Spherical Harmonics Treatment of Epithermal Neutron Spectra in Reactor Lattices

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A procedure has been developed to solve the slowing down transport equation for neutrons in a cylindricalized reactor lattice cell. Treating the anisotropy of the epithermal neutron flux by the spherical harmonics formalism, which reduces the space-angle-lethargy-dependent transport equation to the matrix integrodifferential equation in space and lethargy, and replacing the lethargy transfer integrals by finite-difference forms, a set of matrix ordinary differential equations, with lethargy and space dependent coefficients, is obtained. In the resonance region this set takes a lower block triangular form and can be directly solved by forward block substitution; in the lethargy range, where the fast fission effects have to be considered, the iterative procedure is introduced. A simple and efficient approximation is then proposed, making possible the analytical solution for the spatial dependence of the spherical harmonics flux moments.

The proposed procedure has been numerically examined and approved. Some typical results are presented and discussed.

I. INTRODUCTION

Several procedures have been reported in the literature for calculating neutron resonance absorptions and epithermal flux spectra in a cylindricalized reactor lattice cell, taking into account detailed spatial variation of the flux. Their common feature is that the neutron slowing down problem is formulated in terms of a Boltzmann integral equation. To solve this equation, first Driggers[1] and later Magier[2] applied the multigroup multiregion approach and the first flight collision probability technique, assuming the flat and isotropic emission densities in each region. In Ref. 2 the work was limited to the study of the 6.7-eV resonance of ^{238}U. Similarly, for the calculation of the fast spectra and the fast fission effects, Helholtz and Rothenstein[3] developed the multigroup procedure which used the collision and escape probabilities for a spatially flat flux.

Instead of using the multigroup approach, Kier[4] and Kier and Robba[5] divided the energy range of interest into extremely narrow intervals of equal lethargy width. The reaction rates and the flux distribution for each interval were again obtained applying the first flight collision probability technique, but supposing that the source distribution in each cell region could be represented by a three term space-dependent polynomial. The effect of the flat-flux approximation and the interference effects in UO_2-ThO_2 mixtures were studied.

A somewhat different approach was made by Lewis and Adler.[6] First the spatial dependence of the flux and emission density were approximated by Lagrange interpolation polynomials through a number of discrete ordinates. The space-lethargy-dependent neutron transport equation was thus reduced to a set of coupled integral equations

[1]F. E. DRIGGERS, *Trans. Am. Nucl. Soc.*, 8, 206 (1965).

[2]J. MAGIER, *J. Nucl. Energy*, 22, 417 (1968).

[3]J. HELHOLTZ and W. ROTHENSTEIN, *Nucl. Sci. Eng.*, 24, 349 (1966).

[4]P. H. KIER, *Nucl. Sci. Eng.*, 26, 230 (1966).

[5]P. H. KIER and A. A. ROBBA, "RABBLE, A Program for Computation of Resonance Absorption in Multiregion Reactor Cells, ANL-7326, Argonne National Laboratory (1967).

[6]E. F. LEWIS and F. T. ADLER, *Nucl. Sci. Eng.*, 31, 117 (1968).

in lethargy, which was then integrated numerically. The validity of the widely used flat-flux and flux recovery assumptions was examined in detail and the necessity for a more accurate treatment of resonance effects established. For practical purposes, however, the above procedure may be time consuming. At resonance energies the space variation of neutron flux in the fuel is difficult to represent by a low order polynomial, while the lethargy-dependent transport coefficients require permanent reevaluation in the course of numerical integration over lethargy. Recently, two more reports[7,8] have appeared, developing further the collision probability treatment of the resonance energy range.

In the present paper, a unified method is provided for computing the neutron spectrum down to the thermal energy range. The neutron slowing down problem is formulated in terms of an integrodifferential Boltzmann equation. The anisotropy of the neutron flux is treated applying the spherical harmonics formalism. This reduces the space-angle-lethargy-dependent transport equation to a matrix integrodifferential equation in space and lethargy. Approximating further the lethargy transfer integrals by finite difference forms, a set of ordinary matrix differential equations is obtained. In the resonance region this set takes a lower block triangular form and can be directly solved by forward block substitution; in the lethargy range, where the fast fission effects have to be considered, the iterative procedure is introduced. As for each lethargy pivotal point a boundary value problem has to be solved for a nonhomogeneous system of ordinary differential equations with space-dependent coefficients, the application of standard numerical methods, like the finite-spatial-difference method[9] or the method of adjoint equations,[10] is too cumbersome and would make the whole procedure impracticable. A simple and efficient approximation is proposed here, allowing an analytical solution for the space dependence of the spherical harmonics flux moments.

[7]Y. ISHIGURO and HIDEKI TAKANO, "PEACO, A Code for Calculation of Group Constants of Resonance Energy Region in Heterogeneous Systems," JAERI-1219, Japan Atomic Energy Research Institute (1971).

[8]A. P. OLSON, "RABID, An Integral Transport Theory Code for Neutron Slowing Down in Slab Cells," ANL-7645, Argonne National Laboratory (1970).

[9]G. I. MARCHUK, V. G. TURCHIN, V. V. SMELOV, and G. A. IL'YASOVA, BNL-719, Vol. II, Brookhaven National Laboratory (1962).

[10]G. N. LANCE, *Numerical Methods for the High Speed Computers*, Iliffe, London (1960).

II. OUTLINE OF THE METHOD

II.A. *Spherical Harmonics Treatment of the Resonance Flux Angular Dependence*

Consider a cylindrically symmetric infinitely long reactor lattice cell, consisting of a number of concentric annular zones. In a material zone composed of I isotopes, having mass number M_i, scattering cross section, Σ_{si}, and the total cross section, Σ_i, the space-angle-lethargy variation of the resonance neutron flux, $\phi(r,u,\mathbf{\Omega})$, will be described by the integrodifferential slowing down transport equation:

$$\mathbf{\Omega}\,\mathrm{grad}\,\phi(r,u,\mathbf{\Omega}) + \Sigma(u)\,\phi(r,u,\mathbf{\Omega})$$

$$= \frac{1}{4\pi}\sum_{i=1}^{I}\int_{u-q_i}^{u}\Sigma_{si}(u')\,\frac{\exp(u'-u)}{1-\alpha_i}\,du'\int_{\mathbf{\Omega}}\phi(r,u,\mathbf{\Omega})\,d\Omega \quad , \tag{1}$$

