the function which gives Eq (53) its smallest value, and $u^*(\hat{r})$ is another function which is almost identical to $u(\hat{r})$. On the problem domain, we regard $u^*(\hat{r})$ to be infinitesimally different from $u(\hat{r})$. Then we define the first variation of $u(\hat{r})$ to be

$$\partial u = u^*(\hat{r}) - u(\hat{r}) = \varepsilon\phi(\hat{r}) \tag{54}$$

and the second variation to be

$$\partial^2 u = \partial(\partial u) \tag{55}$$

where ε tends to zero, and $\phi(\hat{r})$ is an arbitrary continuous differentiable function. Therefore, the variation of $u(\hat{r})$ is a measure of a very small change in $u(\hat{r})$ for a given value of $\hat{r}$. In taking the variation we consider the independent variable $\hat{r}$ to be a constant whereby

$$\partial \hat{r} = 0 \tag{56}$$

We can also show (Huebner, 1975) that

$$\nabla(\partial u(\hat{r})) = \partial(\nabla u(\hat{r})) \tag{57}$$

and

$$\partial \int_R u(\hat{r}) dr = \int_R \partial u(\hat{r}) d\hat{r} \tag{58}$$

where R represents some volume in phase space.

To find the stationary point of a functional I(u), we require that the first variation vanishes. If the second variation is positive then the stationary point is a minimum: if it is a negative then the stationary point is a maximum. The second variational derivative therefore determines whether we have a maximum or minimum variational problem. In either case we need to take the first variation of the functional in order to determine the conditions that $u(\hat{r})$ must satisfy so as to insure that I(u) has its extremum.

These conditions are just the Euler-Lagrange equation and the natural boundary conditions for the variational problem (Gelfand and Fomin, 1963). The Euler-Lagrange equation is the partial differential equation of the boundary value problem. For the functional of Eq (53) the Euler-Lagrange equation and natural boundary conditions are Eqs (50) and (52).

In Appendix A we have derived general expressions for the first and second variation of an arbitrary first order functional. In Appendix B we use these expressions to show that if $a(\hat{r}_s) = p(\hat{r}_s)$, Eqs (50) and (52) are indeed the Euler-Lagrange equation and natural boundary condition of Eq (53). Furthermore, it can be shown that the usual Neumann boundary condition is also a natural boundary condition. However, the Dirichlet condition is essential and must be satisfied by the trial space.

The Raleigh-Ritz Method. The usual numerical procedure for finding the function $u(\hat{r})$ which makes the functional I(u) stationary is the classical Raleigh-Ritz method (Miklin, 1964). For the model Sturm-Liouville problem this stationary point is a minimum. Therefore, the solution to this problem requires that we find the minimum of Eq (50). This minimum is approximated by the Raleigh-Ritz method. Because of the nature of the variational problem (Eq (53)),

the Raleigh-Ritz method will provide us with an upper bound to the minimum of I(u); or at best, we will compute this minimum exactly. However, in practice, this is never the case and our approximate solution bounds the true minimum from above. For some problems (in elasticity theory) the minimum of the functional represents the minimum potential energy of the system and therefore it is physically meaningful. However, for most problems a physically pleasing interpretation of I(u) is not available.

In the Raleigh-Ritz procedure we minimize I(u) with a linear combination of functions called a minimizing sequence (Courant and Hilbert, 1953). These are really trial functions with unknown coefficients and for the finite element method, they can be expressed in the form of Eq (20), i.e.

$$u(\hat{r}) \simeq \sum_{i=0}^{M} \phi_i N_i(\hat{r}) \tag{59}$$

Then we select the coefficients ϕ_i so that I(u) is a minimum by requiring that

$$\frac{\partial I(u)}{\partial \phi_i} = 0 \quad o \leq i \leq M \tag{60}$$

Eq (60) produces a set of linear algebraic equations in the unknown coefficients ϕ_i. We can then solve this linear system and thus determine the minimizing function of I(u).

For the model problem, Eqs (59) and (60) when inserted into Eq (53) gives

$$2\int_V \left\{ p(\hat{r}) \nabla u \cdot \nabla N_i + [q(\hat{r})u - f(\hat{r})] N_i \right\} d\hat{r}$$

$$+ 2\oint_S [b(\hat{r}_s)u + c(\hat{r}_s)] N_i d\hat{s} = 0 \quad o \leq i \leq M \tag{61}$$

where we can now solve for the ϕ_i's. Furthermore, the matrix problem of Eq (61) is positive definite symmetric (Huebner, 1975) and therefore a numerical solution can be obtained.

The Parity Equation

The parity equations are similar to our model Sturm-Liouville problem in that the operators are positive definite and self-adjoint (Kaplan and Davis, 1967). Because of this we would like to duplicate our variational treatment of the previous section for the second order transport problem. Specifically, we will provide a variational formalism for the even parity transport equation to include the general boundary conditions of Eqs (46) to (48). We have chosen to use the even parity equation for reasons to be discussed later. However, the odd parity development, except for a change of notation, is similar to that for the even parity equation.

Variational principles for the parity equations already exist (Kaplan, et al., 1967). These principles usually treat the vacuum boundary condition as a natural condition. However, a treatment and discussion of general boundary conditions have not been accomplished. To date, these variational principles have been used to primarily provide a theoretical basis for the Marshack boundary conditions of the P_n method (Davis, 1966); and to develop numerical schemes for eliminating ray effects (Briggs, et al., 1975). The variational principle of Vladimirov (1963) is also in this category. Furthermore the

Roussopoulos principles of Cobb (1971) and Selegnut (1959) are based on the non-self-adjoint first order transport equation. These and other variational principles have also been used to accurately compute integral or average quantities such as reaction rates, cross-sections and eigenvalues (Duderstadt and Martin, 1979).

We begin by using experience, insight, trial and error, and finally good judgment to write a functional for the even parity transport equation as follows

$$I(\Psi^g) = \int_R [<\hat{\Omega}\cdot\nabla\Psi^g, K^u(\hat{\Omega}\cdot\nabla^g)> + <\Psi^g, G^g\Psi^g>$$

$$- 2<\hat{\Omega}\cdot\nabla\Psi^g, K^uQ^u> - 2<\Psi^g, Q^g>]d\hat{r}$$

$$+ \oint_S [<|\hat{\Omega}\cdot\hat{n}|Q_{eb}, \Psi^g(\hat{r}_s, \hat{\Omega})>]d\hat{s} \qquad (62)$$

where $<\cdot,\cdot>$ represents the usual inner product in angle (4π steradians), and $|\cdot|$ means the absolute value, and $\hat{n}$

is the outward unit normal to the problem boundaries. The parity operators and sources have the usual meaning and

$$Q_{eb} = a\Psi^{g}(\hat{r}_s,\hat{\Omega}) - bq_s(\hat{r}_s,\hat{\Omega}) \tag{63}$$

Therefore, Q_{eb} is a function of Ψ^{g}, $\hat{r}$, and $\hat{\Omega}$, and we let

$$a = \frac{1 - \alpha(\hat{r}_s)}{\alpha(\hat{r}_s) + 1} \tag{64}$$

where $o \leq \alpha(\hat{r}_s) \leq 1$, and b and α depend on the boundary condition. They are defined as

1. Vacuum boundary

$$\alpha(\hat{r}_s) = 0 \; ; \; b = 0 \tag{64a}$$

2. Incident source

$$\alpha(\hat{r}_s) = 0 \; ; \; b = 2 \tag{64b}$$

3. Albedo condition

$$o < \alpha(\hat{r}_s) \leq 1 \; ; \; b = 0 \tag{64c}$$

4. Mixed condition

$$o \leq \alpha(\hat{r}_s) \leq 1 \; ; \; b = \frac{2}{1+\alpha(\hat{r}_s)} \tag{64d}$$

and

5. Dirichlet condition

$$o < \alpha(\hat{r}_s) \leq 1 \; ; \; b = o \text{ or } \frac{2}{1+\alpha(\hat{r}_s)} \tag{64e}$$

where we require that $\psi^g(\hat{r}_s,\hat{\Omega})$ be a constant in some or all of the independent variables, and also satisfy one of the above mentioned conditions.

We now prove that our postulate is correct and that the functional of Eq (62) is indeed the variational problem corresponding to the second order (even parity) transport problem. This proof which is an extension of that for the model Sturm-Liouville problem, is carried out in Appendix C. There we also show that the boundary conditions (1) to (4) are natural conditions and that the Dirichlet condition is an essential condition.

It is important to note that with vacuum boundary conditions the functional of Eq (62) reduces to that of

Kaplan and Davis (1967) with Marshack boundary conditions (Davis, 1966). However, we have now included the albedo, incident source, mixed and interface conditions as natural boundary conditions. We have also rigorously shown that this concept of natural and essential boundary conditions is indeed valid. Furthermore, we have developed a quadratic functional which can be used to provide a numerical solution to general particle transport problems. This functional has mathematical and numerical properties which are similar to that of our model problem.

Therefore, we could seek a solution (minimum) based on the usual Raleigh-Ritz procedure and expect that our numerical problem would be positive definite and symmetric (Wills, 1981). Applying the Raleigh-Ritz method to Eq (62) we get with

$$\psi^g(\hat{r},\hat{\Omega}) = \sum_{i=0}^{M} \phi_i N_i(\hat{r},\hat{\Omega}) \tag{65}$$

$$2\oint_R [<\hat{\Omega}\cdot\nabla\psi^g, K^u(\hat{\Omega}\cdot\nabla N_i)> + <\psi^g, G^g N_i> - <\hat{\Omega}\cdot\nabla N_i, K^u Q^u> - <N_i, Q^g>]d\hat{r}$$

$$+ \oint_S [<|\hat{\Omega}\cdot\hat{n}|[2a\psi^g - bq_s], N_i(\hat{r}_s,\hat{\Omega})>]d\hat{s} = 0 \tag{66}$$

where we can solve for the ϕ_i's. The variational problem has been reduced to a matrix problem which is positive definite and symmetric.

CHAPTER VI

PROJECTION METHODS AND WEAK FORMS

Projection methods can be used to provide approximate solutions to a large number of problems. They have been used extensively to solve boundary value and other problems which are described by differential and integral equations. These methods are important in that they facilitate the recasting of general problems into a form more suitable for a numerical solution. Most projection methods involve the use of a contraction mapping (Stakgold, 1979). The original problem is usually projected unto a reduced finite dimensional subspace and a solution is then sought in this new and restricted space.

Projection methods include such techniques as collocation, Galerkin, the method of moments and least squares (Golberg, 1978). These methods are sometimes called the method of weighted residuals (Finlayson and Scriven, 1966). However, they all begin with the use of a projection operator defined as (Atkinson, 1976)

$$P_n(x)x = x \quad \text{for all } x \in X_n \tag{67}$$

where P_n is a bounded projection operator from X unto X_n. X is a Banach space and X_n a finite dimensional subspace of X. Then

$$P_n^2 = P_n \tag{68}$$

and

$$||P_n|| = ||P_n^2|| \leq ||P_n||^2 \tag{69}$$

where $||\cdot||$ represents the usual definition of a norm and Eq (69) implies that $||P_n|| \geq 1$ (Atkinson, 1976).

Therefore, a projection operator maps every element of a general space X into X_n, a subspace of X. It also maps each element of X_n unto itself. This projected space X_n is usually the n-dimensional space in which we seek to find a solution.

If P_n is a projection operator then $(I - P_n)$ is also a projection operator where I represents the identity operator (Wouk, 1979). Furthermore, in a Hilbert space we can

introduce the concept of orthogonal projections where the projection operator involves the inner product of two functions. An orthogonal projection operator P_n is symmetric and orthogonal to $(I - P_n)$. Therefore,

$$\langle P_n x, (I - P_n) y \rangle = o \quad \text{for } x, y \in X \tag{70}$$

where $(I - P_n)$ is a projection operator unto the orthogonal *complement of* X_n. *Finally, for an* orthogonal projection P_n

$$||x||^2 = ||P_n x||^2 + ||(I - P_n)x||^2 \tag{71}$$

and

$$||P_n|| = 1 \tag{72}$$

The projection method for solving a problem of the form

$$Ly(x) = f(x) \tag{73}$$

is to approximate $y(x)$ on a finite dimensional space by

$$y(x) \simeq y_n(x) = \sum_{j=1}^{n} \alpha_j \phi_j(x) \tag{74}$$

and define

$$R(x) = Ly_n(x) - f(x) \tag{75}$$

where $R(x)$ would be identically equal to zero if $y(x) = y_n(x)$. However, since in general this is not true, we try to choose $y_n(x)$ so that $R(x)$ is small. We accomplish

this by making the projection of R(x) unto $Y_n(x)$ equal to zero, i.e.,

$$P_n L y_n(x) - P_n f(x) = P_n R(x) = 0 \qquad (76)$$

where $y_n \in Y_n$ and Y_n is the finite dimensional subspace of the Banach space Y. Therefore, the projection method for solving Eq (73) is to pick $y_n(x) \in Y_n(x)$ in accordance with Eq (76) such that the components in $y_n(x)$ of $Ly_n(x)$ agree with f(x).

Eq (76) represents a set of coupled algebraic equations. However, before we can seek a numerical solution we must first choose a projection operator P_n. There are a number of possibilities, but the usual selections lead to the well-known methods of collocation, Galerkin, least squares and the method of moments. In the collocation method we require that the residual vanish at selected node points. Thus we determine the α_j's of Eq (74) by requiring that

$$R(x_i) = 0 \quad 1 \leq i \leq N \qquad (77)$$

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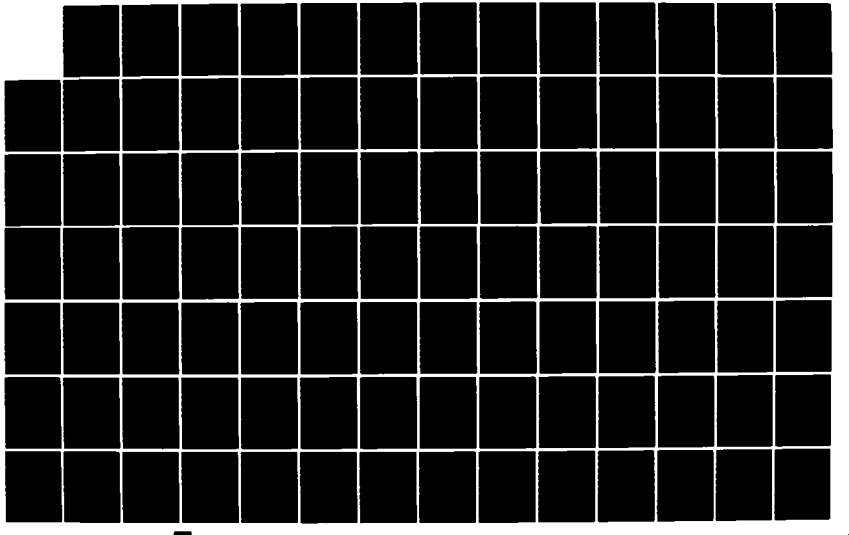

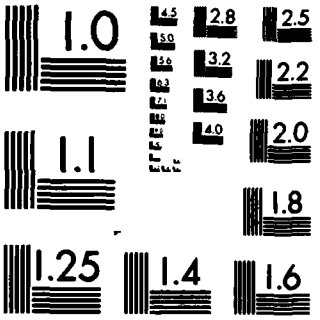

or equivalently by

$$\int R(x)w_i(x)dx = 0 \quad 1 \leq i \leq N \tag{78}$$

where $w_i(x) = \delta(x - x_i)$. The Dirac delta function $w_i(x)$ represents the test or weight function of the collocation method (Finlayson and Scriven, 1966). Therefore, we have defined or chosen our projection operator with respect to the weight function $w_i(x)$ and in accordance with Eq (78) or (77).

For the methods of Galerkin, least squares and the method of moments we can also require, as in the case of collocation, that the residual be orthogonal to some weight function. This in turn leads to the algebraic problem (Eq (78)), and with a proper choice of the subspace Y_n, to a solution for the α's of Eq (74). The weight functions are selected as follows (Prenter, 1975).

a. Galerkin. The residual is required to be orthogonal to the trial space. Here we take the weight functions to be the same as the trial functions of Eq (74), i.e.

$$w_i(x) = \phi_i(x) \tag{79}$$

b. Least Squares. We minimize the two-norm of the residual by choosing our weight functions to be

$$w_i(x) = \frac{\partial R(x)}{\partial \alpha_i} \tag{80}$$

c. Method of Moments. The residual is made orthogonal to the monomial basis $\{x^n\}$. We choose the weight functions to be

$$w_i(x) = x^i \quad o \le i \le N \tag{81a}$$

Weak Forms

The most widely used projection methods are collocation and Galerkin. However, the Galerkin method is a

generalization of the Raleigh-Ritz method for problems which are positive definite and self-adjoint. For these problems we can obtain a Raleigh-Ritz solution without having to develop a variational formalism. Furthermore, the Galerkin method is more general than this in that it can be applied to problems which are not positive definite.

In applying the Galerkin method to two point boundary value problems the normal procedure is to use integration by parts to produce the Galerkin weak form (Strang and Fix, 1973). This procedure lowers the continuity restriction of the trial space and allows for the inclusion of natural boundary conditions. We can then establish a precise equivalence with the Raleigh-Ritz variational problem. This equivalence is important for reasons which we have already mentioned.

For the Sturm-Liouville boundary value problem of Eq (50) we can use the divergence theorem to derive the weak form. Assuming a trial space in the form of Eq (59), the Galerkin projection can be written as

$$\int_V [-\nabla\cdot p(\hat{r})\nabla\cdot u(\hat{r}) + q(\hat{r}) - f(\hat{r})]N_i(\hat{r})d\hat{r} = 0$$

$$\text{for } 0 \le i \le M \qquad (81b)$$

Then, applying the Gauss divergence theorem to the first term of Eq (81b), we get

$$\int_V \{p(\hat{r})\nabla u\cdot\nabla N_i + [q(\hat{r})u - f(\hat{r})]N_i\}d\hat{r} - \int_S [p(\hat{r}_s)\nabla u(\hat{r}_s)\cdot\hat{n}]N_i d\hat{s} = 0 \quad 1\le i\le M \tag{82}$$

and using Eq (52) we can rewrite Eq (82) as

$$\int_V \{p(\hat{r})\nabla u\cdot\nabla N_i + [q(\hat{r})u - f(\hat{r})]N_i\}d\hat{r} + \int_S [b(\hat{r}_s)u(\hat{r}_s) + c(\hat{r}_s)]N_i d\hat{s} = 0 \quad 1\le i\le M \tag{83}$$

Eq (83) is identical to Eq (61). We have therefore established the equivalence of the Raleigh-Ritz solution and the Galerkin weak form. The boundary conditions of Eq (52) can now be treated as natural boundary conditions. Furthermore all boundary conditions for a Galerkin weak form solution to Eq (50) can be treated within the context of the variational problem, as either natural or essential conditions.

CHAPTER VII

THE FINITE ELEMENT PROJECTION METHOD

In Chapter V we presented a variational formulation of the second order transport problem. However, we would like to provide a numerical treatment that is straightforward and avoids the explicit use of a variational principle. The projection methods which we discussed in Chapter VI can be used to provide this alternate numerical treatment. Furthermore, for the Galerkin method we can establish an equivalence to the variational problem. The purpose of this Chapter is to establish this equivalence and to outline a finite element Galerkin method for solving general particle transport problems.

Our intent is to provide a numerical solution to the even parity second order transport equation. In doing so we will treat the boundary conditions within the context of a classical Raleigh-Ritz solution, as essential or natural conditions. This classical solution was presented in Chapter V, where we discussed in detail the concept of natural and essential boundary conditions.

We begin by referring to Chapter IV where the angular flux was written in terms of odd and even components as

$$\phi(\hat{r},\hat{\Omega}) = \psi^g(\hat{r},\hat{\Omega}) + \psi^u(\hat{r},\hat{\Omega}) \tag{84}$$

where the even and odd parity flux ψ^g and ψ^u can be obtained by solving Eqs (35) and (36). Therefore, a solution to these equations provide a solution for the particle angular flux. Furthermore, because ψ^g and ψ^u are even and odd on the unit sphere they represent the scalar or reaction rate flux and the particle current respectively (Miller et al., 1973). For most problems we are interested in an accurate description of the scalar flux and thus a solution to Eq (35) is all that is required. Because of this, our solution will be presented in terms of the even parity transport equation. Nonetheless the solution strategy can be applied to either problem.

The Galerkin Weak Form

Our solution is based on a finite element Galerkin solution of the even parity transport equation. We have chosen this approach because solutions to Eq (35) by use of a variational principle or the Galerkin method are equivalent (Wills, 1981). To show this, we can expand the even parity flux as in Eq (65). Using the Galerkin projection operator we can then write Eq (35) as

$$\int_R [\langle -\hat{\Omega}\cdot\nabla K^u \hat{\Omega}\cdot\nabla \psi^g, N_i\rangle + \langle G^g \psi^g, N_i\rangle - \langle Q^g, N_i\rangle$$

$$+ \langle \hat{\Omega}\cdot\nabla K^u Q^u, N_i\rangle] d\hat{r} = 0 \quad (85)$$

We can now use the divergence theorem (Kaplan and Davis, 1967)

$$\int_R \langle \hat{\Omega}\cdot\nabla f, g\rangle d\hat{r} = -\int_R \langle f, \hat{\Omega}\cdot\nabla g\rangle d\hat{r} + \oint_S \langle (\hat{\Omega}\cdot\hat{n}) f, g\rangle d\hat{s} \quad (86)$$

to include the boundary terms of Eqs (46) and (47). This then allows us to rewrite Eq (85) as

$$2\int_R [\langle \hat{\Omega}\cdot\nabla \psi^g, K^u(\hat{\Omega}\cdot\nabla N_i)\rangle + \langle \psi^g, G^g N_i\rangle - \langle \hat{\Omega}\cdot\nabla N_i, K^u Q^u\rangle$$

$$- \langle N_i, Q^g\rangle] d\hat{r} + \oint_S \langle |\hat{\Omega}\cdot\hat{n}| [2a\psi^g - bq_s], N_i(\hat{r}_s, \hat{\Omega})\rangle d\hat{s} = 0 \quad (87)$$

where a and b are defined by Eqs (64a) to Eq (64e).

Eq (87) is a set of coupled algebraic equations which represent the Galerkin weak form of the even parity transport equation. It is identical to the Raleigh-Ritz system

of equations, Eq (66). Therefore, we have established the equivalence of the Raleigh-Ritz solution and the Galerkin weak form. Furthermore, we can now consider the boundary conditions of Eqs (46) and (47) to be natural conditions and the Dirichlet condition to be essential.

This treatment of the boundary conditions and a numerical solution of Eq (87) is our finite element projection method. This zig-zag between a variational principle and the Galerkin method allows us to rigorously treat the boundary and interface conditions as natural or essential. In effect, we need a variational principle in order to explain our treatment of the boundary terms. We also need a variational principle in order to determine which boundary conditions are essential or natural.

Solution Strategy

At this point of the development we have reduced the problem to a set of algebraic equations once we define the trial basis, Eq (65). The problem as represented by Eq (87) is therefore a matrix problem for the flux expansion coefficients (ϕ_i). Furthermore, for a general time dependent multigroup treatment (see Chapter IV) we have to solve a number of these matrix problems, which are then coupled in time and energy. However, a solution to Eq (87) is still a formidable task.

Nonetheless, we can develop a solution strategy which is based on the special properties of the problem matrix. These properties together with the parity (odd, even) characteristics of the even parity flux should ease some of the computational difficulties. Also, by a judicious choice of the trial functions we can effectively treat the spatial and angular dependences.

Trial Functions. For the most general particle transport problems the steady state one group problem of Eq (87) is a five dimensional problem. The particle flux has three independent spatial variables in $\hat{r}$ and two angular variables in $\hat{\Omega}$. A spatial solution is usually carried out in rectangular, cylindrical or spherical geometries. The gradient or streaming operator $(\hat{\Omega}\cdot\nabla\Psi)$ for these orthogonal geometries are well-known and can be found in Bell and Glasstone (1970). Our intent is to discuss a general solution strategy applicable to these geometries. Here we will omit some of the specific algebraic details. However, we will address some of them in cylindrical coordinates and as they apply to the air-over-ground problem which is discussed in Chapter VIII.

In Chapter II we wrote the particle velocity or vector dependence in terms of particle energy and the

direction vector $\hat{\Omega}$. This vector is related to the spatial problem coordinates and is usually specified by two independent angle variables μ and χ (Duderstadt and Martin, 1979). These angles are defined with respect to the particular problem geometry. In rectangular geometry they are defined as in Figure 3 where $u = \cos\theta$ and θ is the angle formed by $\hat{\Omega}$ and the z-axis. χ is the angle between the x-z plane and the plane formed by the $\hat{\Omega}$ vector and the z-axis.

