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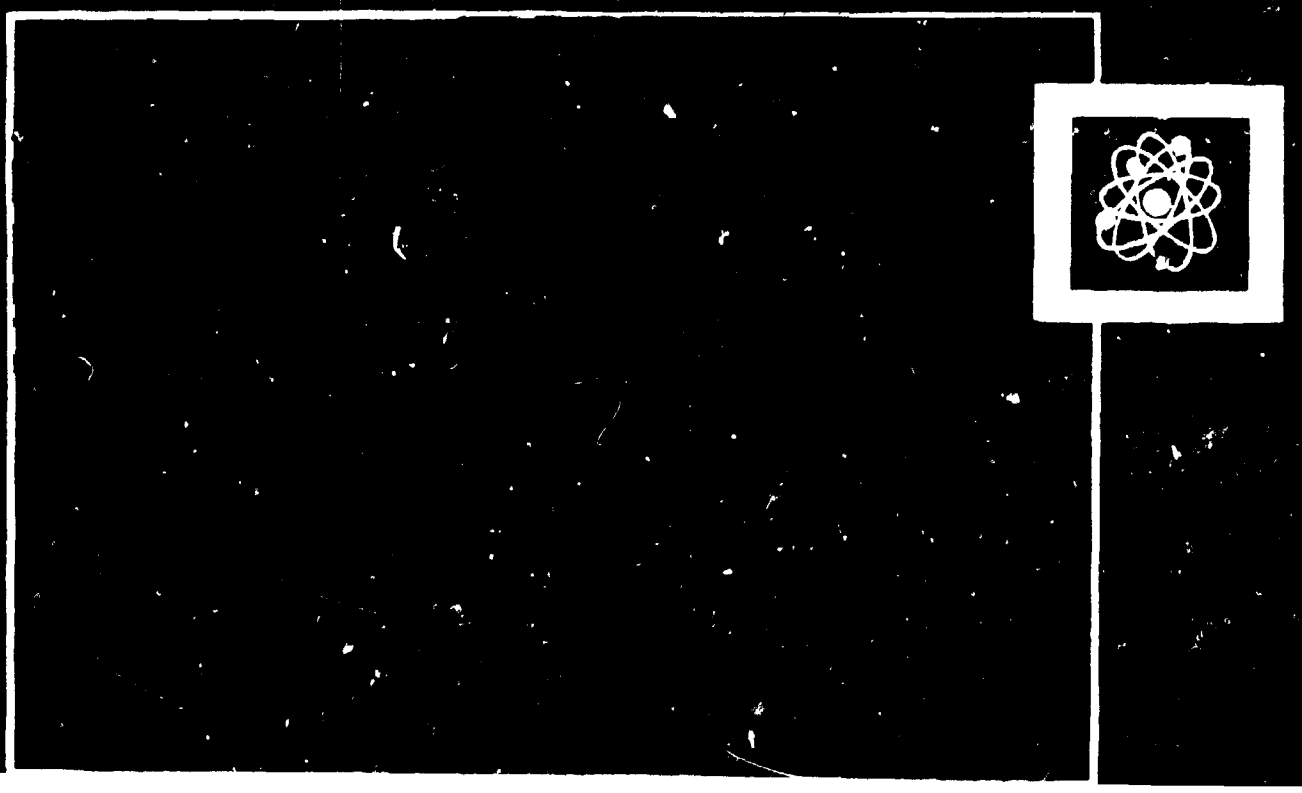

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DIFFERENCE METHOD OF SOLUTION OF TWO-DIMENSIONAL MULTIGROUP TIME-INDEPENDENT DIFFUSION EQUATIONS

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ABSTRACT

The project of nuclear reactors is still based on the solution of multi-group diffusion equations. This report gives a numerical solution of a two-dimensional system of time independent multigroup diffusion equations. On principle it is very simple to expand this method for a three-dimensional problem, but in such a case from the point of view of economical solution it is more advantageous to use the synthesis technique.

The system of partial differential equations is being replaced by a system of difference linear algebraical equations. Following this paper the DIFFIT - code procedure in ELLIOT - AUTOCODE for NE 803 B and NE 503 has been worked out. This procedure serves mainly for calculations of the reactor core. Further the REDIFFIT - code variant for radiation shielding calculations by using the removal-diffusion method has been worked out.

The number of mesh-points for the computers named above is 1000, the number of chosen groups is 30. The slowing-down of neutrons from the given group into all lower groups has been taken into consideration. By a suitable choice of the boundary conditions it is possible to use these procedures for one-dimensional problems (plane and cylinder).

Printed by
Czechoslovak Atomic Energy Commission
Centre for Scientific and Technical Information
Zbraslav nad Vltavou

1. Formulation of the Problem

The following system of multi-group equations is being solved:

$$\left\{ -\operatorname{div}\left[D_i(\vec{r})\ \operatorname{grad}\ \phi_i(\vec{r}) \right] + \Sigma_i(\vec{r})\ \phi_i(\vec{r}) = \right.$$

$$\left. = \sum_{j=1}^{i-1} \Sigma^{r}_{j \to i}(\vec{r})\ \phi_j(\vec{r}) + \frac{\nu_i(\vec{r})}{k_{eff}}\ Q(\vec{r}) + S_i(\vec{r}) \right\}_{i=1}^{G} \qquad (1)$$

where:

$\phi_i(\vec{r})$ . . . the integral of neutron flux in the ranges of the i-th group

