THE FINITE ELEMENT METHOD
APPLIED TO
NEUTRON DIFFUSION PROBLEMS

by

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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

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BIOGRAPHICAL NOTE

The outhor, Lothario Olavo Deppe, was born on September 3, 1940 in Nova Petrópolis, state of Rio Grande do Sul, Brazil. He 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 Pesquizas 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.

The author is married to the former Alzira Soares Lourenço and has a son.

CHAPTER I

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 pratical 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_l.

$$\Omega = \bigcup_{l=1}^{L} \Omega_l$$

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

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

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

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

$$-\underline{\nabla}\cdot D(\underline{r},E)\underline{\nabla}\phi(\underline{r},E) + \Sigma_t(\underline{r},E)\phi(\underline{r},E)$$

$$= \int_\xi dE'\ \Sigma_s(\underline{r},E'\to E)\phi(\underline{r},E') + \frac{\chi(E)}{\lambda}\int_\xi dE'\,\nu\Sigma_f(\underline{r},E')\phi(\underline{r},E') \qquad (1.1.a)$$

We will impose any of the following homogeneous boundary conditions:

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

$$\text{or } \frac{\partial}{\partial \underline{n}}\ \phi(\underline{r},E) = 0 \qquad \text{for } E \in \xi \text{ and } \underline{r} \in \partial_e\Omega \qquad (1.1.b)$$

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

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

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

$$\text{for } E \in \xi \text{ and } \underline{r} \in \partial_i\Omega \qquad (1.1.c)$$

The symbols have the following meaning:

$\underline{r}$ - generalized spatial variable

E - energy variable

$\phi(\underline{r},E)$ - scalar neutron flux (/cm^2.s)

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

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

$\Sigma_s(\underline{r},E' \to E)$ - 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)

$\lambda = 1/k_{eff}$ - 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 $d\underline{r}$ about $\underline{r}$ 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 ($\varepsilon_1,\ldots,\varepsilon_G$) of contiguous subdomains and builds up a coupled set of differential equations resulting from the balance condition applied to each subdomain, or energy group.

$$A_1\phi_1 = -\underline{\nabla}\cdot D_1\underline{\nabla}\phi_1 + \Sigma_{r1}\phi_1 = \frac{1}{\lambda}\sum_{g=1}^{G}\nu\Sigma_{fg}\phi_g$$

$$A_2\phi_2 = -\underline{\nabla}\cdot D_2\underline{\nabla}\phi_2 + \Sigma_{r2}\phi_2 = \Sigma_{s1}\phi_1$$

$$A_G\phi_G = -\underline{\nabla}\cdot D_G\underline{\nabla}\phi_G + \Sigma_{rG}\phi_G = \Sigma_{s(G-1)}\,\phi_{G-1} \qquad (1.2)$$

Where the spatial variable $\underline{r}$ 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 multidimensional 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_l, the collection of interfaces $\partial_i\Omega$ 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:

$$-\underline{\nabla}^2 \phi = L\phi = f \qquad (1.3)$$

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

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

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

An integration by parts yields

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

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

$$(\underline{\nabla}\phi, \underline{\nabla}u) - (u,f) = 0 \qquad (1.5)$$

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).

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

The Galerkin method would require that

$$(u_i, L\hat{\phi}) = (u_i, f) \qquad i = 1,2,\ldots,N$$

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

$$(\underline{\nabla} u_i, \underline{\nabla}\hat{\phi}) = (u_i, f) \qquad i = 1,2,\ldots,N \tag{1.7}$$

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.

$$A_1 \phi_1 = \frac{1}{\lambda} \sum_{g=1}^{G} \nu\Sigma_{fg}\phi_g$$

$$A_g \phi_g = \Sigma_{sg-1} \phi_{g-1} \qquad g = 2,3,\ldots,G \qquad (1.2)$$

with boundary conditions

$$\phi_g = 0$$

$$\frac{\partial}{\partial \underline{n}} \phi_g = 0 \qquad g = 1,2,\ldots,G$$

$$r \in \partial_e \Omega$$

and continuity conditions

$$\phi_g^- = \phi_g^+$$

$$D_g^- \frac{\partial}{\partial \underline{n}} \phi_g^- = D_g^+ \frac{\partial}{\partial \underline{n}} \phi_g^+ \qquad g = 1,2,\ldots,G$$

$$r \in \partial_i \Omega$$

The spatial variable is implied in the notation.

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

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

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

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

where $\underline{A}$ and $\underline{F}$ are G x 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 x G piecewise functions, continuous in each Ω_1. The expansion coefficients a_i^g are not to be confused with the elements of the matrix $\underline{A}$, which are never used in the following discussion.

$$\underline{\hat{\Phi}}(\underline{r}) = \sum_{i=1}^{N} \underline{U}_i(\underline{r})\,\underline{a}_i = [\hat{\Phi}_1(\underline{r}) \ldots \hat{\Phi}(\underline{r})]^T \qquad (2.2)$$

where

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

are the unknown coefficient vectors and

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

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

$$(\underline{U}_i,\ \underline{A}\,\underline{\hat{\Phi}} - \frac{1}{\lambda}\,\underline{F}\,\underline{\hat{\Phi}}) = 0 \qquad i = 1,2,\ldots,N \qquad (2.3)$$

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 $D\,\underline{\nabla}\,\hat{\Phi}$ be continuous (which is, in fact, the current continuity condition) so that the $(u_i, \underline{\nabla}\cdot D\,\underline{\nabla}\,\hat{\Phi})$ 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 $\underline{\phi}$ to be a solution to Eq. (2.1). Then, for any compatible diagonal matrix $\underline{W}$ we must have

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

Integrate the leakage term by parts to obtain

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

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

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

where

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

$$\underline{\Sigma_r} = [\Sigma_{r1} \ \ldots\ \Sigma_{rG}]^T$$

In order for the terms of the bilinear form (2.4) to exist we must only require that $\underline{\phi}$ 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 $\hat{\underline{\Phi}}$ be an approximate solution to the "weak" form Eq. (2.4), the Galerkin method requires that

$$a(\underline{U}_i, \hat{\underline{\Phi}}) = 0 \qquad i = 1, 2, \ldots, N \qquad (2.5)$$

This scheme thus does enlarge considerably the number of piecewise functions u_i 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.

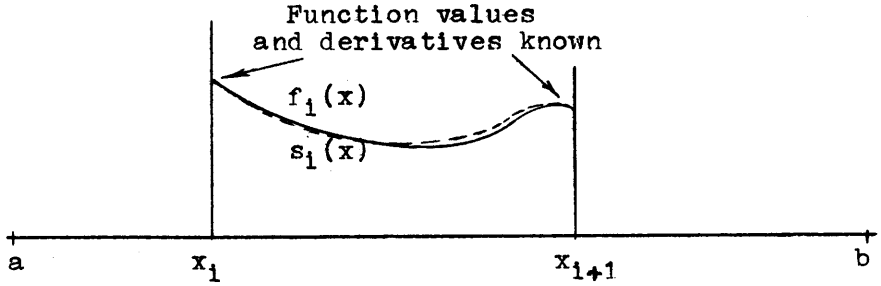


Fig.2.1 - Function $f_i(x)$ and uniquely determined cubic interpolate in region (x_i, x_{i+1}).

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:

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

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

Where μ in our case is

$$\mu = 2m$$

K is a positive constant independent of $\left| x_{i+1} - x_i \right|$, 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:

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

$$+ f(x_i)\, u_i^{1+}(x) + f(x_{i+1})\, U_{i+1}^{1-}(x)$$

where the primes denote x-differentiation.

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

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

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

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

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

In Fig. 2.2 we plot these functions.

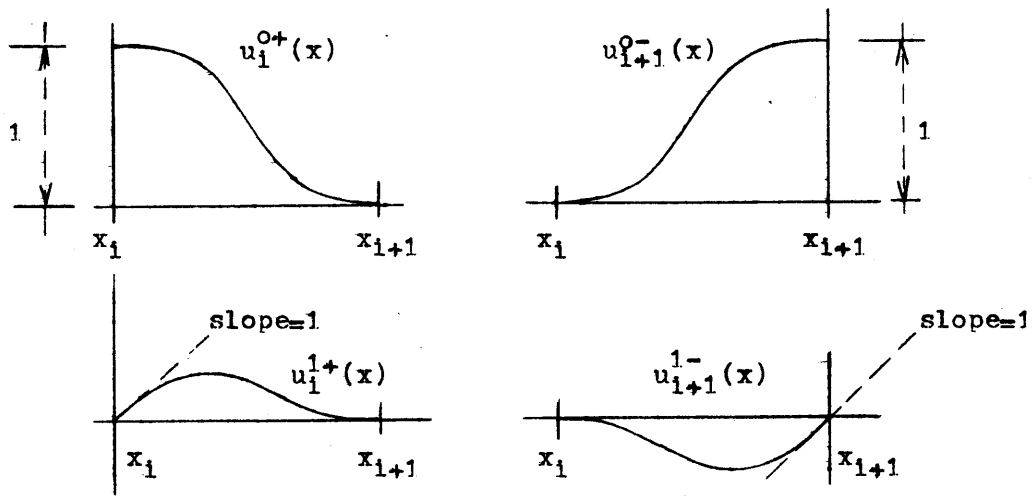


Fig.2.2 - One-dimensional cubic element functions

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.

$$s(x) = \sum_{i=1}^{n-1} s_i(x)$$

$$= \sum_{i=1}^{n-1} [f(x_i^+)\, u_i^{0+}(x) + f(x_{i+1}^-)\, u_{i+1}^{0-}(x)$$

$$+ f'(x_i^+)\, u_i^{1+}(x) + f'(x_{i+1}^-)\, u_{i+1}^{1-}(x)]$$

where the f's are unknowns to be determined.

Function and derivative continuity are naturally preserved by making

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

$$f'(x_i^+) = f'(x_i^-) = f'(x_i) \qquad i = 2, N-1 \qquad (2.7)$$

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

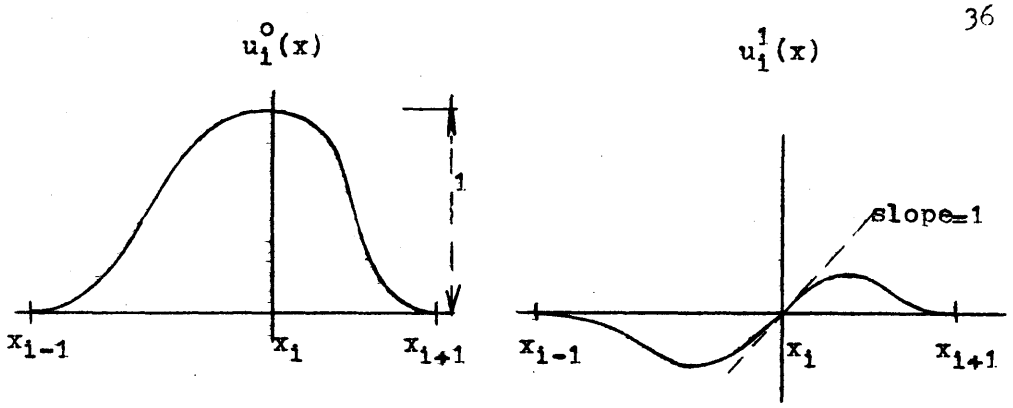


Fig.2.3 - Cubic basis functions appropriate for function and derivative continuity

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).

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

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

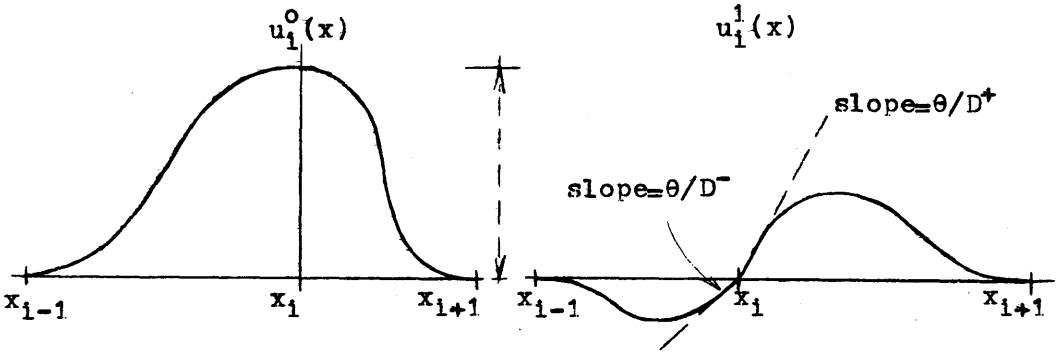


Fig.2.4 - Cubic basis functions appropriate for flux and current continuity across interfaces for a neutron diffusion problem.

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)

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

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

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.

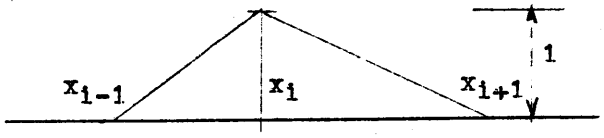


Fig. 2.5 - Linear basis function appropriate for flux continuity across interfaces.

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

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

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.

$$\left\| f(x) - s(x) \right\| \leq K_l \, \overline{\Delta x}^{2} \qquad \text{(linear)}$$

$$\leq K_c \, \overline{\Delta x}^{4} \qquad \text{(cubic)}$$

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:

$$s_i(x,y) = \sum_{px=o}^{1} \sum_{py=o}^{1} \Big[f_{i,j}^{(px+py)} u_i^{px+}(x) u_j^{py+}(y) + f_{i+1,j}^{(px+py)} u_{i+1}^{px-}(x) u_j^{py+}(y) + f_{i,j+1}^{(px+py)} u_i^{px+}(x) u_{j+1}^{py-}(y) + f_{i+1,j+1}^{(px+py)} u_{i+1}^{px-}(x) u_{j+1}^{py-}(y) \Big]$$

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.

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

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

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

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:

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

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

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.

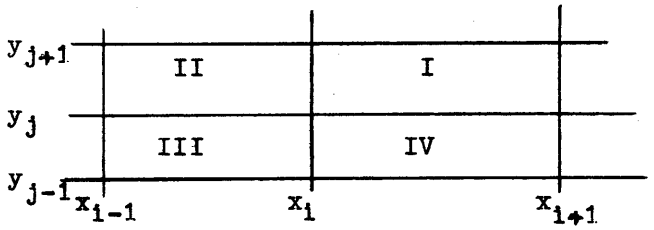


Fig. 2.6 - Two-dimensional partition

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 i and j lines are Eq. (2.10)

$$u_{ij}^{00}(x,y) = \begin{cases} u_i^{0+}(x)\, u_j^{0+}(y) & , \quad \text{I} \\ u_i^{0-}(x)\, u_j^{0+}(y) & , \quad \text{II} \\ u_i^{0+}(x)\, u_j^{0-}(y) & , \quad \text{III} \\ u_i^{0-}(x)\, u_j^{0-}(y) & , \quad \text{IV} \end{cases} \tag{2.10a}$$

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

$$u_{ij}^{01}(x,y) = \begin{cases} \frac{\theta}{D_I}\, u_i^{0+}(x)\, u_j^{1+}(y) & , \quad \text{I} \\ \frac{\theta}{D_{II}}\, u_i^{0-}(x)\, u_j^{i+}(y) & , \quad \text{II} \\ \frac{\theta}{D_{III}}\, u_i^{0+}(x)\, u_j^{1-}(y) & , \quad \text{III} \\ \frac{\theta}{D_{IV}}\, u_i^{0-}(x)\, u_j^{1-}(y) & , \quad \text{IV} \end{cases} \tag{2.10c}$$

$$u_{ij}^{ll}(x,y) = \begin{cases} \frac{\theta}{D_I} u_i^{l+}(x)\, u_j^{l+}(y) & , \text{I} \\ \frac{\theta}{D_{II}} u_i^{l-}(x)\, u_j^{l+}(y) & , \text{II} \\ \frac{\theta}{D_{III}} u_i^{l+}(x)\, u_j^{l-}(y) & , \text{III} \\ \frac{\theta}{D_{IV}} u_i^{l-}(x)\, u_j^{l-}(y) & , \text{IV} \end{cases} \qquad (2.10d)$$

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

Case 2

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

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.

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

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

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

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

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

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

Still another possibility would be to impose the zero derivatives conditions by droping 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

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

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

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

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

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

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

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

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:

$$\phi \simeq \hat{\phi} = \sum_{n=1}^{N}\sum_{m=1}^{M}\sum_{i=1}^{I(n,m)} a^1_{n,m,i}u^1_{n,m,i}(x,y)$$

$$\phi \simeq \hat{\phi} = \sum_{n=1}^{N}\sum_{m=1}^{M}\sum_{i=1}^{I(n,m)} a^2_{n,m,i}u^2_{n,m,i}(x,y)$$

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.

$$\int_V \left[D_1 \underline{\nabla}\hat{\phi}_1 \cdot \underline{\nabla} u^1_{n,m,i} + \left[\Sigma_{r1}\hat{\phi}_1 - \frac{1}{\hat{\lambda}} \left(\nu\Sigma_{f1}\hat{\phi}_1 + \nu\Sigma_{f2}\hat{\phi}_2\right)\right] u^1_{n,m,i}\right] dV = 0$$

$$\int_V \left[D_2 \underline{\nabla}\hat{\phi}_2 \cdot \underline{\nabla} u^2_{n,m,i} + \left[\Sigma_{r2}\hat{\phi}_2 - \Sigma_{s1}\hat{\phi}_1\right] u^2_{n,m,i}\right] dV$$

$$\text{for } \begin{array}{l} n = 1,N \\ m = 1,M \\ i = 1,\ I(n,m) \end{array} \qquad (2.11)$$

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

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

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

Where the $\underline{A}$ are matrices which incorporate the diffusion and removal terms, the $\underline{F}$ incorporate the fission terms and 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 = 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 x 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. 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.

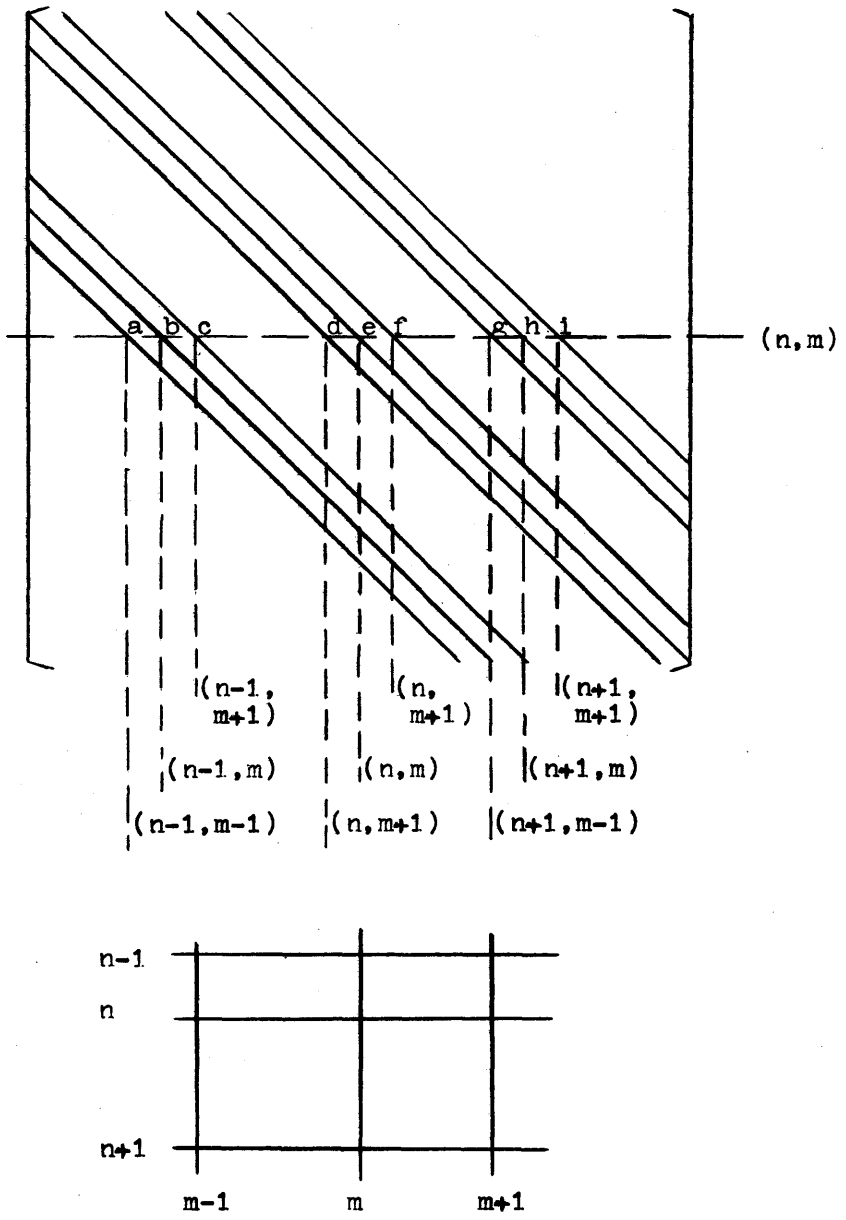


Fig. 2.7 - Two-dimensional partition and matrix form for unknowns ordered as: 1) all unknowns at each point; 2) all columns; 3) all rows.

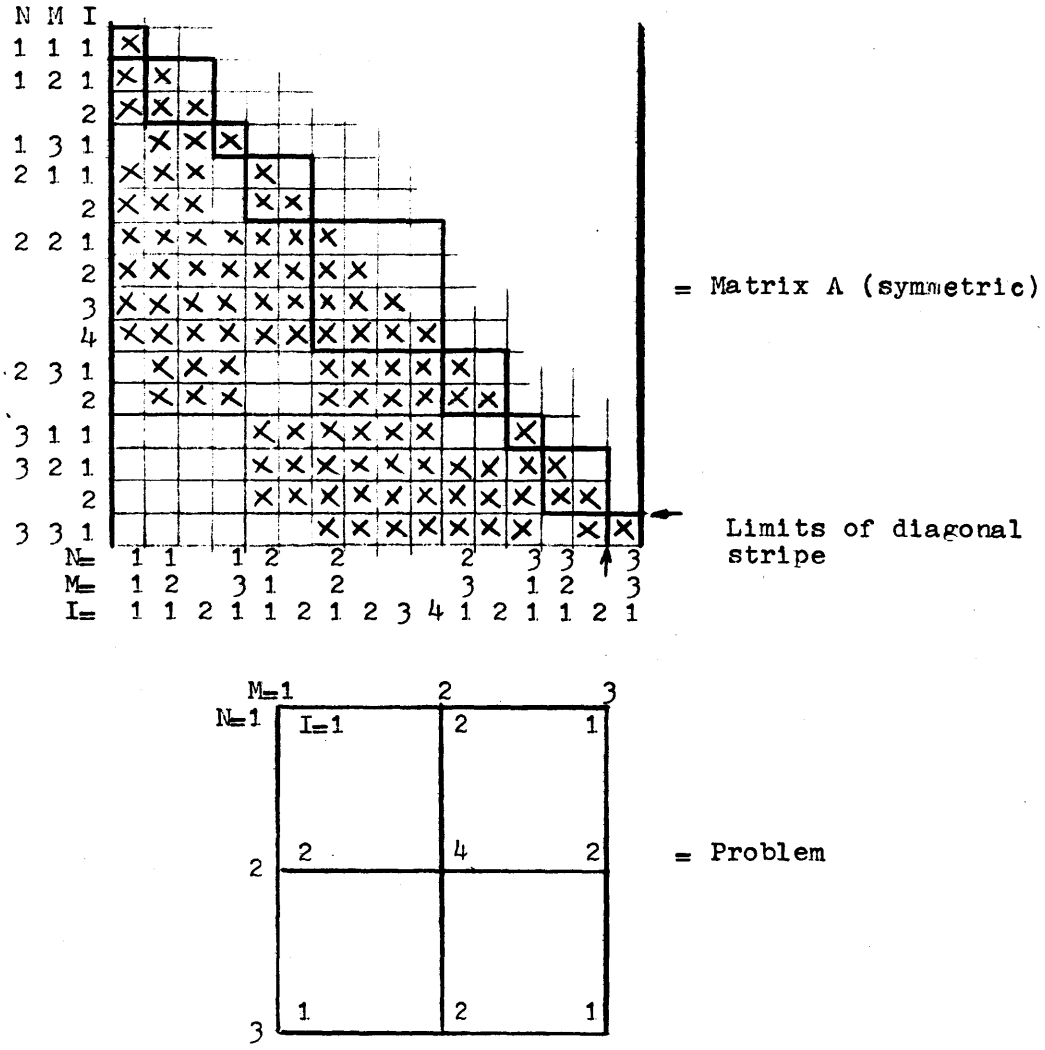


Fig. 2.8 - Two-dimensional partition and corresponding matrix structure

The power iteration method requires the following iteration procedure.

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

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

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

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

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

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 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

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

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

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.

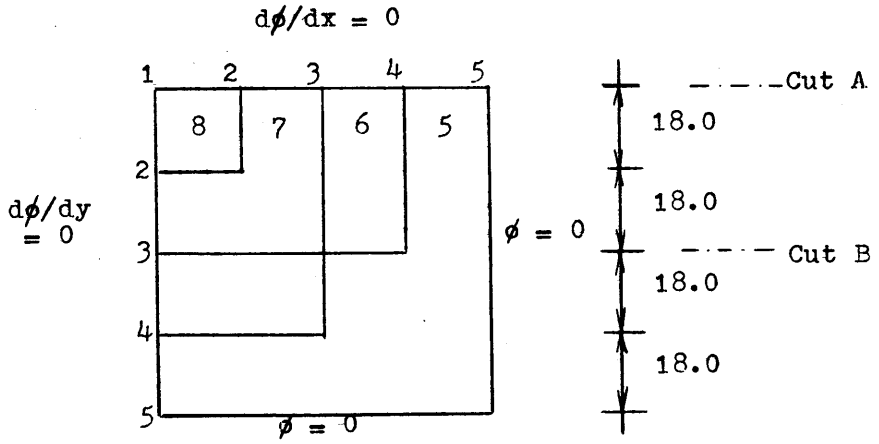


Fig. 3.1 - The 4-composition problem geometry

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 untolerable 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 derivatives continuity. (41 sets)	64	1.07825	0.25740 0.44611
3	CHD (18.0)	First derivatives uncoupled. (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.