By expressing the problem in an orthogonal spatial coordinate as in Figure 3 we can easily derive expressions for the streaming operator. We can also derive expressions for the surface normal term $\hat{\Omega}\cdot\hat{n}$ (Wills, 1981). Furthermore, we can easily demonstrate the odd-even properties of our second order formulation. These properties are important in determining the scalar flux and particle current. They also show that this second order formulation is just a separation of the odd and even components of the angular flux. The even parity equation and flux carries the even information which is important in determining the scalar or reaction rate flux. However, the odd parity equation and flux has the odd information which is important in determining the net current.

In order to see that this is indeed the case the reader can easily verify that in any orthogonal coordinate

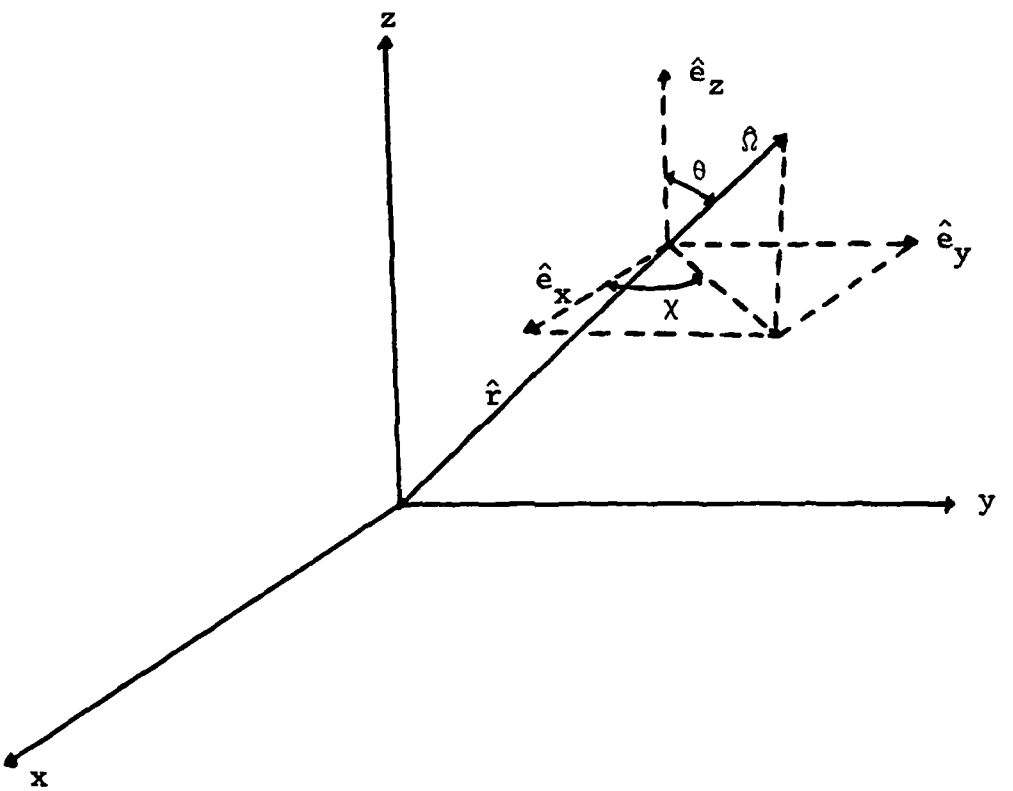

Figure 3. Rectangular Coordinates

system the surface term $\hat{\Omega}\cdot\hat{n}$ is an odd function on the unit sphere. It is an odd function in the direction $\hat{\Omega}$ or equivalently in the angles μ and χ. Then, by writing the angular flux as in Eq (84) and the parity flux as in Eqs (29) and (30), he can show (Wills, 1981) that

$$\int_{4\pi}\psi^{u}(\hat{r},\hat{\Omega})d\hat{r} = 0 \tag{88}$$

where

$$\int_{4\pi}\phi(\hat{r},\hat{\Omega})d\hat{\Omega} = \int_{4\pi}\phi(\hat{r},-\hat{\Omega})d\hat{\Omega} \tag{89}$$

and the integration is carried out over all directions (4π steradians). Therefore

$$\int_{4\pi}\phi(\hat{r},\hat{\Omega})d\hat{\Omega} = \int_{4\pi}\psi^{g}(\hat{r},\hat{\Omega})d\hat{\Omega} \tag{90}$$

Furthermore, since the term $\hat{\Omega}\cdot\hat{n}$ is represented by odd spherical harmonic functions (Wills, 1981) we can write

$$\int_{4\pi}(\hat{\Omega}\cdot\hat{n})\psi^{g}(\hat{r},\hat{\Omega})d\hat{\Omega} = 0 \tag{91}$$

and the particle current as

$$\int_{4\pi}(\hat{\Omega}\cdot\hat{n})\phi(\hat{r},\hat{\Omega})d\hat{\Omega} = \int_{4\pi}(\hat{\Omega}\cdot\hat{n})\psi^{u}(\hat{r},\hat{\Omega})d\hat{\Omega} \qquad (92)$$

where we used the fact that $\hat{\Omega}\cdot\hat{n}$ and $\psi^{u}(\hat{r},\hat{\Omega})$ are odd, whereas $\psi^{g}(\hat{r},\hat{\Omega})$ is even on the unit sphere.

This odd-even property of the second order formulation is also important in the choice of a finite element trial basis. We propose to use a dual basis -- a piecewise polynomial (spline) basis in the spatial variables and spherical harmonics in angle. Our choice of spherical harmonics, or an equivalent tensor product of surface harmonics (Sansone, 1977) in the angular variables is based on the following:

i. The odd-even properties of the second order flux and equations.

ii. The usual practice of expanding the scattering cross-sections in spherical harmonics (Bell and Glasstone, 1970).

iii. The streaming and surface normal terms are expanded by the use of Legendre functions.

iv. The orthogonal and parity characteristic of spherical and surface harmonics.

v. Spherical harmonic functions have been successful in mitigating ray effects (Reed, 1972).

We also chose a spatial finite element basis in order to ease the computational burden of the five-dimensional problem. A finite element basis can easily model difficult and complicated geometries. Furthermore, a finite element spline basis is easy to construct and their piecewise nature facilitates the evaluation of the many integrals in the Galerkin weak form. There is also a wide selection of spline basis functions and element shapes to choose from (Prenter, 1975). This provides the flexibility which is required in solving general particle transport problems.

Expanding our solution in this dual basis of polynomial splines and spherical harmonics we can now write the trial function expansion of Eq (65) and Eq (87) with

$$N_i(\hat{r},\hat{\Omega}) = Y_{\ell,m}(\hat{\Omega})B_j(\hat{r}) \qquad (93)$$

where $-\ell \leq m \leq +\ell$ and the index i varies with ℓ, m and j.

This is a global basis of harmonic functions in angle and a local finite element basis in the spatial variables which represent $\hat{r}$. Referring to Figure 3, these could be the x, y, z variables in rectangular geometry where the angle or direction variables are u and χ. Furthermore, if there is symmetry in the problem we could eliminate some of the independent variables and thus reduce the dimension of the trial space.

Spherical Harmonics and Surface Harmonic Tensors. Spherical harmonics are complex functions in the direction variables of $\hat{\Omega}$. These variables are usually denoted by the symbols μ and χ. In rectangular geometry they are defined as in Figure 3. Their definition in other orthogonal geometries can be found in Bell and Glasstone (1970). They specify directions or points on a unit sphere where $u \in [-1, 1]$ and $\chi \in [0, 2\pi]$. The normalized spherical harmonic functions are defined as (Wills, 1981)

$$Y_{\ell,m}(\hat{\Omega}) = C_{\ell,m} P_{\ell,m}(u) e^{im\chi}$$

$$= Q^{c}_{\ell,m} + iQ^{s}_{\ell,m} \qquad (94)$$

where $P_{\ell m}(u)$ are the associate Legendre functions (MacRobert, 1967) and

$$C_{\ell,m} = \sqrt{\frac{2\ell+1}{4\pi} \cdot \frac{(\ell-m)!}{(\ell+m)!}} \tag{95}$$

We have also defined $Q^c_{\ell m}$ and $Q^s_{\ell m}$ to be the even and odd surface harmonic tensors

$$Q^c_{\ell m} = C_{\ell m} P_{\ell m}(u)\cos(m\chi) \tag{96}$$

and

$$Q^s_{\ell m} = C_{\ell m} P_{\ell m}(u)\sin(m\chi) \tag{97}$$

The usual spherical harmonic expansion of a function $f(\hat{\Omega})$ is written as

$$f(\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{+\ell} f_{\ell m} Y_{\ell m}(\hat{\Omega}) \tag{98}$$

where $f_{\ell,m}$ are the expansion coefficients which are determined by the inner product

$$f_{\ell m} = \langle f(\hat{\Omega}), Y_{\ell m}(\hat{\Omega}) \rangle = \int_{4\pi} f(\hat{\Omega}) Y^{*}_{\ell m}(\hat{\Omega}) d\hat{\Omega} \tag{99}$$

and $Y^{*}_{\ell m}$ is the complex conjugate. We can rewrite Eq (98) without a loss of generality (Wills, 1981) as

$$f(\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} f^{e}_{\ell m} Q^{c}_{\ell m} + i f^{o}_{\ell m} Q^{s}_{\ell m} \tag{100}$$

where $f^{e}_{\ell,m} \neq f^{o}_{\ell,m}$ and we have used the fact that

$$Y_{\ell,-m} = (-1)^{m} Y^{*}_{\ell m} = (-1)^{m} Q^{c}_{\ell m} + i(-1)^{m+1} Q^{s}_{\ell m} \tag{101}$$

Using a spherical harmonic expansion in Eqs (65) and (87) produces a matrix problem which is complex if there is no symmetry in the angle χ (Blomquist and Lewis, 1980). The matrix of the Galerkin weak form is then a Hermetian matrix and the computations must be carried out in complex arithmetic. However, since we know that the sources are all real and that the solution is real, we could use an alternate and equivalent real trial space (Fletcher, 1983). This trial space is just the surface harmonic tensors of Eq (94) where the expansion of Eq (100) is now written as

$$f(\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} \left\{ f^{c}_{\ell m} Q^{c}_{\ell m} + f^{s}_{\ell m} Q^{s}_{\ell m} \right\} \qquad (102)$$

and the trial function of Eq (93) as

$$N_i(\hat{r},\hat{\Omega}) = \left[Q^{c}_{\ell m} + Q^{s}_{\ell m} \right] B_j(\hat{r}) \qquad \text{with } 0 \le m \le \ell \qquad (102a)$$

In order to see that the expansions of Eqs (98) and (102) are equivalent, we need to separate the spherical harmonic coefficients into their real and imaginary parts (Courant and Hilbert, 1953) as

$$f_{\ell m} = \begin{cases} f^{c}_{\ell m} - i f^{s}_{\ell m} & \text{for } m>0 \\ (f^{c}_{\ell m} + i f^{s}_{\ell m}) * (-1)^{m} & \text{for } m<0 \end{cases} \qquad (103)$$

By substituting Eq (103) into Eq (98) we can derive the real expansion, Eq (102). These harmonic functions are complete and converge uniformly and in the mean (Churchill and Brown, 1978). They are also orthogonal in that for $\ell \neq \ell'$ and $m \neq m'$

$$\begin{aligned} \langle Y_{\ell m}(\hat{\Omega}), Y_{\ell' m'}(\hat{\Omega}) \rangle &= \langle Q^{c}_{\ell m}, Q^{c}_{\ell' m'} \rangle \\ &= \langle Q^{c}_{\ell m}, Q^{s}_{\ell' m'} \rangle \\ &= \langle Q^{s}_{\ell m}, Q^{s}_{\ell' m'} \rangle \\ &= 0 \end{aligned} \qquad (104)$$

Another important property of these harmonic functions is that they have special parity characteristics. This is a very important property computationally and in choosing the angular trial space. It allows us to construct a basis which is best suited to accomodate the odd-even (parity) properties of the even and odd parity fluxes. In solving the even or odd parity equations we

need to use a trial space which is complete in either the even or odd functions on the unit sphere. In effect, we need to limit our trial space to either even or odd functions. This restriction is implicit in our definition of the parity flux (Eqs (29) and (30)). There we separated the angular flux into a sum of components (the even and odd parity fluxes) which are even and odd on the unit sphere.

Therefore, in solving Eq (87), we need to use an angular trial space of even functions. By our definition, the odd components in this function space are all zero. Using the parity characteristic of spherical harmonics this trial space is just the expansion of Eqs (98) or (102) where the index ℓ is restricted to be even (Davis, 1966). For a solution to the odd parity problem we could construct a similar reduced trial space where ℓ is odd. In either case we have reduced our trial space to a subset of the larger solution space which is required in the P_n method (Greenspan et al., 1968). Furthermore, this smaller trial space reduces the size of the matrix problem which must be solved. This in turn reduces the computational effort which is required.

In order to demonstrate that these harmonic functions have parity we need to show that

$$Y_{\ell m}(-\hat{\Omega}) = (-1)^{\ell} Y_{\ell m}(\hat{\Omega}) \tag{105}$$

or equivalently that

$$Q^{c}_{\ell m}(-\hat{\Omega}) = (-1)^{\ell} Q^{c}_{\ell m}(\hat{\Omega}) \tag{106}$$

and

$$Q^{s}_{\ell m}(-\hat{\Omega}) = (-1)^{\ell} Q^{s}_{\ell m}(\hat{\Omega}) \tag{107}$$

Here, $-\hat{\Omega}$ specifies the direction opposite to $\hat{\Omega}$ and can be represented by $-\mu$ and $\pi + \chi$ (See Figure 3). The proof of these relationships is straightforward. It includes the fact (Hobson, 1965) that

$$P_{\ell m}(-u) = (-1)^{\ell - m} P_{\ell m}(u) \tag{108}$$

$$e^{im(\pi + \chi)} = (-1)^m e^{im\chi} \tag{109}$$

$$\sin[m(\pi + \chi)] = (-1)^m \sin(m\chi) \tag{110a}$$

and

$$\cos[m(\pi + \chi)] = (-1)^m \cos(m\chi) \tag{110b}$$

Finally, we can show that in the limit of diffusion theory, the Galerkin second order equations reduce to the diffusion equation and Fick's law. This equivalence is important in that it shows the relationship between our finite element projection method and the P_1 method. It also shows that our approach, in the limit of a linearly anisotropic approximation, is consistent with these established and proven techniques. This equivalence is presented and discussed in Appendix D. Furthermore, we can also expand the streaming operators and cross-sections of the second order forms by using the well-known recursive properties of spherical harmonics. These relationships are included in Appendix E.

The Muitigroup Solution. A complete solution of general particle transport problems must include a rigorous treatment of the time and energy dependences. As shown in Chapter IV, the usual approach is simply to extend the steady-state and time-independent solution to energy and time dependent problems. For the second order transport equations this includes the usual multigroup approach in energy and a weighted difference or Crank-Nicholson scheme in time (Duderstadt and Martin, 1979).

In order to keep the algebra and notation to a minimum and at a manageable level we will not rewrite the Galerkin weak form with an explicit time and energy dependent notation (subscript). Instead, we will refer the reader to Duderstadt and Martin (1979) and to Chapter IV. However, we will discuss a time and energy dependent solution within the context of Eq (87). Our intent is to discuss the important aspects of a general solution which includes the usual time and energy dependent treatment.

The discrete time and energy dependent equations are just the system of Eq (87) with redefined operators, cross-sections and source terms (See Chapter IV). The even parity flux is now defined with an explicit time and energy (multi-

group) dependence. The source terms will include known flux values from a previous time step and sources from other energy groups. This problem will be implicit in time with the solutions at a given time step being dependent on those at previous times. Furthermore, the multigroup equations are coupled by the source terms whereby the sources in a given group are dependent on the flux in other groups.

The general solution strategy is to begin with some initial condition and to proceed by a marching scheme in time. At each time step we then solve the multigroup energy dependent problem by the usual iterative procedure. This multigroup problem is a set of coupled one group problems where the parity sources of Eq (87) are energy and time dependent sources. These sources can be written in a form similar to Eq (26) as

$$Q_b^g = S_d^g + S_u^g + S_b^g + K(\Delta t, \psi_b^g) \tag{111}$$

and

$$Q_b^u = S_d^u + S_u^u + S_b^u + K(\Delta t, \psi_b^u) \tag{112}$$

Here we have omitted the explicit time index and included fissions and group scatter sources. $K(\nabla t, \psi_b^g)$ and $K(\nabla t, \psi_b^u)$ represent terms which depend on the time discretization that is used and b is the energy group index. ψ_b^g and ψ_b^u are the even and odd parity fluxes from the previous time step or initial conditions, and

S_d^g = even parity downscatter source.

S_u^g = even parity upscatter source.

S_f^g = even parity fission source.

S_d^u = odd parity downscatter source.

S_u^u = odd parity upscatter source.

S_b^g = even parity inhomogenous source.

S_b^u = odd parity inhomogenous source.

These sources are similar to the usual multigroup sources where, for example, the odd parity downscatter source for energy group b can be written as

$$S_d^u = \sum_{b'=1}^{b-1} \int_{4\pi} \sigma_{sb'\to b}^u(\hat{r}, \hat{\Omega}\cdot\hat{\Omega}')\psi_{b'}^u(\hat{r}, \hat{\Omega}')d\hat{\Omega}' \qquad (113)$$

where $1 \leq b \leq G$ and group one has the most energetic particles. The other sources can be similarly defined where the scattering cross-sections are defined by Eqs (33) and (34).

It is important to note that because fissions occur isotropically they only contribute to the even parity source term. Furthermore, with isotropic inhomogenous sources and scattering the odd parity sources are all zero. However, for problems with anisotropic scattering we must include and compute the odd parity downscatter and upscatter sources. These and the $K(\nabla t, \Psi_b^u)$ term of Eq (112) are expressed in terms of the odd parity flux. Therefore we must compute the odd parity group fluxes in order to determine the source terms for anisotropic and time dependent problems.

This is a disadvantage of our second order formulation. If we are only interested in scalar flux values and thus a solution to the even parity equation then for anisotropic and time dependent problems, we must indirectly compute the odd parity flux. This can be accomplished by inserting Eq (37) into Eqs (112) and (113). However, this increases the computational work, especially for problems with upscatter sources. Nonetheless, we are not computing Ψ_b^u explicitly, and a solution can be obtained without having to solve the odd parity equations.

Except for the extra effort which is required in computing the multigroup and time dependent sources the solution approach is similar to that which is normally used to solve the first order transport equation (Sanchez and McCormick, 1982). This involves an inner and outer iteration strategy. At each time step we carry out a multigroup solution where we solve the one group steady state matrix problem for each energy group. This is the inner iteration where we calculate the space and angle flux distribution $\Psi_b^g(\hat{r},\hat{\Omega})$ for each energy group b. The usual practice for solving the diffusion equation is to use an iterative (indirect) solver to solve the matrix problem (Bell and Glasstone, 1970). This practice, together with the iterative procedure of the discrete ordinate method, has led to the concept of an "inner iteration strategy."

An outer iteration provides a solution for the group fluxes $\Psi_b^g(\hat{r},\hat{\Omega})$ for <u>all</u> of the energy groups. It involves a sweep through all energy groups in order of decreasing energy to provide an updated steady state solution. The outer iteration is then repeated until some convergence criteria is satisfied or a prescribed number of iterations are performed. For problems which do not have fissions or upscatter sources, only one outer iteration is required. The group flux $\Psi_b^g(\hat{r},\hat{\Omega})$ converges in one outer iteration. However, fissions and upscatter sources depend on the un-

known and to be computed flux in lower energy groups. Therefore, the usual practice is to begin with an initial flux guess for all of the energy groups and to perform a number of outer iterations before convergence is achieved. At each outer iteration the fissions and upscatter sources are computed by using the flux solutions of the previous outer iteration.

The Matrix Problem. A numerical solution of the second order transport problem requires that we solve a matrix problem. This matrix problem is obtained by expanding, evaluating and assembling the individual terms of the Galerkin weak form, Eq (87). This involves the evaluation of a number of integrals and the construction of a problem matrix and source vector. Finally we must solve this system for the flux expansion coefficients (ϕ_i). These coefficients can then be substituted into Eq (65) to give the even parity flux.

The matrix problem can be written as

$$\left[A\right]\left[\phi\right] = \left[S\right] \tag{114}$$

where

A = positive definite symmetric problem matrix

ϕ = flux expansion coefficient vector

S = right hand side or source vector

To get from Eq (87) to (114) we will follow the usual finite element practice (Huebner, 1975) of evaluating the integrals by Gauss-Legendre quadrature. Numerical integration with Gauss quadrature can be written as (Atkinson, 1978)

$$\int_a^b f(x)dx = \sum_{j=1}^{n} w_j f(x_j) \tag{115}$$

where the w_j's are the Gauss Legendre weights and x_j's are the zeros of the nth degree Legendre polynomial. The quadrature formulae Eq (115) integrates all polynomials of degree $\leq 2n-1$ exactly.

In order to reduce the computational effort a complete expansion of the Galerkin weak form and identification of the distinct integrals is required (Wills, 1981). These integrals are evaluated once and then used to assemble the problem matrix and source vector. We can then use an indirect solver (Hageman and Young, 1981), or Cholesky decomposition (Stewart, 1973) to solve this positive de-

finite symmetric system. Furthermore, the problem matrix will have a large number of zeros due to the use of finite elements. Therefore, we could use a sparse matrix storage scheme (Jennings, 1977) to reduce the problem size. This, coupled with the fact that the problem matrix is symmetric, will decrease the computer storage requirements and costs.

CHAPTER VIII

THE AIR-OVER-GROUND PROBLEM

We now apply our method to a real and difficult problem -- the air-over-ground problem. This problem involves the deep penetration of particles in the atmosphere along with reflection and propagation into the ground. These particles are neutrons, gamma rays and x-rays. They propagate away from a point source in a two-dimensional air-over-ground geometry. Solutions to this problem have a variety of applications. These applications include the prediction of collateral damage and radiation exposure in a nuclear environment.

The air-over-ground problem increases in complexity because it has point sources, forward peaked anisotropic scattering, an exponentially varying atmosphere, and an air-ground interface (Pace et al., 1975). Numerical solutions to this problem already exist. The main solution techniques are Monte Carlo and discrete ordinates. However, both Monte Carlo and discrete ordinates have severe difficulties and limitations (Loewe et al., 1983). A Monte Carlo solution has statistical errors. These are expected uncertain-

ties in the approximate solution. However, these uncertainties become large as the problem dimensions increase. Therefore, over large space regions the Monte Carlo solution has poor statistics and unacceptable errors. It also requires many hours of computer execution time. Discrete ordinates is also limited by deficiencies in the difference scheme, ray effects and long execution times.

Because of these difficulties many researchers have investigated and developed alternate solution techniques for solving the air-over-ground problem. Roberds and Bridgman (1977) have used a projection of "specially tailored" trial functions to solve this problem. Shulstad (1976), Eamon (1976) and Sacenti and Jacobsen (1975) have used a mass integral scaling technique. In this approach scale factors are used to correct infinite homogenous air results. Souders (1981) has also applied projection methods to the even parity transport equation. He attempted a collocation and Galerkin solution and concluded that these methods could not be successfully used to solve this problem. In contrast to our use of spherical harmonics he used Lagrange polynomials and special ellipsoid trial functions to model the angular dependences. He did not include the air-ground interface or a nonhomogenous atmosphere.

The most general solution of the air-over-ground problem can be obtained in a three dimensional spatial geometry. This is a time and energy dependent problem with two angle variables (u,χ). Therefore, the general air-over-ground problem requires a detailed seven dimensional solution. However, if in cylindrical geometry, we confine the point sources to the z-axis, then the problem becomes two dimensional in the spatial variables. It has azimuthal symmetry and can be solved as a six dimensional problem in a cylindrical (r,z) geometry.

It is not our purpose to provide the most general solution to the air-over-ground problem here. Instead, we will reduce the problem further to a monoenergetic steady-state problem in cylindrical geometry. The point sources will be confined to the z-axis. However, we will include first scatter sources, anisotropic scattering, an exponentially varying atmosphere and the air-ground interface. Furthermore, our solution can be easily extended to the general time and energy dependent (multigroup) problem. As was pointed out in Chapter VII, this is a straightforward extension which requires the solution of a number of coupled steady-state, monoenergetic problems. Therefore, our primary objective is to demonstrate that the finite element projection method can be used to solve the steady-state one group air-over-ground problem.

