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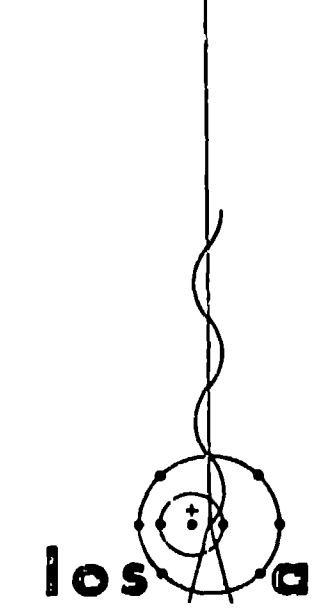

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ABSTRACT

The effectiveness of the energy dependent finite element method (EDFEM) as applied to two-dimensional multigroup diffusion problems is investigated. The EDFEM couples the finite element method (FEM) formalism with the energy dependent element size scheme. The EDFEM allows the elements to straddle material interfaces if certain conditions are satisfied; this makes this method especially suitable for heterogeneous reactor calculations. Comaprisons of the results obtained by the EDFEM, the FEM, and the finite difference method for a ZION-I PWR model are presented. A significant reduction of the total number of unknowns involved in the problem is accomplished using the EDFEM which yields a reduction of the computing time by 30%.

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I. INTRODUCTION

The numerical solution of the neutron diffusion equation is frequently required for reactor analysis. Consequently, there are continuing efforts to reduce the computer running time required for these solutions while maintaining the degree of accuracy needed in nuclear reactor analysis. Specifically, finite element methods (FEM) have been investigated as a potential method for reducing computation time.[1-5] Since the FEM has been observed to yield a high order of convergence for practical mesh sizes, the FEM is ideally suited for coarse-mesh calculations.

Energy dependent spatial mesh schemes have also been investigated as a method for reducing computing time.[6-8] In these schemes, fine-mesh arrangements are used in the lower energy neutron groups while relatively coarse meshes are used in the fast groups. This scaling is used because the neutron diffusion length, a characteristic scale length, is generally smallest in the lower energy groups and largest in the fast groups. In this fashion the ratio of mesh size to group diffusion length may be maintained roughly constant from group to group. Energy dependent spatial mesh schemes using either the FEM[8,9] or the finite difference method (FDM)[6,7] have been developed for one-dimensional diffusion problems. Results obtained using the energy dependent finite element method (EDFFM) as applied to one-dimensional problems in Refs. 8 and 9 demonstrated that reduced computing times could be obtained without sacrificing accuracy using this new method. This paper reports the results obtained by applying the method to a

pair of two-dimensional problems.[2] The two-group equations are solved using Lagrange piecewise biquadratic functions as a basis.

II. MATHEMATICAL FORMULATION

The FEM is an extension of Rayleigh-Ritz-Galerkin methods for approximation solutions to problems involving differential equations. Instead of solving the differential equation directly this method casts the equation in a variational or weak form. The functional for a given equation is not unique. The determination of the associated functional for a given problem is the first step is generating the solution. The basic formalism of the EDFEM is identical to that of the FEM.

Considered the generalized matrix representation of the multigroup diffusion equations,

$$-\nabla\cdot D\nabla\Phi + \Sigma\Phi = \frac{\chi S^{T}\Phi}{k}; \tag{1}$$

and of the multigroup adjoint equation

$$-\nabla\cdot D\nabla\Phi^{\dagger} + \Sigma^{T}\Phi^{\dagger} = S\chi^{T}\Phi^{\dagger} \tag{2}$$

for G groups where,

$\Phi = \text{col}(\phi^1,\phi^2, \ldots, \phi^G)$	direct neutron flux
$\Phi^{\dagger} = \text{col}\ (\phi^{\dagger 1}, \phi^{\dagger 2}, \ldots, \phi^{\dagger G})$	adjoint neutron flux
$D = \text{diag}\ (D^1,D^2, \ldots, D^G)$	the diffusion coefficients
$\Sigma = \text{diag}\ (\Sigma^1,\Sigma^2, \ldots, \Sigma^G)$	group removal and scattering cross sections
$\chi = \text{col}\ (\chi^1,\chi^2, \ldots, \chi^G)$	the prompt neutron spectrum

$S = \text{col}\ (S^1, S^2, \ldots, S^G)$ the product of fission cross section and number of neutron per fission

k neutron multiplication constant.