where

$$\Sigma(u) = \sum_{i=1}^{I}\Sigma_i(u)$$

$$\alpha_i = (M_i - 1)^2/(M_i + 1)^2$$

$$q_i = \ln(1/\alpha_i) \quad .$$

In the above equation it is assumed that scattering of resonance neutrons is isotropic in the laboratory system. Still, due to the extreme differences in the cross-section values for particular reactor cell zones, the neutron flux becomes anisotropic and application of the spherical harmonics formalism is justified. In the P-3 approximation, and for a cylindrically symmetric system, only six spherical harmonics flux moments exist.[11] These are regarded as components of the flux vector:

$$\boldsymbol{F}(r,u) = \begin{bmatrix}\phi_{00}(r,u)\\ \phi_{20}(r,u)\\ \phi_{22}(r,u)\\ \phi_{11}(r,u)\\ \phi_{31}(r,u)\\ \phi_{33}(r,u)\end{bmatrix} \tag{2}$$

satisfying the equation

$$\mathbf{T}(r,u)\,\boldsymbol{F}(r,u)$$

$$= \boldsymbol{E}\sum_{i=1}^{I}\int_{u-q_i}^{u}\Sigma_{si}(u')\,\frac{\exp(u'-u)}{1-\alpha_i}\,\phi_{00}(r,u')\,du' \quad . \tag{3}$$

[11]B. DAVISON, *Neutron Transport Theory*, Oxford University Press, London (1958).

T is a matrix differential operator in r, with space and lethargy dependent coefficients:

$$\mathbf{T}(r,u) = \begin{bmatrix} \Sigma_0(u) & 0 & 0 & \frac{1}{r}\frac{\partial}{\partial r}r & 0 & 0 \\ 0 & 5\Sigma(u) & 0 & -\frac{1}{r}\frac{\partial}{\partial r}r & \frac{1}{r}\frac{\partial}{\partial r}r & 0 \\ 0 & 0 & \frac{5}{6}\Sigma(u) & r\frac{\partial}{\partial r}\frac{1}{r} - \frac{r}{6}\frac{\partial}{\partial r}\frac{1}{r} & & \frac{1}{12\,r^3}\frac{\partial}{\partial r}r^3 \\ \frac{\partial}{\partial r} & -\frac{\partial}{\partial r} & \frac{1}{2\,r^2}\frac{\partial}{\partial r}r^2 & 3\Sigma(u) & 0 & 0 \\ 0 & \frac{\partial}{\partial r} & -\frac{1}{12r^2}\frac{\partial}{\partial r}r^2 & 0 & \frac{7}{6}\Sigma(u) & 0 \\ 0 & 0 & r^2\frac{\partial}{\partial r}\frac{1}{r^2} & 0 & 0 & \frac{7}{15}\Sigma(u) \end{bmatrix} \qquad (4)$$

$\boldsymbol{E}$ is a column vector, $\boldsymbol{E} = (1\ 0\ 0\ 0\ 0\ 0)^T$ and at this stage $\Sigma_0(u) = \Sigma(u)$.

The related boundary conditions, which provide satisfactory results even for small cells, are finite flux everywhere in the cell, continuity of all flux moments at cell zone interfaces, zero integral current, and zero neutron flux gradient at the outer cell boundary.

II.B. Numerical Treatment of the Resonance Flux Lethargy Variation

Through the application of the P-3 spherical harmonics formalism the original space-angle-lethargy-dependent transport Eq. (1) is reduced to the matrix, space- and lethargy-dependent Eq. (3). This will now be integrated numerically to provide the lethargy variation of the spherical harmonics flux moments.

Let the lethargy interval under consideration, $(u_{\min}, u_{\max})$, be partitioned by N equally spaced pivotal points, u_n. For a given cell composition, the step size $\Delta u = u_n - u_{n-1}$ should not be greater than the minimum value of the maximum lethargy gain per collision. Replacing further the lethargy transfer integrals in Eq. (3) by finite difference forms, a set of matrix ordinary differential equations is obtained:

$$\mathbf{T}(r,u_n)\boldsymbol{F}(r,u_n) = \boldsymbol{E}\sum_{i=1}^{I}\left[\frac{\Delta u}{2}\frac{\Sigma_{si}(u_n)}{1-\alpha_i}\phi_{00}(r,u_n) + \sum_{l=1}^{L_i-1}\Delta u\exp(-l\Delta u)\frac{\Sigma_s(u_{n-l})}{1-\alpha_i}\phi_{00}(r,u_{n-l}) + \frac{\Delta u}{2}\exp(-L_i\Delta u)\frac{\Sigma_s(u_{n-L_i})}{1-\alpha_i}\phi_{00}(r,u_{n-L_i}) + C_i\right] \quad ; (5)$$

$n = 1,2,\ldots,N$; $\quad u_n = u_{\min} + n\Delta u$;

$u_{\max} = u_{\min} + N\Delta u$.

L_i is the largest integer value of the quotient $q_i/\Delta u$; C_i is the difference corrector of the trapezoidal formula, referring to the i'th isotope.

If the pivotal points u_n are sufficiently dense, so that the difference correction may be ignored, the system of matrix differential Eqs. (5) takes a lower block triangular form and can be directly solved by forward block substitution. Knowing, or assuming, the space-lethargy flux variation at and below $u_{\min}$, the spatial distribution of the resonance flux at $u_n > u_{\min}$ can be determined by successive solution of the nonhomogeneous ordinary differential equations:

$$\mathbf{T}'(r,u_n)\boldsymbol{F}(r,u_n) \cong \boldsymbol{E}\sum_{i=1}^{I}\left[\sum_{l=1}^{L_i-1}\Delta u\exp(-l\Delta u)\frac{\Sigma_{si}(u_{n-l})}{1-\alpha_i}\phi_{00}(r,u_{n-l}) + \frac{\Delta u}{2}\exp(-L_i\Delta u)\frac{\Sigma_{si}(u_{n-L_i})}{1-\alpha_i}\phi_{00}(r,u_{n-L_i})\right] \ ; \quad n = 1,2,\ldots,N \ . \qquad (6)$$

$\mathbf{T}'$ is a matrix differential operator given by Eq. (4), but with modified Σ_0:

$$\Sigma_0(u_n) = \Sigma(u_n) - \frac{\Delta u}{2}\sum_{i=1}^{I}\frac{\Sigma_{si}(u_n)}{1-\alpha_i} \ . \qquad (7)$$

II.C. Approximate Analytical Solution for the Space Variation of Resonance Flux

In each step of numerical integration over lethargy a boundary value problem has to be solved for a nonhomogeneous system of ordinary differential Eqs. (7). To avoid difficulties associated with standard numerical methods, which could make the whole procedure impracticable, the attention is turned to a combination of numerical and analytical techniques.