Problem Geometry and Boundary Conditions

This problem will be modeled in cylindrical (r,z) geometry with vacuum boundary conditions. It is a steady-state, monoenergetic (one group) four-dimensional problem with two spatial (r,z) and two angle (u,χ) variables. The coordinate system and directional angles of this geometry and the air-over-ground problem are shown in Figure (4). μ is the cosine of the angle formed by the z-axis and the particle velocity vector $\hat{\Omega}$. χ is the angle between the planes formed by the $\hat{r}$ vector and z-axis and that of the $\hat{\Omega}$ vector and z-axis.

For the air-over-ground problem the scattering cross-sections will be highly peaked in the forward direction (Bartine et al., 1977). This is due to the scattering properties of air and the high particle energies which exist in this problem. Because of this the exterior boundary condition for this problem will be approximated by a vacuum boundary condition (Burgio, 1975). This boundary condition is represented by Eq (9) and for the second order transport equation by Eqs (46) and (47). In the Galerkin weak form and the equivalent variational problem it is defined by Eq (64a).

Furthermore, in two-dimensional cylindrical (r,z) geometry there is symmetry in the angle χ. This symmetry

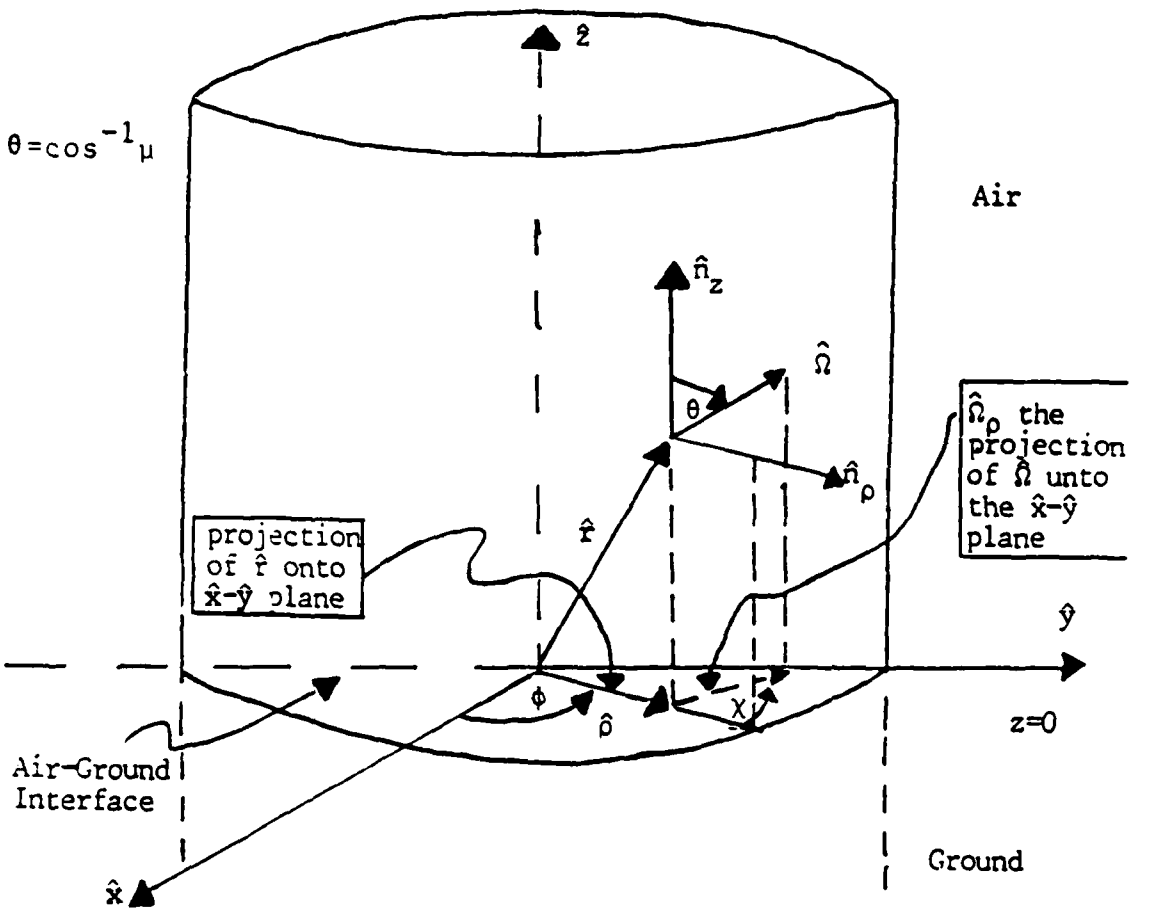

Figure 4. Air-Over-Ground Problem Geometry and Coordinate System.

can be written as

$$\phi(\hat{r},\hat{\Omega}_1) = \phi(\hat{r},\hat{\Omega}_2) \quad \text{for } \hat{\Omega}_{p2} = \hat{\Omega}_{p1} - 2(\hat{n}\cdot\hat{\Omega}_{p1})\hat{n} \tag{116}$$

or as

$$\phi(\hat{r},\mu,\chi) = \phi(\hat{r},\mu,-\chi) = \phi(\hat{r},\mu,2\pi-\chi) \tag{117}$$

The symmetry χ is shown in Figure 5, where the vectors $\hat{n}$ and $\hat{\rho}$ are perpendicular.

Note that because of the problem geometry and the exponentially varying air density (in the z direction), only azimuthal symmetry in the angle χ is assured. There is no symmetry in $\mu(\cos\theta)$ and therefore $\phi(\hat{r},\hat{\Omega})$ will not be equal to $\phi(\hat{r},-\hat{\Omega})$. The symmetry condition, Eqs (116) and (117), implies that

$$\phi(\hat{r},\mu,\chi) = \text{even functions in } \chi \tag{118}$$

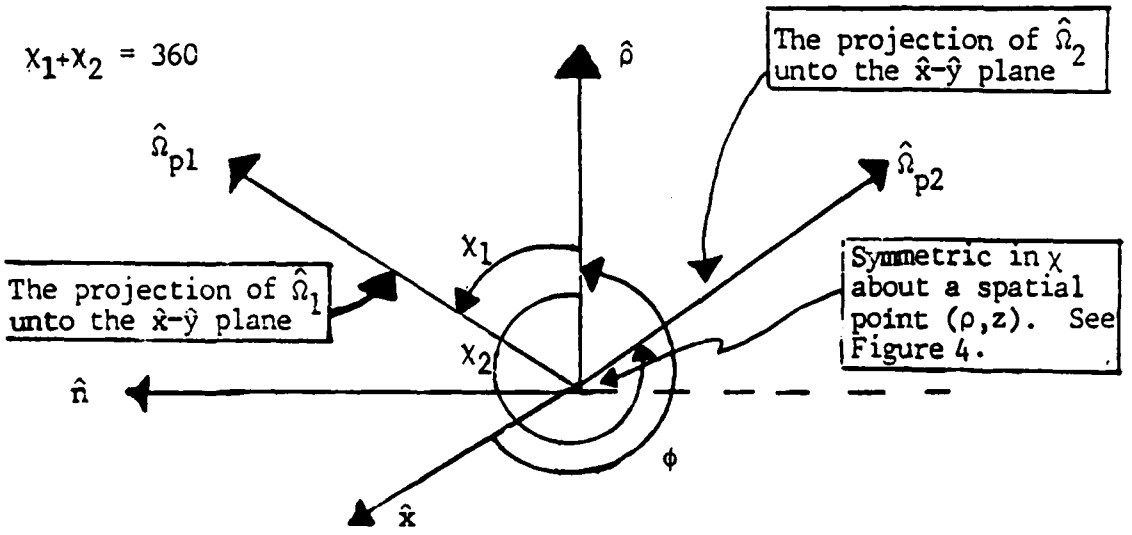

Figure 5. A Schematic of the Angular Symmetry.

The problem geometry and coordinate system as shown in Figure 4, together with the symmetry in χ requires that when ρ is equal to zero the solution is a constant in χ. This also implies that at $\rho = 0$ the angle χ must be equal to zero. Therefore, along the z-axis we have that

$$\frac{\partial}{\partial \chi} \phi(\hat{r},\hat{\Omega}) = 0 \quad \text{for } \rho = 0 \text{ and } \chi \equiv 0 \tag{120}$$

At the air-ground interface the angular flux is continuous in the spatial variable $\hat{r}$. This interface condition which is represented by Eq (13) is a natural condition of the Galerkin weak form (See Appendix C). However, this is a plane interface for which it can be shown (Bell and Glasstone, 1970) that the angular flux is discontinuous in the variable μ. This discontinuity exists at $\mu = 0$ and depends primarily upon the problem geometry, sources and material properties. The most severe cases are those of a vacuum boundary and interfaces where the adjoining materials are very dissimilar in terms of sources and cross-section data. The air-over-ground problem is in this later category.

It is important to note that this discontinuity does not present a difficulty in the Galerkin weak form. This formulation treats the interface condition as a natural condition and would provide an approximate solution to the problem. However, our trial space must be complete and in this case completeness includes the ability to approximate discontinuous functions. For problems where this discontinuity is severe the choice of a reasonable and "admissible" trial space is important.

Our trial space of harmonic functions is complete. The associated Legendre polynomials are also complete. They can approximate discontinuous functions in the mean by an infinite series where the number of functions (N) tend to ∞ (Bell and Glasstone, 1970). However, we can get a better approximation with a smaller trial space (N), if we include functions which are discontinuous at $\mu = 0$. This is the basic idea of the Double P_n approximation (Duderstadt and Martin, 1979). We simply separate the trial space in two half ranges in μ and use separate Legendre expansions on each range, i.e., $\mu \epsilon [-1,0)$ and $\mu \epsilon [0,1]$. With this approach we can easily treat problems with severe interface discontinuities. A very accurate solution of the air-over-ground problem may require such a treatment.

The Finite Element Basis and Problem Equations

Applying the finite element projection method of Chapter VII to the air-over-ground problem requires a numerical (computer) solution of the Galerkin weak form Eq (87). However, we must further define and choose our trial space in accordance with the problem symmetries and boundary conditions. In this solution we will follow the usual practice of not using a Double P_n approximation in angle. This approximation may only be needed for those problems where a very accurate solution at the air-ground interface is desired.

The general solution strategy of Chapter VII employs a dual basis of global harmonic functions in angle and finite elements in the spatial variables. We could also use four dimensional finite elements in both space and angle (Miller et al., 1973). However, these four dimensional phase-space finite elements will be very costly (computer costs) and inefficient (Wheaton, 1978). This is due to the added complexity of anisotropic scattering. Anisotropic scattering increases the data management and computational difficulties. A local basis in angle requires that the scattering contribution to each element must be computed on an element by element basis for all space and angle elements within the problem domain. Therefore, a

four-dimensional phase-space finite element formulation of this problem is not a very attractive or realistic approach.

We will use a dual basis of spherical harmonics and splines. The global nature of the spherical harmonic functions would facilitate the treatment of anisotropic scattering. This expansion which must also satisfy the symmetry conditions of Eqs (117) and (120) can be written as

$$\psi^g(z,\rho,\mu,\chi) = \sum_{iz=1}^{IZ} \sum_{ir=1}^{IR} \sum_{\ell=0}^{L} \sum_{m=0}^{\ell} A_i B_{iz}(z) B_{ir}(\rho) Q^c_{\ell m} \qquad (121)$$

where A_i are the expansion coefficients and $B_{iz}(z)B_{ir}(\rho)$ form a tensor product of normalized B-splines on a rectangular (ρ,z) grid (Deboor, 1978). $Q^c_{\ell m}$ is a surface harmonic function which is defined by Eq (96) with ℓ restricted to be even.

The definition of a polynomial B-spline is

$$B(x)_{i,k,t} = (t_{i+k} - t_i)[t_i \ldots\ldots t_{i+k}]G_k(x,t) \qquad (122)$$

where

$$G_k(x,t) = (t - x)_+^{k-1} = \begin{cases} (t-x)^{k-1} & \text{for } t \geq x \\ 0 & \text{for } t \leq x \end{cases} \qquad (123)$$

and

k = 1,2....= order of the B-spline

i = index of the i-th normalized B-spline

t_i and t_{i+k} represent the node points and $[t_i.....t_{i+k}]$ defines the usual k-th Newton divided difference. The graph of an unnormalized cubic spline function with evenly spaced nodes (knots) is shown in Figure 6. High order splines ($k \geq 2$) are (k-2) times continuously differentiable. These are very smooth functions, however, we can also construct low order linear splines and splines (k = 1) with jump discontinuities at the nodes (Schultz, 1973).

B-splines have been used extensively as interpolation functions (Schumaker, 1981). Spline interpolation requires the solution of a smaller system of equations than interpolation with Hermite or Lagrange polynomials. The usual practice is to use normalized B-splines in a N-

$$x_{i+2} - x_{i+1} = x_{i+1} - x_i$$
$$= x_i - x_{i-1} = x_{i-1} - x_{i-2} = h$$

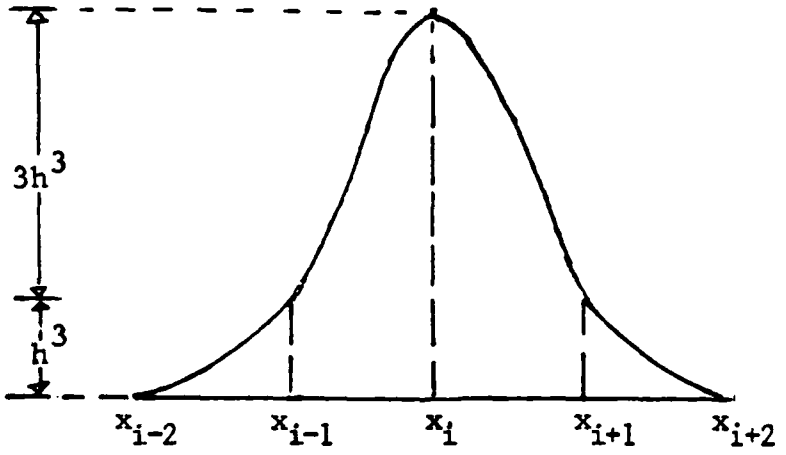

Figure 6. Cubic Spline With Evenly Spaced Nodes

dimensional space whereby

$$\sum_{i=1}^{N} B_{i,k,t}(x) = 1 \quad \text{for all } x \tag{124}$$

A tensor product of B-splines is being used here for the following reasons:

1. They are piecewise continuous and form a local basis such that the integral $\int_R B_i(x)B_j(x)\,dx$ is zero if $|i - j| \geq k$ where k is the order of the B-splines. This reduces the number of integrals which must be evaluated and also produces a sparse and banded coefficient matrix.
2. A separation of the ρ and z integration variables is possible.
3. For a given problem partition (mesh spacing) polynomial splines will produce a coefficient (problem) matrix that is smaller but less sparse than Hermites or Lagrange polynomials.

In the Galerkin weak form of Eq (87) the test or weight functions can now be defined as

$$N_i(z,\rho,\mu,\chi) = B_{jz}(z)B_{jr}(\rho)Q^c_{kn} \tag{125}$$

The spatial trial functions of B-splines are defined in the global problem coordinates. In this solution a local element coordinate system and a parametric reoresentation will not be used. Instead we will use ring type axisymmetric rectangular elements which are defined in the problem coordinates. These are four node two-dimensional elements with axial symmetry. They will be constructed on a non-uniform mesh in the (ρ,z) plane. Furthermore, in this representation the expansion coefficients of Eq (121) do not represent the solution values at the nodes except when linear B-splines (k = 2) are used. In the terminology of Chapter III and with this exception, these coefficients are generalized coordinates.

By substituting Eqs (125), (121) and (64a) into Eq (87) we get

$$\sum_{iz=1}^{IZ}\sum_{ir=1}^{IR}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell} A_i\Big[\int_R\Big\{\langle\hat{\Omega}\cdot\nabla(B_j\cdot Q^c_{kn}),K^u(\hat{\Omega}\cdot\nabla(B_iQ^c_{\ell m}))\rangle$$

$$+\ \langle B_jQ^c_{kn},G^g(B_iQ^c_{\ell m})\rangle\Big\}d\hat{r}\ +\ \int_s\oint_{4\pi}|\hat{\Omega}\cdot\hat{n}|B_jQ^c_{kn}B_iQ^c_{\ell m}d\hat{\Omega}d\hat{s}\Big]$$

$$=\int_R\Big\{\langle\hat{\Omega}\cdot\nabla(B_jQ^c_{kn}),K^uQ^u\rangle\ +\ \langle B_jQ^c_{kn},Q^g\rangle\Big\}d\hat{r} \tag{126}$$

Here ℓ and k are even integers and for simplicity the ρ, z, μ, χ dependences are omitted and

$$B_i = B_{iz}(z)B_{ir}(\rho) \tag{127}$$

$$B_j = B_{jz}(z)B_{jr}(\rho) \tag{128}$$

Eq (126) can be written as a matrix problem in the form of Eq (114) where the A_i's are the flux expansion coefficients. The elements of the problem matrix and source vector are obtained by evaluating and summing the individual expanded terms of Eq (126). Details of this expansion are carried out in Appendix F where the surface normal and (streaming) gradient operators are defined in cylindrical geometries.

The directional gradient operator in cylindrical geometry is defined as (Bell and Glasstone, 1970)

$$\hat{\Omega}\cdot\nabla\phi = \sqrt{1-\mu^2}\cos(\chi)\frac{\partial(\rho\phi)}{\partial\rho} - \frac{1}{\rho}\frac{\partial\left\{\phi\sqrt{1-\mu^2}\sin\chi\right\}}{\partial\chi} + \mu\frac{\partial\phi}{\partial z} \tag{129}$$

This is the conservative form of the directional derivative in two dimensional (ρ,z) geometry with azimuthal symmetry. The K^u and G^g operators have been defined in Eqs (42) and (39). The scalar product of the velocity and normal vectors can be written as

$$\hat{\Omega}\cdot\hat{n} = \begin{cases} \hat{\Omega}\cdot\hat{n}_z & \text{for the horizontal outer surfaces (top or bottom) of the problem cylinder, and as} \\ \hat{\Omega}\cdot\hat{n}_\rho & \text{for the vertical surface (side) of the cylinder} \end{cases} \tag{130}$$

where

$$\hat{\Omega}\cdot\hat{n}_z = \begin{cases} \mu \text{ on the top surface, and} \\ -\mu \text{ on the bottom surface} \end{cases} \tag{131}$$

and

$$\hat{\Omega}\cdot\hat{n}_\rho = \sqrt{1-\mu^2}\cos\chi \tag{132}$$

The normal unit vectors $\hat{n}_\rho$ and $\hat{n}_z$ are shown in Figure 7.

Expanding the expressions in Eq (126) produces an integral-differential equation which has twenty-eight terms (See Appendix F). These terms, except for the source terms, can easily be separated into a product of z, ρ, μ and χ

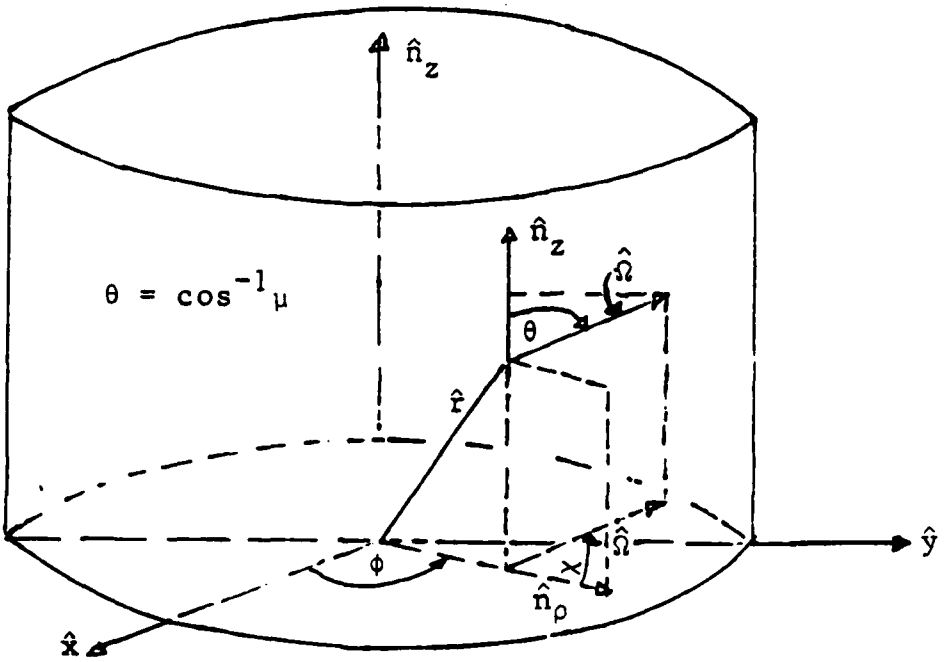

Figure 7. Surface Normal and Particle Velocity Direction Vectors.

integrals. This is an integral separation of variables which is a direct result of Eq (121); where it is assumed that the solution can be expressed in a form where the dependent variables are separable. This separation property simplifies the individual integrals which have to be evaluated. It allows for the evaluation of only single integrals and not the more complicated double, triple or quadruple integrals. By this separation of variables it may be possible to integrate most of these single integrals analytically and thus avoid a numerical integration process.

The term by term expansion of Eq (126) has produced thirty-seven distinct single integrals. These integrals can be found in Appendix G. The angle integrals are only dependent on the degree of the spherical harmonic trial function expansion which is used. They are not dependent on the problem parameters and therefore they can be independently evaluated. They can be evaluated once, and thereafter, used as a part of the problem input data. The source integrals are derived from an interpolation of the first scatter air-over-ground source over the entire spatial problem domain. This first scatter source is derived in the next section.

The Source Terms

A numerical solution of the second order transport equation requires that the source terms (right hand side of Eq (126) must be evaluated. These terms form the individual elements of the problem source vector in Eq (114). The even and odd parity sources Q^g and Q^u are comprised of the relevant terms of Eqs (111) and (112). For this steady-state monoenergetic solution these are the even and odd parity inhomogenous sources S^g and S^u where we have dropped the explicit multigroup index. These sources will be defined as the first scatter or collision even and odd parity sources. For the air-over-ground problem the first scatter source $S(\hat{r},\hat{\Omega})$ is the number density of particles which leave the source point and undergo only one collision before being scattered into direction $\hat{\Omega}$ at position $\hat{r}$. Streaming neutrons which leave the source point and do not collide before reaching position $(\hat{r},\hat{\Omega})$ are not included in the collision source.

The use of a first scatter source makes the air-over-ground problem more isotropic. It removes the strongly anisotropic streaming particles from being a part of the problem. Therefore, the solution fluence of Eq (126) will be the scattered even parity fluence $\psi_s^g(\hat{r},\hat{\Omega})$ and not the total even parity fluence $\psi_t^g(\hat{r},\hat{\Omega})$. Following

the derivation of Wills (1981), the total even parity fluence can be defined as

$$\Psi_t(\hat{r},\hat{\Omega}) = \Psi_s(\hat{r},\hat{\Omega}) + \Psi_d(\hat{r},\hat{\Omega}) \tag{133}$$

where

$$\Psi_d(\hat{r},\hat{\Omega}) = \text{streaming uncollided particles at position } (\hat{r},\hat{\Omega}).$$

A precise mathematical definition of the S^g and S^u sources will now be developed. Also a source interpolation procedure will be outlined. This source interpolation is used in order to simplify the source integrals of Appendix F.

The First Scatter Source. The even and odd parity sources have been defined as

$$S^u(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{S(\hat{r},\hat{\Omega}) - S(\hat{r},-\hat{\Omega})\right\} \tag{134}$$

$$S^g(\hat{r},\hat{\Omega}) = \tfrac{1}{2}\left\{S(\hat{r},\hat{\Omega}) + S(\hat{r},-\hat{\Omega})\right\} \tag{135}$$

If S^u and S^g are first scatter source densities then $S(\hat{r},\hat{\Omega})$ and $S(\hat{r},-\hat{\Omega})$ must also be defined as first scatter source particles/unit volume. If a position (ρ,z) in the problem domain is chosen then a unit vector from the source point $(0,zb)$ can be defined as

$$\hat{\Omega}'(\rho,z) = \frac{\rho\hat{e}_\rho + (z-zb)\hat{e}_z}{\{\rho^2 + (z-zb)^2\}^{\frac{1}{2}}} \tag{136}$$

Figure 8 shows the direction vectors of this first scatter (collision) source. $\hat{\Omega}'$ is the direction that all streaming (uncollided) particles have at point (ρ,z).