The Dirichlet condition is

$$\Phi^\dagger(r),\Phi(r) = 0 \text{ for } r\varepsilon\partial\Omega_e \tag{3}$$

where $\partial\Omega_e$ is the external boundary of domain Ω.

The associated functional is

$$J = \int_\Omega [\Phi^{\dagger T}(\Sigma - \chi S^T/k)\Phi + \nabla\Phi^{\dagger T}\cdot D\nabla\Phi]d\Omega, \tag{4}$$

or

$$a(\phi^{\dagger T}\phi) - b(\phi^{\dagger T}\phi)/k = J. \tag{5}$$

The functional, Eq. (4), is not a quadratic functional but a bilinear functional. The bilinear forms are

$$a(\Phi^{\dagger T},\Phi) = \int_\Omega (\nabla\Phi^\dagger\cdot{}^T D\nabla\Phi + \Phi^{\dagger T}\Sigma\Phi)d\Omega, \tag{6}$$

$$b(\Phi^{\dagger T},\Phi) = \int_\Omega \Phi^{\dagger T}\chi S^T\Phi d\Omega \tag{7}$$

The weak form of the problem is now an eigenvalue problem. Both Φ and $\Phi^\dagger$ have the same properties. $\phi^\dagger$ and $\phi\varepsilon H$, where $H = H_o^1(\Omega) \times H_o^1(\Omega) \times \ldots \times H_1^1(\Omega)$ G times. H_o^1 is the Sobolev space of functions which vanish on $\partial\Omega$ and whose first derivatives are square integrible in Ω.

In terms of trial functions $\hat{\Phi},\hat{\phi}^\dagger$, Eq. (5) is rewritten

$$a(\hat{\Phi}^{\dagger T},\hat{\Phi}) - b(\hat{\Phi}^{\dagger T}\hat{\Phi})/k = \hat{J}, \tag{8}$$

where

$$\phi = \sum_{i=1}^{N} \hat{\phi}_i u_i, \tag{9}$$

$$\hat{\phi}^\dagger = \sum_{i=1}^{N} \hat{\phi}^\dagger u_i . \tag{10}$$

The u_i are the basis functions often called the element functions and the expansion functions $\hat{\phi}_i$ are the nodal values of the fluxes.

The variation of $\hat{J}$ with respect to $\phi^{\dagger T}$ is required to vanish. Then

$$a(u_i\hat{\phi}) - b(u_i\hat{\phi})/k = 0, \qquad i = 1, 2, \ldots, N. \tag{11}$$

Therefore the function which minimizes the functional, Eq. (4) is also a solution of the weak form, Eq. (11). After the discretization procedure is performed, Eq. (1) yields the matrix equation

$$A^g\phi^g = Q^g \tag{12}$$

for each energy group g where A^g is given by N x N matrix Q in an N x 1 matrix; and ϕ^g is a column vector for N space point unknowns.

Each element A^g_{ij} of A^g is obtained from

$$A^g_{ij} = \int D^g \nabla u_i \cdot \nabla u_j d\Omega + \int \Sigma_a u_i u_j d\Omega, \qquad j = i, i\pm\tfrac{1}{2}, i\pm1; \tag{13}$$

and Q_1 from

$$Q^g_1 = \frac{\chi^g}{k} \sum_{h=1}^{G} \nu^h \Sigma^h_f \int \hat{\phi}^h u_i d\Omega. \tag{14}$$

The rationale behind the EDFEM is to keep the size of A minimal as an alternative method of reducing the computing time. In the steady state problem, the coefficient matrix A for each energy group needs be assembled and inverted only once. However, for time dependent cases, the computing time required to assemble and invert A(t) for each time step becomes a major concern.

The characteristic features of matrix A are that it is symmetric, positive definite, diagonally dominant, and highly banded. Any one or more of these characteristics can be used advantageously to speed up the numerical computation. The Choleski direct inversion method is used here.

Conventionally, the FEM maintains the element sizes the same in all energy groups so that the spatial arrangement of nodal points is identical for all groups. Elements are refined uniformly through all energy groups. The philosophy of the EDFEM is to refine only those energy groups whose characteristic diffusion length are small compared with the diffusion length of other energy groups. Since the EDFEM requires inner products of element functions whose supports Ω_i and Ω_j are not equal, the larger element edge size is always an integer multiple of the smaller one for simplicity.