To initiate the numerical integration over lethargy, suppose that below and at u_{min} the neutron flux is spatially flat in each cell zone. Then, at the first pivotal point u_1, Eq. (6) takes a simple form:

$$\mathbf{T}'(r,u_1)\boldsymbol{F}(r,u_1) = EC_0 \ , \tag{8}$$

where the value of the constant C_0 depends on the normalization factor. The exact analytical solution of Eq. (8) is known[11]:

$$\phi_{st}(r,u_1) = \frac{\delta_{s+t,0}C_0}{\Sigma_0(u_1)} + \sum_{k=1}^{3} A_{st}^k(u_1)$$

$$\times \{a^k(u_1)I_t[\nu^k(u_1)r] + (-1)^t b^k(u_1)K_t[\nu^k(u_1)r]\} \ ;$$

$$\delta_{s+t,0} = \begin{cases} 0 \text{ for } s+t\neq 0 \\ 1 \text{ for } s+t=0 \end{cases} ;$$

$$st = 00,\ 20,\ 22,\ 11,\ 31,\ 33 \ , \tag{9}$$

where

I_t and K_t = modified Bessel functions of the first and second kind of the order t

$\nu^k(u_1)$ = eigenvalues of the operator $\mathbf{T}'(r,u_1)$

$A_{st}^k(u_1)$ = known coefficients[11] depending on the cross sections $\Sigma(u_1)$ and $\Sigma_0(u_1)$

$a^k(u_1)$ and $b^k(u_1)$ = unknown integration constants determined by specifying the boundary conditions.

At the next lethargy point u_2, Eq. (6) is of the form

$$\mathbf{T}'(r,u_2)\boldsymbol{F}(r,u_2)$$

$$= E\left(C_1 + C_2\sum_{k=1}^{2}\{a^k(u_1)I_0[\nu^k(u_1)r] + b^k(u_1)K_0[\nu^k(u_1)r]\}\right) . \tag{10}$$

If $\nu^k(u_1)$ are not the eigenvalues of the operator $\mathbf{T}'(r,u_2)$, the exact analytical solution of Eq. (10) can again be expressed in terms of Bessel functions:

$$\phi_{st}(r,u_2) = \frac{\delta_{s+t,0}C_1}{\Sigma_0(u_2)} + \sum_{k=1}^{2}\{\alpha_{st}^k(u_1,u_2)I_t[\nu^k(u_1)r] + (-1)^t\beta_{st}^k(u_1,u_2)K_t[\nu^k(u_1)r]\}$$

$$+ \sum_{k=1}^{3} A_{st}^k(u_2)\{a^k(u_2)I_t[\nu^k(u_2)r] + (-1)^t b^k(u_2)K_t[\nu^k(u_2)r]\} \ , \tag{11}$$

where $\alpha_{st}^k(u_1,u_2)$ and $\beta_{st}^k(u_1,u_2)$ are the solutions of the following algebraic equations:

$$\boldsymbol{N}^k(u_1,u_2)\,\boldsymbol{\alpha}^k(u_1,u_2) = EC_2a^k(u_1) \ ;$$

$$\boldsymbol{N}^k(u_1,u_2)\,\boldsymbol{\beta}^k(u_1,u_2) = EC_2b^k(u_1) \ ; \quad k = 1,2 \ . \tag{12}$$

Here $\boldsymbol{\alpha}^k$ and $\boldsymbol{\beta}^k$ are column vectors:

$$\boldsymbol{\alpha}^k = (\alpha_{00}^k\ \alpha_{20}^k\ \alpha_{22}^k\ \alpha_{11}^k\ \alpha_{31}^k\ \alpha_{33}^k)^T \ ,$$

$$\boldsymbol{\beta}^k = (\beta_{00}^k\ \beta_{20}^k\ \beta_{22}^k\ \beta_{11}^k\ \beta_{31}^k\ \beta_{33}^k)^T \ , \tag{13}$$

and $\boldsymbol{N}^k(u_1,u_2)$ is a matrix:

$$\boldsymbol{N}^k(u_1,u_2) = \begin{bmatrix} \Sigma_0(u_2) & 0 & 0 & \nu^k(u_1) & 0 & 0 \\ 0 & 5\Sigma(u_2) & 0 & -\nu^k(u_1) & \nu^k(u_1) & 0 \\ 0 & 0 & \frac{5}{6}\Sigma(u_2) & \nu^k(u_1) & -\frac{1}{6}\nu^k(u_1) & \frac{1}{12}\nu^k(u_1) \\ \nu^k(u_1) & -\nu^k(u_1) & \frac{1}{2}\nu^k(u_1) & 3\Sigma(u_2) & 0 & 0 \\ 0 & \nu^k(u_1) & -\frac{1}{12}\nu^k(u_1) & 0 & \frac{7}{6}\Sigma(u_2) & 0 \\ 0 & 0 & \nu^k(u_1) & 0 & 0 & \frac{7}{15}\Sigma(u_2) \end{bmatrix} \tag{14}$$

It is not possible to continue the numerical integration over lethargy in the above manner and the exact analytical solution of Eq. (10), which in the general case cannot be expressed in the form of Eq. (11), will only be used here to introduce and examine a new approximate procedure based on a convenient combination of numerical and analytical treatment.