By definition only particles which are streaming radially outward from the source point can be included in the direction fluence. Therefore the direct fluence at point (ρ,z) is in the $\hat{\Omega}'$ direction and can be written as

$$\phi_d(\rho,z,\hat{\Omega}') = \frac{Y}{4\pi s^2} \exp\left\{-\int_o^s \sigma_t(z)ds\right\} \tag{137}$$

where

$$s = \left\{\rho^2 + (z-zb)^2\right\}^{\frac{1}{2}} \tag{138}$$

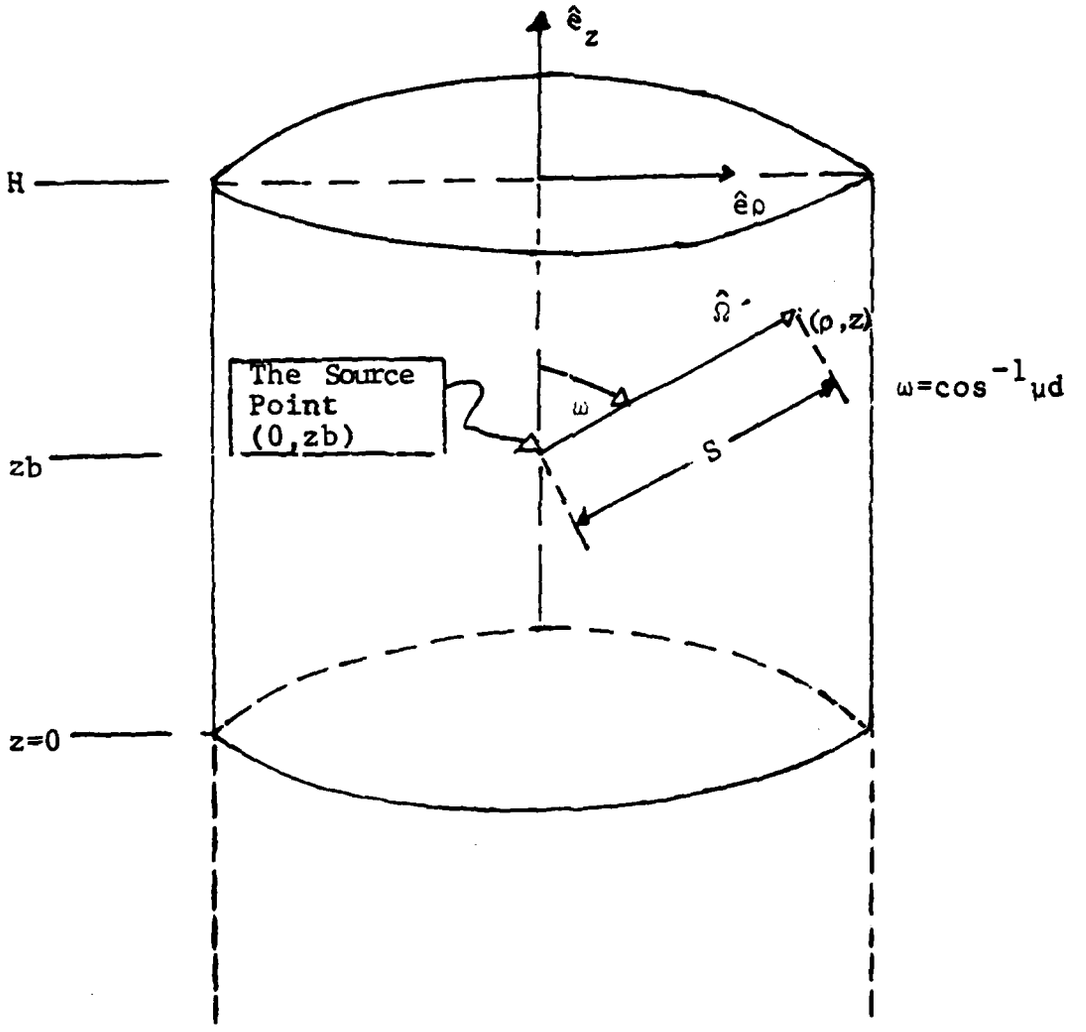

Figure 8. First Scatter (Collision) Source Direction Vectors.

and $\int ds$ means that the integration is carried out along the path s (See Figure 8).

Y = Total number of source particles.

$$\sigma_t(z) = \begin{cases} \sigma_t(0)e^{-z/sh} & \text{for } z \geq 0 \\ \sigma_t \text{ (ground)} & \text{for } z < 0 \end{cases} \qquad (139)$$

sh = atmospheric scale height

The term $\int_o^s \sigma_t(z)ds$ is the average number of collisions which a particle undergoes in traveling from the source point (o, zb) to point (ρ,z). From Figure 8 the distance s can also be written as

$$s = (z-zb)/\mu d \qquad (140)$$

and therefore by changing variables

$$ds = dz/\mu d \qquad (141)$$

where μd is a function of ρ and z (but constant along a path length) and,

$$\mu d(\rho,z) = \cos(\omega) = (z-zb)/s = \frac{(z-zb)}{\{\rho^2 + (z-zb)^2\}^{\frac{1}{2}}} \quad (142)$$

The integral term of Eq (137) can now be written for $z > 0$ as

$$\tau(\rho,z) = \int_o^s \sigma_t(z)ds = \frac{\sigma_t(0)}{\mu d}\int_{zb}^{z} e^{-z/sh}dz \quad (143)$$

and finally as

$$\tau(\rho,z) = \frac{\sigma_t(0)}{\mu d}\left\{e^{-zb/sh} - e^{-z/sh}\right\}\bullet sh$$

$$= \left\{\sigma_t(zb) - \sigma_t(z)\right\}\bullet \frac{sh}{\mu d} \quad (144)$$

From the above derivation it follows that

$$\tau(\rho,z) = \begin{cases} \left\{\sigma_t(zb) - \sigma_t(z)\right\}\bullet \frac{sh}{\mu d} & \text{for } z > 0 \\ \left\{\sigma_t(zb) - \sigma_t(0)\right\}\bullet \frac{sh}{\mu d} - \frac{\sigma_t z}{\mu d} & \text{for } z < 0 \end{cases} \quad (145)$$

also

$$\phi_d(\rho,z,\hat{\Omega}') = \frac{Y}{4\pi s^2}\exp(-\tau(\rho,z)) \tag{146}$$

Note that $\phi_d(\rho,z,\hat{\Omega}')$ is only a function of ρ and z.

The first scatter source at (ρ,z) and with direction μd are those particles which undergo their first collision at (ρ,z) and are scattered from direction $\hat{\Omega}'$ to $\hat{\Omega}$. Therefore the first scatter source can now be defined as

$$S(\rho,z,\hat{\Omega}) = \sigma^s(z,\hat{\Omega}\cdot\hat{\Omega}')\phi_d(\rho,z,\hat{\Omega}') \tag{147}$$

where σ^s is not a function of $\hat{\Omega}'$ but of the scattering angle $\hat{\Omega}\cdot\hat{\Omega}'(\mu_o)$ and z. From Figure 8 and Figure 4 $\hat{\Omega}'$ is defined by μd and $\chi = 0$ i.e., $\Omega' = (\mu',\chi')$ where $\mu' = \mu d$ and $\chi' = 0$.

By use of the addition theorem it is shown in Appendix H that Eq (147) can be written as

$$S(\rho,z,\hat{\Omega}) = 2\phi_d(\hat{r},z,\hat{\Omega})e^{-z/sh}\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2 P_{\ell m}(\mu d)\cos(m\chi) \tag{148}$$

and that the even and odd parity first scatter sources are

$$S^{g}(\rho,z,\hat{\Omega}) = \phi_{d}(\rho,z,\hat{\Omega}')\, e^{-z/sh} \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_{\ell}^{s}(0) C_{\ell m}^{2} \Big\{1 + (-1)^{\ell}\Big\} P_{\ell m}(\mu) P_{\ell m}(\mu d) \cos(m\chi) \qquad (149)$$

and

$$S^{u}(\rho,z,\hat{\Omega}) = \phi_{d}(\rho,z,\hat{\Omega}') e^{-z/sh} \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_{\ell}^{s}(0) C_{\ell m}^{2} \Big\{1 - (-1)^{\ell}\Big\} P_{\ell m}(\mu) P_{\ell m}(\mu d) \cos(m\chi) \qquad (150)$$

where m* means that all terms with an m = 0 subscript must be divided by two.

Source Interpolation. Because of the complicated nature of the source expressions, Eqs (149) and (150), and the need to integrate the source terms of Appendix F, a spatial source interpolation will be used. This interpolation which simplifies the source integrals is necessary if a very tedious (double or quadruple) integration is to be avoided. By this interpolation process the source terms of Appendix F can all be separated into a product of single integrals.

It is important to note that μd which is given by Eq (142) is a function of ρ and z. Furthermore, $\phi_d(\rho,z,\hat{\Omega}')$ of Eq (146) is a function of ρ and z. Beginning with Eqs (149) and (150) they can be rewritten as

$$S^g(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_\ell^s(0) C_{\ell m}^2 \left\{1 + (-1)^\ell\right\} A_{\ell m}(\rho,z) P_{\ell m}(\mu) \cos(m\chi) \tag{151}$$

and

$$S^u(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L} \sum_{m^*=0}^{\ell} \sigma_\ell^s(0) C_{\ell m}^2 \left\{1 - (-1)^\ell\right\} A_{\ell m}(\rho,z) P_{\ell m}(\mu) \cos(m\chi) \tag{152}$$

where

$$A_{\ell m}(\rho,z) = \phi_d(\rho,z,\hat{\Omega}') P_{\ell m}(\mu d) e^{-z/sh} \tag{153}$$

A spatial (ρ,z) interpolation of the even and odd parity sources, Eqs (151) and (152), is therefore an inter-

polation of $A_{\ell m}(\rho,z)$. In this project these first scatter second order sources will be interpolated by a combination of piecewise bilinear Lagrange polynomial functions. Specifically, S^g is approximated by a tensor product of linear Lagrange polynomials as follows

$$S^g(\rho,z,\hat{\Omega}) = \sum_{i=1}^{NZ}\sum_{j=1}^{NR} S^g(\rho_j,z_i,\hat{\Omega})H_j(\rho)H_i(z) \qquad (154)$$

where

$S^g(\rho_j,z_i,\hat{\Omega})$ = the even parity source, Eq (149) evaluated at the spatial nodes (ρ_j,z_i)

NZ = total number of z-nodes

NR = total number of R-nodes

$H(\rho)$ = ρ-linear Lagrange polynomial

$H(z)$ = z-linear Lagrange polynomial

These linear polynomials (See Figure 9) are defined as

$$H_i(x) = \begin{cases} \dfrac{x_{i-1} - x}{x_{i-1} - x_i} & \text{for } x_{i-1} \le x \le x_i \\ \dfrac{x_{i+1} - x}{x_{i+1} - x_i} & \text{for } x_i \le x \le x_{i+1} \end{cases} \qquad (155)$$

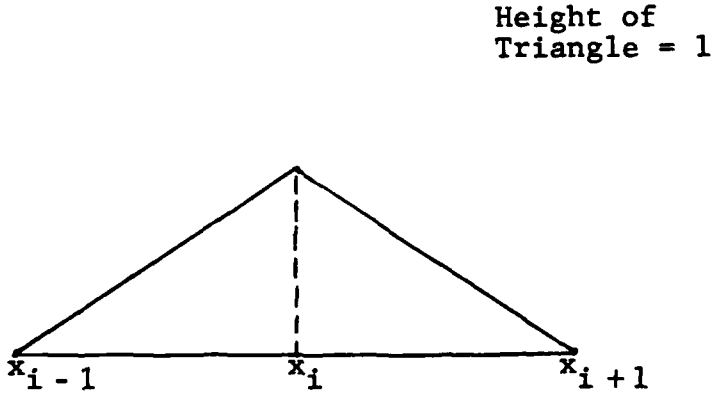

Figure 9. A Linear Lagrange Polynomial Function.

The product $H_j(\rho)\cdot H_i(z)$ of Eq (154) forms a tensor product space on a rectangular grid, in the ρ, z plane (Prenter, 1975)

Substituting Eq (149) for $S^g(\rho_j,z_i,\hat{\Omega})$ in Eq (154) gives

$$S^g(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\left[\sigma_\ell^s(0)C_{\ell m}^2\left\{1 + (-1)^\ell\right\}P_{\ell m}(\mu)\cos(m\chi)*\right.$$

$$\left.\sum_{i=1}^{NZ}\sum_{j=1}^{NR}A_{\ell m}(\rho_j,z_i)H_j(\rho)H_i(z)\right] \qquad (156)$$

Similarly the odd parity source can also be expressed as

$$S^u(\rho,z,\hat{\Omega}) = \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\left[\sigma_\ell^s(0)C_{\ell m}^2\left\{1 - (-1)^\ell\right\}P_{\ell m}(\mu)\cos(m\chi)*\right.$$

$$\left.\sum_{i=1}^{NZ}\sum_{j=1}^{NR}A_{\ell m}(\rho_j,z_i)H_j(\rho)H_i(z)\right] \qquad (157)$$

Eqs (156) and (157) can now be substituted into the source terms of Eq (126). This substitution and a separation of the integration variables produced a number of source intergrals. These integrals are listed in Appendix G.

Computer Solution and Results

A finite element projected solution of the air-over ground problem can be obtained from a computer solution to a system of coupled algebraic equations, which are in the form of Eq (126). In order to validate, evaluate and demonstrate the potential of our finite element formalism, a computer program was developed to solve the steady-state monoenergetic problem. This solution involves a computer assemblage and solution of the matrix problem of Eq (126).

Our solution is basically a computer implementation of the problem equations and expansions of the previous section. We developed a computer code to solve the even parity Galerkin equation with vacuum boundary conditions, first scatter sources, and an exponentially varying atmosphere. This is a solution to Eq (126) with the source terms of Eqs (156) and (157), and in an air-ground cylindrical geometry where the point sources are confined to the z-axis. A tensor product of cubic splines ($k = 4$) is used to represent the spatial (ρ,z) variables.

This is a four-dimensional problem with two spatial and two angular (μ,χ) variables. The ground is modeled as a homogenous cylinder with constant material properties (density and cross-sections). However, in keeping with

the exponentially varying density of the atmosphere (Messier, 1971) the cross-section of air is modeled with an exponential dependence where

$$\sigma_{air}(r) = \sigma_{air}(0)e^{-z/H} \tag{158}$$

and

$\sigma_{air}(0)$ = cross-section of air at sea level

H = atmospheric scale height

z = height above sea level.

In order to compare and validate our solution with other methods (codes) we also included an option ($H \to \infty$) which models a homogenous atmosphere.

The Computer Program. This is a straightforward computer implementation of the problem equations which were developed in the previous section. These equations are expanded in Appendix F. The integrals which must be evaluated are in Appendix G.

This finite element transport (FET) code computes the even parity flux and the scalar or total reaction rate flux for the air-over-ground problem. It was developed

specifically to solve this problem. The structure, format and design of the FET program are based upon the special features and difficulties of the air-over-ground problem. Therefore, the FET code is designed for a specific research application and not as a general particle transport code.

The FET program consists of over 1800 lines and twenty subprograms. We used a modular programming style and separated the computational tasks into five main areas. In each of these areas we developed function and subroutine subprograms to carry out specific tasks. We also used an eight point Gauss-Legendre adaptive quadrature routine to numerically evaluate the integrals of Appendix G. This integration program is a part of a system library of mathematical subroutines and functions. It belongs to the SLATEC (Sandia-Los Alamos-Air Force Weapons Laboratory Technical Exchange Committee) common mathematical subprogram library (Allen and Funk, 1981).

The main computational tasks in the order in which they were performed by FET are as follows:

1. Program Initialization and Input

   The problem parameters and data are read from an input file by the main program driver. This program determines the problem size and computes the problem mesh (elements).

2. Evaluation of the Integrals

The integrals of Appendix C are evaluated for each of the trial function expansion subscripts.

3. Computation of the Source Vector

The first collision source is computed and the source vector (right hand side of Eq (126)) is assembled. The individual elements of the source vector are computed and stored as a singly subscripted real array.

4. Compute the Problem Matrix

The individual terms of the left hand side of Eq (126) are computed. These terms are then added and subtracted to form the problem matrix. This is a doubly subscripted N x N array. However, because the problem matrix is positive definite symmetric only those elements on or above the diagonal are computed. Furthermore, a special sparse symmetric storage scheme is used (Bathe, 1982), and the problem matrix is stored as a singly subscripted array.

5. Solution of the Matrix Problem

Having assembled the problem matrix and source vector the FET code solves a matrix problem for the even

parity expansion coefficients (the A_i's) of Eq (121). Because the problem matrix is positive definite symmetric we could use an indirect (iterative) solver (Hageman and Young, 1980). We can also use a Gauss-Jordan elimination process or some other direct method (Atkinson, 1978). FET uses Cholesky decomposition which is a variant of Gauss-Jordan elimination for positive definite symmetric matrices. A subprogram which is based on the routine Colsol of Bathe (1982) is used in the FET code. This subprogram carries out a Cholesky decomposition of the problem matrix and a back-substitution of the source vector (Jennings, 1977).

Results and Comparisons. The evaluation and validation of our finite element projection technique was accomplished by using the FET code to solve a number of sample problems. These solutions show that our solution technique is capable of solving difficult problems of physical and engineering interest. They are not meant to be a complete and exact solution of the air-over-ground problem but, rather a demonstration of the potential of our solution approach to solve general particle transport problems. However, they do show that for the air-over-ground problem our method can serve as a feasible and com-

plementary alternative to Monte Carlo and discrete ordinates.

The air-over-ground problem was chosen because of its inherent difficulties and the limitations of presently available solution techniques (Loewe, et al., 1983). In order to validate our solution approach and the FET code a number of P_3 homogenous air calculations were performed. These calculations afforded a comparison of our results to those of other methods. We compared our results with those of diffusion theory and discrete ordinates. We also carried out homogenous and inhomogenous P_3 air-over-ground calculations. These calculations demonstrate the potential of our method for providing detailed and accurate solutions to the air-over-ground problem. We will now present these results and comparisons.

One group neutron cross-sections from the DLC-31 cross-section set of Oak Ridge National Laboratory (ORNL) were used. These cross-sections are a part of the Radiation Shielding Information Center (RSIC) data library. Two sets of one-group cross-sections were used to perform the calculations. These cross-sections were assembled by ORNL from the Evaluated Nuclear Data File IV (ENDF-IV). A uniform 1/E weighting function was used to average and collapse the cross-sections to 37 groups.

The cross-sections are approximated by a 4th order (P_3) Legendre polynomial expansion. The two sets of one group cross-sections which we will label group one and two reflects the anisotropic (forward peak) scattering of air. These cross-sections are for homogenous air at an air density of 1.11 mg/cc and with mean free paths of 0.16 km and 0.11 km for groups one and two respectively. The group two scattering P_3 cross-sections are more anisotropic and forward peaked than those of group one.

In order to validate our method and debug the computer code FET we compared our results to those of an analytic diffusion theory solution. This analytic solution is based on a point source of one particle in a finite homogenous sphere. It can be shown (Glasstone and Edlund, 1952) that the diffusion solution of this problem with vacuum boundary conditions is given by

$$\phi(r) = \frac{S_o\left[e^{-r/L} - e^{(r-2R_o)/L}\right]}{4\pi D(1 - e^{-2R_o/L})r} \qquad (159)$$

where

r = distance from the point source (center of sphere)

R_o = radius of sphere

L = diffusion length

D = diffusion coefficient

S_o = source strength

Diffusion theory is inappropriate to model this problem exactly, especially close to the boundaries and point sources (Duderstadt and Hamilton, 1976). Furthermore because the FET code provides the solution to a point source on the z-axis in a cylindrical geometry an exact comparison cannot be made. However, we can compare these two results in an approximate way.

Both the FET code and analytic diffusion results are for a point source of one particle and the group one and two homogenous air cross-sections. These results for a sphere and cylinder with vacuum boundaries are shown in Figures 10 and 11. The diffusion calculations are performed in a sphere with a radius of 2km and with the point sources at the origin. The FET calculations are for a cylinder of radius and height equal to 2km respectively. The source is located at the center of the cylinder. For the group one calculation the cylinder is subdivided into 256 rectangular elements (cells). However, for the group two calculation it is partitioned into 324 (rectangular) elements. These (FET) results are presented for radial points at the source altitude.

