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AN ADVANCED METHOD OF HETEROGENEOUS REACTOR THEORY

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Boris P. KOCHUROV*

日本原子力研究所
Japan Atomic Energy Research Institute

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An Advanced Method of Heterogeneous Reactor Theory

Boris P. KOCHUROV*

Department of Reactor Engineering
Tokai Research Establishment
Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun, Ibaraki-ken

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Recent approaches to heterogeneous reactor theory for numerical applications were presented in the course of 8 lectures given in JAERI. The limitations of initial theory known after the First Conference on Peacefull Uses of Atomic Energy held in Geneva in 1955 as Galanine-Feinberg heterogeneous theory:-matrix from of equations, -lack of consistent theory for heterogeneous parameters for reactor cell, -were overcome by a transformation of heterogeneous reactor equations to a difference form and by a development of a consistent theory for the characteristics of a reactor cell based on detailed space-energy calculations.

General few group (G-number of groups) heterogeneous reactor equations in dipole approximation are formulated with the extension of two-dimensional problem to three-dimensions by finite Furie expansion of axial dependence of neutron fluxes. A transformation of initial matrix reactor equations to a difference form is presented.

The methods for calculation of heterogeneous reactor cell characteristics giving the relation between vector-flux and vector-current on a cell boundary are based on a set of detailed space-energy neutron flux distribution calculations with zero current across cell boundary and G calculations with linearly independent currents across the cell boundary. The equations for reaction rate matrices are formulated. Specific methods were developed for description of neutron migration in axial and radial

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Course of lectures given in JAERI in the period April 1 -June 24, 1994

* Visiting researcher from the Institute for Theoretical and Experimental Physics, B. Cheremushkinskaya, 25, Moscow, 117259, Russia

directions. The methods for resonance level's approach for numerous high-energy resonances. On the basis of these approaches the theory, methods and computer codes were developed for 3D space-time react or problems including simulation of slow processes with fuel burn-up, control rod movemets, Xe poisoning and fast transients depending on prompt and delayed neutrons. As a result reactors with several thousands of channels having non-uniform axial structure can be feasibly treated.

Keywords: Heterogeneous Reactor, Neutron migration, Resonance Absorption, Reaction Rates, Collision Probability.

非均質炉理論の新解法

日本原子力研究所東海研究所原子炉工学部

Boris P. KOCHUROV*

(1994年7月15日受理)

数値計算を目指す非均質炉理論の新手法について8章にわたる講義を原研で行った。1955年ジュネーブで行われた第1回原子力平和利用会議以来Galaninne-Feinbergの非均質炉理論として知られている、方程式をマトリックスで表現した初期の理論では原子炉の格子の非均質パラメータは一貫性に欠けているが、この問題を階差式に変換し、エネルギーと空間を変数とする格子パラメータに関する統一的な理論を展開した。

一般的な双極近似を用いた少数群非均質炉理論を2次元問題から有限フーリエ変換により3次元問題へ拡張した。初期のマトリックスで表現した方程式群を階差式で表現した。つまり格子の境界でのベクトル中性子束とベクトル中性子流との関係を与える非均質格子の特性方程式は、境界で中性子流はゼロだが詳細なエネルギー空間依存の中性子束の計算と境界を横切る線形で独立な中性子流の計算の合成からなっている。また反応率を与える式を行列で表現した。軸方向および径方向への中性子移動を記述する方法も開発した。共鳴吸収の計算は非均一のレサジー分割と数多い高エネルギー共鳴に対する実効共鳴準位近似に基づいている。以上述べた理論や方法に基づいて燃焼、制御棒の移動やゼノン毒作用のような遅い事象や即発遅発中性子に依存する速い事象の模擬を扱う3次元空間依存動特性コードを開発した。これによって軸方向に非均質な数千のチャンネルを有する原子炉の解析が可能となった。

東海研究所：〒319-11　茨城県那珂郡東海村白方字白根2－4

* 研究者招聘制度により平成6年4月より3ヶ月原研に滞在した。

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Introduction

Heterogeneous theory is applicable to the reactors with arbitrary positions of channels having different axially non-uniform properties, with axises parallel to some fixed direction (fuel assemblies, control rods etc.) . The main supposition is that the channels are well separated relative to neutron mean free paths, so that there are regions between channels where the diffusion approximation is applicable. The properties of channels are supposed to be derived from the solutions of neutron transport equations , the influence of channel to channel is determined by Green functions based on diffusion approximation.

The basic idea of heterogeneous reactor theory belongs to academician L.D.Landau and first systematic formulation of theory was presented in an unpublished work by Achiezer A.I., Pomerantchuk I.Ya.(Introduction to the theory of neutron multiplication systems , 1947). The theory called lately as Galanine-Feinberg theory became well known after the First Conference on Peaceful Uses of Atomic Energy held in Geneva in 1955 [1,2]. Methods of summation developed by Galanine let it possible to solve some heterogeneous reactor problems, for example, concerning thermal utilization factor.

Next stage of theory development - introduction to the theory the first asimuthal mode of neutron distribution around channels that made it possible to develop the theory of neutron migration in uniform lattices (in axial and radial directions).

Yet two obstacles prevented wide practical application of heterogeneous methods :
-matrix form of equations ;
- lack of consistent theory for heterogeneous parameters for reactor cells.

The first obstacle was overcome by a transformation of heterogeneous reactor equations to a *difference* form [3,4,5,6]. The second - by the development of a *consistent theory* for the characteristics of reactor channel or a cell based on detailed space-energy calculations of a cell [7].

Other approaches to the development of heteroheneous reactor theory can be found in [8-12].

As a result the reactors with some thousands of channels having non-uniform axial structure can be feasibly treated. The problem becomes even simpler than for so called homogeneous reactor equations due to a simpler structure of an operator used in inner iterations. The extension to 3 dimensions is reached by finite Furie transformation relative to axial dependence that leads formally to the same form of equations as for the case of 2 dimensions.

For the second part of the problem a theory for heterogeneous parameters - effective boundary conditions on the surface of a reactor cell - was formulated. In a few group theory (with G groups) the main characteristic is GxG Λ-matrix relating a vector-flux to a vector-current on a cell surface. The calculation is based on a series of G+1 solutions of detailed space-energy multi-group problems with linearly independent neutron currents across cell surface. Some weak suppositions concerning fission sources distribution and superposition principle make it possible to separate absorption and slowing down from fission processes and to construct Λ-matrix consisting of two parts and depending on (1+G)*G/2+2*G parameters. Numerical methods for reactor cells with an arbitrary isotopic composition were developed. Specific methods for resonance absorption calculation are based on non-uniform subdivision of lethargy scale and effective resonance level's approach for numerous high-energy resonances including unresolved regions.

Specific methods are needed for Λ_z and Λ_r - matrices describing neutron migration in axial and radial directions. Besides the theory for reaction rate matrices was developed. The theory, methods and computer codes were developed for 3D space-time reactor problems including simulation of slow processes with fuel burn-up, control rod movements (or a change of boric acid concentration), Xe poisoning and fast transients depending on prompt and delayed neutrons.

In *lecture* 1 general heterogeneous reactor equations are formulated.
Few group theory is used instead of age-diffusion theory in the moderator.
The solution is presented as a superposition of neutron fields due to point monopoles and dipoles around each channel.
It is shown that 3 equivalent forms of heterogeneous equations are possible based on the utilization of different variables:
1)amplitudes of external neutron fields at channel centers
2)amplitudes of singular fields at channel centers
3)neutron fluxes on channel or cell boundaries.
Addition theorems for Bessel functions are used for the formulation of heterogeneous reactor equations for the case of channels of finite radii.
It is shown how to convert initial equations given in complex values to equations in real values (by linear transformations).
Elementary symmetry relations are used for simplification of the problem.

The 2nd *lecture* is devoted to one of the central points of the theory developments:
transformation of initial reactor equations to a difference form.
Initial matrix equations have limited applications - for small dimensional problems (reactors or critical assemblies with no more than *hundreds* of channels).
Approximate difference form make heterogeneous equations applicable to reactors with *thousands* of fuel assemblies having non-uniform structure in axial direction. The extension of two-dimensional problem to 3 dimensions is obtained by finite Furie expansion of axial dependence of channel characteristics and neutron fluxes. Symbolically the equations remain of the same form (with extended dimension). Different approaches are possible for the choice of difference equations parameters and they are based on some best elimination of matrix elements outside some fixed set of indices around a given node.

Lecture 3 deals with the heterogeneous characteristics of a reactor cell.
Calculation of these characteristics is based on a detailed space-energy neutron flux distribution calculation with zero current across cell boundary and G calculations with linearly independent currents across the cell boundary (G- number of few groups for reactor calculation).
Closed functional relations can be obtained for boundary parameters - monopole, axial dipole and radial dipole.
The integral equation (collision probability for the case of monopole) is modified for the case of calculation of neutron migration parameters.
Calculations of neutron flux distribution in a cell are based on detailed multi-group calculations with special treatment of resonance absorption (direct calculation with non-uniform division of lethargy scale [7], effective resonance levels [13,14]) and the solution of thermalization problem [15,16] in thermal region of energies.

In *lecture* 4 the methods of heterogeneous reactor equation solutions are considered:

direct calculation of matrix equations with some preliminary matrix transformations leading to an application of operator with some positivity properties; iterative method of solution of direct heterogeneous reactor equations based on line by line multiplications.

Group-theoretical analysis is used for reduction of problem dimension [17].

The solution of heterogeneous reactor equations in difference form is based on a combination of inner iterations (symmetric succesive over-relaxation method) and two-stage Chebyshev's method for outer iterations [18].

Sub critical systems with external sources are solved by a modified iteration method [19].

Lecture 5 describes the methods for the solution of space-energy-time problems:

Space-time kinetics in a reactor cell is based on nuclear chain transformations (capture, fission, decay, (n,2n) reactions), with step by step re-calculations of space-energy distributions . Some interpolation procedures are used for increasing the time intervals between this re-calculations.

3-dimensional burn up processes in a reactor (with control rod movements , fuel reloadings and Xe poisoning) are simulated with time being simply a parameter [20]. For fast transients (including the effects of prompt and delayed neutrons) a decomposition on slowly varying and fast varying functions is applied , with a new cell characteristic Λ_t-matrix (describing time-dependence)[21].

Lecture 6 is devoted to the application of perturbation and optimization theory to the solution of some heterogeneous reactor problem [5,22]. General approach is based on a Lagrange principle for the systems with constrains and application of sequential linearization method. A special approach is used for the solution of power distribution flattening by control rods (change of variables from control rod positions to reactivities immersed by control rods).

Lecture 7 is devoted to a description of some computer codes based on the above theory and methods (for reactor cell, for calculation of reactors by direct heterogeneous methods, for 3-dimensional calculations of a reactor by the solution of heterogeneous equations in difference form, for simulation of slow and fast time processes in a 3-dimensional model of a reactor).

Some numerical results - calculation of reactor cell characteristics, simulation of burnup in a reactor cell, space distribution of reaction rates in critical assemblies, numerical analysis of critical experiments, intercomparison of solutions of matrix heterogeneous reactor equations and solutions of heterogeneous reactor equations in difference form, monopole and dipole one-velocity parameters, simulation of Xe poisoning transients and transients taking account of prompt and delayed neutrons - are presented in the last 8th *lecture*.

1. Heterogeneous Reactor Equations

1.1 *Suppositions*

Reactors with uniform moderator is considered (in the theory developed below this supposition can be practically omitted since boundary conditions can be applied to cell boundaries). The channels have arbitrary disposition with axises supposed to be parallel to a fixed axis for example z-axis,; usually in a regular lattice - square or hexagonal. Between the channels some regions exist where diffusion approximation is applicable. The properties of each channel are supposed to be independent of the properties and positions of other channels and can be determined separately. Reactor neutron problem is divided into 2 parts:
determination of properties of channels;
solution of reactor equations with the properties of channels pre calculated.

1.2 *Source-sink heterogeneous reactor equations*

A reactor system with large distances between channels: $\exp(-R/l)<<1$, where
R - a typical distance between channel surfaces, l-mean free path of neutron travel;
and small dimensions of channels:

$$c=V_{chan}/V_{cell} << 1,$$

is considered.
The neutron flux distribution in the vicinity of each channel is supposed to be independent of azimuthal angle and every channel is characterized by 2 parameters:
γ -constant - the ratio of neutron current to asymptotic value of neutron flux on the channel boundary;
η - multiplication constant - the ratio of number of fast neutrons born in the channel to the number of neutrons absorbed by this channel.

Neutron transport in the reactor is described by 2 Green functions, giving the influence at a given point $\mathbf{r}$ of unit point source at the point $\mathbf{r}_0$ of fast neutrons and thermal neutron sink correspondingly.

The neutron flux distribution at the point $\mathbf{r}$ is a superposition of these sources and sinks influences at points $\mathbf{r}_k$

$$N(\mathbf{r})=\sum_{\mathbf{K}} [G_f(\mathbf{r},\mathbf{r}_k)\eta_k-G_s(\mathbf{r},\mathbf{r}_k)]\gamma_k N(\mathbf{r}_k)$$

$N(\mathbf{r}_k)$ - neutron flux on the surface of channel with the center of axis at $\mathbf{r}_k$.
For a reactor with cylindrical channels and infinite moderator age-diffusion Green functions supposing $\mathbf{r} = \mathbf{r}_l$ are as follows:

$$G_s(\mathbf{r}_l,\mathbf{r}_k)=(1/2\pi D)K_0(|\mathbf{r}_l-\mathbf{r}_k|/L);\ G_s(\mathbf{r}_k,\mathbf{r}_k)=(1/2\pi D)K_0(\rho_k/L);$$

$$G_f(\mathbf{r}_l,\mathbf{r}_k)=(1/4\pi D)\exp(\tau/L^2)\int_{\tau/L^2}^{\infty}\exp[-(z+(\mathbf{r}_l-\mathbf{r}_k)^2/4zL^2)]dz/z$$

where D, τ, L^2 - diffusion coefficient, age and square of diffusion length correspondingly, ρ_k- radius of channel with number $\mathbf{k}$, K_0- modified Bessel function, and we get a system of uniform algebraic equations:

$$N(\mathbf{r}_i)=\sum_{K} H(\mathbf{r}_i,\mathbf{r}_k)N(\mathbf{r}_k);\quad H(\mathbf{r}_i,\mathbf{r}_k)=[G_f(\mathbf{r}_i,\mathbf{r}_k)\,\eta_k-G_s(\mathbf{r}_i,\mathbf{r}_k)]\gamma_k$$

having non trivial solution in the case if the next critical condition is fulfilled:

$$\det(H-1)=0$$

1.3 *General solution of few-group equations in monopole and dipole approximations*

Instead of age-diffusion approximation few-group diffusion approximation in the moderator is supposed. Group fluxes in the moderator φ_i (after a change of variables to n_i) obey the equations:

$$(-\Delta+1/\tau_i+1/L_i^2)n_i=\sum_{j<i} t_{ij}n_j/\tau_j; \qquad (1.3.1)$$

where $n_i=(D_{i_i}/D_G)\varphi_i U_i$;

$$\varphi_i=\int_{U_i}\varphi du/U;\ t_{ij}=\Sigma_{ij}/\Sigma_{Rj};\ 1/L^2_j=\Sigma_{ai}/D_i;\ 1/\tau_i=\Sigma_{Ri}/D_i\ ;$$

G - number of groups, D_i, D_G - diffusion coefficient, Σ_{Ri}, Σ_{ai} slowing -down macroscopic cross-section and absorption macroscopic cross-section in group i correspondingly; Σ_{ij} - scattering cross-section from group j to group I; U_i - lethargy interval in the group i.

