RECEIVED BY TIC FEB 28 1973

COO-2262-1

MITNE-145

THE FINITE ELEMENT METHOD APPLIED TO NEUTRON DIFFUSION PROBLEMS

by

Lothario O. Deppe, K.F. Hansen

February 1973

Department of Nuclear Engineering
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

AEC Research and Development Report
Contract AT(11-1)-2262
U.S. Atomic Energy Commission

20624
MASTER

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

DEPARTMENT OF NUCLEAR ENGINEERING

Cambridge, Massachusetts 02139

THE FINITE ELEMENT METHOD
APPLIED TO
NEUTRON DIFFUSION PROBLEMS

by

Lothario O. Deppe, K. F. Hansen

February, 1973

COO - 2262 - 1

MITNE - 145

AEC Research and Development Report

Contract AT(11-1) - 2262

U.S. Atomic Energy Commission

MASTER

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Atomic Energy Commission, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

PATENT REVIEW APPROVES RELEASE PROCEDURES
GOVERNING PATENT REVIEW AND RELEASE ARE OF
SEE IN RECEIVING SECTION.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

THE FINITE ELEMENT METHOD APPLIED TO
NEUTRON DIFFUSION PROBLEMS

by

Lothario O. Deppe

Submitted to the Department of Nuclear Engineering on February 10, 1971, in partial fulfillment of the requirements for the degrees of Master of Science and Nuclear Engineer.

ABSTRACT

The time-independent, multigroup, two-dimensional neutron diffusion equations are solved in the particular case of a piecewise expansion of the unknown flux solutions in bicubic Hermite polynomials. The matrix formulation is achieved by applying the Galerkin method to the "weak" form of the multigroup equations; the matrix problem is solved through the power iteration method and a Cholesky factorization.

Numerical results are presented, as evaluated through a code (CHD), for several small problems and for a 1000 Mw(e) PWR, beginning-of-life core. The main conclusions arrived at through the numerical analysis show the feasibility of extending the domain of the piecewise expansion functions over heterogeneous regions, the actual spatial behavior of the cross sections being accounted for in the inner products arising from the application of the Galerkin method. Results are shown which indicate the accuracy and utility of the particular approach developed in this thesis.

Thesis Supervisor: Kent F. Hansen
Title: Professor of Nuclear Engineering

TABLE OF CONTENTS

	Page
ABSTRACT	2
LIST OF FIGURES	5
LIST OF TABLES	8
ACKNOWLEDGEMENTS	9
BIOGRAPHICAL NOTE	10
Chapter I - INTRODUCTION	11
1.1 The time-independent neutron diffusion equation and the multigroup approximation	12
1.2 Finite Element Methods	19
Chapter II - A FINITE ELEMENT APPROXIMATION TO THE MULTIGROUP NEUTRON DIFFUSION EQUATIONS	26
2.1 The "weak" form corresponding to the neutron diffusion equations	26
2.2 Construction of a basis for the piecewise expansion in one dimension	32
2.3 The basis functions in two dimensions	38
2.4 Varying cross sections inside the expansion elements	46
2.5 Matrix formulation of the two-group diffusion problem and numerical methods	47
Chapter III - SAMPLE PROBLEMS AND RESULTS	55
3.1 Comparisons between CHD and EXTERMINATOR 2 for a 4-composition problem	56
3.2 The one-dimensional, ten-region problem	63
3.3 The basic two-dimensional, two-composition problem	67
3.4 The basic two-dimensional problem with baffle surrounding the fuel region	72

3.5 The basic two-dimensional problem with varying cross sections inside the fuel region	77
3.6 Results for Zion 1 in two dimensions	84
Chapter IV - CONCLUSIONS AND RECOMMENDATIONS	95
4.1 Conclusions	95
4.2 Recommendations	97
REFERENCES	99
Appendix A - MACROSCOPIC CROSS SECTIONS	101
Appendix B - INNER PRODUCTS BETWEEN FINE LIMITS FOR CUBIC HERMITE POLYNOMIALS	102
Appendix C - THE CODE CHD	107
C.1 General description	107
C.2 Input preparation	114
Appendix D - SOURCE LISTING OF CHD, SAMPLE INPUT AND OUTPUT (Only in MIT library copies)	124

LIST OF FIGURES

	Page
2.1 Function $f_1(x_0)$ and uniquely determined cubic interpolate in region (x_1, x_{1+1})	32
2.2 One-dimensional cubic element functions	34
2.3 Cubic basis functions appropriate for function and derivative continuity	36
2.4 Cubic basis functions appropriate for flux and current continuity across interfaces for a neutron diffusion problem	37
2.5 Linear basis function appropriate for flux continuity across interfaces	38
2.6 Two-dimensional partition	40
2.7 Two-dimensional partition and matrix form for unknowns ordered as: 1) all unknowns at each point; 2) all columns; 3) all rows	51
2.8 Two-dimensional partition and corresponding matrix structure.	52
3.1 The 4-composition problem geometry	56
3.2 Flux plots for 4-composition problem as evaluated through EXTERMINATOR 2 and CHD (cut A)	60
3.3 Flux plots for 4-composition problem as evaluated through EXTERMINATOR 2 and CHD (cut B)	61
3.4 Element averaged results for 4-composition problem as evaluated with EXTERMINATOR 2 and CHD	62
3.4a One-dimensional, ten-region problem	64
3.5 Flux plots for one-dimensional, ten-region problem	66
3.6 The basic two-dimensional, two-composition problem	69

3.7a Thermal flux plots for basic two-dimensional problem at $x=0.0$	70
3.7b Thermal flux plots for basic two-dimensional problem at $x=20.0$ cm	71
3.8 Geometry for the basic two-dimensional problem with baffle surrounding the fuel region	72
3.9a Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region ($y=0.0$)	74
3.9b Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region ($y=20.0$)	75
3.10 Geometry for the basic two-dimensional problem with varying cross sections inside the fuel region	77
3.11a Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=0.0$)	79
3.11b Fast fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=0.0$)	80
3.12a Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=20.0$)	81
3.12b Fast fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=20.0$)	82
3.13 Zion 1 first core layout	85
3.14 Mesh arrangement for CHD runs (Zion 1)	85
3.15 Zion 1 - Region averaged to core averaged power ratios (finest CHD mesh)	88
3.16 Zion 1 - Region averaged to core averaged power ratios (intermediate CHD mesh)	89
3.17 Zion 1 - Region averaged to core averaged power ratios (coarsest CHD mesh)	90

3.18 Flux plots for Zion 1 as evaluated through PDQ-5 (44 x 44) and CHD (10 x 10)	92
3.19 Flux plots for Zion 1 as evaluated through PDQ-5 (44 x 44), CHD (7 x 7) and CHD (6 x 6)	93
4.1 Regular and virtual mesh lines and points in two dimensions	97
C.1 CHD basic logic	108
C.2 Coordinate system orientation assumed by CHD	109

LIST OF TABLES

	Page
3.1 Overall results for EXTERMINATOR 2 and CHD for the 4-composition problem	58
3.2 Eigenvalues for the one-dimensional, ten-region problem	65
3.3 Element averaged results for the one-dimensional, ten-region problem	65
3.4 Eigenvalues for the basic two-dimensional problem	69
3.6 Overall results for the basic two-dimensional problem with baffle surrounding the fuel region	73
3.7 Overall results for the basic two-dimensional problem with varying cross sections inside the fuel region	78
3.8 Overall results for Zion 1 as evaluated through PDQ-5, CITATION and CHD with several mesh sizes	87
3.9 Relative differences of average power in expansion elements of Zion 1 as evaluated through CHD relative to PDQ-5 and CITATION	91
C.1 Some variable values for CHD runs	111
C.2 Expansion functions option definition	118
C.3 Default sets for expansion functions	120

ACKNOWLEDGEMENTS

The author wishes to express his respect and most grateful appreciation to Professor Kent F. Hansen, his thesis supervisor, for the constant guidance and encouragement provided during the course of this work. Prof. Hansen's accessibility and informality are considered most valuable.

Most of all, this work should be a tribute to the author's wife, Alzira, and to his son, Rodrigo. Encouragement and understanding were always found in them.

The author also wishes to make use of this opportunity to express his respect and gratitude to Mr. Sergio de Salvo Brito, who's enthusiasm and far-reaching views have motivated many Brazilians, the author among them.

Dr. Chang Mu Kang provided valuable guidance in some occasions. The author wishes to thank him for it.

Special thanks are for Furnas Centrais Elétricas S.A. (Rio de Janeiro, Brazil), the authors employer, for providing full support during the author's stay at MIT.

The work was performed under USAEC Contract AT(11-1)-2262, with the computations performed at the MIT Information Processing Center.

Finally, the author wishes to thank Miss Linda Wildman for typing this report with skill and patience.

BIOGRAPHICAL NOTE

The outhor, Lothario Olavo Deppe,

received elementary school education in his home town and graduated from High School in December, 1959.

In March, 1961 he enrolled at the School of Engineering, University of Rio Grande do Sul, and received his Bachelor of Science Degree, in Electrical Engineering, in December 1965. In 1966 he attended an extension course in Nuclear Engineering at the Military Institute of Engineering in Rio de Janeiro.

In 1967 he joined the Brazilian Nuclear Energy Commission where he was mostly connected with economic studies regarding the introduction of nuclear plants in brazilian power systems. In 1969 he worked briefly as an independent consultant to Instituto de Pesquisas Radioativas from Minas Gerais, Brazil, and in May of this year he joined the staff of Furnas Centrais Eletricas S.A. from Rio de Janeiro, where he has recently been appointed as head of the nuclear section in the Planning Department.

He enrolled at the Massachusetts Institute of Technology as a candidate for the degree of Nuclear Engineer in September, 1970.

INTRODUCTION

Nuclear reactor physics problems have an inherent numerical connotation, in the sense that they are so complex that no practical problem can be solved by analytic solution of the relevant equations. Consequently, approximation methods are of paramount importance in solving reactor physics problems. Conversely, given some convenient numerical procedure to find an approximate solution to an equation, the accuracy of the solution is strongly dependent upon the computer capacity available to carry out the computations. As a consequence, two ways are open to improve the accuracy with which the behavior of a nuclear reactor can be predicted: better computer performance and inherently more accurate numerical methods.

The present thesis deals with the second alternative and tries to demonstrate that the Finite Element Method has a potential to improve, at least in one particular form, the accuracy with which present, practical, time-independent neutron diffusion equations can be solved.

Neutron diffusion equations are characterized by heterogeneities in the regions in which solutions are sought. If the maximum mesh size of the finite element method were to be limited by the size of the heterogeneity, we would have a natural minimum to the number of unknowns of the problem, and would not be able to take full advantage of the method's inherent high accuracy. In addition it is to be expected that finite element methods will ultimately compare advantageously with finite difference methods if they

result in a considerably lower number of unknowns. Therefore, one would like to have the possibility of defining larger meshes than the heterogeneities themselves (for a PWR in two dimensions, for instance, over 4, 9 or even 16 fuel elements). This possibility is investigated in this thesis for practical problems.

In the remainder of this Chapter we will present the basic, time-independent, continuous energy, homogeneous neutron diffusion equation; we will discuss its meaning and present some of the methods most often used in its solution; finally we will introduce the Finite Element Method itself.

In Chapter II we will discuss the mathematical preliminaries leading to the final matrix equations that have to be solved, and the numerical methods used to achieve this.

In Chapter III we present a series of actual results that were obtained by the use of the computer code CHD, written in order to implement the method in two dimensions and to test the use of coarse meshes on realistic systems. Results are obtained for numerous test problems; in particular we examine in some detail a representation of the Zion 1 reactor in two dimensions, and for three different coarse meshes: one fuel element, 4 fuel elements in some locations, and up to 16 fuel elements in the innermost region.

1.1) The time-independent neutron diffusion equation and the multigroup approximation

We define a closed energy domain $\xi = [E_{\min}, E_{\max}]$, where $E_{\min}$ and $E_{\max}$ are conveniently chosen, in terms of the physical characteristics of the system, as lower and upper bounds of the neutron energy.

In usual reactor problems the mathematical model to the physical problem is defined so that all the problem parameters are at least piecewise continuous, discontinuities being allowed across the interfaces. Therefore, we define the open volume domain Ω , which is the union of a finite number (L) of contiguous open subdomains Ω_1 .

$$\Omega = \bigcup_{i=1}^L \Omega_i$$

The collection of interfaces is denoted $\partial_i \Omega$, and the boundary $\partial \Omega$ is the union of the exterior boundary and the interfaces

$$\partial \Omega = \partial_e \Omega \cup \partial_i \Omega$$

In each Ω_i the properties are assumed to be continuous with discontinuities allowed at $\partial_i \Omega$.

We also define the open domain $\bar{\Omega}$

$$\bar{\Omega} = \Omega \cup \partial_i \Omega$$

The continuous energy, homogeneous, time-independent neutron diffusion equation can be written as (ref. 1):

$$\begin{aligned} & -\nabla \cdot D(\underline{r}, E) \nabla \phi(\underline{r}, E) + \Sigma_t(\underline{r}, E) \phi(\underline{r}, E) \\ & = \int_{\xi} dE' \Sigma_s(\underline{r}, E' \rightarrow E) \phi(\underline{r}, E') + \frac{\chi(E)}{\lambda} \int_{\xi} dE' \nu \Sigma_f(\underline{r}, E') \phi(\underline{r}, E') \end{aligned} \quad (1.1.a)$$

We will impose any of the following homogeneous boundary conditions:

$$\phi(\underline{r}, E) = 0$$

$$\text{or } \frac{\partial}{\partial \underline{n}} \phi(\underline{r}, E) = 0$$

$$\begin{aligned} &\text{for } E \in \xi \\ &\text{and } \underline{r} \in \partial_e \Omega \end{aligned}$$

(1.1.b)

In addition, for all interface points we require flux and current continuity, i.e.

$$\phi(\underline{r}^-, E) = \phi(\underline{r}^+, E)$$

$$D(\underline{r}^-, E) \frac{\partial}{\partial \underline{n}} \phi(\underline{r}^-, E) = D(\underline{r}^+, E) \frac{\partial}{\partial \underline{n}} \phi(\underline{r}^+, E)$$

$$\begin{aligned} &\text{for } E \in \xi \\ &\text{and } \underline{r} \in \partial_i \Omega \end{aligned}$$

(1.1.c)

The symbols have the following meaning:

$\underline{r}$ - generalized spatial variable

E - energy variable

$\phi(\underline{r}, E)$ - scalar neutron flux (/cm².s)

$D(\underline{r}, E)$ - diffusion coefficient (cm)

$\Sigma_t(\underline{r}, E)$ - macroscopic total cross section (/cm)

$\Sigma_s(\underline{r}, E' \rightarrow E)$ - macroscopic scattering cross section from E' to E (/cm)

$\chi(E)$ - prompt fission neutron spectrum

$\nu \Sigma_f(\underline{r}, E)$ - fission neutron production macroscopic cross section (/cm)

$\lambda = 1/k_{\text{eff}}$ - eigenvalue introduced to define an eigenvalue problem

k_{eff} - system multiplication factor

$\partial/\partial \underline{n}$ - outward normal derivative at a surface.

Eq. (1.1.a) results from a balance condition applied to a volume $d\mathbf{r}$ about $\mathbf{r}$ and to an energy interval dE about E . The left-hand side specifies losses (or gains) by net leakage and by removal; the right-hand side specifies births by inscattering from other energies or by fissions in the whole energy domain.

To simplify notation, Eq. (1.1) will henceforth be expressed as

$$L \phi = 0$$

where L is a linear operator.