$D_i(\vec{r})$ . . . the diffusion coefficient for the i-th group

$$\Sigma_i(\vec{r}) = \Sigma^{v}_i(\vec{r}) + D_i(\vec{r})\ B^2(\vec{r})$$

$$\Sigma^{v}_i(\vec{r}) = \Sigma^{c}_i(\vec{r}) + \Sigma^{f}_i(\vec{r}) + \sum_{j=i+1}^{G} \Sigma^{r}_{i \to j}(\vec{r})$$

$\Sigma^{v}_i(\vec{r})$ . . . the group removal cross-section

$\Sigma^{c}_i(\vec{r})$ . . . the radiation-absorption cross-section

$\Sigma^{f}_i(\vec{r})$ . . . the fission-absorption cross-section

$$\Sigma^{r}_{i \to j}(\vec{r}) = \Sigma^{r\ el.}_{i \to j}(\vec{r}) + \Sigma^{r\ in.}_{i \to j}(\vec{r})$$

$\Sigma^{r\ el.}_{i \to j}(\vec{r}), \Sigma^{r\ in.}_{i \to j}(\vec{r})$ . . . the elements of the scattering matrix

$B^2(\vec{r})$ . . . the buckling (it is beeing found out during the process of the separation of the variables)

$$Q(\vec{r}) = \sum_{j=1}^{G} \nu_j(\vec{r})\ \Sigma^{f}_j(\vec{r})\ \phi_j(\vec{r})$$

$\nu_j(\vec{r})$ . . . the average number of neutrons released by fission

$\psi_i(\vec{r})$ ... the integral of the fission spectrum in the ranges of the i-th group

$$\sum_{i=1}^{G} \psi_i(\vec{r}) = 1$$

$S_i(\vec{r})$ ... the external neutron-source in the i-th group (i.e. a source independent on $\phi_j(\vec{r})$ for $j = 1 \div 6$). In the removal-diffusion method this source is given by the uncollided flux of neutrons from the actual source into the given point and by slowing-down of neutrons in this point

$\lambda = k_{eff}$ ... $k_{eff} = 1$ for $S_i(\vec{r}) \neq 0$, k_{eff} is the searched eigenvalue of the problem, i.e. such a value, which the discussed set is just critical for.

G ... the number of groups (groups are numbered in the direction of falling of energy).

$E^f(\vec{r})$ ... the energy released per fission

$E^c(\vec{r})$ ... the energy released per radiation absorption

2. Transfer of the Diffusion Equations into the Difference Equations for Individual Geometries

The discussed set is being devided into the individual regions of the volume V and the surface S and the equations (1) are being integrated through the volume of each region.

By using the Gauss-furmula we get for each region

$$\left\{ -\iint_S \left[D_i(\vec{r}) \operatorname{grad} \phi_i(\vec{r}) \right] \cdot \vec{n} \, dS + \iiint_V \Sigma_i(\vec{r}) \phi_i(\vec{r}) \, dV = \right.$$

$$= \sum_{\substack{j=1 \\ j \neq i}}^{i-1} \iiint_V \Sigma^r_{j \to i}(\vec{r}) \phi_j(\vec{r}) \, dV + \frac{1}{k_{eff}} \iiint_V \psi(\vec{r}) Q(\vec{r}) \, dV + \tag{2}$$

$$\left. + \iiint_V S_i(\vec{r}) \, dV \right\}_{i=1}^{G}$$

where $\vec{n}$ is the unit vector of the outward going normal to the boundary of the discussed region.

To be able to realize the integration (2), the following assumptions should be taken into consideration:

a) Inside each of the regions a mesh-point p is to be chosen. The value of the flux in the point p is the mean value of the flux in the discussed region:

$$\phi_p^i = \frac{\iiint_V \phi_i(\vec{r}) \cdot dV}{V}$$

b) The scalar product $(grad\ \phi_i(\vec{r}) \cdot \vec{n})$ on the surface between two regions is expressed using the fluxes in the mesh-points inside these regions.

c) The physical properties are constant inside an individual subregion of the discussed region.

So we get a "m-point" formula, where m is the number of the regions surrounding the discussed region, enlarged by one. In the three-dimensional space using the rectangular and cylindrical coordinates we get $m = 7$.
If some of the variables are separable, the fluxes in two-dimensional (or one-dimensional) space may be expressed. The corresponding buckling is to be calculated using the following formulae:

1) For $\phi_i(\vec{r}) = \phi_i(\vec{r}_{x,y}) \cdot \varphi(z)$ and $S_i(\vec{r}) = S_i(\vec{r}_{x,y}) \cdot \varphi(z)$

for $z \in \langle -\frac{H}{2}, \frac{H}{2} \rangle$

is $$B^2 = -\frac{\left(\frac{d\varphi}{dz}\right)_{H/2} - \left(\frac{d\varphi}{dz}\right)_{-H/2}}{\int_{-H/2}^{H/2} \varphi(z)\, dz}$$

Specially for $\varphi(x) = \cos \frac{\pi}{H_{extr.}} x$ is $B^2 = \left(\frac{\pi}{H_{extr.}}\right)^2$