In a reactor of finite height after the separation of variables: $n \rightarrow n\exp(i\alpha z)$

where $\alpha=\pi/H$, H - reactor height , the system of equations becomes as follows:

$$(-\Delta_i+\kappa^2_i)n_i=\sum_{j<i} t_{ij}\xi^2_j n_{j_j}\quad \kappa^2_i=1/\tau_i+1/L_i^2+\alpha^2;\ \kappa^2_G=1/L_G^2+\alpha^2;\ \xi_j^2\equiv 1/\tau_j. \quad (1.3.2)$$

General solution with logatithmic singuliarities is consructed of Bessel functions:

$$n_i=c_{ij}f_j^0;\ f_j^0=K_0(\kappa_j r);\qquad (\kappa^2_i-\kappa^2_j)\,c_{ij}f_j^0=\sum_{k<i} t_{ik}\xi^2_k c_{kj}f_j^0;\ i=j+1,\ldots,G$$

with the system of recurrence relations for c_{ij}

$$c_{jj}=1;\ c_{ij}=(1/(\kappa^2_i-\kappa^2_j))\sum_{k<i} t_{ik}\xi^2_k c_{kj} \qquad (1.3.3)$$

If the loss of energy is less than group widths only neighbor groups are related to each other by recurrence relations:

$$c_{jj}=1;\ c_{ij}=v_{ij}c_{i-1,j};\ v_{ij}=\xi_{i-1}^2/(\kappa^2_i-\kappa^2_j) \qquad (1.3.4)$$

A triangular matrix can be constructed:

$$C=\begin{bmatrix} 1 & & 0 \\ & \cdot & \\ & & \cdot \\ c_{ij},\ i>j & & 1 \end{bmatrix} \qquad (1.3.5)$$

and general solution presented as

$N=C\mathcal{J}_0A_0$;

$\mathcal{J}_0$- a diagonal G×G matrix with functions f_j^0 at the diagonal, A_0 - vector of arbitrary constants. Green function is constructed as follows.
Suppose a unit source is placed in the center of coordinates

$$(r)e_j / D_G; e_j = \begin{bmatrix} 0 \\ 0 \\ \cdot \\ 1 \\ \cdot \\ 0 \end{bmatrix} \leftarrow$$

Taking an integral to the boundary of a circle of small radius and for the limit of this radius $\rightarrow 0$, we get

$$2\pi CA_0=e_j/D_G \quad A_0=C^{-1}\, e_j/2\pi D_G\ ;$$
$$G^j_0(\,|\mathbf{r}-\mathbf{r}_0|\,)=(1/2\pi D_G)C\,\mathcal{J}_0(\,|\mathbf{r}-\mathbf{r}_0|\,)C^{-1}e_j; \qquad (1.3.6)$$

In 2-group approximation $(\kappa_1^2=1/\tau+\alpha^2;\ \kappa_2^2=1/L^2+\alpha^2)$:

$$G_0^1(r)=(1/2\pi D_G)\begin{vmatrix} K_0(\kappa_1 r) & \\ (K_0(\kappa_2 r)-K_0(\kappa_1 r))/(1-\tau/L^2) & \end{vmatrix};\quad G_0^2(r)=(1/2\pi D_G)\begin{vmatrix} 0 & \\ (K_0(\kappa_2 r) & \end{vmatrix}$$

Addition theorem for Bessel functions is given by the next relation (Fig. 1.1):

$$\exp(in\psi_1)K_n(a|\mathbf{r}-\mathbf{r}_1|)=\sum_{m=-\infty}^{\infty} I_m(a|\mathbf{r}-\mathbf{r}_0|)\,K_{n+m}(a|\mathbf{r}_0-\mathbf{r}_1|)\exp(im(\pi-\psi_0) \qquad (1.3.7)$$

Let angle φ_0 is measured from the direction of unit vector α_0, φ_1 - from α_1 .
Following definitions, shown in the picture,

$\psi_1=\varphi_1-\chi_{01}$; $\pi-\psi_0=\chi_{10}-\varphi_0$; $\chi_{10}=\theta_{10}+\chi_{01}+\pi$;
θ_{10} - the angle between α_0 and α_1 ; χ_{01} -the angle measured from α_1 to $\mathbf{r}_0$-$\mathbf{r}_1$;
χ_{10} -the angle measured from α_0 to $\mathbf{r}_1$-$\mathbf{r}_0$; addition theorem is rewritten in the form:

$$\exp(in\varphi_1)K_n(a|\mathbf{r}-\mathbf{r}_1|)=(-1)^n\exp(-in\theta_{10}) \qquad (1.3.8)$$

$$\sum_{m=-\infty}^{\infty} I_m(a|\mathbf{r}-\mathbf{r}_0|)\,K_{n-m}(a|\mathbf{r}_0-\mathbf{r}_1|)\exp(i(n-m)\chi_{10}\exp(im\,\varphi_0)$$

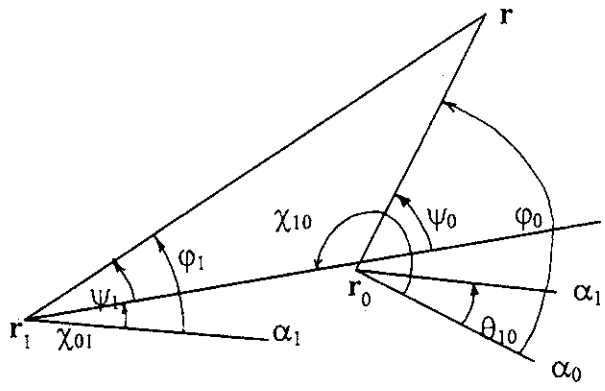


Fig. 1.1. Addition theorem for Bessel functions
$\psi_1=\varphi_1-\chi_{01}$; $\pi-\psi_0=\chi_{10}-\varphi_0$; $\chi_{10}=\theta_{10}+\chi_{01}+\pi$;
$|\mathbf{r}-\mathbf{r}_0|<|\mathbf{r}_1-\mathbf{r}_0|$

Suppose a source and sink of equal strength S are placed at the points $\mathbf{r}_0+d\mathbf{n}$, $\mathbf{r}_0-d\mathbf{n}$. The resulting neutron flux is next (Fig. 1.2):

$$S[G_0^j(|\mathbf{r}_0-\mathbf{r}_1+d\mathbf{n}|)- G_0^j(|\mathbf{r}_0-\mathbf{r}_1-d\mathbf{n}|)]$$

After application of addition theorem to functions $K_0(\kappa_i|\mathbf{r}_0-\mathbf{r}_1+d\mathbf{n}|)$, $K_0(\kappa_i|\mathbf{r}_0-\mathbf{r}_1-d\mathbf{n}|)$ (assuming $\alpha_0=\alpha_1=\mathbf{n}$) we get:

$$\sum_m I_m(\kappa_i d)\, K_m(\kappa_i|\mathbf{r}_0-\mathbf{r}_1|)=\sum_{m=-\infty}^{\infty} I_m(\kappa_i d)\, K_m(\kappa_i|\mathbf{r}_0-\mathbf{r}_1|)\exp(-im\chi_{10})[1-(-1)^m]$$

the angle χ_{10} is measured from $\mathbf{n}$ to $\mathbf{r}_1-\mathbf{r}_0$. Taking a limit $d\to 0$, and assuming $2Sd=P$ to be constant, instead of the last sum the following expression is obtained:

$$P\kappa_j K_1(\kappa_j|\mathbf{r}_1-\mathbf{r}_0|)\cos\psi;\ \cos\psi=(\mathbf{r}_1-\mathbf{r}_0,\mathbf{n})/|\mathbf{r}_1-\mathbf{r}_0|$$

with the Green function giving the influence of dipole at point $\mathbf{r}$, having the direction $\mathbf{n}$:

$$G_1^j(\mathbf{r}-\mathbf{r}_0,\mathbf{n})=CF_1(|\mathbf{r}-\mathbf{r}_0|)C^{-1}[(\mathbf{r}-\mathbf{r}_0,\mathbf{n})/|\mathbf{r}-\mathbf{r}_0|]e_j/(2\pi D_G)$$

$$F_1(|\mathbf{r}-\mathbf{r}_0|)=\mathrm{diag}\{\kappa_j K_1(\kappa_j|\mathbf{r}-\mathbf{r}_0|)\}$$

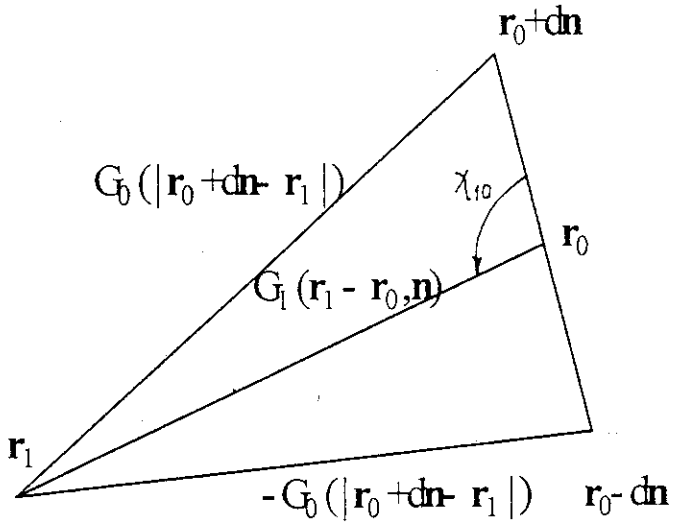


Fig. 1.2. Green function for dipole; $\alpha_0=\alpha_1=\mathbf{n}$

Interchanging $\mathbf{r}$ and $\mathbf{r}_0$ and taking the derivative of $G_0(|\mathbf{r}-\mathbf{r}_0|)$ in the direction $\mathbf{n}$, we can get a relation

$$(\partial/\partial|\mathbf{r}-\mathbf{r}_0|)G_0^j(|\mathbf{r}-\mathbf{r}_0|)|_n = -G_1^j(\mathbf{r}-\mathbf{r}_0, \mathbf{n})$$

$G_1^j(\mathbf{r}-\mathbf{r}_0, \mathbf{n})$ -Green function of a unit dipole in the direction $\mathbf{n}$ at point $\mathbf{r}$.

Taking a limit

$$\lim_{\rho\to 0}[G_1^j(\mathbf{r}+\mathbf{m}\rho-\mathbf{r}_0, \mathbf{n})- G_1^j(\mathbf{r}-\mathbf{r}_0, \mathbf{n})]/\rho = (dG_1, \mathbf{m})$$

we get an expression

$$(dG_1^j,\bullet)=(C\mathcal{J}_2C^{-1}e_j/2\pi D, \bullet); \qquad (1.3.10)$$

$$\mathcal{J}_2(\mathbf{r}-\mathbf{r}_0,\mathbf{n})=\operatorname{diag}_j\{\kappa_jK_1(\kappa_j|\mathbf{r}-\mathbf{r}_0|)\mathbf{n}/|\mathbf{r}-\mathbf{r}_0|-(\kappa_j^2/|\mathbf{r}-\mathbf{r}_0|^2)K_2(\kappa_j|\mathbf{r}-\mathbf{r}_0|)(\mathbf{r}-\mathbf{r}_0,\mathbf{n})(\mathbf{r}-\mathbf{r}_0)$$

Reactor with infinite moderator

General solution in a dipole approximation is presented by the next expression:

$$N(\mathbf{r}-\mathbf{r}_k) = \sum_k [G_0(|\mathbf{r}-\mathbf{r}_k|)A_k + G_1(\mathbf{r}-\mathbf{r}_k,\mathbf{B}_k]$$

A - a vector of arbitrary constants $a_{k,j}$, j=1,...G; $\mathbf{B}_k=\{ b_{k,j} \}$ - 2-dimensional vector , $\mathbf{k}=(k_1,k_2)$ -two-dimensiona vector, pointing the positions of channel centers.

For a Green function $G_0^j(|\mathbf{r}-\mathbf{r}_k|)$ function $K_0^j(\kappa_i|\mathbf{r}-\mathbf{r}_k|)$

according to addition theorem is equal:

$$K_0(\kappa_i|\mathbf{r}-\mathbf{r}_k|)=I_0(\kappa_i|\mathbf{r}-\mathbf{r}_l|)K_0(\kappa_i|\mathbf{r}_k-\mathbf{r}_l|)+$$
$$+2I_1(\kappa_i|\mathbf{r}-\mathbf{r}_l|)K_1(\kappa_i|\mathbf{r}_k-\mathbf{r}_l|)(\mathbf{r}-\mathbf{r}_l,\mathbf{r}_k-\mathbf{r}_l)/(|\mathbf{r}-\mathbf{r}_l||\mathbf{r}_k-\mathbf{r}_l|)+.....$$

so that in the vicinity of every channel neutron field is as follows:

$$G_0(|\mathbf{r}-\mathbf{r}_l|)\delta_{lk}A_l+\sum_k(1-\delta_{lk})\{I_0G_0(|\mathbf{r}_k-\mathbf{r}_l|)+2(I_1/\kappa)G_1(\mathbf{r}_k-\mathbf{r}_l,(\mathbf{r}-\mathbf{r}_l)/|\mathbf{r}-\mathbf{r}_l|)A_k;$$
$I_0=\mathrm{diag}\{I_0(\kappa_j|\mathbf{r}-\mathbf{r}_l|)\}$; $I_1/\kappa=\mathrm{diag}\{I_0(\kappa_j|\mathbf{r}-\mathbf{r}_l|)/\kappa_j\}$.

The influence of the second term is calculated in a similar way. The resulting neutron distribution near the channel **l** is given by expression

$$N_0(|\mathbf{r}-\mathbf{r}_l|)=[G_0(|\mathbf{r}-\mathbf{r}_l|)A_l+G_1(\mathbf{r}-\mathbf{r}_l,\mathbf{B}_l)]\delta_{lk}+ \qquad (1.3.11)$$
$$+\sum_k(1-\delta_{lk})\{I_0G_0(|\mathbf{r}_k-\mathbf{r}_l|)+2(I_1/\kappa)G_1(\mathbf{r}_k-\mathbf{r}_l,(\mathbf{r}-\mathbf{r}_l)/|\mathbf{r}-\mathbf{r}_l|)A_k+$$
$$+I_0G_1(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k)+2(I_1/\kappa)(G_2(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k),(\mathbf{r}-\mathbf{r}_l)/|\mathbf{r}-\mathbf{r}_l|)\}$$

$$G_2(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k)=(C\mathcal{J}_2C^{-1}/2\pi D);\ \mathcal{J}_2(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k)= \qquad (1.3.12)$$

$$=\mathrm{diag}_j\{\kappa_jK_1(\kappa_j|\mathbf{r}_l-\mathbf{r}_k|)\mathbf{B}_k/|\mathbf{r}_l-\mathbf{r}_k|-(\kappa_j^2/|\mathbf{r}_l-\mathbf{r}_k|^2)K_2(\kappa_j|\mathbf{r}_l-\mathbf{r}_k|)(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k)(\mathbf{r}_l-\mathbf{r}_k)\}$$

The 4 terms determine the influence:
monopole-monopole, monopole-dipole, dipole-monopole, dipole-dipole. Function G_2 is the same as the derivative of $G_1(\mathbf{r}_l-\mathbf{r}_k,\mathbf{B}_k)$ in the direction $\mathbf{r}-\mathbf{r}_l$.

Cylindrical reactor of finite dimensions

For a cylindrical reactor of finite radius R general solution after a change of variables (B to A) can be written in a form:

$$N(\mathbf{r})=C\mathcal{F}C^{-1}B;\ C^{-1}B\equiv A;\ A=\{A^n_{k,j}\}; \qquad (1.3.13)$$
$$F^j(\mathbf{r})A_j=\sum_k\sum_n K_n(\kappa_j|\mathbf{r}-\mathbf{r}_k|)\exp(in\varphi_k)A^n_{k,j}+$$
$$+\sum_\nu C_j^\nu I_\nu(\kappa_j r)\exp(i\nu\vartheta)$$

and includes a regular part taking account of finite dimensions (the last term) . The angle θ is measured from some fixed direction , for example direction of x-axis (Fig 1.3).
Suppose a boundary condition on the external surface of the reactor:

$$(1-s)N(R)-sR\partial N(R)/\partial R=0 \qquad (1.3.14)$$

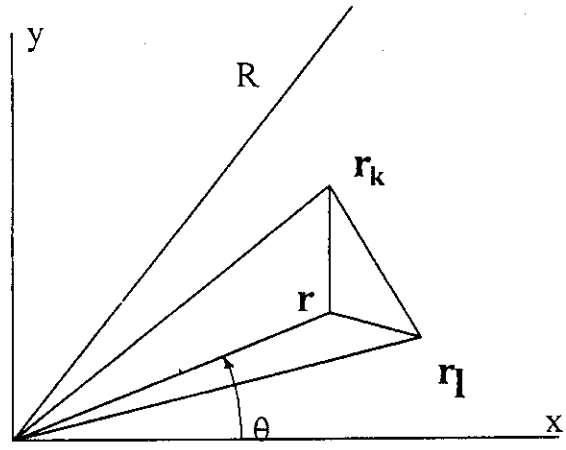


Fig.1.3 Finite reactor of radius R

Represent addition theorem in the next form

$$\exp(in\varphi_k)K_n(a|\mathbf{r}_k-\mathbf{r}|)=\exp(-in\vartheta_k)\times \\ \times\sum_{\nu=-\infty}^{\infty}I_{\nu-n}(ar_k)K_\nu(aR)\exp(i\nu\vartheta+i(n-\nu)\chi_k) \qquad (1.3.15)$$

and put the above expression into the equation for general solution

$$F^j(\mathbf{r})A_j=\sum_n\exp(in\varphi_k)A^n_{k,j}\sum_\nu I_{\nu-n}(\kappa_j r_k)K_\nu(\kappa_j R)\times \\ \times\exp(in\vartheta+i(n-\nu)\chi_k)+\sum C^\nu_j I_\nu(\kappa_j R)\exp(i\nu\vartheta).$$

Applying operator $D\equiv(1-s)-sR\partial/\partial R$ to the expression of neutron flux and gathering together the terms for the mode $\exp(i\nu\varphi)$, we get

$$C^\nu_j DI_\nu(\kappa_j R)=-\sum_n\sum_k\exp(-in\vartheta_k)I_{\nu-n}(\kappa_j r_k)DK_\nu(\kappa_j R)\times \\ \times\exp(i(n-\nu)\chi_k)A^n_{k,j},$$

$$C^\nu_j=-d^\nu_j\sum_n\sum_k\exp(i(n-\nu)\chi_k-in\vartheta_k)I_{\nu-n}(\kappa_j r_k)A^n_{k,j}; \\ d^\nu_j=\frac{[(1-s)-sR\partial/\partial R]K_\nu(\kappa_j R)}{[(1-s)-sR\partial/\partial R]I_\nu(\kappa_j R)}. \qquad (1.3.16)$$

The influence of every mode $\exp(iv\theta)I_v(\kappa_j r)$ on the solution near channel l is determined with the next addition theorem (Fig. 1.4):

$(|\mathbf{r}-\mathbf{r}_l| < r_l)$

$$\exp(iv\vartheta)I_v(\kappa_j r) =$$

$$= \sum_m \exp(im\vartheta_l)I_m(\kappa_j|\mathbf{r}-\mathbf{r}_l|)I_{v-m}(\kappa_j r_l) \times \qquad (1.3.17)$$

$$\times \exp(i(v-m)\chi_l + im\varphi_l),$$

so that

$$\sum C_j^v \exp(iv\vartheta)I_v(\kappa_j r) = -\sum_m \sum_v \sum_k \sum_n \exp(im\varphi_l)I_m \times$$

$$\times(\kappa_j|\mathbf{r}-\mathbf{r}_l|)I_{v-m}(\kappa_j r_k)d_j^v \exp(i(v-m)\chi_l + i(n-v)\chi_k) \times$$

$$\times \exp(im\vartheta_l - in\vartheta_k)$$

The first term for the neutron flux is calculated by addition theorem (Fig. 1.5):

$$\sum_n \sum_k K_n(\kappa_j|\mathbf{r}-\mathbf{r}_k|)\exp(in\varphi_k)A_{k,j}^n =$$

$$= \sum_m \exp(im\varphi_l)I_m(\kappa_j|\mathbf{r}-\mathbf{r}_l|)\sum_n \sum_k (-1)^n \exp(-in\vartheta_{kl}) \times$$

$$\times K_{n-m}(\kappa_j|\mathbf{r}_l-\mathbf{r}_k|\exp(i(n-m)\kappa_{kl})A_{k,j}^n$$