The exact solution of the boundary value problem (1.1) is impossible for any real life case. To begin with, there exists no analytic function representing the detailed energy dependence of any of the cross sections throughout the energy domain. This complexity leads to the necessity of a multigroup formalism for the energy variable: one partitions the energy domain into a finite set $(\epsilon_1, \dots, \epsilon_G)$ of contiguous subdomains and builds up a coupled set of differential equations resulting from the balance condition applied to each subdomain, or energy group.

$$\begin{aligned} A_1 \phi_1 &= -\nabla \cdot D_1 \nabla \phi_1 + \Sigma_{r1} \phi_1 = \frac{1}{\lambda} \sum_{g=1}^G v \Sigma_{fg} \phi_g \\ A_2 \phi_2 &= -\nabla \cdot D_2 \nabla \phi_2 + \Sigma_{r2} \phi_2 = \Sigma_{s1} \phi_1 \\ A_G \phi_G &= -\nabla \cdot D_G \nabla \phi_G + \Sigma_{rG} \phi_G = \Sigma_{s(G-1)} \phi_{G-1} \end{aligned} \quad (1.2)$$

Where the spatial variable $\mathbf{r}$ is implied in the notation, and the groups are numbered by beginning with the highest energies. The A_g are linear, self-adjoint operators.

The group solutions ϕ_g in Eq. (1.2) are all required to satisfy the continuity and boundary conditions (1.1.b) and (1.1.c).

The lower indices used in (1.2) specify energy group. Otherwise the symbols have identical meanings as in (1.1), except for Σ_{rg} which means the total removal cross section from group g and Σ_{sg} which means the outscattering cross sections for group g .

In building up Eq. (1.2) we have assumed (and we will do so henceforth) that all fission events give birth to neutrons in group 1 and that outscattering from any group (g) leads to group ($g+1$). None of these assumptions are essential, in any sense, to the application of the finite element method to Eq.(1.2). However, they simplify calculations and data handling. The first one arises frequently from the few-group structure with which multi-dimensional diffusion calculations are usually made for thermal reactors; the second one is very accurate in most practical cases and is used in PDQ-5 (ref.2) and PDQ-7 (ref.3), for instance.

It is assumed also that it has been possible to do a reasonable homogenization by auxiliary means in order to find the group parameters.

The most important method existing for the solution of Eq. (1.2) is based on the finite difference approximation to the relevant differential operators with the coupling coefficients generated by the "box integration" method (ref 4). This technique is used in the PDQ codes with few groups and yields low order accuracy. Consequently a very fine mesh has to be imposed on the system if reasonably accurate results are to be obtained. The resultant system of simultaneous equations is very large so that not all data can be held in the fast memory of the computers and sophisticated

iterative techniques have to be used in the solution.

Nodal methods have been developed for cases when speed of execution rather than accuracy is the relevant factor. The FLARE code (ref.5) is a good example of this approach: it is essentially a one-group, three-dimensional model, using a very coarse mesh, and thus requiring few unknowns. The loose coupling between the coarse nodes requires that FLARE be "normalized" to more accurate codes for each type of problem; this procedure introduces an "ad hoc" component and is a serious drawback of the method. However, the code is very fast running and satisfactory for some calculations.

Synthesis methods are now being tried for the solution of detailed, three-dimensional problems. In this approach one tries to break the solution of a three-dimensional problem into two pieces. First, a series of two-dimensional solutions is obtained for typical cross sections of the reactor in the third dimension. Next, the overall, three-dimensional solution is assumed to be a linear combination of the two-dimensional solutions, and one "hopes" the procedure to be accurate.

The drawback of the synthesis methods is the lack of error bounds on the solution: one cannot be sure to improve the results by decreasing the mesh. In the finite difference methods, on the other hand, one can be sure to improve the solution by decreasing the mesh, although the convergence rate is very low. Finite element methods also show this nice property, the convergence rate being usually much higher than for the finite difference method.

Methods based on Monte Carlo simulations have also been used in reactor analysis, and have sometimes drawn great enthusiasm as being the ultimate method. It is based on the idea of following "histories" of neutrons, with the several possible events chosen in a random way. The accuracy which can be achieved is thus dependent on the number of "histories" that can be followed, and this number may be very high if a very fine detail is desired. Even on modern computers, such a calculation may become too costly, and it is therefore not likely that Monte Carlo methods will ultimately displace all other methods.

It seems clear that there still is room for improvement in reactor analysis. There exist many codes available and for numerous calculations the speed and precision attained is acceptable. However, there exist also areas where the present state is not satisfactory: three-dimensional, fine mesh, multigroup, static calculations are not yet feasible in modern computers, and three-dimensional, time-dependent problems have barely been touched. On the other hand, the increased concern with reactor safety today, and the increased cost of the incorporation of safety margins in designs, will undoubtedly require the prediction of performances with ever higher accuracy, if possible at low cost.

The solution of the static diffusion equation is probably the single most important calculation in the whole field known as reactor analysis, because it is an inherent part of depletion and kinetics methods, because it is intrinsically three-dimensional, and because it has to be done so often. In this thesis we will show that finite element methods are feasible in some real-life, static, two-dimensional diffusion problems and, furthermore, that they show a potential for the development of faster codes.

1.2) Finite element methods

Finite element methods have been successfully applied in many practical problems where natural discontinuities exist in the domain where solutions are to be found. The general idea behind the method is very simple: given the equation of a problem, one seeks to find approximate solutions which are defined only over subdomains (or finite elements) of the problem domain. When put together, these piecewise solutions form an approximate solution over the whole problem domain. Methods exist by which one can provide some continuity over the interfaces of the elements; this requirement may not be a necessity, although it is often used because it results in the reduction of the number of unknowns.

One central problem consists, then, in finding appropriate, piecewise continuous functions to use as trial functions in an appropriate space, where the approximate solutions will be sought. Polynomials are a natural choice because they are easily integrated and differentiated, they are familiar, and can be made complete. Other trial functions (such as sines and cosines) can be used with relative ease and it is not clear yet whether their use may improve the method for neutron diffusion problems.

Among the possible polynomial spaces, those based upon Lagrange and Hermite methods have been applied to diffusion problems: the first ones are generated by using function values at internal points, whereas Hermite polynomials are generated by values of the function and derivatives at the boundary of the subdomains. A desirable property of Hermite polynomials is the fact that derivatives and/or function continuities can be naturally imposed on the trial functions, depending on our desire to do so and on the degree of the polynomials.

The reduction from the continuous to the discrete form is generally achieved by the application of the Galerkin method to the "weak" form of the equation. The resultant matrix equation appears as

$$\underline{A} \underline{x} = \frac{\underline{F}}{\lambda} \underline{x}$$

where $\underline{x}$ is the unknown vector solution, λ an eigenvalue, and $\underline{A}$ and $\underline{F}$ are the coefficient matrices.

Sparse coefficient matrices are a general consequence of the application of the method, because the piecewise character of the expansion functions assures that only neighboring points couple together. This is a desirable property because it makes the matrices relatively well-conditioned for inversions, and reduces the number of computer operations.

In some problems there exist natural physical regions where it is to be expected that the solution be continuous and relatively smooth within the region. When this is the case one will probably choose such natural regions as the expansion elements. Nuclear reactors, in particular, present such features: in the beginning-of-life case of a PWR, for instance, natural expansion elements are the fuel elements themselves, which are taken as having constant cross sections. As the reactor is depleted, flux shapes tend to get smoother but one may still expect to find discontinuities of cross sections across the interfaces of the fuel elements. These facts and the need, which was discussed earlier, for more accurate and less expensive ways of solving the neutron diffusion equation, makes the application of the finite element method look attractive

beforehand. The amount of work that has been carried out to date in this area is not as large as, for instance, has been done in the area of structural engineering. Several questions remain unclear, and experiences are not completely conclusive yet.

Ref. 6 and ref. 7 present a very good discussion of the method when applied to static and time-dependent neutron diffusion problems, and to slowing down problems in infinite homogeneous media, using Hermite piecewise expansion. Numerical examples are presented for the one and two-dimensional static diffusion equations, as well as for the zero, one and two-dimensional kinetics equations.

A rectangular partition of the space domain is always assumed, and the cross sections are not allowed to vary inside the elements. The relevant mathematical implications of the method are very well analysed. Trial functions are presented which naturally preserve flux and current continuity in neutron diffusion problems, whereas practical ways of accounting for singularities are tested.

A Lagrangian approximation for a triangular partition is presented in ref. 8. Results are shown for four problems in two energy groups, including a 5-region LMFBR configuration. The results are highly encouraging both in execution time and in the accuracy achieved in the prediction of k_{eff} .

A Lagrangian approximation with linear functions is also considered in ref. 9, both for a mixed rectangular-triangular partition and for a pure rectangular partition. The desirability of the mixed partition is demonstrated.

Triangular partitions are in general very flexible in locating expansion elements. The introduction of a new triangle at a region where more detail is desired will not automatically require the introduction of nodes at regions where they are not desired. In addition, curved geometries are easily followed.

Other ideas have been tried elsewhere; e.g. in ref. 10 results are presented for "modulated" piecewise polynomials. Detailed element solutions, obtained by imposing zero derivative conditions on the boundaries of a heterogeneous region, are modified by piecewise Hermite polynomials and used directly as trial functions in coarse mesh, one-dimensional, two-group calculations. The coarse mesh is defined over the whole heterogeneous region for which the detailed solution was obtained, so that the method does actually yield great flux shape details with coarse meshes. No error bounds were found for this scheme but the numerical results were encouraging.

Except for ref. 10, nowhere has there been made any attempt to allow for the variation of parameters inside the expansion elements so as to take full advantage of the finite element method's inherent high accuracy. In the present thesis this interesting possibility will be investigated in a general way. We will see that when the approximation to the "weak" form of the diffusion equation is sought, the spatial variation of the parameters can be taken into account very naturally; furthermore, we will see that numerous numerical experiments indicate that the scheme is worthwhile pursuing.

We will next outline in very general terms the application of the finite element method in order to set up the general structure of Chapter II. Given the equation of a problem, it involves usually a 4 - step procedure.

a) Define a convenient partition of the problem domain, on a bona fide basis, taking into consideration the characteristics of the system, so as to arrive at expansion elements with reasonably constant properties. This choice is frequently natural, as in the case of neutron diffusion problems.

Define, consequently, the open expansion elements Ω_1 , the collection of interfaces $\partial_1\Omega$ and the exterior boundary $\partial_e\Omega$.

b) Choose convenient trial functions for the expansion inside the elements. At this stage considerable freedom exists and the choice will depend on what the user expects to be the general behavior of the solution inside the elements, and on the desirability (or not) of some continuity across the interfaces. Cubic Hermite polynomials, for instance, should be chosen when one expects to be able to preserve function and first derivative continuity. A Lagrangian approximation will only preserve function continuity.

Error bounds of the approximation can be found at this stage.

c) Select a procedure to set up the algebraic set of coupled equations which will permit the solution of the system. The Galerkin method has been widely and successfully used, in general in connection with the "weak" formulation which we will proceed to introduce.

Let the model problem, for instance, be the following:

$$-\nabla^2 \phi = L\phi = f \quad (1.3)$$

where L is a linear operator over the region $\bar{\Omega}$. The usual continuity and boundary conditions are imposed: function and first derivative continuity across interfaces and homogeneous boundary conditions.

The boundary problem can be formulated in a variational form. The functional

$$J = (\phi, L\phi) - 2(\phi, f)$$

is stationary provided

$$(u, L\phi) - (u, f) = 0 \quad (1.4)$$

for all u in the same space as ϕ itself. The $(,)$ indicate the inner products.

An integration by parts yields

$$(\nabla\phi, \nabla u) - \int_S u \frac{\partial}{\partial n} \phi ds - (u, f) = 0$$

Since homogeneous boundary and derivative continuity conditions have been imposed we see that the surface integral vanishes and we are left with

$$(\nabla\phi, \nabla u) - (u, f) = 0 \quad (1.5)$$

Eq. (1.5) is called the "weak" form of Eq. (1.4).

We next seek an approximate solution, in the convenient space of piecewise functions $u_i(\underline{r})$, to Eq. (1.3).

$$\hat{\phi} = \sum_{i=1}^N a_i u_i(\underline{r}) \quad (1.6)$$

The Galerkin method would require that

$$(u_1, L\phi) = (u_1, f) \quad i = 1, 2, \dots, N$$

There are serious drawbacks in this scheme. The expansion functions are required to be twice differentiable and the interface conditions are imposed on the approximate solution. Thus, in order to increase our degree of freedom in choosing the expansion functions we seek instead an approximate solution to the "weak" form Eq. (1.5). The Galerkin method then requires

$$(\nabla u_1, \nabla \phi) = (u_1, f) \quad i = 1, 2, \dots, N$$

(1.7)

The crucial fact in this step is that the space of trial functions is enlarged. Linear functions, for instance, are allowed in the "weak" form, and the approximate solution is not required to obey the derivative continuity conditions.

d) The fourth step in the application of the finite element method is the solution of the set of coupled equations (1.7) and the regeneration of the approximate solution through Eq. (1.6).

CHAPTER II
A FINITE ELEMENT APPROXIMATION
TO THE MULTIGROUP NEUTRON DIFFUSION EQUATIONS

In this chapter we will apply piecewise Hermite polynomial approximations to the multigroup diffusion equations. We first show how the Galerkin method is applied when the multigroup solutions are expanded in terms of piecewise trial functions; we further show the derivation of the "weak" forms corresponding to the equations, and discuss its implications and advantages.

Next we shall show the development of the convenient basis functions for the Hermite piecewise approximation of the multigroup neutron diffusion equations. We then discuss methods to preserve continuities of the solution and "ad hoc" ways to take into account the singularities.

We also discuss the application of the method to cases when the cross sections are allowed to vary inside the expansion elements, and show what the implications of this fact are.

Finally we show the matrix formulation of the problem and the numerical methods used for the solution of the system in the computer code CHD written to implement the method in two-dimensional, multigroup diffusion problems.

2.1) The "weak" form corresponding to the neutron diffusion equations

In this section we develop the coupled "weak" form of the multigroup diffusion equations, arrived at when Eqs. (1.2) are

multiplied by any allowed weighting functions and integrated over the problem domain. We then show the inherent advantages of seeking approximate solutions to the "weak" form instead of to the diffusion equations themselves.

We first draw our attention back to Eqs. (1.2), the basic multigroup diffusion equations, which are repeated here together with the boundary and continuity conditions.

$$\begin{aligned} A_1 \phi_1 &= \frac{1}{\lambda} \sum_{g=1}^G v \Sigma_{fg} \phi_g \\ A_g \phi_g &= \Sigma_{sg-1} \phi_{g-1} \quad g = 2, 3, \dots, G \end{aligned} \quad (1.2)$$

with boundary conditions

$$\begin{aligned} \phi_g &= 0 \\ \frac{\partial}{\partial \underline{n}} \phi_g &= 0 \quad g = 1, 2, \dots, G \\ r &\in \partial_e \Omega \end{aligned}$$

and continuity conditions

$$\begin{aligned} \phi_g^- &= \phi_g^+ \\ D_g^- \frac{\partial}{\partial \underline{n}} \phi_g^- &= D_g^+ \frac{\partial}{\partial \underline{n}} \phi_g^+ \quad g = 1, 2, \dots, G \\ r &\in \partial_i \Omega \end{aligned}$$

The spatial variable is implied in the notation.

In a more compact matrix notation the multigroup diffusion equations can be written as

$$\underline{A} \underline{\phi}(\underline{r}) = \frac{1}{\lambda} \underline{F} \underline{\phi}(\underline{r}) \quad (2.1)$$

where $\underline{\phi}$ is the group flux vector

$$\underline{\phi} = [\phi_1 \ \phi_2 \ \dots \ \phi_G]^T$$

where $\underline{A}$ and $\underline{F}$ are $G \times G$ matrices, and $\underline{\phi}$ is required to satisfy the same continuity and boundary conditions as Eq. (1.2).