2) For $\phi_i(\vec{r}) = \phi_i(x)\,\varphi(r)$ and $S_i(\vec{r}) = S_i(x)\,\varphi(r)$ for $r \in \langle 0, R \rangle$

is $$B^2 = -\frac{\left(\frac{d\varphi}{dr}\right)_R}{\int_0^R \varphi(r)\,dr}$$

Specially for $\varphi(r) = J_0\left(\frac{\alpha_0}{R_{extr.}} r\right)$ is $B^2 = \left(\frac{\alpha_0}{R_{extr.}}\right)^2$

where $J_0(\alpha_0) = 0$ i.e. $\alpha_0 = 2,404825\,56$

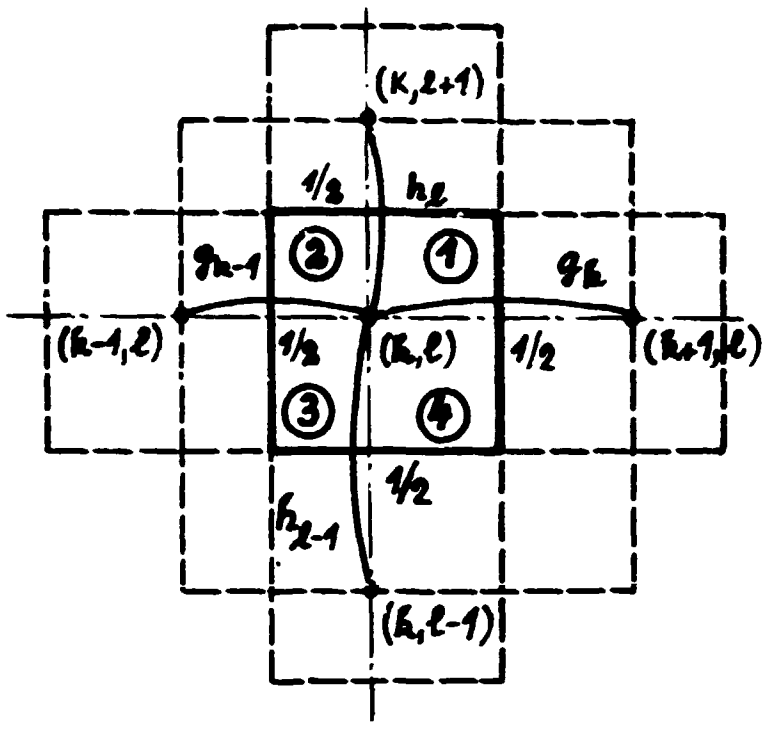
Remark: For the general two-dimensional r, z-geometry is $B^2 \equiv 0$.

Further we shall confine ourselves to the basic geometries in the two-dimensional space. The relation between the fluxes in the neighbouring regions is usually expressed by a "5-point" formula:

$$-a^i_{k,\ell}\,\phi^i_{k+1,\ell} - b^i_{k,\ell}\,\phi^i_{k-1,\ell} - c^i_{k,\ell}\,\phi^i_{k,\ell+1} - d^i_{k,\ell}\,\phi^i_{k,\ell-1} + p^i_{k,\ell}\,\phi_{k,\ell} = f^i_{k,\ell} \qquad (3)$$

The reactor is to be devided so that the mesh-points are chosen arbitraryly and the boundries of the individual regions pass through the medium point between each of the two neighbouring mesh-points.

The physical properties of individual subregions may differ (in the ranges of the individual subregions the physical properties are constant). For the x, y and r, z geometries the following picture is valid :



In the following expressions the group-index i is being omitted :

$$a_{k,\ell} = \frac{1}{g_k}\left(D^1_{k+\frac{1}{2},\ell}\,\frac{h_\ell}{2} + D^4_{k+\frac{1}{2},\ell}\,\frac{h_{\ell-1}}{2}\right)\left[\gamma_k + \frac{g_k}{2}\right]^\sigma$$

$$b_{k,\ell} = \frac{1}{g_{k-1}}\left(D^2_{k-\frac{1}{2},\ell}\,\frac{h_\ell}{2} + D^3_{k-\frac{1}{2},\ell}\,\frac{h_{\ell-1}}{2}\right)\left[\gamma_k - \frac{g_{k-1}}{2}\right]^\sigma = a_{k-1,\ell}$$

$$c_{k,\ell} = \frac{1}{h_\ell}\left(D^1_{k,\ell+\frac{1}{2}}\,\frac{g_k}{2}\left[\gamma_k + \frac{g_k}{4}\right]^\sigma + D^2_{k,\ell+\frac{1}{2}}\,\frac{g_{k-1}}{2}\left[\gamma_k - \frac{g_{k-1}}{4}\right]^\sigma\right)$$

$$d_{k,\ell} = \frac{1}{h_{\ell-1}}\left(D^4_{k,\ell-\frac{1}{2}}\,\frac{g_k}{2}\left[\gamma_k + \frac{g_k}{4}\right]^\sigma + D^3_{k,\ell-\frac{1}{2}}\,\frac{g_{k-1}}{2}\left[\gamma_k - \frac{g_{k-1}}{4}\right]^\sigma\right) = c_{k,\ell-1}$$

$$e_{k,\ell} = \sum_{q=1}^{4} \alpha^q_{k,\ell}\,\Sigma^q_{k,\ell}$$

$$\alpha^1_{k,\ell} = \frac{g_k\,h_\ell}{4}\left[\gamma_k + \frac{g_k}{4}\right]^\sigma \qquad \alpha^2_{k,\ell} = \frac{g_{k-1}\,h_\ell}{4}\left[\gamma_k - \frac{g_{k-1}}{4}\right]^\sigma$$

$$\alpha^3_{k,\ell} = -\frac{g_{k-1}\,h_{\ell-1}}{4}\left[\gamma_k - \frac{g_{k-1}}{4}\right]^\sigma \qquad \alpha^4_{k,\ell} = \frac{g_k\,h_{\ell-1}}{4}\left[\gamma_k + \frac{g_k}{4}\right]^\sigma$$

where $\sigma = \begin{cases} 0 \ldots \text{for x, y geometry} \\ 1 \ldots \text{for r, z geometry} \end{cases}$