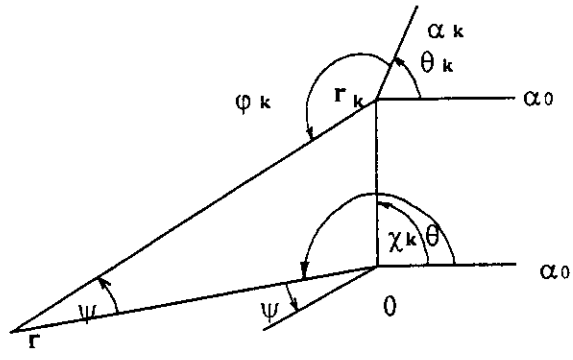


Fig. 1.4. Addition theorem for Bessel functions;

$\psi+\theta=\theta_k+\varphi_k$

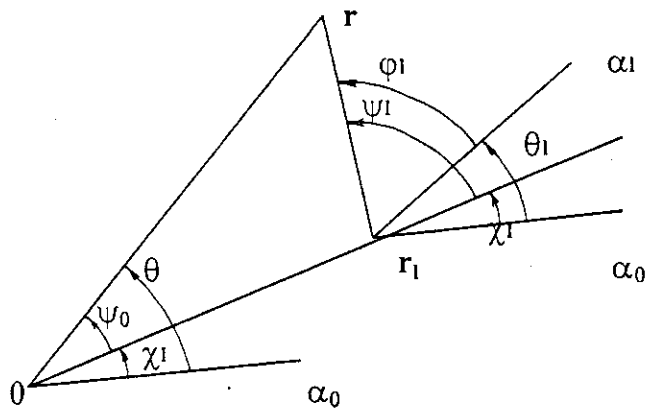


Fig. 1.5 Addition theorem for Bessel functions;

$\psi_0=\theta-\chi_l$; $\psi_l+\chi_l=\varphi_l+\theta_l$

Finally, taking account of both terms we get the solution in the vicinity of channel l:

$$F^{j}(\mathbf{r})A=\sum_{m}\exp(im\varphi_l)\sum_{k}\{\delta_{lk}K_m(\kappa_j|\mathbf{r}-\mathbf{r}_l|+ \\ +(1-\delta_{lk})I_m(\kappa_j|\mathbf{r}-\mathbf{r}_l|)\sum_{n}F_{lk}^{mn,j}\}A_{k,j}^{n} \qquad (1.3.18)$$

$$F_{lk}^{mn,j}=F_{lk,inf}^{mn,j}+F_{lk,fin}^{mn,j}$$

$$F_{lk,inf}^{mn,j}=(-1)^n\exp(in\vartheta_{kl})K_{n-m}(\kappa_j|\mathbf{r}_k-\mathbf{r}_l|)\exp(i(n-m)\chi_{kl});$$

$$F_{lk,fin}^{mn,j}=-\sum_{\nu}\exp(im\vartheta_l)d_j^{\nu}I_{\nu-n}(\kappa_j\mathbf{r}_k)I_{\nu-m}(\kappa_j\mathbf{r}_l)\times \\ \times\exp(i(n-\nu)\chi_k+i(\nu-m)\chi_l-in\vartheta_k).$$

$F_{lk,inf}^{mn,j}$

$F_{lk,fin}^{mn,j}$

- the kernal for the reactor of finite radius and the part responsible for finite radius of reactor correspondingly.

1.4 *Different forms of few-group heterogeneous reactor equations*

The solution near l th channel is presented by expression:

$$N(\mathbf{r}) = C(K + IF)C^{-1}B, \qquad (1.4.1)$$

$$K = \underset{k,j}{\text{diag}}\{K_m(\kappa_j|\mathbf{r}-\mathbf{r}_k|)\}, \; I = \underset{k,j}{\text{diag}}\{I_m(\kappa_j|\mathbf{r}-\mathbf{r}_k|)\}$$

Introducing a vector $\Phi_l \equiv [CFC^{-1}B]_l = \{\Phi^m_{l,j}\}$

rewrite the above equation: $N_l = C[KC^{-1}B_l + IC^{-1}\Phi_l]$

Suppose a linear dependence exists: $B_l = u_l\Phi_l$

then

$$\Phi = CFC^{-1}u\Phi \qquad (1.4.2)$$

and the solution is transformed as follows:

$$N_l(\mathbf{r}) = [CKC^{-1}u + CIC^{-1}]\Phi_l \qquad (1.4.3)$$

The above equation (1.4.2) is a uniform system of linear equations relative to vector Φ, having the dimension KxGxH; K - number of channels, G - number of groups, H - number of modes near channel surfaces (H=1 - monopole, H=3 - dipole approximation); (j=1,...,G).
The second equation gives the relation between regular and non regular parts of solutions near channel l which is determined by matrix u . For each angular mode matrix u can be determined from the solutions in an infinite media (with regular parts imposed) for determination of non regular parts:
$CI_mC^{-1}e_j \exp(im\varphi_l)$;

$CK_mC^{-1}u_l^{me_j} \exp(im\varphi_l)$

$\{u_{l,ij}^{me_j}\}$
An other equivalent approach : instead of u-matrix the relations on channel boundaries are given as:

$$\rho\partial N / \partial\rho = \Lambda N,$$

N - KxGxH - vector; ρ - radii of channels; Λ - matrix composed of GxG sub matrices for each channel.

Apply the operator

$$\partial \equiv \rho\partial / \partial\rho$$

to both parts of equation (1.4.1) and use the relation

$$C(\partial K + \partial IF)C^{-1}B = \Lambda N \qquad (1.4.4)$$

Do equivalent transformations
$FC^{-1}B$:

$$FC^{-1}B = I^{-1}FC^{-1}B = I^{-1}C^{-1}C(-K + K + IF)C^{-1}B =$$
$$= -I^{-1}KC^{-1}B + I^{-1}C^{-1}N$$

and put the result into (1.4.4)

$$C(\partial K - \partial II^{-1}K)C^{-1}B = [-C\partial II^{-1}C^{-1} + \Lambda]N \qquad \text{so that} \qquad C^{-1}B = C^{-1}\gamma N,$$

with $C^{-1}\gamma=(\partial K-\partial II^{-1}K)[C^{-1}\Lambda-\partial II^{-1}C^{-1}]$.

Using the expression for Bessel functions Wronskian one obtains:

$$\gamma = C(-IC^{-1}\Lambda + \partial IC^{-1}). \qquad (1.4.5)$$

Again using expression for B in (1.4.1) one gets:

$$N=C(K+IF)C^{-1}\gamma N \qquad (1.4.6)$$

Comparing the above expression with the expression for the solution by Green functions we see that γ is determined in such a way that the term

$2\pi D_G\gamma N(\rho)$ gives the strength of sinks and sources on channel axises

Using the relations:

$$u\Phi = \gamma(CKC^{-1}u + CIC^{-1})\Phi,$$

we find the relations between equivalent values γ and u:

$$\gamma = u(CKC^{-1}u + CIC^{-1})^{-1};$$
$$u = (1 - \gamma CKC^{-1})^{-1}\gamma CIC^{-1} = \gamma(1 - CKC^{-1}\gamma)^{-1}CIC^{-1} \qquad (1.4.7)$$

For the case of channels of small dimensions, monopole approximation, I=1, ∂I=0,

$$N = -C(K + F)C^{-1}\Lambda N,$$

and at the supposition of no slowing-down inside channels:

$$\Lambda = \begin{bmatrix} 0 & -\eta\gamma \\ 0 & \gamma \end{bmatrix}\frac{1}{2\pi D};(G = 2)$$

one gets

$$n_{l,1} = \frac{1}{2\pi D}[K_0(\kappa_1\rho_l)(\eta\gamma)_l n_{l,2} + \sum_k (1-\delta_{lk})K_0(\kappa_1|\mathbf{r}_l - \mathbf{r}_k|)(\eta\gamma)_k n_{k,2}]$$

$$n_{l,2} = \frac{1}{2\pi D_G}\{[K_0(\kappa_2\rho_l) - K_0(\kappa_1\rho_l)(1-\tau/L^2)^{-1}(\eta\gamma)_l - -K_0(\kappa_2\rho_l)\gamma_l]n_{l,2} + \sum_k (1-\delta_{lk})[(K_0(\kappa_2|\mathbf{r}_l - \mathbf{r}_k|) - -K_0(\kappa_1|\mathbf{r}_l - \mathbf{r}_k|))(1-\tau/L^2)^{-1}(\eta\gamma)_k - -K_0(\kappa_2|\mathbf{r}_l - \mathbf{r}_k|)\gamma_k]n_{k,2}\}.$$

The latter expression is the same as in the initial theory with 2-group Green functions instead of age-diffusion Green functions.

Let us separate the terms depending on the number of secondary neutrons emitted in fissions ν:

$$u=(1-\nu f)^{-1}u_1\nu - u_2 \qquad (1.4.8)$$

Matrix u_2 is provided by absorption and slowing-down of neutrons;
u_1 - by neutron fissions induced by the external neutron field $CIC^{-1}\Phi$;
Rewrite:

$$B=[(1-\nu f)^{-1}u_1\nu - u_2]\,\Phi; \quad (1-\nu f)B=[u_1\nu-(1-\nu f)u_2]\,\Phi$$

Thus 3 equivalent forms of heterogeneous reactor equations are obtained (λ, k - eigenvalues; k - effective multiplication factor):

$$B=(\nu/k)[f+(u_2+fu_2)CFC^{-1}]B - u_2\,CFC^{-1}B \qquad (1.4.9)$$

$$N = C(K+IF)C^{-1}(\gamma_1(\nu)/\lambda - \gamma_2)N \qquad (1.4.10)$$

$$\Phi = CFC^{-1}[(1-\nu f)^{-1}\nu u_1/\lambda - u_2]\,\Phi \qquad (1.4.11)$$

B- amplitudes of singular parts of equations

$CKC^{-1}B$;
Φ - amplitudes of external fields on channel axises

$CIC^{-1}\Phi$;
N - neutron fluxes on channel surfaces (extrapolated from the moderator, asymptotic)

$$N=N(\rho)=[CKC^{-1}B+CIC^{-1}\Phi]_{(r=\rho)}.$$

As it will be shown later matrix Λ can be presented as:

$\Lambda=\Lambda_1+\Lambda_2$; $\Lambda_1=-\Lambda_1'/(1-\upsilon)$; $\upsilon=k_0-q\Lambda_2N_0$;

Λ_1' and υ linearly depend on the number of neutrons born in fissions. Introduce a critical parameter - effective multiplication factor k and devide by k both of these values:

$\Lambda_1' \rightarrow \Lambda_1'/k$ and $\upsilon \rightarrow \upsilon/k$

After the change of variable

$N \rightarrow N'=N/(1-\upsilon/k)$

equation (1.4.6) (or (1.4.10)) transforms to the next form:

$$N'=(\upsilon+C\mathcal{J}C^{-1}\gamma_1')N'/k-C\mathcal{J}C^{-1}\gamma_2N' \; ; \; \mathcal{J}=K+IF; \qquad (1.4.12)$$

$\gamma_1'=CIC^{-1}\Lambda_1'+\upsilon\gamma_2$; $\gamma_2=C(IC^{-1}\Lambda_2-\partial IC^{-1})$

Equation (1.4.12) has simple linear dependence on k.

1.5 *Real representation of equations*

For computational applications general equations given in complex form are to be transformed to real form. Matrix elements were given in an arbitrary fixed directions for angles near each channel. These angles for the reactor can be counted from one fixed direction (say x-axis). In that case
$\vartheta_k = \vartheta_{kl} = 0$.
For a cylindrical reactor, and a lattice having a symmetry center, it is better to take a direction of radius-vector connecting the center of symmetry and the point $\mathbf{r}_k$ of $\mathbf{k}$ channel center, t.i. (for the central channel α can be chosen in the direction of x-axis)

$$\alpha_k = \mathbf{n}_k = \mathbf{r}_k / |\mathbf{r}_k|$$

In the expression for matrix elements now

$$\vartheta_l = \chi_l; \vartheta_k = \chi_k; \vartheta_{kl} = \chi_k - \chi_l;$$

Changing the meaning of variables (see picture), and using the relation (Fig. 1.6, 1.7):

$$\psi_{kl}=\psi_{lk}+\chi_k-\chi_l-\pi \qquad (1.5.1)$$

next relations are obtained for matrix elements:

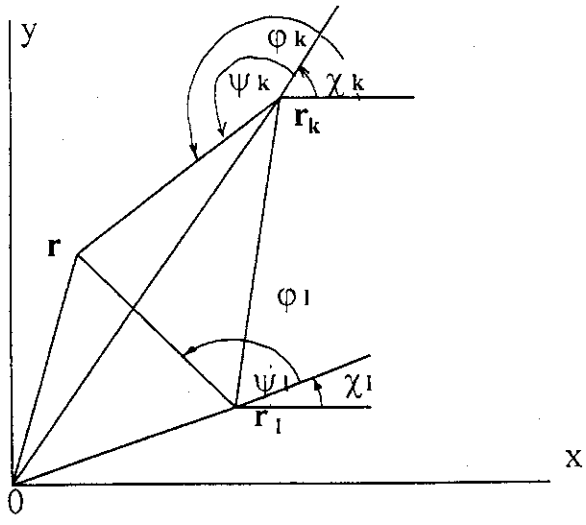


Fig. 1.6. Change of variables: $\psi_k=\varphi_k-\chi_k$, $\psi_l=\varphi_l-\chi_l$

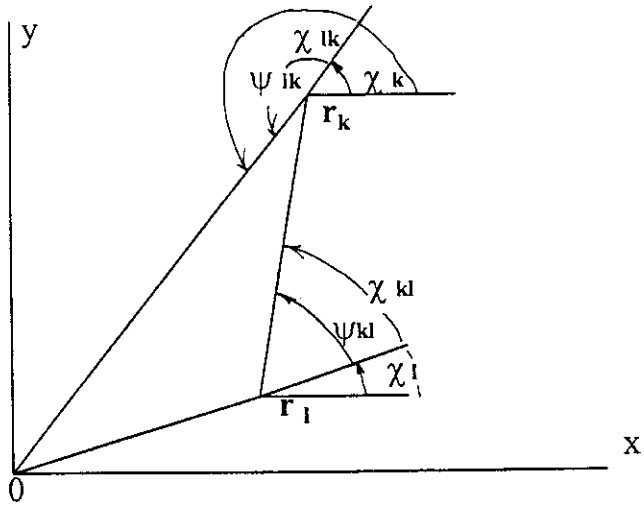


Fig. 1.7. The angles between $\mathbf{r}_k$, $\mathbf{r}_l$ and $\mathbf{r}_k$-$\mathbf{r}_l$;

$\chi_{kl}=\chi_{lk}-\pi$; $\psi_{kl}=\chi_{lk}-\chi_l$; $\psi_{lk}=\chi_{lk}-\chi_k$

$$F_{lk,inf} = K_{n-m}(\chi_j|r_l - r_k|)\exp(i(n\psi_{lk} - m\psi_{kl}))$$
$$F^{mn,j}_{lk,fin} = -\sum_{\nu} d^{\nu}_{j} I_{\nu-m}(\chi_j r_l) I_{\nu-n}(\chi_j r_k)\exp(i\nu(\chi_l - \chi_k)) \qquad (1.5.2)$$

Formal algebraic transformation with the changes of basis

$e = \{e^{m,\mu}_k\} = \{\exp(-im\mu\psi_k)\}$
to basis
$f = \{f^{m,\mu}_k\} = \{f^{00}_k = 1, f^{m,1}_k = \cos m\psi_k, f^{m,-1}_k = \sin m\psi_k\}$

leads to a real form by the next matrix transformation:

$$e = Qf; Q = \begin{bmatrix} 1 & & & \\ & \cdot & & \\ & & \cdot & \\ & & & q^m_k \end{bmatrix};$$

$$q^m_k = \begin{bmatrix} 1 & -i \\ 1 & i \end{bmatrix}$$

The presentation of an arbitrary vector in basis e must coincide with its presentation in basis f:

$$\langle f, y\rangle = \langle e, x\rangle = \langle Qf, x\rangle = \langle f, Q^+x\rangle; \langle e, x\rangle = \sum e_n x_n,$$
$$y = Q^+x,$$

Q^+ - conjugate-Hermite.
For a linear transformation $\mathcal{J}$ in basis e its representation in basis f is as follows:
$x' = Fx$

$$\langle e, x'\rangle = \langle e, Fx\rangle = \langle Qf, F(Q^+)^{-1}y\rangle =$$
$$\langle f, Q^+F(Q^+)^{-1}y\rangle = \langle f, \Phi y\rangle$$

that is two matrices in different basises are related to each other by following relation:

$$\Phi = Q^+F(Q^+)^-$$

For $\nu=\mu$ the transformations of matrix elements are as follows:

$$\mu, \nu: \begin{bmatrix} (1,1) & (1,-1) \\ (-1,1) & (-1,-1) \end{bmatrix};$$

$$\Phi^{m,\mu;n,\nu}_{lk}\} =$$
$$= \begin{bmatrix} \mathrm{Re}\,U + \mathrm{Re}\,V & \mathrm{Im}\,U - \mathrm{Im}\,V \\ -\mathrm{Im}\,U - \mathrm{Im}\,V & \mathrm{Re}\,U - \mathrm{Re}\,V \end{bmatrix};$$

$$U = \mathcal{J}^{mn}_{lk}; V = \mathcal{J}^{m,-n}_{lk}$$

For the case m=0, or n=0, or m=n=0 the next expression is valid:

$$\{\Phi_{lk}^{0;n,\nu}\} = \{\mathrm{Re}\,U; \mathrm{Im}\,U\};$$

$$\{\Phi_{lk}^{m,\mu;0}\} = \begin{bmatrix} 2\,\mathrm{Re}\,V \\ -2\,\mathrm{Im}\,V \end{bmatrix};$$

$$\Phi_{lk}^{0;0} = \mathcal{J}_{lk}^{0;0}$$

For the infinite part of the kernel:

$$\mathrm{Re}U \pm \mathrm{Re}V =$$
$$= \cos(n\psi_{lk} - m\psi_{kl})K_{n-m}(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|) \pm$$
$$\pm\cos(n\psi_{lk} + m\psi_{kl})K_{n+m}(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|);$$

$$\mathrm{Im}U \pm \mathrm{Im}V =$$
$$= \sin(n\psi_{lk} - m\psi_{kl})K_{n-m}(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|) \mp$$
$$\mp\sin(n\psi_{lk} + m\psi_{kl})K_{n+m}(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|)$$