It can be shown (ref. 7) that the multigroup "weak" form corresponding to the multigroup equations (1.2) can be derived directly from the continuous energy diffusion equation (1.1) by defining convenient weighting functions. In this thesis we will not use this rigorous procedure, because it is not a crucial step. Instead, we will assume the multigroup equations as arrived at independently and we will seek approximations to the group solutions themselves. In using this approach we will be unable to present any measure of the error bounds on the solution in the energy variable, so that in Sections 2.2 and 2.3, where error bounds will be presented for the Hermite approximation, we will be concerned only with the spatial variables.

In particular, we will not be able to evaluate error bounds on the eigenvalue of the system. However, the multigroup formalism is a well-established approximation and there exist many homogenization procedures which have been shown to present sufficiently accurate results. The main problem in the solution of a diffusion equation lies in the spatial approximation, and it is with this problem that this thesis is concerned with.

We next seek approximate solutions to the G coupled equations implied in Eq. (2.1) by an expansion in some conveniently chosen $N \times G$ piecewise functions, continuous in each Ω_1 . The expansion coefficients a_1^g are not to be confused with the elements of the matrix $\underline{A}$, which are never used in the following discussion.

$$\hat{\phi}(\underline{r}) = \sum_{i=1}^N \underline{U}_i(\underline{r}) \underline{a}_i = [\hat{\phi}_1(\underline{r}) \dots \hat{\phi}_N(\underline{r})]^T \quad (2.2)$$

where

$$\underline{a}_i = [a_i^1 \dots a_i^G]^T \quad i = 1, 2, \dots, N$$

are the unknown coefficient vectors and

$$\underline{U}_i = \text{Diag} [u_i^1(\underline{r}) \dots u_i^G(\underline{r})] \quad i = 1, 2, \dots, N$$

are the expansion matrices.

We have seen earlier (Ch.I) that we would be very limited in the choice of the expansion function if we were to seek approximate solutions directly to Eq. (2.1), because of the interface conditions implied in this equation. The use of the Galerkin method would require that the introduction of Eq. (2.2) into Eq. (2.1) result in

$$(\underline{U}_i, \underline{A} \hat{\phi} - \frac{1}{\lambda} \underline{F} \hat{\phi}) = 0 \quad i = 1, 2, \dots, N \quad (2.3)$$

where (,) means the inner product.

We will now focus attention on what would be required for the terms of (2.3) to exist. The nature of the operator $\underline{A}$ is such that we must require that the $\underline{D} \nabla \hat{\phi}$ be continuous (which is, in fact, the current continuity condition) so that the $(u_i, \underline{V} \cdot \underline{D} \nabla \hat{\phi})$ exist. We will have great difficulties in finding expansion functions which will provide this continuity: piecewise linear functions are excluded at once; furthermore, we will see that in the vicinity of singular points we do not, in fact, want to preserve current continuity.

These facts lead to the desirability of seeking solutions in the "weak" form of Eq. (2.1) where the continuity conditions can be relaxed. To achieve this we assume ϕ to be a solution to Eq. (2.1). Then, for any compatible diagonal matrix $\underline{W}$ we must have

$$(\underline{W}, \underline{A} \phi - \frac{1}{\lambda} \underline{F} \phi) = 0$$

Integrate the leakage term by parts to obtain

$$(\nabla \underline{W}, \underline{D} \nabla \phi) + (\underline{W}, \underline{\Sigma}_r \phi) + \int_S ds \underline{W} \underline{D} \nabla \phi = (\underline{W}, \frac{1}{\lambda} \underline{F} \phi)$$

Because of the continuity and boundary conditions the integrals vanish and we are left with a bilinear form

$$a(\underline{W}, \phi) = (\nabla \underline{W}, \underline{D} \nabla \phi) + (\underline{W}, \underline{\Sigma}_r \phi) - (\underline{W}, \frac{1}{\lambda} \underline{F} \phi) = 0 \quad (2.4)$$

where

$$\underline{D} = [D_1 \dots D_G]^T$$

$$\underline{\Sigma}_r = [\Sigma_{r1} \dots \Sigma_{rG}]^T$$

In order for the terms of the bilinear form (2.4) to exist we must only require that ϕ and $\underline{W}$ and their first spatial derivatives be squared integrable. The space of functions which satisfy these conditions is called a Sobolev space.

In order that $\hat{\phi}$ be an approximate solution to the "weak" form Eq. (2.4), the Galerkin method requires that

$$a(\underline{U}_1, \hat{\phi}) = 0 \quad i = 1, 2, \dots, N \quad (2.5)$$

This scheme thus does enlarge considerably the number of piecewise functions u_1 that can be used in the expansion: in particular, linear piecewise functions can be used and the interface current continuity conditions do not have necessarily to be met. We will only require function continuity.

In the next two sections we will summarize the construction of a complete basis for the piecewise expansion of the solution to the "weak" form of the multigroup neutron diffusion equations, in one and two dimensions, and in terms of the Hermite polynomials of the first and third degrees.

Ref. 6 and Ref. 7 discuss in great detail the construction of such bases. We will present it in a more intuitive way, summarize the highlights and present final conclusions.

In neutron diffusion problems we are generally faced with regions whose properties are piecewise smooth. For a beginning-of-life core of a PWR, for instance, the fuel elements are generally considered as homogenized mixtures of the actual elements, the mixture being defined with constant nuclear properties throughout the element. Once the reactor is depleted, the properties will change in a non-uniform way inside the elements. However, they will still be relatively smooth and we probably will have to consider discontinuities at interfaces.

Furthermore, we have imposed flux and current continuity conditions to Eq. (2.1). These conditions are natural for neutron diffusion equations and this fact, when taken together with the piecewise smoothness of the nuclear properties leads naturally to the use of the Hermite interpolation. In this scheme, interpolating polynomials (called Hermite polynomials) are generated inside the interpolation domain by the use of function values and derivatives at the boundaries.

2.2) Construction of a basis for the piecewise expansion in one dimension

We will now focus attention on the construction of the Hermite cubic basis appropriate for the expansion of the unknown solution in a one-dimensional space and indicate afterwards the use of linear bases and, in the next section, the extension to two-dimensions. Thus consider a one-dimensional interval (x_i, x_{i+1}) as shown in Fig. (2.1), part of a region (a,b) , where we want to interpolate an unknown function, knowing the values of the function and of the first derivatives at both ends. It is easily seen that the cubic polynomial is uniquely determined by these values inside the region of interest.

Fig.2.1 - Function $f_i(x)$ and uniquely determined cubic interpolate in region (x_i, x_{i+1}) .

The pointwise error bound of the general Hermite interpolation is well known and stated in ref. 6 and 7. In the maximum norm inside (x_i, x_{i+1}) and for one-dimensional neutron diffusion problems the interpolation error is bounded by:

$$\left\| \frac{d^q}{dx^q} [f_i(x) - s_i(x)] \right\| \leq K |x_{i+1} - x_i|^{(\mu-q)}$$

$$0 \leq q \leq m-1$$

Where μ in our case is

$$\mu = 2m$$

K is a positive constant independent of $|x_{i+1} - x_i|$, and m is such that $(2m-1)$ is the degree of the interpolating polynomial.

We further realize that $s_i(x)$ can be expressed in the following way, by a sum of four polynomials:

$$\begin{aligned} s_i(x) = & f(x_i) u_i^{0+}(x) + f(x_{i+1}) u_{i+1}^{0-}(x) \\ & + f(x_i) u_i^{1+}(x) + f(x_{i+1}) u_{i+1}^{1-}(x) \end{aligned}$$

where the primes denote x -differentiation.

Each of the u 's is uniquely defined; they are called element functions in refs. 6 and 7, form a complete piecewise basis inside (x_i, x_{i+1}) , and are expressed by

$$u_{i+1}^{0-}(x) = \begin{cases} 3\left[\frac{x-x_1}{x_{i+1}-x_1}\right]^2 - 2\left[\frac{x-x_1}{x_{i+1}-x_1}\right]^3 & , x_1 \leq x \leq x_{i+1} \\ 0 & , \text{Otherwise} \end{cases} \quad (2.6.a)$$

$$u_i^{0+}(x) = \begin{cases} 3\left[\frac{x_{i+1}-x}{x_{i+1}-x_1}\right]^2 - 2\left[\frac{x_{i+1}-x}{x_{i+1}-x_1}\right]^3 & , x_1 \leq x \leq x_{i+1} \\ 0 & , \text{Otherwise} \end{cases} \quad (2.6.b)$$

$$u_{i+1}^{1-}(x) = \begin{cases} \left[-\left(\frac{x-x_1}{x_{i+1}-x_1}\right)^2 + \left(\frac{x-x_1}{x_{i+1}-x_1}\right)^3 \right] (x_{i+1}-x_1) & , x_1 \leq x \leq x_{i+1} \\ 0 & , \text{Otherwise} \end{cases} \quad (2.6.c)$$

$$u_i^{1+}(x) = \begin{cases} \left[\left(\frac{x_{i+1}-x}{x_{i+1}-x_1}\right)^2 - \left(\frac{x_{i+1}-x}{x_{i+1}-x_1}\right)^3 \right] (x_{i+1}-x_1) & , x_1 \leq x \leq x_{i+1} \\ 0 & , \text{Otherwise} \end{cases} \quad (2.6.c)$$

In Fig. 2.2 we plot these functions.

Fig.2.2 - One-dimensional cubic element functions

If, now, the region (a,b) is considered as partitioned in $(N-1)$ contiguous sub-domains, we can approximate the unknown solution of a problem over the whole interval by a sum of piecewise approximations with the use of a set of u -functions in each sub-domain.

$$\begin{aligned}
 s(x) &= \sum_{i=1}^{n-1} s_i(x) \\
 &= \sum_{i=1}^{n-1} [f(x_i^+) u_i^{0+}(x) + f(x_{i+1}^-) u_{i+1}^{0-}(x) \\
 &\quad + f'(x_i^+) u_i^{1+}(x) + f'(x_{i+1}^-) u_{i+1}^{1-}(x)]
 \end{aligned}$$

where the f 's are unknowns to be determined.

Function and derivative continuity are naturally preserved by making

$$f(x_i^+) = f(x_i^-) = f(x_i)$$

$$f'(x_i^+) = f'(x_i^-) = f'(x_i)$$

$$i = 2, N-1$$

(2.7)

Conditions (2.7) lead to the generation of the basis functions appropriate for the approximation of an unknown solution inside the interval (a,b) , preserving function and derivative continuity across the interfaces. They are shown in Fig. 2.3

Fig.2.3 - Cubic basis functions appropriate for function and derivative continuity

In neutron diffusion problems, however, we want to require current continuity across the partition interfaces. This condition can be readily met if we redefine slightly the 1-type element functions in the following way, in two contiguous subdomains (see Fig. 2.4).

$$u_i^1(x) = \begin{cases} (\frac{\theta}{D^-}) u_i^{1-}(x), & x_{i-1} \leq x \leq x_i \\ (\frac{\theta}{D^+}) u_i^{1+}(x), & x_i \leq x \leq x_{i+1} \end{cases} \quad (2.8)$$

θ is a constant introduced so as to make (θ/D^-) and (θ/D^+) close to 1, for numerical reasons.

Fig.2.4 - Cubic basis functions appropriate for flux and current continuity across interfaces for a neutron diffusion problem.

In the case of piecewise linear functions we will be able to preserve function continuity across interfaces. The element functions are expressed by Eq. (2.9)

$$u_{i+1}^{0-}(x) = \begin{cases} \frac{x-x_i}{x_{i+1}-x_i} & , x_i \leq x \leq x_{i+1} \\ 0 & , \text{otherwise} \end{cases} \quad (2.9.a)$$

$$u_i^{0+}(x) = \begin{cases} \frac{x_{i+1}-x}{x_{i+1}-x_i} & , x_i \leq x \leq x_{i+1} \\ 0 & , \text{otherwise} \end{cases} \quad (2.9.b)$$

When the proper coupling conditions (function continuity) are imposed we will have defined the basis functions for the expansion, as shown in Fig. 2.5.

Fig. 2.5 - Linear basis function appropriate for flux continuity across interfaces.

It is shown in ref. 7 that, if the solution is approximated through the "weak" form, and this "weak" form is positive definite, then the error bounds of a neutron diffusion source problem are

$$\|f(x) - s(x)\| \leq K \overline{\Delta x}^{2m}$$

where $\overline{\Delta x}$ is an upper bound of the mesh sizes, and K is a constant independent of $\overline{\Delta x}$.

So, in the cases considered we will have the following error bounds.

$$\begin{aligned} \|f(x) - s(x)\| &\leq K_1 \overline{\Delta x}^2 && \text{(linear)} \\ &\leq K_c \overline{\Delta x}^4 && \text{(cubic)} \end{aligned}$$

2.3) The basis functions in two dimensions

The element functions in two dimensions are generated by taking products of the one-dimensional ones in each direction. For instance, the two-dimensional bicubic interpolate in one element (see Fig. 2.6, element IV) is given by:

$$\begin{aligned} s_1(x, y) = \sum_{px=0}^1 \sum_{py=0}^1 &\left[f_{1,j}^{(px+py)} u_i^{px+}(x) u_j^{py+}(y) + f_{1+1,j}^{(px+py)} u_{i+1}^{px-}(x) \right. \\ &u_j^{py+}(y) + f_{1,j+1}^{(px+py)} u_i^{px+}(x) u_{j+1}^{py-}(y) + \\ &\left. f_{1+1,j+1}^{(px+py)} u_{i+1}^{px-}(x) u_{j+1}^{py-}(y) \right] \end{aligned}$$

where $f_{i,j}$ means the value of the function at point (i,j) , and

where the superscript $(px+py)$ on f means the px^{th} derivative in the X direction and the py^{th} derivative in the y direction.

There are, consequently, 16 values to be known at the 4 corner points: function values, the first derivative in each direction, and the 4 mixed derivatives $\partial^2/\partial x \partial y$.

It is shown in refs. 6 and 7 that a two-dimensional polynomial interpolate $s_1(x,y)$ is uniquely determined, given the appropriate corner values, and for sufficiently smooth functions satisfies the following pointwise error bound in any norm.

$$\left\| \frac{\partial^{(px+py)}}{\partial^{px} \partial^{py}} (f(x,y) - s(x,y)) \right\| \leq K_x \Delta x^{(2mx-px)} + K_y \Delta y^{(2my-py)}$$

$$\text{for } 0 \leq px \leq mx-1$$

$$\text{and } 0 \leq py \leq my-1$$

Where, K_x and K_y are positive constants independent of Δx and Δy respectively, and where $(2mx-1)$ and $(2my-1)$ specify the degree of the one-dimensional polynomials in each direction.

Consequently, in the case of bilinear and bicubic interpolation we have the following interpolation error bounds:

$$\left\| f(x,y) - s(x,y) \right\| \leq K_1 (\Delta x^2 + \Delta y^2) \quad (\text{linear})$$

$$\leq K_c (\Delta x^4 + \Delta y^4) \quad (\text{cubic})$$

where K is an upper bound of K_x and K_y .

As in the one-dimensional case, basic functions for neutron diffusion problems can be defined by imposing appropriate coupling conditions to the element functions. The unknown solution of a two-dimensional problem can then be approximated by considering a convenient partition of the problem domain.

We will show the procedure for construction of the basis functions for the case of bicubic element functions.