The solution is obtained by first solving the fast-group equation on its coarse mesh. The thermal group term in the fast source is handled in a straight forward manner. The fast-group flux is represented by biquadratic polynomials in each element, and therefore quadratic interpolation can be used to obtain fast group fluxes at spatial points corresponding to the finer thermal mesh nodes. These values are then

used to generate new fast elements having the same support as the thermal elements. This representation is used for fast group fluxes which appear in the thermal group source.

The treatment of element sizes is clearly an important difference between FEM and the EDFEM. The EDFE also allows element boundaries to cross more material interfaces than does the FEM. However, element boundaries must lie on the material interfaces when adjacent diffusion coefficients differ drastically. In the fast groups, jumps in the diffusion coefficient are generally smaller from region to region while in the thermal groups this is not the case. Since an energy dependent mesh is used, the coarse fast elements may encompass several material interfaces while the finer thermal elements do not. The solution then does not possess a continuous first derivative inside the coarse fast element.

Assume that a finite element subspace $S_C^h H$ of degree k - 1 is used with the forms a(u,v), b(u,v) given in Eq. (11). If the coefficients in the multigroup Eq. (1) are smooth, then[10]

$$||\Phi - \Phi||_s \leq C_1 h^{k-s}$$

and

$$(k - \hat{k}) \leq C_2 h^{2k-2}.$$

Since the smoothness condition is violated in heterogeneous elements, these estimates for order of convergence do not hold.

When the fast element is inhomogeneous, the diffusion coefficients and other cross sections differ within the element, errors are introduced into the computed fast flux. Since the multigroup equations are coupled this error propagates into all other group fluxes. It is expected however, that the accuracy of the solution will not be severely degraded when the discontinuities are small. Therefore, the placement of fast group elements requires a careful study of problem configuration.

III. RESULTS AND DISCUSSION

The two thermal reactor problems investigated are (i) a simple two region model consisting of a core and reflector, and (ii) an inhomogeneous model of the ZION-I PWR core. Quadratic Lagrange polynomials are selected for basis functions. The EDFE computer program was used for numerical experimentation on the Burroughs 6700 computer.

The basic data for the first problem is given in Table I. This reactor configuration was examined in the x-y domain shown in Fig. 1. This problem is a two-dimensional extension of the problem discussed in Ref. 8. Notice the existence of a singular point, a so called "corner singularity".

The L/N 1-1 designation refers to the case in which the fast and thermal group element edges are of equal length. The L/N 1-2 case is the refinement applied only to the thermal group whose element edges are one half the size of those in the fast group.

An important observation can be made from Figs. 2a and 2b. The L/4 1-2 thermal flux distribution agrees well with the L/8 1-1 thermal flux distribution. In addition, the L/4 1-2 flux profile exhibits better agreement with the L/8 1-1 flux profile than does the L/6 1-1 profile. It is important to recognize the total number of unknowns involved in these runs. There are 320 unknowns involved in the L/4 1-2 computation whereas 518 unknowns are involved in the L/8 1-1 computation; accordingly, this reduction of nearly 38% in the total number of unknowns leads to a reduction of approximately 33% computing time required to set up the problem by the EDFE program. Eigenvalue results are indicated in Table III.

The ZION-1 PWR model represents a more stringent numerical test if the EDFEM because of its heterogeneity which is expected to dictate the slow/fast mesh ratio rather than a simple, ratio of diffusion lengths. The model contains several core reflector corners which introduce "strong" singularities in the flux. In all cases fast group elements include several fuel regions. The model configuration is indicated in Fig. 3, and the cross sections appear in Table III.

The thermal neutron flux along the core center line is shown in Fig. 4. The L/4 1-1 case consists of a 4 x 4 element arrangement in both groups. Here L is the half width of the reactor. The intervals on the abscissa correspond to fuel enrichment zones with the exception of the last interval which is the water reflector. The near perfect agreement between the thermal flux shapes of the L/4 1-2 run and L/8 1-1 run is evident in Fig. 4. The value of k_{eff} corresponding to the L/8 1-1 run is 1.275 02; the L/4 1-2 valve is 1.274 53, and the L/4 1-1 value is 1.275 29. These can be compared to a benchmark value

of 1.275 08 resulting from a fine mesh Citation run with 5 624 unknowns/ group.