For $m=1$, $n=1$ $F^{m,n}_{l,k;inf}$ are given by the next formulas:

$$\begin{bmatrix} c^-K_0 + c^+K_2 & s^-K_0 + s^+K_2 \\ -s^-K_0 + s^+K_2 & c^-K_0 - c^+K_2 \end{bmatrix}; \qquad (1.5.3)$$

$$c^\pm = \cos(\psi_{lk} \pm \psi_{kl});$$
$$s^\pm = \sin(\psi_{lk} \pm \psi_{kl}).$$

Taking account of (1.5.1) and the following equality

$$K_0(z) = -\frac{2}{z}K_1(z) + K_2(z)$$

instead (1.5.3) we obtain:

$$\frac{2}{\chi_j|\mathbf{r}_k - \mathbf{r}_l|}K_1(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|)\cdot \qquad (1.5.4)$$
$$\begin{bmatrix} \cos(\chi_k - \chi_l) & -\sin(\chi_k - \chi_l) \\ \sin(\chi_k - \chi_l) & \cos(\chi_k - \chi_l) \end{bmatrix} +$$
$$+2K_2(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|)\begin{bmatrix} \cos\psi_{kl} & 0 \\ 0 & \sin\psi_{kl} \end{bmatrix}\cdot$$
$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} \cos\psi_{lk} & 0 \\ 0 & \sin\psi_{lk} \end{bmatrix}$$

Matrix elements correspond to function $\mathcal{J}_2$; if **B** is decomposed along unit vectors $\mathbf{n}_k$, τ_k in the direction of channel **k** and orthogonal to it correspondingly, and the vector $\mathbf{r}$-$\mathbf{r}_l$ along $\mathbf{n}_l$, τ_l.The infinite part in dipole approximation

$$F_{lk,\,inf}^{m,\mu;n,\nu}$$

in correspondence with indices:

m,μ; n,ν:

$$\begin{pmatrix} 0;0 & 0;1,1 & 0;1,-1 \\ 1,1;0 & 1,1;1,1 & 1,1;1,-1 \\ 1,-1;0 & 1,-1;1,1 & 1,-1;1,-1 \end{pmatrix}$$ is as following:

$$F_{lk,\,inf}^{m,\mu;n,\nu} = \mathrm{diag}(1,2\cos a,2\sin a)\begin{pmatrix} K_0 & S & S \\ S & T & T \\ S & T & T \end{pmatrix}\cdot\mathrm{diag}(1,\cos b,\sin b)+$$

$$+2(S/\chi_j|\mathbf{r}_k-\mathbf{r}_l|)\mathrm{diag}(0,\sin a,\cos a)\cdot\begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \end{pmatrix}\mathrm{diag}(0,\sin b,\cos b) \quad (1.5.5)$$

$a \equiv \psi_{kl}; \quad b \equiv \psi_{lk}; S \equiv K_1(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|);$

$$T = K_0(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|) + \frac{K_1(\kappa_j|\mathbf{r}_k - \mathbf{r}_l|)}{\kappa_j|\mathbf{r}_k - \mathbf{r}_l|}$$

The result for finite part of matrix elements:

$$F_{lk,\,fin}^{m,\mu;n,\nu;j} =$$

$$= -\delta_m \sum_{\nu\geq 0} d_\nu^j \delta_\nu P_m \begin{pmatrix} \partial_m^+ I_\nu^l & 0 \\ 0 & \partial_m^- I_\nu^l \end{pmatrix} \begin{pmatrix} c_\nu & -s_\nu \\ s_\nu & c_\nu \end{pmatrix} \begin{pmatrix} \partial_n^+ I_\nu^k & 0 \\ 0 & \partial_n^- I_\nu^k \end{pmatrix} P_n, \qquad (1.5.6)$$

m,n=0,1;

$$\delta_m = \begin{matrix} 1/2; m = \\ 1; m > 0 \end{matrix}$$

d_ν^j - a coefficient that depends on the boundary condition on the reactor surface;

$P_m = \begin{pmatrix} 1 & 0 \\ 0 & (1-\delta_{m0}) \end{pmatrix}$ - a projection operator on the first coordinate , if m=0;

$\partial_m^+, \partial_m^-$ are defined by the relations:

$$\partial_m : I_\nu \to I_{\nu-m} + I_{\nu+m};$$
$$\partial_m^- : I_\nu \to I_{\nu-m} - I_{\nu+m};$$

By definition, $c_\nu \equiv \cos\nu(\chi_k - \chi_l); s_\nu \equiv \sin\nu(\chi_k - \chi_l); I_\nu^l \equiv I_\nu(\chi_j r_l)$

Some formulas for trigonomertic functions in matrix elements.

Let θ be the angle between axises of fixed system of coordinates. Vector **k** considered as a complex value in the Decart coordinate system $k=k_1+ik_2$ has the next components

$\mathbf{l} = (l_1, l_2); \quad k_1 = l_1 + l_2\cos\theta; \quad k_2 = l_2\sin\theta;$

For 2 vectors $k = r\exp(i\varphi), k' = \rho\exp(i\Psi)$
the product of complex conjugate $\bar{k} = r\exp(-i\varphi)$ by k' is:

$$\bar{k}k' = r\rho[\cos(\psi - \varphi) + i\sin(\psi - \varphi)] =$$

$$l_1 l_1' + l_2 l_2' + (l_1 l_2' + l_2 l_1')\cos\theta + i(l_1 l_2' - l_2 l_1')\sin\theta$$

that is $\cos(\psi-\varphi) = [l_1 l_1' + l_2 l_2' + (l_1 l_2' + l_2 l_1')\cos\theta]/(r\rho);$

$\sin(\psi-\varphi) = (l_1 l_2' - l_2 l_1')\sin\theta/(r\rho)$

$r = (l_1^2 + l_2^2 + 2l_1 l_2\cos\theta)^{1/2}; \qquad \rho = (l_1'^2 + l_1'^2 + 2l_1' l_2'\cos\theta)^{1/2}$

The above formulas give the expresions for trigonometric functions depending on the angles between the vectors in an arbitrary coordinate system; for the case of hexagonal lattice:

$\mathbf{l} = (l_1, l_2)$; $\mathbf{l}' = (l_1', l_2')$; $\cos\theta = 1/2$; $\sin\theta = \sqrt{3}/2$

1.6 *Reactor symmetry. Elementary relations*

Let the loading in a heterogeneous reactor with a square or hexagonal lattice has some symmetry.
Let c corresponds to a rotation around the center of symmetry by the angle $2\pi/M$, M=4, 6 for square, hexagonal lattice correspondingly. Double rotation is given by the product

$cc=c^2$ $c^M = e$;
M rotations superimpose the lattice with itself. The rotation in back direction is given by

c^{-1}, $cc^{-1} = e$.

Another symmetry transformation - reflection relative to bissectrissa between the angles x and y

$$\sigma_1, \sigma_1 \cdot \sigma_1 = \sigma_1^2 = e$$

The set of elements and its products presentes a finite group G.
The group with elements c, σ is defined as $C_{Mv} = \{c^m \sigma_1^n\}$
and includes 2M different elements.

Let **k** be a position of some channel , **gk** - the position after applying transformation g.
Neutron flux should be the same for all the channels **gk** ;

$g \subset G = C_{Mv}$

In this case the number of unknown values decreases in 2M times. The above group is a maximal symmetry point group possible. In other cases the symmetry can be described by some subgroup of group C_{Mv}.
To take account of all the channels having symmetric positions the next sum is taken:

$$F_{l,k} \rightarrow \sum_{g \in G} F_{l,gk},$$

for F_{inf} the calculations should be fulfilled for all the pairs: **l**, **gk.** For finite parts of matrix elements F_{fin}

$$\partial_n^{\pm} I_v^{gk} = \partial_n^{\pm} I_v^{k}$$

since the distance from symmetry center is the same for these channels, and the dependence on g exists only in functions:

$\cos\nu(\chi_{gk} - \chi_l); \sin\nu(\chi_{gk} - \chi_l)$
Let

$q = pM + d; d < M; \psi \equiv \chi_k - \chi_l$

Then

$$\sum_{g\in C_M}\exp(iq(\chi_{gk}-\chi_l))=\sum_{m=1}\exp(iq\psi+i(pM+d)\times$$

$$\times\frac{2\pi m}{M})=\exp(iq\psi)\sum_{m=1}^{M}\exp(id\frac{2\pi m}{M})=$$

$$=\exp(iq\psi)\exp(id\frac{2\pi}{M})\sum_{m=0}^{M-1}\exp(id\frac{2\pi m}{M})=$$

$$=\exp(iq\psi)\exp(id\frac{2\pi}{M})\sum_{m=1}^{M}\exp(id\frac{2\pi m}{M})\rightarrow$$

$$\rightarrow\exp(i\frac{2\pi}{M}d)=1, d<M.$$

The 3d number of this chain of equations is equal to the last if and only if d=0; in this case the sum (dependent on all m) is equal M. Consequently, if a subgroup C_M is included in the symmetry group, then q=pM, p - integer value.
Thus in this case matrix elements become:

$$F_{l,k,fin}\rightarrow M\sum_{s\in Q}F_{l,sk,fin},$$

the subgroup Q include unity e and possibly reflection σ;
the sum (1.5.6) includes only ν values of the type: ν=pM; p - an integer.

1.7 *Justification of heterogeneous method and introduction of heterogeneous parameters for a channel or a reactor cell*

Justification of heterogeneous theory can be done in few-group approximation. In the initial heterogeneous theory with small fuel rods every channel was characterized by a thermal constant giving the relation between thermal flux (asymptotic) and the current at the rod boundary

$$\gamma=2\pi D\rho(\partial N/\partial\rho)N \qquad (1.6.1)$$

In a few- group theory vector-flux is composed of G components and the general relation between flux and current on the channel boundary must be given by a G×G matrix Λ:

$$\rho\partial N/\partial\rho=\Lambda N \qquad (1.6.2)$$

In a few-group approximation the flux in the reactor
can be considered as obeying a system of integral equations:

$$N_i(\mathbf{r})=\sum_j\int K_i(\mathbf{r},\mathbf{r}')[\Sigma_{ij}+\chi_{ij}\nu_j\Sigma_j^f](\mathbf{r}')N_j(\mathbf{r}')d\mathbf{r}' \qquad (1.6.3)$$

$$i,j=1,2,\ldots,G$$

$$K_i(\mathbf{r},\mathbf{r}')=\exp[-s_i(\mathbf{r},\mathbf{r}')]/4\pi R^2, R=|\mathbf{r}-\mathbf{r}'| \qquad (1.6.4)$$

Let $\mathcal{L}$ be the operator in equation (1.6.3), and $\mathcal{L}_0$ corresponds to the same reactor without channels ,
that is to the case of moderator in full volume.

The equation (1.6.3) can be rewritten in a form:

$$N = \ell N \qquad (1.6.5)$$

$$N = \ell_0 N + Q; \qquad Q = (\ell - \ell_0) N \qquad (1.6.6)$$

Let N be an arbitrary vector-function, defined for all the reactor volume . If the ray (**r**,**r'**) does not intersects any channel than the result of integration for Q is zero since ℓ coincides with ℓ_0 for these cases.

If the ray intersects some channels than the result of integration decreases as

$$\exp(-R\Sigma_{i\,mod}) << 1, \; i,j = 1,...G \qquad (1.6.7)$$

with the increase of the distance from channels (due to the behavior of kernel in integral equations).

The function Q can be presented as superposition of functions

$$Q(\mathbf{r}) = \sum_k Q_k(\mathbf{r}) \qquad (1.6.8)$$

where function Q_k differs from zero in some vicinity of channel **k** at the distances of order of mean free path from it.

Let G^i be Green function for moderator, that is the solution of the equation:

$$G^i(\mathbf{r}, \mathbf{r}_0) = \ell_0 G^i(\mathbf{r}, \mathbf{r}_0) + \delta(\mathbf{r} - \mathbf{r}_0)e_i \qquad (1.6.9)$$

The solution of the equation (1.6.3) can be presented as superposition:

$$N(\mathbf{r}) = \sum_k \int < G(\mathbf{r}, \mathbf{r}_0) Q_k(\mathbf{r}_0) > d\,\mathbf{r}_0 \qquad (1.6.10)$$

symbol < > means scalar product for G-vectors.

In one-group case the regular solution of the equation

$$N^{(0)} = \ell_0 N^{(0)} \qquad (1.6.11)$$

can be found as a superposition of plane waves:

$$N^{(0)}(\mathbf{r}) = \int C(\mathbf{n}) \exp[p(\mathbf{rn})] d\mathbf{n} \qquad (1.6.12)$$

Insert the function

$$\exp[p(\mathbf{rn})$$

into equation (1.6.11), then we get an expression

$$1 = \int (\exp[-\Sigma\,|\mathbf{r}-\mathbf{r}'| - p(\mathbf{r}-\mathbf{r}', \mathbf{n})]/4\pi R^2)\Sigma_s R^2 dR d\varphi \sin\theta d\theta$$

$$1 = \int \exp(-\Sigma R - pR\cos\theta)\Sigma_s R^2 dR \sin\theta d\theta =$$

$$= -(1/2)\,\Sigma_s \int_{-1}^{1} du/(pu - \Sigma) = (\Sigma_s/2p)\ln[(1+p\Sigma)/(1-p\Sigma)]$$

$$1=(\Sigma_s/2p)\ln[(1+p/\Sigma)/(1-p/\Sigma)]=(\Sigma_s/p)\mathrm{arcth}(p/\Sigma) \qquad (1.6.13)$$

that is the plane wave is the solution of equation (1.6.11) if p is the root of equation (1.6.13).

Suppose $C(\mathbf{n})=1/4\pi$; then function $I_0(p_0|\mathbf{r}|)$ is the solution of equation (1.6.13). The function
$I_n(p_0|\mathbf{r}|)\exp(in\varphi)$ ($|n|=1,2,...$) is also a solution of equation (1.6.11).

In a few-group approximation we have solutions of the type $\exp[p_i(\mathbf{rn})]$, p_i being the root of equation:

$$1=(\Sigma_{jj}/p_j)\mathrm{arcth}(p_j/\Sigma_j) \qquad (1.6.14)$$

For i>j the solution can be found in a form,

$$N_i=b_{ij}N_j=b_{ij}\exp[p_j(\mathbf{rn}) \qquad (1.6.15)$$

or after substitution in equation (1.6.13) and after integration we get a system of equations for b_{ij}:

$$b_{ij}=a_{ij}\left[\sum_m \Sigma_{im}b_{mj}+\Sigma_{ii}b_{ij}\right];$$
$$a_{ij}\equiv(1/p_j)\mathrm{arcth}(p_j/\Sigma_i)$$

with recurrence relations for their determination:

$$b_{ij}=w_{ij}\sum_m \Sigma_{im}b_{mj}, i>j; b_{jj}=1; \qquad (1.6.16)$$
$$w_{ij}=\left[p_j/\mathrm{arcth}(p_j/\Sigma_i)-\Sigma_{ii}\right]^{-1}$$
$$c_{ij}=w_{ij}(p_{i-1}^2/p_i^2\,\Sigma_{i+1,i}c_{i-1,j}; c_{jj}= \qquad (1.6.17)$$

For one-group case (j=G=1) Green function, that is the solution with line source $\delta(\mathbf{r}-\mathbf{r}_o)$ can be obtained by Furie transform:

$$G(r)=a(c,l)K_0(p_0r)+\int_1^\infty f(p)K_0(pr\Sigma)dp \qquad (1.6.18)$$
$$l\equiv 1/\Sigma; c=\Sigma_s/\Sigma; a(c,l)=p_0^2(1-l^2p_0^2)/\pi(c-1+l^2p_0^2)$$

that is Green function is presented as a sum of asymptotic part and the part decreasing exponentially at the distances of the order of several mean free paths:

$$G_{as}(r)\approx K_0(p_0r)$$
$$\exp(-r\Sigma)$$
$$f(p)-$$

a bounded function. Similar presentation is valid in few-group theory.
The solution in the vicinity of channel l can be presented as:

$$N(\mathbf{r})=\int <G(\mathbf{r},\mathbf{r}_0)Q_l(\mathbf{r}_0)>d\,\mathbf{r}_0+\sum\int <G(\mathbf{r},\mathbf{r}_0)Q_k(\mathbf{r}_0)>d\,\mathbf{r}_0 \quad (6.19)$$

But if the distances between channels exceed several mean free paths we can take asymptotic parts of Green functions:

$$N(\mathbf{r}) = \int < G(\mathbf{r}, \mathbf{r}_0) Q_l(\mathbf{r}_0) > d\,\mathbf{r}_0 + \sum_{k \neq l} \int < G_{as}(\mathbf{r}, \mathbf{r}_0) Q_k(\mathbf{r}_0) > d\,\mathbf{r}_0 \quad (6.20)$$

Applying addition theorem for Bessel functions in $G_{as}(\mathbf{r},\mathbf{r}_0)$ for the sets of points $(\mathbf{r},\mathbf{r}_0,\mathbf{r}_k)$ and $(\mathbf{r},\mathbf{r}_l,\mathbf{r}_k)$ we see that the second term can be presented as a sum

$$N_i^{(0)}(\mathbf{r}) = \sum_n \sum_{j=1}^{G} c_{ij} \exp(in\varphi_l) I_n(\chi_j |\mathbf{r} - \mathbf{r}_l|) A_{l,j}^n \quad (1.6.21)$$

Thus the influence of neighbor channels leads to the presence of a regular part of solution in the vicinity of a given channel **l**. By definition the function Q_l is:

$$Q_l = (\ell - \ell_0)N = (\ell_l - \ell_0)N \quad (1.6.22)$$

and the first term in (1.6.20) behaves as $G_{as}(|\mathbf{r}-\mathbf{r}_l|)$ at large distances $|\mathbf{r}-\mathbf{r}_l|$. Thus function (1.6.20) can be presented as a sum:

$$N(\mathbf{r}) = N^{(1)}(\mathbf{r}) + N^{(0)}(\mathbf{r}) \quad (1.6.23)$$

Applying operator $(1-\ell_0)$ we get

$$(1-\ell_0)(N^{(1)}+N^{(0)}) = (\ell_1-\ell_0)(N^{(1)}+N^{(0)})$$

But since $N^{(0)}$ - is a regular solution $(1-\ell_0)N^{(0)}=0$
we get an equation

$$N^{(1)} = \ell_1 N^{(1)} + (\ell_1 - \ell_0)N^{(0)} \quad (1.6.24)$$

The behavior of $N^{(0)}$ is known and depends only on the coefficients $A^n_{l,j}$. The solution $N^{(1)}$ can only linearly depend on these coefficients and its behavior at the distances of several mean free paths is as follows:

$$N_i^{(1)} = \sum_n \sum_{j=1}^{G} c_{ij} \exp(in\varphi_l) K_n(\chi_j |\mathbf{r} - \mathbf{r}_l|) B_{l,j}^n \quad (1.6.25)$$

and the relation between A and B must be given by a G×G matrix u:

$$B_l^n = u_l^n A_l^n \quad (1.6.26)$$

$$A_l^n = \{A_{l,j}^n\}; B_l^n = \{B_{l,j}^n\}, j = 1,\ldots,G \quad (1.6.27)$$

The equation (1.6.24) can also be written in an equivalent form:

$$(N^{(1)}+N^{(0)}) = \ell_1(N^{(1)}+N^{(0)}) \quad (1.6.28)$$

Matrix u can be found from G solutions with linearly independent A-coefficients. Matrix u is uniquely related to matrix Λ.