Let each cell zone be divided into a number of subzones and suppose that in a subzone z, having outer radius r_z, the right side of Eq. (10) is approximated by its volume averaged value:

$$T'(r, u_2)F_z(r,u_2) \simeq E\,\gamma_z(u_1) \quad \text{for } r_{z-1} \le r \le r_z \;; \tag{15}$$

$$\gamma_z(u_1) = C_1 + \frac{C_2}{r_z^2 - r_{z-1}^2} \int_{r_{z-1}}^{r_z} \sum_{k=1}^{2} \{a_z^k(u_1) I_0[\nu^k(u_1)r] + b_z^k(u_1) K_0[\nu^k(u_1)r]\}\, r\, dr \;. \tag{16}$$

For each of the subzones, the approximate analytical solution of Eq. (10) is then

$$\phi_{z,st}(r,u_2) = \frac{\delta_{s+t,0}\,\gamma_z(u_1)}{\Sigma_0(u_2)} + \sum_{k=1}^{3} A_{st}^k(u_2)\{a_z^k(u_2) I_t[\nu^k(u_2)r] + (-1)^t\, b_z^k(u_2)\, K_t[\nu^k(u_2)r]\} \;, \quad r_{z-1} \le r \le r_z \;. \tag{17}$$

The integration constants a_z^k and b_z^k are allowed to have different values in each subzone to provide continuous flux moments everywhere in the cell. They are determined by the interface conditions

$$F_z(r_z, u_2) = F_{z+1}(r_z, u_2) \;. \tag{18}$$

It has been numerically examined and approved, for numerous cell configurations and different parameter values, that the approximate solution of Eq. (17) rapidly converges to the exact solution of Eq. (11). One typical example of this convergence is illustrated by Figs. 1 and 2 and Table I. For a two-zone fuel moderator cell, the right side of Eq. (10), assumed to be zero in the fuel (moderation neglected), is represented by the full line in Fig. 1. The corresponding exact solutions of Eq. (10), for the flux moments ϕ_{00} and ϕ_{11}, are given by full lines in Fig. 2. The right side of Eq. (10) is then approximated as shown in Fig. 1 (dashed-dotted lines), and the corresponding solutions of Eqs. (15) and (16) are presented in Fig. 2. The rapid convergence to the exact solution is observable and the details are presented in Table I.

By extending the above formalism to the whole slowing down region, the set of matrix ordinary differential Eqs. (6), governing the space-lethargy flux distribution in a subzone, is approximated as

$$T(r,u_n)F(r,u_n) \simeq E\,\gamma_n \;, \quad n = 1, 2, \ldots, N \;; \tag{19}$$

$$\gamma_n = \sum_{i=1}^{I} \left[\sum_{l=1}^{L_i - 1} \Delta u \exp(-l\Delta u) \frac{\Sigma_{si}(u_{n-l})}{1 - \alpha_i} \overline{\phi_{00}}(u_{n-l}) + \frac{\Delta u}{2} \exp(-L_i \Delta u) \frac{\Sigma_{si}(u_{n-L_i})}{1 - \alpha_i} \overline{\phi_{00}}(u_{n-L_i}) \right] \;. \tag{20}$$

TABLE I

Convergence of the Proposed Approximate Solution, Eq. (17), to the Exact Analytical Solution, Eq. (11)

(Parameter values the same as for Figs. 1 and 2)

Number of Subzones	Scalar Neutron Flux (arbitrary units)		
	At the Center of the Cell	At the Fuel Moderator Interface	At the Effective Cell Boundary
1	2.80975	8.75208	13.5055
2	2.69758	8.32817	13.9469
3	2.65126	8.13180	14.0045
4	2.62993	8.03614	14.0239
5	2.61874	7.98453	14.0329
6	2.61224	7.95407	14.0378
7	2.60816	7.93477	14.0407
8	2.60544	7.92185	14.0427
9	2.60355	7.91280	14.0440
Exact Solution	2.59616	7.87722	14.0490

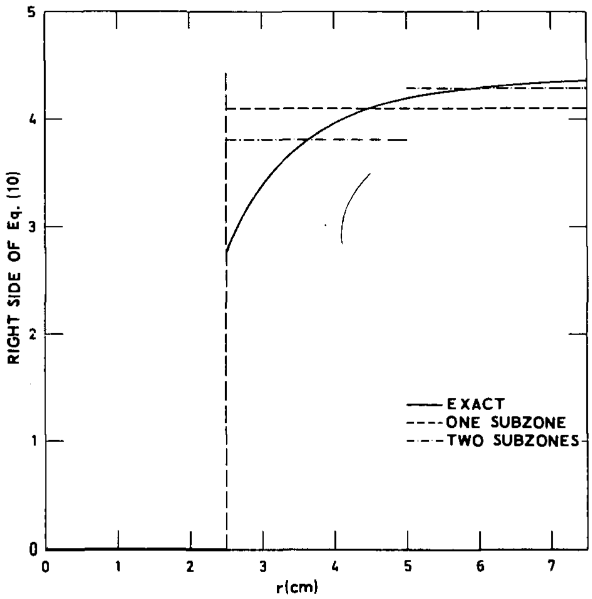

Fig. 1. Graphic representation of the right side of Eq. (10). Two-zone fuel moderator cell, r_1 = 2.5 cm, r_2 = 7.5 cm. Parameter values: C_1 = 4.44, C_2 = 1, ν^1 = 1.09, ν^2 = 0.44, a^1 = 0.0001, a^2 = -0.0151, b^1 = -18.43, b^2 = -2.194.

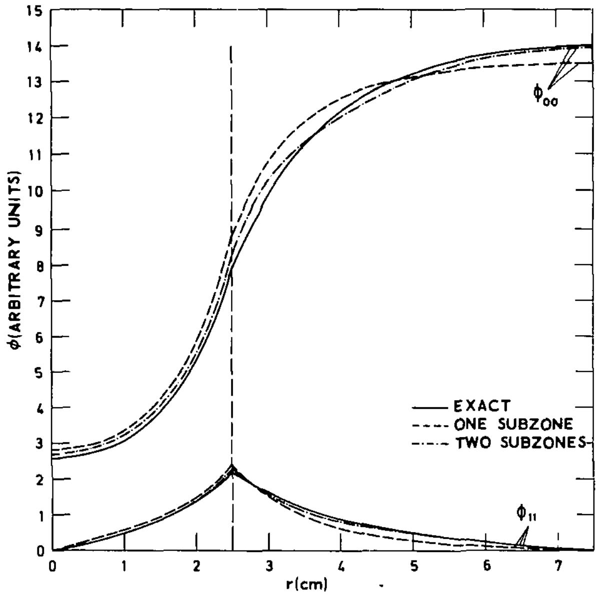

Fig. 2. Comparison of the exact and approximate analytical solutions of Eq. (10) for the flux moments ϕ_{00} and ϕ_{11}. Parameter values: $C_1 = 4.44$, $C_2 = 1$, $\nu^1 = 1.09$, $\nu^2 = 0.44$, $a^1 = 0.0001$, $a^2 = -0.0151$, $b^1 = -18.43$, $b^2 = -2.194$.