The fast flux shapes obtained with the L/4 1-1, L/4 1-2, and L/8 1-1 runs are observed to be "smooth", as compared to the thermal flux, and in good agreement with one another. This indicates that the L/4 refinement is sufficient for the fast group. The L/4 1-1 thermal group flux plot of Fig. 4 indicates that the refinement is not sufficiently fine for the thermal group. Notice that even though the flux eigenfunction of the L/4 1-1 run is not highly accurate the value of k_{eff} is. This is a result of the variational principal embodied in the FEM.

For the L/8 1-1 run there are 256 unknowns in each group while for the L/4 1-2 run there are 256 unknowns in the thermal group and 64 in the fast group. It is observed that a reduction in total execution time of 35% is achieved in the EDFE L/4 1-2 run as compared to the conventional L/8 1-1 run. These comments refer to the use of direct inversion. When inner iterations are used, as they are for problems with a large number of unknowns, the time savings will be even greater.[7]

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TABLE I

Two-Group Macroscopic Cross Sections

Fast Group

Thermal Group

	Fuel	Reflector
D	1.5	1.2
	0.4	0.15
Σ_T	0.0623	0.101
	0.2	0.02
$\nu\Sigma_f$	0.0	0.0
	0.218	0.0
$\Sigma_{1\to2}$	0.06	0.1

$\nu_1 = 1.0 \times 10^8$ cm/sec

$\nu_2 = 2.2 \times 10^5$ cm/sec

TABLE II

Eigenvalues $1/K_{eff}$: Two-Dimensional, Two-Region, Two-Group Problem.
(Benchmark $1/K_{eff}$=1.1140943 for m=2, Δx=L/6)*

Δx	Quadratic Lagrange(1-1)	Quadratic Lagrange(1-2)	Quadratic Lagrange(1-4)	Linear* Hermite(m=1)	Cubic* Hermite(m=2)	Finite* Difference
L/2	1.09230613	1.11792116	1.12232815	1.0802150	1.1082321	1.0783013
L/4	1.10852172	1.11360767	-	1.0962251	1.1134916	1.0797120
L/6	1.11225374	1.11369092	-	1.1040456	1.1140943	1.0895577
L/8	1.11341751	-	-	-	-	-
L/20	-	-	-	-	-	1.1105031

*See Ref. 2.

TABLE III

Macroscopic Cross Sections

Group 1

Group 2

Composition	D(cm)	Σ_r(cm^{-1})	$\nu\Sigma_f$(cm^{-1})	Σ_s(cm^{-1}) (k→k+1)	Comments
3	1.02130 0.33548	0.00322 0.14596	0.0 0.0	0.0	Zion I (Core Baffle)
11	1.41760 0.37335	0.02597 0.06669	0.00536 0.10433	0.01742	Zion I (2.25%)
12	1.41970 0.37370	0.02576 0.07606	0.00601 0.12472	0.01694	Zion I (2.8%)
13	1.42650 0.37424	0.02560 0.08359	0.00653 0.14120	0.01658	Zion I (3.3%)
15	1.45540 0.28994	0.02950 0.00949	0.0 0.0	0.02903	Zion I (Water)