Fig. 2.6 - Two-dimensional partition

Case 1

$$D_I D_{III} = D_{II} D_{IV}$$

This condition is satisfied at any interior or interface points, except singular points. The basis functions which allow current or simply derivative continuity across the $\underline{i}$ and $\underline{j}$ lines are Eq. (2.10)

$$u_{ij}^{00}(x,y) = \left[\begin{array}{ll} u_i^{0+}(x) u_j^{0+}(y) & , \quad \text{I} \\ u_i^{0-}(x) u_j^{0+}(y) & , \quad \text{II} \\ u_i^{0+}(x) u_j^{0-}(y) & , \quad \text{III} \\ u_i^{0-}(x) u_j^{0-}(y) & , \quad \text{IV} \end{array} \right. \quad (2.10a)$$

$$u_{ij}^{10}(x,y) = \left[\begin{array}{ll} \frac{\theta}{D_I} u_i^{1+}(x) u_j^{0+}(y) & , \quad \text{I} \\ \frac{\theta}{D_{II}} u_i^{1-}(x) u_j^{0+}(y) & , \quad \text{II} \\ \frac{\theta}{D_{III}} u_i^{1+}(x) u_j^{0-}(y) & , \quad \text{III} \\ \frac{\theta}{D_{IV}} u_i^{1-}(x) u_j^{0-}(y) & , \quad \text{IV} \end{array} \right. \quad (2.10b)$$

$$u_{ij}^{01}(x,y) = \left[\begin{array}{ll} \frac{\theta}{D_I} u_i^{0+}(x) u_j^{1+}(y) & , \quad \text{I} \\ \frac{\theta}{D_{II}} u_i^{0-}(x) u_j^{1+}(y) & , \quad \text{II} \\ \frac{\theta}{D_{III}} u_i^{0+}(x) u_j^{1-}(y) & , \quad \text{III} \\ \frac{\theta}{D_{IV}} u_i^{0-}(x) u_j^{1-}(y) & , \quad \text{IV} \end{array} \right. \quad (2.10c)$$

$$u_{ij}^{11}(x,y) = \left[\begin{array}{ll} \frac{\theta}{D_I} u_i^{1+}(x) u_j^{1+}(y) & , I \\ \frac{\theta}{D_{II}} u_i^{1-}(x) u_j^{1+}(y) & , II \\ \frac{\theta}{D_{III}} u_i^{1+}(x) u_j^{1-}(y) & , III \\ \frac{\theta}{D_{IV}} u_i^{1-}(x) u_j^{1-}(y) & , IV \end{array} \right. \quad (2.10d)$$

In these equations, θ is a normalization constant chosen so that $\theta/D = 1$.

Case 2

$$D_I D_{III} \neq D_{II} D_{IV} \quad (\text{singular points})$$

It is easy to see that at singular points the current continuity condition of the diffusion problem can be met by specifying

$$\frac{\partial}{\partial x} \phi(x,y) = \frac{\partial}{\partial y} \phi(x,y) = 0$$

for (x,y) - singular point

However, we know that the analytic solution at a singular point does not satisfy the above conditions. Further some results to be shown later indicate that imposition of the above condition gives poor approximate solutions.

As mentioned previously, diffusion theory itself is not valid at corners with discontinuities. We do not expect analytic

solutions near singularities to truly represent the physical neutron distribution. Furthermore, on a practical point of view, in many problems one is more interested in overall measures of core performance (k_{eff} , region-wise reaction rates). In these cases one may argue that, whatever the analytic singular component of the solution, it is a localized effect and its contribution to overall features should be very small.

On the other hand, in real life two-dimensional calculations one will have some kind of scattered pattern of zones with different enrichments inside a reactor, so that most of the actual points will be singular ones. We expect the singularity to be a function of the magnitude of the material discontinuities. It will have a greater influence at water-fuel interfaces than at interfaces between fuels of different enrichments.

One of the purposes of the present thesis was to investigate how one might proceed in dealing with singular points in problems where one is mainly concerned with regionwise, averaged behaviors (such as a depletion analysis). One might, for instance, arbitrarily specify first derivative continuity by making all $\theta/D = 1$ at Eq. (2.12b) and (2.12c). This approach seems intuitively convenient for "fuel only" singular points, where the diffusion coefficients do not change drastically.

On the other hand one may also uncouple completely the first derivatives by "opening" Eq. (2.10b) and (2.10c) into four equations.

$$u_{ij}^{\bar{1}0}(x,y) = \begin{cases} u_1^{1-}(x) u_j^{0+}(y) & , & \text{II} \\ u_1^{1-}(x) u_j^{0-}(y) & , & \text{III} \quad (2.10b-) \\ 0 & , & \text{I \& IV} \end{cases}$$

$$u_{ij}^{+10}(x,y) = \begin{cases} u_1^{1+}(x) u_j^{0+}(y) & , & \text{I} \\ u_1^{1+}(x) u_j^{0-}(y) & , & \text{IV} \quad (2.10b+) \\ 0 & , & \text{II \& III} \end{cases}$$

$$u_{ij}^{0\bar{1}}(x,y) = \begin{cases} u_1^{0-}(x) u_j^{1-}(y) & , & \text{III} \\ u_1^{0+}(x) u_j^{1-}(y) & , & \text{IV} \quad (2.10c-) \\ 0 & , & \text{I \& II} \end{cases}$$

$$u_{ij}^{+0\bar{1}}(x,y) = \begin{cases} u_1^{0+}(x) u_j^{1+}(y) & , & \text{I} \\ u_1^{0-}(x) u_j^{1+}(y) & , & \text{II} \quad (2.10c+) \\ 0 & , & \text{III \& IV} \end{cases}$$

$$u_{ij}^{00}(x,y) - \text{Eq. (2.10a)}$$

$$u_{ij}^{11}(x,y) - \text{Eq. (2.10d)}$$

Still another possibility would be to impose the zero derivatives conditions by dropping Eq. (2.10b) and (2.10c) completely from the set of expansion functions. This approach, however, leads to intolerable distortions both in flux shape near the singular points and in the overall characteristics.

In Ch. III we will show results arrived at for different problems and ways of dealing with singular points.

The generation of basic functions at the boundaries of the domain can be easily shown to be special cases of the expressions given by Eq. (2.10), arrived at by coupling element functions whose supports are non-zero.

As in the one-dimensional case, refs. 6 and 7 show that, if the solution to the diffusion problem is approximated through the weak form, and the weak form is positive definite, then the error bounds of a neutron diffusion source problem, for $f(x,y)$ sufficiently differentiable, are

$$\left\| \left\| f(x,y) - s(x,y) \right\| \right\|_{\infty} \leq K_x \overline{\Delta x}^{2m} + K_y \overline{\Delta y}^{2m}$$

Where $\overline{\Delta x}$ and $\overline{\Delta y}$ are upper bounds of the mesh sizes in each direction, and K_x and K_y are constants independent of $\overline{\Delta x}$ and $\overline{\Delta y}$ respectively.

In the bilinear and bicubic cases consequently

$$\begin{aligned} \left\| \left\| f(x,y) - s(x,y) \right\| \right\|_{\infty} &\leq K_l (\overline{\Delta x}^2 + \overline{\Delta y}^2) \text{ (linear)} \\ &\leq K_c (\overline{\Delta x}^4 + \overline{\Delta y}^4) \text{ (cubic)} \end{aligned}$$

Where the K are convenient upper bounds of K_x and K_y in each case.

2.4) Varying cross sections inside the expansion element

Up to this point we have tacitly assumed that the diffusion coefficient was a piecewise constant function. The weak form of the problem is properly posed for more general behavior of the diffusion coefficient. In particular, a unique solution to the problem will exist if $D(\underline{r})$ is allowed to be a piecewise continuous, rather than piecewise constant, function.

From a theoretical view piecewise continuous diffusion coefficients present no difficulties. From the view of the approximation methods the inclusion merely changes the evaluation of elements in the coefficient matrix.

The number of basis functions (and consequently the number of unknowns) is approximately equal to some integer times the number of mesh points. We have assumed that mesh lines are always located at interfaces. If the system has many discontinuities then we will have many unknowns. It is evident that if the spacing between discontinuities is very small, then finite difference methods may be adequate for the problem, and one need not consider higher-order methods. Conversely, it is of interest to attempt to use coarse meshes, and higher order methods, in an attempt to find accurate solutions with a small computing burden. Clearly then, for highly heterogeneous systems, we must consider the problem of mesh intervals which extend through discontinuities. It is just this problem that we consider in some detail in this thesis.

Our approach will be the following: We will use element and/or basis functions which are themselves smooth within their interval of definition. Discontinuities in properties, within the interval, will be accounted for in all inner products. The approximate solution will be smoother than the actual solution; however the effects of the discontinuities will be averaged into the approximate solution through the elements of the coefficient matrix.

2.5) Matrix formulation of the two-group diffusion problem and numerical methods

In this section we present the matrix equation which results from the application of the finite element method to the two-group diffusion problem. We further present the numerical methods used in the actual solution of the system with the computer code CHD. We will exemplify the procedure with a simple, two-dimensional, two-group problem, with the realization that an extension to more groups is straightforward.

We consider a partition of the problem domain in Cartesian coordinates on a "bone fide" basis. In a PWR, for instance, a partition along fuel element interfaces will provide surprisingly accurate results. Let N be the number of rows and M be the number of columns resulting from the partition.

We next preassign some order to the unknowns and define two column vectors $\underline{a}_1$ and $\underline{a}_2$ as the ordered set of the unknown solutions in each group. Although it is not crucial, the form of the matrices is easier to visualize and it will be assumed in this

thesis that the ordering is done by assigning to each point all its associated unknowns (flux, first derivatives, mixed derivative for bicubic expansion, for instance) in some order, before moving to the next point.

Consider now Eq. (1.2) specialized for two dimensions and two groups

$$A_1 \phi_1(x,y) = \frac{1}{\lambda} [\nu \Sigma_{f1} \phi_1(x,y) + \nu \Sigma_{f2} \phi_2(x,y)]$$

$$A_2 \phi_2(x,y) = \Sigma_{s1} \phi_1(x,y)$$

where the spatial variation of the operators is implied.

We next approximate the fluxes by means of the piecewise Hermite polynomials (u) defined in the previous sections:

$$\phi = \hat{\phi} = \sum_{n=1}^N \sum_{m=1}^M \sum_{i=1}^{I(n,m)} a_{n,m,i}^1 u_{n,m,i}^1(x,y)$$

$$\phi = \hat{\phi} = \sum_{n=1}^N \sum_{m=1}^M \sum_{i=1}^{I(n,m)} a_{n,m,i}^2 u_{n,m,i}^2(x,y)$$

where $I(n,m)$ is the number of basis functions at point (n,m) , and where $N, M, I(n,m)$ are taken as being the same for both groups for simplicity of notation.

We seek the approximate solutions in the coupled "weak" form of the two-group equations. The Galerkin method requires that we apply Eq. (2.5), the overall result being that the following set of coupled linear equations be solved.

$$\int_V \left[D_1 \nabla \phi_1 \cdot \nabla u_{n,m,i}^1 + [\Sigma_{r1} \phi_1 - \frac{1}{\lambda} (v \Sigma_{f1} \phi_1 + v \Sigma_{f2} \phi_2)] u_{n,m,i}^1 \right] dV = 0$$

$$\int_V \left[D_2 \nabla \phi_2 \cdot \nabla u_{n,m,i}^2 + [\Sigma_{r2} \phi_2 - \Sigma_{s1} \phi_1] u_{n,m,i}^2 \right] dV$$

$$\begin{aligned} \text{for } n &= 1, N \\ m &= 1, M \\ i &= 1, I(n, m) \end{aligned} \quad (2.11)$$

Where $\hat{\lambda}$ is introduced as an approximation to λ .

When the necessary products of the Hermite functions are performed, we end up with two coupled matrix equations of the form

$$\underline{A}_1 \underline{a}_1 = \frac{1}{\lambda} [\underline{F}_1 \underline{a}_1 + \underline{F}_2 \underline{a}_2]$$

$$\underline{A}_2 \underline{a}_2 = \underline{S}_1 \underline{a}_1 \quad (2.12)$$

Where the $\underline{A}$ are matrices which incorporate the diffusion and removal terms, the $\underline{F}$ incorporate the fission terms and $\underline{S}_1$ incorporates the group 1 downscattering terms.

It is useful to focus some attention on the forms of the matrices of Eq. (2.12). They will all show an overall stripe structure, the number of stripes depending on the dimensions of the problem.

$$\text{Number of stripes} = 3^k$$

$$k = \text{No. of spatial dimensions (1, 2 or 3)}$$

Additionally, the stripes themselves are formed by block matrices whose size will depend on the number of coupling expansion functions associated with the relevant points.

In Fig. (2.7) we show the general form of these block matrices for a two-dimensional problem. Each position $(a,b...i)$ represents a block matrix, the size depending on the number of basis functions existing at each of the coupling points. The coupling between a general point (n,m) and its immediate neighbors (and with itself) is shown.

In Fig. (2.8) the structure of one of the A matrices is shown for a simple 3×3 two-dimensional partition. The problem is too small so that the stripes are not evident and we show just the limits of the diagonal.

It can be shown (ref. 6 and 7) that the matrices $\underline{A}_1$ and $\underline{A}_2$ are always symmetric and positive definite. $\underline{F}_2$ and $\underline{S}_1$ are not symmetric in the general case and, in fact, may even not be square if the total number of expansion functions in the fast group is not the same as in the thermal group. Matrix $\underline{F}_1$ is also always symmetric.

We choose to solve Eq.(2.12) by uncoupling the system through the power iteration method (ref. 11). This method has been used successfully in conjunction with finite difference methods and can be shown to yield, in these cases, solutions which are everywhere positive (the fundamental modes) for any positive initial guess, and the corresponding eigenvalue which can thus be identified with the k_{eff} of the system. On practical grounds we have reasons to expect that the same will be true in the present case, for any initial guess corresponding to everywhere positive fluxes.

Fig. 2.7 - Two-dimensional partition and matrix form for unknowns ordered as: 1) all unknowns at each point; 2) all columns; 3) all rows.

Fig. 2.8 - Two-dimensional partition and corresponding matrix structure

The power iteration method requires the following iteration procedure.

$$\underline{A}_1 \underline{b}_1^{(t)} = \underline{F}_1 \underline{a}_1^{(t-1)} + \underline{F}_2 \underline{a}_2^{(t-1)}$$

$$\underline{A}_2 \underline{b}_2^{(t)} = \underline{S}_1 \underline{b}_1^{(t)}$$

$$\hat{\lambda}^{(t)} = \frac{(\underline{b}_1^{(t)}, \underline{b}_1^{(t)}) + (\underline{b}_2^{(t)}, \underline{b}_2^{(t)})}{(\underline{b}_1^{(t)}, \underline{a}_1^{(t-1)}) + (\underline{b}_2^{(t)}, \underline{a}_2^{(t-1)})}$$

$$\underline{a}_1^{(t)} = \frac{\underline{b}_1^{(t)}}{\hat{\lambda}^{(t)}}$$

$$\underline{a}_2^{(t)} = \frac{\underline{b}_2^{(t)}}{\hat{\lambda}^{(t)}} \quad (2.13)$$

Where the parenthesis indicate inner products.

We next will show the numerical scheme used to solve each of Eq. (2.13) that is, the problems

$$\underline{b}_1^{(t)} = \underline{A}_1^{-1} [\underline{F}_1 \underline{a}_1^{(t-1)} + \underline{F}_2 \underline{a}_2^{(t-1)}]$$

$$\underline{b}_2^{(t)} = \underline{A}_2^{-1} \underline{S}_1 \underline{b}_1^{(t)}$$

When the matrices $\underline{A}_1$ and $\underline{A}_2$ are positive definite and not too large the Cholesky factorization scheme (ref. 12) can be conveniently utilized^(*). It is shown that in this case the A's can be factorized as

$$A = \underline{E} \underline{E}^T$$

where $\underline{E}$ is a lower triangular matrix.