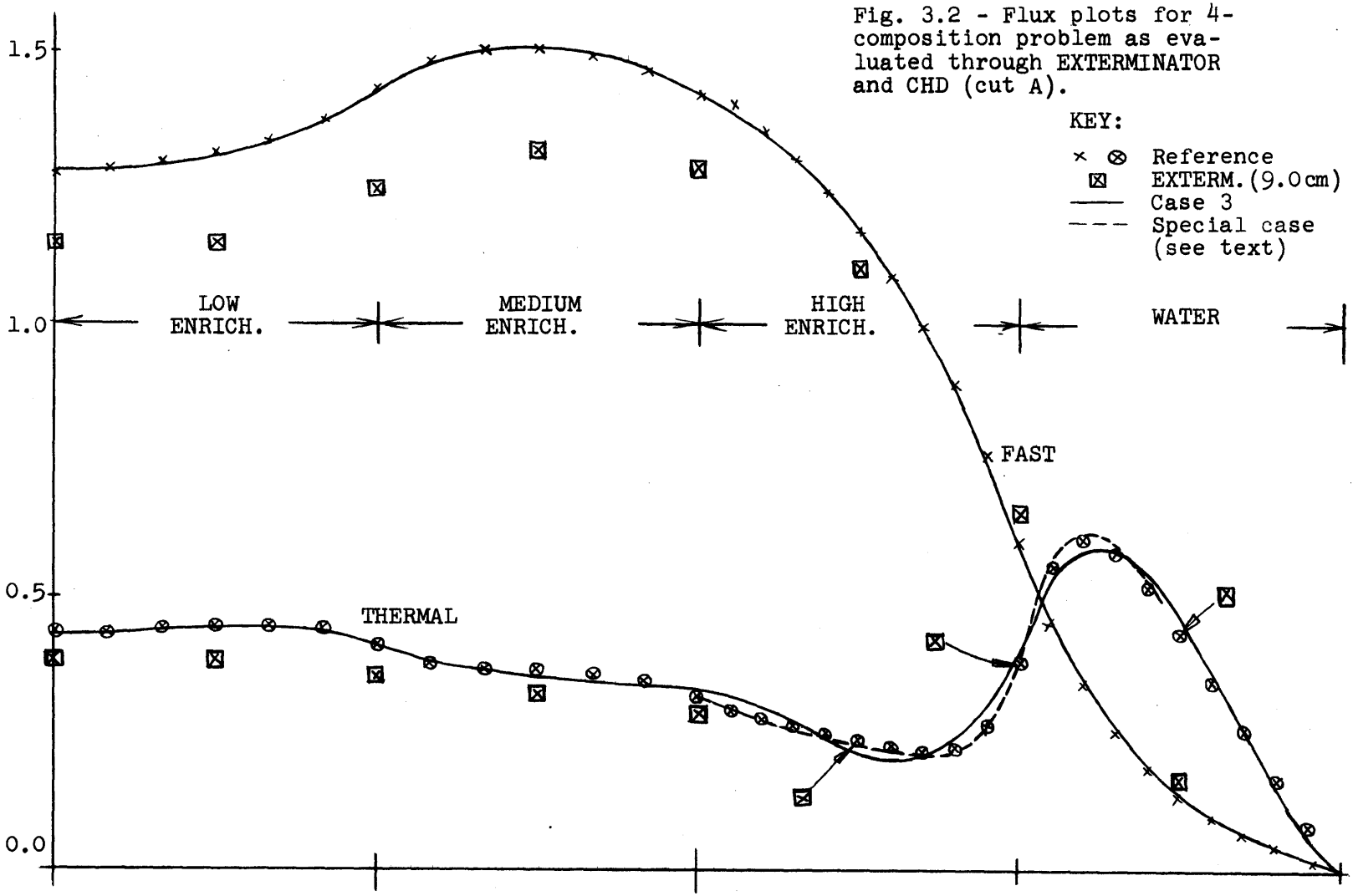


Fig. 3.2 - Flux plots for 4-composition problem as evaluated through EXTERMINATOR and CHD (cut A).

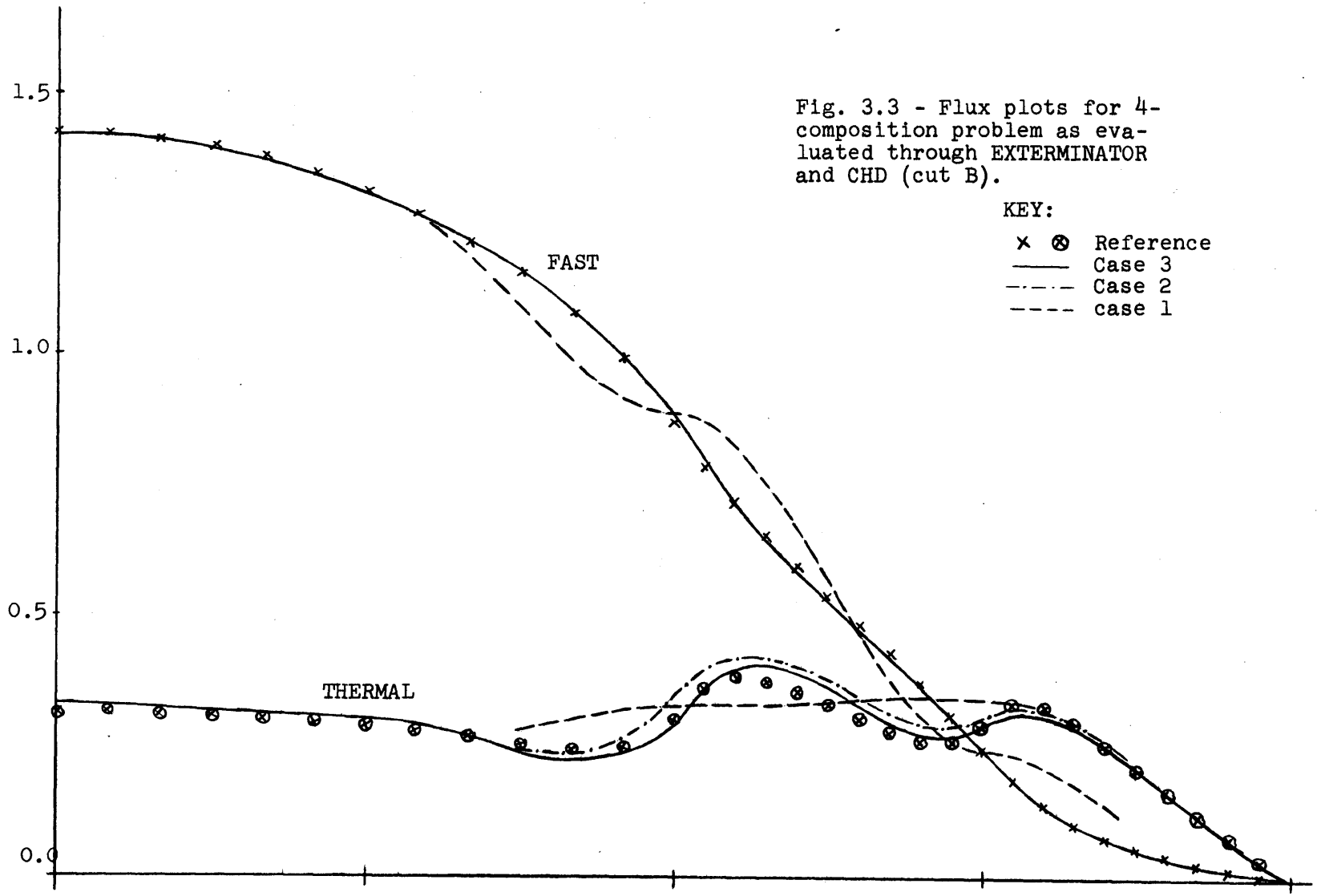


Fig. 3.3 - Flux plots for 4-composition problem as evaluated through EXTERMINATOR and CHD (cut B).

KEY:

× ⊗ Reference
—— Case 3
-·-·- Case 2
---- case 1

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 continuinity 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.

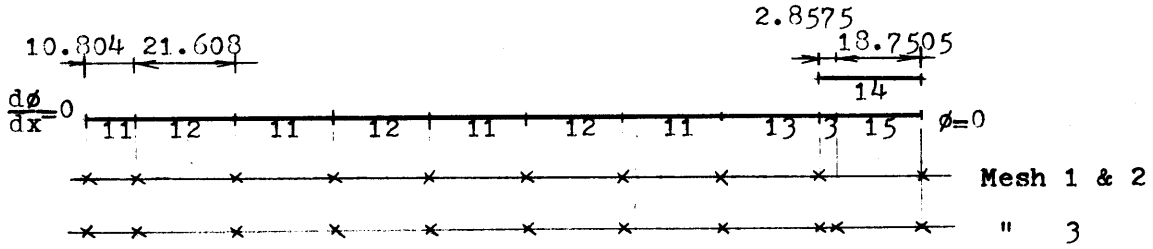


Fig. 3.4a - One-dimensional, ten-region problem.

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.

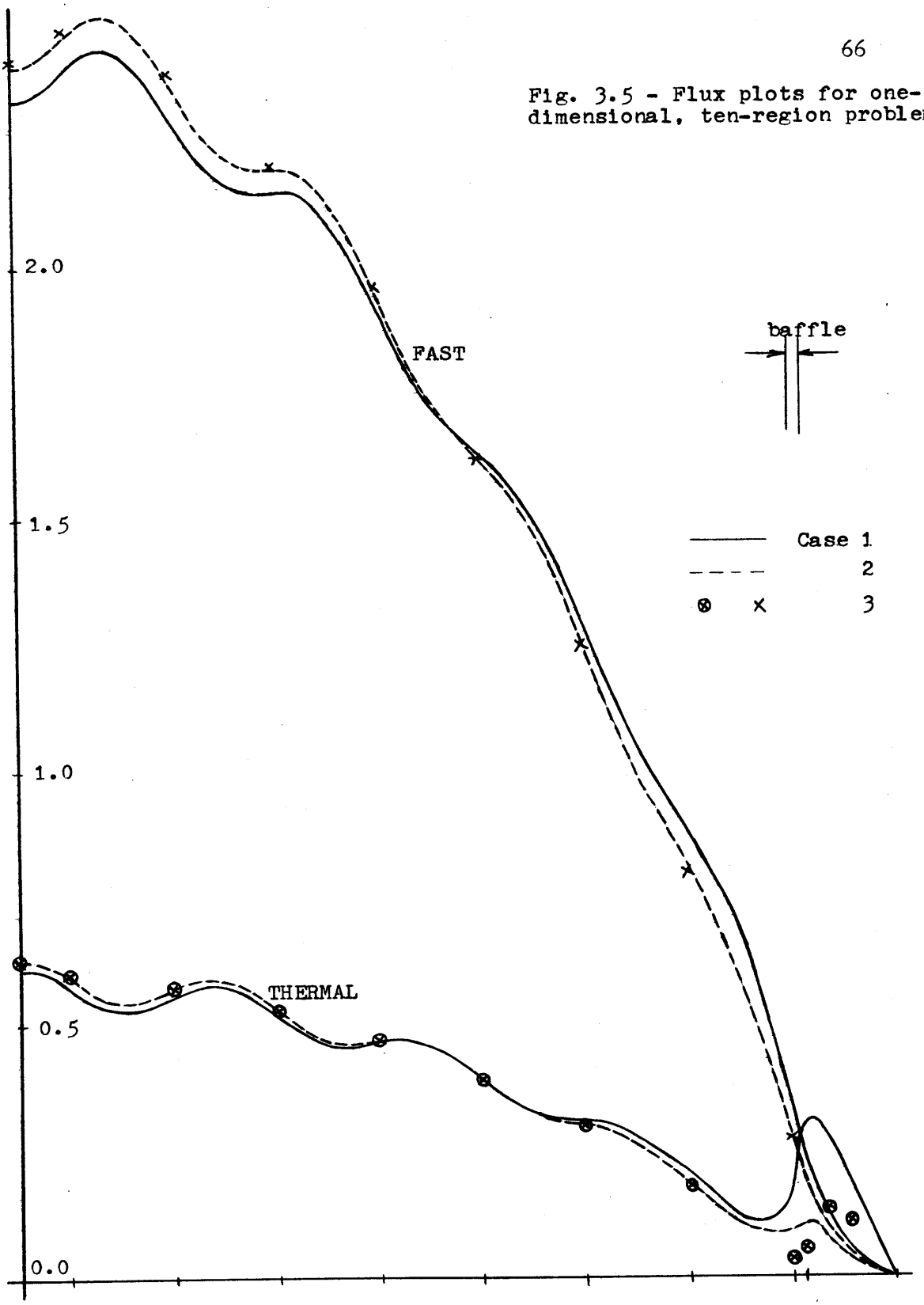
Case	1	2	3
Description	No baffle	Baffle and water homogenized.	Baffle explicitly considered.
k_{eff}	1.27912	1.27873	1.27866

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

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

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

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.

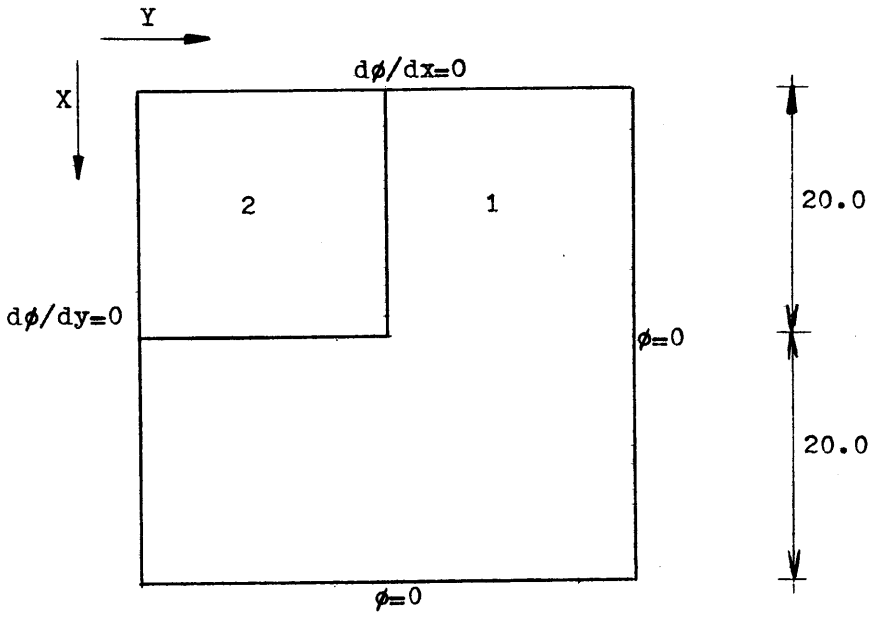
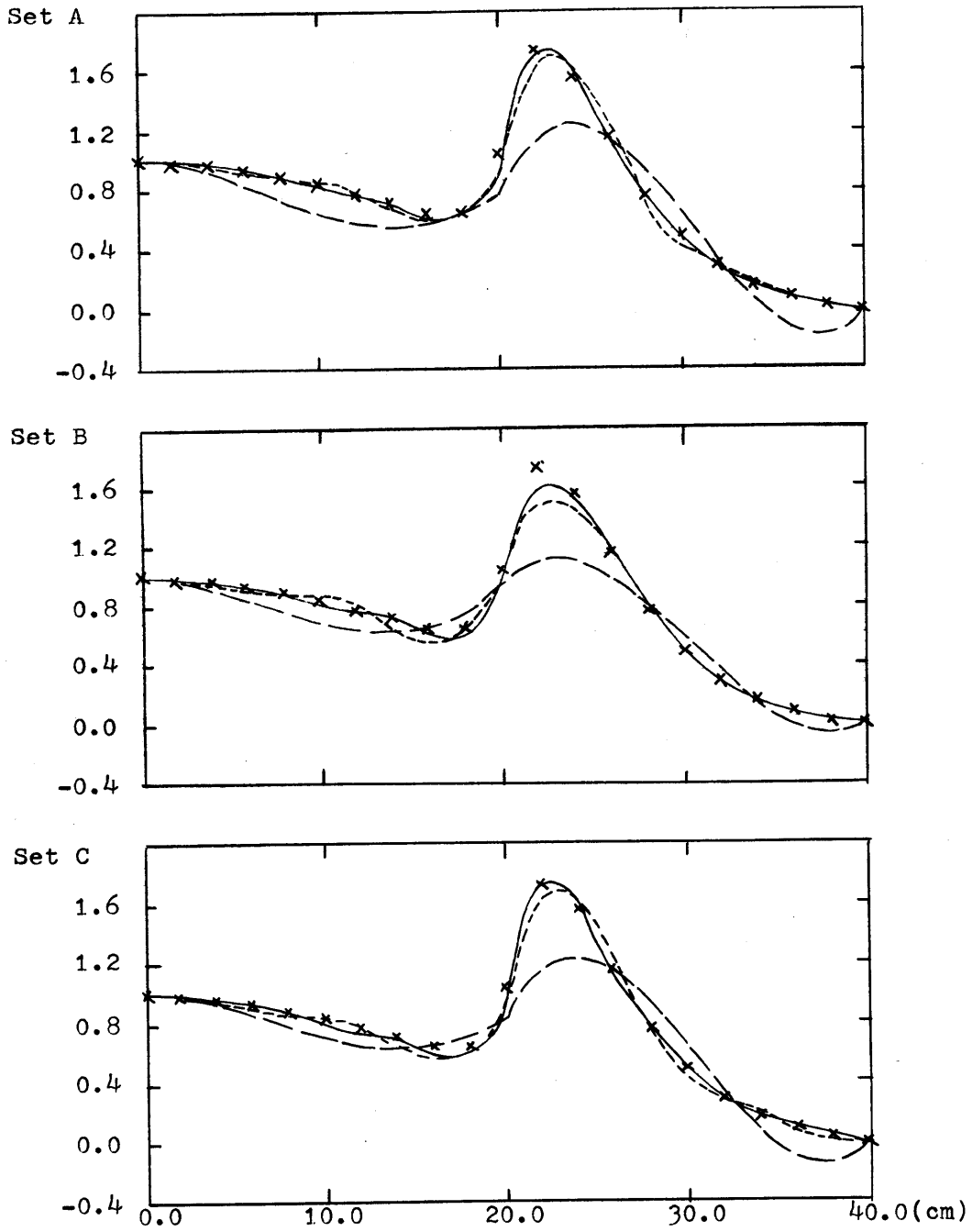


Table 3.4 - Eigenvalues for the basic two-dimensional problem.

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



KEY: Bicubic Hermite: — — Δx=20.0; ---- Δx=13.333; —— Δx=6.667;
Finite difference: Δx=2.0

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

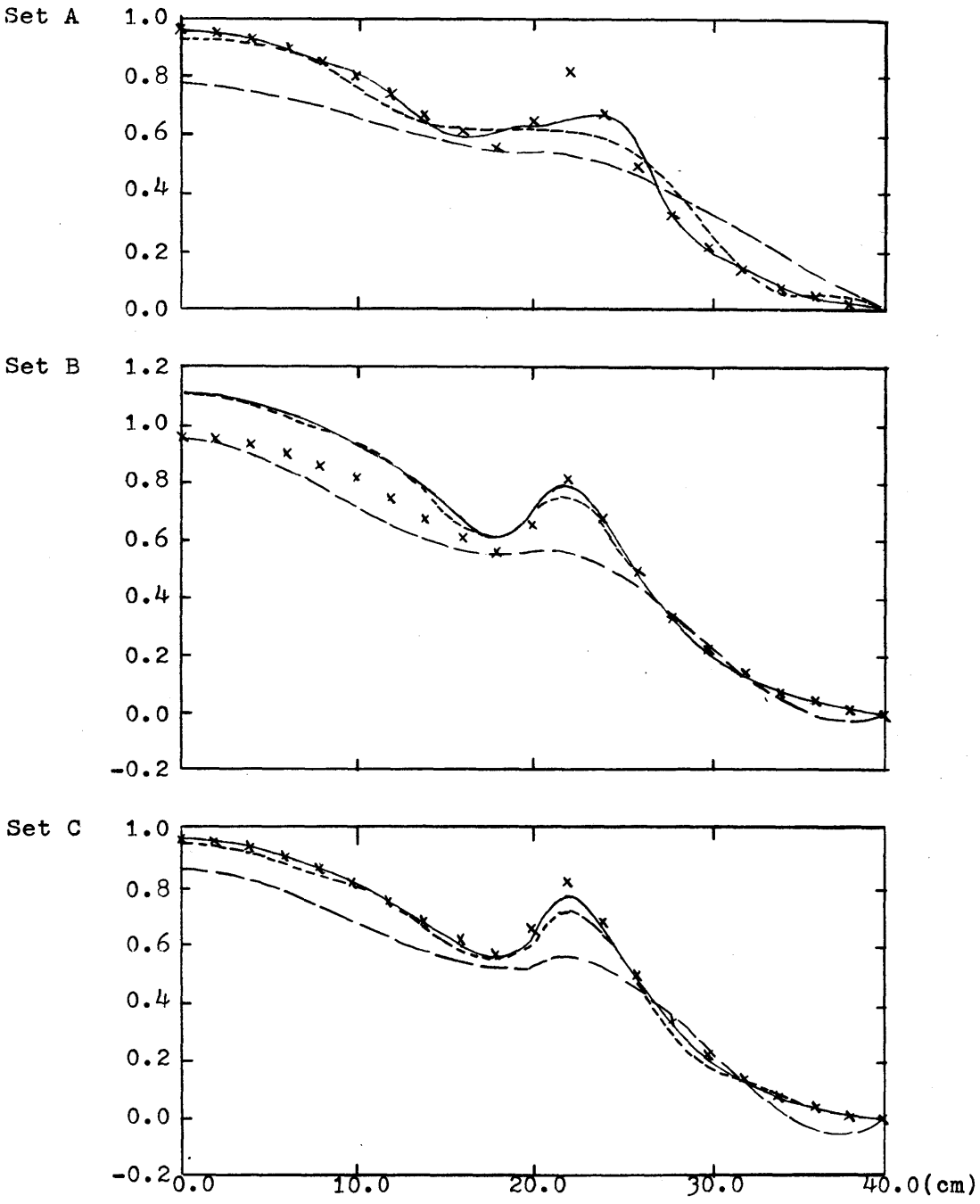


Fig. 3.7.b - Thermal flux plots for basic two-dimensional problem at x=20.0

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.

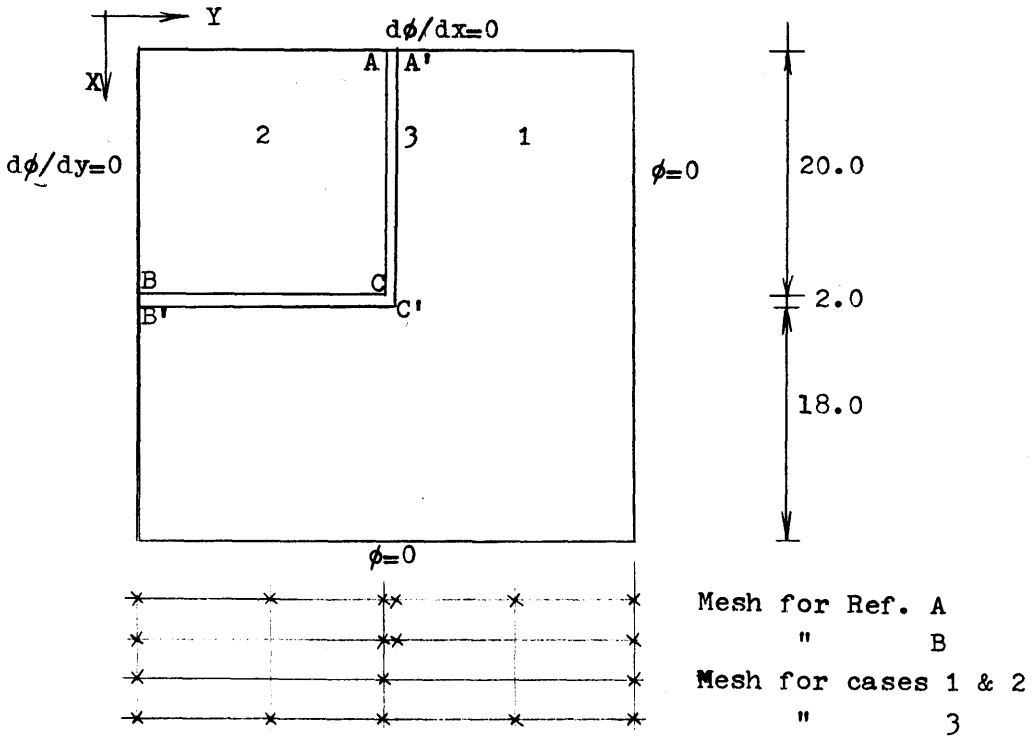


Fig. 3.8 - Geometry for the basic two-dimensional problem with baffle surrounding the fuel region.

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 explicitely. 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 ploted 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	

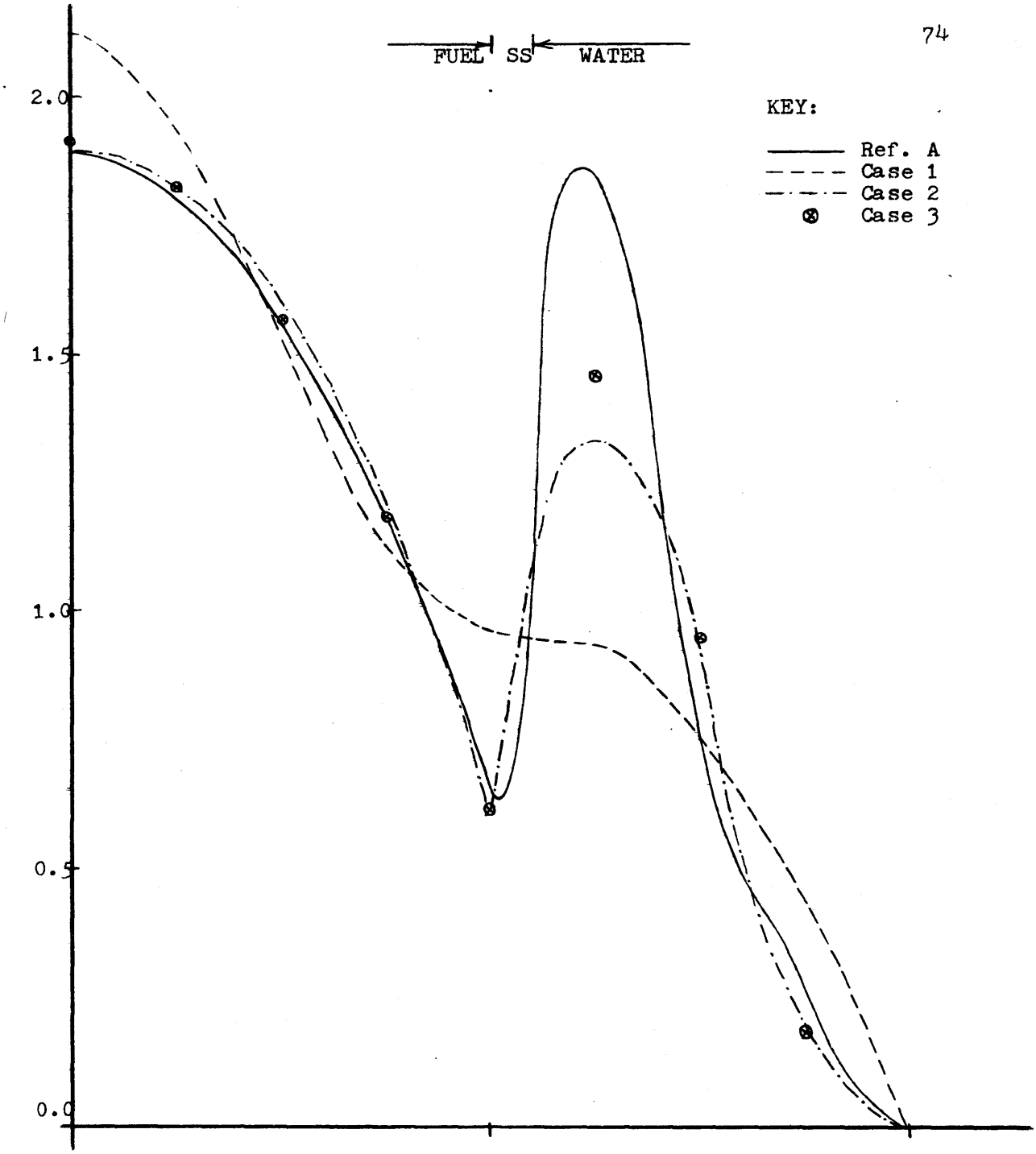


Fig. 3.9.a - Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region (y=0.0)

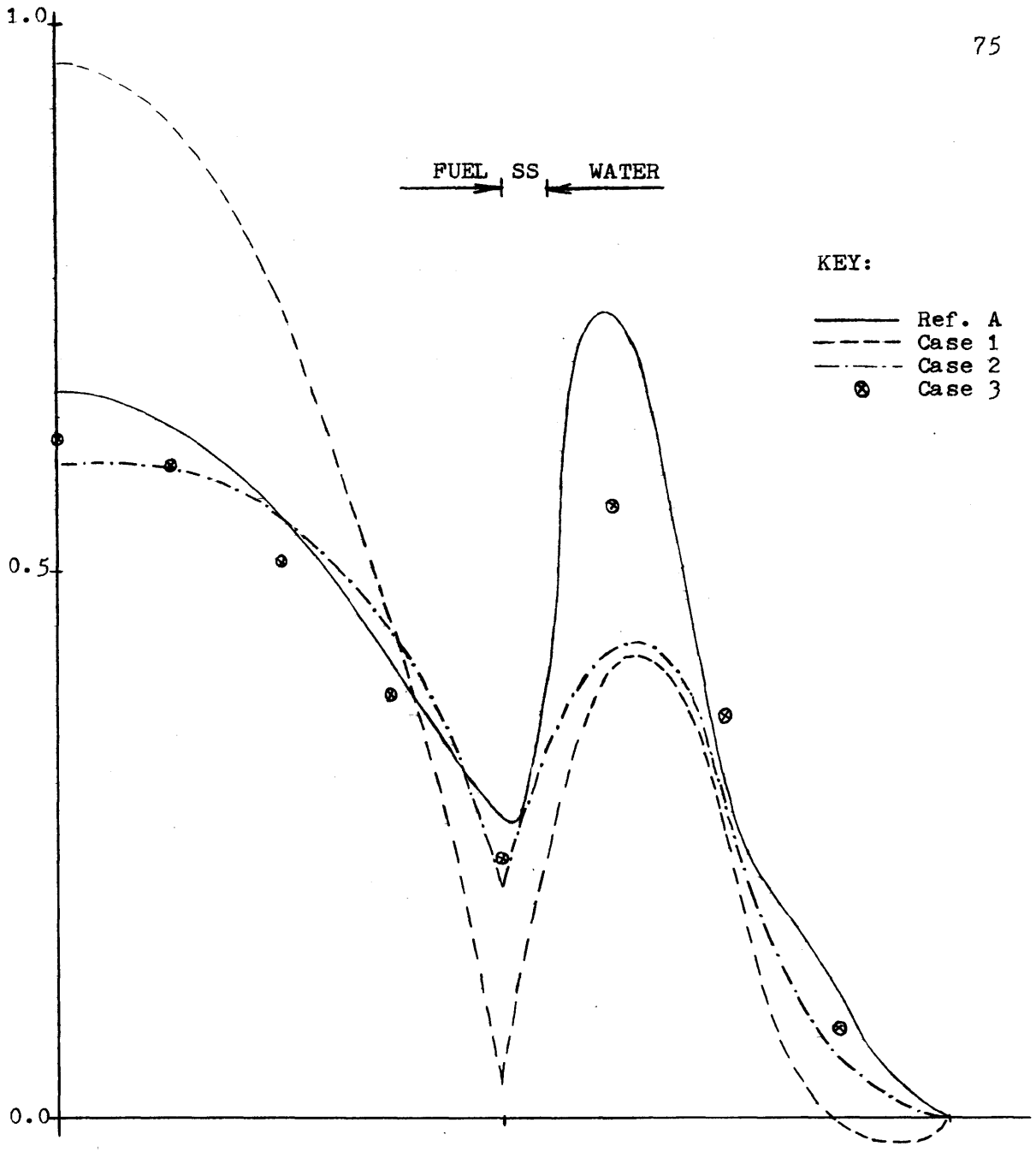


Fig. 3.9.b - Thermal fluxes for basic two-dimensional problem with baffle surrounding fuel region (y=20.0)

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 <u>inside</u> baffle and reflector but rather in their <u>effect</u> 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).