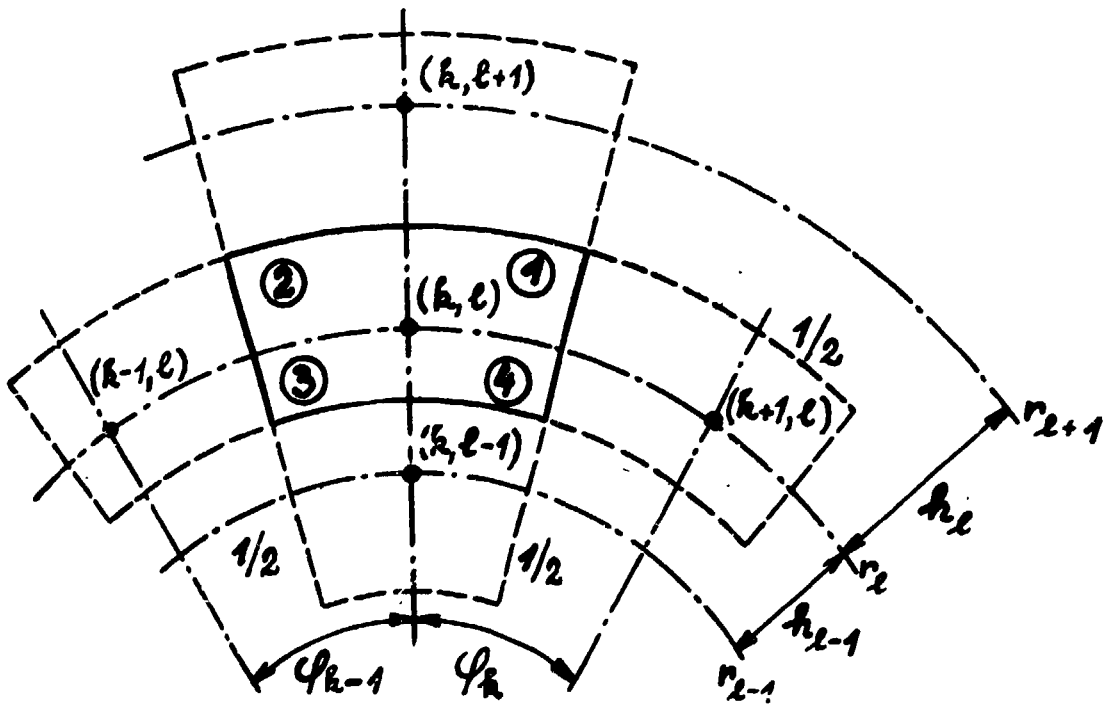
For r, z geometry is

$$\gamma_k = \sum_{m=1}^{k-1} g_m$$

For the points $(1,1)$ on the axis is valid :

$$g_0 = 0 \qquad \gamma_1 = 0 \qquad b_{1,\ell} = 0$$

For r, φ geometry is valid :



$$a_{k,\ell} = \frac{1}{r_\ell \varphi_k} \left(D^1_{k+\frac{1}{2},\ell} \frac{h_\ell}{2} + D^4_{k+\frac{1}{2},\ell} \frac{h_{\ell-1}}{2} \right)$$

$$b_{k,\ell} = \frac{1}{r_\ell \varphi_{k-1}} \left(D^2_{k-\frac{1}{2},\ell} \frac{h_\ell}{2} + D^3_{k-\frac{1}{2},\ell} \frac{h_{\ell-1}}{2} \right) = a_{k-1,\ell}$$

$$c_{k,\ell} = \frac{1}{h_\ell} \left(D^1_{k,\ell+\frac{1}{2}} \frac{\varphi_k}{2} + D^2_{k,\ell+\frac{1}{2}} \frac{\varphi_{k-1}}{2} \right) \left[r_\ell + \frac{h_\ell}{2} \right]$$

$$d_{k,\ell} = \frac{1}{h_{\ell-1}} \left(D^4_{k,\ell-\frac{1}{2}} \frac{\varphi_k}{2} + D^3_{k,\ell-\frac{1}{2}} \frac{\varphi_{k-1}}{2} \right) \left[r_\ell - \frac{h_{\ell-1}}{2} \right] = c_{k,\ell-1}$$

$$e_{k,\ell} = \sum_{q=1}^{4} \alpha^q_{k,\ell} \; \Sigma^q_{k,\ell}$$

$$\alpha^1_{k,\ell} = \frac{\varphi_k \, h_\ell}{4} \left[r_\ell + \frac{h_\ell}{4} \right] \qquad \alpha^2_{k,\ell} = \frac{\varphi_{k-1} \, h_\ell}{4} \left[r_\ell + \frac{h_\ell}{4} \right]$$

$$\alpha^3_{k,\ell} = \frac{\varphi_{k-1} \, h_{\ell-1}}{4} \left[r_\ell - \frac{h_{\ell-1}}{4} \right] \qquad \alpha^4_{k,\ell} = \frac{\varphi_k \, h_{\ell-1}}{4} \left[r_\ell - \frac{h_{\ell-1}}{4} \right]$$