The elements of $\underline{E}$ can be determined by using the algorithm

$$e_{jj} = [a_{jj} - \sum_{k=1}^{j-1} e_{jk}^2]^{1/2}$$

$$e_{ij} = \frac{a_{ij} - \sum_{k=1}^{j-1} e_{ik} e_{jk}}{e_{jj}}$$

The problem can then be solved in two sweeps, one forward and one backward to insert $\underline{E}$ and $\underline{E}^T$ respectively.

(*) Matrices of up to 350 x 350 elements have been inverted without problems in double precision.

CHAPTER III

SAMPLE PROBLEMS AND RESULTS

The final aim of this chapter is to present some results on the approximate solution of realistic, two-dimensional reactor problems as they were evaluated with CHD. The most important example chosen was the first-loading, beginning-of-life core of the Zion 1 reactor (ref.13) the evaluation being done with 3 different kinds of coarse meshes, on a quarter-core symmetry basis. The results are compared to conventional finite difference results, as obtained with the use of the EXTERMINATOR 2, PDQ-5 and CITATION codes. For the finite element examples the finest mesh used corresponds to a full fuel element (about 22 cm). Subsequently, some meshes were defined over 4 fuel elements and, finally, a very coarse mesh was defined over the innermost 16 fuel elements.

Several questions arise when coarse meshes are used. For instance, when two regions with varying cross sections have a common interface, it is not at all clear whether the best continuity condition should actually preserve current across the interface. The same reasoning is actually valid for any mesh point surrounded by regions with varying parameters.

Even in the simplest case, when cross sections are constant inside the expansion elements, it is not clear which conditions should be imposed across singular points. Zero first derivative conditions, for instance, are known to preserve the appropriate continuity conditions of the diffusion problem. However, it is

also known that the diffusion approximation itself does not hold in the vicinity of these points, so that it may be appropriate to relax such conditions.

All these questions were investigated through a set of appropriately defined smaller problems. In some cases the results are compared with finite difference results, through the use of the EXTERMINATOR 2 code, and in other cases they are compared to very fine mesh results of CHD, which are known to be very accurate.

The order in which the results are presented in the following sections corresponds to an increasing complexity of the problems.

All cross sections are listed in Appendix A.

3.1) Comparisons between CHD and EXTERMINATOR 2 for a 4-composition problem.

In its earliest versions, CHD was tested against EXTERMINATOR 2 for the small problem shown in Fig. 3.1. The basic 18 cm measure corresponds approximately to the width of a PWR fuel element.

Fig. 3.1 - The 4-composition problem geometry

EXTERMINATOR 2 was developed at Oak Ridge, and the version used at MIT corresponds essentially to ORNL 4078 (ref. 14). It is a standard finite difference code, using periodic extrapolation as acceleration technique for the outer iterations, and row or column successive overrelaxation in the inner iterations.

Several EXTERMINATOR 2 and CHD runs were made, the purpose being mainly to investigate what kind of derivative continuity condition (if any) should be used at singular points such as 22, 33, 43 and 34. It was to be expected beforehand that at singular points surrounded by fuel elements one could get sufficiently accurate results by requiring simply derivative continuity, because the diffusion coefficients are not very different for homogenized fuel elements of different enrichments. For singular points where there are fuel-water interfaces one might expect that uncoupling the first derivatives should improve the results. Continuities imposed directly on the expansion functions result in less unknowns, whereas each uncoupling increases the number of unknowns by 1. Thus the problem consists basically in determining if the imposition of continuities will not distort the results in a way intolerable for the purpose of the calculation.

Various combinations of element functions were used throughout the work. They are identified by code numbers, and are described in detail in App. C.

Macroscopic two-group cross sections were taken from ref. 10, Table 5.1, and are close to low, medium and highly enriched, homogenized PWR fuel element properties.

In Table 3.1 we compare overall features for all the runs.

Table 3.1 Overall results for EXTERMINATOR 2 and CHD for the 4-composition problem

Case	Code (mesh.cm)	Solution condition at singular points	# of unknowns per group	k_{eff}	Average fluxes at reentrant water region (fast/th.)
	EXTERM. (9.0)	-	81	1.09472	
	EXTERM. (4.5)	..	289	1.08260	
	EXTERM. (3.0)	-	625	1.07972	
Ref.	EXTERM. (3.0 & 1.8)	-	1156	1.07840	0.25973 0.44608
1	CHD (18.0)	Zero first derivatives	56	1.07598	0.30615 0.45573
2	CHD (18.0)	First deri- vatives con- tinuity. (41 sets)	64	1.07825	0.25740 0.44611
3	CHD (18.0)	First deri- vatives un- coupled. (61 sets)	72	1.07812	0.25564 0.44631

It can be seen that, except for the case of zero derivatives at all singular points, we can reproduce k_{eff} up to four decimal places with CHD, using a whole fuel element as a mesh and thus requiring much fewer unknowns, in general by a factor over 10. On the other hand, the significant deviation of the EXTERMINATOR result from the reference k_{eff} , as the finite difference mesh is increased, is also very clear. In particular, the 9.0 cm EXTERMINATOR mesh requires 81 unknowns per group, about the same as all the CHD runs: whereas the finite element method yields k_{eff} within less than 0.03% in cases 2 and 3, the finite difference result is off by 1.63%.

We have also included in the last column a measure of the average fluxes at the reentrant water regions, where one may expect the largest errors to occur. In the finite element cases 2 and 3 fast fluxes are represented within less than 1.6% whereas thermal fluxes are represented within less than 0.05%.

It should also be realized that the distortion due to the singular points is a very localized effect and its influence on the overall core performance (exemplified here by k_{eff}) is rather small.

In Figs. 3.2 and 3.3 we have plotted fast and thermal fluxes for cuts through positions A and B, and in Fig. 3.4 we present element-averaged results.

It is evident from Fig. 3.3 that case 1, where we have imposed zero derivative across the singular points, is not a realistic assumption and does not yield accurate pointwise results. For this reason, none of the following examples was ever evaluated with this option.

11.0455 1.36019 0.43627	12.3315 1.45922 0.35520	10.0330 1.08427 0.25101
	10.8738 1.30455 0.31100	8.4419 0.83480 0.21987
		1.58602 0.25973 0.44608

Reference (EXTERMINATOR)

11.022 1.3556 0.43558	12.265 1.4523 0.35318	9.9761 1.0755 0.24986
	10.959 1.2653 0.31958	8.4350 0.81152 0.22220
		1.6245 0.30615 0.45573

Case 1 (CHD)

11.041 1.3568 0.43651	12.305 1.4606 0.35385	10.033 1.0843 0.25098
	10.863 1.3069 0.31023	8.4753 0.83484 0.22103
		1.5860 0.25740 0.44611

Case 2 (CHD)

11.055 1.3585 0.43707	12.321 1.4621 0.35437	10.048 1.0851 0.25146
	10.849 1.3071 0.30959	8.4510 0.83493 0.22017
		1.5866 0.25564 0.44631

Case 3 (CHD)

KEY

Absorp. rate
Avg. fast flux
Avg. ther. flux

Fig. 3.4 - Element averaged results
for 4-composition problem as evaluated with EXTERMINATOR and CHD

In case 3 we uncouple the first derivatives at all singular points. It is clear that the pointwise fluxes are better matched in this case. Further the element-averaged results are well-matched in case 2, where first derivative continuity is imposed across the singular points, as well as in case 3.

In Fig. 3.2 we have also included a thermal flux plot labeled (S) for Special Case, at the fuel water interface. For this case two extra mesh points were included at each side of the fuel water interface at $x = 0.0$, 4.5 cm to each side of the interface. The pointwise error is negligible in this case. Clearly thus we can improve local accuracy by refining the mesh slightly in the region of large gradients.

3.2) The one-dimensional, ten-region problem

When one tries to represent a core such as Zion 1 on a coarse mesh, the core baffle arises as an anomaly perturbing the regular structure of the fuel elements, which would otherwise provide an excellent partition for the problem. The explicit representation introduces undesired fine meshes at several points of the region.

On the other hand, the baffle has a relatively strong influence on the system (mainly in the thermal flux distribution of adjacent elements) so that it cannot be neglected. In order to account for the baffle's presence in the finite element method (an inherently coarse mesh method) one can either homogenize it with some portion of the reflector, or define a region with varying parameters on the outside of the core, which would include the baffle and water.

In order to investigate how accurate a solution one could get by homogenizing the baffle in a real reactor, a series of one-dimensional (*) runs were made with the dimensions, compositions and number of regions of the Zion 1 reactor. The geometry shown in Fig. 3.4a was used, with cross sections corresponding to values arrived at for these fuel elements (ref. 13).

All the results presented were obtained from CHD.

Fig. 3.4a - One-dimensional, ten-region problem.

In Tables 3.2 and 3.3 we present some overall results, and in Fig. 3.5 we present flux plots. It can be seen, in general, that the baffle causes relatively important changes in the system. Although k_{eff} can be fairly well corrected by smearing the SS into the adjacent reflector region, pointwise flux deviations of 100% from the correct answer occur at fuel-baffle interface.

(*) Actually, CHD does not have a one-dimensional option incorporated. However, 1D can be simulated by using zero derivative conditions at two opposite boundaries of a convenient two-dimensional problem.

Table 3.2 - Eigenvalues for one-dimensional, ten-region problem.

Case	1	2	3
Description	No baffle	Baffle and water homogenized.	Baffle explicitly considered.
k_{eff}	1.27912	1.27873	1.27866

Table 3.3 - Element averaged results for one-dimensional, ten-region problem.

Case	Composition								
	11	12	11	12	11	12	11	13	¹⁵ ₁₄ 3 & 15
1	7.02	14.58	13.13	12.68	10.48	9.07	6.38	4.28	0.427
	0.602	0.543	0.562	0.472	0.450	0.338	0.273	0.148	
2	7.23	15.00	13.45	12.90	10.54	8.94	6.06	3.58	0.431
	0.620	0.558	0.576	0.480	0.451	0.333	0.259	0.121	
3	7.28	15.09	13.53	12.96	10.56	8.93	6.01	3.37	0.378
	0.624	0.562	0.579	0.483	0.452	0.333	0.257	0.112	

KEY Absorp. rate
Thermal flux

Fig. 3.5 - Flux plots for one-dimensional, ten-region problem.

From these runs we draw the conclusion that for a real reactor one can probably arrive at sufficiently accurate results, as far as average properties are concerned, by smearing the baffle in the nearby moderator region. The coarse mesh structure can thus be maintained throughout the problem domain.

Pointwise flux results however show significant deviations which one would like to reduce. Therefore, we will try to account for the baffle's presence by incorporating it into a region with varying parameters together with some portion of the nearby reflector.

In the following sections all the implications that arise when defining regions with varying parameters will be evaluated through small, two-dimensional problems. First, ways will be shown to deal with cases such as the baffle, when one is interested just in the influence of an outside region on a core and not in the detailed flux behavior inside the perturbing region. Second, solutions will be shown for cases in which varying cross sections are specified inside a fuel region .

We begin by showing in Sec. (3.3) a simple two-dimensional problem, in which modifications will be introduced in Sec. (3.4) and (3.5) to allow investigation of the problems we have mentioned..

3.3) The basic two-dimensional two-composition problem

One of the sample two-dimensional problems used in ref. 7 was the two-composition core shown in Fig. 3.6.

In ref. 7 a fine finite difference result (2 cm mesh) is compared with results from Hermite polynomials expansions for the cases of linear and cubic basis functions and, in the latter case, for 3 ways of taking into account the singularity. Some of the k_{eff} are shown in Table 3.4, and in Figs. 3.7 we show thermal flux plots for $x = 0$ and $x = 20$ cm.

Set A of the expansion functions is defined so as to preserve currents across the singular point by making

$$\frac{\partial \phi}{\partial x} = \frac{\partial \phi}{\partial y} = 0 \quad \text{for } x = y = 20 \text{ cm}$$

As we have already seen, this option is not interesting in actual practice, because the zero derivatives introduce great distortions in the flux shapes. It is no longer an option in CHD.

Set B specifies derivative continuity across the singular point and corresponds to option 41 in CHD.

Set C uncouples the first derivatives and corresponds to option 61 in CHD.

As was to be expected, the best pointwise flux distribution was achieved with set C, although for a 20 cm mesh none of the solutions

Fig. 3.6 - The basic two-dimensional,
two-composition problem.

69

Table 3.4 - Eigenvalues for the basic
two-dimensional problem.

Δh (cm)	Bicubic expansion			Finite difference
	Set A	Set B	Set C	
20.0	0.8962196	0.9041992	0.9023381	0.9004928
10.0	0.8965491	0.9008425	0.8980759	
6.667	0.8968995	0.8999750	0.8975901	
2.0

Fig. 3.7.a - Thermal flux plots for basic two-dimensional problem at $x=0.0$

FIG. 3.7.b - Thermal flux plots for basic two-dimensional problem at $x=20.0$

compares very well with the finite difference one. For a 10 cm mesh, however, set C predicts very accurate pointwise results.

3.4 The basic two-dimensional problem with baffle surrounding the fuel region

The basic two-dimensional two-composition problem shown in Sec. (3.3) was first modified by the introduction of a SS baffle between fuel and reflector. Comparisons were then made between results achieved by treating the baffle explicitly (that is, by defining it explicitly as an expansion element) and by treating it implicitly (that is, by taking it as part of an overall baffle reflector expansion element where the cross sections are allowed to vary spatially).

The geometry used is shown in Fig. 3.8.

Fig. 3.8 - Geometry for the basic two-dimensional problem with baffle surrounding the fuel region.

For case 1 the set of functions was defined so as to explicitly preserve current between fuel and SS across points A and B (a set of 421 and a set of 422 type functions, consequently) whereas at the singular point the first derivatives were uncoupled (a 61-type set).

For cases 2 and 3 the first derivatives were uncoupled in the Y and X directions, respectively at points A and B (two 51-type sets, consequently).

Reference solutions A and B were obtained by treating the baffle region explicitly. Ref. A is the most accurate one and was obtained by uncoupling the first derivatives at all singular points (C and C'). Ref. B was obtained with a coarser mesh but with the same treatment for singular points C and C'.

Some results are presented in Table 3.6 and fluxes are plotted in Figs. 3.9.

Table 3.6 - Overall results for the basic two-dimensional problem with baffle surrounding the fuel region.

Case	Ref. A	Ref. B	11	2	3
k_{eff}	0.88385	0.88395	0.87931	0.88042	0.88142
# unknowns (/group)	104	40	18	20	70
Abs.rate (baffle + water)	17.4275	17.09072	18.0478	17.7249	17.7682
Fast/Thermal ratio (avg. fuel fluxes)	3.39073	3.38603	3.38638	3.40373	3.40571
Rel. running time	45			5

Fig. 3.9.a - Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region ($y=0.0$)

Fig. 3.9.b.- Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region ($y=20.0$)

In Table 3.6 we can see that the effect of the baffle on the k_{eff} of the system (a reduction from about 0.9 to about 0.884) can be taken into account approximately through the implicit treatment of the baffle, although with an error of about 0.3% in the best case. It should be realized however that in a real reactor the influence of the baffle would not be as important as in the present case, so that the error might be acceptable.

Through the plots in Figs. 3.9 we clearly see how, in case 1, the method preserves current continuity at points A and B, this fact leading to distortions in the flux. At the singular point, however, where we do not try to preserve current, the solutions try to accommodate themselves. A logical extension then is to uncouple the derivatives in the Y direction at point A, and in the X direction at point B, because as we cannot represent the flux behavior with sufficient accuracy through baffle and water anyway there is no reason in preserving current at fuel-ss interfaces. This is done in cases 2 and 3: case 2 proved to be very accurate (within about 10% at interface points) for the fuel region, but less accurate at the reflector-baffle region; case 3 improved the plot a little bit, especially in the reflector. However, since we are not interested in the detailed flux behavior inside baffle and reflector but rather in their effect on fuel, we will probably get sufficient accuracy by using the case.2 setup.