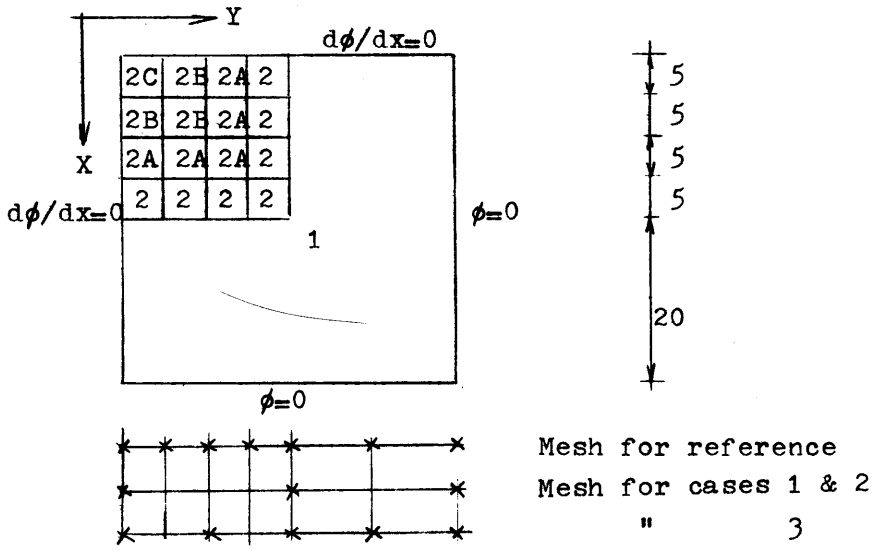


Fig. 3.10 - Geometry for the basic two-dimensional problem with varying cross sections inside the fuel region.

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

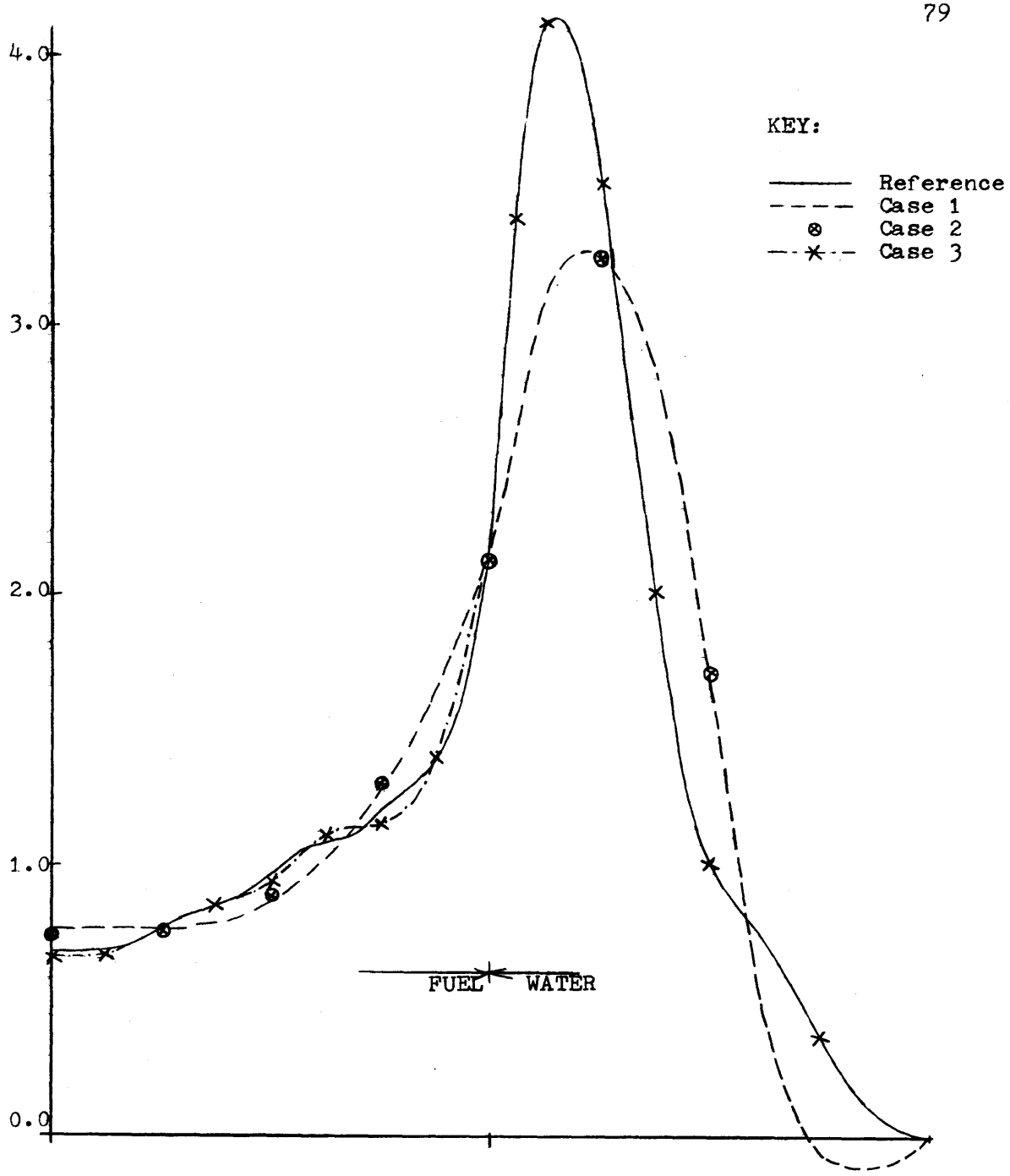


Fig. 3.11.a - Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region (x=0.0)

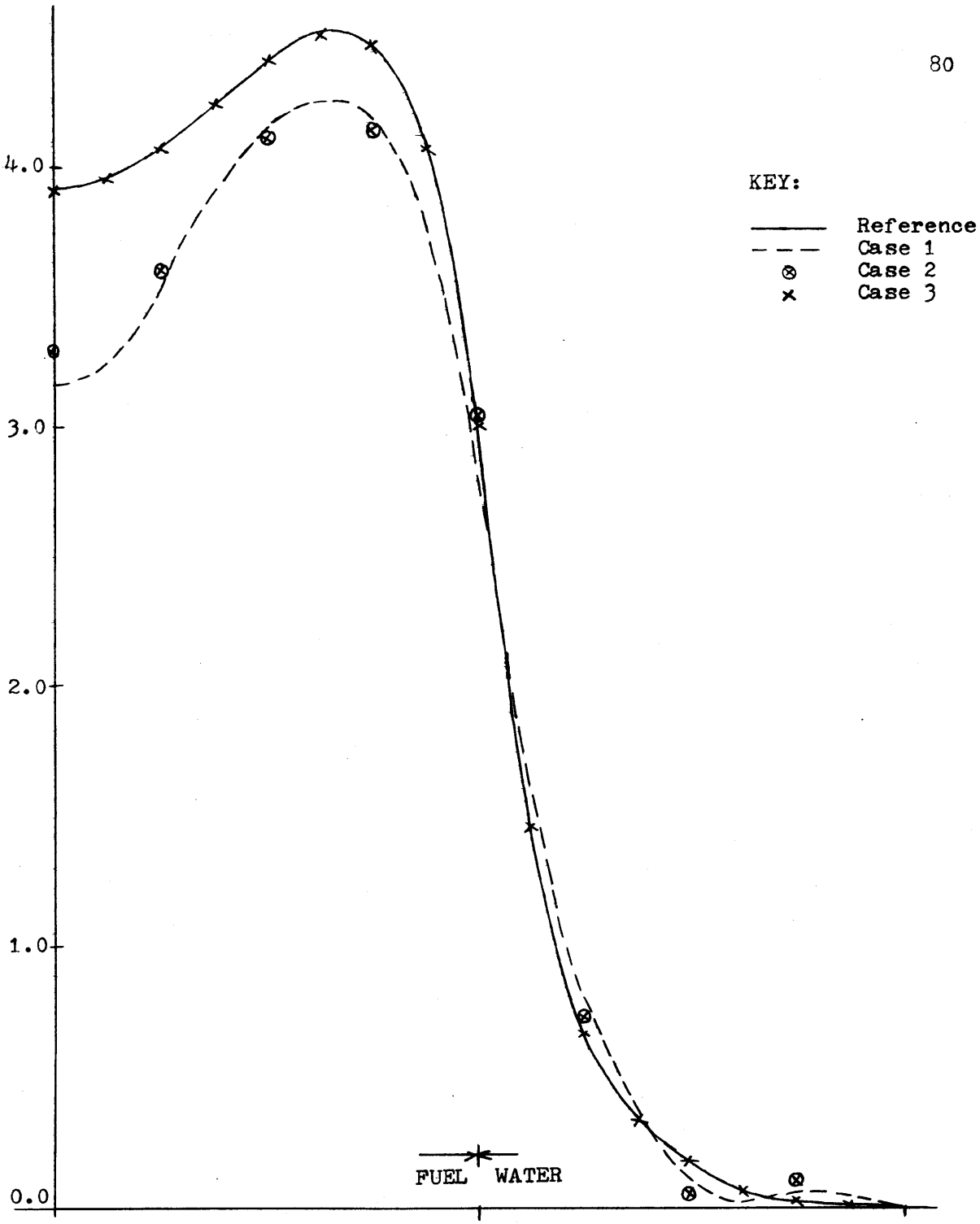


Fig. 3.11.b - Fast fluxes for two-dimensional problem with varying cross sections inside fuel region (x=0.0)

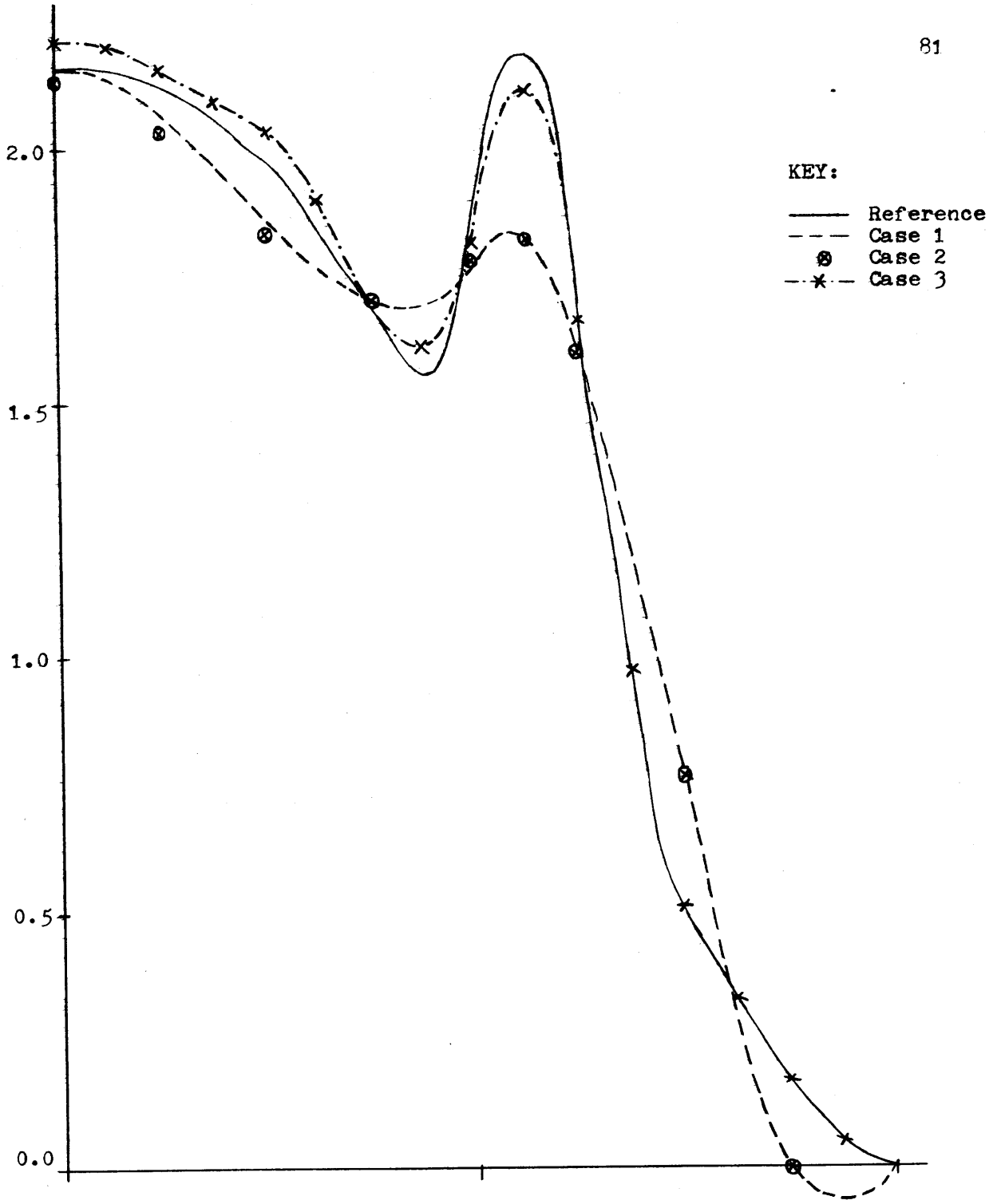


Fig. 3.12.a - Thermal fluxes for two-dimensional problem with varying cross sections inside fuel region (x=20.0)

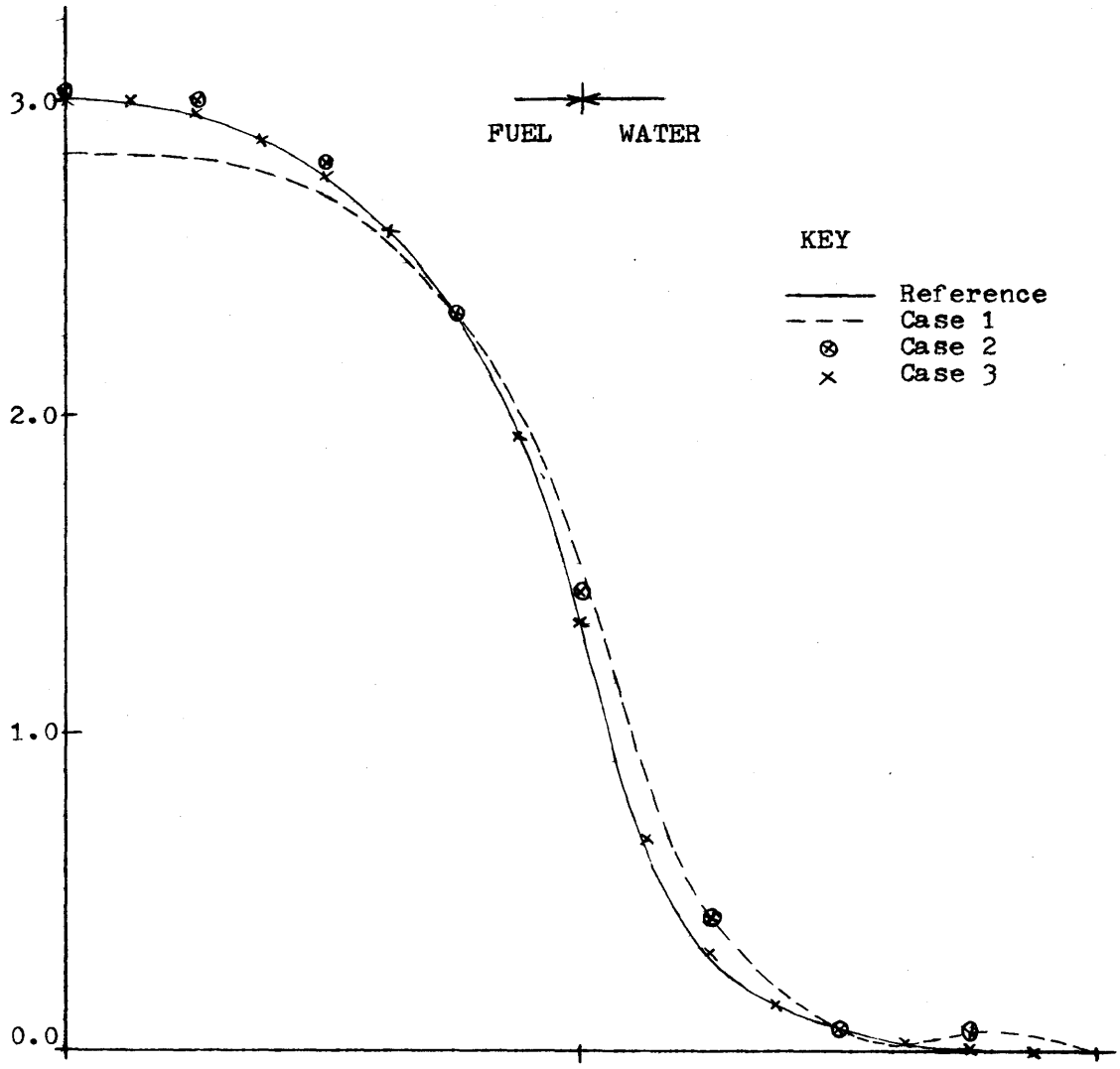


Fig. 3.12.b - Fast fluxes for two-dimensional problem with varying cross sections inside fuel region (x=20.0)

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.

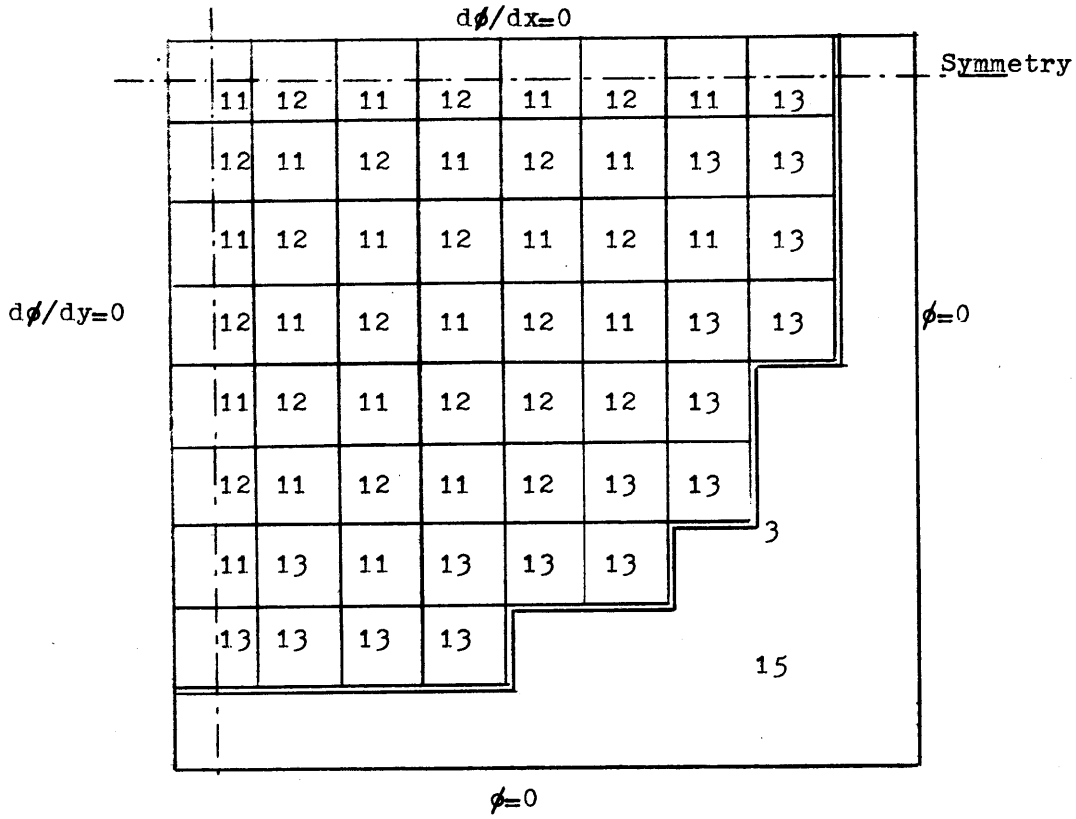


Fig. 3.13 - Zion 1 first core layout.

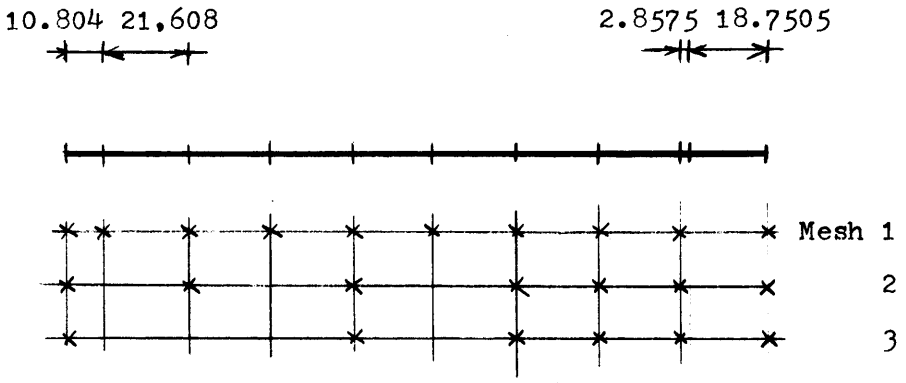


Fig. 3.14 - Mesh arrangement for CHD runs (Zion 1)

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 elements facing baf.)	5.133			5.191	5.181	5.183
Relative running cost (MIT conditions)	51			36		

ZION 1

	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								

KEY

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

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

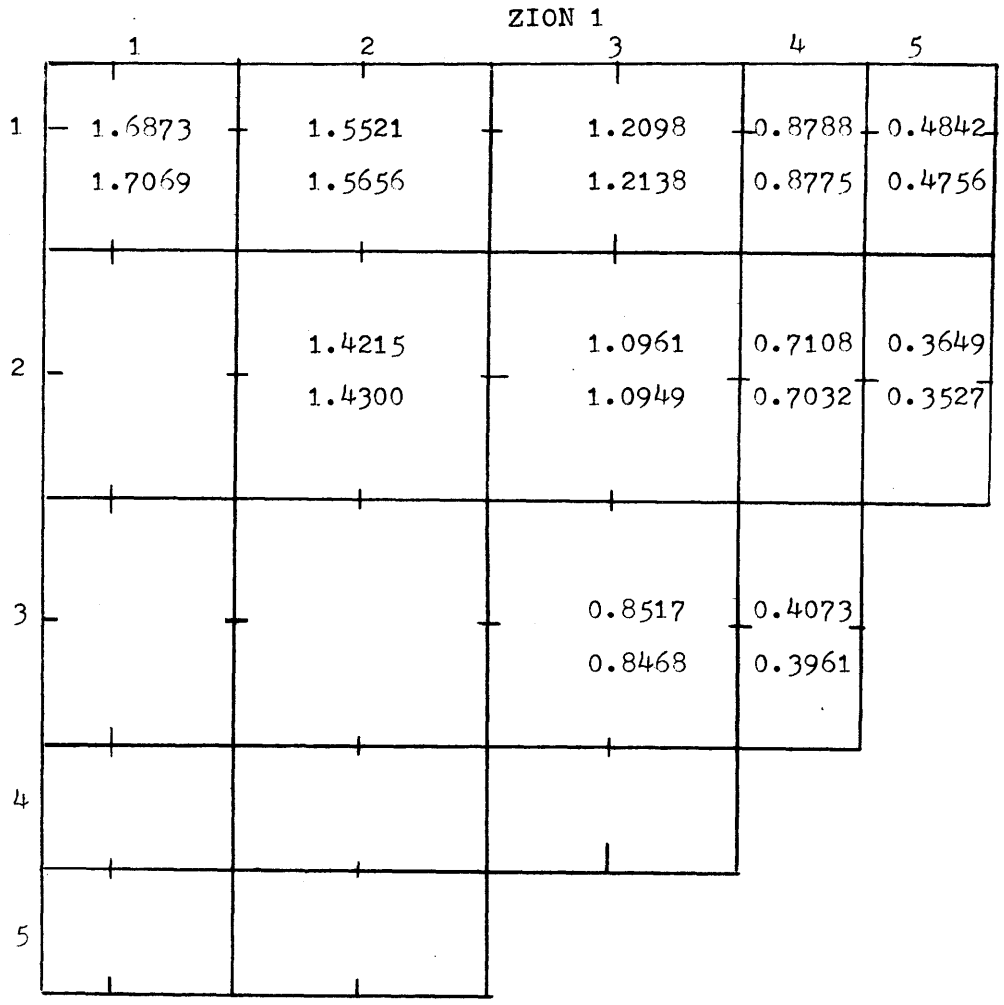


Fig. 3.16 - Region averaged to core averaged power ratios.