$$r_\ell = \sum_{m=1}^{\ell-1} h_m \qquad h_0 = 0 \qquad r_1 = 0$$

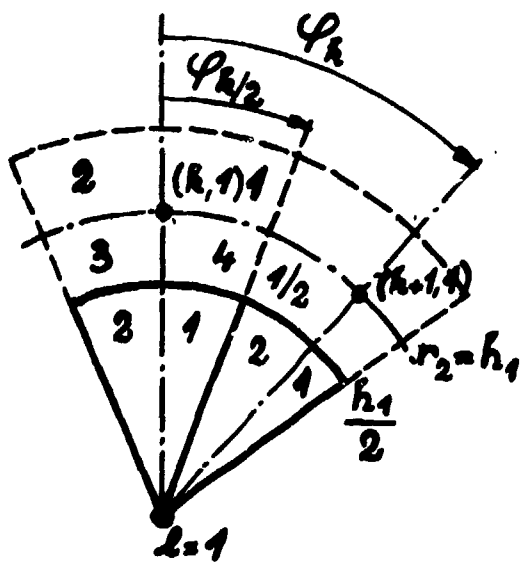
For the medium point $(k,1)$ is valid :

$$a_{k,1} = b_{k,1} = d_{k,1} = 0$$

$$c_{k,1} = \frac{1}{h_1} \left(D^1_{k,1/2} \frac{\varphi_k}{2} + D^2_{k,1/2} \frac{\varphi_{k-1}}{2} \right) \frac{h_1}{2}$$

$$e_{k,1} = \sum_{k=1}^{n} \sum_{q=1}^{2} \alpha^q_{k,1} \; \Sigma^q_{k,1}$$

$$\alpha^1_{k,1} = \frac{\varphi_k \, h_1}{4} \frac{h_1}{4} \qquad \alpha^2_{k,1} = \frac{\varphi_{k-1} \, h_1}{4} \frac{h_1}{4}$$



Further for all geometries we get :

$$p_{k,\ell} = a_{k,\ell} + b_{k,\ell} + c_{k,\ell} + d_{k,\ell} + e_{k,\ell}$$

$$D^{1}_{k,\ell+\frac{1}{2}} = 2/(1/D^{4}_{k,\ell+1} + 1/D^{1}_{k,\ell})$$

$$D^{2}_{k,\ell+\frac{1}{2}} = 2/(1/D^{3}_{k,\ell+1} + 1/D^{2}_{k,\ell})$$

$$D^{3}_{k,\ell-\frac{1}{2}} = 2/(1/D^{2}_{k,\ell-1} + 1/D^{3}_{k,\ell})$$

$$D^{4}_{k,\ell-\frac{1}{2}} = 2/(1/D^{1}_{k,\ell-1} + 1/D^{4}_{k,\ell})$$

$$D^{1}_{k+\frac{1}{2},\ell} = 2/(1/D^{2}_{k+1,\ell} + 1/D^{1}_{k,\ell})$$

$$D^{2}_{k-\frac{1}{2},\ell} = 2/(1/D^{1}_{k-1,\ell} + 1/D^{2}_{k,\ell})$$

$$D^{3}_{k-\frac{1}{2},\ell} = 2/(1/D^{4}_{k-1,\ell} + 1/D^{3}_{k,\ell})$$

$$D^{4}_{k+\frac{1}{2},\ell} = 2/(1/D^{3}_{k+1,\ell} + 1/D^{4}_{k,\ell})$$

$$f^{i}_{k,\ell} = f^{r,i}_{k,\ell} + f^{f,i}_{k,\ell} + f^{s,i}_{k}$$

$$f^{r,i}_{k,\ell} = \sum_{\substack{j=1 \\ i+1}}^{i-1} \left\{ \sum_{q=1}^{4} \alpha^{q}_{k,\ell} \; \Sigma^{r,q}_{k,\ell} \; j \to i \right\} \phi^{j}_{k,\ell}$$

Further we shall suppose that

$$\left\{ \psi^{q,i}_{k,\ell} = \psi^{i}_{k,\ell} \right\}_{q=1}^{4}$$

Then

$$f^{f,i}_{k,\ell} = \frac{\psi^{i}_{k,\ell}}{\lambda} Q_{k,\ell} \quad ; \quad Q_{k,\ell} = \sum_{j=1}^{6} \left\{ \sum_{q=1}^{4} \alpha^{q}_{k,\ell} \, \nu^{q,j}_{k,\ell} \, \Sigma^{f\,q,j}_{k,\ell} \right\} \phi_{k,\ell}$$

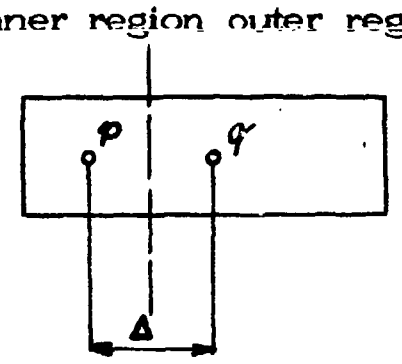
$$f^{s,i}_{k,\ell} = \sum_{q=1}^{4} \alpha^{q}_{k,\ell} \; S^{q,i}_{k,\ell}$$

3. Boundary Conditions

In general the boundary conditions may be chosen as follows :

$$\gamma_i(\vec{r})\,\phi_i(\vec{r}) + \xi_i(\vec{r})\,\frac{\partial \phi_i(\vec{r})}{\partial n} = \sigma_i(\vec{r}) \qquad (i = 1,2,\ldots,6)$$

where $\frac{\partial \phi_i(\vec{r})}{\partial n}$ is the derivative of the flux $\phi_i(\vec{r})$ taken in the direction of the outer normal to the surface of the set in the point $\vec{r}$.
In the difference shape is this condition expressed by the following formula



$$\gamma_i(p,q)\,\frac{\phi_p^i + \phi_q}{2} + \xi_i(p,q)\,\frac{\phi_q^i - \phi_p^i}{\Delta} = \sigma_i(p,q)$$