2. Difference Formulation of Heterogeneous Reactor Equations

2.1 A difference approach

An approximate method has been developed leading to heterogeneous reactor problem formulation in terms of a difference equation so that numerical solution for nuclear reactors with several thousands of lattice elements can be obtained. The method has high accuracy as it can be shown by a comparison with the solutions by direct method.

The method is based on a direct transformation of the heterogeneous equation to a difference form. Application of a difference operator with free parameters which are determined from the requirement of the "best" elimination of far distant terms immediately lead to a difference equation which is directly related to initial heterogeneous equation.

The resulting difference operator providing sufficient (and really rather high) accuracy of solutions appears to be broader than conventional Laplace operator (the difference scheme for square lattice should include 9 points) that makes some widely used homogeneous codes inapplicable. Chebyshev's iterative metod for outer iteration combined with succesive over-relaxation method for inner iteration were successfully used for the solution of derived equations.

2.2 Transformation of heterogeneous reactor equations to a difference form

Boundary conditions are supposed to be given on channel surfaces in the form of a Λ-matrix:

$$\rho \partial N / \partial \rho = \Lambda N,$$

N - KxG- vector of neutron fluxes on channel surfaces (extrapolated from the moderator, asymptotic)
K - number of rods, G -number of groups;
ρ - radii of channels;
Λ - **k** - diagonal matrix is composed of GxG sub matrices for each channel, and consists of two parts - Λ_1 and Λ_2 -depending on neutron fissions and on neutron absorbtion and slowing down correspondingly:

$$\Lambda=\Lambda_1+\Lambda_2;\ \Lambda_1=-\Lambda_1'/(1-\upsilon);\ \upsilon= k_0-q\Lambda_2 N_0;$$

Λ_1' and υ linearly depend on the number of neutrons born in fissions. After introduction of a critical parameter - effective multiplication factor *k*:

$$\Lambda_1' \rightarrow \Lambda_1'/k \text{ and } \upsilon \rightarrow \upsilon/k$$

and a a-change of variables

$$N \rightarrow N'=N/(1-\upsilon/k)$$

the equation for neutron flux becomes as follows:

$$N'=(\upsilon+C\mathcal{J}C^{-1}\gamma_1')N'/k-C\mathcal{J}C^{-1}\gamma_2N' \; ; \qquad (2.2.1)$$

$$\mathcal{J}=K+IF; \qquad (2.2.2)$$

$$\gamma_1'=CIC^{-1}\Lambda_1'+\upsilon\gamma_2; \quad \gamma_2=C(IC^{-1}\Lambda_2-\partial IC^{-1}) \qquad (2.2.3)$$

Triangular matrix C depends on moderator properties;

$$K=\underset{g,k}{\mathrm{diag}}\{K_0(\kappa_g\,\rho_k);\ I=\underset{g,,k}{\mathrm{diag}}\{I_0(\kappa_g\rho_k)\}$$

$\kappa_g^2=\xi_g+\alpha^2$; K_0, I_0 - modified Bessel functions,
$\alpha=\pi/H$; H – effective reactor height .

The (GxK)x(GxK) g-diagonal matrix F is composed of influence functions, which depend, generally, on the boundary conditions on the outer reactor surface. Keeping in mind that the latter can be formed by fictitious sources and sinks outside the reactor in infinitely expanded moderator and in difference formulation the boundary conditions are taken into account directly, it is enough for our purposes to take these functions for infinite moderator. In this case and F -matrix elements are taken as:

$$F_{kl}^{g}=K_0(\kappa_g|\mathbf{r}_k-\mathbf{r}_l|)(1-\delta_{kl}) \qquad (2.2.4)$$

A difference form of heterogeneous reactor equation is derived as follows (first consider monopole approximation).
Introducing an arbirary matrix D (diagonal by **k** and g) and taking account of (2.2.2), equation (2.2.1) can be transformed to the following

$$UN'=[U\upsilon/k+(I_0^{-1}K_0+F)(\gamma'_1/k-\gamma_2)]N'$$

$$U=I_0^{-1}C^{-1} \qquad (2.2.5)$$

For N''=UN'' the following equation is obtained

$$N''=[\upsilon/k+(I_0^{-1}K_0-D+F+D)(\gamma_1''/k-\gamma_2')]N''; \qquad (2.2.6)$$

$$\gamma_1''=\gamma_1'U^{-1}; \ \gamma_2'=\gamma_2U^{-1};$$

The aim of transformations leading to equation (2.2.6) was to bring the matrix F (2.2.4) on the left. If instead of $\mathbf{r}_k$ one takes an arbirary vector **r** in the elements of matrix F, then each of them will satisfy an equation

$$(-\Delta_r+\kappa_g^2\,a^2)F^{g}(\mathbf{r},\mathbf{r}_l)=0 \qquad (2.2.7)$$

a - lattice pitch.
Approximately the same is correct if one operates on $\mathbf{r}_k$ by a difference operator including an operator Δ_l which substitutes the Laplace operator on the reactor lattice:

$$(-\Delta_1 + \kappa_g^{\,2} a^2) F^g_{kl} \cong 0; | \mathbf{k} - \mathbf{l} | > 0 \qquad (2.2.8)$$

$$\Delta_1 : f_k \Rightarrow \sum_Q (f_{k+Qe1} - 4 f_k),$$

$\mathbf{e}_1 = (1,0)$, Q rotates a vector on the angles 0 , 90 ,180 , 270 (for square lattice).

Now let it be some other operator instead of operator in (2.2.8) , only some properties being preserved: it must be of "local" type, that is it must connect only some neighbor points, besides it must be symmetric relative to rotations around point **k**, superimposing the lattice with itself. Thus for a square lattice for example one can take an operator (g-diagonal with elements $\wp_g$) which relates to each other the values of a discrete function in some neighbor points:

$$\wp_g : f_k \Rightarrow (-\alpha_1\Delta_1 - \alpha_2\Delta_2 - ... + \beta\kappa_g^{\,2} a^{\,2}) f_k ; \sum \alpha_i = 1, \qquad (2.2.9)$$

The operator Δ_2 differs from Δ_1 in that $\mathbf{e}_2 = (1,1)$ is substituted for $\mathbf{e}_1 = (1,0)$ so that Δ_2 embraces the next to **k** set of points and so on. For example, in a 9-point scheme $\wp$ includes only Δ_1 and Δ_2 and $\alpha=(\alpha_1)$, $\alpha_2=1-\alpha_1$. The set of indices appearing after operating by $\wp$ in the point **k** is denoted by U_k (Fig. 2.1.).

It is naturally to make such a choice of α and β in (2.2.9) that provides the best elimination of the elements outside U_k. Since F_{kl} are invariant relatively to shifts of the lattice it is enough for determination of α and β to set $\mathbf{k}=0$.

Various criteria could be recommended for the choice of α and β. The result of application of criteria :

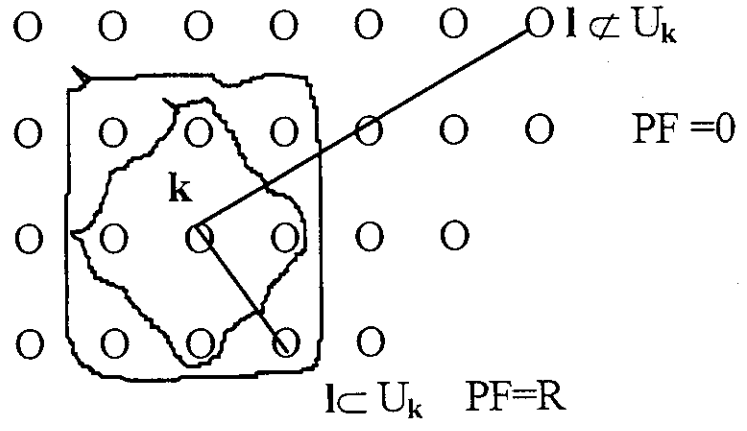


Fig. 2.1. The set of indices near **k**, U_k

$$\max_{l} |\mathcal{P}_g(\alpha,\beta)F_{0l}^g| \to \min \qquad (2.2.10)$$

for some rather wide set of points l surrounding point 0 is shown in table 2.1.
If one operates on both parts of the eqution (2.2.6) by $\mathcal{P}(\alpha,\beta)$ with the parameters α,β derived for example as above then for every **k** it approximately eliminates all the elements in (2.2.6) outside every set U_k . On the contrary, the elements F_{kl}, $l \subset U_k$, are not eliminated. The result of operating by $\mathcal{P}(\alpha,\beta)$ on F, $l \subset U_k$, is denoted as R:

$$R = \mathcal{P}(\alpha,\beta)\,(F+D) \qquad (2.2.11)$$

2.3 2D monopole equations

Thus instead of (2.2.6) the following equation is obtained

$$\mathcal{P}N'' = [\,\mathcal{P}\upsilon/k + (\mathcal{P}\,(I_0^{-1}K_0 - D) + R)(\gamma_1''/k - \gamma_2')]N'' \qquad (2.2.12)$$

if the elements $\mathcal{P}F_{kl}$, $l \not\subset U_k$, are neglected.

Relation has a form of a difference equation: for every **k** $\mathcal{P}$ and R connect only the points inside U_k , the other matrices γ, I_0, K_0, D - being **k**- diagonal .
It should be noted that matrix $R\gamma_2'$ is triangular relative to g.

Expanding the set U_k , t.i. adding the neighbor points and adding correspondingly new parameters to the set α,β it is possible to eliminate F outside U_k with a higher accuracy. If F^g operates in a short distance itself (as in epithermal groups), it can be retained in a form stated in initial heterogeneous equation.
The solution of the problem stated above for determination of parameters α, β depends on a single parameter

$$z \equiv \kappa_g a.$$

The results of application of criteria (2.2.10) for a 9-point scheme are presented in the table below: the optimal parameters α_1 and β as well as elements of R-operator in points 0, $\mathbf{e}_1$, $\mathbf{e}_2$, Bessel function $K_0(z)$ and the maximal error

$\varepsilon = \max |\mathcal{P}F|$, $l \not\subset U_k$.

The deviation of β from 1 shows how large is the difference between $\mathcal{P}$ - operator and operator $(\Delta_1 - z^2)$. It should be noted that the signs of R-operator are inverse to that of operator $\mathcal{P}$.

Table 2.1. Parameters of 9-point difference scheme for square lattice.

z	α_1	β	R_0	R_1	R_2	K_0	δ
0.1	0.6425	0.9966	-7.730	2.732	0.7614	2.427	1.634-3
0.5	0.6437	1.020	-2.846	1.706	0.4719	0.924	1.535-3
1.0	0.6477	1.086	-1.259	1.283	0.4210	0.421	1.279-3
2.0	0.6624	1.385	-0.330	0.906	0.2122	0.114	0.667-3
3.0	0.6834	2.039	-0.100	0.731	0.1362	0.035	0.259-3
4.0	0.7080	3.381	-0.032	0.636	0.0876	0.011	0.081-3

2.4 2D dipole equations

Generally in dipole approximation besides monopole component additional - dipole components are added. If however the interaction between dipole terms is neglected (monopole-dipole approximation) it is possible to derive a difference equation relative only to one - monopole component. Consider one of the forms of heterogeneous equations : for Φ variable (F^{xx}... are neglected) -

$$\varphi = Fw\varphi;\ \varphi \equiv C^{-1}\Phi;\ w = C^{-1}uC$$

$$\varphi \equiv \begin{bmatrix}\varphi^0\\ \varphi^x\\ \varphi^y\end{bmatrix} = \begin{bmatrix}F^{00} & F^{0x} & F^{0y}\\ F^{x0} & 0 & 0\\ F^{yo} & 0 & 0\end{bmatrix} \cdot \begin{bmatrix}w^0 & 0 & 0\\ 0 & w^1 & 0\\ 0 & 0 & w^1\end{bmatrix}\begin{bmatrix}\varphi^0\\ \varphi^x\\ \varphi^y\end{bmatrix} \qquad (2.4.1)$$

Rewrite the equation for each component:

$$\varphi^0 = F^{00}w^0\varphi^0 + F^{0x}w^1\varphi^x + F^{0y}w^1\varphi^y;$$
$$\varphi^x = F^{x0}w^0\varphi^0;\ \varphi^y = F^{y0}w^0\varphi^0; \qquad (2.4.2)$$

and put the values for φ^x, φ^y into the first equation:

$$\varphi = F^{00}w^0\varphi + F^{0x}w^1F^{x0}w^0\varphi + F^{0y}w^1F^{y0}w^0\varphi \qquad (2.4.3)$$

The terms $F^{x0}w^0\varphi^0$, $F^{y0}w^0\varphi^0$ can be estimated by taking a derivative of an approximate expression for φ^0:

$$\varphi^0 = F^{00}w^0\varphi^0 \qquad (2.4.4)$$

For a fixed **l** consider a sum:

$$\varphi_l^x = \sum_{k\notin U_l} F_{lk}^{x0}w_k^0\varphi_k^0 + \sum_{k\in U_l} F_{lk}^{x0}w_k^0\varphi_k^0 \qquad (2.4.5)$$

The set of indices $k\subset U_l$ is defined in a difference scheme. Green function G_l can be expressed as a derivative of G_0. Thus if instead of $\mathbf{r}_l$ an arbitrary point **r** is taken then

$$\partial F^{00}(\mathbf{r}-\mathbf{r}_k)/\partial x = F^{x0}(\mathbf{r}-\mathbf{r}_k) \qquad (2.4.6)$$

If $\mathbf{k}\notin U_l$ then approximately we have an equality:

$$F_{lk}^{x0} \approx \frac{1}{2\alpha\chi_j|\mathbf{e}_x|}(F_{l+e_x,k}^{00} - F_{l-e_x,k}^{00}) \qquad (2.4.7)$$

Therefore approximately:

$$\varphi_l^x = \sum_{k\subset U_l} (1/2\alpha k|\mathbf{e}_x|)(F_{l+e_x,k}^{00} - F_{l-e_x,k}^{00})w_k^0\varphi_k^0 + \sum_{k\subset U_x} F_{lk}^{x0}w^{k0}\varphi^{k0}$$

Expanding the first sum for all $\mathbf{k}$ and taking account of (2.4.4), the last equality can be written in the form:

$$\varphi_l^x = \partial_x \varphi_l^0 \qquad (2.4.8)$$

$$\partial_x: \varphi_l^0 \to (1/(2a\kappa|\mathbf{e}_x|)\cdot (\varphi^0_{l+e_x} - \varphi^0_{l-e_x}) +$$

$$\sum_{k\subset U_l}[F_{lk}^{x0} - \frac{1}{2a\kappa|\mathbf{e}_x|}(F^{00}_{l+e_x,k} - F^{00}_{l-e_x,k})]w_k^0\varphi_k^0$$

Operator ∂_x can be chosen from the condition of best presentation of F_{lk}^{x0} by a linear combination of the differencies (2.4.7) along different directions:

$$\partial_x \to \partial_x(\varepsilon)$$
$$\varepsilon = \{\varepsilon_i\}$$
$$\mathbf{e}_i\,(i = 1,\ldots,I)$$

If R_x^1, R_x^1 is the product of $P(\alpha,\beta)$ by F^{0x}, F^{0y} within U_l then we can derive an equation:

$$P\varphi^0 = R^0 w^0 \varphi^0 + (\mathbf{R}^1 w^1 \partial)\varphi^0 \qquad (2.4.9)$$
$$\mathbf{R}^1 \equiv (R_x^1, R_y^1); \partial \equiv (\partial_x, \partial_y)$$

2.5 Extention to 3 dimensions

For the case of axially nonuniform properties of channels take a Green function for point source:

$$G_0^j(|\mathbf{r}-\mathbf{r}_0|) = (1/4\pi D_G)C\mathcal{J}_0C^{-1}e_j \qquad (2.5.1)$$

function $\mathcal{J}_0$ depends on

$$(1/|\mathbf{r}-\mathbf{r}_0|)\exp(-\kappa_i|\mathbf{r}-\mathbf{r}_0|);\ \mathbf{r} = (x,y,z)$$

For the equation (one of the forms of heterogeneous equations)

$$\Phi = F\omega\Phi;\ \omega = C^{-1}uC \qquad (2.5.2)$$

matrix F depends on the elements

$$F_{lk}^j = (1/2|\mathbf{r}_l-\mathbf{r}_k|)\exp(-\kappa_i|\mathbf{r}_l-\mathbf{r}_k|)$$

Present the solution as finite expansion by trigonometric functions:

$$\Phi = \sum_{m=-M}^{m=M} \Phi_m \exp(i\alpha m z),\ \alpha = \pi/H; \qquad (2.5.3)$$

Multiplying the equation for Φ by exp(-iαnz) and taking the integral over z we have:

$$\Phi_n = \sum_{m=-M}^{m=M} \int \exp[-i\alpha n(z-z')]F(|\mathbf{r}-\mathbf{r}'|)\exp[i\alpha(n-m)z']\,\omega(z')dzdz'\Phi_m$$

Matrix element

$$F_{nn}^{j} = \sum_{m=-M}^{m=M} \int \exp[-i\alpha n(z-z')-\kappa_j(\rho^2+(z-z')^2)^{1/2}]dz/(\rho^2+(z-z')^2)^{1/2} = K_0(\rho(\kappa_j^2+\alpha^2n^2)^{1/2}) \quad (2.5.4)$$