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

ZION 1

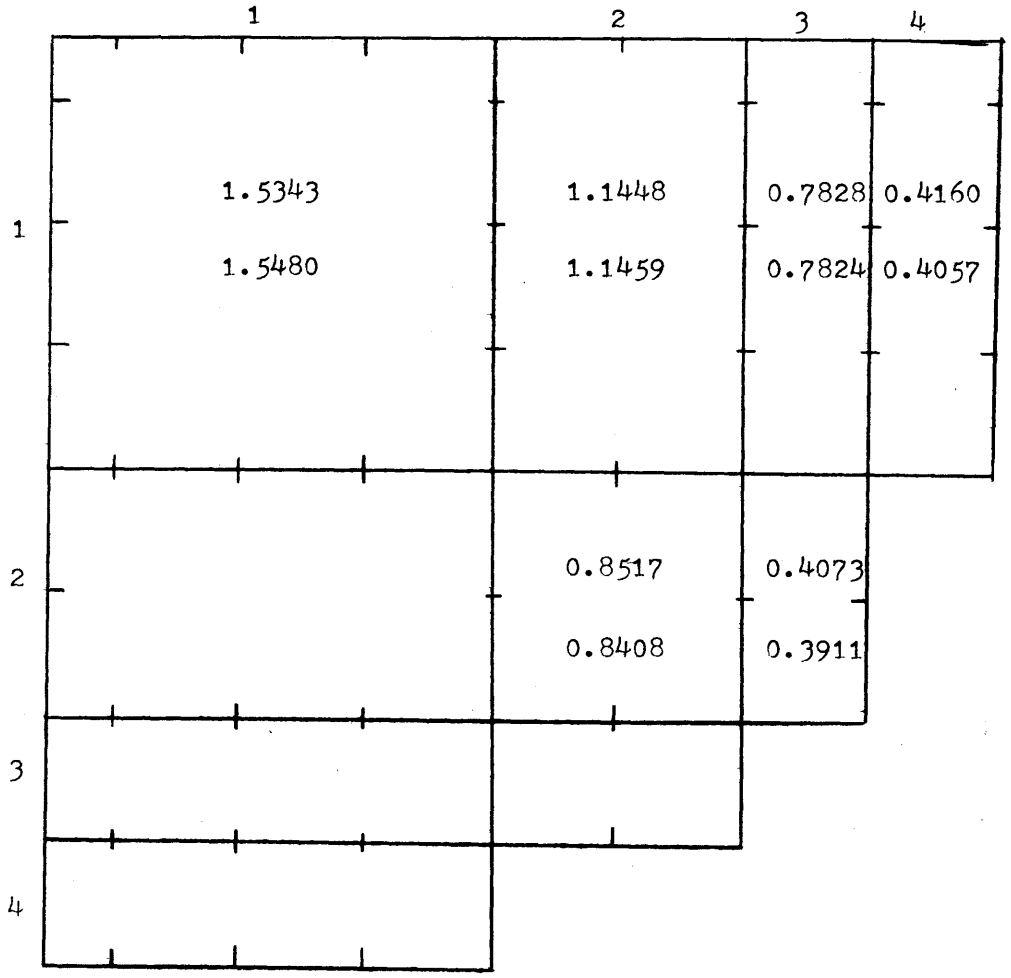


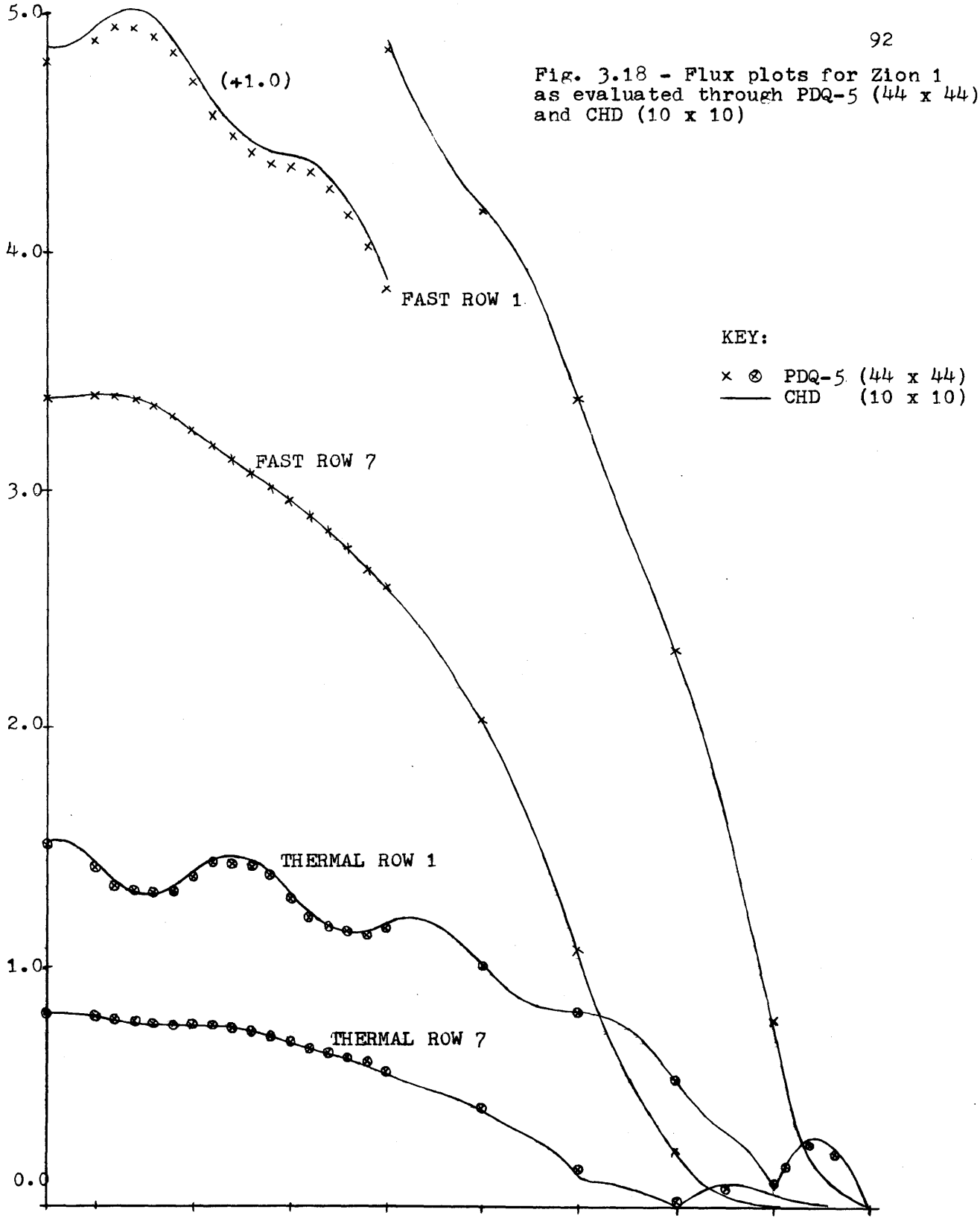
Fig. 3.17 - Region averaged to core averaged power ratios.

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)



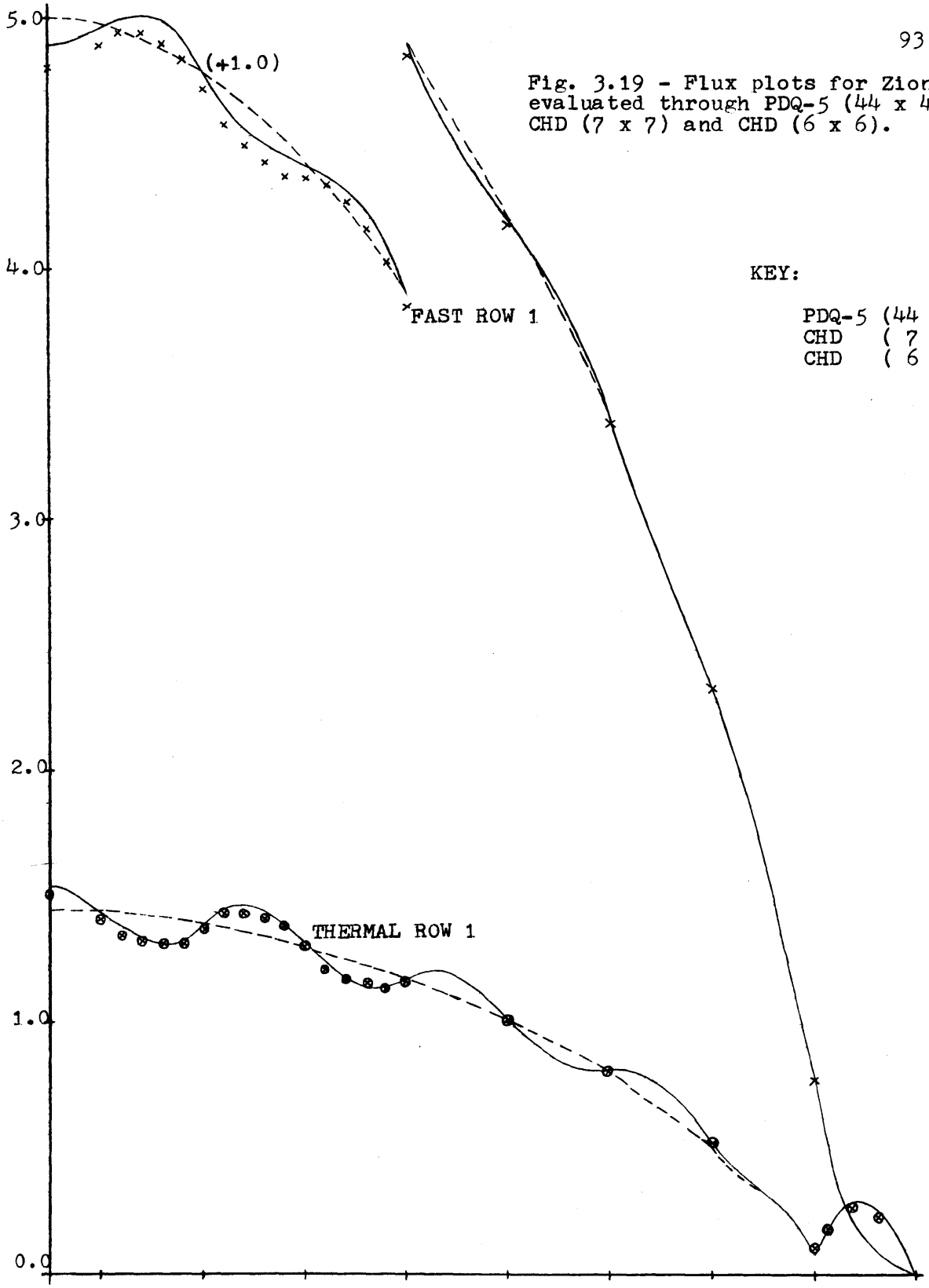


Fig. 3.19 - Flux plots for Zion 1 as evaluated through PDQ-5 (44 x 44), CHD (7 x 7) and CHD (6 x 6).

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 RECOMMENDATIONS

4.1) 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.

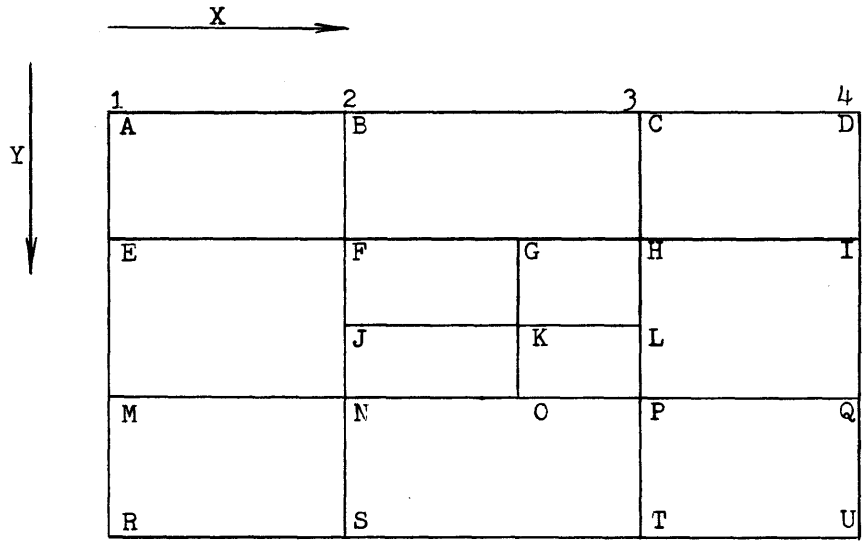


Fig. 4.1 - Regular and virtual mesh lines and points in two dimensions

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 achive this we define the following expansion functions:

Point	Interval of definition
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

$$\phi(J_x^-) = \phi(J_x^+)$$
$$\partial\phi/\partial x(J^-) = \partial\phi/\partial x(J^+)$$

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.

APPENDIX A

MACROSCOPIC CROSS SECTIONS

Group 1
Group 2

Composition	D(cm)	$\Sigma_r(cm^{-1})$	$\nu\Sigma_f(cm^{-1})$	$\Sigma_s(cm^{-1})$ $(k \rightarrow k+1)$	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 LIMITS FOR CUBIC HERMITE POLYNOMIALS

$h_- \equiv x_i - x_{i-1}$

$h_+ \equiv x_{i+1} - x_i$

$x_2 > x_i$

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

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

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

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

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

$$(u_i^{0+}, u_{i+1}^{0-})_{x_1}^{x_2} = -\frac{4}{7} h_+^{-6} (x)^7 + 2h_+^{-5} (x)^6 - \frac{9}{5} h_+^{-4} (x)^5$$
$$-\frac{1}{2} h_+^{-3} (x)^4 + h_+^{-2} (x)^3$$

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

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

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

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

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

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

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

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

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

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

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

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

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

$$(\tfrac{d}{dx}\,u_i^{0-},\ \tfrac{d}{dx}\,u_{i-1}^{0+})_{x_1}^{x_2} = \int_{x_1}^{x_2} \tfrac{d}{dx}\,u_i^{0-}\,(x)\ \tfrac{d}{dx}\,u_{i-1}^{0+}\,(x)\,dx =$$

$$= -\frac{36}{5}\,h_-^{-6}\,(x)^5 + 18\,h_-^{-5}\,(x)^4 - 12\,h_-^{-4}\,(x)^3$$

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

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

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

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

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

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

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

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

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

$$(\frac{d}{dx} u_i^{1+}, \frac{d}{dx} u_{i+1}^{0-})_{x_1}^{x_2} = -\frac{18}{5} h_+^{-5} (x)^5 + \frac{21}{2} h_+^{-4} (x)^4 - 10 h_+^{-3} (x)^3 + 3h_+^{-2} (x)^2$$

$$(\frac{d}{dx} u_i^{0-}, \frac{d}{dx} u_{i-1}^{1+})_{x_1}^{x_2} = -\frac{18}{5} h_-^{-5} (x)^5 + \frac{21}{5} h_-^{-4} (x)^4 - 10 h_-^{-3} (x)^3 + 3h_-^{-2} (x)^2$$

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

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

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

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

APPENDIX C

THE CODE CHD

C.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.

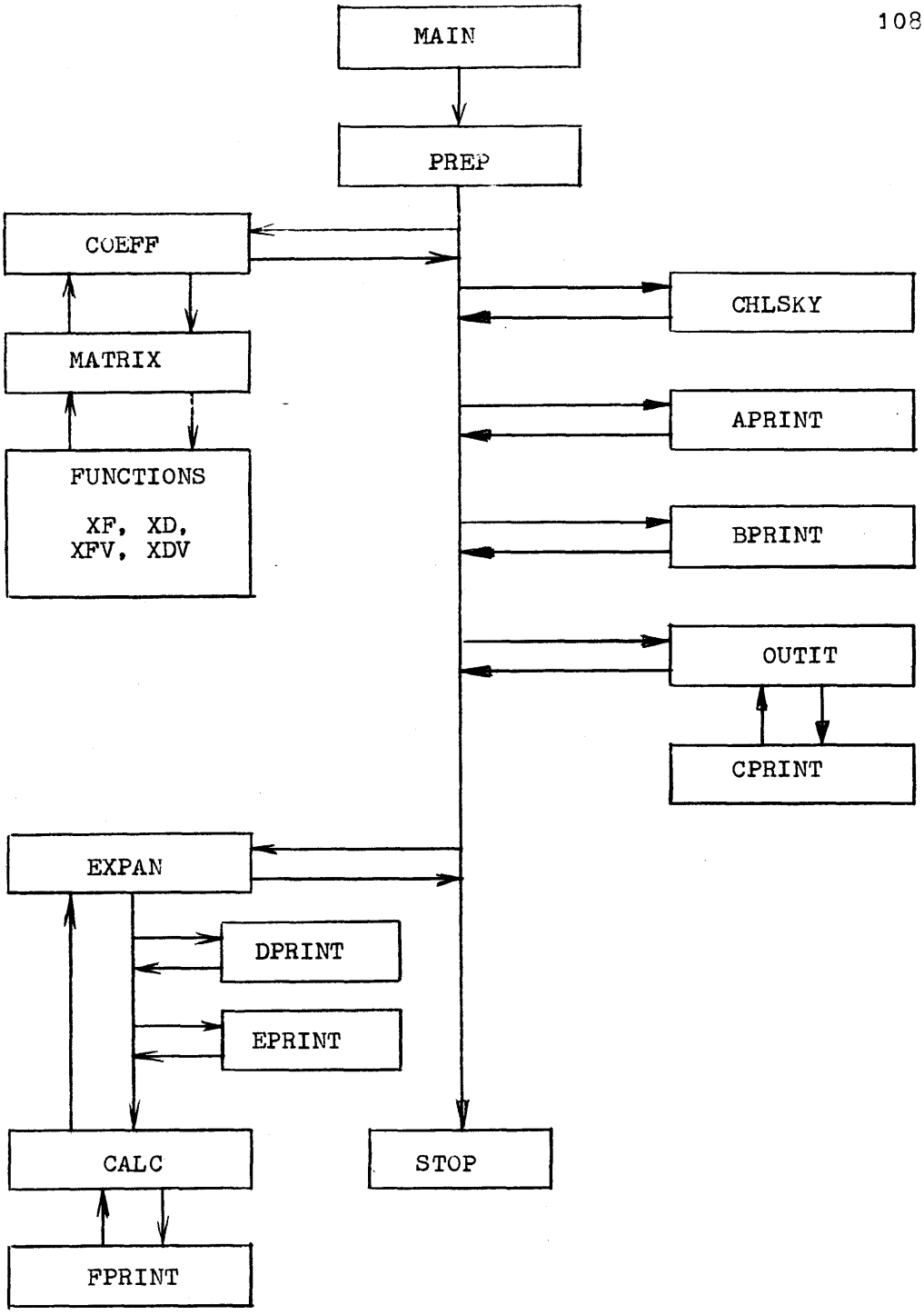


Fig. C.1 - CHD basic logic

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

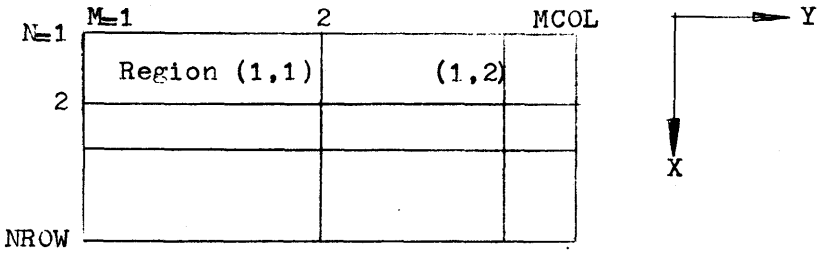


Fig. C.2 - Coordinate system orientation assumed by CHD.

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
- 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).

$$\begin{aligned} M(\min) = {} & LMAX\,(\,6\,KGROUP + 1.5) + 1.5\,LXMAX \\ & + LXCMAX\,(\,2\,KGROUP + 0.5) \\ & + LXFMAX\,(\,2\,KGROUP - 1.5) + JMAX\,(\,4\,KGROUP - 1) \\ & + JVMAX\,(\,NVN * MVM/2 + NVN + MVM + 1) \\ & + NROW * MCOL\,(\,KGROUP + 7) \\ & + (NROW + MCOL)\,/2 + 7\,KGROUP + 4 \end{aligned} \qquad (C.1)$$

Neglect any fraction.

The statement

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

Problems	LMAX	LXMAX	LXCMAX	LXFMAX	M Size (mim.)
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

Fast core (bytes) = 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: Performes 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

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

$$+ \int_V \Sigma r(KG,\underline{r})\phi(KG,\underline{r})d\underline{r}$$

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

Where KG ≡ KGROUP

A collapsed macroscopic cross section is defined as

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

with the average flux defined as

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

The collapsed diffusion coefficient is defined as

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

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 if 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 - ($\leq$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.

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

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

($\geq$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.

($\geq$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

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

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	$(\theta/D)\ (\partial/\partial x)$	$\partial / \partial y$	$(\theta/D)(\theta^2/\partial x \partial y)$
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 ot 50 and 51 sets, respectively, in these cases. The latter should be used.

c) When inputing 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)
$D_1D_2 \neq D_3D_4$	$D_I(\underline{r})$ and $D_{II}(\underline{r})$ and $D_{III}(\underline{r})$ and $D_{IV}(r)$ 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 = 0 and 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.