It should also be realized that case 2 corresponds to a very coarse mesh and is probably intrinsically off a correct solution in the same measure as Ref. B is off Ref. A.

Fast flux plots are not shown but are very accurate in all cases.

3.5) The basic two-dimensional problem with varying cross sections inside the fuel region

The basic two-dimensional, two-composition problem shown in Sec. (3.3) is now modified by changing cross sections inside the fuel region. Comparisons will be made between results obtained by treating each sub-composition as a separate expansion element, and results obtained by treating the variations implicitly, that is by allowing them to occur inside coarse expansion elements. The results should give an idea about whether it is possible (or not) to define expansion elements over more than one fuel element in a real reactor.

The geometry used is shown in Fig. 3.10. The cross sections were changed in concentric "rings": the fast and thermal diffusion coefficients were increased by 10% whereas the thermal absorption cross section was almost doubled, from the outermost "ring" toward the inside (see Appendix A).

Fig. 3.10 - Geometry for the basic two-dimensional problem with varying cross sections inside the fuel region.

In case 1 we explicitly preserved current across points A and B, and in cases 2 and 3 this requirement is relaxed by uncoupling the derivatives in the Y direction (point A) and X direction (point B). In all the cases first derivatives were completely uncoupled at the singular point.

The reference solution was obtained with a very fine mesh, as shown. First derivatives were uncoupled at the fuel-water singular point, whereas derivative continuity was specified at all fuel-fuel singular points.

In Table 3.7 we shown some overall results, and in Figs. 3.11 and 3.12 fluxes are plotted.

Table 3.7 - Overall results for the basic two-dimensional problem with varying cross sections inside the fuel region.

Case	Reference	1	2(*)	3
k_{eff}	0.72936	0.74164	0.74271	0.72906
# unknowns(/group)	146	18	20	74
Abs. rate (fuel)	111.4182	109.94	109.98	111.423
Fast/thermal rat. (avg. fuel flux)	3.49786	3.346	3.3445	3.4912

(*) This case is presented as a sample problem in App.D

Fig. 3.11.a - Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=0.0$)

Fig. 3.11.b - Fast fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=0.0$)

Fig. 3.12.a - Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=20.0$)

Fig. 3.12.b - Fast fluxes for two-dimensional problem with varying cross sections inside fuel region ($x=20.0$)

As it can be seen, cases 1 and 2 incorporate too coarse a mesh for the detailed flux behavior to be represented satisfactorily, whereas case 3 is probably an adequate setup for most applications: fast fluxes cannot be separated in the graphs, and thermal fluxes show perfectly the general behavior of the reference solution, even across singular points.

In these runs it is to be noted that it is not essential that the solution first derivatives be uncoupled across regular points such as A and B, a more important parameter being the number of subregions in the expansion element. This can be seen in the behavior of runs 1 and 2: whereas the number of unknowns is increased by one for each "opening", the results (mainly the overall ones) are very close. This is due to the fact that the flux solution is smoother in this case than in the baffle case shown in Sec. 3.4.

A series of runs was also made with this same geometry but with the diffusion coefficients kept constant throughout the region. The results were similar to the ones just shown and will not be presented here.

We can state now two conclusions from all the previous runs. First, when representing a real reactor we will probably be able to account adequately for the baffle's presence by treating it implicitly as part of an overall baffle-moderator expansion element. We should however uncouple appropriately the first derivatives of the solution at the baffle surface.

Second, we will probably be able to achieve reasonable results by defining one expansion element over four adjacent fuel elements. In this case, it is not essential that the first derivative be uncoupled. This conclusion is based upon the relatively small changes in D between regions.

We next proceed to show the results that were arrived at for the Zion 1 reactor in 3 different cases of region partition.

3.6) Results for Zion-1 in two-dimensions

Zion 1 is a modern PWR with a nominal capacity of 3250 Mw(th). The first cycle, quarter-core layout is shown in Fig. 3.13 (ref. 13). Once the fuel elements are homogenized, a quarter core, two-dimensional diffusion calculation may involve something between 2000 and 5000 unknowns per group or more, depending on the desired accuracy. In the present section, comparisons are made between CHD and PDQ-5 (ref. 2) and CITATION (ref. 15), for different mesh sizes.

PDQ-5 and CITATION are both standard diffusion-depletion codes. The first code considers the discrete points where flux is to be calculated as located at the borders of the finite difference volumes, whereas the second considers them located at the center of the volumes. This means that in the first code fluxes are calculated at material interfaces, but not so in the second code, since material properties have to be constant inside the finite difference volumes. This fact may cause the results to be slightly different for otherwise identical problems.

Three runs were made with CHD, the mesh spacing being as shown in Fig. 3.14.

Fig. 3.13 - Zion 1 first core layout.

Fig. 3.14 - Mesh arrangement for CHD runs (Zion 1)

In all the runs the baffle was implicitly accounted for as a sub-region of an overall baffle-moderator expansion element. In these cases, as has been seen earlier, current continuity across the fuel-baffle interface is expected to introduce large distortions in the flux shape. We have, therefore, uncoupled the first derivatives of the solution at all these interface points (using sets 51 or 61, whichever is appropriate).

Run 1 was made by specifying set 41 (derivative continuity) for any singular point completely surrounded by fuel elements, and 61 (first derivatives uncoupling) otherwise.

For runs 2 and 3 first derivatives were uncoupled at all appropriate points.

Results are shown in Tables 3.8 and 3.9, and in Figs. 3.15 to 3.19.

We will first draw some conclusions from Table 3.8. All CHD runs do yield k_{eff} which are less than 0.04% off the most accurate finite difference value, in general with a number of unknowns between 5 and 10 times smaller. In particular we notice that CITATION (44 x 44) yields k_{eff} less accurately than CHD with the coarsest mesh. Under the computing environment at MIT we were able to run CHD with the finest mesh at a considerably lower cost as compared to PDQ-5, in spite of the fact that CHD does not incorporate any iteration acceleration technique.

Power ratios are shown in Figs. 3.15-17, whereas in Table 3.9 some relative differences are presented. We realize first that CHD (10 x 10) is remarkably accurate when compared to PDQ-5, whereas it is up to 10% off at the corner elements when compared to CITATION (75 x 75). However, PDQ-5 is also off

Table 3.8 - Overall results for Zion 1 as evaluated through PDQ-5, CITATION and CHD with several mesh sizes.

Code	PDQ-5	CITAT.	CITAT.	CHD	CHD	CHD
# unknowns(/group (mesh)	1936 (44-44)	1936 (44-44)	5625 (75-75)	348 (10-10)	190 (7-7)	128 (6-6)
k_{eff}	1.2749	1.27313	1.27508	1.27469	1.27474	1.27554
Pointwise flux convergence (10^{-4})	4.0	4.0	4.0	1.7	1.76	1.0
Fast/thermal flux ratio (mid point)	3.835	3.922		3.820	3.820	4.16
Fast/thermal flux ratio (fuel ele- ments facing baf.)	5.133			5.191	5.181	5.183
Relative running cost (MIT condi- tions)	51			36		

	1	2	3	4	5	6	7	8
1	1.6271 1.6361 1.6524	1.7590 1.8002 1.8108	1.5320 1.5387 1.5524	1.5519 1.5856 1.5918	1.2537 1.2560 1.2623	1.1587 1.1758 1.1742	0.8039 0.7904 0.7896	0.5115 0.4954 0.4871
2		1.5800 1.5873 1.6025	1.6563 1.6051 1.7038	1.3945 1.3990 1.4087	1.3556 1.3818 1.3841	1.0372 1.0318 1.0339	0.9166 0.9230 0.9186	0.4970 0.4786 0.4705
3			1.4452 1.4490 1.4603	1.4664 1.4966 1.5023	1.1831 1.1813 1.1859	1.0779 1.0903 1.0878	0.7262 0.7092 0.7078	0.4455 0.4285 0.4206
4				1.2447 1.2439 1.2493	1.2123 1.2255 1.2257	0.9001 0.8872 0.8869	0.7216 0.7123 0.7067	0.3233 0.3013 0.2911
5					1.0777 1.0749 1.0747	0.8526 0.8401 0.8379	0.5340 0.5104 0.5019	
6						0.6682 0.6516 0.6462	0.3277 0.3042 0.2947	
7								
8								

Fig. 3.15 - Region averaged to core averaged power ratios.

KEY

CITAT.	(75 x 75)
PDQ-5	(44 x 44)
CHD	(10 x 10)

89

	ZION 1				
	1	2	3	4	5
1	1.6873 1.7069	1.5521 1.5656	1.2098 1.2138	0.8788 0.8775	0.4842 0.4756
2		1.4215 1.4300	1.0961 1.0949	0.7108 0.7032	0.3649 0.3527
3			0.8517 0.8468	0.4073 0.3961	
4					
5					

Fig. 3.16 - Region averaged to core averaged power ratios.

PDQ-5	(44 x 44)
CHD	(7 x 7)

	1	2	3	4
1	1.5343 1.5480	1.1448 1.1459	0.7828 0.7824	0.4160 0.4057
2		0.8517 0.8408	0.4073 0.3911	
3				
4				

Fig. 3.17 - Region averaged to core
averaged power ratios.

PDQ-5 (44 x 44)
CHD (6 x 6)

Table 3.9 - Relative differences of average power in expansion elements of Zion 1 as evaluated through CHD relative to PDQ-5 and CITATION.

Position (see Figs. 3.15 through 3.17)	CHD mesh	CHD off relative to (%)	
		PDQ-5 (44-44)	CITAT.(75-75)
1-1 (3.15)	10-10	+ 0.996	+ 1.555
1-1 (3.16)	7-7	+ 1.162	
1-1 (3.17)	6-6	+ 0.893	
1-8 (3.15)	10-10	- 1.675	- 4.770
1.5 (3.16)	7-7	- 1.776	
1.4 (3.17)	6-6	- 2.476	
6-7 (3.15)	10-10	- 3.123	- 10.070
3-4 (3.16)	7-7	- 2.750	
2-3 (3.17)	6-6	- 3.977	

Fig. 3.18 - Flux plots for Zion 1
as evaluated through PDQ-5 (44 x 44)
and CHD (10 x 10)

Fig. 3.19 - Flux plots for Zion 1 as evaluated through PDQ-5 (44 x 44), CHD (7 x 7) and CHD (6 x 6).

CITATION by about 7% in the worst case, so that we are lead to conclude that, very roughly, CHD (10 x 10) and PDQ-5 (44 x 44) show the same order of accuracy.

The coarser meshes CHD runs show larger differences when compared to PDQ-5. However, the very largest mesh CHD set up might provide basis for the development of reactor simulators of the FLARE type, without the inconveniences of this code.

Flux shapes are shown in Figs. 3.18 and 3.19. It is clear that the shape yielded by the smallest mesh CHD run is essentially correct with differences of the same order as those shown in Table 3.9 for the power ratios. The shape detail achieved by CHD (7 x 7) where expansion elements are defined over up to 4 fuel elements are remarkably accurate. However, when the mesh is opened still more for CHD (6 x 6) we are no longer able to follow the fine spatial oscillations of the solution.

CHAPTER IV

CONCLUSIONS AND RECOMMENDATIONS4.1) Conclusions

From the results presented in Ch. III we draw several general conclusions. We have demonstrated that it is possible to represent a multi-region reactor, in two-dimensional cartesian geometry, with a fair accuracy, using Hermite bicubic polynomials expansion on a coarse mesh partition equivalent to a PWR fuel element. The resultant system of equations requires at least 5 times fewer unknowns, for equivalent accuracy, than a system based on the finite difference method, and thus offers the potential of faster codes. These conclusions are drawn from Sec. 3.1 where EXTERMINATOR 2 is compared with CHD for a 4-composition problem, and from Sec. 3.6 (case 1) where PDQ-5 and CITATION are compared with CHD for the Zion 1 reactor. In particular for this latter case we state the following numerical results:

a) CHD yields k_{eff} which is 0.03% off a value obtained with a very fine finite difference mesh (CITATION) using 15 times more unknowns.

b) CHD yields fuel element averaged fission rates which are 1% and 3.2% (for the innermost and an outside element, respectively) off the values predicted by PDQ-5 using 6 times more unknowns.

We have further shown that it is possible to define expansion elements over regions with varying cross sections, by implicitly accounting for the variation in the construction of the coefficient matrices. This conclusion is drawn from Secs. 3.4 and 3.5, where

some convenient small two-dimensional problems are investigated, and from Sec. 3.6 (cases 1, 2 and 3), where PDQ-5 and CITATION results are compared to coarse mesh CHD results for the Zion 1 reactor. In particular we state the following results.

a) The core baffle of a PWR can be accounted for by implicitly treating it as a sub-region of an overall expansion region incorporating baffle and the nearby reflector. The baffle's influence on the core can be well accounted for in this way, the pointwise flux distribution in the nearby fuel elements being remarkably accurate.

b) The definition of one expansion element over 4 fuel elements in some regions yields very accurate results both in pointwise flux distributions and in overall reactor characteristics. With a number of unknowns 10 times smaller CHD was able to follow very closely pointwise flux distributions obtained with PDQ-5; further, region-averaged fission rates were less than 3% off and k_{eff} was less than 0.03% off the most accurate value.

c) Very coarse meshes (up to 16 fuel elements) are feasible for PWR's. The results are reasonably accurate (k_{eff} less than 0.04% off the most accurate value) and the number of unknowns is remarkably small (128 per group for the Zion 1 reactor on a quarter core symmetry).

In all cases the differences in material properties were close to what one would find in real reactors. In particular we have used actual Zion 1, homogenized cross sections (see App. A) whenever the Zion 1 reactor was represented.

All these results seem to indicate that it is possible to

build a few-group, three-dimensional, reflected reactor simulator of the FLARE type without any of the inconveniences of present nodal methods.

4.2) Recommendations

Problems that should be investigated following this thesis are:

- a) Acceleration of convergence through Chebyshev polynomials.
- b) Desirability and feasibility of using different mesh sizes for the thermal and fast groups.

- c) Mesh lines that do not extend over the whole problem domain (call it virtual mesh lines and virtual mesh points).

Assume a mesh as shown in Fig. 4.1.

Fig. 4.1 - Regular and virtual mesh lines and points in two dimensions

Points (11), (21), ..., (44) are part of a regular mesh. The virtual point K can be incorporated into the mesh structure without extending lines JL and GO throughout the domain. To achieve this we define the following expansion functions:

<u>Point</u>	<u>Interval of definition</u>
N	RSTPOKJFEMR
J	FGKONJF
F	AEMNJKGHCBA
K	NOPLHGFJN

If we want to preserve continuities across point J (for instance) we assume the corresponding unknowns to be determined by conditions at N and F. In other words, we make

$$\begin{aligned}\phi(J_x^-) &= \phi(J_x^+) \\ \partial\phi/\partial x(J^-) &= \partial\phi/\partial x(J^+)\end{aligned}$$

d) Zero flux boundaries which are not straight lines but which follow the core shape.

e) Determination of the maximum size of matrices that can be handled with a Cholesky factorization for normal problems.

f) When these questions are answered it will probably be worthwhile to develop a coarse mesh reactor simulator using the general setup shown in Sec. 3.6 (case 2 or 3), still with a direct inversion in the in-group solutions.

REFERENCES

- 1) A. F. Henry; Nuclear Reactor Physics II, MIT Lecture Notes; Spring, 1971.
- 2) L. A. Hageman, C. J. Pfeifer; The Utilization of the Neutron Diffusion Program PDQ-5; WAPD-TM-395; January, 1965.
- 3) W. R. Cadwell; PDQ-7 Reference Manual; WAPD-TM-678; January, 1967
- 4) Richard S. Varga; Matrix Iterative Analysis, Sec. 6.3; Prentice-Hall inc.; 1962.
- 5) D. L. Delp, et al.; FLARE - A Three - Dimensional Boiling Water Simulator; GEAP-4598; July, 1964.
- 6) K. F. Hansen, C. M. Kang; Finite Element Methods in Reactor Physics Analysis; to be published in Advances in Nuclear Science and Technology.
- 7) Chang Mu Kang, K. F. Hansen; Finite Element Methods for Space - Time Reactor Analysis; U.S.AEC Report MIT - 3903 - 5, November, 1971.