($|\mathbf{r}-\mathbf{r}'|=(\rho^2+(z-z')^2)^{1/2}$) differs from the matrix element of axially uniform reactor by the change of argument:

$$\kappa_j^2 \rightarrow \kappa_{j,n}^2 = \kappa_j^2+\alpha^2n^2 \quad (2.5.5)$$

Thus the system of equations is obtained:

$$\Phi_n = \sum_{m=-M}^{m=M} F_{nn}\omega_{nm}\Phi_m; \quad (2.5.6)$$

where

$$\omega_{nm} \equiv \omega_{n-m} = \int \exp[i\alpha(n-m)z]\omega(z)dz$$

Since the solution is to be a real value the next equality is valid for complex conjugate (') value:

$$\Phi'_n = -\Phi_n,$$

so that

$$\Phi_{-n} = -\Phi_n\,,\ \Phi_0 = 0$$

and the above equation can be rewritten as follows:

$$\Phi_n = \sum_{m=1}^{M} F_{nn}(\omega_{nm} - \omega_{n,-m})\,\Phi_m$$

or

$$\Phi_{-n} = -\Phi_n = \sum_{m=1}^{M} F_{nn}(\omega_{-n,m} - \omega_{-n,-m})\,\Phi_m;$$

Subtracting equations one from another and changing the order of summation we get:

$$\Phi_n = F_{nn} \sum_{m=1}^{M} \omega_m^c(\Phi_{n-m} - \Phi_{m-n}); \quad (2.5.7)$$

where

$$\omega_m^c = \int_0^H \omega(z)\cos m\alpha z dz; \quad (2.5.8)$$

The indices m in the above sum have the limits:

$1 \le n-m \le M$; $1 \le m-n \le M$;

Since $1 \le n \le M$

and $\omega_m^c = \omega_{-m}^c$ it follows that m changes in the limits:

$$0 \le m \le 2M \ .$$

Thus though the dimension of equation is M^2, really the dimension of the problem is lower: matrix F consists only of diagonal elements and matrix elements ω_m^c for channel parameters are to be calculated for

$$0 \le m \le 2M;$$

The equation for 3 dimensions differs from the similiar equation for 2 dimensions by the dimension of the problem and by the arguments ($\kappa_{j,n}$) of matrix elements F_{nn} ; so transformation to a difference form is applicable in this case also , P and R operators depend now on arguments

$$z_{j,n}=a\,\kappa_{j,n};\ \ a \text{ - lattice pitch.}$$

2.6 3D dipole equations

A general few-group heterogeneous reactor equation formulation is used:

$$N' = (\upsilon + C\mathcal{J}C^{-1}\,\gamma_1')\,N'/k - C\mathcal{J}C^{-1}\,\gamma_2\,N' \qquad (2.6.1)$$

where

$N' = N/(1-\upsilon/k)$;
$\gamma_1' = CIC^{-1}\,\Lambda_1 + \gamma_2\upsilon$,
$\gamma_2 = CIC^{-1}\,\Lambda_2 - C\partial IC^{-1}$;

Matrices γ depend on GxG Λ-matrices of effective boundary conditions relating vector-flux to vector-current on a channel or cell boundary (of radius ρ) :

$$dN = \Lambda N\ ;\quad d \equiv \rho\, d/dr\,\big|_{r=\rho} \qquad (2.6.2)$$

$\rho = \{\rho_k\}$, ρ_k - radius of kth channel (or cell),

Taking account of azimuthal angle dependence of neutron flux near each channel surface one gets a dipole approximation with 3-component vector-flux on the surface of each channel : $N(N^0, \mathbf{N}^1)$, N^0 - scalar monopole component, $\mathbf{N}^1$ - 2-dimensional dipole component $\mathbf{N}^1 = (N^x, N^y)$.
Finite Furie expansion taking account of axial dependence

$N_g(r,z)=\sum_{m=1}^{M}\psi_{gm}(r)\,\mathrm{sinamz}$, $\alpha=\pi/H$; H - effective height,

leads symbolically to the same form of equations as above with $\mathcal{J}$, K , I, F depending on axial index m (and m-diagonal),ψ-HxGxKxM - vector, γ - (HxMxGxK) x (HxMxGxK) - **k**-diagonal matrix with Λ elements calculated as follows (2M+1 instead of MxM elements):

$$\Lambda^{0}_{mn}=\Lambda^{0C}_{m-n}-\Lambda^{0C}_{m+n}+\alpha^2n^2(\Lambda^{0C}_{z,m-n}-\Lambda^{0C}_{z,m+n}) \quad (2.6.3)$$

$$\Lambda^{1}_{mn}=\Lambda^{1C}_{m-n}-\Lambda^{1C}_{m+n}$$

$$\Lambda^{C}_{m}=(\alpha/\pi)\int_{o}^{\pi/\alpha}\Lambda(z)\cos\alpha mz\,dz\;;$$

K - number of channels in a regular lattice pointed by vectors $\mathbf{k}(k_1,k_2)$, G - number of groups, g = 1,..G, M -number of axial modes, H - number of asimuthal modes : H= 1 - monopole, H=3 - dipole.

Matrix $\mathcal{J}$ has a structure:

$$\mathcal{J}=K+IF; \quad (2.6.4)$$

$$K=\underset{g,m,k}{\mathrm{diag}}(K_0,K_1,K_1);\ I=\underset{g,m,k}{\mathrm{diag}}(I_0,I_1,I_1)$$

K_0,K_1,I_0,I_1 - modified Bessel functions, depending on arguments

$$\kappa_{g,m}\rho_k;\ \kappa_{g,m}^2=\xi_g+\alpha^2m^2$$

F - (HxGxMxK)x(HxGxMxK) h,g,m-diagonal matrix with zero elements on **k** - diagonal. Neglecting the interaction between dipole components we can write F - matrix in the next form:

$$F=\begin{pmatrix}F^{00} & F^{0x} & F^{0y}\\ F^{x0} & 0 & 0\\ F^{y0} & 0 & 0\end{pmatrix} \quad (2.6.5)$$

$$F^{00}=K_0;\quad F^{0x}=-K_1(c+\theta s);\quad F^{x0}=2K_1c;$$
$$F^{0y}=-K_1(\theta c+s);\quad F^{y0}=2K_1s;$$

$c=\cos(\chi_{lk})$; $s=\sin(\chi_{lk})$, χ_{lk} - the angle between $\mathbf{r}_{lk}$ and x-axis;

$$\theta=\begin{cases}0 & \text{for square,}\\ 1/2 & \text{for hexagonal lattice;}\end{cases}$$

Bessel function are defined for arguments $\kappa_{gm}r_{lk}$.

$$\Lambda=\underset{k}{\mathrm{diag}}\,\underset{h}{\mathrm{diag}}\,(\Lambda^0,\Lambda^1,\Lambda^1);\quad \gamma=\underset{k}{\mathrm{diag}}\,\underset{h}{\mathrm{diag}}\,(\gamma^0,\gamma^1,\gamma^1)$$

A difference form of heterogeneous reactor equation is derived as follows (first consider monopole approximation).

The elements F approximately obey the equation :

$$(-\Delta_l + \kappa_g{}^2\alpha^2)\, F^g_{kl} \cong 0 \qquad |\mathbf{k} - \mathbf{l}| > 1 \qquad (2.6.6)$$

$$\Delta_l : f_k \Rightarrow \sum_Q (f_{k+Qe1} - 4 f_k)$$

$\mathbf{e}_l = (1,0)$, Q rotates a vector on the angles 0 , 90 ,180 , 270 (for square lattice). After some transformations of equation (2.6.1) and change of variables, operating on both its sides by an operator $\wp(\alpha,\beta)$ with elements:

$$\wp_g : f_k \Rightarrow (-\alpha_1\Delta_1 - \alpha_2\Delta_2 - ... + \beta\kappa_g{}^2\alpha^2)\, f_k ; \sum \alpha_i = 1, \qquad (2.6.7)$$

with best fitted parameters α, β, which effectively eliminate F-matrix elements outside some fixed local set U_k of indices surrounding **k**, one obtains an approximate difference form of heterogeneous equation:

$$\wp\, \varphi = Q\, \gamma\, \varphi$$

In dipole approximation the equation can be presented as follows:

$$\begin{aligned}
\varphi^0 &= \upsilon/\kappa + (D^0 - \delta)\, \gamma^0 \varphi^0 + F'^{00}\, \gamma^0 \varphi^0 + F^{0x}\, \gamma^1 \varphi^x + F^{0y}\, \gamma^1 \varphi^y \\
\varphi^x &= D^1 \varphi^x + F^{x0}\, \gamma^0 \varphi^0 \\
\varphi^y &= D^1 \varphi^y + F^{y0}\, \gamma^0 \varphi^0
\end{aligned} \qquad (2.6.8)$$

$$\begin{aligned}
F'^{00} &= F^{00} + \delta ; \\
D^i &= I_i{}^{-1} K_i .
\end{aligned}$$

with $(-\Delta + \kappa^2)\, F^{0\,s}(\mathbf{r},\mathbf{r}_l) = 0 ;\ s = 0,x,y.$

On the basis of equations

$$F^{x0} = -(2\kappa^{-1}/(1-\theta^2))\, (\partial F^{00}(\mathbf{r},\mathbf{r}_l)/\partial x - \theta\, \partial F^{00}(\mathbf{r},\mathbf{r}_l)/\partial y)$$

$$F^{y0} = -(2\kappa^{-1}/(1-\theta^2))\, (\partial F^{00}(\mathbf{r},\mathbf{r}_l)/\partial y - \theta\, \partial F^{00}(\mathbf{r},\mathbf{r}_l)/\partial x)$$

$$\kappa \equiv \operatorname*{diag}_{g,m} \{\kappa_{g,m}\} \qquad (2.6.9)$$

introduce difference operators with approximate relations

$$\begin{aligned}
&\wp_0 F^{00'} = R^{00}; \\
&\wp_0 F^{0x} = R^{0x} ; \wp_0 F^{0y} = R^{0y} ; \\
&\wp_x F^{00'} = F^{x0} - R^{x0}; \wp_y F^{00'} = F^{y0} - R^{y0}.
\end{aligned} \qquad (2.6.10)$$

Use an approximate relation

$$\varphi^0 = \upsilon/\kappa + (D^0 - \delta)\, \gamma^0 \varphi^0 + F'^{00}\, \gamma^0 \varphi^0$$

to exclude F and F from the second and third equations of (2.6.8) by means the raslations (2.6.10).
Then we can get a difference equation:

$$\mathcal{P}\varphi = \mathcal{P}\upsilon/k\varphi + Q\gamma\varphi \; ; \qquad (2.6.11)$$
$$\varphi = (\varphi^0, \varphi^x, \varphi^y)$$

$$\mathcal{P} = \begin{matrix} \mathcal{P}_0 & 0 & 0 \\ -\mathcal{P}_x & E & 0 \\ -\mathcal{P}_y & 0 & E \end{matrix} \qquad Q = \begin{matrix} \mathcal{P}_0 D_0 + R^{00} & R^{x0} & R^{y0} \\ -\mathcal{P}_x D_0 + R^{x0} & D_1 & 0 \\ -\mathcal{P}_y D_0 + R^{y0} & 0 & D_1 \end{matrix}$$

with $\mathcal{P}$, Q - local (difference) operators depending on axial index m and group index g (and m,g-diagonal), γ - (HxMxGxK) x (HxMxGxK) - h, **k** - diagonal matrix (γ matrix is related now by simple transformations to the initial γ–matrix; $\gamma = (\gamma^0, \gamma^1, \gamma^1)$) , φ -HxGxKxM - vector; difference operators are defined by approximate relations (2.6.10).

2.7 The choice of difference equations parameters

a)Square lattice (9-point scheme)

Consider addition theorem for Bessel functions (see Fig. 2.2):

$$\exp(in\psi_1)K_n(a|\mathbf{r'}|) = \sum_{-\infty}^{\infty} I_m(a|\mathbf{r'} - \mathbf{r}|)K_{n+m}(a|\mathbf{r}|)\exp(im\psi_0) \quad (2.7.1)$$

Consider P^0-operator for 9-point scheme (square lattice).
Let **r** be some fixed vector
Take the next sums:

$$S_1^{00} = \sum_{j=1}^{4} K_0(\kappa r_{1j}'); \; S_2^{00} = \sum_{j=1}^{4} K_0(\kappa r_{2j}'); \qquad (2.7.2)$$

The sum S_1 is determined for channels at the distance a;
sum S_2 - for channels at the distance $\sqrt{2}a$;
$\mathbf{r}_{ij} = \mathbf{r} - a\mathbf{e}_{ij}$
where a - lattice pitch.
$\mathbf{e}_{ij}$ (i=1,2; j=1,2,3,4) -unit vectors with the angles (relative to x-axis):

$\chi_{ij} = (j-1)\pi/2 + (i-1)\pi/4$

By means of addition theorem for Bessel functions we have:

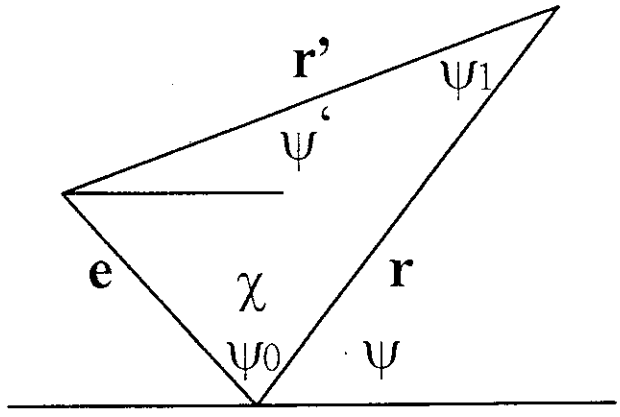


Fig. 2.2. Addition theorem for the choice of difference scheme parameters

$$K_0(\kappa r) = \sum_{m=-\infty}^{\infty} I_m(h) K_m(\kappa r) e^{im(\chi-\psi)} \qquad (2.7.3)$$

and the first sum can be presented as follows:

$$S_1^{00} = \sum_{m=-\infty}^{\infty} I_m(h) K_m(\kappa r) e^{-im\psi} \sum_{j=1}^{3} e^{i\frac{m\pi j}{2}} =$$

$$= 4 \sum_{m=-\infty}^{\infty} I_{4m}(h) K_{4m}(\kappa r) e^{-i4m\psi}.$$

or after summing the terms with positive and negative m
we get an expression (and a similar expression for the second sum):

$$S_1^{00} = 4I_0(h)K_0(\kappa r) + 8 \sum_{m=-\infty}^{\infty} I_{4m}(h) K_{4m}(\chi r) \cos 4m\psi.$$

$$S_2^{00} = 4I_0(\sqrt{2}h)K_0(\kappa r) + 8 \sum_{m=1}^{\infty} (-1)^m I_{4m}(\sqrt{2}h) K_{4m}(\kappa r) \cos 4m\psi.$$

Define the next sum:

$$S^{00} = S_1^{00} + \beta^0 S_2^{00} = 4[I_0(h) + \beta^0 I_0(\sqrt{2}h)]K_0(\kappa r) + \qquad (2.7.4)$$
$$+8\,[I_4(h) - \beta^0 I_4(\sqrt{2}h)]K_4(\kappa r)\cos 4\psi + 8 \sum_{m=1}^{\infty} [I_{4m}(h) + (-1)^m \beta^0 I_{4m}(\sqrt{2}h)]K_{4m}(\kappa r)\cos 4m\psi$$

Parameter β^0 can be chosen from the requirements to set the second term to zero:

$$\beta^0 = \frac{I_4(h)}{I_4(\sqrt{2}h)} \qquad (2.7.5)$$

Define the elements of operator P as follows (Fig. 2.3.):

$$P^0: P_0^0=4[I_0(h)+\beta^0 I_0(\sqrt{2}h)]; P_k^0 = -1; |\mathbf{k}|=1; P_k^0 = -\beta^0; |\mathbf{k}|=\sqrt{2}; \quad (2.7.6)$$

P_0^0; P_k^0 $|\mathbf{k}|=1; |\mathbf{k}|=\sqrt{2}$; - diagonal element of operator P and the elements for the first and second rows of channels around the central channel.