APPENDIX D

SOURCE LISTING OF CHD, SAMPLE INPUT AND OUTPUT (only in MIT library copies)

```
 1
 3     3     2     5   150 2100 4000 4100     1     3     3
50    -4     0     0    -1
     1.0         0.0          1.0          0.0
1.0E-06    1.0E-04    1.0E-04

  100.0
    1.0          1.0
 1
    1.2         0.15
  0.101         0.02

    0.1
 2
    1.5          0.4
 0.0623          0.2
    0.0        0.218
   0.06
 3
   1.55       0.4133
 0.0623         0.25
    0.0        0.218
   0.06
 4
   1.60       0.4267
 0.0623          0.3
    0.0        0.218
   0.06
 5
   1.65         0.44
 0.0623         0.35
    0.0        0.218
   0.06
   20.0         20.0
   20.0         20.0
 1    -1
-1    -1
 1     3     3
    5.0          5.0          5.0          5.0
    5.0          5.0          5.0          5.0
 5     4     3     2
 4     4     3     2
 3     3     3     2
 2     2     2     2
```

```
    $JOB            DEPPE,TIME=2
 1        DIMENSION A(40000)
 2        MSIZE=40000
 3        READ(5,1000)NRUN
 4        NRUN1=0
 5      990 NRUN1=NRUN1+1
 6        READ(5,1000) NROW,MCOL,KGROUP,JMAX,LMAX,LXMAX,LXCMAX,LXFMAX,JVMAX,
         1NVN,MVM
 7     1000 FORMAT(14I5)
 8        NROW1=NROW-1
 9        MCOL1=MCCL-1
10        K1=KGROUP-1
11        K2=3*KGROUP*LMAX
12        NVN=NVN+1
13        MVM=MVM+1
14        IF(JVMAX.EQ.0) JVMAX=1
15        L1=1
16        L2=L1+2*KGROUP*LXCMAX
17        L3=L2+6*KGROUP*LMAX
18        L4=L3+LXMAX
19        L5=L4+LXFMAX*K1
20        L6=L5+LXFMAX*K1
21        L7=L6+KGROUP
22        L8=L7+JMAX*KGROUP
23        L9=L8+JMAX*KGROUP
24        L10=L9+JMAX*KGROUP
25        L11=L10+JMAX*K1
26        L12=L11+NROW1
27        L12A=L12+MCOL1
28        L12B=L12A+JVMAX*NVN
29        L12C=L12B+JVMAX*MVM
30        L12D=L12C+KGROUP
31        L12E=L12D+KGROUP
32        L12F=L12E+KGROUP
33        L12G=L12F+KGROUP
34        L12H=L12G+KGROUP
35        L13=L12H+KGROUP
36        L14=L13+NROW*MCOL*6
37        L15=L14+NROW*MCOL*KGROUP
38        L16=L15+(LMAX+1)/2
39        L17=L16+(LMAX+1)/2
40        L18=L17+(LMAX+1)/2
41        L19=L18+(LXMAX+1)/2
42        L20=L19+(LXCMAX+1)/2
43        L21=L20+(LXFMAX+1)/2
44        L22=L21+(NROW1*MCOL1+1)/2
45        L23=L22+(JVMAX*NVN*MVM+1)/2
46        L24=L23+(JVMAX+1)/2
47        L25=L24+(JVMAX+1)/2
48        MSIZE1=L25+(NROW*MCOL+1)/2
49        IF(MSIZE.LT.MSIZE1) GOTO 1100
50        CALL  PREP(NRUN1,K2,
         1MSIZE,MSIZE1,   NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
         1JVMAX,NVN,MVM,LMAX,LXMAX,
         1LXCMAX,LXFMAX,A(L1),A(L2),A(L3),A(L4),A(L5),A(L6),A(L7),A(L8),
         1A(L9),A(L10),A(L11),A(L12),A(L12A),A(L12B),A(L12C),A(L12D),
```

```
     2A(L12E),A(L12F),A(L12G),A(L12H),
     2                        A(L13),A(L14),A(L15),A(L16),A(L17),A(L18),
     3A(L19),A(L20),A(L21),A(L22),A(L23),A(L24),A(L25))
51         IF(NRUN1.LT.NRUN) GOTO 990
52         GOTO 1200
53   1100 M=MSIZE1-MSIZE
54         WRITE(6,1150) M
55   1150 FORMAT(1H1,'***ERROR*** SIZE OF ARRAY A IS TOO SMALL BY',I 6,3X,
     1'WORDS')
56   1200 STOP
57         END
```

```
      SUBROUTINE PREP(NRUN1,K2,MSIZE,MSIZE1,NROW,NROW1,MCOL,MCOL1,
     1KGROUP,K1,JMAX,JVMAX,NVN,MVM,LMAX,
     1LXMAX,LXCMAX,LXFMAX,A,AR,F1,F,S,XI,DI,SR,SF,ST,HN,HM,HNV,HMV,
     2DA,DAA,DB,DBB,D1,D2,IND,TH,LXD,
     2LXDC,LXDF,LLX,LLXC,LLXF,JC,JCV,NVMAX,MVMAX,IP)
      REAL*8 A(KGROUP,LXCMAX),AR(K2)
      INTEGER*2 LXD(LMAX),LXDC(LMAX),LXDF(LMAX),LLX(LXMAX),LLXC(LXCMAX),
     1LLXF(LXFMAX),JC(NROW1,MCOL1)
      INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
      INTEGER*2 IP(NROW,MCOL)
      DIMENSION XI(KGROUP),DI(KGROUP,JMAX),SR(KGROUP,JMAX),
     1SF(KGROUP,JMAX),ST(K1,JMAX)
      DIMENSION HN(NROW1),HM(MCOL1)
      DIMENSION IND(NROW,MCOL,6),TH(KGROUP,NROW,MCOL)
      DIMENSION F1(LXMAX),F(K1,LXFMAX),S(K1,LXFMAX)
      DIMENSION HNV(JVMAX,NVN),HMV(JVMAX,MVM),DA(KGROUP),DAA(KGROUP),
     1DB(KGROUP),DBB(KGROUP),D1(KGROUP),D2(KGROUP)
      READ(5,1000) NCONV,      ICMAX,NP,IOUT,ICLPS
 1000 FORMAT(16I5)
      READ(5,1010)BL,BR,BT,BB
      READ(5,1010)EPSCH,EPSF,EPSL
 1010 FORMAT(8E10.8)
      DO 1012 N=1,NROW
      DO 1012 M=1,MCOL
      IP(N,M)=42
      IND(N,M,1)=110
      IND(N,M,2)=210
      IND(N,M,3)=0
      IND(N,M,4)=120
      IND(N,M,5)=0
 1012 IND(N,M,6)=220
      IP(1,1)=40
      IP(1,MCOL)=40
      IP(NROW,1)=40
      IP(NROW,MCOL)=40
      ISMAX=NROW*MCOL+10
      DO 1024 IS=1,ISMAX
      READ(5,1000)N,M,IPP
      IF(N.EQ.0) GOTO 1025
      IP(N,M)=IPP
      II=IP(N,M)/10
      IF(II.EQ.4) GOTO 1024
      IND(N,M,2)=211
      IND(N,M,3)=212
      IND(N,M,4)=121
      IND(N,M,5)=122
 1024 CONTINUE
 1025 CONTINUE
      READ(5,1010)XNORM
      READ(5,1010)(XI(K),K=1,KGROUP)
      DO 1050 JJ=1,JMAX
      READ(5,1000) J
      READ(5,1010)(DI(K,J),K=1,KGROUP)
      READ(5,1010)(SR(K,J),K=1,KGROUP)
      READ(5,1010)(SF(K,J),K=1,KGROUP)
      READ(5,1010)(ST(K,J),K=1,K1)
```

```
1050 CONTINUE
     READ(5,1010)(HN(N),N=1,NROW1)
     READ(5,1010)(HM(M),M=1,MCOL1)
     DO 1060 N=1,NROW1
1060 READ(5,1000)(JC(N,M),M=1,MCOL1)
     IF(JVMAX.EQ.1.AND.NVN.EQ.1.AND.MVM.EQ.1) GOTO 1083
     DO 1082 JJ=1,JVMAX
     READ(5,1000) J,NVMAX(J),MVMAX(J)
     NVMAX1=NVMAX(J)+1
     MVMAX1=MVMAX(J)+1
     READ(5,1010)(HNV(J,NV),NV=1,NVMAX1)
     READ(5,1010)(HMV(J,MV),MV=1,MVMAX1)
     DO 1082 NV=1,NVMAX1
     READ(5,1000)(JCV(J,NV,MV),MV=1,MVMAX1)
1082 CONTINUE
1083 CONTINUE
     DO 1421 K=1,KGROUP
     DO 1421 N=1,NROW
     DO 1421 M=1,MCOL
1421 TH(K,N,M)=-1000.
     IF(NROW1.LT.2.OR.MCOL1.LT.2) GOTO 1750
     DO 1700 N=2,NROW1
     DO 1700 M=2,MCOL1
     IF(IP(N,M).EQ.40.OR.IP(N,M).EQ.60) GOTO 1700
     JA=JC(N,M-1)
     JAA=JC(N-1,M-1)
     JB=JC(N,M)
     JBB=JC(N-1,M)
     IF(JA    ) 1430,1430,1450
1430 DO 1440 K=1,KGROUP
1440 DA(K)=DI(K,-JA)
     GOTO 1470
1450 MVA=MVMAX(JA    )+1
     JA=JCV(JA,1,MVA)
     DO 1460 K=1,KGROUP
1460 DA(K)=DI (K,JA)
1470 IF(JAA    ) 1480,1480,1500
1480 DO 1490 K=1,KGROUP
1490 DAA(K)=DI(K,-JAA)
     GOTO 1520
1500 NVA=NVMAX(JAA    )+1
     MVA=MVMAX(JAA    )+1
     JAA=JCV(JAA,NVA,MVA)
     DO 1510 K=1,KGROUP
1510 DAA(K)=DI (K,JAA)
1520 IF(JB    ) 1530,1530,1550
1530 DO 1540 K=1,KGROUP
1540 DB(K)=DI(K,-JB)
     GOTO 1570
1550 JB=JCV(JB,1,1)
     DO 1560 K=1,KGROUP
1560 DB(K)=DI (K,JB)
1570 IF(JBB    ) 1580,1580,1600
1580 DO 1590 K=1,KGROUP
1590 DBB(K)=DI(K,-JBB)
     GOTO 1620
```

```
163     1600 NVA=NVMAX(JBB    )+1
164          JBB=JCV(JBB,NVA,1)
165          DO 1610 K=1,KGROUP
166     1610 DBB(K)=DI (K,JBB)
167     1620 IF(IP(N,M).EQ.50.OR.IP(N,M).EQ.51.OR.IP(N,M).EQ.61) GOTO 1670
168          IF(IP(N,M).EQ.41) GOTO 1675
169          IF(IP(N,M).EQ.421) GOTO 1655
170          IF(IP(N,M).EQ.422) GOTO 1635
171          ABS1=DA(KGROUP)/DB(KGROUP)
172          ABS2=DAA(KGROUP)/DBB(KGROUP)
173          IF(ABS(ABS1-ABS2).GT.1.0E-04) GOTO 1663
174          IF(ABS(1.0-ABS1).GT.1.0E-04) GOTO 1630
175          ABS1=DA(KGROUP)/DAA(KGROUP)
176          IF(ABS(1.0-ABS1).GT.1.0E-04) GOTO 1650
177          IP(N,M)=40
178          GOTO 1700
179     1630 IP(N,M)=422
180          IF(JA.LT.0.AND.JB.LT.0) GOTO 1635
181          IP(N,M)=51
182          IND(N,M,4)=121
183          IND(N,M,5)=122
184     1635 DO 1640 K=1,KGROUP
185     1640 TH(K,N,M)=(DA(K)+DB(K))/2.0
186          GOTO 1700
187     1650 IP(N,M)=421
188          IF(JA.LT.0.AND.JAA.LT.0) GOTO 1655
189          IP(N,M)=51
190          IND(N,M,2)=211
191          IND(N,M,3)=212
192     1655 DO 1660 K=1,KGROUP
193     1660 TH(K,N,M)=(DA(K)+DAA(K))/2.0
194          GOTO 1700
195     1663 IP(N,M)=41
196          IF(JA.LT.0.AND.JAA.LT.0.AND.JB.LT.0.AND.JBB.LT.0) GOTO 1675
197          IP(N,M)=61
198          IND(N,M,2)=211
199          IND(N,M,3)=212
200          IND(N,M,4)=121
201          IND(N,M,5)=122
202          GOTO 1675
203     1670 IF(IP(N,M).EQ.61) GOTO 1675
204          IF(ABS(DA(KGROUP)-DAA(KGROUP)).LT.1.0E-04) GOTO 1672
205          IND(N,M,4)=120
206          IND(N,M,5)=0
207          GOTO 1673
208     1672 IND(N,M,2)=210
209          IND(N,M,3)=0
210     1673 IF(IP(N,M).EQ.50) GOTO 1700
211     1675 DO 1680 K=1,KGROUP
212     1680 TH(K,N,M)=(DA(K)+DAA(K)+DB(K)+DBB(K))/4.0
213     1700 CONTINUE
214     1750 CONTINUE
215          IF(MCOL1.LT.2) GOTO 2150
216          DO 2100 M=2,MCOL1
217          IF(IP(1,M).EQ.40) GOTO 1930
218          IF(IP(1,M).EQ.50) GOTO 1925
```

```
219          JA=JC(1,M-1)
220          JB=JC(1,M)
221          IF(JA    ) 1810,1810,1830
222      1810 DO 1820 K=1,KGROUP
223      1820 DA(K)=DI(K,-JA)
224          GOTO 1850
225      1830 MVA=MVMAX(JA    )+1
226          JA=JCV(JA,1,MVA)
227          DO 1840 K=1,KGROUP
228      1840 DA(K)=DI (K,JA)
229      1850 IF(JB    ) 1860,1860,1880
230      1860 DO 1870 K=1,KGROUP
231      1870 DB(K)=DI(K,-JB)
232          GOTO 1900
233      1880 JB=JCV(JB,1,1)
234          DO 1890 K=1,KGROUP
235      1890 DB(K)=DI (K,JB)
236      1900 IF(IP(1,M).EQ.41.OR.IP(1,M).EQ.51) GOTO 1915
237          IF(IP(1,M).EQ.422) GOTO 1915
238          IF(ABS(DA(KGROUP)-DB(KGROUP)).GT.1.0E-04.AND.BT.GT.0.5)GOTO 1910
239          IP(1,M)=40
240          GOTO 1930
241      1910 IP(1,M)=422
242          IF(JA.LT.0.AND.JB.LT.0) GOTO 1915
243          IP(1,M)=51
244          IND(1,M,4)=121
245          IND(1,M,5)=122
246      1915 DO 1920 K=1,KGROUP
247      1920 TH(K,1,M)=(DA(K)+DB(K))/2.0
248      1925 IND(1,M,2)=210
249          IND(1,M,3)=0
250      1930 CONTINUE
251          IF(IP(NROW,M).EQ.40) GOTO 2100
252          IF(IP(NROW,M).EQ.50) GOTO 2095
253          JA=JC(NROW1,M-1)
254          JB=JC(NROW1,M)
255          IF(JA    ) 1950,1950,1970
256      1950 DO 1960 K=1,KGROUP
257      1960 DA(K)=DI(K,-JA)
258          GOTO 1990
259      1970 NVA=NVMAX(JA    )+1
260          MVA=MVMAX(JA    )+1
261          JA=JCV(JA,NVA,MVA)
262          DO 1980 K=1,KGROUP
263      1980 DA(K)=DI (K,JA)
264      1990 IF(JB    ) 2000,2000,2020
265      2000 DO 2010 K=1,KGROUP
266      2010 DB(K)=DI(K,-JB)
267          GOTO 2040
268      2020 NVA=NVMAX(JB    )+1
269          JB=JCV(JB,NVA,1)
270          DO 2030 K=1,KGROUP
271      2030 DB(K)=DI (K,JB)
272      2040 IF(IP(NROW,M).EQ.41.OR.IP(NROW,M).EQ.51) GOTO 2055
273          IF(IP(NROW,M).EQ.422) GOTO 2055
274          IF(ABS(DA(KGROUP)-DB(KGROUP)).GT.1.0E-04.AND.BB.GT.0.5) GOTO 2050
```

```
      IP(NROW,M)=40
      GOTO 2100
 2050 IP(NROW,M)=422
      IF(JA.LT.0.AND.JB.LT.0) GOTO 2055
      IP(NROW,M)=51
      IND(NROW,M,4)=121
      IND(NROW,M,5)=122
 2055 DO 2060 K=1,KGROUP
 2060 TH(K,NROW,M)=(DA(K)+DB(K))/2.0
 2095 IND(NROW,M,2)=210
      IND(NROW,M,3)=0
 2100 CONTINUE
 2150 CONTINUE
      IF(NROW1.LT.2) GOTO 2500
      DO 2480 N=2,NROW1
      IF(IP(N,1).EQ.40) GOTO 2350
      IF(IP(N,1).EQ.50) GOTO 2345
      JA=JC(N-1,1)
      JB=JC(N,1)
      IF(JA    ) 2210,2210,2230
 2210 DO 2220 K=1,KGROUP
 2220 DA(K)=DI(K,-JA)
      GOTO 2250
 2230 NVA=NVMAX(JA    )+1
      JA=JCV(JA,NVA,1)
      DO 2240 K=1,KGROUP
 2240 DA(K)=DI (K,JA)
 2250 IF(JB    ) 2260,2260,2280
 2260 DO 2270 K=1,KGROUP
 2270 DB(K)=DI(K,-JB)
      GOTO 2300
 2280 JB=JCV(JB,1,1)
      DO 2290 K=1,KGROUP
 2290 DB(K)=DI (K,JB)
 2300 IF(IP(N,1).EQ.41.OR.IP(N,1).EQ.51) GOTO 2315
      IF(IP(N,1).EQ.421) GOTO 2315
      IF(ABS(DA(KGROUP)-DB(KGROUP)).GT.1.0E-04.AND.BL.GT.0.5) GOTO 2310
      IP(N,1)=40
      GOTO 2350
 2310 IP(N,1)=421
      IF(JA.LT.0.AND.JB.LT.0) GOTO 2315
      IP(N,1)=51
      IND(N,1,2)=211
      IND(N,1,3)=212
 2315 DO 2320 K=1,KGROUP
 2320 TH(K,N,1)=(DA(K)+DB(K))/2.0
 2345 IND(N,1,4)=120
      IND(N,1,5)=0
 2350 CONTINUE
      IF(IP(N,MCOL).EQ.40) GOTO 2480
      IF(IP(N,MCOL).EQ.50) GOTO 2475
      JA=JC(N-1,MCOL1)
      JB=JC(N,MCOL1)
      IF(JA    ) 2370,2370,2390
 2370 DO 2380 K=1,KGROUP
 2380 DA(K)=DI(K,-JA)
```

```
331           GOTO 2400
332       2390 NVA=NVMAX(JA    )+1
333           MVA=MVMAX(JA    )+1
334           JA=JCV(JA,NVA,MVA)
335           DO 2395 K=1,KGROUP
336       2395 DA(K)=DI (K,JA)
337       2400 IF(JB    ) 2410,2410,2430
338       2410 DO 2420 K=1,KGROUP
339       2420 DB(K)=DI(K,-JB)
340           GOTO 2450
341       2430 MVA=MVMAX(JB    )+1
342           JB=JCV(JB,1,MVA)
343           DO 2440 K=1,KGROUP
344       2440 DB(K)=DI (K,JB)
345       2450 IF(IP(N,MCOL).EQ.41.OR.IP(N,MCOL).EQ.51) GOTO 2475
346           IF(IP(N,MCOL).EQ.421) GOTO 2465
347           IF(ABS(DA(KGROUP)-DB(KGROUP)).GT.1.0E-04.AND.BR.GT.0.5) GOTO 2460
348           IP(N,MCOL)=40
349           GOTO 2480
350       2460 IP(N,MCOL)=421
351           IF(JA.LT.0.AND.JB.LT.0) GOTO 2465
352           IP(N,MCOL)=51
353           IND(N,MCOL,2)=211
354           IND(N,MCOL,3)=212
355       2465 DO 2470 K=1,KGROUP
356       2470 TH(K,N,MCOL)=(DA(K)+DB(K))/2.0
357       2475 IND(N,MCOL,4)=120
358           IND(N,MCOL,5)=0
359       2480 CCNTINUE
360       2500 CONTINUE
361           DO 2560 M=1,MCOL
362           IF(BT-0.5)2510,2510,2520
363       2510 IND(1,M,1)=0
364           IND(1,M,3)=0
365           IND(1,M,4)=0
366           IND(1,M,5)=0
367           GOTO 2530
368       2520 IND(1,M,2)=0
369           IND(1,M,3)=0
370           IND(1,M,6)=0
371       2530 IF(BB-0.5)2540,2540,2550
372       2540 IND(NROW,M,1)=0
373           IND(NROW,M,3)=0
374           IND(NROW,M,4)=0
375           IND(NROW,M,5)=0
376           GOTO 2560
377       2550 IND(NROW,M,2)=0
378           IND(NROW,M,3)=0
379           IND(NROW,M,6)=0
380       2560 CONTINUE
381           DO 2620 N=1,NROW
382           IF(BL-0.5)2570,2570,2580
383       2570 IND(N,1,1)=0
384           IND(N,1,2)=0
385           IND(N,1,3)=0
386           IND(N,1,5)=0
```

```
387           GOTO 2590
388       2580 IND(N,1,4)=0
389           IND(N,1,5)=0
390           IND(N,1,6)=0
391       2590 IF(BR-0.5)2600,2600,2610
392       2600 IND(N,MCOL,1)=0
393           IND(N,MCOL,2)=0
394           IND(N,MCOL,3)=0
395           IND(N,MCOL,5)=0
396           GOTO 2620
397       2610 IND(N,MCOL,4)=0
398           IND(N,MCOL,5)=0
399           IND(N,MCOL,6)=0
400       2620 CONTINUE
401           L=0
402           DO 2800 N=1,NROW
403           DO 2800 M=1,MCOL
404           DO 2800 I=1,6
405           IF(IND(N,M,I).LE.0) GOTO 2800
406           L=L+1
407           IND(N,M,I)=IND(N,M,I)+1000*L
408       2800 CONTINUE
409           LMAX=L
410           LMAX1=LMAX-1
411           L1=1
412           L2=L1+KGROUP*LMAX
413           L3=L2+ KGROUP*LMAX
414           L4=L3+ K1*LMAX
415           CALL COEFF(LXIN,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
          1JVMAX,NVN,MVM,LMAX,LXMAX,
          1LXCMAX,LXFMAX,A,AR(L1),AR(L2),AR(L3),AR(L4),F1,F,S,DI,SR,SF,ST,HN,
          2HM,HNV,HMV,DA,DAA,DB,DBB,D1,D2,
          3                    IND,TH,LXD,LXDF,LLX,LLXF,JC,JCV,NVMAX,MVMAX,IP)
416           CALL CHLSKY(LXIN,EPSCH,KGROUP,LMAX,LXMAX,LXCMAX,A,AR(L1),AR(L3),
          1LXD,LXDC,LLX,LLXC)
417           CALL APRINT(MSIZE,MSIZE1,NRUN1,ICMAX,NCONV,EPSF,EPSL,EPSCH,BL,BR,
          1BT,BB,JMAX,XNORM,NROW,MCOL,KGROUP,LMAX,LXMAX,LXCMAX,LXFMAX,
          2JVMAX,NVN,MVM,IND,IP)
418           CALL BPRINT(NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,JVMAX,NVN,MVM,
          1        AR(L1),XI,DI,SR,SF,ST,HN,HM,HNV,HMV,JC,JCV,NVMAX,MVMAX)
419           L3=L2+LMAX
420           L4=L3+LMAX
421           CALL OUTIT(NP,IOUT,NCONV,EPSF,EPSL,NROW,MCOL,KGROUP,K1,
          1LMAX,LXMAX,
          1LXCMAX,LXFMAX,A,AR(L1),AR(L2),AR(L3),AR(L4),F1,F,S,IND,LXD,LXDC,
          2LXDF,LLX,LLXC,LLXF)
422           L=LXMAX/2
423           LC=LXCMAX/2
424           LF=LXFMAX/2
425           LS=KGROUP*NROW1*MCOL1+5
426           ICMAX1=ICMAX
427           IF(ICMAX.LE.0) ICMAX1=1
428           CALL EXPAN(ICMAX,ICMAX1,XNORM,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,
          1JMAX,JVMAX,NVN,MVM,LMAX,ICLPS,
          1      A(1,1),AR(L1),AR(L2),AR(L3),AR(L4),F1(1),F1(L),F(1,1),
          2F(1,LF),S(1,1),S(1,LS),XI,DI,SR,SF,ST,HN,HM,HNV,HMV,
```

```
     3 IND,TH,JC,JCV,NVMAX,MVMAX,LXD,LXDC,LXDF,LLX,LLXC,IP)
429    RETURN
430    END
```

```
      SUBROUTINE COEFF(LXIN,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
     1JVMAX,NVN,MVM,LMAX,
     1LXMAX,LXCMAX,LXFMAX,A,AA,AF,AS,IFLAG,F1,F,S,DI,SR,SF,ST,HN,HM,
     2HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,
     2IND,TH,LXD,LXDF,LLX,LLXF,JC,JCV,NVMAX,MVMAX,IP)
      REAL*8 A(KGROUP,LXCMAX),AA(KGROUP,LMAX),AF(KGROUP,LMAX),
     1AS(K1,LMAX)
      INTEGER*2 LXD(LMAX),LXDF(LMAX),LLX(LXMAX),LLXF(LXFMAX),
     1JC(NROW1,MCOL1)
      INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
      INTEGER*2 IP(NROW,MCOL)
      COMMON/COM11/L,LL,NI,NNI,MI,MMI,NS,NNS,MS,MMS,NA,MA,LLMIN,LLMAX
      DIMENSION DI(KGROUP,JMAX),SR(KGROUP,JMAX),SF(KGROUP,JMAX),
     1ST(K1,JMAX)
      DIMENSION HN(NROW1),HM(MCOL1)
      DIMENSION IND(NROW,MCOL,6),TH(KGROUP,NROW,MCOL)
      DIMENSION F1(LXMAX),F(K1,LXFMAX),S(K1,LXFMAX)
      DIMENSION IFLAG(LMAX)
      DIMENSION HNV(JVMAX,NVN),HMV(JVMAX,MVM),D1(KGROUP),D2(KGROUP),
     1TDN1(KGROUP),TDN2(KGROUP),TDM1(KGROUP),TDM2(KGROUP)
      DO 1000 LL=1,LMAX
      IFLAG(LL)=0
      DO 1000 K=1,KGROUP
      AA(K,LL)=0.0
      AF(K,LL)=0.0
 1000 IF(K.LE.K1) AS(K,LL)=0.0
      LX=0
      LXF=0
      DO 1500 N=1,NROW
      DO 1500 M=1,MCOL
      DO 1500 I=1,6
      L=IND(N,M,I)/1000
      IF(L.LE.0) GOTO 1500
      NI=(IND(N,M,I) -1000*L)/100
      MI=(IND(N,M,I)-1000*L-100*NI)/10
      NMIN=N-1
      NMAX=N+1
      IF(NMIN.LT.1) NMIN=1
      IF(NMAX.GT.NROW) NMAX=NROW
      MMIN=M-1
      MMAX=M+1
      IF(MMIN.LT.1) MMIN=1
      IF(MMAX.GT.MCOL) MMAX=MCOL
      NSMIN=1
      NSMAX=2
      MSMIN=1
      MSMAX=2
      IS=IND(N,M,I)-1000*L-100*NI-10*MI
      IF(IS.GT.0.AND.NI.EQ.2) GOTO 1010
      IF(IS.GT.0.AND.MI.EQ.2) GOTO 1020
      GOTO 1030
 1010 NSMIN=IS
      NSMAX=IS
      NMIN=N+(2*IS-3)
      NMAX=NMIN
      GOTO 1030
```

```
479     1020 MSMIN=IS
480          MSMAX=IS
481          MMIN=M+(2*IS-3)
482          MMAX=MMIN
483     1030 CONTINUE
484          LLMIN=L
485          LLMAX=1
486          DO 1180 NS=NSMIN,NSMAX
487          NB=N+(2*NS-3)
488          IF(NB.LT.1.OR.NB.GT.NROW) GOTO 1180
489          NA=N
490          IF(NB.GT.N)NA=NB
491          DO 1160 MS=MSMIN,MSMAX
492          NNS=NS
493          MMS=MS
494          MB=M+(2*MS-3)
495          IF(MB.LT.1.OR.MB.GT.MCOL) GOTO 1160
496          MA=M
497          IF(MB.GT.M)MA=MB
498          DO 1080 II=1,6
499          LL=IND(N,M,II)/1000
500          IF(LL.LE.0) GOTO 1080
501          NNI=(IND(N,M,II)-1000*LL)/100
502          MMI=(IND(N,M,II)-1000*LL-100*NNI)/10
503          IS=IND(N,M,II)-1000*LL-100*NNI-10*MMI
504          IF(IS.GT.0.AND.NNI.EQ.2.AND.IS.NE.NNS) GOTO 1080
505          IF(IS.GT.0.AND.MMI.EQ.2.AND.IS.NE.MMS) GOTO 1080
506          CALL MATRIX(N,M,I,N ,M ,II,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
            1JVMAX,NVN,MVM,
            1      LMAX,AA,AF,AS,IFLAG,DI,SR,SF,ST,HN,HM,
            1 HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,IND,TH,JC,JCV,NVMAX,MVMAX,IP)
507     1080 CONTINUE
508          NNS=(N-NB+3)/2
509          MMS=(M-MB+3)/2
510          DO 1140 II=1,6
511          LL=IND(NB,MB,II)/1000
512          IF(LL.LE.0) GOTO 1140
513          NNI=(IND(NB,MB,II)-1000*LL)/100
514          MMI=(IND(NB,MB,II)-1000*LL-100*NNI)/10
515          IS=IND(NB,MB,II)-1000*LL-100*NNI-10*MMI
516          IF(IS.GT.0.AND.NNI.EQ.2.AND.IS.NE.NNS) GOTO 1140
517          IF(IS.GT.0.AND.MMI.EQ.2.AND.IS.NE.MMS) GOTO 1140
518          CALL MATRIX(N,M,I,NB,MB,II,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
            1JVMAX,NVN,MVM,
            1      LMAX,AA,AF,AS,IFLAG,DI,SR,SF,ST,HN,HM,
            1 HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,IND,TH,JC,JCV,NVMAX,MVMAX,IP)
519     1140 CONTINUE
520     1160 CONTINUE
521     1180 CONTINUE
522          DO 1280 NS=NSMIN,NSMAX
523          NNS=NS
524          NB=N+(2*NS-3)
525          IF(NB.LT.1.OR.NB.GT.NROW) GOTO 1280
526          NA=N
527          IF(NB.GT.N)NA=NB
528          DO 1260 MM=MMIN,MMAX
```

```
529           IF(M.EQ.MM) GOTO 1260
530           MA=M
531           IF(MM.GT.M)MA=MM
532           MS=(MM-M+3)/2
533           MMS=(M-MM+3)/2
534           DO 1240 II=1,6
535           LL=IND(N,MM,II)/1000
536           IF(LL.LE.0) GOTO 1240
537           NNI=(IND(N,MM,II)-1000*LL)/100
538           MMI=(IND(N,MM,II)-1000*LL-100*NNI)/10
539           IS=IND(N,MM,II)-1000*LL-100*NNI-10*MMI
540           IF(IS.GT.0.AND.NNI.EQ.2.AND.IS.NE.NNS) GOTO 1240
541           IF(IS.GT.0.AND.MMI.EQ.2.AND.IS.NE.MMS) GOTO 1240
542           CALL MATRIX(N,M,I,N ,MM,II,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
             1JVMAX,NVN,MVM,
             1      LMAX,AA,AF,AS,IFLAG,DI,SR,SF,ST,HN,HM,
             1 HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,IND,TH,JC,JCV,NVMAX,MVMAX,IP)
543       1240 CONTINUE
544       1260 CONTINUE
545       1280 CONTINUE
546           DO 1440 MS=MSMIN,MSMAX
547           MMS=MS
548           MB=M+(2*MS-3)
549           IF(MB.LT.1.OR.MB.GT.MCOL) GOTO 1440
550           MA=M
551           IF(MB.GT.M)MA=MB
552           DO 1420 NN=NMIN,NMAX
553           IF(N.EQ.NN) GOTO 1420
554           NA=N
555           IF(NN.GT.N)NA=NN
556           NS=(NN-N+3)/2
557           NNS=(N-NN+3)/2
558           DO 1400 II=1,6
559           LL=IND(NN,M,II)/1000
560           IF(LL.LE.0) GOTO 1400
561           NNI=(IND(NN,M,II)-1000*LL)/100
562           MMI=(IND(NN,M,II)-1000*LL-100*NNI)/10
563           IS=IND(NN,M,II)-1000*LL-100*NNI-10*MMI
564           IF(IS.GT.0.AND.NNI.EQ.2.AND.IS.NE.NNS) GOTO 1400
565           IF(IS.GT.0.AND.MMI.EQ.2.AND.IS.NE.MMS) GOTO 1400
566           CALL MATRIX(N,M,I,NN,M ,II,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,
             1JVMAX,NVN,MVM,
             1      LMAX,AA,AF,AS,IFLAG,DI,SR,SF,ST,HN,HM,
             1 HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,IND,TH,JC,JCV,NVMAX,MVMAX,IP)
567       1400 CONTINUE
568       1420 CONTINUE
569       1440 CONTINUE
570           DO 1490 LL=LLMIN,L
571           IF(IFLAG(LL).LT.1) GOTO 1490
572           IFLAG(LL)=0
573           LX=LX+1
574           LXF=LXF+1
575           LLX(LX)=LL
576           LLXF(LXF)=LL
577           DO 1480 K=1,KGROUP
578           A(K,LX     )=AA(K,LL)
```

```
579           AA(K,LL)=0.0
580           IF(K-1) 1450,1450,1460
581      1450 F1(LX)=AF(K,LL)
582           GOTO 1470
583      1460 F(K-1,LXF)=AF(K,LL)
584      1470 AF(K,LL)=0.0
585           IF(K.EQ.KGROUP) GOTO 1480
586           S(K,LXF)=AS(K,LL)
587           AS(K,LL)=0.0
588      1480 CONTINUE
589      1490 CONTINUE
590           LXD(L)=LX
591           IF(L.EQ.LMAX) GOTO 1498