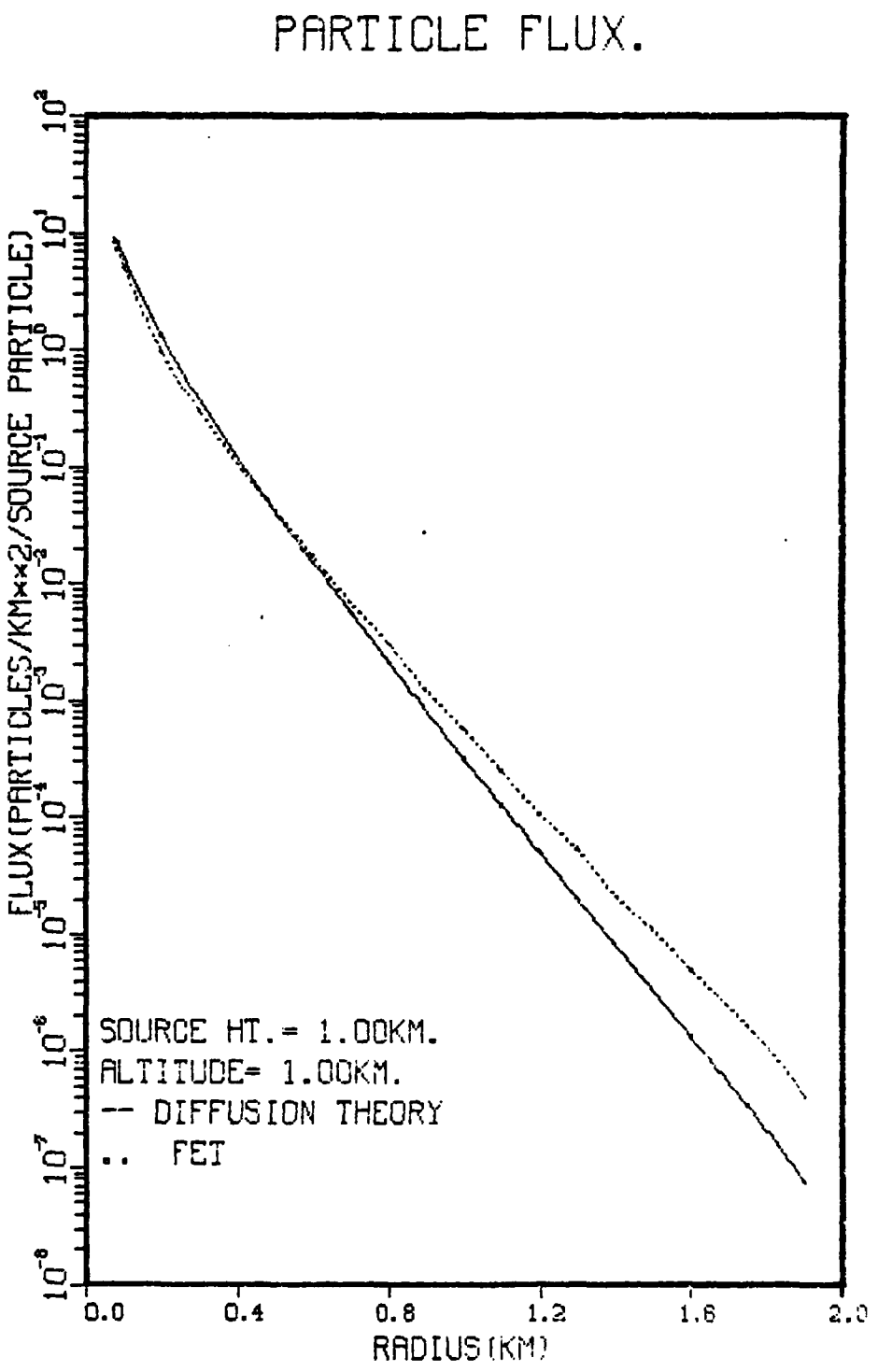

Figure 10. Group 1 -- Diffusion Theory Comparison

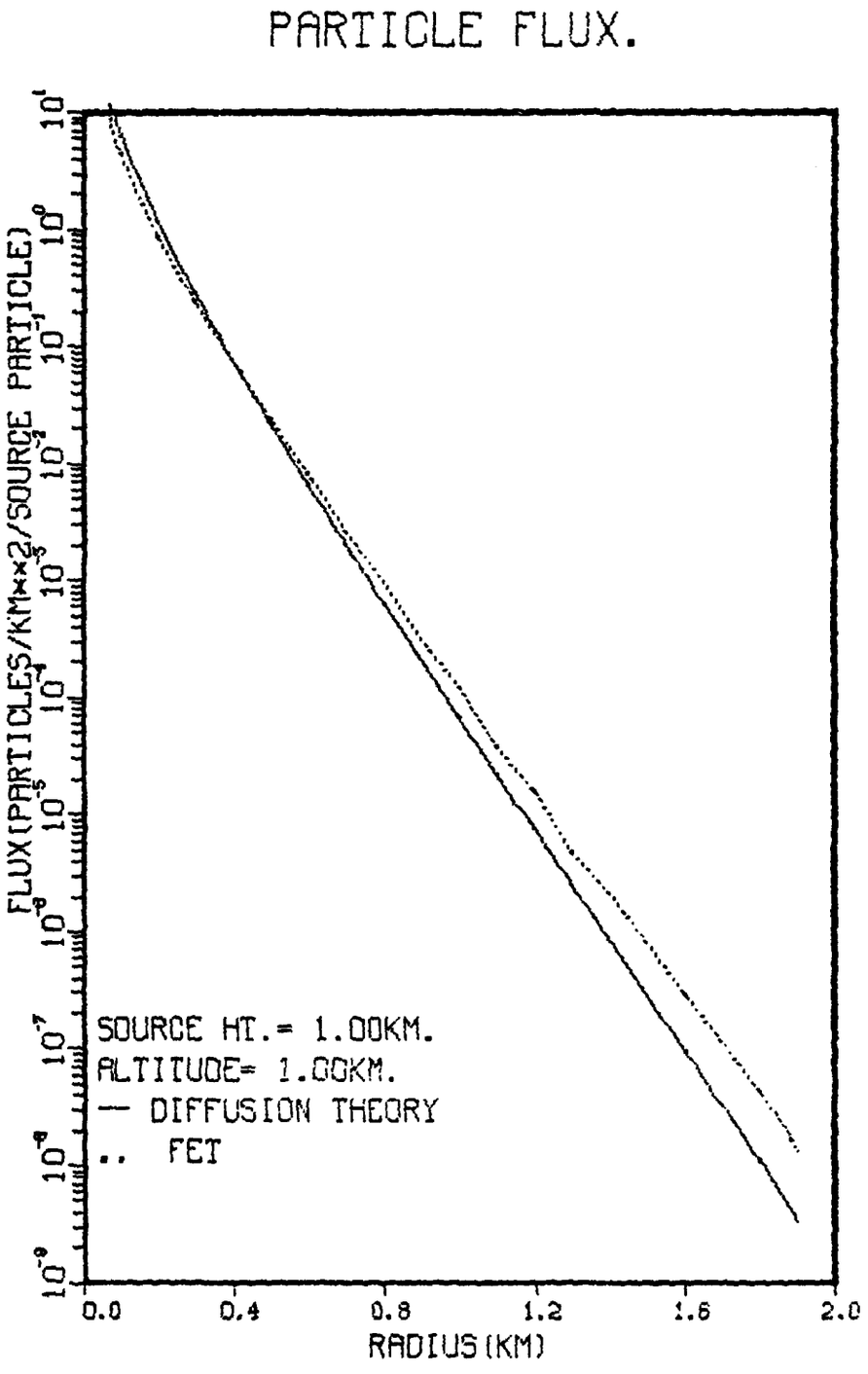

Figure 11. Group 2 -- Diffusion Theory Comparison

To further examine and validate our results we also made two comparisons with discrete ordinate solutions. These solutions were independently obtained by using the discrete ordinates (S_n) code ANISN (Burgio, 1975). Infinite homogenous air calculations in spherical geometry were performed with point sources at the origin and an S_{32} angular quadrature. These are published results for a number of one group problems. We have presented, in Figures 12 and 13, a comparison of these results for the cross-sections of groups one and two. The FET results are for a 2km x 2km homogenous cylinder with vacuum boundary conditions. Here again the cylinder is partitioned into 256 and 324 rectangular elements for the groups one and two calculations respectively. The point source is at the cylinder center and the flux values are for radial points which are at the source altitude. Because of the differences in the geometry of the FET and S_n calculations an exact comparison cannot be made. However, we are able to provide an approximate comparison and thus demonstrate that our results are appropriate and valid.

We also performed a number of air-over-ground calculations. The homogenous ground cross-sections for group one and two are larger and less anisotropic than for that of air. Furthermore, the ground cross-sections for group two are more anisotropic than the group one

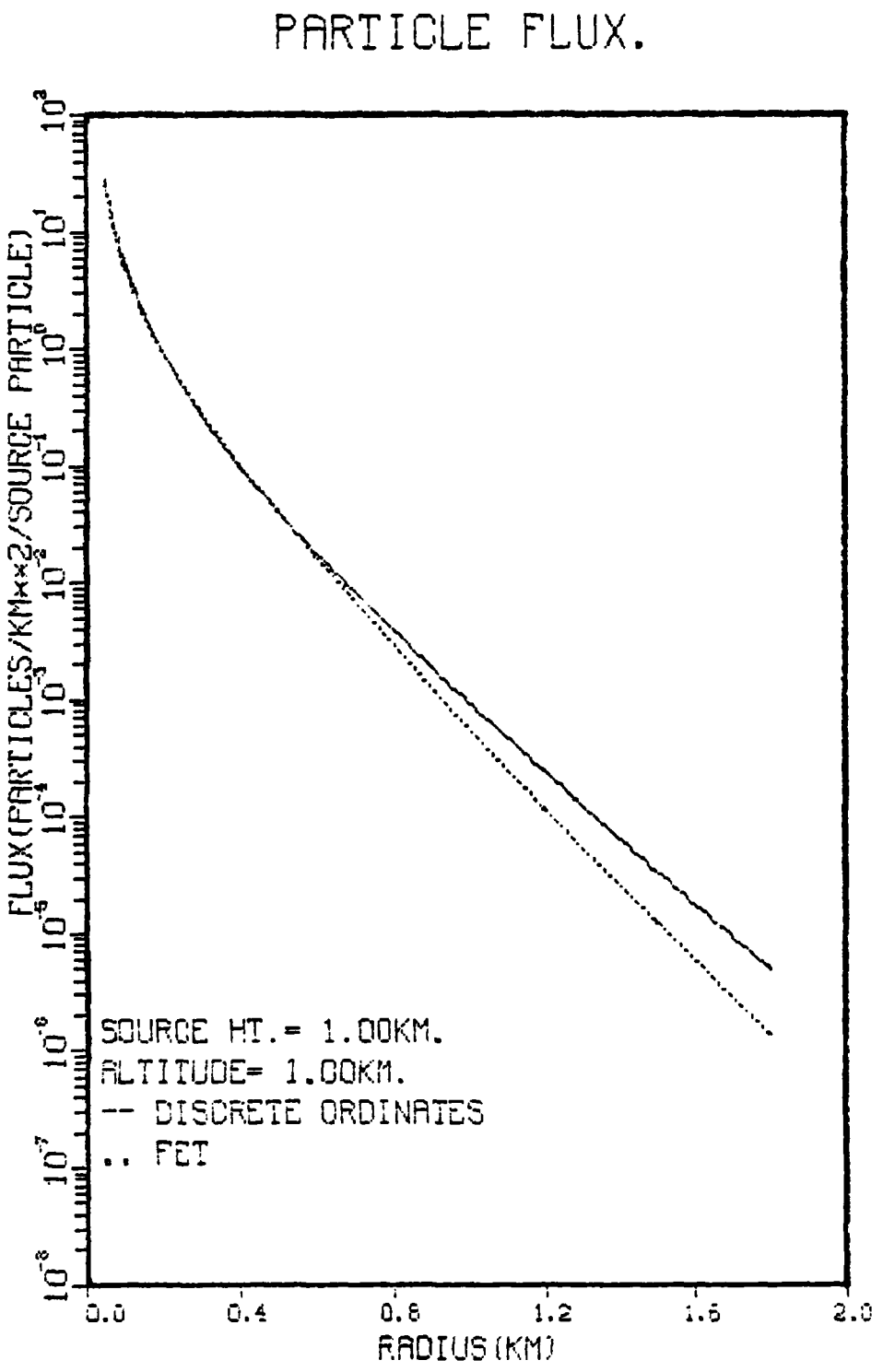

Figure 12. Group 1 -- Discrete Ordinates Comparison

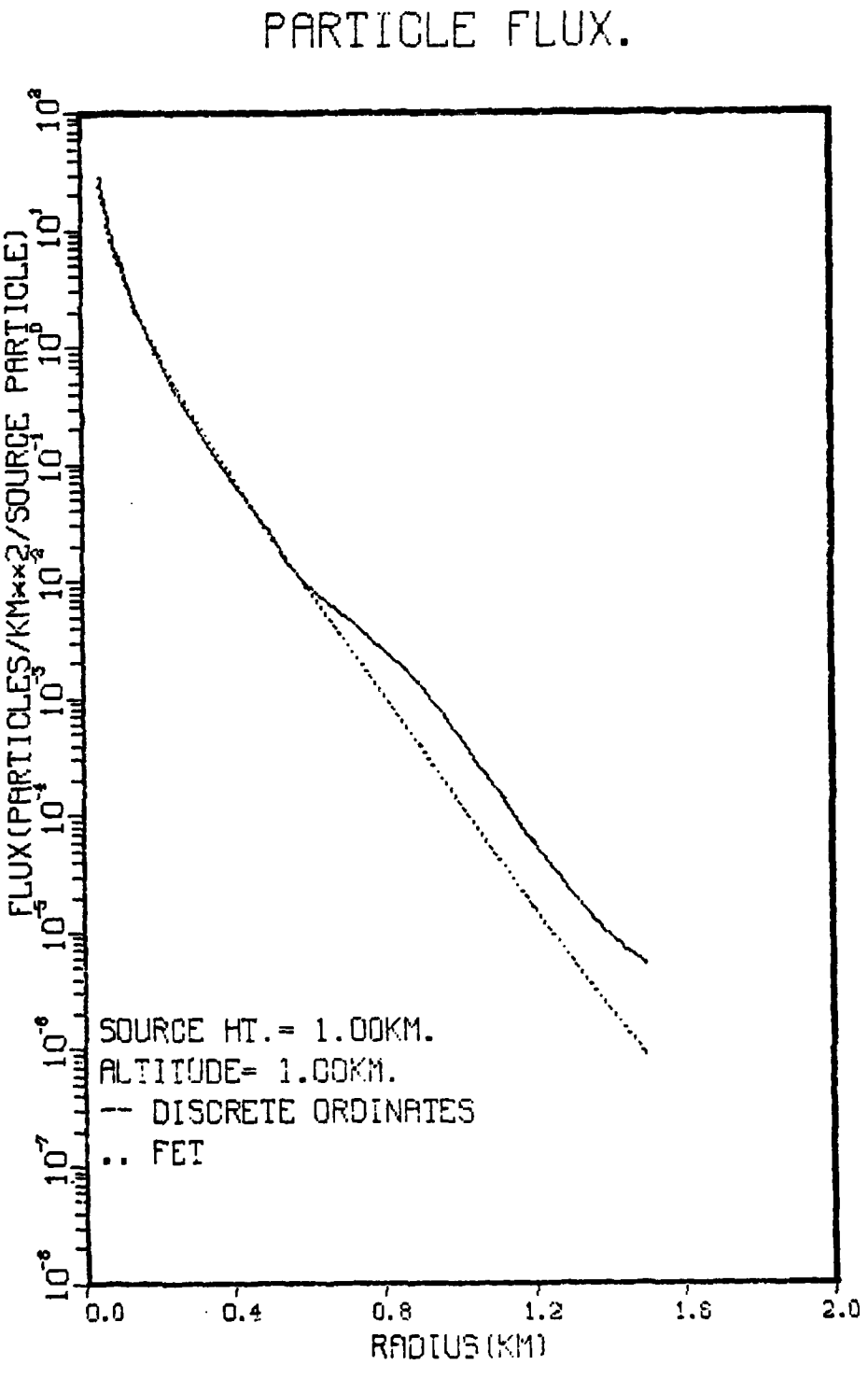

Figure 13. Group 2 -- Discrete Ordinates Comparison

ground cross-sections. The ground mean free paths for group one and two are 1.05E-4 and 7.42E-5 kilometers. At the air-ground interface the material properties and cross-section data are rapidly varying. The air and ground cross-sections vary by three orders of magnitude. This presents special difficulties and a severe test for most numerical solution techniques (Lowe, et al., 1983).

The difficulties in solving the air-over-ground problem are also due to the presence of point sources and an exponentially varying atmosphere. These difficulties are further compounded by the need to properly treat the air-ground interface condition. This is an important consideration, especially when a solution is required at the interface. For many applications a solution is required at ground level or very close to the interface (Pace, et al., 1975). Therefore, we are primarily interested in a solution to the air-over-ground problem for radial points (ground range) along this interface.

This interface condition is treated as a natural condition in our finite element projected solution. Therefore, our solution also demonstrates the ability of our method to model the air-ground interface. Solutions for the homogenous and exponentially varying problems are presented in Figures 14 through 17. The group one and two cross-sections were used to calculate scalar flux values