Also appears as:

Chang Mu Kang; ScD Thesis, Nuclear Engineering Department, MIT; November, 1971.
- 8) H. G. Kaper, G. K. Leaf, A. J. Lindeman; Applications of Finite Element Methods in Reactor Mathematics. Numerical Solution of the Neutron Diffusion Equation; ANL-7925; February, 1972.
- 9) L. A. Semenza, E. E. Lewis, E. C. Rossow; The Application of the Finite Element Method to the Multigroup Neutron Diffusion Equation; Nucl. Sci. Eng., 47, 302-310 (1972).
- 10) Patrick G. Bailey, A. F. Henry; Variational Derivation of Modal-Nodal Finite Difference Equations in Spatial Reactor Physics; U.S.AEC Report COO-3052-5; July, 1972.
- 11) L. A. Hageman; Numerical Methods and Techniques Used in the Two-Dimensional Neutron Diffusion Program PDQ-5; WAPD-TM-364; February, 1963.

- 12) V. N. Faddeeva; Computational Methods of Linear Algebra; Dower Publications, Inc.; New York; 1959.
- 13) Terrance A. Rieck; The Engineering Feasibility and Fuel Cost Analysis of Variable Nuclear Refueling Intervals; PhD Thesis in progress, Nuclear Engineering Dpt., MIT.
- 14) T. B. Fowler, M. L. Tobias, D. R. Vondy; EXTERMINATOR 2 - a Fortran IV Code for Solving Multigroup Neutron Diffusion Equations in Two Dimensions; ORNL 4078; April, 1967.
- 15) T. B. Fowler, D. R. Vondy, G. W. Cunningham; Nuclear Reactor Core Analysis Code: CITATION; ORNL-TM-2496, Rev. 2; July, 1969.

MACROSCOPIC CROSS SECTIONSGroup 1
Group 2

Compo- sition	D(cm)	$\Sigma_r(\text{cm}^{-1})$	$v\Sigma_f(\text{cm}^{-1})$	$\Sigma_s(\text{cm}^{-1})$ ($k \rightarrow k+1$)	Comments
1	1.20 0.15	0.101 0.020	0.0 0.0	0.1	C.M.Kang (water)
2	1.5 0.4	0.0623 0.2	0.0 0.218	0.06	C.M.Kang (fuel)
2A	1.55 0.4133	0.0623 0.25	0.0 0.218	0.06	
2B	1.60 0.4267	0.0623 0.30	0.0 0.218	0.06	
2C	1.65 0.44	0.0623 0.35	0.0 0.218	0.06	
3	1.02130 0.33548	0.00322 0.14596	0.0 0.0	0.0	Zion 1 (core baffle)
5	1.63 0.275	0.0383 0.0108	0.0 0.0	0.0380	Water
6	1.399 0.387	0.0261 0.0832	0.00659 0.129	0.0168	Fuel (high enrich.)
7	1.397 0.389	0.0260 0.071	0.00553 0.102	0.0172	Fuel (medium enrich.)
8	1.397 0.388	0.0259 0.0532	0.00485 0.0636	0.0179	Fuel (low enrich.)
11	1.41760 0.37335	0.02597 0.06669	0.00536 0.10433	0.01742	Zion 1 (2.25 %)
12	1.41970 0.37370	0.02576 0.07606	0.00601 0.12472	0.01694	Zion 1 (2.8 %)
13	1.42650 0.37424	0.02560 0.08359	0.00653 0.14120	0.01658	Zion 1 (3.3 %)
14	1.38377 0.29745	0.025164 0.032006	0.0 0.0	0.024241	16.5 % SS + 83.5 % water
15	1.45540 0.28994	0.02950 0.00949	0.0 0.0	0.02903	Zion 1 (water)

APPENDIX B

INNER PRODUCTS BETWEEN FINE LIMITSFOR CUBIC HERMITE POLYNOMIALS

$$h_- \equiv x_1 - x_{1-1}$$

$$h_+ \equiv x_{1+1} - x_1$$

$$x_2 > x_1$$

$$(x)^k \equiv (x_2^k - x_1^k)$$

$$(h-x)^k \equiv [(h-x_2)^k - (h-x_1)^k]$$

$$(u_1^{0-}, u_{1-1}^{0+})_{x_1}^{x_2} \equiv \int_{x_1}^{x_2} u_1^{0-}(x) u_{1-1}^{0+}(x) dx =$$

$$= -\frac{4}{7} h_-^{-6} (x)^7 + 2h_-^{-5} (x)^6 - \frac{9}{5} h_-^{-4} (x)^5 \\ - \frac{1}{2} h_-^{-3} (x)^4 + h_-^{-2} (x)^3$$

$$(u_1^{0-}, u_{1-1}^{0-})_{x_1}^{x_2} = \frac{4}{7} h_-^{-6} (x)^7 - 2h_-^{-5} (x)^6 + \frac{9}{5} h_-^{-4} (x)^5$$

$$(u_1^{0+}, u_{1+1}^{0-})_{x_1}^{x_2} = -\frac{4}{7} h_+^{-6} (x)^7 + 2h_+^{-5} (x)^6 - \frac{9}{5} h_+^{-4} (x)^5$$

$$- \frac{1}{2} h_+^{-3} (x)^4 + h_+^{-2} (x)^3$$

$$(u_1^{0+}, u_{1+1}^{0+})_{x_1}^{x_2} = -\frac{4}{7} h_+^{-6} (h_+-x)^7 + 2h_+^{-5} (h_+-x)^6 - \frac{9}{5} h_+^{-4} (h_+-x)^5$$

$$(u_{i-1}^{0-}, u_{i-1}^{1+})_{x_1}^{x_2} = -\frac{2}{7} h_-^{-5} (x)^7 + \frac{7}{6} h_-^{-4} (x)^6 - \frac{8}{5} h_-^{-3} (x)^5 + \frac{3}{4} h_-^{-2} (x)^4$$

$$(u_i^{1+}, u_{i+1}^{0-})_{x_1}^{x_2} = -\frac{2}{7} h_+^{-5} (x)^7 + \frac{7}{6} h_+^{-4} (x)^6 - \frac{8}{5} h_+^{-3} (x)^5 + \frac{3}{4} h_+^{-2} (x)^4$$

$$(u_i^{0+}, u_{i+1}^{1-})_{x_1}^{x_2} = \frac{2}{7} h_+^{-5} (x)^7 - \frac{5}{6} h_+^{-4} (x)^6 + \frac{3}{5} h_+^{-3} (x)^5 + \frac{1}{4} h_+^{-2} (x)^4 - \frac{1}{3} h_+^{-1} (x)^3$$

$$(u_i^{1-}, u_{i-1}^{0+})_{x_1}^{x_2} = \frac{2}{7} h_-^{-5} (x)^7 - \frac{5}{6} h_-^{-4} (x)^6 + \frac{3}{5} h_-^{-3} (x)^5 + \frac{1}{4} h_-^{-2} (x)^4 - \frac{1}{3} h_-^{-1} (x)^3$$

$$(u_i^{0-}, u_i^{1-})_{x_1}^{x_2} = -\frac{2}{7} h_-^{-5} (x)^7 + \frac{5}{6} h_-^{-4} (x)^6 - \frac{3}{5} h_-^{-3} (x)^5$$

$$(u_i^{1-}, u_i^{0-})_{x_1}^{x_2} = (u_i^{0-}, u_i^{1-})_{x_1}^{x_2}$$

$$(u_i^{0+}, u_i^{1+})_{x_1}^{x_2} = -\frac{2}{7} h_+^{-5} (h_+ - x)^7 + \frac{5}{6} h_+^{-4} (h_+ - x)^6 - \frac{3}{5} h_+^{-3} (h_+ - x)^5$$

$$(u_i^{1+}, u_i^{0+})_{x_1}^{x_2} = (u_i^{0+}, u_i^{1+})_{x_1}^{x_2}$$

$$(u_1^{1-}, u_{1-1}^{1+})_{x_1}^{x_2} = \frac{1}{7} h_-^{-4} (x)^7 - \frac{1}{2} h_-^{-3} (x)^6 + \frac{3}{5} h_-^{-2} (x)^5 - \frac{1}{4} h_-^{-1} (x)^4$$

$$(u_1^{1+}, u_{1+1}^{1-})_{x_1}^{x_2} = \frac{1}{7} h_+^{-4} (x)^7 - \frac{1}{2} h_+^{-3} (x)^6 + \frac{3}{5} h_+^{-2} (x)^5 - \frac{1}{4} h_+^{-1} (x)^4$$

$$(u_1^{1-}, u_1^{1-})_{x_1}^{x_2} = \frac{1}{7} h_-^{-4} (x)^7 - \frac{1}{3} h_-^{-3} (x)^6 + \frac{1}{5} h_-^{-2} (x)^5$$

$$(u_1^{1+}, u_1^{1+})_{x_1}^{x_2} = -\frac{1}{7} h_+^{-4} (h_+ - x)^7 + \frac{1}{3} h_+^{-3} (h_+ - x)^6 - \frac{1}{5} h_+^{-2} (h_+ - x)^5$$

$$\begin{aligned} \left(\frac{d}{dx} u_1^{0-}, \frac{d}{dx} u_{1-1}^{0+} \right)_{x_1}^{x_2} &= \int_{x_1}^{x_2} \frac{d}{dx} u_1^{0-} (x) \frac{d}{dx} u_{1-1}^{0+} (x) dx = \\ &= -\frac{36}{5} h_-^{-6} (x)^5 + 18 h_-^{-5} (x)^4 - 12 h_-^{-4} (x)^3 \end{aligned}$$

$$\left(\frac{d}{dx} u_1^{0+}, \frac{d}{dx} u_{1+1}^{0-} \right)_{x_1}^{x_2} = -\frac{36}{5} h_+^{-6} (x)^5 + 18 h_+^{-5} (x)^4 - 12 h_+^{-4} (x)^3$$

$$\left(\frac{d}{dx} u_1^{0-}, \frac{d}{dx} u_1^{0-} \right)_{x_1}^{x_2} = \frac{36}{5} h_-^{-6} (x)^5 - 18 h_-^{-5} (x)^4 + 12 h_-^{-4} (x)^3$$

$$\left(\frac{d}{dx} u_1^{0+}, \frac{d}{dx} u_1^{0+} \right)_{x_1}^{x_2} = -\frac{36}{5} h_+^{-6} (h_+ - x)^5 + 18 h_+^{-5} (h_+ - x)^4 - 12 h_+^{-4} (h_+ - x)^3$$

$$\left(\frac{d}{dx} u_1^{1-}, \frac{d}{dx} u_{1-1}^{0+}\right)_{x_1}^{x_2} = \frac{18}{5} h_-^{-5} (x)^5 - \frac{15}{2} h_-^{-4} (x)^4 + 4h_-^{-3} (x)^3$$

$$\left(\frac{d}{dx} u_1^{0+}, \frac{d}{dx} u_{1+1}^{1-}\right)_{x_1}^{x_2} = \frac{18}{5} h_+^{-5} (x)^5 - \frac{15}{2} h_+^{-4} (x)^4 + 4h_+^{-3} (x)^3$$

$$\left(\frac{d}{dx} u_1^{1+}, \frac{d}{dx} u_1^{0+}\right)_{x_1}^{x_2} = -\frac{18}{5} h_+^{-5} (h_+-x)^5 + \frac{15}{2} h_+^{-4} (h_+-x)^4 - 4h_+^{-3} (h_+-x)^3$$

$$\left(\frac{d}{dx} u_1^{0+}, \frac{d}{dx} u_1^{1+}\right)_{x_1}^{x_2} = \left(\frac{d}{dx} u_1^{1+}, \frac{d}{dx} u_1^{0+}\right)_{x_1}^{x_2}$$

$$\left(\frac{d}{dx} u_1^{1-}, \frac{d}{dx} u_1^{0-}\right)_{x_1}^{x_2} = -\frac{18}{5} h_-^{-5} (x)^5 + \frac{15}{2} h_-^{-4} (x)^4 - 4h_-^{-3} (x)^3$$

$$\left(\frac{d}{dx} u_1^{0-}, \frac{d}{dx} u_1^{1-}\right)_{x_1}^{x_2} = \left(\frac{d}{dx} u_1^{1-}, \frac{d}{dx} u_1^{0-}\right)_{x_1}^{x_2}$$

$$\begin{aligned} \left(\frac{d}{dx} u_1^{1+}, \frac{d}{dx} u_{1+1}^{0-}\right)_{x_1}^{x_2} = & -\frac{18}{5} h_+^{-5} (x)^5 + \frac{21}{2} h_+^{-4} (x)^4 - 10 h_+^{-3} (x)^3 + \\ & 3h_+^{-2} (x)^2 \end{aligned}$$

$$\begin{aligned} \left(\frac{d}{dx} u_1^{0-}, \frac{d}{dx} u_{1-1}^{1+}\right)_{x_1}^{x_2} = & -\frac{18}{5} h_-^{-5} (x)^5 + \frac{21}{5} h_-^{-4} (x)^4 - 10 h_-^{-3} \\ & (x)^3 + 3h_-^{-2} (x)^2 \end{aligned}$$

$$\left(\frac{d}{dx} u_1^{1-}, \frac{d}{dx} u_{1-1}^{1+}\right)_{x_1}^{x_2} = \frac{9}{5} h_-^{-4} (x)^5 - \frac{9}{2} h_-^{-3} (x)^4 + \frac{11}{3} h_-^{-2} (x)^3 - h_-^{-1} (x)^2$$

$$\left(\frac{d}{dx} u_1^{1+}, \frac{d}{dx} u_{1+1}^{1-}\right)_{x_1}^{x_2} = \frac{9}{5} h_+^{-4} (x)^5 - \frac{9}{2} h_+^{-3} (x)^4 + \frac{11}{3} h_+^{-2} (x)^3 - h_+^{-1} (x)^2$$

$$\left(\frac{d}{dx} u_1^{1-}, \frac{d}{dx} u_1^{1-}\right)_{x_1}^{x_2} = \frac{9}{5} h_+^{-4} (x)^5 - 3 h_-^{-3} (x)^4 + \frac{4}{3} h_-^{-2} (x)^3$$

$$\left(\frac{d}{dx} u_1^{1+}, \frac{d}{dx} u_1^{1+}\right)_{x_1}^{x_2} = -\frac{9}{5} h_+^{-4} (h_+ - x)^5 + 3 h_+^{-3} (h_- - x)^4 - \frac{4}{3} h_+^{-2} (h_- - x)^3$$

APPENDIX C

THE CODE CHDC.1) General description

CHD (Cubic Hermite Diffusion) solves the multigroup diffusion equations in a two-dimensional, rectangular geometry by expanding piecewisely the unknown solutions in bicubic Hermite polynomials and using the Galerkin method to arrive at a discrete formulation. The resulting equations are uncoupled through the power iteration method, and the in-group solutions are achieved by direct inversion (Cholesky factorization).

When the solution is converged several output options are available: fine flux expansion inside the coarse mesh, cross sections averaging, reaction rates and average fluxes calculations. All these outputs are normalized to an specified overall fission rate.

In Fig. C.1 we show the general code logic.

The variable dimensioning techniques available in Fortran IV are used in CHD. Practically all dimensioned variables are stored in a general, one-dimensional array called A and dimensioned in a small main program.