592           L1=L+1
593           DO 1495 LL=L1,LLMAX
594           IF(IFLAG(LL).LT.1) GOTO 1495
595           IFLAG(LL)=0
596           LXF=LXF+1
597           LLXF(LXF)=LL
598           DO 1493 K=1,K1
599           F(K,LXF)=AF(K+1,LL)
600           AF(K+1,LL)=0.0
601           S(K,LXF)=AS(K,LL)
602      1493 AS(K,LL)=0.0
603      1495 CONTINUE
604      1498 LXDF(L)=LXF
605      1500 CONTINUE
606           LXMAX=LX
607           LXFMAX=LXF
608           LXIN=LXCMAX-LXMAX
609           DO 1600 LXM=1,LXMAX
610           LX=LXMAX-LXM+1
611           DO 1600 K=1,KGROUP
612           A(K,LX+LXIN)=A(K,LX)
613      1600 A(K,LX)=0.0
614           RETURN
615           END
```

```
616          SUBROUTINE MATRIX(N,M,I,NN,MM,II,NROW,NRCW1,MCOL,MCOL1,KGROUP,K1,
            1JMAX,JVMAX,NVN,MVM,LMAX,AA,AF,AS,IFLAG,
            2DI,SR,SF,ST,HN,HM,HNV,HMV,D1,D2,TDN1,TDN2,TDM1,TDM2,
            3IND,TH,JC,JCV,NVMAX,MVMAX,IP)
617          REAL*8 AA(KGROUP,LMAX),AF(KGROUP,LMAX),AS(K1,LMAX)
618          REAL*8 HNV1,HNV2,HMV1,HMV2,XN,XDN,XM,XDM,XF,XD,XFV,XDV
619          INTEGER*2 JC(NROW1,MCOL1)
620          INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
621          INTEGER*2 IP(NROW,MCOL)
622          COMMON/COM11/L,LL,NI,NNI,MI,MMI,NS,NNS,MS,MMS,NA,MA,LLMIN,LLMAX
623          DIMENSION IFLAG(LMAX)
624          DIMENSION DI(KGROUP,JMAX),SR(KGROUP,JMAX),SF(KGROUP,JMAX),
            1ST(K1,JMAX)
625          DIMENSION HN(NROW1),HM(MCOL1)
626          DIMENSION IND(NROW,MCOL,6),TH(KGROUP,NROW,MCOL)
627          DIMENSION HNV(JVMAX,NVN),HMV(JVMAX,MVM),D1(KGROUP),D2(KGROUP),
            1TDN1(KGROUP),TDN2(KGROUP),TDM1(KGROUP),TDM2(KGROUP)
628          IF(LL.LT.LLMIN) LLMIN=LL
629          IF(LL.GT.LLMAX) LLMAX=LL
630          IFLAG(LL)=1
631          JA=JC(NA-1,MA-1)
632          IF(JA    ) 900,900,920
633      900 DO 910 K=1,KGROUP
634          D1(K)=DI(K,-JA)
635      910 D2(K)=DI(K,-JA)
636          GOTO 940
637      920 NV1=1
638          NV2=1
639          MV1=1
640          MV2=1
641          NVMAX1=NVMAX(JA    )+1
642          MVMAX1=MVMAX(JA    )+1
643          IF((NA-1).LT.N) NV1=NVMAX1
644          IF((NA-1).LT.NN) NV2=NVMAX1
645          IF((MA-1).LT.M) MV1=MVMAX1
646          IF((MA-1).LT.MM) MV2=MVMAX1
647          JA1=JCV(JA,NV1,MV1)
648          JA2=JCV(JA,NV2,MV2)
649          DO 930 K=1,KGROUP
650          D1(K)=DI (K,JA1)
651      930 D2(K)=DI (K,JA2)
652      940 DO 1020 K=1,KGROUP
653          TDN1(K)=1.0
654          TDM1(K)=1.0
655          TDN2(K)=1.0
656          TDM2(K)=1.0
657          GOTO (1010,1002,1010,1004,1010,1006), I
658     1002 IF(IP(N,M).EQ.421)                          TDN1(K)=TH(K,N,M)/D1(K)
659          GOTO 1010
660     1004 IF(IP(N,M).EQ.422)                          TDM1(K)=TH(K,N,M)/D1(K)
661          GOTO 1010
662     1006 IF(TH(K,N,M).GT..0) TDN1(K)=TH(K,N,M)/D1(K)
663     1010 CONTINUE
664          GOTO (1020,1012,1020,1014,1020,1016), II
665     1012 IF(IP(NN,MM).EQ.421)
            2TDN2(K)=TH(K,NN,MM)/D2(K)
```

```
666           GOTO 1020
667     1014  IF(IP(NN,MM).EQ.422)
             2TDM2(K)=TH(K,NN,MM)/D2(K)
668           GOTO 1020
669     1016  IF(TH(K,NN,MM).GT..0)
             2TDN2(K)=TH(K,NN,MM)/D2(K)
670     1020  CONTINUE
671           DO 1100 K=1,KGROUP
672           IF(LL.GT.L) GOTO 1021
673           IF(JA    ) 10201,10201,10203
674    10201  XN=XF(NI,NS,NNI  , NNS,TDN1(K),TDN2(K))*HN(NA-1)**(NI+NNI -1)
675           XDN=XD(NI,NS,NNI,NNS,TDN1(K),TDN2(K))*HN(NA-1)**(NI+NNI-3)
676           XM=XF(MI,MS,MMI  , MMS,TDM1(K),TDM2(K))*HM(MA-1)**(MI+MMI -1)
677           XDM=XD(MI,MS,MMI,MMS,TDM1(K),TDM2(K))*HM(MA-1)**(MI+MMI-3)
678           AA(K,LL )=AA(K,LL)+ SR(K,-JA)*XN*XM+DI(K,-JA)*(XN*XDM+XM*XDN)
679           GOTO 1021
680    10203  HNV1=0.0
681           DO 10208 NV=1,NVMAX1
682           HNV2=HNV1+HNV(JA    ,NV)
683           HMV1=0.0
684           DO 10205 MV=1,MVMAX1
685           HMV2=HMV1+HMV(JA    ,MV)
686           XN =XFV(NI,NS,NNI,NNS,HN(NA-1),HNV1,HNV2,TDN1(K),TDN2(K))
687           XDN=XDV(NI,NS,NNI,NNS,HN(NA-1),HNV1,HNV2,TDN1(K),TDN2(K))
688           XM =XFV(MI,MS,MMI,MMS,HM(MA-1),HMV1,HMV2,TDM1(K),TDM2(K))
689           XDM=XDV(MI,MS,MMI,MMS,HM(MA-1),HMV1,HMV2,TDM1(K),TDM2(K))
690           JAV=JCV(JA,NV,MV)
691           AA(K,LL)=AA(K,LL)+SR (K,JAV         )*XN*XM + DI (K,JAV         )*
             1(XN*XDM+XM*XDN)
692    10205  HMV1=HMV2
693    10208  HNV1=HNV2
694     1021  IF(K.NE.1) GOTO 1050
695           IF(JA    ) 1031,1031,1033
696     1031  DO 1032 KK=1,KGROUP
697           IF(KK. EQ.1.AND.LL.GT.L) GOTO 1032
698           XN=XF(NI,NS,NNI  , NNS,TDN1(K),TDN2(KK))*HN(NA-1)**(NI+NNI -1)
699           XM=XF(MI,MS,MMI  , MMS,TDM1(K),TDM2(KK))*HM(MA-1)**(MI+MMI -1)
700           AF(KK,LL)=AF(KK,LL)+SF(KK,-JA)*XN*XM
701     1032  CONTINUE
702           GOTO 1040
703     1033  DO 1039 KK=1,KGROUP
704           IF(KK.EQ.1.AND.LL.GT.L) GOTO 1039
705           HNV1=0.0
706           DO 1038 NV=1,NVMAX1
707           HNV2=HNV1+HNV(JA    ,NV)
708           HMV1=0.0
709           DO 1035 MV=1,MVMAX1
710           HMV2=HMV1+HMV(JA    ,MV)
711           JAV=JCV(JA,NV,MV)
712           IF(SF(KK,JAV).LT.1.0E-04) GOTO 1035
713           XN =XFV(NI,NS,NNI,NNS,HN(NA-1),HNV1,HNV2,TDN1(K),TDN2(KK))
714           XM =XFV(MI,MS,MMI,MMS,HM(MA-1),HMV1,HMV2,TDM1(K),TDM2(KK))
715           AF(KK,LL)=AF(KK,LL)+SF (KK,JAV         )*XN*XM
716     1035  HMV1=HMV2
717     1038  HNV1=HNV2
718     1039  CONTINUE
```

```
719     1040 CONTINUE
720          GOTO 1100
721     1050 CONTINUE
722          IF(JA    ) 1061,1061,1062
723     1061 XN=XF(NI,NS,NNI  , NNS,TDN1(K),TDN2(K-1))*HN(NA-1)**(NI+NNI -1)
724          XM=XF(MI,MS,MMI  , MMS,TDM1(K),TDM2(K-1))*HM(MA-1)**(MI+MMI -1)
725          AS(K-1,LL)=AS(K-1,LL)+ST(K-1,-JA)*XN*XM
726          GOTO 1100
727     1062 HNV1=0.0
728          DO 1068 NV=1,NVMAX1
729          HNV2=HNV1+HNV(JA    ,NV)
730          HMV1=0.0
731          DO 1065 MV=1,MVMAX1
732          HMV2=HMV1+HMV(JA    ,MV)
733          XN =XFV(NI,NS,NNI,NNS,HN(NA-1),HNV1,HNV2,TDN1(K),TDN2(K-1))
734          XM =XFV(MI,MS,MMI,MMS,HM(MA-1),HMV1,HMV2,TDM1(K),TDM2(K-1))
735          JAV=JCV(JA,NV,MV)
736          AS(K-1,LL)=AS(K-1,LL)+ST (K-1,JAV          )*XN*XM
737     1065 HMV1=HMV2
738     1068 HNV1=HNV2
739     1100 CONTINUE
740          RETURN
741          END
```

```
      SUBROUTINE CHLSKY(LXIN,EPSCH,KGROUP,LMAX,LXMAX,LXCMAX,E,SUM,EAUX,
     1LXD,LXDC,LLX,LLXC)
      REAL*8 E(KGROUP,LXCMAX)
      REAL*8 SUM(KGROUP,LMAX),EAUX(KGROUP),DSQRT,DABS
      INTEGER*2 LXD(LMAX),LXDC(LMAX),LLX(LXMAX),LLXC(LXCMAX)
      DO 1050 K=1,KGROUP
      DO 1050 LL=1,LMAX
1050  SUM(K,LL)=0.0
      LXC=1
      LXDC(1)=1
      LLXC(1)=1
      DO 1100 K=1,KGROUP
1100  E(K,1)=DSQRT(E(K,LXIN+1))
      DO 1500 L=2,LMAX
      LXA=LXD(L-1)+2
      LLMIN=LLX(LXA-1)
      DO 1120 K=1,KGROUP
      DO 1120 LL=LLMIN,L
1120  SUM(K,LL)=0.0
      LXB=LXD(L)
      LXCA=LXDC(L-1)+1
      IFLAG=0
      LL=LLX(LXA-1)
      LXC1=LXDC(LL)
      LXC=LXC+1
      LLXC(LXC)=LL
      DO 1110 K=1,KGROUP
1110  E(K,LXC)=E(K,LXA-1+LXIN)/E(K,LXC1)
      DO 1500 LLX1=LXA,LXB
      LLMAX=LLX(LLX1)
      LLMIN=LLMIN+1
      DO 1470 LL=LLMIN,LLMAX
      IF(L-LL)1140,1125,1140
1125  DO 1130 LLLX1=LXCA,LXC
      DO 1130 K=1,KGROUP
      SUM(K,LL)=SUM(K,LL)+E(K,LLLX1)**2
1130  EAUX(K)=DSQRT(E(K,LXB+LXIN)-SUM(K,LL))
      LXC=LXC+1
      LXDC(L)=LXC
      GOTO 1220
1140  LLXB=LXDC(LL)
      LLXA=LXDC(LL-1)+1
      IF(LLXC(LLXA).GT.LLXC(LXC)) GOTO 1165
      DO 1160 LLLX1=LLXA,LLXB
      LLL1=LLXC(LLLX1)
      IF(LLL1.GT.LLXC(LXC)) GOTO 1165
      DO 1160 LLLX2=LXCA,LXC
      IF(LLL1.NE.LLXC(LLLX2)) GOTO 1160
      DO 1150 K=1,KGROUP
1150  SUM(K,LL)=SUM(K,LL)+E(K,LLLX1)*E(K,LLLX2)
1160  CONTINUE
1165  IF(LL-LLMAX)1170,1190,1170
1170  DO 1180 K=1,KGROUP
      EAUX(K)=-SUM(K,LL)/E(K,LLXB)
1180  IF(DABS(EAUX(K)).GT.EPSCH) IFLAG=1
      GOTO 1210
```

```
1190 DO 1200 K=1,KGROUP
     EAUX(K)=(E(K,LLX1+LXIN)-SUM(K,LL))/E(K,LLXB)
1200 IF(DABS(EAUX(K)).GT.EPSCH) IFLAG=1
1210 IF(IFLAG.EQ.0) GOTO 1470
     LXC=LXC+1
1220 LLXC(LXC)=LL
     DO 1450 K=1,KGROUP
1450 E(K,LXC)=EAUX(K)
1470 CONTINUE
     LLMIN=LLMAX
1500 CONTINUE
     LXCMAX=LXC
     RETURN
     END
```

```
811          SUBROUTINE OUTIT(NP,IOUT,NCONV,EPSF,EPSL,NROW,MCOL,KGROUP,K1,LMAX,
            1LXMAX,LXCMAX,LXFMAX,E,Y,SS,YI,SUM,F1,F,S,IND,LXD,LXDC,LXDF,LLX,
            2LLXC,LLXF)
812          REAL*8 E(KGROUP,LXCMAX),Y(KGROUP,LMAX),SS(LMAX),YI(LMAX),SUM(LMAX)
813          REAL*8 YNUM,DEN,YLMD1,YLMD2,DABS
814          INTEGER*2 LXD(LMAX),LXDC(LMAX),LXDF(LMAX),LLX(LXMAX),LLXC(LXCMAX),
            1LLXF(LXFMAX)
815          DIMENSION F1(LXMAX),F(K1,LXFMAX),S(K1,LXFMAX)
816          DIMENSION IND(NROW,MCOL,6)
817          LMAX1=LMAX-1
818          IF(NP.GT.0) GOTO 1020
819          DO 1000 KK=1,KGROUP
820          DO 1000 LL=1,LMAX
821     1000 Y(KK,LL)=0.0
822          DO 1011 N=1,NROW
823          DO 1011 M=1,MCOL
824          LL=IND(N,M,1)/1000
825          IF(LL.LE.0) GOTO 1011
826          DO 1010 KK=1,KGROUP
827     1010 Y(KK,LL)=1.0
828     1011 CONTINUE
829          YLIM1=1.0
830          GOTO 1060
831     1020 YLIM1=0.0
832          DO 1030 KK=1,KGROUP
833     1030 READ(5,1040)(Y(KK,LL),LL=1,LMAX)
834     1040 FORMAT(6E12.5)
835          DO 1050 KK=1,KGROUP
836          DO 1050 LL=1,LMAX
837     1050 IF(YLIM1.LT.DABS(Y(KK,LL)))YLIM1=DABS(Y(KK,LL))
838     1060 YLMD1=1.0E 20
839          YLIM2=0.0
840          NCONV1=0
841     1100 NCONV1=NCONV1+1
842          IF(NCONV1.GT.NCONV) GOTO 1500
843          YNUM=0.0
844          DEN=0.0
845          DO 1300 K=1,KGROUP
846          DO 1110 L=1,LMAX
847          SS(L)=0.0
848     1110 YI(  L)=Y(K,L)
849          IF(K.NE.1) GOTO 1210
       C COMPUTATION OF FISSION SOURCE
850          DO 1150 L=1,LMAX
851          LX=LXD(L)
852          SS(L)=SS(L)+F1(LX)*Y(1,L)
853          IF(L.EQ.1) GOTO 1130
854          LX1=LXD(L-1)+1
855          LX2=LX-1
856          DO 1120 LX=LX1,LX2
857          LL=LLX(LX)
858          SS(L)=SS(L)+F1(LX)*Y(1,LL)
859     1120 SS(LL)=SS(LL)+F1(LX)*Y(1,L)
860     1130 LXF1=1
861          IF(L.GT.1) LXF1=LXDF(L-1)+1
862          LXF2=LXDF(L)
```

```
      DO 1150 LXF=LXF1,LXF2
      LL=LLXF(LXF)
      DO 1150 KK=2,KGROUP
 1150 SS(L)=SS(L)+F(KK-1,LXF)*Y(KK,LL)
      GOTO 1250
C COMPUTATION OF SCATTERING SOURCE
 1210 DO 1230 L=1,LMAX
      LXF1=1
      IF(L.GT.1) LXF1=LXDF(L-1)+1
      LXF2=LXDF(L)
      DO 1230 LXF=LXF1,LXF2
      LL=LLXF(LXF)
 1230 SS(L)=SS(L)+S(K-1,LXF)*Y(K-1,LL)
 1250 Y(K,1)=SS(1)/E(K,1)
      DO 1270 L=2,LMAX
      SUM(L)=0.0
      LXC1=LXDC(L-1)+1
      LXC2=LXDC(L)-1
      DO 1260 LXC=LXC1,LXC2
      LL=LLXC(LXC)
 1260 SUM(L)=SUM(L)+E(K,LXC)*Y(K,LL)
      LXC=LXDC(L)
 1270 Y(K,L)=(SS(L)-SUM(L))/E(K,LXC)
      DO 1275 L=1,LMAX
      SUM(L)=0.0
 1275 SS(L)=Y(K,L)
      Y(K,LMAX)=SS(LMAX)/E(K,LXCMAX)
      DO 1285 LA=1,LMAX1
      L=LMAX-LA+1
      LXC1=LXDC(L-1)+1
      LXC2=LXDC(L)-1
      DO 1280 LXC=LXC1,LXC2
      LL=LLXC(LXC)
 1280 SUM(LL)=SUM(LL)+E(K,LXC)*Y(K,L)
      LXC=LXDC(L-1)
      Y(K,L-1)=(SS(L-1)-SUM(L-1))/E(K,LXC)
 1285 CONTINUE
      DO 1290 L=1,LMAX
      YNUM=YNUM+Y(K,L)**2
 1290 DEN=DEN+YI(  L)*Y(K,L)
 1300 CONTINUE
      YLMD2=YNUM/DEN
      DO 1400 K=1,KGROUP
      DO 1400 L=1,LMAX
      Y(K,L)=Y(K,L)/YLMD2
      IF(YLIM2.LT.DABS(Y(K,L)))YLIM2=DABS(Y(K,L))
 1400 CONTINUE
      CALL CPRINT(NCONV1,YLIM1,YLIM2,YLMD1,YLMD2)
      IF(ABS(YLIM2-YLIM1)/YLIM1.LT.EPSF.AND.DABS(YLMD2-YLMD1)/YLMD1
     1.LT.EPSL) GOTO 1500
      YLIM1=YLIM2
      YLIM2=0.0
      YLMD1=YLMD2
      GOTO 1100
 1500 IF(IOUT.LE.0) GOTO 1600
      DO 1550 KK=1,KGROUP
```

```
917     1550 PUNCH 1040, (Y(KK,LL),LL=1,LMAX)
918     1600 RETURN
919          END
```

```
      SUBROUTINE EXPAN(ICMAX,
     1                 ICMAX1,XNORM,NROW,NROW1,MCOL,MCOL1,KGROUP,K1,
     1JMAX,JVMAX,NVN,MVM,LMAX,
     1ICLPS,   X,Y,TDN,TDM,TD,AVS,AVA,AVF,AVD,XINT,FL,XI,DI,SR,SF,ST,HN,
     1HM,HNV,HMV,IND,TH,JC,JCV,NVMAX,MVMAX,ISTR,ISTC,MINR,MINC,KC,IP)
      REAL*8 Y(KGROUP,LMAX)
      INTEGER*2 ISTR(ICMAX1),ISTC(ICMAX1),MINR(ICMAX1),MINC(ICMAX1),
     1KC(ICMAX1),JC(NROW1,MCOL1)
      INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
      INTEGER*2 IP(NROW,MCOL)
      DIMENSION X(KGROUP,NROW,MCOL,6)
      DIMENSION TDN(2,2),TDM(2,2),TD(2,2)
      DIMENSION DI(KGROUP,JMAX),SR(KGROUP,JMAX),SF(KGROUP,JMAX),
     1ST(K1,JMAX),XI(KGROUP)
      DIMENSION AVA(KGROUP,NROW1,MCOL1),AVF(KGROUP,NROW1,MCOL1),
     1AVD(KGROUP,NROW1,MCOL1),AVS(KGROUP,NROW1,MCOL1)
      DIMENSION HN(NROW1),HM(MCOL1)
      DIMENSION IND(NROW,MCOL,6),TH(KGROUP,NROW,MCOL)
      DIMENSION XINT(KGROUP,NROW1,MCOL1)
      DIMENSION HNV(JVMAX,NVN),HMV(JVMAX,MVM)
      DIMENSION FL(13,13)
      IF(ICMAX.LE.0) GOTO 1005
      DO 1003 J=1,ICMAX
 1003 READ(5,1004)JJ,ISTR(JJ),ISTC(JJ),MINR(JJ),MINC(JJ),KC(JJ)
 1004 FORMAT(14I5)
 1005 CONTINUE
      DO 1100 N=1,NROW
      DO 1100 M=1,MCOL
      DO 1100 I=1,6
      L=IND(N,M,I)/1000
      IF(L)1010,1010,1030
 1010 DO 1020 K=1,KGROUP
 1020 X(K,N,M,I)=0.0
      GOTO 1100
 1030 DO 1040 K=1,KGROUP
 1040 X(K,N,M,I)=Y(K,L)
 1100 CONTINUE
      CALL DPRINT(NROW,MCOL,KGROUP,X,IND,IP)
      FISS=0.0
      DO 1205 N=1,NROW1
      DO 1205 M=1,MCOL1
      J =JC(N,M)
      IF(J.LT.0) JA=-J
      DO 1200 K=1,KGROUP
      DO 1108 NI=1,2
      NS=N+NI-1
      IF(J.LT.0) GOTO 1103
      NV=1
      IF(NS.GT.N) NV=NVMAX(J)+1
 1103 CONTINUE
      DO 1108 MI=1,2
      MS=M+MI-1
      IF(J.LT.0) GOTO 1105
      MV=1
      IF(MS.GT.M) MV=MVMAX(J)+1
      JA=JCV(J,NV,MV)
```

```
 969    1105 CONTINUE
 970         TDN(NI,MI)=1.0
 971         TDM(NI,MI)=1.0
 972         TD (NI,MI)=1.0
 973         IF(IP(NS,MS).EQ.421)
            1TDN(NI,MI)=TH(K,NS,MS)/DI(K,JA)
 974         IF(IP(NS,MS).EQ.422)
            1TDM(NI,MI)=TH(K,NS,MS)/DI(K,JA)
 975         IF(TH(K,NS,MS).GT..0)
            1TD(NI,MI)=TH(K,NS,MS)/DI(K,JA)
 976    1108 CONTINUE
 977         XA21=X(K,N,M,2)
 978         IF(IND(N,M,3).GT.0) XA21=X(K,N,M,3)
 979         XB21=X(K,N,M+1,2)
 980         IF(IND(N,M+1,3).GT.0) XB21=X(K,N,M+1,3)
 981         XA12=X(K,N,M,4)
 982         IF(IND(N,M,5).GT.0) XA12=X(K,N,M,5)
 983         XC12=X(K,N+1,M,4)
 984         IF(IND(N+1,M,5).GT.0) XC12=X(K,N+1,M,5)
 985         XINT(K,N,M)=(X(K,N,M,1)+X(K,N,M+1,1)+X(K,N+1,M,1)+X(K,N+1,M+1,1))
            1*HN(N)*HM(M)/4. + (XA21*TDN(1,1)+XB21*TDN(1,2)-X(K,N+1,M,2)*TDN(2,
            21)-X(K,N+1,M+1,2)*TDN(2,2))*(HN(N)**2*HM(M))/24. + (XA12*TDM(1,1)-
            3X(K,N,M+1,4)*TDM(1,2)+XC12*TDM(2,1)-X(K,N+1,M+1,4)*TDM(2,2))*(HN
            4(N)*HM(M)**2)/24. + (X(K,N,M,6)*TD(1,1)-X(K,N,M+1,6)*TD(1,2)-X(K,
            5N+1,M,6)*TD(2,1)+X(K,N+1,M+1,6)*TD(2,2))*(HN(N)**2*HM(M)**2)/144.
 986         IF(J)1110,1110,1140
 987    1110 FISS=FISS+XINT(K,N,M)*SF(K,-J)/XI(K)
 988         AVF(K,N,M)=          SF(K,-J)*XINT(K,N,M)
 989         AVD(K,N,M)=          XINT(K,N,M)/DI(K,-J)
 990         IF(K-KGROUP)1115,1120,1120
 991    1115 SA=SR(K,-J)-ST(K,-J)
 992         AVS(K,N,M)=ST(K,-J)*XINT(K,N,M)
 993         GOTO 1125
 994    1120 SA=SR(K,-J)
 995    1125 AVA(K,N,M)=          SA*XINT(K,N,M)
 996         GOTO 1200
 997    1140 AVA(K,N,M)=0.0
 998         AVF(K,N,M)=0.0
 999         AVD(K,N,M)=0.0
1000         IF(K.LE.K1) AVS(K,N,M)=0.0
1001         NVMAX1=NVMAX(J)+1
1002         MVMAX1=MVMAX(J)+1
1003         HNV1=0.0
1004         DO 1190 NV=1,NVMAX1
1005         HNV2=HNV1+HNV(J,NV)
1006         U1N1 = 1./(HN(N)**2)*(HNV2**3-HNV1**3)-1./(2.*HN(N)**3)*(HNV2**4-
            1         HNV1**4)
1007         U1N2 = -1./(HN(N)**2)*((HN(N)-HNV2)**3- (HN(N)-HNV1)**3)
            1         +1./(2.*HN(N)**3)*((HN(N)-HNV2)**4-(HN(N)-HNV1)**4)
1008         U2N1 = -1./(3.*HN(N))*(HNV2**3-HNV1**3)+1./(4.*HN(N)**2)*(HNV2**4-
            1         HNV1**4)
1009         U2N2 = -1./(3.*HN(N))*((HN(N)-HNV2)**3-(HN(N)-HNV1)**3)
            1         +1./(4.*HN(N)**2)*((HN(N)-HNV2)**4-(HN(N)-HNV1)**4)
1010         HMV1=0.0
1011         DO 1180 MV=1,MVMAX1
1012         HMV2=HMV1+HMV(J,MV)
```

```
1013          U1M1 = 1./(HM(M)**2)*(HMV2**3-HMV1**3)-1./(2.*HM(M)**3)*(HMV2**4-
             1        HMV1**4)
1014          U1M2 = -1./(HM(M)**2)*((HM(M)-HMV2)**3- (HM(M)-HMV1)**3)
             1        +1./(2.*HM(M)**3)*((HM(M)-HMV2)**4-(HM(M)-HMV1)**4)
1015          U2M1 = -1./(3.*HM(M))*(HMV2**3-HMV1**3)+1./(4.*HM(M)**2)*(HMV2**4-
             1        HMV1**4)
1016          U2M2 = -1./(3.*HM(M))*((HM(M)-HMV2)**3-(HM(M)-HMV1)**3)
             1        +1./(4.*HM(M)**2)*((HM(M)-HMV2)**4-(HM(M)-HMV1)**4)
1017          T11=X(K,N,M,1)*U1N2*U1M2 + X(K,N,M+1,1)*U1N2*U1M1 + X(K,N+1,M,1)*
             1U1N1*U1M2 + X(K,N+1,M+1,1)*U1N1*U1M1
1018          T21=XA21*U2N2*U1M2*TDN(1,1)+XB21*U2N2*U1M1*TDN(1,2)+X(K,N+1,M,2)
             1*U2N1*U1M2*TDN(2,1)+X(K,N+1,M+1,2)*U2N1*U1M1*TDN(2,2)
1019          T12=XA12*U1N2*U2M2*TDM(1,1)+X(K,N,M+1,4)*U1N2*U2M1*TDM(1,2)
             1+XC12*U1N1*U2M2*TDM(2,1)+X(K,N+1,M+1,4)*U1N1*U2M1*TDM(2,2)
1020          T22=X(K,N,M,6)*U2N2*U2M2*TD(1,1)+X(K,N,M+1,6)*U2N2*U2M1*TD(1,2)
             1+X(K,N+1,M,6)*U2N1*U2M2*TD(2,1)+X(K,N+1,M+1,6)*U2N1*U2M1*TD(2,2)
1021          T=T11+T21+T12+T22
1022          JAV=JCV(J,NV,MV)
1023          FISS=FISS+T*SF(K,JAV)/XI(K)
1024          AVF(K,N,M)=AVF(K,N,M)+SF(K,JAV)*T
1025          AVD(K,N,M)=AVD(K,N,M)+T/DI(K,JAV)
1026          IF(K-KGROUP)1150,1160,1160
1027     1150 SA=SR(K,JAV)-ST(K,JAV)
1028          AVS(K,N,M)=AVS(K,N,M)+ST(K,JAV)*T
1029          GOTO 1170
1030     1160 SA=SR(K,JAV)
1031     1170 AVA(K,N,M)=AVA(K,N,M)+T*SA
1032     1180 HMV1=HMV2
1033     1190 HNV1=HNV2
1034     1200 CONTINUE
1035     1205 CONTINUE
1036          XNORM=XNORM/FISS
1037          DO 1208 N=1,NROW1
1038          DO 1208 M=1,MCOL1
1039          DO 1208 K=1,KGROUP
1040          AVA(K,N,M)=AVA(K,N,M)*XNORM
1041          AVF(K,N,M)=AVF(K,N,M)*XNORM
1042          AVD(K,N,M)=AVD(K,N,M)*XNORM
1043          IF(K.LE.K1) AVS(K,N,M)=AVS(K,N,M)*XNORM
1044     1208 XINT(K,N,M)=XINT(K,N,M)*XNORM/(HN(N)*HM(M))
1045          CALL EPRINT(NROW,NROW1,MCOL,MCOL1,KGROUP,K1,ICLPS,AVA,AVF,AVD,
             1AVS,XINT,HN,HM,JC)
1046          JJ=0
1047          IF(ICMAX)1210,1600,1550
1048     1210 INMAX=-ICMAX+2
1049          IMMAX=-ICMAX+2
1050          DO 1500 K=1,KGROUP
1051          DO 1500 N=1,NROW1
1052          DO 1500 M=1,MCOL1
1053          JA=JC(N,M)
1054          JJ=JJ+1
1055     1500 CALL CALC(XNORM,NROW,MCOL,KGROUP,JMAX,
             1                                JVMAX,      NVN,MVM,JA,JJ,INMAX,IMMAX,
             1K,N,M,HN(N),HM(M),X,TDN,TDM,TD,IND,TH,FL,DI,NVMAX,MVMAX,JCV,IP)
1056          GOTO 1600
1057     1550 DO 1590 K=1,KGROUP
```

```
1058          DO 1590 N=1,NROW1
1059          DO 1590 M=1,MCOL1
1060          JA=JC(N,M)
1061          INMAX=5
1062          IMMAX=5
1063          DO 1560 JB=1,ICMAX
1064          IF(MINR(JB).EQ.N.AND.MINC(JB).EQ.M.AND.KC(JB).EQ.K) GOTO 1570
1065      1560 CONTINUE
1066          GOTO 1580
1067      1570 INMAX=ISTR(JB)+2
1068          IMMAX=ISTC(JB)+2
1069      1580 JJ=JJ+1
1070      1590 CALL CALC(XNORM,NROW,MCOL,KGROUP,JMAX,
             1                                  JVMAX,     NVN,MVM,JA,JJ,INMAX,IMMAX,
             1K,N,M,HN(N),HM(M),X,TDN,TDM,TD,IND,TH,FL,DI,NVMAX,MVMAX,JCV,IP)
1071      1600 RETURN
1072          END
```

```
1073          SUBROUTINE CALC(XNORM,NROW,MCOL,KGROUP,JMAX,
             1                                        JVMAX,NVN,MVM,JA,JJ,INMAX,
             1IMMAX,K,N,M,HNN,HMM,X,TDN,TDM,TD,IND,TH,FL,DI,NVMAX,MVMAX,JCV,IP)
1074          INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
1075          INTEGER*2 IP(NROW,MCOL)
1076          DIMENSION DI(KGROUP,JMAX)
1077          DIMENSION X(KGROUP,NROW,MCOL,6)
1078          DIMENSION TDN(2,2),TDM(2,2),TD(2,2)
1079          DIMENSION IND(NROW,MCOL,6),TH(KGROUP,NROW,MCOL)
1080          DIMENSION FL(13,13)
1081          J=10000*K+100*N+M
1082          IF(JA.LT.0) DA=DI(K,-JA)
1083          DO 1108 NI=1,2
1084          NS=N+NI-1
1085          IF(JA.LT.0) GOTO 1103
1086          NV=1
1087          IF(NS.GT.N) NV=NVMAX(JA)+1
1088      1103 CONTINUE
1089          DO 1108 MI=1,2
1090          MS=M+MI-1
1091          IF(JA.LT.0) GOTO 1105
1092          MV=1
1093          IF(MS.GT.M) MV=MVMAX(JA)+1
1094          JAV=JCV(JA,NV,MV)
1095          DA=DI(K,JAV)
1096      1105 CONTINUE
1097          TDN(NI,MI)=1.0
1098          TDM(NI,MI)=1.0
1099          TD (NI,MI)=1.0
1100          IF(IP(NS,MS).EQ.421)
             1TDN(NI,MI)=TH(K,NS,MS)/DA
1101          IF(IP(NS,MS).EQ.422)
             1TDM(NI,MI)=TH(K,NS,MS)/DA
1102          IF(TH(K,NS,MS).GT..0)
             1TD(NI,MI)=TH(K,NS,MS)/DA
1103      1108 CONTINUE
1104          XA21=X(K,N,M,2)
1105          IF(IND(N,M,3).GT.0) XA21=X(K,N,M,3)
1106          XB21=X(K,N,M+1,2)
1107          IF(IND(N,M+1,3).GT.0) XB21=X(K,N,M+1,3)
1108          XA12=X(K,N,M,4)
1109          IF(IND(N,M,5).GT.0) XA12=X(K,N,M,5)
1110          XC12=X(K,N+1,M,4)
1111          IF(IND(N+1,M,5).GT.0) XC12=X(K,N+1,M,5)
1112          DO 1450 IN=1,INMAX
1113          Z=HNN*(IN-1)/(INMAX-1)
1114          H=HNN
1115          U1N1=3*(Z/H)**2-2*(Z/H)**3
1116          U1N2=3*((H-Z)/H)**2-2*((H-Z)/H)**3
1117          U2N1=(-(Z/H)**2+(Z/H)**3)*H
1118          U2N2=(((H-Z)/H)**2-((H-Z)/H)**3)*H
1119          DO 1450 IM=1,IMMAX
1120          Z=HMM*(IM-1)/(IMMAX-1)
1121          H=HMM
1122          U1M1=3*(Z/H)**2-2*(Z/H)**3
1123          U1M2=3*((H-Z)/H)**2-2*((H-Z)/H)**3
```

```
1124          U2M1=(-(Z/H)**2+(Z/H)**3)*H
1125          U2M2=(((H-Z)/H)**2-((H-Z)/H)**3)*H
1126          T11=X(K,N,M,1)*U1N2*U1M2 + X(K,N,M+1,1)*U1N2*U1M1 + X(K,N+1,M,1)*
             1U1N1*U1M2 + X(K,N+1,M+1,1)*U1N1*U1M1
1127          T21=XA21*U2N2*U1M2*TDN(1,1)+XB21*U2N2*U1M1*TDN(1,2)+X(K,N+1,M,2)
             1*U2N1*U1M2*TDN(2,1)+X(K,N+1,M+1,2)*U2N1*U1M1*TDN(2,2)
1128          T12=XA12*U1N2*U2M2*TDM(1,1)+X(K,N,M+1,4)*U1N2*U2M1*TDM(1,2)
             1+XC12*U1N1*U2M2*TDM(2,1)+X(K,N+1,M+1,4)*U1N1*U2M1*TDM(2,2)
1129          T22=X(K,N,M,6)*U2N2*U2M2*TD(1,1)+X(K,N,M+1,6)*U2N2*U2M1*TD(1,2)
             1+X(K,N+1,M,6)*U2N1*U2M2*TD(2,1)+X(K,N+1,M+1,6)*U2N1*U2M1*TD(2,2)
1130          FL(IN,IM)=(T11+T21+T12+T22)*XNORM
1131      1450 CONTINUE
1132          CALL FPRINT(J,JJ,INMAX,IMMAX,FL)
1133          RETURN
1134          END
```

```
      SUBROUTINE APRINT(MSIZE,MSIZE1, NRUN1,ICMAX,NCONV,EPSF,EPSL,EPSCH,
     1BL,BR,BT,BB,JMAX,XNORM,NROW,MCOL,KGROUP,LMAX,LXMAX,LXCMAX,LXFMAX,
     2JVMAX,NVN,MVM,IND,IP)
      INTEGER*2 IP(NROW,MCOL)
      DIMENSION IND(NROW,MCOL,6)
      WRITE(6,1000)