From here

$$\phi_q^i = \frac{\frac{\xi_i(p,q)}{\Delta} - \frac{\gamma_i(p,q)}{2}}{\frac{\xi_i(p,q)}{\Delta} + \frac{\gamma_i(p,q)}{2}}\,\phi_p^i + \frac{\sigma_i(p,q)}{\frac{\xi_i(p,q)}{\Delta} + \frac{\gamma_i(p,q)}{2}} \qquad (4)$$

For $\sigma_i(p,q) \neq 0$ it is necessary to put $k_{eff} = 1$, because (following (4)) this case turns into a problem with a given external source in the regions next to the outside of the discussed set. In the case of a free surface of the set (i.e. any radiation on the surface of the set coming from the outside is omitted) is $\sigma_i(\vec{r}) = 0$ and the boundary condition turns into the form

$$\phi_q^i = \varkappa^i(p,q)\,\phi_p^i$$

For the interface with vacuum is valid :

$$\frac{\phi_i}{-\frac{\partial \phi_i}{\partial n}} = .71\,\lambda_{tr.}^i = 2.13 D^i \Rightarrow \xi_i = 2.13\,D^i \qquad \gamma_i = 1$$

$$\alpha_i = \frac{\frac{4.26}{\Delta} D^i - 1}{\frac{4.26}{\Delta} D^i + 1}$$

In general for any point (k,ℓ) in the vicinity of the boundary the boundary conditions expressed by any constants $\alpha^a_{k,\ell}$; $\alpha^d_{k,\ell}$; $\alpha^b_{k,\ell}$; $\alpha^c_{k,\ell}$, where a; b; c; d express the direction of the normal to the boundary (in conformity with (3)), are valid.

4. Solution of the Matrix - Form Problem

Using the expressions (4) (or (4a)) and (3) we get a system of equations for $\phi^i_{k,\ell}$. This system may be written for each group in a matrix form :

$$\hat{A}\phi = F \qquad (5)$$

where

$\hat{A}$ ... is a symmetrical square quazitridiagonal matrix of coefficients which are eventually modified by the boundary conditions

ϕ ... is a column vector

F ... is a column vector

The solution of the system may be found directly using a "direct method" or by using an iteration method (an "inner iteration").

4.1 Direct Method

With regard to that fact the matrix $\hat{A}$ is a symmetrical zone matrix it is advantageous to solve the system (5) by using the "Banachiewitcz's root square-method" (/3/) :

The matrix $\hat{A}$ is to be divided intc a product of two reciprocally transposed matrices :

$$\hat{A} = \hat{S}' \hat{S} \qquad (6)$$

Then the matrix equation (5) desintegrates into a system of two matrix equations :

$$\begin{aligned} \hat{S}' Z &= F \\ \hat{S} \phi &= Z \end{aligned} \qquad (7)$$

where Z is an auxiliary vector.

Let us mark :

$$\hat{A} \equiv \{a_{i,j}\} \qquad \hat{S} \equiv \{s_{i,j}\} \qquad F \equiv \{f_i\}$$

$$Z \equiv \{z_i\} \qquad \phi \equiv \{\phi_i\}$$

Then

$$s_{11} = \sqrt{a_{11}} \qquad s_{1j} = \frac{a_{1j}}{s_{11}}$$

$$s_{ii} = \sqrt{a_{ii} - \sum_{l=1}^{i-1} s_{li}^2} \qquad (i > 1)$$

$$s_{ij} = \frac{1}{s_{ii}} \left(a_{ij} - \sum_{l=1}^{i-1} s_{li}\, s_{lj} \right) \qquad (j > i)$$

$$s_{ij} = 0 \qquad (j < i)$$

$$z_1 = \frac{f_1}{s_{11}} \qquad z_i = \frac{f_i - \sum_{l=1}^{i-1} s_{li}\, z_l}{s_{ii}} \qquad (i > 1)$$

$$\phi_n = \frac{z_n}{s_{nn}} \qquad \phi_i = \frac{z_i - \sum_{l=i+1}^{n} s_{il}\, \phi_l}{s_{ii}} \qquad (i < n)$$

Using this method it is necessary to reserve the computer-store only for one half of the zone of the matrix including the diagonal. The matrix $\hat{S}$ is to be calculated only once because during the outer iteration (see

further) changes only the right side F of the matrix equation (5). If for definite i we obtain $S_{ii}^2 < 0$, the calculation may be formally continued by using the imaginary unit. In this case the resulting flux values are real, but they have no physical meaning (i.e. for such a case does not exist any solution of the problem).

4.2 Inner Iteration

For the given type of the matrix $\hat{A}$ an iteration method in /1/ is described (the Young-Frenkel's successive overrelaxation method) :

$$\phi_{k,\ell}^{i(m)} = \phi_{k,\ell}^{i(m-1)} + \omega^i \left[\phi_{k,\ell}^{*i(m)} - \phi_{k,\ell}^{i(m-1)} \right]$$

$$\phi_{k,\ell}^{*i(m)} = \frac{1}{p_{k,\ell}^i} \left[a_{k,\ell}^i \, \phi_{k+1,\ell}^{i(m-1)} + b_{k,\ell}^i \, \phi_{k-1,\ell}^{i(m)} + \right. \qquad (8)$$

$$\left. + c_{k,\ell}^i \, \phi_{k,\ell+1}^{i(m-1)} + d_{k,\ell}^i \, \phi_{k,\ell-1}^{i(m)} + f_{k,\ell}^i \right]$$

i ... is an overrelaxation factor, the value of which lies in the ranges 1 ÷ 2 and depends on the energy group.