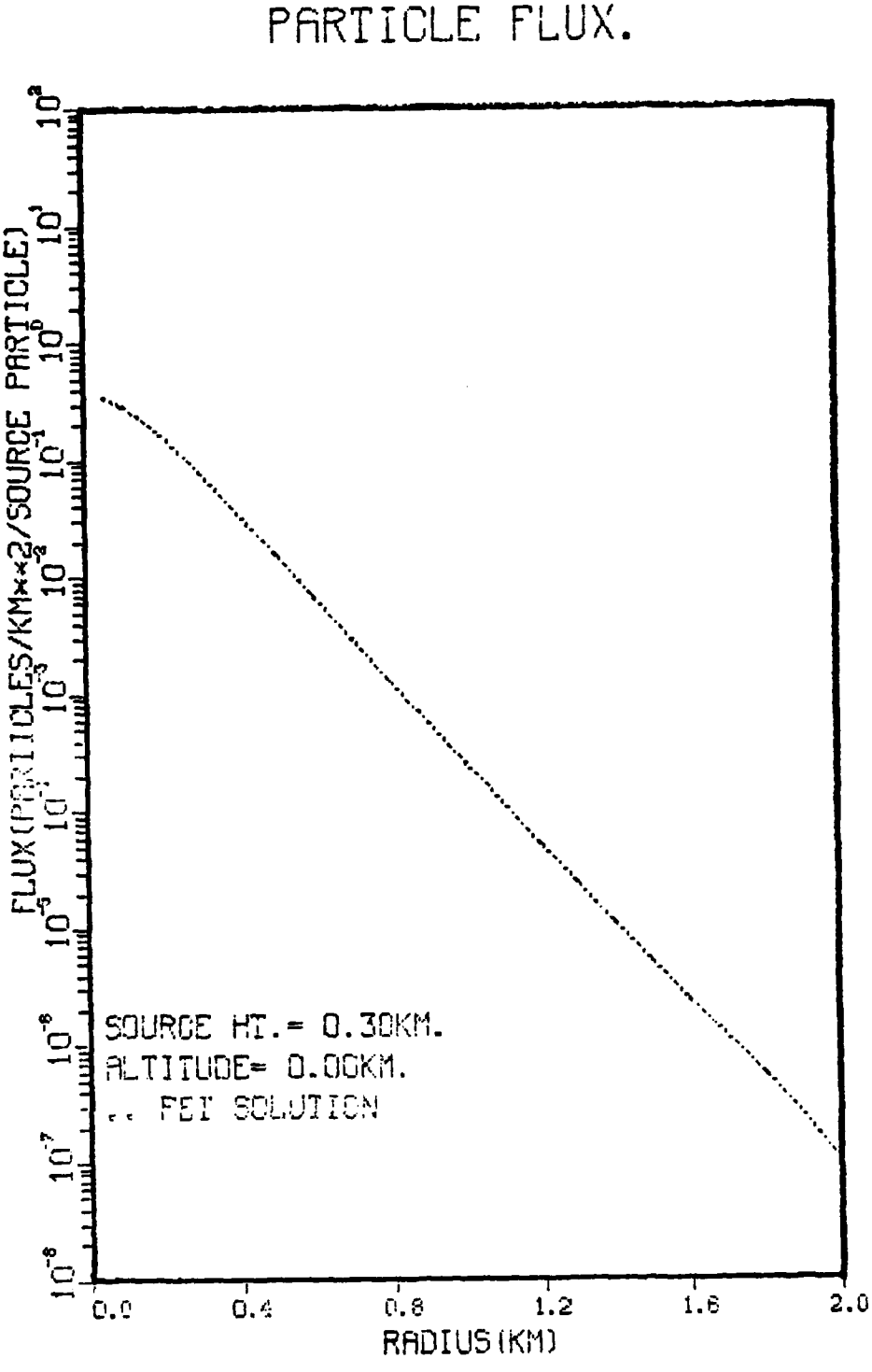

Figure 14. Group 1 -- Homogenous Air-Over-Ground Solution

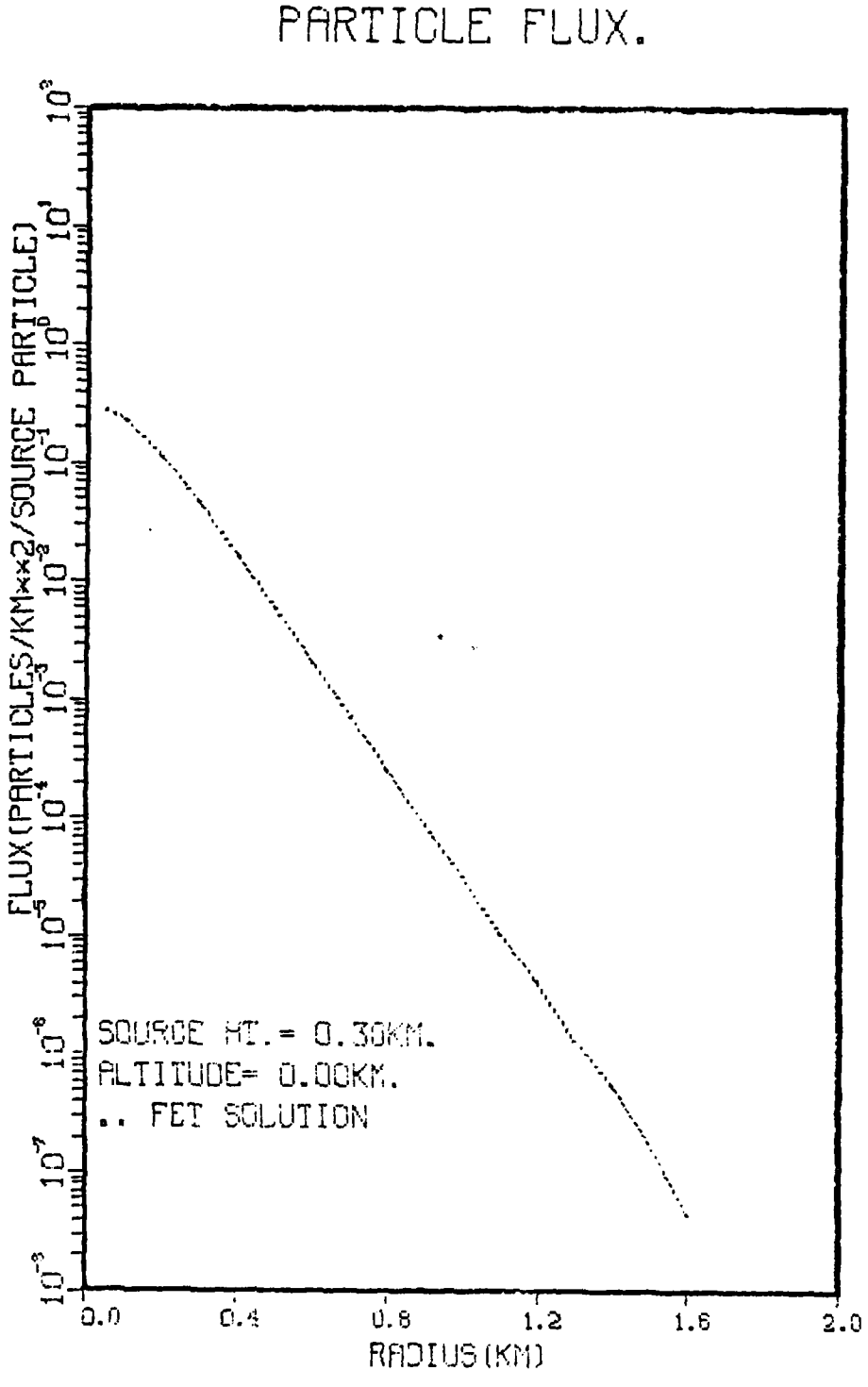

Figure 15. Group 2 -- Homogenous Air-Over-Ground Solution

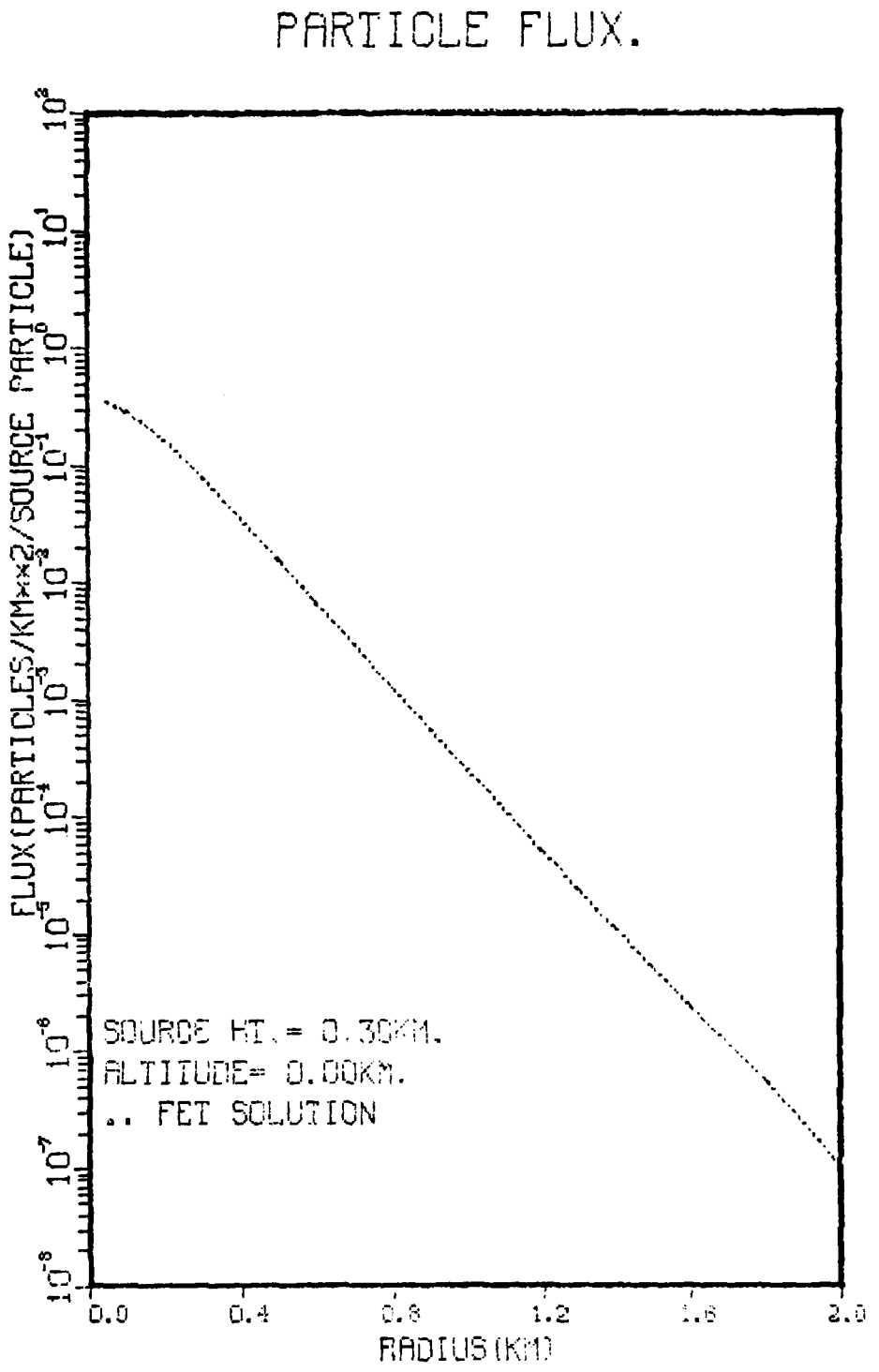

Figure 16. Group 1 --Exponential Air-Over-Ground Solution

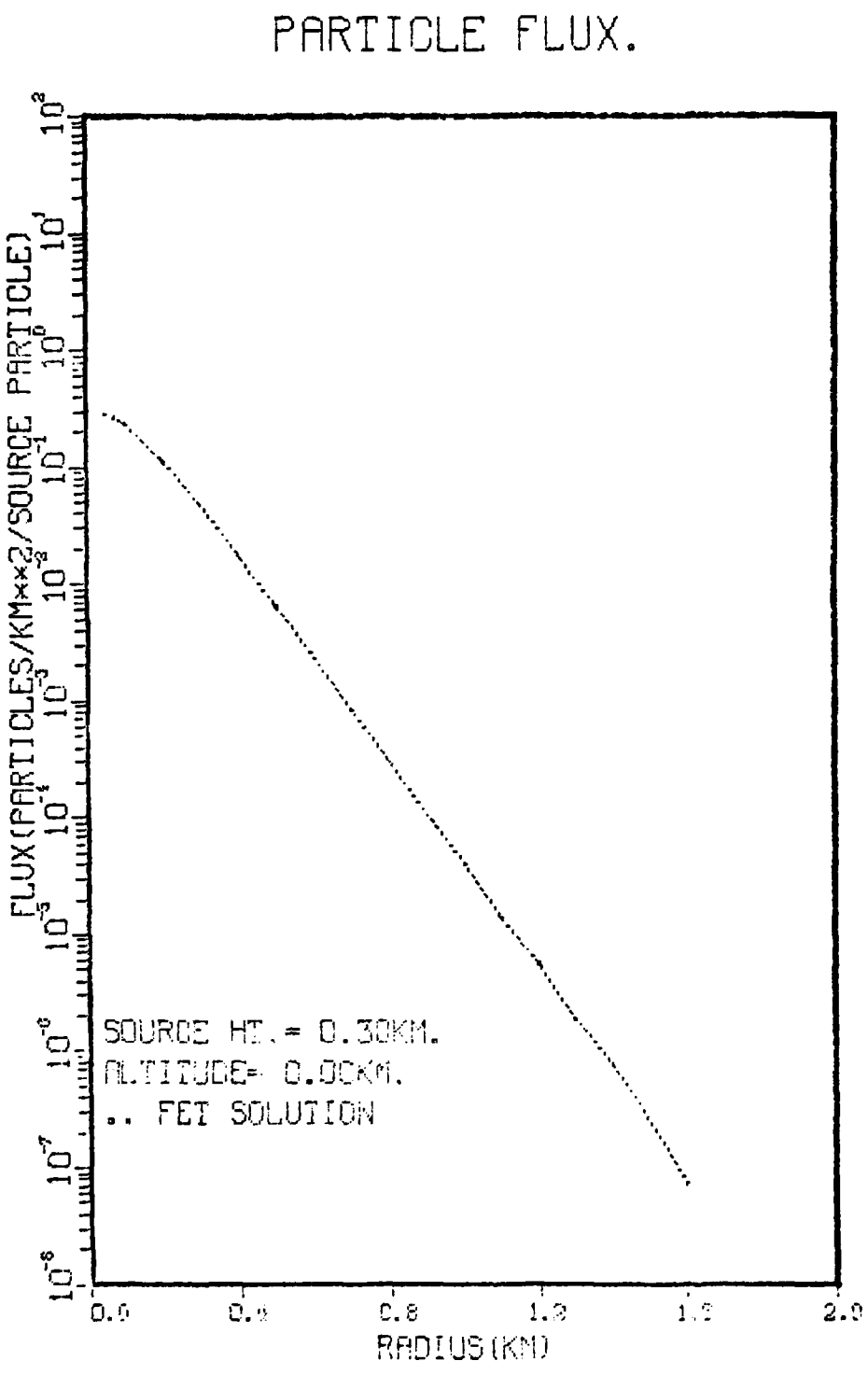

Figure 17. Group 2 -- Exponential Air-Over-Ground Solution

at the air-ground interface. The problem domain is a 2km x 2km cylinder with vacuum boundary conditions. The cylinder has 304 cells for the group one problem and 381 cells for group two. A scale height (H) of 7km is used in the exponentially varying air-over-ground calculations. In Figures 18 and 19 we show the variation of the group one homogenous air-over-ground solution across the interface. This (air-ground) interface is located at 4.5E-4 kilometers from the bottom of the problem cylinder.

Finally, we examined contour plots for the homogenous air (only) problem and the convergence of the FET solution. Figure 20 shows an example of this convergence. These are results at points along the air-ground interface for the group one homogenous air-over-ground problem. The problem domain is a 1km x 1km cylinder which is partitioned into a nonuniform mesh with an equal number of mesh points along the z and ρ axes.

In Figure 21 we present a contour plot of the group one FET homogenous air solution. This plot is intended to show any deviation of the solution from the physical symmetries of the problem. Such deviations or distortions of the solution is usually an indication of ray effect in the discrete ordinate solution (Loewe, et al., 1983). Figure 21 shows that the FET solution does not suffer from the anomalous ray effect problem of discrete ordinates.

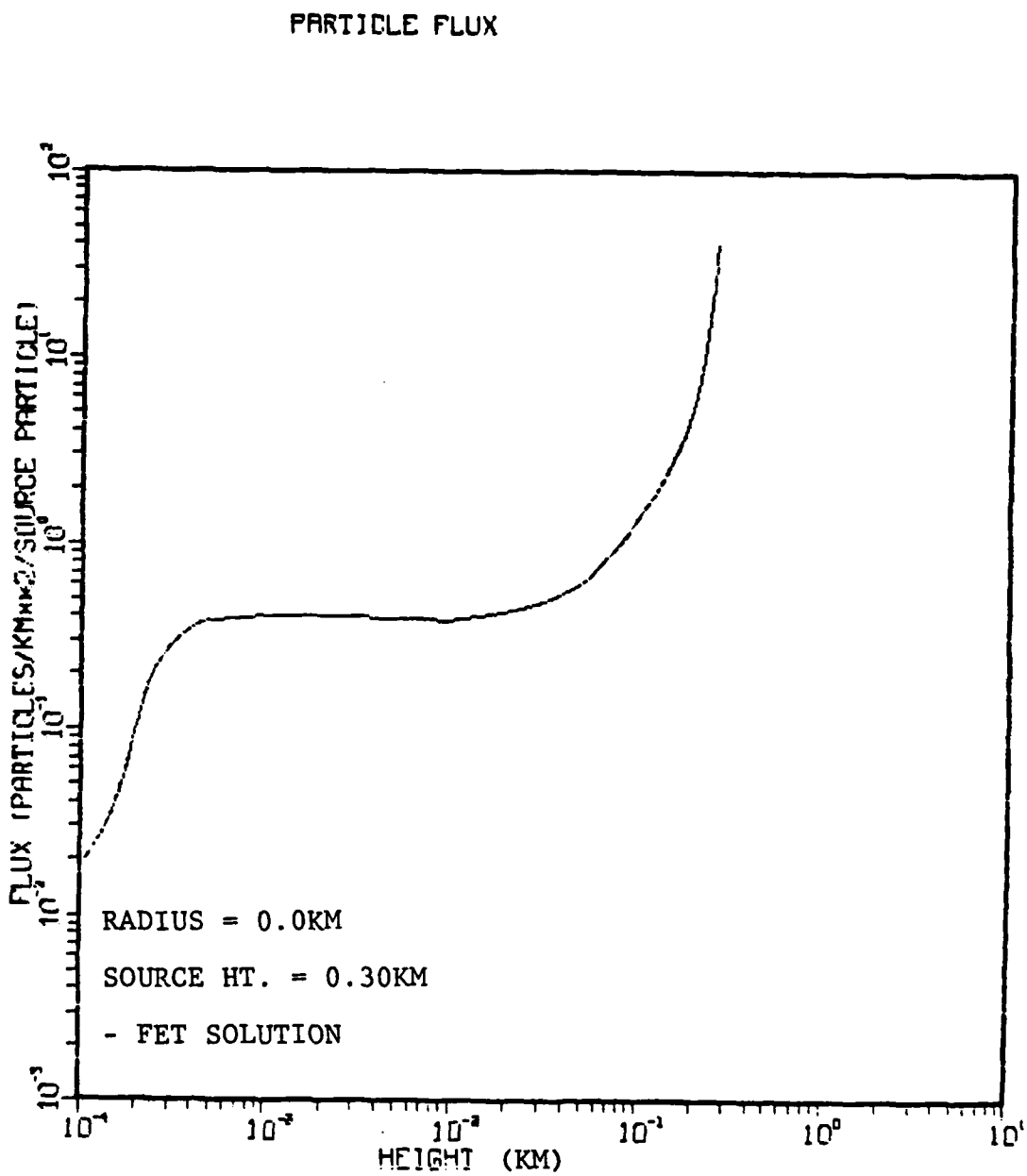

Figure 18. Group 1 -- Homogenous Air-Over-Ground Solution at Radius = 0.0km

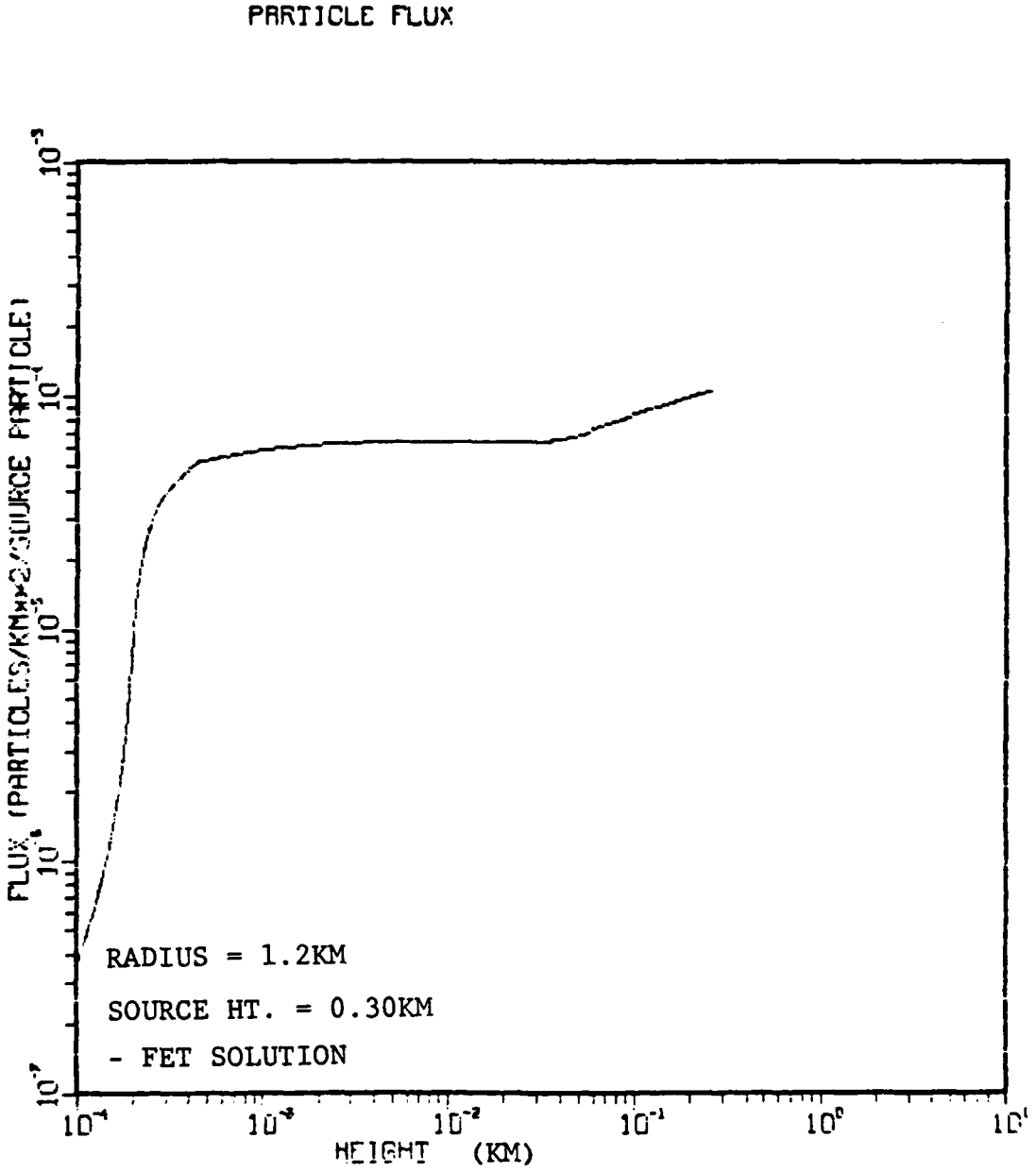

Figure 19. Group 1 -- Homogenous Air-Over-Ground Solution at Radius = 1.2km

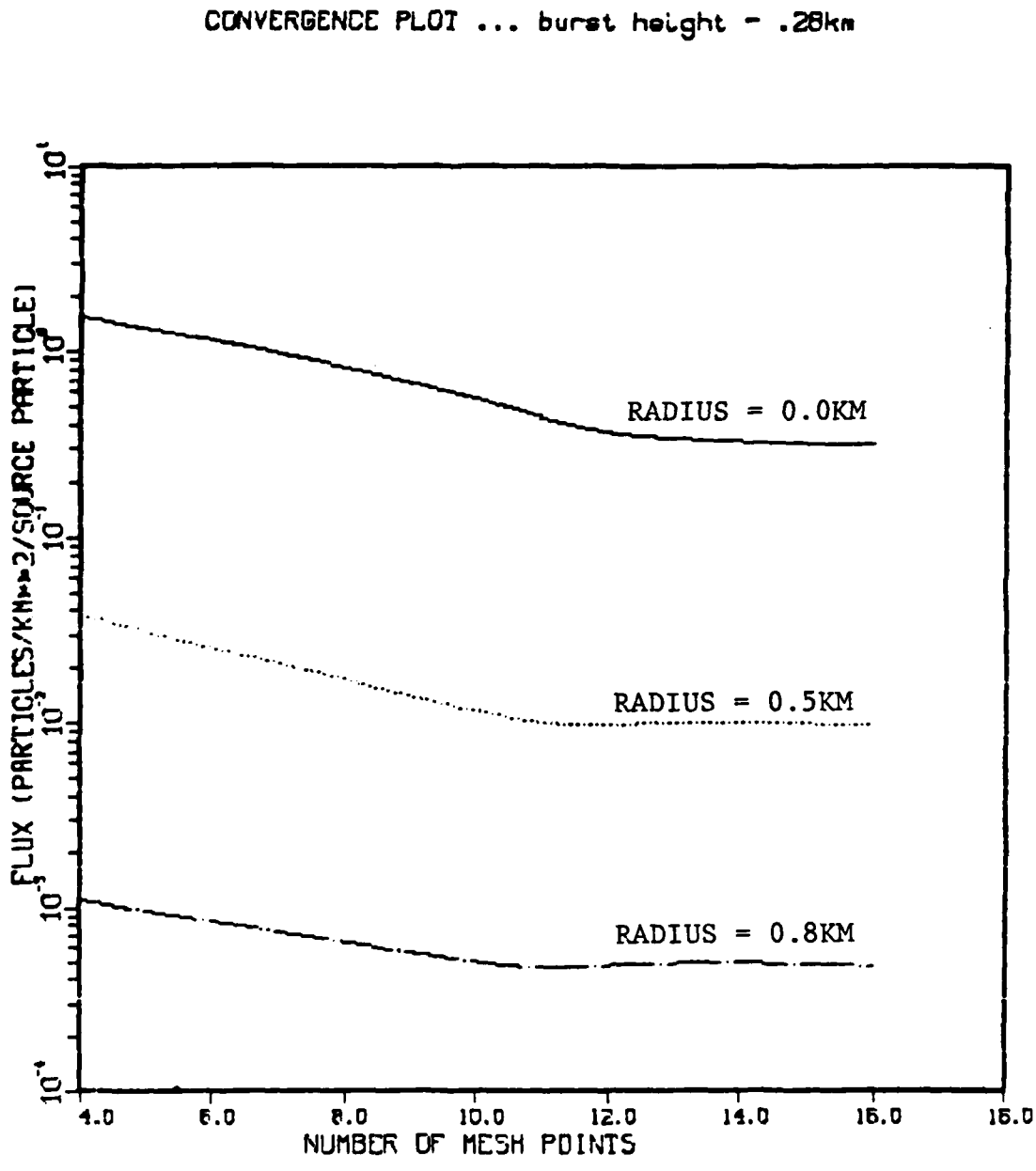

Figure 20. FET Convergence

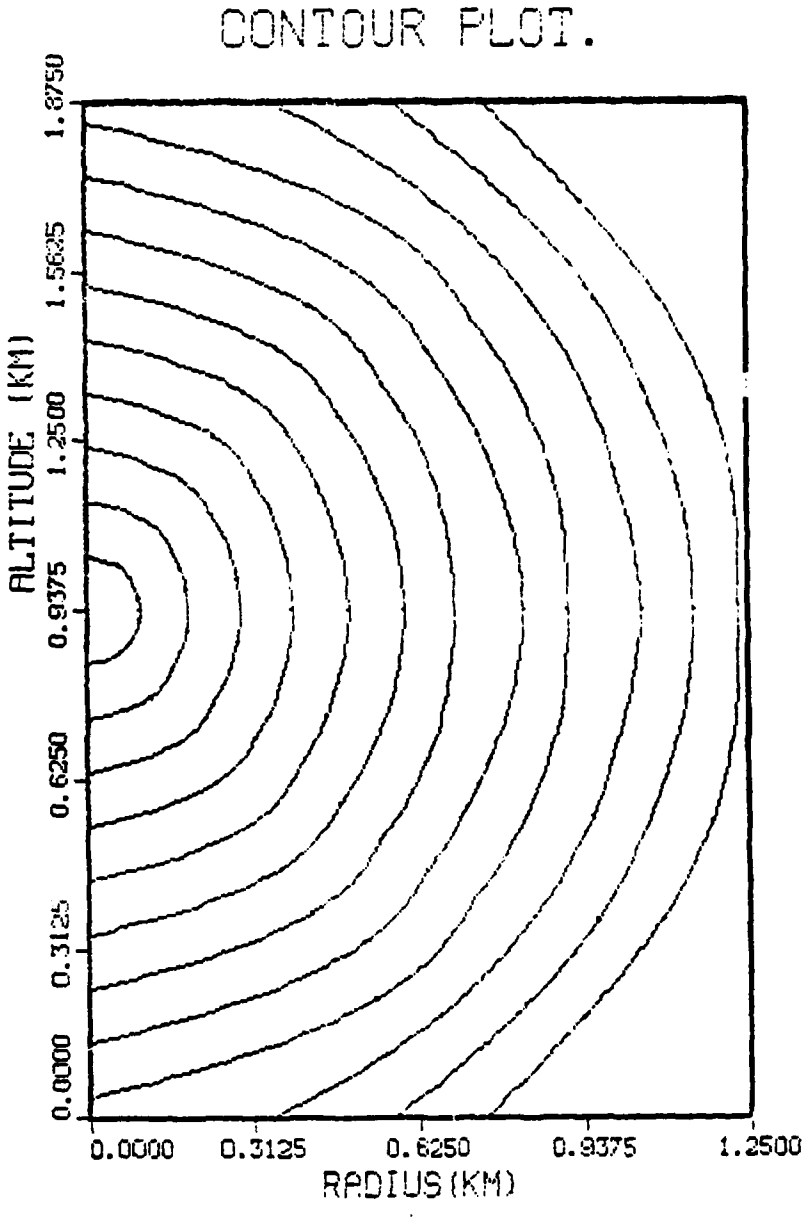

Figure 21. Contour Plot of FET Solution

These steady-state one group results show the potential of this solution technique to provide a complete solution to the air-over-ground problem. However, an energy dependent multigroup solution is required for most applications. For others a complete time and energy dependent solution will be needed. In either case, these solutions can be obtained by solving a number of coupled one group problems. Therefore, our steady-state one group solution can be extended to the general air-over-ground problem.

All of our computations were carried out on a Cray-I computer. The FET code was written in Fortran 77 and it is not optimized in terms of storage requirements or efficiency. The calculations were all carried out in-core (central memory). The computer storage requirements were such that special auxillary or disc storage was not needed. Furthermore, the maximum execution time which was required was less than ten minutes. However, for larger problems we expect the storage requirements and execution times to increase.

CHAPTER IX

CONCLUSION AND RECOMMENDATION

A method for solving general particle transport problems has been developed. This method is based on a mathematical formalism which includes a rigorous treatment of general boundary conditions. These boundary conditions are dealt with within the context of a classical energy minimization (variational) principle and an equivalent Bubnov-Galerkin solution. Using the second order forms of the transport equation, this equivalence is established and the resulting matrix problem is positive definite symmetric.

The mathematical formalism also includes an explicit forward or weighted difference in time and a piecewise constant energy dependence. This is the usual multigroup treatment of the energy dependence. With these approximations of the time and energy dependences, the transport problem (equations) is reduced to a set of coupled steady-state monoenergetic problems.

The numerical technique involves a finite element projected solution of the transport equation. A finite

element trial space of spherical harmonics and polynomial splines is used. The particle flux is expressed as a linear and separable sum of even and odd components on the unit sphere. Then, a numerical solution using the parity (odd, even) characteristics of spherical harmonics was developed. In this development we included anisotropic sources and scattering. Furthermore, we established that in the diffusion limit our method reduces to the P_1 method or diffusion theory.

A validation of the method has been obtained by a computer solution to the air-over-ground problem. This problem is modeled in cylindrical (r,z) geometry with an exponentially varying atmosphere, anisotropic scattering and anisotropic first scatter sources. The ground was treated as a homogenous mixture and vacuum boundary conditions were used. The computer code FET was developed and used to solve the problem.

Comparisons of the FET solutions to those of diffusion theory and discrete ordinates validated our solution technique. These comparisons show the ability of our method to solve general and difficult particle transport problems. Furthermore, the potential of this solution approach to serve as a complementary alternative to the standard techniques of Monte Carlo, discrete ordinates and

the P_n method was demonstrated. However, the use and validation of this method by solving other particle transport problems is required.

Further work is also required in the computer implementation of this method. The applications of this technique to general time and energy dependent problems is required. A number of different finite element types and shapes should be used and examined as to their potential to model other problems of physical and engineering interest.

Because of the special properties of the problem matrices the method should be examined in terms of computational efficiency and costs. Furthermore, other comparisons should be made. Comparisons for problems where solutions by other methods are available and can be easily obtained are required. For problems with angular singularities, the issues of convergence and stability of the solution should be examined.

In this regard, we feel that our method can be easily applied to problems with difficult and complicated geometries. Nuclear reactors and radiation shielding problems are in this category. However, many of these problems have singular points. These are points where the solution has unbounded derivatives (Strang and Fix, 1973). Furthermore, these angular singularities may reduce the

accuracy and rate of convergence of our finite element method.

The equivalence of this technique to diffusion theory should be further examined. In the limit of diffusion theory, this method, with a finite element basis of linear splines, should produce the diffusion theory finite difference matrix. This is a Stieltjes matrix which guarantees an all positive solution. Furthermore, a solution by other projection methods such as collocation, least squares and the method of moments should be examined. Collocation is especially attractive in that there exists an equivalence between the Galerkin and collocation methods (Prenter, 1975).

Finally, a Double P_n aproximation should be applied to the air-over-ground problem. The effects of this approximation on the solution accuracy, especially at the air-ground interface, should be examined. This approximation would also be able to better model the vacuum boundary conditions. However, the determination of a local reflection coefficient and use of the albedo boundary condition might be more appropriate. Furthermore, the applicability of our solution technique to specific charge particle transport problems should be investigated. This would entail the inclusion of the Fokker-Planck collision terms into the mathematical and numerical models.

APPENDIX A

VARIATIONS OF A FIRST ORDER FUNCTIONAL

First order functionals provide the variational model for many physical systems. These functionals which are usually quadratic (as in Eq (53)), can be used to provide solutions to a large number of problems. These solutions are obtained by determining the stationary point or extremum of the functional. The classical Raleigh-Ritz method is usually used to numerically determine this extremum.

However, before obtaining a numerical solution we are oftentimes interested in determining the analytic conditions that would make the functional stationary. These conditions are obtained by using the calculus of variations to extremize the functional. We are required to take variations (derivatives) of the functional which in turn provide us with information about the problem and its solution.

Following the discussion of Chapter V we will begin with a first order functional (Gelfand and Fomin, 1963).

$$I(u) = \int_R F(\hat{r},u(\hat{r}),\nabla u(\hat{r}))d\hat{r} \qquad (160)$$

where ∇ is the usual gradient operator in some n-dimensional phase space and we note that the variational problem is independent (invariant) of the coordinate system (Courant and Hilbert, 1953).