Here $\overline{\phi_{00}}$ denotes the scalar flux at the relevant lethargy, averaged over the volume of the subzone (the subzone index z is omitted for brevity). An approximate analytical expression can now be written for the space dependence of the spherical harmonics flux moments:

$$\phi_{st}(r,u_n) = \frac{\delta_{s+t,0}\,\gamma_n}{\Sigma_0(u_n)} + \sum_{k=1}^{3} A^k_{st,n}\,[a^k_n I_t(\nu^k_n r) + (-1)^t b^k_n K_t(\nu^k_n r)] \quad , \qquad (21)$$

where a^k_n and b^k_n are the unknown integration constants to be determined from the boundary condition equations at each lethargy pivotal point u_n. For γ_n the following recurrence relation applies:

$$\gamma_n = \exp(-\Delta u)\gamma_{n-1} + \Delta u \sum_{i=1}^{I} \frac{1}{1-\alpha_i} \times \left[\exp(-\Delta u)\,\Sigma_{si}(u_{n-1})\,\overline{\phi_{00}}(u_{n-1}) - \frac{\exp(-L_i\Delta u)}{2}\,\Sigma_{si}(u_{n-L_i})\,\overline{\phi_{00}}(u_{n-L_i}) - \frac{\exp[-(L_i-1)\Delta u]}{2}\,\Sigma_{si}(u_{n-L_i-1})\,\overline{\phi_{00}}(u_{n-L_i-1})\right] \quad . \qquad (22)$$

For purely hydrogenous moderator, Eq. (22) takes a simple form:

$$\gamma_n = \exp(-\Delta u)\,[\gamma_{n-1} + \Delta u\,\Sigma_s \overline{\phi_{00}}(u_{n-1})] \quad , \qquad (23)$$

while for the cell zones where moderation can be neglected, γ_n becomes zero and Σ_0 equals the macroscopic absorption cross section.

Equation (21) cannot be directly applied at lethargies near the very strong resonances, where large arguments of I and K functions cause machine overflow and underflow and make it impossible to determine the unknown integration constants. Thus, for large arguments, the expression for the flux moments is modified using the asymptotic expansions for Bessel functions.[12] Let r_1 and r_2 be the inner and the outer radii of the cell zone considered. Then, for $\nu r_1 \gg 1$ and $\nu r_2 \gg 1$:

$$\phi_{st}(r,u_n) = \frac{\delta_{s+t,0}\,\gamma_n}{\Sigma_0(u_n)} + \sum_{k=1}^{3} A^k_{st,n}\,\{a'^k_n \exp[-\nu^k_n(r_2 - r)]\,P_t(\nu^k_n r) + (-1)^t b'^k_n \exp[-\nu^k_n(r - r_1)]\,Q_t(\nu^k_n r)\} \quad , \qquad (24)$$

where a'^k_n and b'^k_n are the new integration constants, to be determined from the boundary condition equations, and

$$P_t(x) = \frac{1}{\sqrt{2\pi x}} \sum_{m=0}^{30} (8x)^{-m} \frac{1}{m!} \prod_{k=1}^{m} [(2k-1)^2 - 4t^2] \quad ;$$

$$Q_0(x) = \frac{\sqrt{\pi}}{\sqrt{2x}}\,G_0(x) \quad ; \quad Q_1(x) = \frac{\sqrt{\pi}}{\sqrt{2x}}\,G_1(x) \quad ;$$

$$Q_{t+1} = \frac{2t}{x}\,Q_t(x) + Q_{t-1}(x) \quad . \quad (t>1) \qquad (25)$$

Here, G_0 and G_1 are polynomials in $1/x$.[13]

Note that the volume averaging of the flux, i.e., calculation of $\overline{\phi_{00}}$ and the related integral quantities, as different reaction rates and resonant integrals, can be performed by integrating expression (21) analytically so that no additional error is introduced at this stage of calculation:

$$\overline{\phi_{00}}(u_n) = \frac{\gamma_n}{\Sigma_0(u_n)} + \frac{2}{r_2^2 - r_1^2} \sum_{k=1}^{2} \frac{1}{\nu^k_n} \{a^k_n[r_2 I_1(\nu^k_n r_2) - r_1 I_1(\nu^k_n r_1)] - b^k_n[r_2 K_1(\nu^k_n r_2) - r_1 K_1(\nu^k_n r_1)]\} \quad . \qquad (26)$$

[12] The same transformation can be used in some diffusion theory calculations, where the machine overflow and underflow are caused either by strong absorption of control rods or by large dimensions of the system.

[13] G. N. WATSON, *A Treatise on the Theory of Bessel Functions*, The Macmillan Company, New York (1944).

The validity and the applicability of the assumption made in Eqs. (19) and (20) depend on how fast the approximate analytical solution of Eq. (21) converges when the number of cell subzones is increased. This has been numerically examined for different cell compositions and various lethargy ranges. Some typical results for a two-zone U-C cell and the lethargy range 1 to 100 eV are presented in Table II. Here, as well as in all the other cases studied, a rapid convergence of the reaction rates calculation, with increasing number of fuel and/or moderator subzones, is observable.

TABLE II

Convergence of the Resonance Reaction Rates Calculation with Increasing Number of Fuel and/or Moderator Subzones

Number of Subzones		Reaction Rates (arbitrary units)		
In Fuel	In Moderator	Absorption in Fuel	Total in Fuel	Total in Moderator
1	1	5.91102	13.9232	166.204
2	1	5.87967	13.8499	166.331
3	1	5.85865	13.8026	166.415
4	1	5.84766	13.7785	166.460
5	1	5.84120	13.7647	166.485
1	1	5.91102	13.9232	166.204
1	2	5.79107	13.6461	167.855
1	3	5.72546	13.4935	168.392
1	4	5.69390	13.4201	168.623
1	5	5.67717	13.3811	168.743
1	1	5.91102	13.9232	166.204
2	2	5.76135	13.5766	167.967
3	3	5.67730	13.3826	168.570
4	4	5.63649	13.2890	168.834
5	5	5.61442	13.2388	168.974