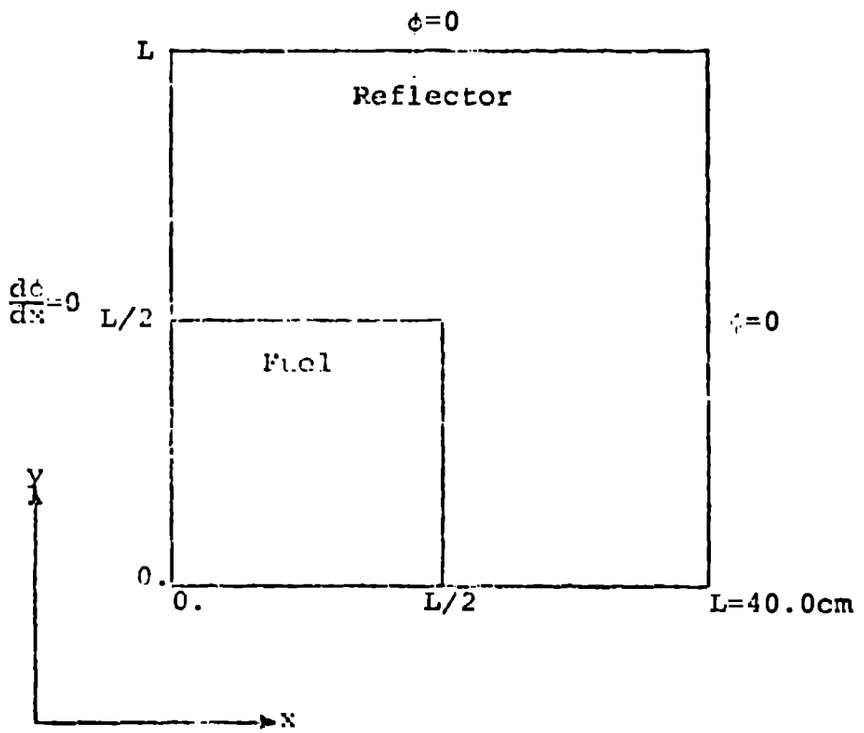

Fig. 1. Reactor Configuration:
Two-Dimensional, Two-Region, Two-Group Problem.

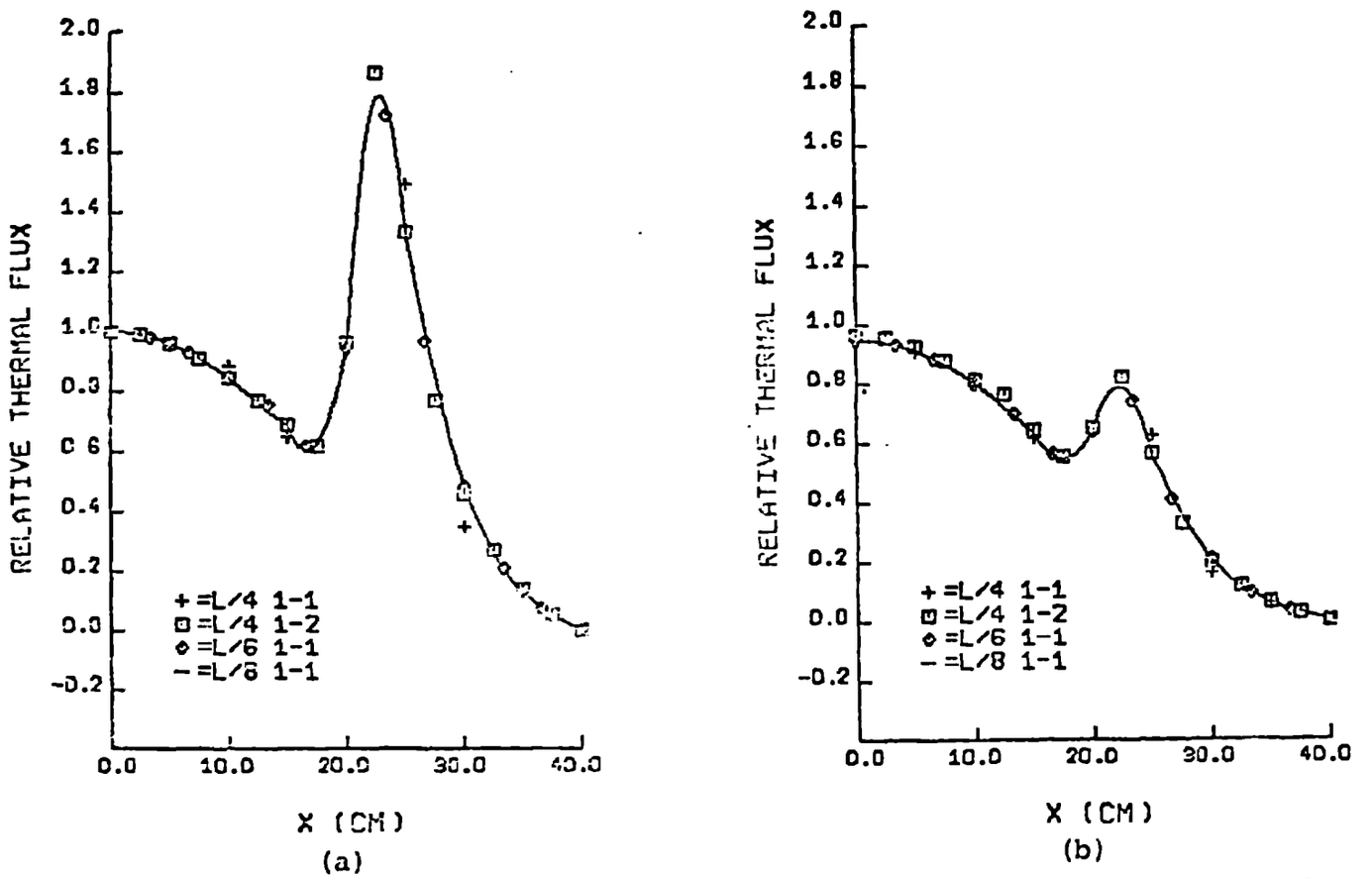

Fig. 2. Relative Thermal Fluxes (a) at y=0.0cm and (b) at y=20.0cm: Two-Dimensional, Two-Region, Two-Group Problem.