Based on our earlier definition of a variation, we can write the first variation of Eq (162) as

$$\partial I(u) = \int_R \partial F(\hat{r}, u(\hat{r}), \nabla u(\hat{r}))\, d\hat{r} \tag{161}$$

and

$$\partial F = F(\hat{r}, u^*(\hat{r}), \nabla u^*(\hat{r})) - F(\hat{r}, u(\hat{r}), \nabla u(\hat{r})) \tag{162}$$

where

$$u^*(\hat{r}) = u(\hat{r}) + \varepsilon\phi(\hat{r}) \tag{163}$$

and

$$\partial u(\hat{r}) = \varepsilon\phi(\hat{r}) \tag{164}$$

Expanding ∂F in a Taylor series and keeping terms of order ε; or taking the variational derivative of F (Lancoz, 1949) we get

$$\partial I(u) = \varepsilon \int_R \left[\phi \frac{\partial F}{\partial u} + \phi' \frac{\partial F}{\partial u'} \right] dr \qquad (165)$$

where we have dropped the explicit $\hat{r}$ dependence and $u' = \nabla u$; $\phi' = \nabla \phi$.

For a stationary point we require that Eq (165) be equal to zero. Then we can expand the individual terms of the integral and discuss the conditions for an extremum to exist. However, to decide on whether Eq (160) is a minimum or maximum principle we must take the second variation. This is

$$\partial^2 I(u) = \partial(\partial I(u)) = \varepsilon \int_R \partial \left[\phi \frac{\partial F}{\partial u} + \phi' \frac{\partial F}{\partial u'} \right] d\hat{r} \qquad (166)$$

$$= \varepsilon^2 \int_R \left[\phi^2 \frac{\partial^2 F}{\partial u^2} + 2\phi\phi' \frac{\partial^2 F}{\partial u' \partial u} + (\phi')^2 \frac{\partial^2 F}{\partial (u')^2} \right] d\hat{r} \qquad (167)$$

APPENDIX B

THE EULER-LAGRANGE EQUATION

The Sturm-Liouville variational problem of Chapter V corresponds to a linear boundary value problem with mixed boundary conditions. This is a natural boundary condition of the variational or equivalent Galerkin problem. In order to show the equivalence between the variational and boundary value problems we will take the first variation of Eq (53). This procedure will produce the Sturm-Liouville equation and identify the natural boundary conditions. In the terminology of variational calculus the partial differential equation which extremizes the functional is called its Euler-Lagrange equation. For the model problem of Chapter V, this is (the Sturm-Liouville equation) Eq (50).

We begin by taking the first variation of Eq (53) in accordance with the derivation of Appendix A. This gives

$$\partial I(u) = \varepsilon \int_V 2\left\{p(\hat{r})\nabla u(\hat{r})\phi' + \left[q(\hat{r})u(\hat{r}) - f(\hat{r})\right]\phi(\hat{r})\right\} d\hat{r}$$

$$+ \varepsilon \oint_S 2\left[b(\hat{r}_s)u(\hat{r}_s) + c(\hat{r}_s)\right]\phi(\hat{r}_s) d\hat{s} \qquad (168)$$

and since $\phi' = \nabla\phi(\hat{r})$ we can use the product rule of differentiation and the Gauss divergence theorem to get

$$\partial I(u) = \varepsilon \int_V 2\left\{-\nabla(p(\hat{r})\nabla u(\hat{r})) + q(\hat{r})u(\hat{r}) - f(\hat{r})\right\}\phi d\hat{r}$$

$$+ \varepsilon \oint_S 2\left[p(\hat{r}_s)\nabla u(\hat{r}_s)\cdot\hat{n} + b(\hat{r}_s)u(\hat{r}_s) + c(\hat{r}_s)\right]\phi(\hat{r}_s)d\hat{s} \tag{169}$$

where $\hat{n}$ is an outward unit normal to the problem boundaries.

For a minimum to exist we require that the first variation should be zero or that the variational derivative

$$\frac{\partial I(u)}{\partial \varepsilon} = \lim_{\varepsilon \to 0} \frac{\partial I(u)}{\varepsilon} \tag{170}$$

be zero. In either case, since ε is small and not equal to zero and $\phi(\hat{r})$ is an arbitrary function, we must have that $\phi(\hat{r})$ is equal to zero everywhere or that

$$-\nabla(p(\hat{r})\nabla u(\hat{r})) + q(\hat{r})u(\hat{r}) - f(\hat{r}) = 0 \tag{171}$$

and

$$p(\hat{r}_s)\nabla u(\hat{r}_s)\cdot\hat{n} + b(\hat{r}_s)u(\hat{r}_s) + c(\hat{r}_s) = 0 \qquad (172)$$

Eq (171) is the Sturm-Liouville problem of Eq (50). It is also the Euler-Lagrange equation of Eq (53). Furthermore, Eq (172) represents the natural boundary conditions which are satisfied automatically by the minimizing sequence. A numerical solution of the Raleigh-Ritz system of Eq (61) will provide a solution to Eqs (171) and (172). This is guaranteed if the solution is also a minimum of the functional of Eq (53). Therefore, we have shown the equivalence between the variational and boundary value problems of Eq (53), (50) and (51).

It is important to note that for the Dirichlet boundary condition we set $a(\hat{r}_s)$ to zero in Eq (51) and then Eq (172) is satisfied if $p(\hat{r}_s)$ is also equal to zero. Since $p(\hat{r}_s)$ must be nonzero in the Sturm-Liouville problem then we must require that $u(\hat{r}_s)$ be a constant on the boundary. This implies that

$$b(\hat{r}_s)u(\hat{r}_s) = -c(\hat{r}_s) = c \qquad (173)$$

and that

$$\phi(\hat{r}_s) = 0 \tag{174}$$

where $c(\hat{r}_s)$ is a constant and there is no variation of $u(\hat{r}_s)$ on the boundary.

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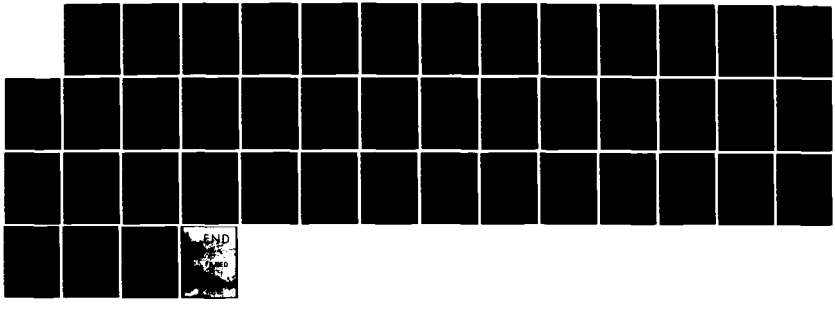

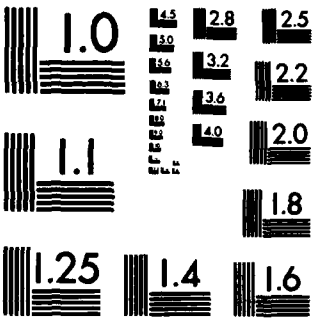

APPENDIX C

THE EVEN PARITY FUNCTIONAL

Based on the self-adjoint nature of the second order transport equation, we can formulate quadratic functionals whose minimum will provide solutions to general particle transport problems. Such a functional in the form of Eq (62) has been proposed. An important aspect of this formulation is the treatment of general boundary conditions as natural conditions. In order to show that the conditions whereby Eq (62) has a minimum are also a solution to the even parity transport problem, we must take the first variation of this functional. Following the arguments of Appendices A and B, we begin by writing the first variation of Eq (62) as

$$\begin{aligned} \partial I(u) &= \int_D \partial F(\hat{r},\hat{\Omega},u,\nabla_a u)\,d\hat{p} \\ &= \varepsilon \int_D \left[\phi \frac{\partial F}{\partial u} + \phi'_a \frac{\partial F}{\partial u'_a}\right] d\hat{p} \end{aligned} \tag{175}$$

where we have dropped the explicit $(\hat{r},\hat{\Omega})$ dependence and $u = \psi^g$; $u'_a = \nabla_a \psi^g = \hat{\Omega}\cdot\nabla\psi^g$; $\phi'_a = \hat{\Omega}\cdot\nabla\phi$ and the integral is to be carried out over the entire volume in phase space. We note that the parity operators are positive definite and self-adjoint, where for a self-adjoint operator L

$$\langle f, Lh\rangle = \langle Lf, h\rangle \tag{176}$$

where f and h are continuous and differentiable functions. Then, after some algebra and use of the divergence theorem

$$\int_R \langle \hat{\Omega}\cdot\nabla f, h\rangle = -\int_R \langle f, \hat{\Omega}\cdot\nabla h\rangle d\hat{r} + \oint_S \langle (\hat{\Omega}\cdot\hat{n}) f, h\rangle d\hat{s} \tag{177}$$

we get

$$\begin{aligned}\frac{\partial I}{\partial \varepsilon} = \int_R \Big[& 2\langle G^g \psi^g, \phi\rangle - 2\langle Q^g, \phi\rangle + 2\langle \hat{\Omega}\cdot\nabla K^u Q^u, \phi\rangle \\ & - 2\langle \hat{\Omega}\cdot\nabla K^u (\hat{\Omega}\cdot\nabla\psi^g), \phi\rangle \Big] d\hat{r} + \oint_S \Big[\langle |\hat{\Omega}\cdot\hat{n}| (Q_{eb} + a\psi^g), \phi\rangle \\ & - 2\langle (\hat{\Omega}\cdot\hat{n})\psi^u, \phi\rangle \Big] d\hat{s}\end{aligned} \tag{178}$$

where we have used the fact that

$$\frac{\partial Q_{eb}}{\partial u} = a \tag{179}$$

and earlier defined $\Psi^u(\hat{r},\hat{\Omega})$ to be the odd parity flux. That is

$$\Psi^u(\hat{r}_s,\hat{\Omega}) = K^u\left[Q^u(\hat{r}_s,\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi^g(\hat{r}_s,\hat{\Omega})\right] \tag{180}$$

We can now rewrite the surface term of Eq (178) as

$$\oint_s \langle(\hat{\Omega}\cdot\hat{n})\left[Q_{eb} + a\Psi^g - 2\Psi^u\right],\phi\rangle_{\hat{\Omega}\cdot\hat{n}>0}d\hat{s}$$

$$+\oint_s \langle(\hat{\Omega}\cdot\hat{n})\left[Q_{eb} + a\Psi^g + 2\Psi^u\right],\phi\rangle_{\hat{\Omega}\cdot\hat{n}<0}d\hat{s} \tag{181}$$

and if ϕ is nonzero we must require that

$$-\hat{\Omega}\cdot\nabla K^u(\hat{\Omega}\cdot\nabla\Psi^g) + G^g\Psi^g - Q^g + \hat{\Omega}\cdot\nabla K^u Q^u = 0 \tag{182}$$

and also that Eq (181) be equal to zero in order for a minimum to exist. Therefore Eq (62) has a minimum if Eq (178) is equal is zero. The conditions for this to occur are that the Euler-Lagrange equation, Eq (182), and the boundary term, Eq (181), should be zero. Eqs (182) and (181) represent the even parity transport equation and boundary conditions of Chapter IV.

We can easily recognize that the Euler-Lagrange equation is just Eq (35). Furthermore, if ϕ is nonzero on the problem boundaries, then from Eq (181) we must require that

$$Q_{eb} + a\psi^{g}(\hat{r}_s,\hat{\Omega}) - 2\psi^{u}(\hat{r}_s,\hat{\Omega}) = 0 \quad \text{for } \hat{\Omega}\cdot\hat{n}>0 \tag{183}$$

and

$$Q_{eb} + a\psi^{g}(\hat{r}_s,\hat{\Omega}) + 2\psi^{u}(\hat{r}_s,\hat{\Omega}) = 0 \quad \text{for } \hat{\Omega}\cdot\hat{n}<0 \tag{184}$$

With Q_{eb} defined (See Chapter V) as

$$Q_{eb} = a\psi^{g}(\hat{r}_s,\hat{\Omega}) - bq_s(\hat{r}_s,\hat{\Omega}) \tag{185}$$

where

$$a = \frac{1 - \alpha(\hat{r}_s)}{\alpha(\hat{r}_s) + 1} \tag{186}$$

and $0 \leq \alpha(r_s) \leq 1$. We can now recognize that the natural boundary conditions are

1. Vacuum boundary

   $\alpha(\hat{r}_s) = 0 \; ; \; b = 0$

2. Incident source

   $\alpha(\hat{r}_s) = 0 \; ; \; b = 2$

3. Albedo condition

   $0 < \alpha(\hat{r}_s) \leq 1 \; ; \; b = 0$

and

4. Mixed condition

   $0 < \alpha(\hat{r}_s) \leq 1 \; ; \; b = \frac{2}{1+\alpha}(\hat{r}_s)$

However, the Dirichlet condition with

$0 \leq \alpha(\hat{r}_s) \leq 1 \; ; \; b = 0$ or $\frac{2}{1+\alpha}(\hat{r}_s)$

and the angular flux completely or partially specified on the boundaries is an essential condition. This condition must be imposed on the trial space in order to insure that it will be included in a solution to the variational problem, Eq (62). There is some flexibility in specifying the Dirichlet condition. Nonetheless, they must be consistent and reflect the physics of the problem.

It is important to note that the vacuum boundary is really a special case of the Dirichlet boundary condition. Furthermore, if we use a global basis in angle (spherical harmonics) we are unable to explicitly enforce the boundary condition as essential. Nonetheless, we are able to treat the vacuum boundary as natural with $\alpha = b = 0$. This approach which is an approximation to the true vacuum boundary results in the usual Marshack boundary condition (Davis, 1966).

We can also treat the usual interface conditions within this variational context (Strang and Fix, 1973). Noting that the variational problem is dependent upon material properties (cross-sections), we divide the problem domain into regions of constant or continuously varying cross-section data. In each region we require that the variational problem and the second order transport equations be satisfied. We then treat discontinuities of material properties as a set of coupled boundary value problems.

Except for those problems with interface singularities (Strang and Fix, 1973) we can proceed by imposing an albedo boundary condition at the interface. At interfaces we set $\alpha(\hat{r}_s) = 1$ and $b = 0$ in the functional of Eq (62). We then write a separate functional for each region and require that the first variation vanishes on the entire problem domain. The boundary conditions are treated in the usual manner as essential or natural conditions. However, upon taking the sum of the individual functionals we require that the interface terms vanish.

The interface terms can be written as

$$\oint_s <\left[(\hat{\Omega}\cdot\hat{n})\psi_+^u(\hat{r}_I,\hat{\Omega}) + (-\hat{\Omega}\cdot\hat{n}_-)\psi_-^u(\hat{r}_I,-\hat{\Omega})\right],\phi> d\hat{s} \qquad (187)$$

where + means in the limit approaching the interface in a given positive $\hat{\Omega}$ direction from the left and - means in the opposite $-\hat{\Omega}$ direction from the right. Then with $\hat{n}$ being the outward normal to the interface we have

$$\hat{n}_- = -\hat{n}_+ \qquad (188)$$

and

$$(\hat{\Omega}\cdot\hat{n}_+) = (-\hat{\Omega}\cdot\hat{n}_-) \qquad (189)$$

We can now rewrite Eq (187) as

$$\oint_s <(\hat{\Omega}\cdot n_+)\left[\psi^u_+(\hat{r}_I,\hat{\Omega}) + \psi^u_-(\hat{r}_I,-\hat{\Omega})\right],\phi>d\hat{s} \qquad (190)$$

and require that for Eq (189) to hold for arbitrary ϕ

$$\psi^u_+(\hat{r}_I,\hat{\Omega}) = -\psi^u_-(\hat{r}_I,-\hat{\Omega})$$

$$= \psi^u_-(\hat{r}_I,\hat{\Omega}) \qquad (191)$$

where we have used the odd-even properties of the odd parity flux.

Furthermore, upon recognizing that ϕ represents the even parity flux ψ^g which is an even function on the unit sphere and $\hat{\Omega}\cdot\hat{n}$ is always odd, we can write Eq (190) as

$$\oint_s <(\hat{\Omega}\cdot\hat{n}_+)\left[\psi_+(\hat{r}_I,\hat{\Omega}) - \psi_-(\hat{r}_I,\hat{\Omega})\right],\phi>d\hat{s} = 0 \qquad (192)$$

where

$$\psi(\hat{r}_I,\hat{\Omega}) = \psi^u(\hat{r}_I,\hat{\Omega}) + \psi^g(\hat{r}_I,\hat{\Omega}) \qquad (193)$$

Then we get

$$\psi_+(\hat{r}_I,\hat{\Omega}) = \psi_-(\hat{r}_I,\hat{\Omega}) \qquad (194)$$

Eq (192) requires that the angular flux be continuous at the interface. This is a continuity requirement in $\hat{r}$ for a given direction $\hat{\Omega}$ which also implies continuity of the particle current across the interface. The usual interface condition is therefore satisfied as a natural condition of the variational problem.

APPENDIX D

THE DIFFUSION LIMIT

In Chapter VII we presented a finite element projection of splines and harmonic functions in a solution strategy for solving the second order transport equation. In this Galerkin solution of Eqs (35) and (36) it can be shown that in the limit of diffusion theory our equations reduce to, and are consistent with the diffusion approximation. The even parity Galerkin equation is just the diffusion equation whereas the odd parity equation reduces to Fick's law.

In the P_1 (diffusion) approximation we assume that all sources are isotropic (Duderstadt and Hamilton, 1976) and that the flux and scattering are linearly anisotropic. Then the even parity flux and the net current can be written as

$$\psi^g(\hat{r},\hat{\Omega}) = \frac{\phi(\hat{r})}{4\pi} \tag{195}$$

and

$$J(\hat{r}) = \int_{4\pi} (\hat{\Omega}\cdot\hat{n})\psi^u(\hat{r},\hat{\Omega})d\hat{\Omega} \tag{196}$$

where, in rectangular coordinates (See Figure 3)

$$\hat{\Omega}\cdot\hat{n} = \hat{\Omega}\cdot[\hat{e}_x + \hat{e}_y + \hat{e}_z]$$

$$= \sum_{\ell=1}^{1}\sum_{m=0}^{\ell} \frac{1}{C_{\ell m}} \left[Q^c_{\ell m} + Q^s_{\ell m}\right] \qquad (197)$$

The parity sources are

$$Q^g(\hat{r},\hat{\Omega}) = \frac{S(\hat{r})}{4\pi} \qquad (198)$$

and

$$Q^u(\hat{r},\hat{\Omega}) = 0 \qquad (199)$$

Then by Eqs (39) and (42) and with the usual cross-section expansion (Wills, 1981) we can carry out the algebra to write the Galerkin projection in angle of Eq (35) as

$$\int_{4\pi}\left[L\phi(\hat{r}) - S(\hat{r})\left(Q_{oo}^{c}\right)^{2}\right]Q_{oo}^{c}\,d\hat{\Omega} \tag{200}$$

where

$$L \cdot = -\left[\frac{\partial}{\partial x}\frac{1}{\sigma_{tR}}\frac{\partial}{\partial x}\left(\frac{Q_{11}^{c}}{C_{11}}\right)^{2} + \frac{\partial}{\partial y}\frac{1}{\sigma_{tR}}\frac{\partial}{\partial y}\left(\frac{Q_{11}^{s}}{C_{11}}\right)^{2}\right.$$

$$\left. + \frac{\partial}{\partial z}\frac{1}{\sigma_{tR}}\frac{\partial}{\partial z}\left(\frac{Q_{10}^{c}}{C_{10}}\right)^{2}\right]\left(Q_{oo}^{c}\right)^{2} - \sigma_{r}\left(Q_{oo}^{c}\right)^{2} \tag{201}$$

$$\sigma_{tR} \approx \sigma_{t} - \sigma_{1} \tag{202}$$

$$\sigma_{r} = \sigma_{t} - \sigma_{o} \tag{203}$$

and σ_1 and σ_o are the Legendre cross-section expansion coefficients.

Upon evaluation of the integrals in Eq (200) we get

$$-\nabla\cdot D\nabla\phi(\hat{r}) + \sigma_r\phi(\hat{r}) = S(r) \tag{204}$$

where

$$D = \frac{1}{3\sigma_{tR}} = \text{diffusion coefficient} \tag{205}$$

We can also rewrite the odd parity equation, Eq (36) as (Wills, 1981)

$$G^u(\hat{r})\Psi^u(\hat{r},\hat{\Omega}) = Q^u(\hat{r},\hat{\Omega}) - \hat{\Omega}\cdot\nabla\Psi^g(\hat{r},\hat{\Omega}) \tag{206}$$

and carry out the Galerkin projection on this equation to get

$$J(\hat{r}) = -D\nabla\phi(\hat{r}) \tag{207}$$

Eq (204) is the diffusion equation and Eq (207) is Fick's law. Therefore, for a linearly anisotropic approximation in angle the Galerkin projection of the second order transport equation is consistent with P_1 or diffusion theory.

APPENDIX E

SURFACE HARMONIC TENSOR

The use of surface harmonic tensors in solving particle transport problems is not a new concept. The P_n method uses spherical harmonic functions to expand and evaluate moments of the first order transport equation. The scattering cross-sections, gradient and surface normal operators are usually expanded in spherical harmonics. Therefore, in a numerical solution of transport problems, the properties and relationships of harmonic functions play a vital role.

In our second order formulation of Chapter VII we have found it necessary to develop and use these properties. Some of the most useful ones will now be presented. The harmonic functions are as defined earlier and in Chapter VII. We begin by writing the usual scattering cross-section and surface normal expansions as

$$\sigma_s(\hat{r},\hat{\Omega}\cdot\hat{\Omega}') = 2\sum_{\ell=0}^{L}\sigma_\ell(\hat{r})\sum_{m^*=0}^{\ell}\left[Q^c_{\ell m}(\hat{\Omega}')Q^c_{\ell m}(\hat{\Omega}) + Q^s_{\ell m}(\hat{\Omega}')Q^s_{\ell m}(\hat{\Omega})\right] \tag{208}$$

and in rectangular geometry

$$\hat{\Omega}\cdot\hat{n} = \hat{\Omega}\cdot\left[\hat{e}_x + \hat{e}_y + \hat{e}_z\right]$$

$$= \sum_{\ell=1}^{1}\sum_{m=0}^{\ell} \frac{1}{C_{\ell m}}\left[Q^c_{\ell m} + Q^s_{\ell m}\right] \qquad (209)$$

where the * in m* means to divide by two when m = 0 and we have used the addition theorem (Bell and Glasstone, 1970) to derive Eq (208). Using Eq (208) we can then rewrite the second order operators in terms of $Q_{\ell m}$'s (Wills, 1981).