II.D. Iterative Treatment of the Fast Fission Effects

In the preceding sections the procedure suitable for calculating the space and lethargy variation of resonance neutron flux in a cylindricalized reactor lattice cell has been developed. It can be easily extended for also treating the fast fission effects. Beside slowing down by elastic scattering, the transport equation governing the fast neutron flux must include the slowing down by inelastic scattering and the neutron yield from both thermal and fast fissions. Let $u = 0$ be the lower and u_f the upper bounds of the lethargy range where fast fission effects are to be considered. Then the equation analogous to Eq. (3) is

$$\mathbf{T}(r,u)\mathbf{F}(r,u) = \mathbf{E}\sum_{i=1}^{I}\Big[\int_{u-q_i}^{u}\Sigma_{si}(u')\frac{\exp(u'-u)}{1-\alpha_i}\phi_{00}(r,u')\,du' + \int_0^u \Sigma_{\text{in},i}(u'\to u)\phi_{00}(r,u')\,du' + \int_0^{u_f}\chi(u)\nu_i(u')\Sigma_{fi}(u')\,\phi_{00}(r,u')\,du'\Big] + \mathbf{E}\,S(r,u) \;, \tag{27}$$

where $\Sigma_{\text{in},i}(u' \to u)$ is the inelastic scattering kernel, Σ_f is the macroscopic fast fission cross section, ν_i is the number of secondaries per a fast fission, $\chi(u)$ is the fission spectrum, $S(r,u)$ is the thermal fission source, supposedly known. The numerical treatment of the neutron lethargy variation, presented in Sec. II.B., would in case of Eq. (27) lead to a coupled system of matrix ordinary differential equations that could not be solved simultaneously. The following iterative procedure is thus introduced:

$$\mathbf{T}(r,u)\mathbf{F}_j(r,u) = \mathbf{E}\sum_{i=1}^{I}\Big\{\int_{u-q_i}^{u}\Sigma_{si}(u')\frac{\exp(u'-u)}{1-\alpha_i}\phi_{00,j}(r,u')\,du' + \int_0^u\left[\Sigma_{\text{in},i}(u'\to u) + \chi(u)\nu_i(u')\Sigma_{fi}(u')\right]\phi_{00,j}(r,u')\,du' + \int_u^{u_f}\chi(u)\nu_i(u')\Sigma_{fi}(u')\phi_{00,j-1}(r,u')\,du'\Big\} + \mathbf{E}\,S(r,u) \;, \tag{28}$$

where j is the iteration index and $\mathbf{F}_j$ is the unknown vector. For $j=1$, $\phi_{00,j-1}$ is the initial guess, for $j>1$ this is the function known from the previous iteration.

Convergence of the above iteration scheme is very good. The total neutron balance condition can serve as the criterion for the completed iteration procedure: the total number of neutrons absorbed in the lethargy region considered, or scattered out of this region, must equal, to the desired accuracy, the total number of neutrons born in thermal and fast fissions.

Further treatment of Eq. (28) can be exactly the same as the one proposed in Secs. II.B. and II.C.

III. RESULTS AND DISCUSSION

According to the procedure developed in the previous sections, FORTRAN IV programs have been written for the CDC-3600 computer. The space and lethargy distribution of epithermal neutrons in a cylindricalized reactor lattice cell,

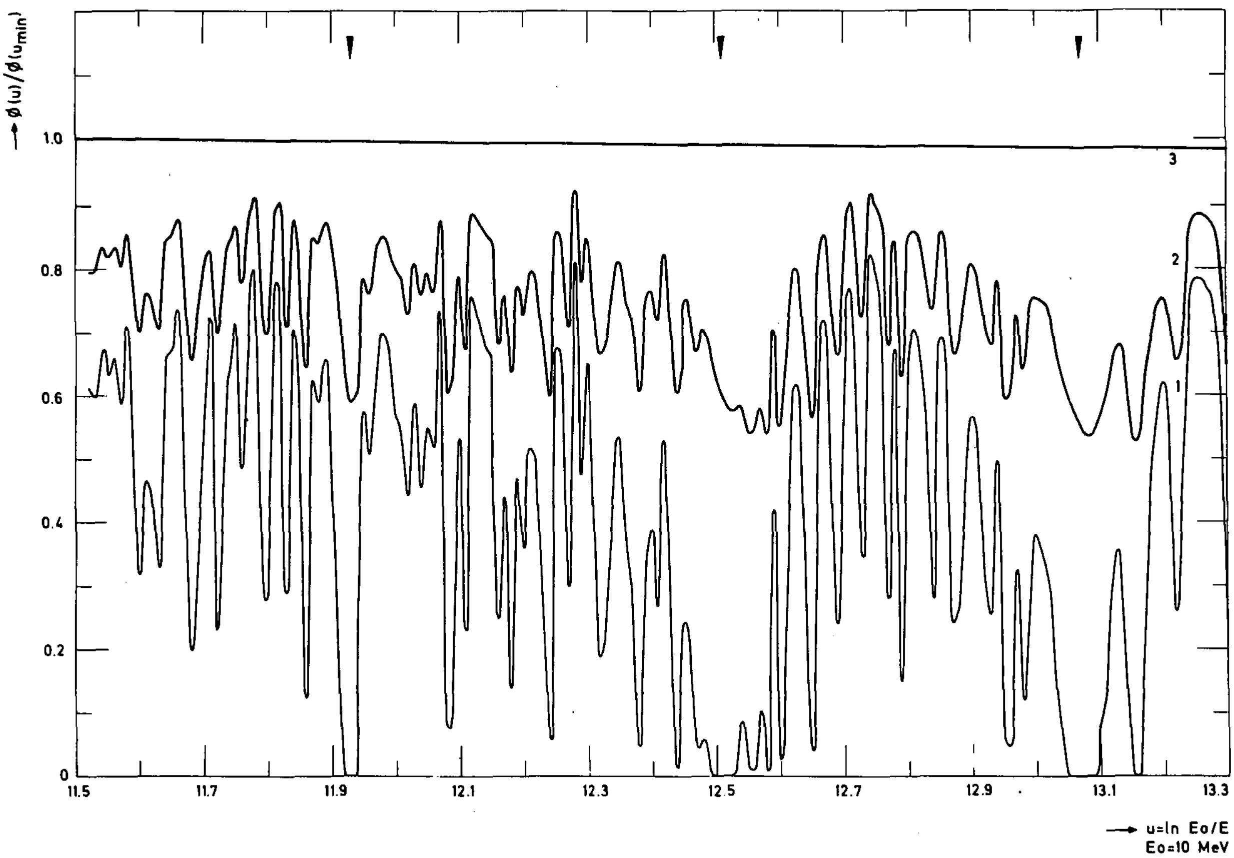

Fig. 3. Lethargy variation of the resonance neutron flux in a two-zone enriched uranium metal-H_2O cell.

and the related integral quantities, can be determined as detailed as the neutron cross sections are known for the materials considered. For the resonance neutrons the KEDAK[14] nuclear data have been used. In the fast energy region, where cross-section variations are rather smooth, the standard multigroup scheme has been adopted and the group data given in Ref. 15 have been used. Some typical results are presented.