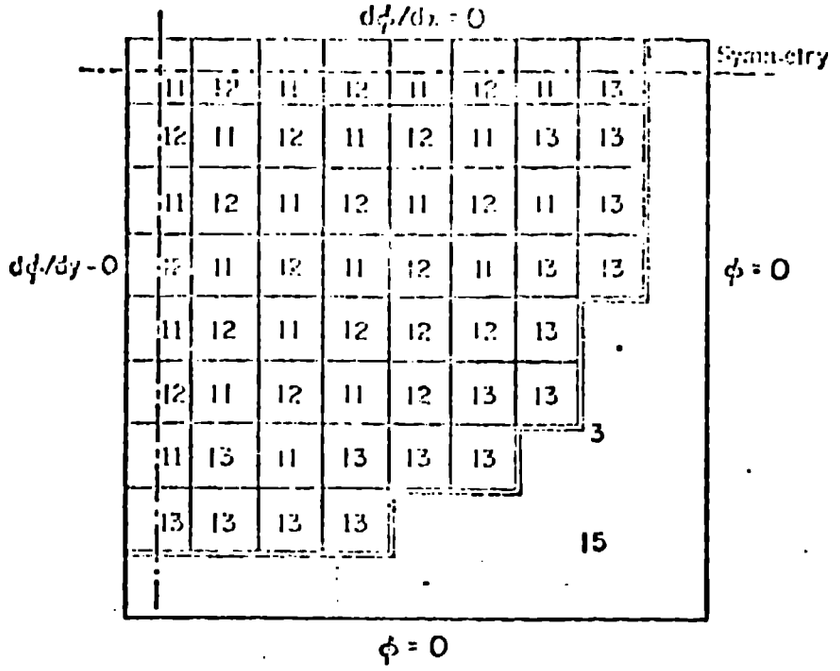

Fig. 3. ZION-1 first core layout.

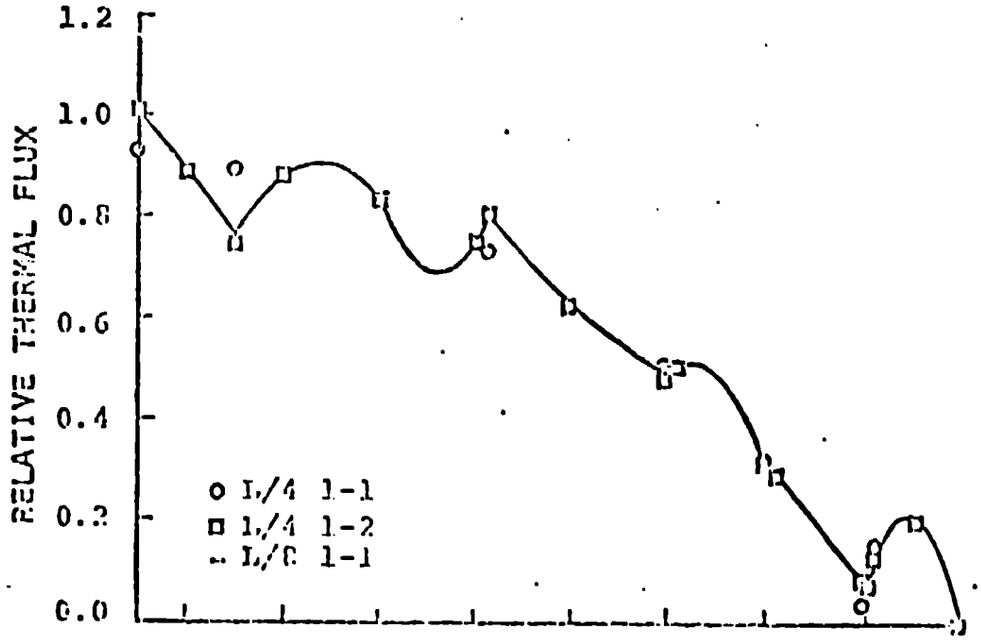

Fig. 4. Thermal flux along core center line.