The product PF'^{00}_{0k} is by definition R^{00} -operator with the elements (δ-matrix elements are taken from the requirement to set parameters R_i^{00} equal zero):

$$R^{00}: R_0^{00}=P_0^0\delta- 4[K_0(h) +\beta^0 K_0(\sqrt{2}h)]; R_k^{00}=0, |\mathbf{k}|=1;$$
$$R_k^{00}= P_0^0 K_0(\sqrt{2}h)]-2[K_0(h)+ K_0(\sqrt{5}h)] -$$
$$- \beta^0[K_0(2\sqrt{2}h)+2 K_0(\sqrt{2}h)+\delta]; |\mathbf{k}|=\sqrt{2}; \qquad (2.7.7)$$
$$\delta=(P_0^0-2\beta^0)K_0(h)-2 K_0(\sqrt{2}h)-K_0(2h) -2\alpha K_0(\sqrt{5}h)$$

The error of difference transformation can be estimated as the difference

$$\varepsilon_k^{00} = P^0 F_{0k}^{oo} - S_1^{00} - \beta^o S_2^{00};$$
$$|\mathbf{k}| \geq 2$$

For small h this error is estimated from the expantion

$$I_m(x) \approx (x/2)^m/m!; K_m(x) \approx (1/2)(x/2)^{-m}(m-1)!; x<<1; \ m>1$$

as

$$|\varepsilon_k^{00}| \approx (5/7!)(h/2)^8 K_8(h|\mathbf{k}|)|\ \cos 8\psi_k\ | < (5/2)(1/|\mathbf{k}|^8)$$

For the other choice of the elements of operator P the above sum would include the terms with m<2 end the error would be larger. For large $|\mathbf{k}|$ the error can be evaluated from asymptotic expansion of Bessel functions:

$$|\varepsilon_k^{00}| \approx (5h^8/7!256)(\pi/2h|\mathbf{k}|)$$

and becomes worse for the other choice of β^0.
Maximal value - at $|\mathbf{k}| = 2$ (for 9-point scheme)

$$|\varepsilon^{00}|_{max}=(5/2^9)\approx 0.00977$$

For 5-point scheme ($\beta^0 =0, |\mathbf{k}|_{min}= \sqrt{2}$)
$|\varepsilon^{00}|_{max}=(1/\sqrt{2})^4= 1/4$

For mixed scheme (P - 5-points, R - 9 points):

$$|\varepsilon^{00}|_{max}=(1/2)^4= 0.0625$$

Now consider the product P^0F^{0x};

$$F^{0x}(o,\mathbf{r}) = -K_1(\kappa r)(x+\theta y)/r = -K_1(\kappa r)\cos\psi; \qquad (2.7.8)$$

Take the sums:

$$S_1^{0x} = \sum_{j=1}^{4} K_1(\kappa r_{1j}')\cos\psi'_{1j};\quad S_2^{0x} = \sum_{j=1}^{4} K_1(\kappa r_{2j}')\cos\psi'_{2j};$$

Taking account of addition theorem (the sum with n and -n) in the above equation

$$K_1(\kappa r') = (1/2)\sum_{m=-\infty}^{\infty} I_m(h)[K_{m-1}(\kappa r)\exp(-i(m-1)\psi) + K_{m+1}(\kappa r)\exp(-i)(m+1)\psi)]\exp(im\chi)$$

we get

$$S_1^{0x} = 4I_0(h)K_1(\kappa r)\cos\psi + 4\sum_{m=1}^{\infty} I_{4m}(h)[K_{4m-1}(\kappa r)\cos((4m-1)\psi) + K_{4m+1}(\kappa r)\cos((4m+1)\psi)]$$

Finally,

$$S^{0x} = S_1^{0x} + \beta^0 S_2^{0x} = 4[I_0(h) + \beta^0 I_0(\sqrt{2}h)]K_1(\kappa r)\cos\psi + +4\sum_{m=1}^{\infty} [I_{4m}(h) + (-1)^m \beta^0 I_{4m}(\sqrt{2}h)]$$
$$[K_{4m-1}(\kappa r)\cos((4m-1)\psi) + K_{4m+1}(\kappa r)\cos((4m+1))\psi] \qquad (2.7.9)$$

The error:

$$P^0 F_{0k}^{0x} = S^{0x} - P_0^0 K_0(h|\mathbf{k}|) = 4\sum_{m=1} [I_{4m}(h) + (-1)^m \beta^0 I_{4m}(\sqrt{2}h)]$$
$$[K_{4m-1}(\kappa r)\cos(4m-1)\psi + K_{4m+1}(\kappa r)\cos(4m+1)\psi]$$

Thus the above choice of P^0 suppress also two first terms in the expression for error $P^0 F_{0k}^{0x}$. For small h:

$$|\varepsilon_k^{0x}| = (40/8!)(h/2)^8 |K_7(h|\mathbf{k}|)\cos 7\psi_k + K_9(h|\mathbf{k}|)\cos 9\psi_k| \quad | < (20/h)(|\mathbf{k}|^9)[1 + k^2h^2/224]$$

and maximal error is:

$$|\varepsilon_k^{0x}| = (20/512)/h \approx 0.039/h.$$

The elements of R-operator also are inversely proportional to h.

Matrix R^{0x} for 9-point scheme , square lattice, is presented by the next formulas (Fig 2.3.):

$$\begin{aligned}
&R^{0x} : R^{0x}{}_0 = 0;\ R_k^{0x} = -r_1^{01}(\mathbf{k},\mathbf{e}_x);\ |\mathbf{k}| = 1 \\
&\qquad\qquad R^{0x} = -r_2^{01}(\mathbf{k},\mathbf{e}_x);\ |\mathbf{k}| = \sqrt{2} \\
&R^{0y} : R_0^{0y} = 0;\ R_k^{0y} = -r_1^{01}(\mathbf{k},\mathbf{e}_y);\ |\mathbf{k}| = 1 \qquad (2.7.10) \\
&\qquad\qquad R_k^{0y} = -r_2^{01}(\mathbf{k},\mathbf{e}_y);\ |\mathbf{k}| = \sqrt{2} \\
&r_1^{01} = P^0{}_0 K_1(h) - K_1(2h) - \sqrt{2}K_1(\sqrt{2}h) - (4\beta^0/\sqrt{5})K_1(\sqrt{5}h) \\
&r_2^{01} = (\sqrt{2}/2)P^0{}_0 K_1(h) - K_1(h) - (3/\sqrt{5})K_1(\sqrt{2}h) - \beta^0[K_1(2h) + \sqrt{2}/2K_1(2\sqrt{2}h)]
\end{aligned}$$

Now define operators P^x and P^y and their products with matrix elements F^{x0}

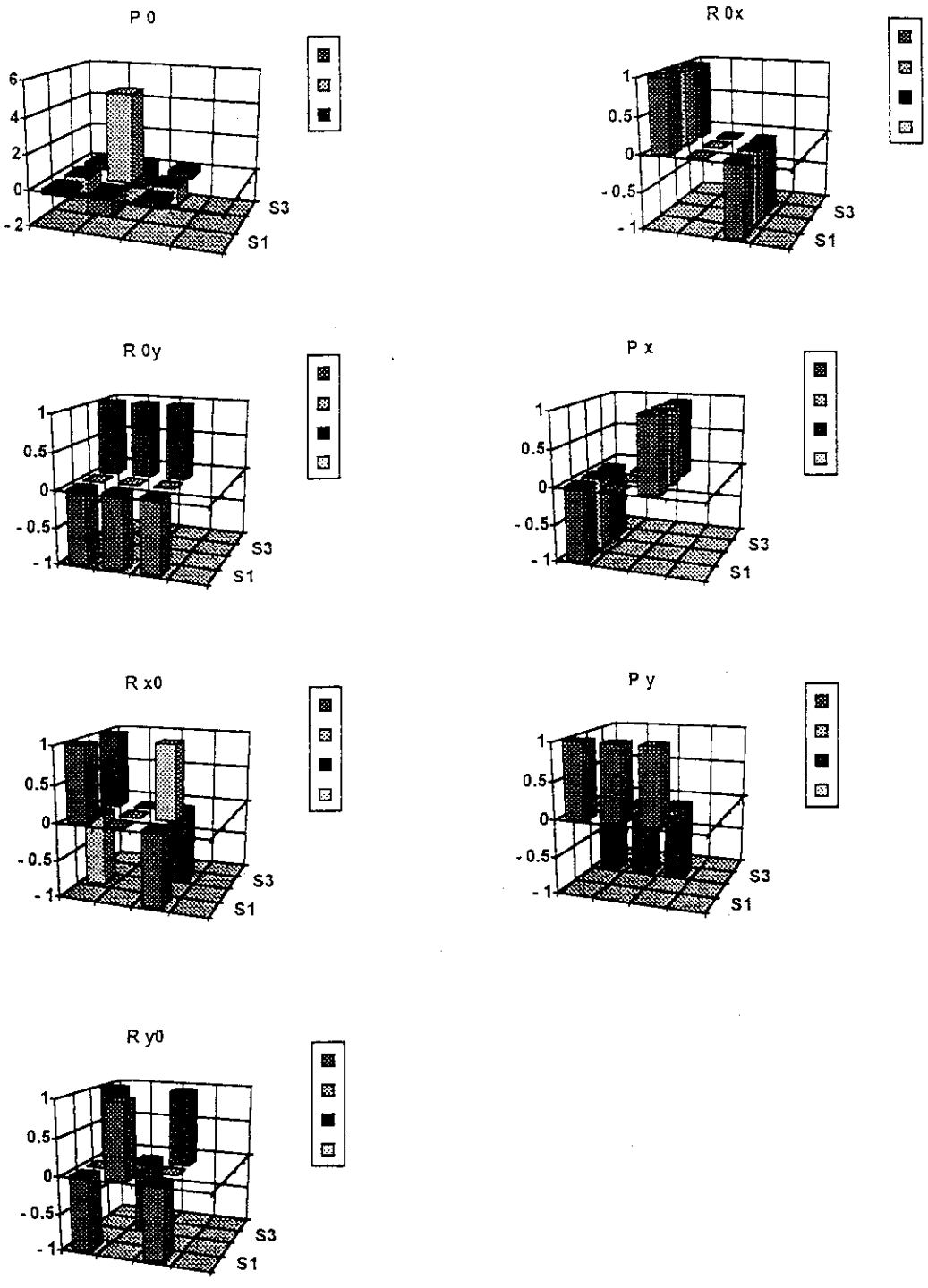


Fig. 2.3. The structure of difference operators square lattice, 9-point scheme

$F^{x0}(0,\mathbf{r}) = 2K_1(\kappa r)\cos\psi$, $F^{y0}(0,\mathbf{r}) = 2K_1(\kappa r)\sin\psi$, (2.7.11)
$\cos\psi = x/r$; $\sin\psi = y/r$.
For 9-point scheme introduce the sums:

$$S_1^{x0} = \sum_{j=1}^{4} K_0(\kappa r_{1j}')x'_{1j}/r'_{1j} = K_0(\kappa r'_{11}) - K_0(\kappa r'_{13});$$

$$S_2^{x0} = \sqrt{2}\sum_{j=1}^{4} K_1(\kappa r_{2j}')\, x'_{2j}/r'_{2j} = = \sum_{j=1}^{2} (-1)^{j-1}[K_0(\kappa r'_{2,j}) - K_0(\kappa r'_{2,j+2})]$$

Taking account of (2.7.3) we get

$$S_1^{x0} = \sum_{m=-\infty}^{\infty} I_m(h)K_m(\kappa r)\exp(-im\psi)[1-\exp(im\pi)] = 4\sum_{m=0}^{\infty} I_{2m+1}(h)K_{2m+1}(\kappa r)\cos((2m+1)\psi)$$

Similarly:

$$S_2^{x0} = \sum_{m=-\infty}^{\infty} I_m(\sqrt{2}h)K_m(\kappa r)\exp(-im\psi)[1-\exp(im\pi/2)] =$$
$$= 4\sum_{m=-\infty}^{\infty} (-1)^m I_{2m+1}(\sqrt{2}h)K_{2m+1}(\kappa r)\sin((2m+1)\pi/4)\exp((-i(2m+1)\psi) =$$
$$= 8\sum_{m=0}^{\infty} (-1)^m I_{2m+1}(\sqrt{2}h)K_{2m+1}(\kappa r)\sin((2m+1)\pi/4)\cos((2m+1)\psi) =$$
$$= 4\sqrt{2}\sum_{m=0}^{\infty} \mathrm{sig}(m)\, I_{2m+1}(\sqrt{2}h)K_{2m+1}(\kappa r)\cos((2m+1)\psi);$$

$\mathrm{sig}(m) = 1$, $m = 0,3,4,7,8....$
$\mathrm{sig}(m) = -1$, $m = 1,2,5,6,9,...$

Introduce the sum:

$$S^{x0} = S_1^{x0} + \beta^1 S_2^{x0} = 4[I_1(h) + \sqrt{2}\beta^1 I_1(\sqrt{2}h)]K_1(\kappa r)\cos\psi +$$
$$+4\,[I_3(h) - \sqrt{2}\beta^1 I_3(\sqrt{2}h)]K_3(\kappa r)\cos 3\psi + \qquad (2.7.12)$$
$$+4\sum_{m=2}^{\infty} [I_{2m+1}(h) + \sqrt{2}\,\mathrm{sig}(m)\beta^1 I_{2m+1}(\sqrt{2}h)]K_{2m+1}(\kappa r)\cos((2m+1)\psi)$$

The expression for S^{y0} differs by the change of cos by sin.
Take the next value for β^1:

$$\beta^1 = I_3(h)/\sqrt{2}I_3(\sqrt{2}h); \qquad (2.7.13)$$

The elements of P^x and P^y are defined by the next expressions:

P^x: $P^x_0 = 0$; $P_k^x = p^1 k_x$; $|\mathbf{k}| = 1$
$P_k^x = \beta^1 p^1 k_x$; $|\mathbf{k}| = \sqrt{2}$
P^y: $P^y_0 = 0$; $P_k^y = p^1 k_y$; $|\mathbf{k}| = 1$ (2.7.14)
$P_k^y = \beta^1 p^1 k_y$; $|\mathbf{k}| = \sqrt{2}$
$p^1 = 1/(2[I_1(h) + \sqrt{2}\beta^1 I_1(h))$;
R^{x0}: $R^{x0}_0 = 0$, $R_k^{x0} = r_1^{x0} k_x$; $|\mathbf{k}| = 1$
$R_k^{x0} = -r_2^{x0} k_x$; $|\mathbf{k}| = \sqrt{2}$

R^{y0}: $R^{y0}_0 = 0$, $R_k^{y0} = r_1^{y0} k_y$; $|\mathbf{k}| = 1$
$R_k^{y0} = -r_2^{y0} k_y$; $|\mathbf{k}| = \sqrt{2}$

$r_1^{10} = 2K_1(h) - p^1[\delta - K_0(\sqrt{2}h) + 2\beta^1(K_0(h) - K_0(\sqrt{3}h))]$

$r_2^{10} = -\sqrt{2}K(\sqrt{2}h) + p^1[K_0(h) - K_0(\sqrt{3}h) + \beta^1(\delta - K_0(2\sqrt{2}h))]$

b) Hexagonale lattice

For hexagonal lattice we take the next sum:

$$S^{00} = \sum_{j=1}^{6} K_0(\kappa r_j')$$

The sum S is determined for channels at the distance *a*:

$\mathbf{r}_j = \mathbf{r} - a\mathbf{e}_j$

where *a* - lattice pitch, $\mathbf{e}_j$ (j=1,2,3,4,5,6) unit vectors with the angles

$\chi_{ij} = (j-1)\pi/3$ (j=1,... 6)

By means of addition theorem:

$$S^{00} = 6I_0(h)K_0(\chi r) + 12\sum_{m=1}^{\infty} I_{6m}(h)K_{6m}(\chi r)\cos 6m\psi$$

The elements of P^0 are defined by equalities:

$$P^0: P_0^0 = 6I_0(h);\ P_k = -1,\ |\mathbf{k}| = 1; \qquad (2.7.15)$$

The elements of operator R are calculated as follows
(the elements of δ –matrix are chosen from the requirement
that R-matrix be diagonal):

$$R^{00}: R_0^0 = P_0^0\delta - 6K_0(h);\ R_k^0 = 0,\ |\mathbf{k}| = 1;$$
$$\delta = (P_0^0 - 2)K_0(h) - 2K_0(\sqrt{3}h) - K_0(2h); \qquad (2.7.16)$$

The error can be estimated as the maximum value of the sum for $|\mathbf{k}| > 1$:

$$\varepsilon_k^{00} = P^0 F_{0k}^{00} = -12\sum_{m=1}^{\infty} I_{6m}(h)K_{6m}(h|\mathbf{k}|)\cos 6m\psi_k$$

For small h (taking account the first term of series expansion -)

$$|\varepsilon_k^{00}| = (2/5!)(h/2)^6 K_6(h|\mathbf{k}|)|\cos 6\psi_k| < (1/|\mathbf{k}|^6)$$

and the maximum value is

$$|\varepsilon^{00}|_{max} = (1/\sqrt{3})^6 = 0.037$$

Direct calculation shows that for h= 0.1; 0.3; 1 the error is

0.0363, 0.0360 and 0.0325 correspondingly.
For the product P^0F^{0x},

$$F^{0x}(0,\mathbf{r})=-K_1(\kappa r)(x+\theta y)/r =-K_1(\kappa r)\cos\psi;$$

introduce the sums:

$$S^{0x}=6I_0(h)K_1(\kappa r)\cos\psi + 6\sum_{m=1}^{\infty} I_{6m}(h)\,[K_{6m-1}(h|\mathbf{k}|)\cos((6m-1)\psi_k)+$$
$$+K_{6m+1}(h|\mathbf{k}|)\cos(6m+1)\psi_k)]$$

Using the expression for P^0 we get the next formulas for R^{0x}, R^{0y}:

$$R^{0x}:\ R_0^{0x}=0;\ R_k^{0x}=-r^{01}(\mathbf{k},\mathbf{e}_x);|\mathbf{k}|=1;$$
$$R^{0y}:\ R_0^{0y}=0;\ R_k^{0x}=-r^{01}(\mathbf{k},\mathbf{e}_y);|\mathbf{k}|=1; \qquad (2.7.17)$$

$$r^{01}=(P_0^0-1)K_1(h)-\sqrt{3}K_1(\sqrt{3}h)$$
$$-K_1(2h);$$

The product P^xF^{x0} ; $F^{x0}=2K_1(\kappa r)x/r$; $F^{y0}=2K_1(\kappa r)y/r$;
is determined after introduction of the sum

$$S^{x0}=\sum_{j=1}^{6} K_0(hr'_j)=\sum_{j=1}^{2}(-1)^{j-1}[K_0(\kappa r'_{2j-1})-K_0(\kappa r'_{2j+1})]=4\sqrt{3}I_1(h)K_1(\kappa r)\sin(\pi/3-\psi)+$$
$$+4\sqrt{3}\sum_{m=2}^{\infty} sig1(m)I_{2m+1}(h)K_{2m+1}(\kappa r)\sin[(2m+1)(\pi/3-\psi)]$$

$$sig1(m)=\begin{cases}1, & m=3l;\\ 0, & m=3l+1;\\ -1, & m=3l+2;\end{cases}$$

Similar expression can be derived for S^{y0} with the change $\pi/3-\psi$ for ψ. Define

$$P^x:\ P_0^x=0;\ P_k^x=p^1k_x,\ |\mathbf{k}|=1; \qquad (2.7.18)$$
$$P^y:\ P_0^y=0;\ P_k^y=p^1k_y,\ |\mathbf{k}|=1;$$
$$p^1=1/(3I_1(h));$$