A rectangular coarse mesh partition of the problem domain is assumed. At each point CHD will construct the appropriate set of bicubic basis functions depending on several conditions such as boundary conditions, user specification, or neighboring regions characteristics. Current continuity is imposed where appropriate.

Fig. C.1 - CHD basic logic

The coordinate system orientation shown in Fig. C.2 is assumed by CHD.

Fig. C.2 - Coordinate system orientation assumed by CHD.

The minimum number of rows or columns allowed is 2, and a column or a row has to be specified at each boundary. Only convex regions are allowed so that the problem domain is always a full rectangle. Zero flux and zero current boundaries are allowed.

The ordering of the unknowns is assumed to be done in the following way:

- 1) All rows
- 2) All columns
- 3) All unknowns at each point

Unknowns at each point are assumed to be ordered as shown below:

- 1.1) Flux
- 1.2) Current in X direction or

[	<ol style="list-style-type: none"> 1.2.1) Current in negative X direction. 1.2.2) Current in positive X direction.
---	--

- 1.3) Current in Y direction or
- 1.3.1) Current in negative Y direction.
 - 1.3.2) Current in positive Y direction.

1.4) Mixed derivative.

At each corner point one will have 1 unknown, at each non-corner boundary point 2 or 3, and in each internal point 4, 5 or 6.

Any number of energy groups greater than, or equal to, 2 may be specified. As restrictions, however, all fissions will lead to neutrons being born in the highest energy group and any outscattering will lead to the group immediately below. Groups are numbered beginning with the highest energy one.

Next we present a summary of the main features of the subroutines.

MAIN: The size of the one-dimensional array A has to be specified according to the following minimum value (see definition of variables in input description).

$$\begin{aligned}
 M(\min) = & LMAX (6 \text{ KGROUP} + 1.5) + 1.5 \text{ LXMAX} \\
 & + \text{LXCMA}X (2 \text{ KGROUP} + 0.5) \\
 & + \text{LXFMA}X (2 \text{ KGROUP} - 1.5) + \text{JMA}X (4 \text{ KGROUP} - 1) \\
 & + \text{JVMA}X (\text{NVN} * \text{MVM} / 2 + \text{NVN} + \text{MVM} + 1) \\
 & + \text{NROW} * \text{MCO}L (\text{KGROUP} + 7) \\
 & + (\text{NROW} + \text{MCO}L) / 2 + 7 \text{ KGROUP} + 4
 \end{aligned}
 \tag{C.1}$$

Neglect any fraction.

The statement

$\text{MSIZE} = M$

should also be set to this value.

We next show some values for variables that were arrived at for problems shown in the thesis in order to provide for some insight.

Table C.1 Some Variable Values

<u>Problems</u>	<u>LMAX</u>	<u>LXMAX</u>	<u>LXCMAx</u>	<u>LXFMAx</u>	<u>M Size (mim.)</u>
Ref. A. sec. 3.4	104	1350	2291	2596	20632
Case 1, sec. 3.4	18	123	145	228	1955
Ref, sec. 3.5	146	2019	3770	3892	33912
Case 3, sec.3.1	72	844	1344	1616	
Zion 1 (6x6)	128	1558	3183	2988	26496
(7x7)	190	2443	5775	4696	44626
(10x10)	348	5223	13814	10098	100945

The CHD object deck requires approximately 106 k bytes, and about all arrays are stored in MSIZE. Thus, the amount of fast core required is, approximately

$$\text{Fast core (bytes)} = \text{MSIZE} * 4 + 106000$$

PREP: Is the preparation and program control subroutine.

- a) Reads almost all data
- b) Calculates number of bicubic functions at each point, normalization factor θ where necessary, imposes boundary conditions at the expansion functions where appropriate, and orders the unknowns.

COEFF: Sweeps through all the unknowns and at each one sets up all the unknowns which will couple with the first one. Then calls MATRIX and sets up one-dimensional (in each group) arrays in which the non-zero elements of all coefficient matrices will be stored. If the matrix is symmetric only the lower diagonal part is stored.

MATRIX: Performs the actual calculations of the coefficients with use of the following functions:

XF - bicubic basis functions inner products over the whole range of the element.

XD - derivative of basis functions inner products over the whole range of the element.

These inner products are listed in Ref. 7 App. B.

XFV - bicubic basis functions inner products over partial intervals of the element.

XDV - derivative of bicubic basis functions inner products, over partial intervals of the element.

The formulae for these last inner products are given in App. B of this thesis.

CHLSKY: Calculates the lower triangular matrices corresponding to the Cholesky factorization.

OUTIT: Reads initial flux guess (if any), iterates according to the power iteration method and inverts the in-group matrices using the factorized Cholesky matrices.

EXPAN: Normalizes the solution to an specified fission rate, calculates region-wise reaction rates and average fluxes. These calculations can only be done over each element, there being no provision for specifying an output region over more than one mesh.

Reaction rates are defined as

$$\text{ABSRP} = \sum_{K=1}^{KG-1} \int_V (\Sigma_r(K, \underline{r}) - \Sigma_s(K, \underline{r})\phi(K, \underline{r})) d\underline{r} \\ + \int_V \Sigma_r(KG, \underline{r})\phi(KG, \underline{r}) d\underline{r}$$

$$\text{TRNSP} = \sum_{K=1}^{KG} \int_V (1/D(K, \underline{r})\phi(K, \underline{r})) d\underline{r}$$

Where $KG \equiv \text{KGROUP}$

A collapsed macroscopic cross section is defined as

$$\bar{\Sigma}(K, V) = \frac{\int_V \Sigma(K, \underline{r})\phi(K, \underline{r}) d\underline{r}}{\bar{\phi}(K, V)V}$$

with the average flux defined as

$$\bar{\phi}(K, V) = \frac{\int_V \phi(K, \underline{r}) d\underline{r}}{V}$$

The collapsed diffusion coefficient is defined as

$$[\bar{D}(K, V)]^{-1} = \frac{\int_V (1/D(K, \underline{r})\phi(K, \underline{r})) d\underline{r}}{\bar{\phi}(K, V)V}$$

CALC: Calculates the fine flux distribution at equally spaced points inside the coarse mesh.

All XPRINT sub-routines do just printing, except EPRINT where the region-wise collapsed cross sections are calculated.

C.2) Input Preparation

Statements 1 and 2 in MAIN

Set dimension of A and value of MSIZE to M or more, according to Eq. (C.1).

Card 1 - Format I5

NRUN - Number of cases to be performed. Every case will require the input of all the data, sequentially.

Card 2 - 14I5

NROW - number of rows (including boundary)

MCOL - number of columns (including boundary)

KGROUP - number of groups

JMAX - number of different material compositions to be read in.

(*,**) LMAX - number of unknowns per group

(*,**) LXMAX - size of the one-dimensional array where the lower triangular part of matrix F1 is stored (see text).

(*,**) LMCMAX - size of the one-dimensional array (in each group) where the lower triangular part of the Cholesky matrices will be stored (see text).

(*,**) LMFMAX - size of the one-dimensional arrays (in each group) where the F(2)...F(KGROUP) and S(1)...S(KGROUP-1) matrices will be stored (see text).

JVMAX - number of regions with varying parameters to be specified.

(*) NVN - maximum number of internal rows specified for any of the JVMAX regions.

(*) MVM - maximum number of internal columns specified for any of the JVMAX regions.

(*) Values used just for dimensioning purposes at this stage.
 (**) Actual values are printed.

CHD will not begin any operation and will print an error message if the required value for M is less than specified in MSIZE.

If no variable parameter region is to be specified, JVMAX, NVN and MVM should be input as zero.

Card 3 - 16I5

NCONV - maximum number of outer iterations allowed.

If this number is reached without convergence, the calculation is terminated with all output.

ICMAX - (=0) - no fine flux is to be calculated inside the coarse meshes.

(<0) - fine flux is calculated at all meshes at (-ICMAX) equally spaced **internal** points.

(>0) - user will specify ICMAX sets where he wants the fine flux to be calculated. In this case, cards 22 have to be specified, and flux at remaining meshes will be calculated at 5 equally spaced internal points.

NP - (≤ 0) - no initial guess of the solution is to be input. Code will start with flat flux at all points except at a boundary with a zero flux boundary condition.

(≥ 0) - user will provide an initial solution guess. Cards 21 have to be input.

IOUT - (< 0) - user does not want the solution punched out.

(≥ 0) - user wants solution to be punched out in Format 6E12.5.

ICLPS - (< 0) - code will collapse all cross sections at all regions with varying parameters.

(≥ 0) - user will specify ICLPS regions where he wants the cross sections to be collapsed. Cards 23 have to be input.

The collapsing has only sense over regions with varying parameters, obviously.

Card 4 - 8E10.8

BL - left boundary condition (1.0 - zero derivative; 0.0 zero flux).

BR - right boundary condition.

BT - top boundary condition

BB - bottom boundary condition.

Card 5-8E10.5

EPSCH - Cholesky rejection criterion. Code will reject any value less than EPSCH in the calculation of the Cholesky matrices.

EPSF - Solution convergence criterion

EPSL - Eigenvalue convergence criterion.

CHD will assume the problem as converged when

$$\frac{\left| \left\| \underline{a}^{(t-1)} \right\|_{\infty} - \left\| \underline{a}^{(t)} \right\|_{\infty} \right|}{\left\| \underline{a}^{(t-1)} \right\|_{\infty}} < \text{EPSF}$$

and

$$\frac{|\lambda^{(t-1)} - \lambda^{(t)}|}{\lambda^{(t-1)}} < \text{EPSL}$$

Cards 6 - 3I5

Through cards 6 the user is able to specify the number and type of the expansion functions he wants at each mesh point, with the few exceptions listed below. In each card one point is specified as:

N - row number

M - column number

IPP - any allowed expansion function option (40,50, 60,41,51,61,421 and 422).

CHD reads type-6 cards until a blank field I5 is found.

If the user wants the code to use its default options (probably a good option when first running a problem) he should input just one blank card.

Expansion Functions Option Definition

The first digit of the option will specify the number of expansion functions at the particular point. The third and/or second digits will specify the type of continuity assumed.

In Table C.1 we show all the allowed options.

Table C.2 - Expansion Functions Option Definition

SET	Continuity Condition for			
	Flux	First derivative in X direction	First derivative in Y direction	Mixed derivative
40	Yes	$\partial / \partial x$	$\partial / \partial y$	$\partial^2 / \partial x \partial y$
41	Yes	$\partial / \partial x$	$\partial / \partial y$	$(\theta/D)(\partial^2 / \partial x \partial y)$
421	Yes	$(\theta/D)(\partial / \partial x)$	$\partial / \partial y$	$(\theta/D)(\partial^2 / \partial x \partial y)$
422	Yes	$\partial / \partial x$	$(\theta/D)(\partial / \partial y)$	$(\theta/D)(\partial^2 / \partial x \partial y)$
50	Yes	Open	∂ / ∂	$\partial^2 / \partial x \partial y$
		$\partial / \partial x$	Open	
51	Yes	Open	$\partial / \partial y$	$(\theta/D)(\partial^2 / \partial x \partial y)$
		$\partial / \partial x$	Open	
60	Yes	Open	Open	$\partial^2 / \partial x \partial y$
61	Yes	Open	Open	$(\theta/D)(\partial^2 / \partial x \partial y)$

In options 50 and 51 the code will decide in which direction the opening should be performed.

Input options which are not allowed

a) Corner points should not be specified because there is no reason for doing so. The code will always assume a 40 set, afterwards neglecting 3 of the 4 functions depending on the boundary conditions.

b) At the remaining boundary points no 60 or 61 sets should be specified because they are equivalent to 50 and 51 sets, respectively, in these cases. The latter should be used.

c) When inputting 421 or 422 options at boundary points the user should be careful in specifying the direction of the bending (defined by the last digit, 1 - x direction, 2 - y direction). If a mistake is made the code will use its default option.

Defaults

The code will use the diffusion coefficients in the immediate surroundings of a point to evaluate its characteristics. In Fig. C.3 we show a general arrangement around a point.

Table C.3 Default sets for expansion functions

Condition		Default set
$D_1 = D_2 = D_3 = D_4$		40
$D_1 = D_4$ $D_2 = D_3$ $D_1 \neq D_2$	$D_I(\underline{r}) = D_{IV}(\underline{r}) = \text{const.}$ and $D_{II}(\underline{r}) = D_{III}(\underline{r}) = \text{const.}$	422
	Otherwise	51 (with uncoupling in X direction).
$D_1 = D_2$ $D_3 = D_4$ $D_1 \neq D_3$	$D_I(\underline{r}) = D_{II}(\underline{r}) = \text{const.}$ and $D_{III}(\underline{r}) = D_{IV}(\underline{r}) = \text{const.}$	421
	Otherwise	51 (with uncoupling in Y direction)
$D_1 D_2 \neq D_3 D_4$	$D_I(\underline{r})$ and $D_{II}(\underline{r})$ and $D_{III}(\underline{r})$ and $D_{IV}(\underline{r})$ are constant	41
	Otherwise	61

Card 7 - 8E10.8

XNORM - Overall fission rate to which all output
will be normalized.

Card 8 - 8E10.8

XI(K), K = 1, KGROUP

- Neutron emission per fission in group K.

These values will be used only to calculate the fission rate
in the normalization process.

Card 9 - I5

J - Composition number.

Card 10 - 8E10.8

DI(K,J), K = 1, KGROUP

- diffusion coefficient (cm) for group K and composition
J.

Card 11 - 8E10.8

SR(K,J), K = 1, KGROUP

- removal cross section (/cm)

Card 12 - 8E10.8

SF(K,J), K = 1, KGROUP

- fission production cross section $\nu\Sigma_f$ (/cm)

Card 13 - 8E10.8

ST(K,J), K = 1, GROUP

- Outscattering cross section (/cm) from group K to
K+1.

JMAX sets of cards 9 through 13 are expected.

Card 20

JCV (J,NV,MV), MV = 1, (MVMAX (J) + 1)

Composition number of sub-region (NV,MV) of region J.

(NVMAX(J) + 1) Cards 20 are expected.

JVMAX sets of cards 17 through 20 are expected.

Cards 21 - 6E12.5 (only present if NP>0)

Y(K,L), L = 1, LMAX

KGROUP sets of cards 21 are expected.

Cards 22 - 14I5 (only present if ICMAX>0)

ISTR (JJ) - number of internal equally spaced sub-rows
to be considered in region JJ.

ISTC (JJ) - number of internal equally spaced sub-columns
to be considered in region JJ.

MINR (JJ) - row identification of region JJ.

MINC (JJ) - column identification of region JJ.

KC (JJ) - energy group.

ICMAX cards 22 are expected.

Cards 23 - 14I5 (only present if ICLPS>0)

N - row identification of region where cross sections
collapsing is to be done.

M - column identification of region where cross sections
collapsing is to be done.

Card 14 - 8E10.8

HN(N), N = 1, (NROW-1)

- mesh spacing in X direction.

Card 15 - 8E10.8

HM(M), M = 1, (MCOL-1)

- mesh spacing in Y direction.

Card 16 - 16I5

JC(N,M), M = 1, (MCOL-1)

- composition characteristics of region N,M.

(<0) - code assumes a region with constant properties
and corresponding to composition (-JC)

(>0) - code assumes a region with varying properties; the
region JC will be specified in cards 17 through 20.

(NROW-1) cards 16 are expected.

Cards 17 through 20 are not required if JVMAX = 0 and NVN = 0and MVM = 0.Card 17 - 3I5

J - region with varying parameters.

NVMAX(J) - number of sub-rows in region J.

MVMAX(J) - number of sub-columns in region J.

Card 18 - 8E10.8

HNV (J,NV), NV = 1, (NVMAX(J) + 1)

- Row sub-mesh.

Card 19 - 8E10.8

HMV (J,MV), MV = 1, (MVMAX(J) + 1)

- Column sub-mesh.