(m) ... is the index (i. e. the order) of the inner iteration.

After each of the inner iteration the following is to be calculated :

$$\Theta_{(m)}^{i2} = \frac{\| \phi^{i(m)} - \phi^{i(m-1)} \|}{\| \phi^{i(m-1)} - \phi^{i(m-2)} \|} \qquad (9)$$

where $\| \varphi \|$ is any canonic norm, for instance

$$\| \varphi \|_m = \max_i |\varphi| \; ; \quad \| \varphi \|_\ell = \sum_i |\varphi_i| \; ; \quad \| \varphi \|_k = \sqrt{\textstyle\sum_i |\varphi_i|^2}$$

The expression (9) limits to the maximum eigenvalue of the iterative matrix, given by the equations (8) for the chosen factor ω_0^i.

After the determination of the optimum value of the factor is the following procedure (according to (4)) advisable :

When $|\theta^{i2}_{(m)} - \theta^{i2}_{(m-1)}| < \varepsilon^2_\theta$ where ε^2_θ is the demanded exactness of θ^i (usually $\varepsilon^2_\theta \leq .001$ is sufficient), then

a) for $\theta^{i2}_{(m)} \leq \omega^i_0 - 1$ we put $\omega^i = \omega^i_0$

b) for $\theta^{i2}_{(m)} > \omega^i_0 - 1$ is

$$\mu_i = \frac{\theta^{i2}_{(m)} + \omega^i_0 - 1}{\omega^i_0\ \theta^i_{(m)}} \qquad \omega^i = \frac{2}{1 + \sqrt{1 - \mu^{i2}}} \rightarrow \omega^i_0 \qquad (10)$$

where μ^i is the maximum eigenvalue of the Jacobian matrix $\hat{B} = \hat{E} - \hat{D}^{-1}\hat{A}$, $\hat{D}$ is a diagonal matrix defined by the diagonal elements of the matrix $\hat{A}$, , and $\hat{E}$ is the unit matrix.

From the upper follows for the optimum value of ω^i : $\theta^{i2} = \omega^i - 1$

This is also the limit for $m \rightarrow \infty$.

The factor ω^i does not depend on the right side F of the equation (5) and therefore its optimum value does not change during the outer iteration process.

The inner iteration in the i-th group is considered to be finished if

$$\max_{k,\ell} \frac{|\phi^{i(m)}_{k,\ell} - \phi^{i(m-1)}_{k,\ell}|}{\phi^{i(m)}_{k,\ell}} < \varepsilon^{i2}_\phi \qquad (11)$$

where ε^{i2}_ϕ is the chosen exactness of the flux values.

4.3 Outer Iteration

For $Q_{k,\ell} \equiv 0$ the outer iteration does not take place. In the contrary case, if the inner iteration in all groups is finished (or after the

termination of the direct method) the obtained flux values may be used for a process of improvement of the previous source-approximation :

$$\hat{Q}^{(t)}_{k,\ell} = \sum_{i=1}^{6} \left\{ \sum_{q=1}^{4} \alpha^{q}_{k,\ell} \; \nu^{q,i}_{k,\ell} \; \Sigma^{fq\,i}_{g,\ell} \right\} \phi^{i(t-1)}_{k,\ell} \qquad (12)$$

where (t) is the index (i. e. the order) of the outer iteration.

If $S^{q,i}_{g,\ell} \equiv 0$ and $\sigma_t(p,q) \equiv 0$ the new approximation of the eigenvalue $\lambda^{(t)}$ and its upper and lower limits $\overline{\lambda}^{(t)}$ and $\underline{\lambda}^{(t)}$ may be expressed :

$$\lambda^{(t)} = \lambda^{(t-1)} \min_{k,\ell} \left\{ \frac{Q^{(t)}_{k,\ell}}{Q^{**(t-1)}_{k,\ell}} \right\}$$

$$\overline{\lambda}^{(t)} = \lambda^{(t-1)} \max_{k,\ell} \left\{ \frac{Q^{(t)}_{k,\ell}}{Q^{**(t-1)}_{k,\ell}} \right\}$$

$$\lambda^{(t)} = \lambda^{(t-1)} \frac{\sum_{k,\ell} \left[Q^{(t)}_{k,\ell} \right]^2}{\sum_{k,\ell} \left[Q^{**(t-1)}_{k,\ell} \cdot Q^{(t)}_{k,\ell} \right]}$$

The outer iteration may be considered to be finished if

$$\left| \frac{\overline{\lambda}^{(t)} - \underline{\lambda}^{(t)}}{2\lambda^{(t)}} \right| < \varepsilon^{2}_{\lambda}$$

where $\varepsilon^{2}_{\lambda}$ is the claimed relative exactness of $\lambda = k_{eff}$ or for $\lambda^{(t)} \equiv 1$:

$$\max_{k,\ell} \frac{\left| Q^{(t)}_{k,\ell} - Q^{(t-1)}_{k,\ell} \right|}{Q^{(t)}_{k,\ell}} < \varepsilon^{2}_{Q} \quad ; \quad \max_{k,\ell} \frac{\left| \phi^{i(t)}_{k,\ell} - \phi^{i(t-1)}_{k,\ell} \right|}{\phi^{i(t)}_{k,\ell}} < \varepsilon^{i2}_{\phi}$$