Figure 3 is an illustration of the lethargy variation of the resonance neutron flux at the center of the fuel element, at the fuel moderator interface and at the outer boundary (curves are denoted by 1, 2, and 3, respectively) of a two-zone enriched uranium-H_2O cell. The figure covers the range 100 to 10 eV, where the strong variations of the flux are caused by a large number of unresolved ^{235}U resonances and also by the strong resolved

[14] I. LANGNER, J. J. SCHMIDT, and D. WOLL, KFK-750, Kernforschungszentrum, Karlsruhe (1968).

[15] L. P. ABAGYAN, N. O. BAZAZYANTS, I. I. BONDARENKO, and M. N. NIKOLAEV, *Group Constants for Nuclear Reactor Calculations*, Consultants Bureau, New York (1964).

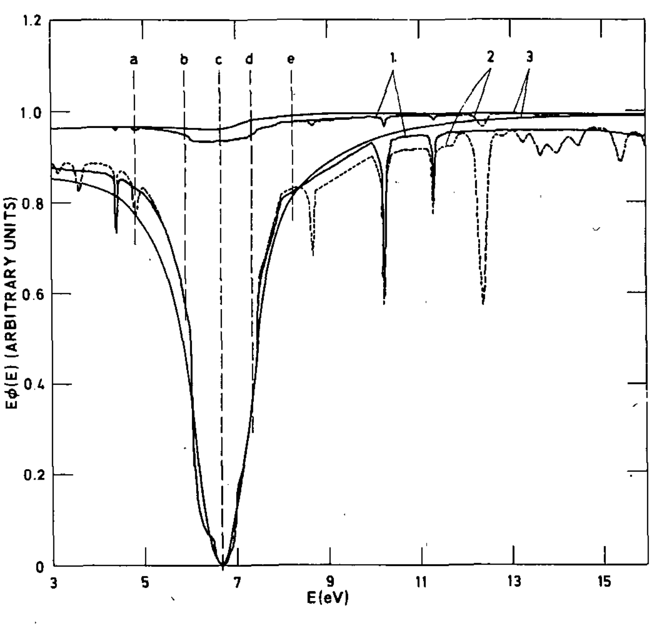

Fig. 4. Energy distribution of the neutron flux through the 6.7-eV resonance of ^{238}U. Uranium-graphite cell studied by Lewis and Adler[6]; r_1 = 1.732 cm, r_2 = 7.2 cm.

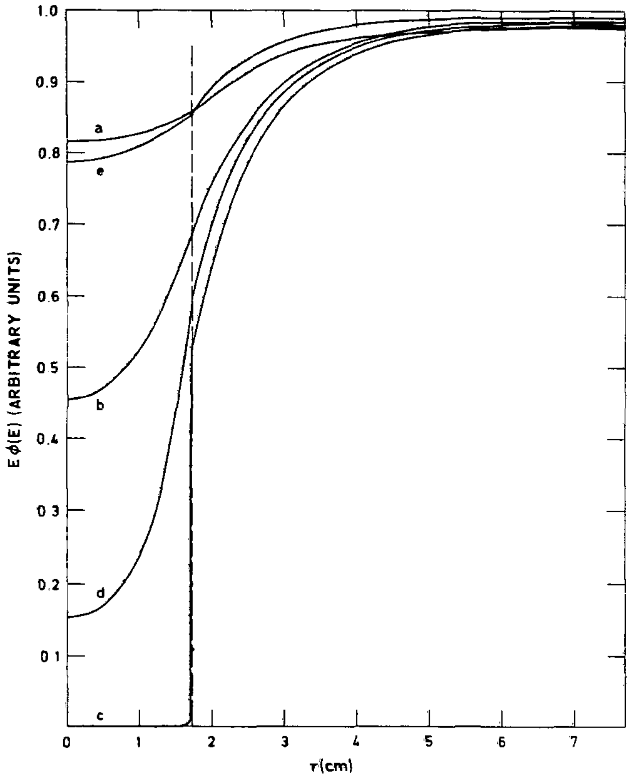

Fig. 5. Spatial distribution of the neutron flux for the energies denoted by (a) through (d) in Fig. 4.

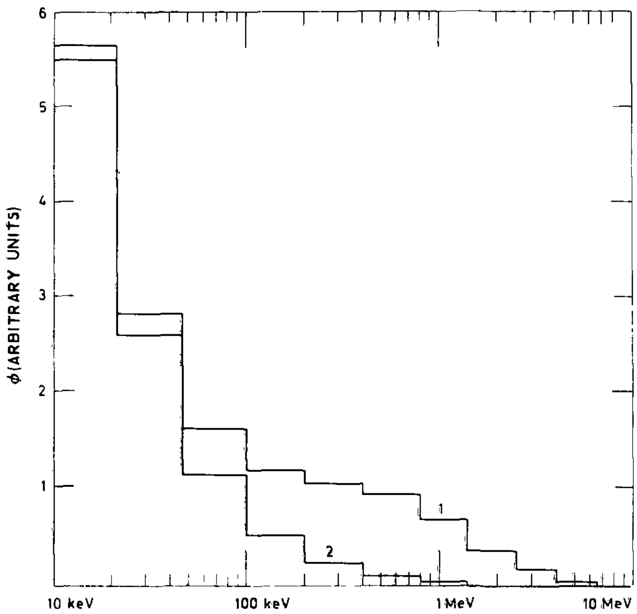

Fig. 6. Energy distribution of the fast-neutron flux at the center (1) and at the outer boundary (2) of a U-D₂O cell; r_1 = 1.193 cm, r_2 = 10 cm.