We can also write the streaming operators in terms of surface harmonic tensors. An example of this is in rectangular coordinates where we can write

$$\hat{\Omega}\cdot\nabla f(\hat{r},\hat{\Omega}) = \left[\frac{Q^c_{11}}{C_{11}}\frac{\partial}{\partial x} + \frac{Q^s_{11}}{C_{11}}\frac{\partial}{\partial y} + \frac{Q^c_{10}}{C_{10}}\frac{\partial}{\partial z}\right] \cdot f(\hat{r},\hat{\Omega}) \qquad (210)$$

Then in the Galerkin weak form we can use the following relationships to expand and simplify the equations

$$Q^c_{10}(\hat{\Omega})Q^c_{\ell m}(\hat{\Omega}) = \frac{C_{10}}{2\ell+1}\left[(\ell-m+1)\frac{C_{\ell m}}{C_{\ell+1,m}}Q^c_{\ell+1,m} + (\ell+m)\frac{C_{\ell m}}{C_{\ell-1,m}}Q^c_{\ell-1,m}\right] \qquad (211)$$

$$Q^c_{10}(\hat{\Omega})Q^s_{\ell m}(\hat{\Omega}) = \frac{C_{10}}{2\ell+1}\left[(\ell - m + 1)\frac{C_{\ell m}}{C_{\ell+1,m}}Q^s_{\ell+1,m} + (\ell + m)\frac{C_{\ell m}}{C_{\ell-1,m}}Q^s_{\ell-1,m}\right] \tag{212}$$

$$Q^c_{11}(\hat{\Omega})Q^c_{\ell m}(\hat{\Omega}) = \frac{C_{11}C_{\ell m}}{2(2\ell+1)}\left[\frac{1}{C^{m+1}_{\ell+1}}Q^c_{\ell+1,m+1} - \frac{1}{C^{m+1}_{\ell-1}}Q^c_{\ell-1,m+1}\right.$$

$$\left. - \frac{(\ell - m + 1)(\ell + m + 2)}{C^{m-1}_{\ell+1}}Q^c_{\ell+1,m-1} + \frac{(\ell+m-1)(\ell+m)}{C^{m-1}_{\ell-1}}Q^c_{\ell-1,m-1}\right] \tag{213}$$

$$Q^c_{11}(\hat{\Omega})Q^s_{\ell m}(\hat{\Omega}) = \frac{C_{11}C_{\ell m}}{2(2\ell+1)}\left[\frac{1}{C^{m+1}_{\ell+1}}Q^s_{\ell+1,m+1} - \frac{1}{C_{\ell-1,m+1}}Q^s_{\ell-1,m+1}\right.$$

$$\left. - \frac{(\ell-m+1)(\ell-m+2)}{C^{m-1}_{\ell+1}}Q^s_{\ell+1,m-1} - \frac{(\ell+m-1)(\ell+m)}{C_{\ell-1,m-1}}Q^s_{\ell-1,m-1}\right] \tag{214}$$

$$Q^s_{11}(\hat{\Omega})Q^c_{\ell m}(\hat{\Omega}) = \frac{C_{11}C_{\ell m}}{2(2\ell+1)}\left[\frac{1}{C_{\ell+1}}\frac{1}{m+1}Q^c_{\ell+1,m+1} - \frac{1}{C_{\ell-1}}\frac{1}{m+1}Q^c_{\ell-1,m+1}\right.$$

$$\left. - \frac{(\ell-m+1)(\ell-m+2)}{C_{\ell+1}}\frac{1}{m-1}Q^c_{\ell+1,m-1} - \frac{(\ell+m-1)(\ell+m)}{C_{\ell-1,m-1}}Q^c_{\ell-1,m-1}\right] \quad (215)$$

To compute the scalar flux and total current we can use the following orthogonal properties, Let

$$g(\hat{\Omega}) = \sum_{\ell=0}^{\infty}\sum_{m=0}^{\ell}\left[Q^c_{\ell m}(\hat{\Omega}) + Q^s_{\ell m}(\hat{\Omega})\right] \quad (216)$$

then

$$\int_{4\pi} g(\hat{\Omega})d\hat{\Omega} = \sqrt{4\pi} \quad (217)$$

$$\int_{4\pi} g(\hat{\Omega})Q^c_{\ell m}(\hat{\Omega})\, d\hat{\Omega} = 1.0 \quad \text{for } m = 0 \quad (218)$$

$$\int_{4\pi} g(\hat{\Omega})Q^c_{\ell m}(\hat{\Omega})\, d\hat{\Omega} = \int_{4\pi} g(\hat{\Omega})Q^s_{\ell m}(\hat{\Omega})\, d\hat{\Omega}$$

$$= \tfrac{1}{2} \text{ for } m \neq 0 \quad (219)$$

APPENDIX F

THE AIR-OVER-GROUND PROBLEM EQUATIONS

In order to obtain a numerical solution to the air-over-ground problem it is necessary to expand the Galerkin weak form of the even parity transport equation. The trial and weight functions of Chapter VII will be used in this expansion. Because this is a very tedious and lengthy derivation, the more obvious algebraic steps will be omitted. The starting point of this formulation is Eq (126) of Chapter VIII.

$$\sum_{iz=1}^{IZ}\sum_{ir=0}^{IR}\sum_{\ell=1}^{L}\sum_{m=0}^{\ell} A_{ij\ell m}\left[\int_R \left\{ \langle \hat{\Omega}\cdot\nabla(B_j Q_{kn}), K^u(\hat{\Omega}\cdot\nabla(B_i Q_{\ell m}))\rangle \right.\right.$$

$$\left.\left. + \langle B_j Q_{kn}, G^g(B_i Q_{\ell m})\rangle \right\} dr + \oint_S \int_{4\pi} |\hat{\Omega}\cdot\hat{n}| B_j Q_{kn} B_i Q_{\ell m} d\hat{\Omega} d\hat{s}\right.$$

$$= \int_R \left\{ \langle \hat{\Omega}\cdot\nabla(B_j Q_{kn}), K^u S^u\rangle + \langle B_j Q_{kn}, S^g\rangle \right\} d\hat{r} \qquad (220)$$

where B_i, B_j, and $Q^c_{\ell m}$ are defined by Eqs (127), (128) and (96), and ℓ and k are restricted to be even integers.

The surface normal terms are defined by Eqs (130) and (131) and we have rewritten the source terms Q^g and Q^u as S^g and S^u. These are given by Eqs (156) and (157). The second order operators K^u and K^g can also be written as

$$K^u f(\hat{\Omega}) = \sigma_t^{-1}\left[f(\hat{\Omega}) - 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\left\{\frac{\sigma^u_\ell}{\sigma_t - \sigma^u_\ell}\right\}\int_{4\pi} T_{\ell m}(\Omega') * f(\hat{\Omega}')d\hat{\Omega}'\right] \quad (221)$$

and

$$G^g f(\hat{\Omega}) = \sigma_t f(\hat{\Omega}) - 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma^g_\ell \int_{4\pi} T_{\ell m}(\hat{\Omega}')f(\hat{\Omega}')d\hat{\Omega}' \quad (222)$$

and

$$T_{\ell m}(\hat{\Omega}') = Q^c_{\ell m}(\mu',\chi')Q^c_{\ell m}(\mu,\chi) + Q^s_{\ell m}(\mu',\chi')Q^s_{\ell m}(\mu,\chi) \quad (223)$$

and $Q^s_{\ell m}$ is defined by Eq (97). Furthermore, we can rewrite the directional derivative, Eq (126) as

$$\hat{\Omega}\cdot\nabla\phi = \frac{\alpha}{\rho}\frac{\partial}{\partial\rho}(\rho\phi) - \frac{1}{\rho}\frac{\partial\{\phi\beta(\mu,\chi)\}}{\partial\chi} + \mu\frac{\partial\phi}{\partial z} \qquad (224)$$

where

$$\alpha = \alpha(\mu,\chi) = \sqrt{1-\mu^2}\cos\chi \qquad (225)$$

and

$$\beta = \beta(\mu,\chi) = \sqrt{1-\mu^2}\sin\chi \qquad (226)$$

Using these relationships and noting that $T_{\ell m}$, $Q_{\ell m}$, B_i, B_j, etc. are all real functions we can expand Eq (220) to get

$$\sum_{iz=1}^{IZ}\sum_{ir=1}^{IR}\sum_{\ell=0}^{L}\sum_{m=0}^{\ell}A_{i,j,\ell,m}\left[\int_R \sigma_t^{-1}\frac{\partial}{\partial\rho}(\rho B_i)\frac{1}{\rho^2}\,dv\int_{4\pi}\alpha^2 Q^c_{\ell m}Q^c_{kn}\,d\hat{\Omega}\right. \qquad (227)$$

$$-\int_R \sigma_t^{-1}\frac{\partial}{\partial\rho}(B_j\rho)\frac{B_i}{\rho^2}\,dv\int\alpha\frac{\partial}{\partial\chi}(\beta Q^c_{\ell m})\,Q^c_{kn}d\hat{\Omega} \tag{228}$$

$$+\int_R \sigma_t^{-1}\frac{\partial}{\partial\rho}\,(\rho B_j)\frac{\partial}{\partial z}(B_i)\,\frac{1}{\rho}\,dv\int_{4\pi}\alpha\mu Q^c_{\ell m}Q^c_{kn}d\hat{\Omega} \tag{229}$$

$$-\int_R \sigma_t^{-1}\frac{1}{\rho}\,\frac{\partial}{\partial\rho}\,(\rho B_i)\frac{B_j}{\rho}\,dv\int_{4\pi}\alpha\frac{\partial}{\partial\chi}(\beta Q^c_{kn})Q^c_{\ell m}d\hat{\Omega} \tag{230}$$

$$+\int_R \sigma_t^{-1}\frac{1}{\rho^2}B_iB_j\,dv\int_{4\pi}\frac{\partial}{\partial\chi}(\beta Q^c_{\ell m})\frac{\partial}{\partial\chi}(\beta Q^c_{kn})\,d\hat{\Omega} \tag{231}$$

$$-\int_R \sigma_t^{-1}\frac{\partial}{\partial z}(B_i)\frac{B_j}{\rho}dv\int_{4\pi}\mu Q^c_{\ell m}\frac{\partial}{\partial\chi}(Q^c_{kn}\beta)\,d\hat{\Omega} \tag{232}$$

$$+\int_R \sigma_t^{-1}\frac{\partial}{\partial\rho}(\rho B_i)\frac{\partial}{\partial z}(B_j)\frac{1}{\rho}\,dv\int_{4\pi}\mu Q^c_{kn}\alpha Q^c_{\ell m}d\hat{\Omega} \tag{233}$$

$$-\int_R \sigma_t^{-1}\frac{\partial}{\partial z}(B_j)\frac{B_i}{\rho}\,dv\int_{4\pi}\mu Q^c_{kn}\,\frac{\partial}{\partial\chi}(\beta Q^c_{\ell m})\,d\hat{\Omega} \tag{234}$$

$$+\int_R \sigma_t^{-1}\frac{\partial}{\partial z}(B_j)\frac{\partial}{\partial z}(B_i)\,dv\int_{4\pi}\mu Q^c_{\ell m}\mu Q^c_{kn}d\hat{\Omega} \tag{235}$$

$$+\;2\sum_{r=0}^{R}\sum_{s=0}^{r}{}^{*}\left|\int_R\sigma^u_{tr}\frac{\partial}{\partial\rho}(\rho B_j)\,\frac{\partial}{\partial\rho}(\rho B_i)\frac{1}{\rho^2}dv\int_{4\pi}\alpha Q^c_{kn}\left\{\int_{4\pi}\alpha Q^c_{\ell m}T_{rs}\,d\hat{\Omega}'\right\}d\hat{\Omega}\right. \tag{236}$$

$$-\int_R\sigma^u_{tr}\,\frac{1}{\rho^2}B_i\frac{\partial}{\partial\rho}(\rho B_j)\,dv\int_{4\pi}\alpha Q^c_{kn}\left\{\int_{4\pi}\frac{\partial}{\partial\chi}(\beta Q^c_{\ell m})T_{rs}\,d\hat{\Omega}'\right\}d\hat{\Omega} \tag{237}$$

$$+\int_R\sigma^u_{tr}\frac{\partial}{\partial z}(B_i)\frac{\partial}{\partial\rho}(\rho B_j)\frac{1}{\rho}dv\int_{4\pi}\alpha Q^c_{kn}\left\{\int_{4\pi}\mu Q^c_{\ell m}T_{rs}\,d\hat{\Omega}'\right\}d\hat{\Omega} \tag{238}$$

$$- \int_R \sigma^u_{tr} \frac{1}{\rho^2} B_j \frac{\partial}{\partial \rho}(\rho B_i)\, dv \int \frac{\partial}{\partial \chi}(\beta Q^c_{kn}) \left\{ \int_{4\pi} \alpha Q^c_{\ell m} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (239)$$

$$+ \int_R \sigma^u_{tr} \frac{1}{\rho} B_i \frac{1}{\rho} B_j\, dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q^c_{kn}) \left\{ \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q^c_{\ell m}) T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (240)$$

$$- \int_R \sigma^u_{tr} \frac{\partial}{\partial z}(B_i) \frac{B_j}{\rho}\, dv \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q^c_{kn}) \left\{ \int_{4\pi} \mu Q^c_{\ell m} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (241)$$

$$+ \int_R \sigma^u_{tr} \frac{\partial}{\partial \rho}(\rho B_i) \frac{\partial}{\partial z}(B_j) \frac{1}{\rho}\, dv \int_{4\pi} \mu Q^c_{kn} \left\{ \int_{4\pi} \mu Q^c_{\ell m} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (242)$$

$$- \int_R \sigma^u_{tr} \frac{B_i}{\rho} \frac{\partial}{\partial z}(B_j)\, dv \int_{4\pi} \mu Q^c_{kn} \left\{ \int_{4\pi} \frac{\partial}{\partial \chi}(\beta Q^c_{\ell m}) T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (243)$$

$$+ \int_R \sigma^u_{tr} \frac{\partial}{\partial z}(B_i) \frac{\partial}{\partial z}(B_j)\, dv \int_{4\pi} \mu Q^c_{kn} \left\{ Q^c_{\ell m} \mu T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \Bigg\} \qquad (244)$$

$$+ \int_R \sigma_t B_j B_i\, dv \int_{4\pi} Q^c_{kn} Q^c_{\ell m}\, d\hat{\Omega} \qquad (245)$$

$$- 2 \sum_{r=0}^{R} \sum_{s=0}^{r} \int_R \sigma^g_r B_j B_i\, dv \int_{4\pi} Q^c_{kn} \left\{ \int_{4\pi} Q^c_{\ell m} T_{rs}\, d\hat{\Omega}' \right\} d\hat{\Omega} \qquad (246)$$

$$+ \oint_S B_i B_j\, ds \int_{4\pi} \left| \mu \underline{\underline{\text{or}}} \sqrt{1 - \mu^2} \cos \chi \right| Q^c_{kn} Q^c_{\ell m}\, d\hat{\Omega} \Bigg] \qquad (247)$$

$$= \int_R \sigma_t^{-1} \frac{1}{\rho} \frac{\partial}{\partial \rho}(\rho B_j)\, dv \int_{4\pi} \alpha Q^c_{kn} S^u\, d\hat{\Omega} \qquad (248)$$

$$- \int_R \sigma_t^{-1} \frac{B_j}{\rho}\, dv \int_{4\pi} \frac{\partial}{\partial \chi}(Q^c_{kn} \beta) S^u\, d\hat{\Omega} \qquad (249)$$

$$+ \int_R \sigma_t^{-1} \frac{\partial}{\partial z}(B_j)\, dv \int_{4\pi} \mu Q^c_{kn} S^u\, d\hat{\Omega} \qquad (250)$$

$$+ 2\sum_{r=0}^{R}\sum_{s^*=0}^{r}\left\{\int_R \sigma_{tr}^u \frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho B_j)dv\int_{4\pi}\alpha Q_{kn}^c\left\{\int_{4\pi} S^u T_{rs}\, d\hat{\Omega}'\right\}d\hat{\Omega}\right. \quad (251)$$

$$- \int_R \sigma_{tr}^u \frac{B_j}{\rho}dv\int_{4\pi}\frac{\partial}{\partial\chi}(\beta Q_{kn}^c)\left\{\int_{4\pi} S^u T_{rs}\, d\hat{\Omega}'\right\}d\hat{\Omega} \quad (252)$$

$$+ \int_R \sigma_{tr}^u \frac{\partial}{\partial z}(B_j)dv\int_{4\pi}\mu Q_{kn}^c\left\{\int_{4\pi} S^u T_{rs}\, d\hat{\Omega}'\right\}\left.d\hat{\Omega}\right\} \quad (253)$$

$$+ \int_R B_j dv\int_{4\pi} Q_{kn}^c S^g d\hat{\Omega} \quad (254)$$

where

$$\sigma_{tr}^u = \sigma_t^{-1}\frac{\sigma_r^u}{\sigma_t - \sigma_r^u} \quad (255)$$

and

$$\int_{4\pi} d\hat{\Omega} = \int_0^{2\pi}\int_{-1} d\mu d\chi \quad (256)$$

Eqs (227) to (244) is an expansion of the first term of Eq (220). Eqs (245) and (246) are expansions of the second term. Eq (247) is an expansion of the third term. Eqs (248) to (254) is an expansion of the right hand side of Eq (220). σ_r^g, σ_t and σ_{tr}^u are functions of z and they must

be included in the spatial or dv integrals. In cylindrical geometry with azimuthal symmetry

$$dv = 2\pi r dr dz \tag{257}$$

and ds means an integration over the surface of the problem cylinder, Figure 7.

For the air-over-ground problem with an exponentially varying air density

$$\sigma_t(z) = \sigma_t(o)e^{-z/sh} \tag{258}$$

$$\sigma_{tr}^{u} = \sigma_{tr}(o)e^{-z/sh} \tag{259}$$

$$\sigma_{r}^{g} = \sigma_{r}^{g}(o)e^{-z/sh} \tag{260}$$

where $\sigma_t(o)$, $\sigma_{tr}^{g}(o)$ are cross-sections of air at sea-level.

z = the height above sea-level

sh = atmospheric scale height ~ 7km

In Eqs (227) to (254) the integrals are separated in the space and angle variables. These are double integrals in space and angle. However, they can be separated into single integrals of the μ, χ, ρ and z variables.

APPENDIX G

INTEGRALS FOR THE AIR-OVER-GROUND PROBLEM

An expansion of the air-over-ground problem equation, Eq (126), has produced twenty-eight integral terms (Appendix F). By a further expansion and separation of the integration variables thirty-seven distinct single integrals are formed. These integrals, to include the source integrals, were numerically integrated for each combination of the expansion subscripts. They were then stored in a matrix and selected products were used to assemble the problem matrices and source vectors.

The thirty-seven angle and spatial integrals are

The Angle Integrals

$$\int_0^{2\pi} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{261}$$

$$\int_0^{2\pi} \cos(\chi)\frac{\partial}{\partial\chi}\left\{\sin(\chi)\cos(m\chi)\right\}\cos(n\chi)\,d\chi \tag{262}$$

$$\int_0^{2\pi} \cos(\chi)\cos(m\chi)\cos(n\chi)\,d\chi \tag{263}$$

$$\int_0^{2\pi} \frac{\partial}{\partial\chi}\left\{\sin(\chi)\cos(m\chi)\right\} \cdot \frac{\partial}{\partial\chi}\left\{\sin(\chi)\cos(n\chi)\right\} d\chi \tag{264}$$

$$\int_0^{2\pi} \cos(m\chi) \cdot \frac{\partial}{\partial\chi}\left\{\sin(\chi)\cdot\cos(n\chi)\right\} d\chi \tag{265}$$

$$\int_0^{2\pi} \cos(m\chi)\cos(n\chi)\, d\chi \tag{266}$$

$$\int_0^{2\pi} \cos(\chi)\cos(n\chi)\sin(m\chi)\, d\chi \tag{267}$$

$$\int_0^{2\pi} \cos(n\chi)\cdot\sin(m\chi)\, d\chi \tag{268}$$

$$\int_0^{2\pi} \frac{\partial}{\partial\chi}\left\{\cos(n\chi)\sin(\chi)\right\}\sin(m\chi)\, d\chi \tag{269}$$

$$\int_0^{\pi/2} \cos(\chi)\cos(m\chi)\cos(n\chi)\, d\chi \tag{270}$$

$$\int_{\pi/2}^{3\pi/2} \cos(\chi)\cos(m\chi)\cos(n\chi)\, d\chi \tag{271}$$

$$\int_{3\pi/2}^{2\pi} \cos(\chi)\cos(m\chi)\cos(n\chi)\, d\chi \tag{272}$$

$$\int_0^1 \mu P_{\ell m}(\mu) P_{kn}(\mu)\, d\mu \tag{273}$$

$$\int_{-1}^0 \mu P_{\ell m}(\mu) P_{kn}(\mu)\, d\mu \tag{274}$$

$$\int_{-1}^{+1} (1-\mu^2) P_{kn}(\mu) P_{\ell m}(\mu)\, d\mu \tag{275}$$

$$\int_{-1}^{+1} \sqrt{1 - \mu^2} \cdot \mu \cdot P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{276}$$

$$\int_{-1}^{+1} \sqrt{1 - \mu^2} \cdot P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{277}$$

$$\int_{-1}^{+1} \mu^2 P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{278}$$

$$\int_{-1}^{+1} \mu P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{279}$$

$$\int_{-1}^{+1} P_{\ell m}(\mu) P_{kn}(\mu) d\mu \tag{280}$$

$P_{\ell m}(\mu)$ and $P_{kn}(\mu)$ are the associated Legendre polynomials.

The Space Integrals

$$\int_0^R \frac{1}{\rho} \cdot \frac{\partial}{\partial \rho} \left\{ \rho B_{jr}(\rho) \right\} \cdot \frac{\partial}{\partial \rho} \left\{ \rho B_{ir}(\rho) \right\} d\rho \tag{281}$$

$$\int_0^R \frac{\partial}{\partial \rho} \left\{ \rho B_{jr}(\rho) \right\} \cdot \frac{B_{ir}(\rho)}{\rho} d\rho \tag{282}$$

$$\int_0^R \frac{1}{\rho} B_{jr}(\rho) B_{ir}(\rho) d\rho \tag{283}$$

$$\int_0^R \frac{\partial}{\partial \rho} \left\{ \rho B_{jr}(\rho) \right\} \cdot B_{ir}(\rho) \, d\rho \tag{284}$$

$$\int_0^R B_{jr}(\rho) \cdot B_{ir}(\rho) d\rho \tag{285}$$

$$\int_0^R B_{jr}(\rho)\cdot B_{ir}(\rho)\rho d\rho \tag{286}$$

$$\int_0^H e^{z/sh} B_{jz}(z)B_{iz}(z)dz \tag{287}$$

$$\int_0^H e^{z/sh} \frac{\partial}{\partial z}\left\{B_{iz}(z)\right\}\cdot B_{jz}(z)dz \tag{288}$$

$$\int_0^H \frac{\partial}{\partial z}\left\{B_{jz}(z)\right\}\cdot \frac{\partial}{\partial z}\left\{B_{iz}(z)\right\}e^{z/sh}dz \tag{289}$$

$$\int_0^H B_{iz}(z)\cdot B_{jz}(z)e^{-z/sh}dz \tag{290}$$

$$\int_0^H B_{iz}(z)\cdot B_{j}(z)dz \tag{291}$$

The Source Integrals

$$\int_0^R \frac{\partial}{\partial \rho}\left\{B_{jr}(\rho)\right\}H_j(\rho)d\rho \tag{292}$$

$$\int_0^R B_{jr}(\rho)\cdot H_j(\rho)d\rho \tag{293}$$

$$\int_0^R B_{jr}(\rho)H_j(\rho)\rho d\rho \tag{294}$$

$$\int_0^H B_{jz}(z)H_i(z)e^{z/sh}dz \tag{295}$$

$$\int_0^H \frac{\partial}{\partial z}\left\{B_{jz}(z)\right\}H_i(z)e^{z/sh}dz \tag{296}$$

$$\int_0^H B_{jz}(z)\cdot H_i(z)dz \tag{297}$$

where

B(z) = cubic polynomial z-spline

B(ρ) = cubic polynomial ρ-spline

sh = atmospheric scale height

R = outer radius of the problem cylinder

H = problem cylinder height

H(z) and H(ρ) are the source interpolating functions (linear Lagrange polynomials).

APPENDIX H

AN EXPANSION OF THE FIRST SCATTER SOURCE IN LEGENDRE POLYNOMIALS

In Chapter VIII the first scatter source was defined as

$$S(\rho,z,\hat{\Omega}) = \sigma^s(z,\hat{\Omega}\cdot\hat{\Omega}')\phi_d(\rho,z,\hat{\Omega}') \qquad (298)$$

where

$\phi_d(r,z,\hat{\Omega}')$ = direct fluence of Chapter VIII, Eq (146)

$\sigma^s(z,\hat{\Omega}\cdot\hat{\Omega}')$ = scattering cross-section

The usual legendre polynomial cross-section expansion will now be carried out. Also the even and odd parity first scatter source expressions of Chapter VIII will be derived. Expanding σ^s in legendre polynomials and using the addition theorem

$$\sigma^s(z,\hat{\Omega}\cdot\hat{\Omega}') = 2\sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(z)P_{\ell m}(\mu')P_{\ell m}(\mu)\cos(m(\chi-\chi')) \qquad (299)$$

where m* means that all terms with an m = 0 subscript must be divided by two, and

$$\sigma_\ell^s(z) = \sigma_\ell^s(0)e^{-z/sh} \tag{300}$$

From Figure 8 and Figure 4 it is apparent that $\mu' = \mu d$ and $\chi' = 0$, therefore

$$S(\rho,z,\hat{\Omega}) = 2\,\phi_d(\rho,z,\hat{\Omega}')e^{-z/sh} * \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0)C_{\ell m}^2 P_{\ell m}(\mu d)P_{\ell m}(\mu)\cos(m\chi) \tag{301}$$

and using the relationships of Eqs (108) and (110b) and a little algebra, the even and odd parity first scatter sources can be written as

$$S^u(\rho,z,\hat{\Omega}) = \tfrac{1}{2}[S(\rho,z,\hat{\Omega}) - S(\rho,z,-\hat{\Omega})] = \phi_d(\rho,z,\hat{\Omega}')e^{-z/sh} * \sum_{\ell=0}^{L}\sum_{m^*=0}^{\ell}\sigma_\ell^s(0) * C_{\ell m}^2\left[1-(-1)^\ell\right]P_{\ell m}(\mu)P_{\ell m}(\mu d)\cos(m\chi) \tag{302}$$

and

$$S^{g}(\rho,z,\hat{\Omega}) = \tfrac{1}{2}[S(\rho,z,\hat{\Omega}) + S(\rho,z,-\hat{\Omega})] = \phi_{d}(\rho,z,\hat{\Omega}')e^{-z/sh} * \sum_{\ell=0}^{L}\sum_{m^{*}=0}^{\ell}\sigma_{\ell}^{s}(0) * C_{\ell m}^{2}\left[1+(-1)^{\ell}\right]P_{\ell m}(\mu)P_{\ell m}(\mu d)\cos(m\chi) \tag{303}$$

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