for $Q_{k,\ell}^{(t)} \neq 0$

If an iteration of k_{eff} takes place the outer iteration may be accelerated by using the Chebyshev polynomials as follows :

$$N^{(t)} = \frac{\sum_{k,\ell} Q_{k,\ell}^{*(t)}}{\lambda^{(t)}}$$

In each point we use the following normalization

$$Q_{k,\ell}^{**(t)} = \frac{N^{(0)}}{N^{(t)}} Q_{k,\ell}^{*(t)} \qquad (15)$$

where $N^{(0)} = \frac{\sum_{k,\ell} Q_{k,\ell}^{(0)}}{\lambda^{(0)}} = \frac{C}{\lambda^{(0)}}$

$$Q_{k,\ell}^{*(t)} = Q_{k,\ell}^{**(t-1)} + \alpha^{(t)} \left[Q_{k,\ell}^{(t)} - Q_{k,\ell}^{**(t-1)} \right] +$$

$$+ \beta^{(t)} \left[Q_{k,\ell}^{**(t-1)} - Q_{k,\ell}^{**(t-2)} \right] \qquad (16)$$

Where $\alpha^{(1)} = \frac{2}{2-\sigma} \qquad \beta^{(1)} = 0$

For $t > 1$

$$\alpha^{(t)} = \frac{4\, ch\,(t-1)\varphi}{\sigma\, ch\, t\varphi} = \frac{4}{5} \frac{1}{e^{\varphi}} \frac{1 + \frac{1}{e^{2\varphi(t-1)}}}{1 + \frac{1}{e^{2\varphi t}}} \qquad (17)$$

$$\beta^{(t)} = \frac{ch\,(t-2)\varphi}{ch\, t\varphi} = \frac{1}{e^{2\varphi}} \frac{1 + \frac{1}{e^{2\varphi(t-2)}}}{1 + \frac{1}{e^{2\varphi t}}}$$

$$\varphi = \operatorname{arg\,cosh}\, x \qquad x = \frac{2}{\sigma} - 1$$

$$e^{\varphi} = x + \sqrt{x^2 - 1} \qquad \sigma = \frac{\lambda_2}{\lambda_1} \qquad \lambda_1 = \lambda = k_{eff}$$

$\lambda_2 < \lambda$ is the nearest of the lower eigenvalues which accommodates to the discussed problem. The ratio 6 may be estimated putting $\alpha^{(t)} = 1$, $\beta^{(t)} = 0$. Then :

$$6 \approx \frac{\sum_{k,\ell} \left| \frac{Q^{**(t)}_{k,\ell}}{\lambda^{(t)}} - Q^{**(t-1)}_{k,\ell} \right|}{\sum_{k,\ell} \left| Q^{**(t-1)}_{k,\ell} - Q^{**(t-2)}_{k,\ell} \right|} \qquad (18)$$

If $\lambda^{(t)} \leq 1$ the normalization does not take place, i.e.

$$N^{(t)} = N^{(0)}$$

Then the value $Q^{**(t)}_{k,\ell}$ is being used for calculation of $f^{f,i}_{k,\ell}$.

5. Determination of Reactor Power

The heat-output P of the reactor in general is determined by using the expression :

$$P = \iiint_V \left[\sum_{i=1}^{a} \left\{ E^f(\vec{r}) \Sigma^f_i(\vec{r}) + E^c(\vec{r}) \Sigma^c_i(\vec{r}) \right\} \phi_i(\vec{r}) \right] dV$$

In a difference form we get

$$P = \omega \sum_{k,\ell} P_{k,\ell} V_{k,\ell}$$

$$P_{k,\ell} = \sum_{i=1}^{a} \phi^i_{k,\ell} \sum_{q=1}^{4} \alpha^q_{k,\ell} \left[E^f \Sigma^f + E^c \Sigma^c \right]^{q,i}_{k,\ell}$$

$$V_{k,\ell} = \sum_{q=1}^{4} \alpha^q_{k,\ell}$$

where ω is

a) for x, y and r, φ geometry :

$$\omega = H \langle \mu_x \rangle = H \frac{2}{\pi} \frac{H_{extr.}}{H} \sin\left(\frac{\pi}{2} \frac{H}{H_{extr.}} \right) \doteq H \frac{2}{\pi}$$

$H_{extr.}$ . . . is the extrapolated height of the reactor core.

H . . . is the actual height of the reactor core.

b) for r, z geometry :

$$\omega = 2\pi$$

which follows from the definition of $\alpha^{q}_{k,\ell}$.

6. Conclusion

Our experience tell us the described method of calculation is convenient for diffusion and removal-diffusion approximations using sufficiently short distances between the mesh-points.
The optimum values of these distances depend on the physical properties of the discussed regions, particularly on $\min_i \left(\frac{D^i}{\Sigma^v_i}\right)$ and on the gradient of the flux and therefore it is difficult to fix them in advance. One of the possible methods of solution is to execute the calculation at least twice with different choice of the mesh-points.

An important question of this method is the speed of convergence. From the present results we can say that for a large number of groups the contributions of neutrons from the slowing-down process into the discussed group are much higher in comparison with the fission neutrons and therefore the outer iteration converges fastly. For such a case the further acceleration of convergence is not necessary because δ stabilizes on a certain value (following (18)) and the iteration is brought to an end. The using of the inner iteration is often problematic. In many cases is the convergence also by using an optimal acceleration very poor.

Therefore we use exclusively the direct method which for the number of mesh-points up to 1000 (i. e. the maximum practicable number of mesh-points used for computers mentioned above) is with regard to time economical and numerical stable.

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