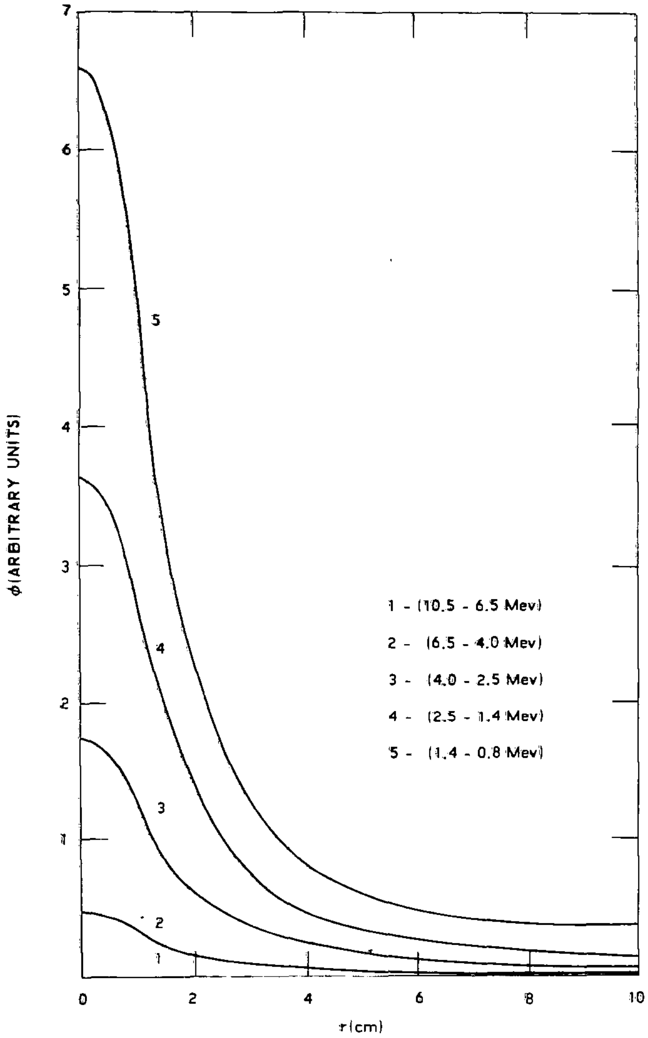

Fig. 7. Spatial distribution of the fast-neutron flux for the five highest energy groups.

resonances of ^{238}U. The arrows in the figure point the positions of these "giant" ^{238}U resonances.

In Fig. 4 the energy distribution of the average flux in the fuel and moderator of a U-C cell, through the 6.7-eV resonance of ^{238}U, obtained by the proposed method supposing the $1/v$ absorption in ^{235}U (curves 1), or taking into account the detailed variation of ^{235}U cross sections (curves 2), is compared with the results of Lewis and Adler[6] (curves 3). The agreement can be considered satisfactory.[16] For the energy values denoted in Fig. 4 by (a) through (d), the radial variation of the

[16]The linear parts of curves 1 and 2 between 7.5 and 10 eV are due to linear interpolation in the tables of the cross section values. Parabolic interpolation, suggested in Ref. 14 for resonance wings, could not be performed since it led to oscillatory results.

flux is given in Fig. 5. Note that at resonance energies polynomial representation, used in Refs. 4 and 6, is very inconvenient for the spatial variation of the neutron flux in the fuel.

In Fig. 6 the energy variation of the fast-neutron flux at the center (step curve 1) and at the outer boundary (step curve 2) of a U-D_2O cell is presented. The calculation has been performed with 11 energy groups covering the energy range from 10.5 MeV to 10 keV. In Fig. 7 the radial distribution of neutron flux, for the 5 energy groups above the fast fission threshold of ^{238}U, is presented.

In Fig. 8 the energy distribution of the fast fission ratio, obtained by the multigroup P-3 procedure of the present paper (step curve), is compared with the distribution obtained using the exact analytical solution of the slowing down equation.[17] The agreement is satisfactory.

The results presented here, as well as the other results obtained, prove that the proposed procedure can be efficiently used to calculate the detailed spatial and lethargy distribution of epithermal neutrons in a multizone cylindrically symmetric lattice cell. The computing time is relatively short, which makes the proposed procedure suitable for practical applications. In the present form the procedure can treat only isotropic scattering. It is believed that at resonance energies a P-3 approximation of the spherical harmonics method is at least as good as the polynomial representation of the spatial flux variation used with the collision probability treatment. The extension of the method to higher order approximations, for instance P-5, would be too complicated and impracticable.

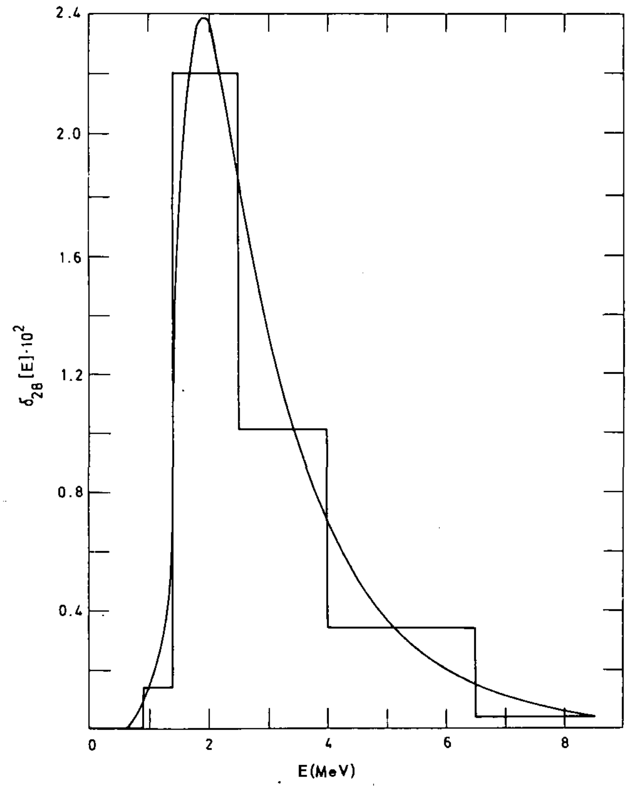

Fig. 8. Energy distribution of the fast fission ratio for a U-D_2O cell; r_1 = 1.193 cm, r_2 = 10 cm.

[17] D. STEFANOVIĆ, *Nucl. Sci. Eng.*, **41**, 349 (1970).