 1000 FORMAT(1H1,      20X,'PROBLEM PARAMETERS')
      WRITE(6,1010)
 1010 FORMAT(21X,18('-'),//)
      WRITE(6,1015) NRUN1
 1015 FORMAT(5X,'RUN NUMBER                          -',I3)
      WRITE(6,1020) NROW
 1020 FORMAT(5X,'NO. OF ROWS                         -',I3)
      WRITE(6,1030) MCOL
 1030 FORMAT(5X,'NO. OF COLUMNS                      -',I3)
      WRITE(6,1040) KGROUP
 1040 FORMAT(5X,'NO. OF GROUPS                       -',I3)
      WRITE(6,1060) NCONV
 1060 FORMAT(/,5X,'OUTER.ITER. - MAX.NO.             -',I3)
      WRITE(6,1070) EPSF
 1070 FORMAT(16X,' - CONV.CRIT.SOL.    -',E10.3)
      WRITE(6,1075)EPSL
 1075 FORMAT(16X,' - CONV.CRIT.K-EFF   -',E10.3)
      WRITE(6,1078) EPSCH
 1078 FORMAT(/,5X,'CHOLESKI REJECTION CRIT.          -',E10.3)
      WRITE(6,1160)
 1160 FORMAT(/,5X,'BOUNDARIES(0.0-ZERO FLUX; 1.0-ZERO DERIV.)')
      WRITE(6,1170) BL
 1170 FORMAT(17X,'- LEFT BND.          -',F4.1)
      WRITE(6,1180) BR
 1180 FORMAT(17X,'- RIGHT BND.         -',F4.1)
      WRITE(6,1190) BT
 1190 FORMAT(17X,'- TOP BND.           -',F4.1)
      WRITE(6,1200) BB
 1200 FORMAT(17X,'- BOTTOM BND.        -',F4.1)
      WRITE(6,1202) XNORM
 1202 FORMAT(/, 5X,'NORMALIZATION(FISSIONS/SEC)     -',E12.5)
      WRITE(6,1210)LMAX
 1210 FORMAT(/,5X,'LMAX  -NO.OF UNKNOWNS(/GROUP)   -',I6)
      WRITE(6,1215)LXMAX
 1215 FORMAT(  5X,'LXMAX -SIZE OF ARRAYS F1,LLX    -',I6)
      WRITE(6,1217)LXCMAX
 1217 FORMAT(  5X,'LXCMAX-SIZE OF ARRAYS E,LLXC    -',I6)
      WRITE(6,1230) LXFMAX
 1230 FORMAT(  5X,'LXFMAX-SIZE OF ARRAYS F,S,LLXF  -',I6)
      WRITE(6,1233) MSIZE
 1233 FORMAT(5X,'MSIZE -SPECIFIED VALUE          -',I8)
      WRITE(6,1235) MSIZE1
 1235 FORMAT(11X,'-ACTUAL VALUE USED        -',I8)
      AL=LMAX
      AK=KGROUP
      AX=LXMAX
      AXC=LXCMAX
      AXF=LXFMAX
      AJ=JMAX
      AJV=JVMAX
```

```
1189          ANV=NVN
1190          AMV=MVM
1191          AN=NROW
1192          AM=MCOL
1193          MSIZE1=AL*(6.*AK+1.5)+AX*1.5+AXC*(2.*AK+0.5)+AXF*(2.*AK-1.5)
             X+AJ*(4.*AK-1.0)+AJV*(ANV*AMV/2.0 +ANV+AMV+1.0)+AN*AM*(AK+7.0)
             X+(AN+AM)/2.0+7.0*AK+4.0
1194          WRITE(6,1238) MSIZE1
1195     1238 FORMAT(11X,'-MINIMUM POSSIBLE VALUE   -',I8)
1196          WRITE(6,1240)
1197     1240 FORMAT(/,5X,'BASIS FUNCTIONS SPECIFICATION',/)
1198          DO 1260 N=1,NROW
1199     1260 WRITE(6,1270)(IP(N,M),M=1,MCOL)
1200     1270 FORMAT(15X,15I6)
1201          RETURN
1202          END
```

```
      SUBROUTINE BPRINT(NROW,NROW1,MCOL,MCOL1,KGROUP,K1,JMAX,JVMAX,NVN,
     1MVM,H,XI,DI,SR,SF,ST,HN,HM,HNV,HMV,JC,JCV,NVMAX,MVMAX)
      INTEGER*2 JC(NROW1,MCOL1)
      INTEGER*2 JCV(JVMAX,NVN,MVM),NVMAX(JVMAX),MVMAX(JVMAX)
      DIMENSION XI(KGROUP),DI(KGROUP,JMAX),SR(KGROUP,JMAX),SF(KGROUP,
     1JMAX),ST(K1,JMAX)
      DIMENSION HN(NROW1),HM(MCOL1),H(MCOL)
      DIMENSION HNV(JVMAX,NVN),HMV(JVMAX,MVM)
      WRITE(6,1000)
 1000 FORMAT(1H1,40X,'C O M P O S I T I O N   P R O P E R T I E S')
      WRITE(6,1010)
 1010 FORMAT(41X,43('-'))
      WRITE(6,1020)
 1020 FORMAT(//,10X,'COMP.',3X,'GROUP',10X,'DIFF.COEFF(CM)',6X,'RMVL.XS(
     1/CM)',6X,'FISS.K->1(/CM)',5X,'SCTT.K->K+1(/CM)')
      WRITE(6,1030)
 1030 FORMAT(10X,5('-'),3X,5('-'),10X,14('-'),6X,12('-'),6X,14('-'),5X,1
     16('-'))
      DO 1080 J=1,JMAX
      K=1
      WRITE(6,1040) J,K,DI(K,J),SR(K,J),SF(K,J),ST(K,J)
 1040 FORMAT(/,10X,I3,5X,I3,12X,F10.5,9X,F10.5,9X,F10.5,9X,F10.5)
      IF(K1.LE.1) GOTO 1065
      DO 1050 K=2,K1
 1050 WRITE(6,1060)   K,DI(K,J),SR(K,J),SF(K,J),ST(K,J)
 1060 FORMAT(18X,        I3,12X,F10.5,9X,F10.5,9X,F10.5,9X,F10.5)
 1065 K=KGROUP
      WRITE(6,1070)   K,DI(K,J),SR(K,J),SF(K,J)
 1070 FORMAT(18X,        I3,12X,F10.5,9X,F10.5,9X,F10.5)
 1080 CONTINUE
      WRITE(6,1090)(XI(K),K=1,KGROUP)
 1090 FORMAT(//,10X,'NEUTRON EMISSION FOR FISSIONS IN GROUP 1,-,KGROUP
     1  -', 4F10.3)
      WRITE(6,1100)
 1100 FORMAT(1H1,40X,'M A T E R I A L S   P I C T U R E')
      WRITE(6,1110)
 1110 FORMAT(41X,33('-'),//)
      H(1)=0.0
      DO 1111 M=2,MCOL
 1111 H(M)=H(M-1)+HM(M-1)
      WRITE(6,1115)(H(M),M=1,MCOL)
 1115 FORMAT(18X,12('(',F7.3,')',1X),//)
      WRITE(6,1120)(M,M=1,MCOL)
 1120 FORMAT(18X,12(I5,5X))
      DO 1121 N=2,NROW
 1121 H(N)=H(N-1)+HN(N-1)
      DO 1180 N=2,NROW
      WRITE(6,1130)(JC(N-1,M),M=1,MCOL1)
 1130 FORMAT(23X,12(I5,5X))
      WRITE(6,1140)H(N),N
 1140 FORMAT(11X,'(',F7.3,')',I3)
 1180 CONTINUE
      WRITE(6,1200)
 1200 FORMAT(1H1,30X,'SPECIFICATIONS FOR REGIONS WITH VARYING PARAMETERS
     1')
      WRITE(6,1210)
```

```
1253    1210 FORMAT(31X,50('-'))
1254         DO 1500 J=1,JVMAX
1255         DO 1250 N=1,NROW1
1256         DO 1250 M=1,MCOL1
1257         IF(JC(N,M).EQ.J) GOTO 1300
1258    1250 CONTINUE
1259         GOTO 1500
1260    1300 WRITE(6,1310) J
1261    1310 FORMAT(///,10X,'REGION NO.',I3)
1262         NVMAX1=NVMAX(J)+1
1263         MVMAX1=MVMAX(J)+1
1264         WRITE(6,1320)(HNV(J,NV),NV=1,NVMAX1)
1265    1320 FORMAT(/,10X,'ROW SUB-MESH',8F10.5)
1266         WRITE(6,1330)(HMV(J,MV),MV=1,MVMAX1)
1267    1330 FORMAT(/,10X,'COL.SUB-MESH',8F10.5)
1268         WRITE(6,1340)
1269    1340 FORMAT(/,10X,'MATERIALS PICTURE OF SUB-MESH',/)
1270         DO 1400 NV=1,NVMAX1
1271    1400 WRITE(6,1410)(JCV(J,NV,MV),MV=1,MVMAX1)
1272    1410 FORMAT(20X,8I5)
1273    1500 CONTINUE
1274         RETURN
1275         END
```

```
      SUBROUTINE CPRINT(NCONV1,YLIM1,YLIM2,YLMD1,YLMD2)
      REAL*8 YLMD1,YLMD2
      IF(NCONV1.NE.1) GOTO 1050
      WRITE(6,1000)
 1000 FORMAT(1H1,33X,'C O N V E R G E N C E   D A T A')
      WRITE(6,1010)
 1010 FORMAT(34X,31('-'),//)
      WRITE(6,1020)
 1020 FORMAT(10X,'OUT.ITER.NO.',3X,'INITIAL AND FINAL SOL. NORMS',4X,
     1'INITIAL AND FINAL K-EFF')
      WRITE(6,1030)
 1030 FORMAT(10X,12('-'),3X,28('-'),4X,23('-'))
 1050 WRITE(6,1060) NCONV1,YLIM1,YLIM2,YLMD1,YLMD2
 1060 FORMAT(10X,I6,4X,2(6X,F10.7,4X,F10.7))
      RETURN
      END
```

```
1291          SUBROUTINE DPRINT(NROW,MCOL,KGROUP,X,IND,IP)
1292          INTEGER*2 IP(NROW,MCOL)
1293          DIMENSION XX(5)
1294          DIMENSION X(KGROUP,NROW,MCOL,6)
1295          DIMENSION IND(NROW,MCOL,6)
1296          WRITE(6,1000)
1297     1000 FORMAT(1H1,30X,'E X P A N S I O N  C O E F F . F O R  F L U X')
1298          WRITE(6,1010)
1299     1010 FORMAT(30X,49('-'),//)
1300          WRITE(6,1020)
1301     1020 FORMAT(5X,'GROUP',3X,'ROW',3X,'COLUMN',8X,'FLUX',11X,'COL.DER(UP)'
            1,5X,'COL.DER(DWN)',5X,'ROW DER(LFT)',5X,'ROW DER(RIT)',4X,'SECOND
            2DERIV.')
1302          WRITE(6,1030)
1303     1030 FORMAT(5X,5('-'),3X,3('-'),3X,6('-'),8X,4('-'),11X,11('-'),5X,
            112('-'),5X,12('-'),5X,12('-'),4X,13('-'))
1304          DO 1100 K=1,KGROUP
1305          DO 1100 N=1,NROW
1306          DO 1100 M=1,MCOL
1307          II=IP(N,M)/10
1308          IF(II.GT.10) II=II/10
1309          II=II-3
1310          GOTO (1034,1035,1036), II
1311     1036 WRITE(6,1120)K,N,M,(X(K,N,M,I),I=1,6)
1312     1120 FORMAT(5X,I3,4X,I3,5X,I3,2X,6(F15.7,2X))
1313          GOTO 1100
1314     1034 XX(1)=X(K,N,M,1)
1315          XX(2)=X(K,N,M,2)
1316          XX(3)=X(K,N,M,4)
1317          XX(4)=X(K,N,M,6)
1318          WRITE(6,1050)K,N,M,(XX(I),I=1,4)
1319     1050 FORMAT(5X,I3,4X,I3,5X,I3,2X,F15.7,2X,2( 9X,F15.7,10X),F15.7,2X)
1320          GOTO 1100
1321     1035 IF(IND(N,M,3).EQ.0) GOTO 1080
1322          XX(1)=X(K,N,M,1)
1323          XX(2)=X(K,N,M,2)
1324          XX(3)=X(K,N,M,3)
1325          XX(4)=X(K,N,M,4)
1326          XX(5)=X(K,N,M,6)
1327          WRITE(6,1070)K,N,M,(XX(I),I=1,5)
1328     1070 FORMAT(5X,I3,4X,I3,5X,I3,2X,3(F15.7,2X),9X,F15.7,10X,F15.7)
1329          GOTO 1100
1330     1080 XX(1)=X(K,N,M,1)
1331          XX(2)=X(K,N,M,2)
1332          XX(3)=X(K,N,M,4)
1333          XX(4)=X(K,N,M,5)
1334          XX(5)=X(K,N,M,6)
1335          WRITE(6,1090)K,N,M,(XX(I),I=1,5)
1336     1090 FORMAT(5X,I3,4X,I3,5X,I3,2X,   F15.7,11X,F15.7,10X,3(F15.7,2X))
1337     1100 CONTINUE
1338          RETURN
1339          END
```

```
1340          SUBROUTINE EPRINT(NROW,NROW1,MCOL,MCOL1,KGROUP,K1,ICLPS,AVA,AVF,
             1AVD,AVS,XINT,HN,HM,JC)
1341          INTEGER*2 JC(NROW1,MCOL1)
1342          DIMENSION AVA(KGROUP,NROW1,MCOL1),AVF(KGROUP,NROW1,MCOL1),
             1AVD(KGROUP,NROW1,MCOL1),AVS(KGROUP,NROW1,MCOL1)
1343          DIMENSION XINT(KGROUP,NROW1,MCOL1),HN(NROW1),HM(MCOL1)
1344          DO 980 N=1,NROW1
1345          DO 980 M=1,MCOL1
1346          DO 980 K=2,KGROUP
1347          AVA(1,N,M)=AVA(1,N,M)+AVA(K,N,M)
1348          AVF(1,N,M)=AVF(1,N,M)+AVF(K,N,M)
1349      980 AVD(1,N,M)=AVD(1,N,M)+AVD(K,N,M)
1350          WRITE(6,1000)
1351     1000 FORMAT(1H1)
1352          WRITE(6,1010)
1353     1010 FORMAT(30X,'REACTION RATES IN REGIONS')
1354          WRITE(6,1020)
1355     1020 FORMAT(30X,25('-'),//)
1356          WRITE(6,1120)(M,M=1,MCOL)
1357     1120 FORMAT(8X,10(I6,6X))
1358          DO 1200 N=2,NROW
1359          WRITE(6,1130)(AVA(1,N-1,M),M=1,MCOL1)
1360     1130 FORMAT(6X,'ABSRP',2X,10E12.5)
1361          WRITE(6,1140)(AVF(1,N-1,M),M=1,MCOL1)
1362     1140 FORMAT(6X,'PRODU',2X,10E12.5)
1363          WRITE(6,1150)(AVD(1,N-1,M),M=1,MCOL1)
1364     1150 FORMAT(6X,'TRNSP',2X,10E12.5)
1365          WRITE(6,1170)N
1366     1170 FORMAT(8X,I6)
1367     1200 CONTINUE
1368          WRITE(6,1000)
1369          WRITE(6,2010)
1370     2010 FORMAT(30X,'AVERAGE FLUXES IN REGIONS')
1371          WRITE(6,2020)
1372     2020 FORMAT(30X,25('-'),//)
1373          WRITE(6,1120)(M,M=1,MCOL)
1374          DO 2200 N=2,NROW
1375          DO 2100 K=1,KGROUP
1376     2100 WRITE(6,2130)K,(XINT(K,N-1,M),M=1,MCOL1)
1377     2130 FORMAT(6X,'GRP.',I1,2X,10E12.5)
1378          WRITE(6,1170) N
1379     2200 CONTINUE
1380          IF(ICLPS.EQ.0) GOTO 2500
1381          DO 2220 N=1,NROW1
1382          DO 2220 M=1,MCOL1
1383          DO 2220 K=2,KGROUP
1384          AVA(1,N,M)=AVA(1,N,M)-AVA(K,N,M)
1385          AVF(1,N,M)=AVF(1,N,M)-AVF(K,N,M)
1386     2220 AVD(1,N,M)=AVD(1,N,M)-AVD(K,N,M)
1387          WRITE(6,2230)
1388     2230 FORMAT(1H1,30X,'FLUX AND VOLUME AVERAGED PROPERTIES')
1389          WRITE(6,2240)
1390     2240 FORMAT(31X,35('-'),//)
1391          WRITE(6,2250)
1392     2250 FORMAT(10X,'ROW COL',3X,'GROUP',10X,'DIFF.COEFF(CM)',6X,'RMVL.XS(/
            1CM)',6X,'FISS.K->1(/CM)',5X,'SCTT.K->K+1(/CM)')
```

```
1393          WRITE(6,2260)
1394     2260 FORMAT(10X,3('-'),1X,3('-'),3X,5('-'),10X,14('-'),6X,12('-'),6X,
                 114('-'),5X,16('-'),/)
1395          DO 2275 N=1,NROW1
1396          DO 2275 M=1,MCOL1
1397          DO 2270 K=1,K1
1398          XX=XINT(K,N,M)*HN(N) *HM(M)
1399          AVA(K,N,M)=(AVA(K,N,M)+AVS(K,N,M))/XX
1400          AVS(K,N,M)=AVS(K,N,M)/XX
1401          AVF(K,N,M)=AVF(K,N,M)/XX
1402     2270 AVD(K,N,M)=XX/AVD(K,N,M)
1403          XX=XINT(KGROUP,N,M)*HN(N)*HM(M)
1404          AVA(KGROUP,N,M)=AVA(KGROUP,N,M)/XX
1405          AVF(KGROUP,N,M)=AVF(KGROUP,N,M)/XX
1406     2275 AVD(KGROUP,N,M)=XX/AVD(KGROUP,N,M)
1407          IF(ICLPS.LT.0) GOTO 2400
1408          DO 2340 NN=1,ICLPS
1409          READ(5,2280) N,M
1410     2280 FORMAT(14I5)
1411          K=1
1412          WRITE(6,2290) N,M,K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M),AVS(K,N,M)
1413     2290 FORMAT(/,8X,2I4,3X,I3,12X,F10.5,9X,F10.5,9X,F10.5,9X,F10.5)
1414          IF(K1.LE.1) GOTO 2330
1415          DO 2310 K=2,K1
1416     2310 WRITE(6,2320)      K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M),AVS(K,N,M)
1417     2320 FORMAT(19X,         I3,12X,F10.5,9X,F10.5,9X,F10.5,9X,F10.5)
1418     2330 K=KGROUP
1419          WRITE(6,2320)      K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M)
1420     2340 CONTINUE
1421          GOTO 2500
1422     2400 CONTINUE
1423          DO 2490 N=1,NROW1
1424          DO 2490 M=1,MCOL1
1425          IF(JC(N,M).LT.0) GOTO 2490
1426          K=1
1427          WRITE(6,2290) N,M,K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M),AVS(K,N,M)
1428          IF(K1.LE.1) GOTO 2430
1429          DO 2410 K=2,K1
1430     2410 WRITE(6,2320)      K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M),AVS(K,N,M)
1431     2430 K=KGROUP
1432          WRITE(6,2320)      K,AVD(K,N,M),AVA(K,N,M),AVF(K,N,M)
1433     2490 CONTINUE
1434     2500 CONTINUE
1435          RETURN
1436          END
```

```
      SUBROUTINE FPRINT(J,JJ,INMAX,IMMAX,FL)
      DIMENSION FL(13,13)
      IF(JJ.NE.1) GOTO 1100
      WRITE(6,1020)
 1020 FORMAT(1H1,      30X,'FLUX VALUES FOR EQUALLY SPACED POINTS INSIDE
     1 THE OUTPUT REGIONS')
      WRITE(6,1030)
 1030 FORMAT(31X,63('-'))
      WRITE(6,1035)
 1035 FORMAT(50X,'(SET=GROUP-ROW-COLUMN)',//)
      WRITE(6,1040)
 1040 FORMAT(3X,'SET',1X,'SUB-ROW',20X,'POINT FLUXES AT SUB-COLUMN')
      WRITE(6,1050)
 1050 FORMAT(3X,3('-'),1X,7('-'),20X,26('-'),/)
      WRITE(6,1060)(JI,JI=1,13)
 1060 FORMAT(16X,13(I5,3X),/)
 1100 CONTINUE
      WRITE(6,1110) J
 1110 FORMAT(1X,I5)
      DO 1200 IN=1,INMAX
 1200 WRITE(6,1210)IN,(FL(IN,IM),IM=1,IMMAX)
 1210 FORMAT( 8X,I3,3X,13(F 8.4))
      RETURN
      END
```

```
1460          REAL FUNCTION XF*8 (JI,JS,JJI,JJS,TD1,TD2)
1461          REAL*8 P
1462          COMMON/COMP/P(2,2,2,2)
1463          M=8*JI+4*JS+2*JJI+JJS-14
1464          GOTO (1111,1112,1121,1122,1211,1212,1221,1222,2111,2112,2121,
             X2122,2211,2212,2221,2222), M
1465      1111 P(1,1,1,1) = 13./35.
1466          GOTO 5000
1467      1112 P(1,1,1,2) = 9./70.
1468          GOTO 5000
1469      1121 P(1,1,2,1) = -11./210.*TD2
1470          GOTO 5000
1471      1122 P(1,1,2,2) = 13./420.*TD2
1472          GOTO 5000
1473      1211 P(1,2,1,1) = 9./70.
1474          GOTO 5000
1475      1212 P(1,2,1,2) = 13./35.
1476          GOTO 5000
1477      1221 P(1,2,2,1) = -13./420.*TD2
1478          GOTO 5000
1479      1222 P(1,2,2,2) = 11./210.*TD2
1480          GOTO 5000
1481      2111 P(2,1,1,1) = -11./210.*TD1
1482          GOTO 5000
1483      2112 P(2,1,1,2) = -13./420.*TD1
1484          GOTO 5000
1485      2121 P(2,1,2,1) = 1./105.*TD1*TD2
1486          GOTO 5000
1487      2122 P(2,1,2,2) = -1./140.*TD1*TD2
1488          GOTO 5000
1489      2211 P(2,2,1,1) = 13./420.*TD1
1490          GOTO 5000
1491      2212 P(2,2,1,2) = 11./210.*TD1
1492          GOTO 5000
1493      2221 P(2,2,2,1) = -1./140.*TD1*TD2
1494          GOTO 5000
1495      2222 P(2,2,2,2) = 1./105.*TD1*TD2
1496      5000 XF=P(JI,JS,JJI,JJS)
1497          RETURN
1498          END
```

```
1499          REAL FUNCTION XD*8 (JI,JS,JJI,JJS,TD1,TD2)
1500          REAL*8 P
1501          COMMON/COMP/P(2,2,2,2)
1502          M=8*JI+4*JS+2*JJI+JJS-14
1503          GOTO (1111,1112,1121,1122,1211,1212,1221,1222,2111,2112,2121,
             X2122,2211,2212,2221,2222), M
1504     1111 P(1,1,1,1) = 6./5.
1505          GOTO 5000
1506     1112 P(1,1,1,2) = -6./5.
1507          GOTO 5000
1508     1121 P(1,1,2,1) = -1./10.*TD2
1509          GOTO 5000
1510     1122 P(1,1,2,2) = -1./10.*TD2
1511          GOTO 5000
1512     1211 P(1,2,1,1) = -6./5.
1513          GOTO 5000
1514     1212 P(1,2,1,2) = 6./5.
1515          GOTO 5000
1516     1221 P(1,2,2,1) = 1./10.*TD2
1517          GOTO 5000
1518     1222 P(1,2,2,2) = 1./10.*TD2
1519          GOTO 5000
1520     2111 P(2,1,1,1) = -1./10.*TD1
1521          GOTO 5000
1522     2112 P(2,1,1,2) = 1./10.*TD1
1523          GOTO 5000
1524     2121 P(2,1,2,1) = 2./15.*TD1*TD2
1525          GOTO 5000
1526     2122 P(2,1,2,2) = -1./30.*TD1*TD2
1527          GOTO 5000
1528     2211 P(2,2,1,1) = -1./10.*TD1
1529          GOTO 5000
1530     2212 P(2,2,1,2) = 1./10.*TD1
1531          GOTO 5000
1532     2221 P(2,2,2,1) = -1./30.*TD1*TD2
1533          GOTO 5000
1534     2222 P(2,2,2,2) = 2./15.*TD1*TD2
1535     5000 XD=P(JI,JS,JJI,JJS)
1536          RETURN
1537          END
```

```
1538          REAL FUNCTION XFV*8(JI,JS,JJI,JJS,AH, X1, X2, TD1, TD2)
1539          REAL*8 H,X1,X2
1540          REAL*8 P
1541          COMMON/COMP/P(2,2,2,2)
1542          H=AH
1543          M=8*JI+4*JS+2*JJI+JJS-14
1544          GOTO (1111,1112,1121,1122,1211,1212,1221,1222,2111,2112,2121,
             X2122,2211,2212,2221,2222), M
1545     1111 P(1,1,1,1)= +4./(7.*H**6)*(X2**7-X1**7)-2./H**5*(X2**6-X1**6)
         2               +9./(5.*H**4)*(X2**5-X1**5)
1546          GOTO 5000
1547     1112 P(1,1,1,2)= -4./(7.*H**6)*(X2**7-X1**7)+2./H**5*(X2**6-X1**6)
         2               -9./(5.*H**4)*(X2**5-X1**5)-1./(2.*H**3)*(X2**4-X1**4)
         3               +1./H**2*(X2**3-X1**3)
1548          GOTO 5000
1549     1121 P(1,1,2,1)=(-2./(7.*H**5)*(X2**7-X1**7)+5./(6.*H**4)*(X2**6-X1**6)
         2               -3./(5.*H**3)*(X2**5-X1**5))*TD2
1550          GOTO 5000
1551     1122 P(1,1,2,2)=(-2./(7.*H**5)*(X2**7-X1**7)+7./(6.*H**4)*(X2**6-X1**6)
         2               -8./(5.*H**3)*(X2**5-X1**5)+3./(4.*H**2)*(X2**4-X1**4)
         3              )*TD2
1552          GOTO 5000
1553     1211 P(1,2,1,1)= -4./(7.*H**6)*(X2**7-X1**7)+2./H**5*(X2**6-X1**6)
         2               -9./(5.*H**4)*(X2**5-X1**5)-1./(2.*H**3)*(X2**4-X1**4)
         3               +1./H**2*(X2**3-X1**3)
1554          GOTO 5000
1555     1212 P(1,2,1,2)= -4./(7.*H**6)*((H-X2)**7-(H-X1)**7)+2./H**5*((H-X2)**6
         2               -(H-X1)**6)-9./(5.*H**4)*((H-X2)**5-(H-X1)**5)
1556          GOTO 5000
1557     1221 P(1,2,2,1)=(+2./(7.*H**5)*(X2**7-X1**7)-5./(6.*H**4)*(X2**6-X1**6)
         2               +3./(5.*H**3)*(X2**5-X1**5)+1./(4.*H**2)*(X2**4-X1**4)
         3               -1./(3.*H)*(X2**3-X1**3))*TD2
1558          GOTO 5000
1559     1222 P(1,2,2,2)=(-2./(7.*H**5)*((H-X2)**7-(H-X1)**7)+5./(6.*H**4)*
         2               ((H-X2)**6-(H-X1)**6)-3./(5.*H**3)*((H-X2)**5-(H-X1)**
         3               5))*TD2
1560          GOTO 5000
1561     2111 P(2,1,1,1)=(-2./(7.*H**5)*(X2**7-X1**7)+5./(6.*H**4)*(X2**6-X1**6)
         2               -3./(5.*H**3)*(X2**5-X1**5))*TD1
1562          GOTO 5000
1563     2112 P(2,1,1,2)=(+2./(7.*H**5)*(X2**7-X1**7)-5./(6.*H**4)*(X2**6-X1**6)
         2               +3./(5.*H**3)*(X2**5-X1**5)+1./(4.*H**2)*(X2**4-X1**4)
         3               -1./(3.*H)*(X2**3-X1**3))*TD1
1564          GOTO 5000
1565     2121 P(2,1,2,1)=(+1./(7.*H**4)*(X2**7-X1**7)-1./(3.*H**3)*(X2**6-X1**6)
         2               +1./(5.*H**2)*(X2**5-X1**5))*TD1*TD2
1566          GOTO 5000
1567     2122 P(2,1,2,2)=(+1./(7.*H**4)*(X2**7-X1**7)-1./(2.*H**3)*(X2**6-X1**6)
         2               +3./(5.*H**2)*(X2**5-X1**5)-1./(4.*H)*(X2**4-X1**4)
         3              )*TD1*TD2
1568          GOTO 5000
1569     2211 P(2,2,1,1)=(-2./(7.*H**5)*(X2**7-X1**7)+7./(6.*H**4)*(X2**6-X1**6)
         2               -8./(5.*H**3)*(X2**5-X1**5)+3./(4.*H**2)*(X2**4-X1**4)
         3              )*TD1
1570          GOTO 5000
1571     2212 P(2,2,1,2)=(-2./(7.*H**5)*((H-X2)**7-(H-X1)**7)+5./(6.*H**4)*
```

```
     2              ((H-X2)**6-(H-X1)**6)-3./(5.*H**3)*((H-X2)**5-(H-X1)**
     3              5))*TD1
1572      GOTO 5000
1573 2221 P(2,2,2,1)=(+1./(7.*H**4)*(X2**7-X1**7)-1./(2.*H**3)*(X2**6-X1**6)
     2              +3./(5.*H**2)*(X2**5-X1**5)-1./(4.*H)*(X2**4-X1**4)
     3             )*TD1*TD2
1574      GOTO 5000
1575 2222 P(2,2,2,2)=(-1./(7.*H**4)*((H-X2)**7-(H-X1)**7)+1./(3.*H**3)*((H-
     2              X2)**6-(H-X1)**6)-1./(5.*H**2)*((H-X2)**5-(H-X1)**5)
     3             )*TD1*TD2
1576 5000 XFV=P(JI,JS,JJI,JJS)
1577      RETURN
1578      END
```

```
1579          REAL FUNCTION XDV*8(JI,JS,JJI,JJS,AH, X1, X2, TD1, TD2)
1580          REAL*8 H,X1,X2
1581          REAL*8 P
1582          COMMON/COMP/P(2,2,2,2)
1583          H=AH
1584          M=8*JI+4*JS+2*JJI+JJS-14
1585          GOTO (1111,1112,1121,1122,1211,1212,1221,1222,2111,2112,2121,
             X2122,2211,2212,2221,2222), M
1586     1111 P(1,1,1,1)= +36./(5.*H**6)*(X2**5-X1**5)-18./H**5*(X2**4-X1**4)
         2                +12./H**4*(X2**3-X1**3)
1587          GOTO 5000
1588     1112 P(1,1,1,2)= -36./(5.*H**6)*(X2**5-X1**5)+18./H**5*(X2**4-X1**4)
         2                -12./H**4*(X2**3-X1**3)
1589          GOTO 5000
1590     1121 P(1,1,2,1)=(-18./(5.*H**5)*(X2**5-X1**5)+15./(2.*H**4)*(X2**4-X1**
         2                4)-4./H**3*(X2**3-X1**3))*TD2
1591          GOTO 5000
1592     1122 P(1,1,2,2)=(-18./(5.*H**5)*(X2**5-X1**5)+21./(2.*H**4)*(X2**4-X1**
         2                4)-10./H**3*(X2**3-X1**3)+3./H**2*(X2**2-X1**2))*TD2
1593          GOTO 5000
1594     1211 P(1,2,1,1)= -36./(5.*H**6)*(X2**5-X1**5)+18./H**5*(X2**4-X1**4)
         2                -12./H**4*(X2**3-X1**3)
1595          GOTO 5000
1596     1212 P(1,2,1,2)= -36./(5.*H**6)*((H-X2)**5-(H-X1)**5)+18./H**5*((H-X2)*
         2                *4-(H-X1)**4)-12./H**4*((H-X2)**3-(H-X1)**3)
1597          GOTO 5000
1598     1221 P(1,2,2,1)=(+18./(5.*H**5)*(X2**5-X1**5)-15./(2.*H**4)*(X2**4-X1**
         2                4)+4./H**3*(X2**3-X1**3))*TD2
1599          GOTO 5000
1600     1222 P(1,2,2,2)=(-18./(5.*H**5)*((H-X2)**5-(H-X1)**5)+15./(2.*H**4)*
         2                ((H-X2)**4-(H-X1)**4)-4./H**3*((H-X2)**3-(H-X1)**3)
         3                )*TD2
1601          GOTO 5000
1602     2111 P(2,1,1,1)=(-18./(5.*H**5)*(X2**5-X1**5)+15./(2.*H**4)*(X2**4-X1**
         2                4)-4./H**3*(X2**3-X1**3))*TD1
1603          GOTO 5000
1604     2112 P(2,1,1,2)=(+18./(5.*H**5)*(X2**5-X1**5)-15./(2.*H**4)*(X2**4-X1**
         2                4)+4./H**3*(X2**3-X1**3))*TD1
1605          GOTO 5000
1606     2121 P(2,1,2,1)=(+9./(5.*H**4)*(X2**5-X1**5)-3./H**3*(X2**4-X1**4)
         2                +4./(3.*H**2)*(X2**3-X1**3))*TD1*TD2
1607          GOTO 5000
1608     2122 P(2,1,2,2)=(+9./(5.*H**4)*(X2**5-X1**5)-9./(2.*H**3)*(X2**4-X1**4)
         2                +11./(3.*H**2)*(X2**3-X1**3)-1./H*(X2**2-X1**2)
         3               )*TD1*TD2
1609          GOTO 5000
1610     2211 P(2,2,1,1)=(-18./(5.*H**5)*(X2**5-X1**5)+21./(2.*H**4)*(X2**4-X1**
         2                4)-10./H**3*(X2**3-X1**3)+3./H**2*(X2**2-X1**2))*TD1
1611          GOTO 5000
1612     2212 P(2,2,1,2)=(-18./(5.*H**5)*((H-X2)**5-(H-X1)**5)+15./(2.*H**4)*
         2                ((H-X2)**4-(H-X1)**4)-4./H**3*((H-X2)**3-(H-X1)**3)
         3               )*TD1
1613          GOTO 5000
1614     2221 P(2,2,2,1)=(+9./(5.*H**4)*(X2**5-X1**5)-9./(2.*H**3)*(X2**4-X1**4)
         2                +11./(3.*H**2)*(X2**3-X1**3)-1./H*(X2**2-X1**2)
         3               )*TD1*TD2
```

```
1615          GOTO 5000
1616     2222 P(2,2,2,2)=(-9./(5.*H**4)*((H-X2)**5-(H-X1)**5)+3./H**3*((H-X2)**4
                2                -(H-X1)**4)-4./(3.*H**2)*((H-X2)**3-(H-X1)**3)
                3              )*TD1*TD2
1617     5000 XDV=P(JI,JS,JJI,JJS)
1618          RETURN
1619          END
```

PROBLEM PARAMETERS

RUN NUMBER - 1
NO. OF ROWS - 3
NO. OF COLUMNS - 3
NO. OF GROUPS - 2

OUTER.ITER. - MAX.NO. - 50
- CONV.CRIT.SOL. - 0.100E-03
- CONV.CRIT.K-EFF - 0.100E-03

CHOLESKI REJECTION CRIT. - 0.100E-05

BOUNDARIES(0.0-ZERO FLUX; 1.0-ZERO DERIV.)
- LEFT BND. - 1.0
- RIGHT BND. - 0.0
- TOP BND. - 1.0
- BOTTOM BND. - 0.0

NORMALIZATION(FISSIONS/SEC) - 0.10000E 03

LMAX -NO.OF UNKNOWNS(/GROUP) - 20
LXMAX -SIZE OF ARRAYS F1,LLX - 133
LXCMAX-SIZE OF ARRAYS E,LLXC - 172
LXFMAX-SIZE OF ARRAYS F,S,LLXF - 246
MSIZE -SPECIFIED VALUE - 40000
-ACTUAL VALUE USED - 33576
-MINIMUM POSSIBLE VALUE - 2012

BASIS FUNCTIONS SPECIFICATION

40	51	40
51	61	40
40	40	40

COMPOSITION PROPERTIES

COMP.	GROUP	DIFF.COEFF(CM)	RMVL.XS(/CM)	FISS.K->1(/CM)	SCTT.K->K+1(/CM)
1	1	1.20000	0.10100	0.00000	0.10000
	2	0.15000	0.02000	0.00000	
2	1	1.50000	0.06230	0.00000	0.06000
	2	0.40000	0.20000	0.21800	
3	1	1.55000	0.06230	0.00000	0.06000
	2	0.41330	0.25000	0.21800	
4	1	1.60000	0.06230	0.00000	0.06000
	2	0.42670	0.30000	0.21800	
5	1	1.65000	0.06230	0.00000	0.06000
	2	0.44000	0.35000	0.21800	

NEUTRON EMISSION FOR FISSIONS IN GROUP 1,-,KGROUP - 1.000 1.000

MATERIALS PICTURE

		(0.000)	(20.000)	(40.000)	(
		1	2	3	
		1	-1		
(20.000)	2				
		-1	-1		
(40.000)	3				

SPECIFICATIONS FOR REGIONS WITH VARYING PARAMETERS

REGION NO. 1

ROW SUB-MESH 5.00000 5.00000 5.00000 5.00000

COL.SUB-MESH 5.00000 5.00000 5.00000 5.00000

MATERIALS PICTURE OF SUB-MESH

5	4	3	2
4	4	3	2
3	3	3	2
2	2	2	2

C O N V E R G E N C E D A T A

OUT.ITER.NO.	INITIAL AND FINAL SOL. NORMS		INITIAL AND FINAL K-EFF	
1	1.0000000	1.7181350	**********	1.8955043
2	1.7181350	1.4432300	1.8955043	0.7529185
3	1.4432300	1.3020120	0.7529185	0.7410499
4	1.3020120	1.2286100	0.7410499	0.7399612
5	1.2286100	1.1901770	0.7399612	0.7406321
6	1.1901770	1.1698290	0.7406321	0.7413442
7	1.1698290	1.1589050	0.7413442	0.7418530
8	1.1589050	1.1529510	0.7418530	0.7421836
9	1.1529510	1.1496600	0.7421836	0.7423912
10	1.1496600	1.1478140	0.7423912	0.7425195
11	1.1478140	1.1467680	0.7425195	0.7425982
12	1.1467680	1.1461680	0.7425982	0.7426460
13	1.1461680	1.1458220	0.7426460	0.7426750
14	1.1458220	1.1456210	0.7426750	0.7426925
15	1.1456210	1.1455030	0.7426925	0.7427031
16	1.1455030	1.1454330	0.7427031	0.7427094

EXPANSION COEFF. FOR FLUX

GROUP	ROW	COLUMN	FLUX	COL.DER(UP)	COL.DER(DWN)	ROW DER(LFT)	ROW DER(RIT)	SECOND DERIV.
1	1	1	1.1454330	0.0000000		0.0000000		0.0000000
1	1	2	1.0562280	0.0000000		-0.1318337	-0.2378771	0.0000000
1	1	3	0.0000000	0.0000000		-0.0348431		0.0000000
1	2	1	1.0562280	-0.1318337	-0.2378771	0.0000000		0.0000000
1	2	2	0.5029880	-0.0780584	-0.1047543	-0.0780584	-0.1047543	0.0188278
1	2	3	0.0000000	0.0000000		-0.0144136		0.0022478
1	3	1	0.0000000	-0.0348431		0.0000000		0.0000000
1	3	2	0.0000000	-0.0144136		0.0000000		0.0022478
1	3	3	0.0000000	0.0000000		0.0000000		0.0003147
2	1	1	0.2573733	0.0000000		0.0000000		0.0000000
2	1	2	0.7405993	0.0000000		0.0756730	0.2156289	0.0000000
2	1	3	0.0000000	0.0000000		0.1251434		0.0000000
2	2	1	0.7405993	0.0756730	0.2156289	0.0000000		0.0000000
2	2	2	0.6186165	0.0164950	0.0268508	0.0164950	0.0268508	-0.0249411
2	2	3	0.0000000	0.0000000		0.0439566		-0.0140185
2	3	1	0.0000000	0.1251434		0.0000000		0.0000000
2	3	2	0.0000000	0.0439566		0.0000000		-0.0140185
2	3	3	0.0000000	0.0000000		0.0000000		-0.0038040

REACTION RATES IN REGIONS

	1	2	3
ABSRP	0.10998E 03	0.10450E 02	
PRODU	0.10000E 03	0.00000E 00	
TRNSP	0.21168E 04	0.35758E 04	
	2		
ABSRP	0.10450E 02	0.22135E 01	
PRODU	0.00000E 00	0.00000E 00	
TRNSP	0.35758E 04	0.74883E 03	
	3		

AVERAGE FLUXES IN REGIONS

	1	2	3
GRP.1	0.38355E 01	0.46288E 00	
GRP.2	0.11468E 01	0.12831E 01	
	2		
GRP.1	0.46288E 00	0.54992E-01	
GRP.2	0.12831E 01	0.27394E 00	
	3		

FLUX AND VOLUME AVERAGED PROPERTIES

COL	GROUP	DIFF.COEFF(CM)	RMVL.XS(/CM)	FISS.K->1(/CM)	SCTT.K
1	1	1.54470	0.06230	0.00000	0.06
	2	0.40824	0.23207	0.21800	

FLUX VALUES FOR EQUALLY SPACED POINTS INSIDE TH

(SET=GROUP-ROW-COLUMN)

SET	SUB-ROW	POINT FLUXES AT SUB-COLUMN							
		1	2	3	4	5	6	7	8
10101									
	1	3.2921	3.5080	3.9294	4.2173	4.0324	3.0358		
	2	3.5080	3.7076	4.0872	4.3176	4.0696	3.0140		
	3	3.9294	4.0872	4.3620	4.4557	4.0700	2.9068		
	4	4.2173	4.3176	4.4557	4.3870	3.8671	2.6515		
	5	4.0324	4.0696	4.0700	3.8671	3.2944	2.1854		
	6	3.0358	3.0140	2.9068	2.6515	2.1854	1.4457		
10102									
	1	3.0358	1.0339	0.1904	0.0443	0.1345	0.0000		
	2	3.0140	1.0208	0.1811	0.0367	0.1291	0.0000		
	3	2.9068	0.9752	0.1609	0.0217	0.1155	0.0000		
	4	2.6515	0.8879	0.1412	0.0112	0.0975	0.0000		
	5	2.1854	0.7497	0.1335	0.0167	0.0789	0.0000		
	6	1.4457	0.5511	0.1492	0.0501	0.0637	0.0000		
10201									
	1	3.0358	3.0140	2.9068	2.6515	2.1854	1.4457		
	2	1.0339	1.0208	0.9752	0.8879	0.7497	0.5511		
	3	0.1904	0.1811	0.1609	0.1412	0.1335	0.1492		
	4	0.0443	0.0367	0.0217	0.0112	0.0167	0.0501		
	5	0.1345	0.1291	0.1155	0.0975	0.0789	0.0637		
	6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
10202									
	1	1.4457	0.5511	0.1492	0.0501	0.0637	0.0000		
	2	0.5511	0.1829	0.0328	0.0116	0.0304	0.0000		
	3	0.1492	0.0328	-0.0049	0.0008	0.0142	0.0000		
	4	0.0501	0.0116	0.0008	0.0042	0.0084	0.0000		
	5	0.0637	0.0304	0.0142	0.0084	0.0059	0.0000		
	6	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000		
20101									
	1	0.7412	0.7463	0.8119	1.0138	1.4275	2.1286		
	2	0.7463	0.7396	0.7789	0.9531	1.3511	2.0618		
	3	0.8119	0.7789	0.7569	0.8616	1.2088	1.9142		
	4	1.0138	0.9531	0.8616	0.8757	1.1313	1.7649		
	5	1.4275	1.3511	1.2088	1.1313	1.2492	1.6931		
	6	2.1286	2.0618	1.9142	1.7649	1.6931	1.7780		
20102									
	1	2.1286	3.2636	2.4736	0.9033	-0.3028	0.0000		
	2	2.0618	3.2247	2.4521	0.8919	-0.3081	0.0000		
	3	1.9142	3.0847	2.3553	0.8492	-0.3103	0.0000		
	4	1.7649	2.8088	2.1352	0.7630	-0.2884	0.0000		
	5	1.6931	2.3622	1.7434	0.6208	-0.2216	0.0000		
	6	1.7780	1.7098	1.1318	0.4102	-0.0891	0.0000		
20201									
	1	2.1286	2.0618	1.9142	1.7649	1.6931	1.7780		
	2	3.2636	3.2247	3.0847	2.8088	2.3622	1.7098		
	3	2.4736	2.4521	2.3553	2.1352	1.7434	1.1318		

```
          4      0.9033   0.8919   0.8492   0.7630   0.6208   0.4102
          5     -0.3028  -0.3081  -0.3103  -0.2884  -0.2216  -0.0891
          6      0.0000   0.0000   0.0000   0.0000   0.0000   0.0000
20202
          1      1.7780   1.7098   1.1318   0.4102  -0.0891   0.0000
          2      1.7098   1.0986   0.5999   0.2359   0.0285   0.0000
          3      1.1318   0.5999   0.2832   0.1194   0.0458   0.0000
          4      0.4102   0.2359   0.1194   0.0490   0.0131   0.0000
          5     -0.0891   0.0285   0.0458   0.0131  -0.0190   0.0000
          6      0.0000   0.0000   0.0000   0.0000   0.0000   0.0000

CORE USAGE       OBJECT CODE=  105264 BYTES,ARRAY AREA=  160240 BYTES,TOTAL AR

COMPILE TIME=     4.07 SEC,EXECUTION TIME=     8.84 SEC,  WATFIV - VERSION 1 L
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