Then

$$R^{x0}:\ R_0^{x0}=0;\ R_k^{x0}=-r^{10}k_x;\ |\mathbf{k}|=1; \qquad (2.7.19)$$
$$R^{y0}:\ R_0^{y0}=0;\ R_k^{y0}=-r^{10}k_y;\ |\mathbf{k}|=1;$$

$$r^{10}=-2K_1(h)+p^1[\delta+K_0(h)-$$
$$-K_0(\sqrt{3}h)-K_0(2h)];$$

3. Heterogeneous Characteristics of a Reactor Cell

3.1 Space-energy distribution of neutrons in a reactor cell

a)Solution of one-group equation

One -group integral neutron transport equation is used for determination of neutron flux distribution:

$$N(\mathbf{r}) = \int K(\mathbf{r},\mathbf{r}')(\Sigma_s N + Q)(\mathbf{r}')d\mathbf{r}$$
$$K(\mathbf{r},\mathbf{r}') = \exp(-s(\mathbf{r},\mathbf{r}'))/4\pi R^2; \qquad (3.1a.1)$$
$$R = |\mathbf{r}-\mathbf{r}'|$$

$N(\mathbf{r})$ - neutron flux , integrated over angles; $N(\mathbf{r})=\int N(\mathbf{r},\mu)d\mu$;
Q - neutron source (isotropic), Σ - total macroscopic cross-section,
Σ_s - scattering macroscopic cross-section, $s(\mathbf{r},\mathbf{r}')$ - optical length.
Consider a multi-layer cylindrical cell of infinite height, surrounded by infinite scattering media with zero absorption cross-section (returning neutrons have isotropic angular distribution). The cell is subdivided by M thin layers, in every layer neutron fluxN is supposed to be constant. After the change of variables (to the density of neutron emission):

$$\Phi = \Sigma N + Q \qquad (3.1a.2)$$

the integral equation transforms to the next:

$$\Phi(\mathbf{r}) = \Sigma_s(\mathbf{r})\int K(\mathbf{r},\mathbf{r}')\Phi(\mathbf{r}')d\mathbf{r}' + Q(\mathbf{r}); \qquad (3.1a.3)$$

$$\Phi_i = (\Sigma_{si}/\Sigma_i V_i)\sum_j P_{ij}V_j\Phi_j + Q_i; i = 1,\ldots,M = 1,$$

Φ_i - mean value :

$$\Phi_i = (1/V_i)\int_{V_i}\Phi(\mathbf{r})d\mathbf{r}$$

Collision probability is defined by an integral:

$$P_{ij} = \int_{V_i} d\mathbf{r}\int_{V_j} d\mathbf{r}'\,\Sigma_i K(\mathbf{r},\mathbf{r}')/V_j \qquad (3.1a.4)$$

The probability of collision in all the volume is 1:

$$\int \Sigma(\mathbf{r})K(\mathbf{r},\mathbf{r}')d\mathbf{r} = \qquad (3.1a.5)$$

that leads to the balance equation:

$$\sum_i P_{ij} = 1; \qquad (3.1a.6)$$

The symmetry of the kernel $K(\mathbf{r},\mathbf{r}')$ leads to the symmetry relation:

$$P_{ij} V_j \Sigma_j = P_{ji} V_i \Sigma_i \qquad (3.1a.7)$$

The two above relations allow to exclude the variable in the last scattering infinite layer:

$$\Phi_i = (\Sigma_{si} / \Sigma_i V_i) \sum_{j=1}^{M} P'_{ij} V_j \Phi_j + Q_i, i = 1,\ldots,M, \qquad (3.1a.8)$$

$$P'_{ij} = P_{ij} + \frac{P_{M+1,i} \Sigma_i V_i P_{M+1,j}}{\sum_{k=1}^{M} P_{M+1,k} V_k \Sigma_k} \theta \qquad (3.1a.9)$$

is a collision probability taking account of neutrons returning from outer scattering region. Parameter θ is introduced for simulation of some albedo conditions (non zero current) on the boundary of the cell.

Calculation of the probabilities.

For an arbitrary unit vector μ its projection on a given plane Π is chosen along y-axis, and x - axis is orthogonal to y. The volume of a flat figure can be written as an integral

$$V = \int dx \int_{s_1(x)}^{s_2(x)} dy \qquad (3.1a.10)$$

with $s_1(x)$, $s_2(x)$ - coordinates of intersection of a straight line parallel to y-axis (Fig.3.1).

The above integral can be written for any direction, so that

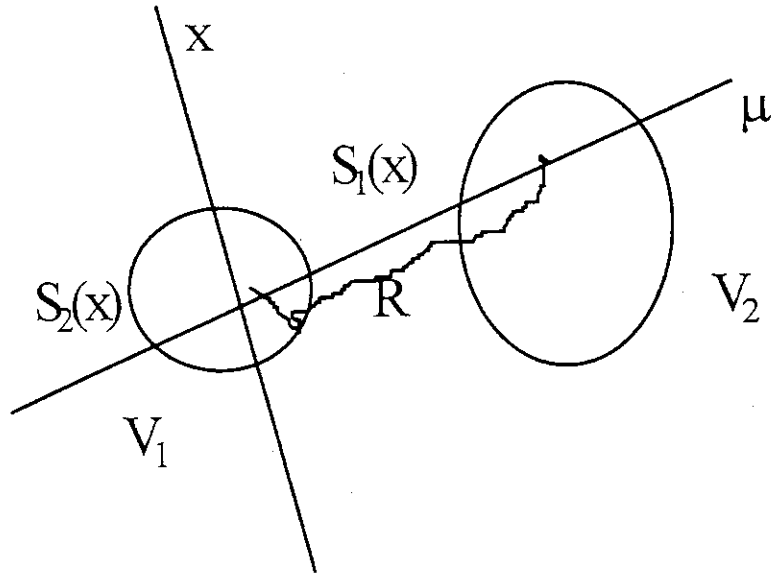


Fig. 3.1. Integrals over V_1 and V_2

$$4\pi V=\int d\mu\int dV = \int d\mu\int dx \int_{s_1(x)}^{s} dy \qquad (3.1a.11)$$

For 2 figures having projections V_1 ,V_2 on Π the integral over two volumes can be presented by an expression:

$$\int dV_2\int dV_1=\int R^2dRd\mu\int dx \int_{s_1(x)}^{s_2(x)} dy \qquad (3.1a.12)$$

For collision probabilities it is necessary to calculate the integral:

$$J=(1/4\pi)\int dR\ \exp(-s(\mathbf{r},\mathbf{r}'))d\mu\int dx \int_{0}^{s_2(x,\mu)-s_1(x,\mu)} du$$

After separation of the parts of the optical lengths in layers i and j:

$$\exp[-s(\mathbf{r},\mathbf{r}')] = \exp(-\Sigma_i R)\exp(-u\Sigma_j / \sin\vartheta)\ \exp(-L_{i-1,j} / \sin\vartheta), \qquad (3.1a.13)$$

the integral J can be presented as a sum:

$$J = (2 / \Sigma_i\Sigma_j)(C_{i,j-1} - C_{i,j} - C_{i-1,j-1} + C_{i-1,j}) \qquad (3.1a.14)$$

where

$$C_{lk}=(1/8\pi)\int \exp(-L_{lk}/\sin\theta)\sin^2\theta d\theta\, d\varphi dx \qquad (3.1a.15)$$

$(d\mu=\sin\theta d\theta d\varphi)$

For cylindrically symmetric regions the integrals do not depend on φ (Fig. 3.2):

$$C_{lk}=(1/8\pi)\int [\exp(-(L_l-L_k)/\sin\theta)- \exp(-(L_l+L_k)/\sin\theta)]\sin^2\theta d\theta \quad (1a.16)$$

By definition of Bicley functions

$$Ki_n(z)=\int_0^{\pi/2} \sin^{n-1}\theta\exp(-z/\sin\theta)d\theta \qquad (3.1a.17)$$

the next formula can be used for collision probabilities :

$$P_{ij} = (2 / \Sigma_j V_j)(C_{i,j-1} - C_{i,j} - C_{i-1,j-1} + C_{i-1,j}), \qquad (3.1a.18)$$

$$C_{lk} = \int_0^{\rho_k} (Ki_3(L_l - L_k) - Ki_3(L_l + L_k))dx \qquad (3.1a.19)$$

where L_l - optical distance from x-axis to the intersection with the circle of radius ρ_l. For integration within a given physical region laying within radii (R_{m-1},R_m) a quadrature formula may be used with a change of variables

$$x = R_m - (R_m - R_{m-1})t^2, t \in [0,1]; \qquad (3.1a.20)$$

$$\int_{R_{m-1}}^{R_m} dx(\cdot) = 2(R_m - R_{m-1})\int_0^1 tdt(\cdot) \qquad (3.1a.21)$$

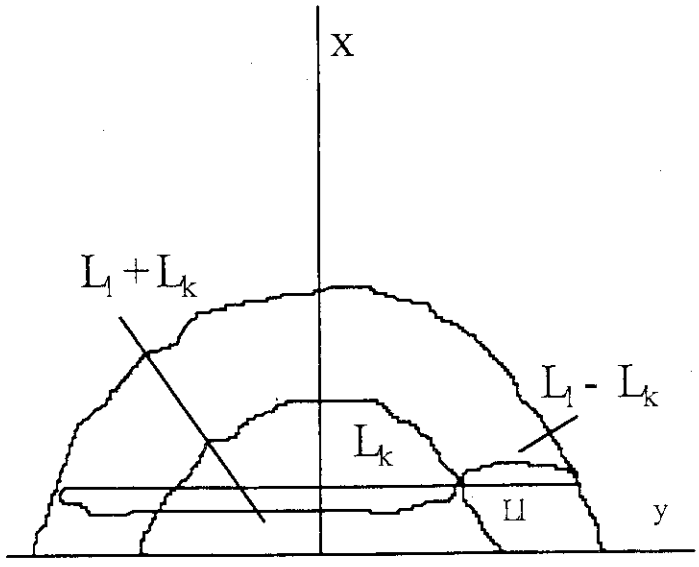


Fig. 3.2. Optical lengths in a cylindrical cell

Modified collision probabilities for axial migration of neutrons

One group migration area of neutrons in axial direction can be calculated by a formula

$$L^2_z \sim (1/2)\Sigma\, \Sigma P^z_{ij} \,(\,\Sigma_s N_0 + q)_j \,/ < \Sigma_a N_0 V >, \qquad (3.1a.22)$$

$$< \Sigma_a N_0 V > = \int_{V_{cell}} \Sigma_a(\rho)\, N\,(\rho)\, d\rho$$

with modified "collision probabilities":

$$P^z_{ij} \equiv P^z_{ij}\, V_j = \Sigma_i/4\pi \int_{V_i} dr \int_{V_j} d\rho \mu^2_z \exp(-\Sigma R) \qquad (3.1a.23)$$

(μ_z - projection of a unit vector in the direction of neutron movement to the axis z), having symmetry relations

$$\Sigma_j P^z_{ij} = \Sigma_i P^z_{ji} \qquad (3.1a.24)$$

These probabilities are determined by integrals:

$$P^z_{ij} = \Sigma_i/4\pi \int dS dx \int R^2\, dR d\mu \mu_z^2 \exp(-\Sigma R) \qquad (3.1a.25)$$

$$P^z_{ij} = T^{ij}_{i-1,j} - T^{ij}_{ij} - T^{ij}_{i-1,j-1} + T^{ij}_{i,j-} \qquad (3.1a.26)$$

where $T_{lk}^{ij} = \Sigma\ a_m^{ij}\ b_m^{lk}$, $l = i-1,i$; $k = j-1,j$; $a_1^{ij} = 2(l_i^2 + l_j^2 + l_i l_j)l_j$;

$a_2^{ij} = 2(l_i + l_j)l_j$; $a_3^{ij} = l_j$; $b_m^{lk} = 2\int_0^{\rho_k} dx(f_m^{lk,-} - f_m^{lk,+})$;

$f_1 = Ki_3(L) - Ki_5(L)$; $f_2 = [Ki_2(L) - Ki_4(L)]Z$; $f_3 = [Ki_1(L) - Ki_3(L)]\ Z^2$ (1a.27)

l_i - mean free path in region i, L - optical length, Z - geometrical length;

the signs +,- mean that lengths are summed or subtracted :

$L = L_l \pm L_k$; L_l - the optical distance from x-axis to the surface with number l.

For uniform media

$$\Sigma\ P^z_{ij} = 2/3\ V_j\ l_j^2 \qquad (3.1a.27)$$

and the diagonal element is equal

$$P^z_{jj} = (2/3)\ V_j l^2_j - P^z_{j-1,j} - P^z_{j+1,j} \qquad (3.1a.28)$$

$$\text{or} \quad P^z_{ij} = (2/3)\ V_j l^2_j + 2T^{ij}_{j-1,j-1} - T^{ij}_{j,j} - T^{ij}_{j-1,j-} ; \qquad (3.1a.29)$$

this formula remains valid and for the case of different properties in neighbor regions. The sum is transformed as follows:

$$P^z_j = \Sigma\Sigma\ a^{ij}_m\ (b_m^{i-1,j} - b_m^{i,j} - b_m^{i-1,j-1} + b_m^{i,j-1}) =$$

$$= \Sigma\Sigma\ c^{ij}_m\ (b_m^{i,j} - b_m^{i,j-1}), \qquad (3.1a.30)$$

where

$c_1^{ij} = a_1^{i+1,j} - a_1^{i,j} = 2(l_{i+1} - l_i)(l_{i+1} + l_i + l_j)\ l_j$; $c_2^{i,j} = a_2^{i+1,j} - a_2^{i,j} = 2(l_{i+1} - l_i)l_j$;

$$c_3^{i,j} = a_3^{i+1,j} - a_3^{i,j} = (1 - 1)l_j = 0. \qquad (3.1a.31)$$

$$P^z_j = \Sigma\ \Sigma\ c_m^{I,j}\ (b_m^{I,j} - b_m^{I,j-1}) + (2/3)\ V_j\ l_j^2 \qquad (3.1a.32)$$

Modified "collision probabilities" are used for determination of axial component Λ^z of (G×G) matrix Λ (section 3.3c).

b)multi-group calculations

For the calculation of heterogeneous reactor cell characteristics a detailed space-energy neutron distribution in a multi-region reactor cell must be found, generally with nuclear chain transformation simulation depending on time variable.

Thus the solution may depend on 3 variables: space - energy -time.

A library of microscopic nuclear data can include:

- multi-group microscopic cross sections,
- parameters of resonances and effective resonances.
- scattering matrices for neutron thermalization.

The data for chain transformations (channels for capture, fissions, decay, (n,2n) reactions) are (and may be) included in the library.

It is desirable that input data include only data for geometry and isotope (nuclear densities) composition (initial for the case of time simulation), power and time points of burnup calculations.

The results of calculations include :

- space energy distribution of neutron flux (depending on time if necessary),
- reaction rates for nuclides in all physical regions,
- multiplication factor,
- few-group cross-sections,
- monopole and dipole (axial and radial) few-group Λ-matrices,
- reaction rate R-matrices or vectors.

The latter data can be used as an input for 2 or 3-dimensional heterogeneous reactor calculations and stored in some exchange files.

Calculation of space-energy neutron flux distribution in a reactor cell

Neutron transport in every group can be evaluated by collision probability method in the solution of a multigroup system of integral neutron transport equations:

$$\Phi^i(r)=\int K^i(r,r'')(\Sigma_s^i\Phi^i+Q^i)(r'')dr'' \qquad (3.1b.1)$$

The source of neutrons Q in every group i in epithermal region consists of two parts:

$$Q^i=Q_s^i+Q_f^i, \qquad Q_s^i=\sum_{j<i}\Sigma^{ij}\Phi^j \qquad (3.1b.2)$$

Q_s^i is due to neutrons scattered from upper groups, i,j=1,2,....

Φ^j - neutron flux in group j; Σ^{ij} - macroscopic scattering cross-section from group j to group i. The source

$$Q_f^i=\theta^i S(r); \qquad (3.1b.3)$$

$$S(r)=\sum_j \nu^j\Sigma_f^j\Phi^j(r); \qquad (3.1b.4)$$

is due to fissions with the normalization:

$$\sum_j \theta^j = 1; \int S(r)dV = 1; \qquad (3.1b.5)$$

Σ_f^j, ν^j - macroscopic fission cross-section and the number of secondary neutrons per fission. The distribution of θ corresponds to fission spectrum.

Thus it is supposed that due to fissions 1 neutron appears in the cell having fission spectrum distribution and some space distribution S(r); the last can estimated according to a pre-calculated distribution of fissions by thermal neutrons. This is a weak supposition since fast neutrons have large mean free paths comparative to cell dimensions, the solution weakly depends on their space distribution and can be improved by iteration procedure.

Energy distribution can be based on multi-group approximation. A library has a fixed group structure. When resonance absorption calculation is included a special subdivision of energy scale allows an effective direct treatment of resonances for prescribed nuclei . In this case lethargy scale is transformed to include a larger number of intervals. Resonance parameters for chosen isotopes are used for calculation of group cross-section for transformed lethargy scale. If both energy intervals i and j lay in the basic library scale, scattering cross-sections are taken from this library; if at least one of these intervals is subdivided for resonance absorption description, then the model of scattering by free atoms is used with the probabilities

$$p_{j\leftarrow i}$$

of elastic scattering from group i to group j , defined by the following set of expressions (A - atomic mass of a nucleus):

(the probabilities are defined by integrals
$(1/(1-\alpha))\int du \int du'\ \exp(-(u-u'))$
over Δu_i and Δu_j ; $u' \in (u-\varepsilon, u)$)
$\alpha=(A-1)^2/(A+1)^2$; $\varepsilon = \ln(1/\alpha)$;

(3.1b.6)

$$p_{j\leftarrow i} = \left[\frac{1}{\Delta u_i}\frac{1}{(1-\alpha)}\left[e^{-(u_j^- - u_i^+)} - e^{-(u_j^- - u_i^-)} - e^{-(u_j^+ - u_i^+)} + e^{-(u_j^+ - u_i^-)}\right]\right], \qquad \varepsilon \geq u_j^+ - u$$

$$p_{j\leftarrow i} = \frac{1}{\Delta u_i}\frac{1}{(1-\alpha)}\left[e^{-(u_j^- - u_i^+)} - e^{-a} - e^{-\varepsilon}(a - u_j^- + u_i^+)\right], \qquad a = \min(\varepsilon, u_j^- - u_i^-, u_j^+ - u_i^+),\ u_j^- - u_i^+ < \varepsilon < u_j^+ - u_i^+ \text{ or } u_j^+ - u_i^+ < \varepsilon < u_j^- - u_i^-;$$

$$p_{j\leftarrow i} = \frac{1}{\Delta u_i}\frac{1}{(1-\alpha)}\left[e^{-(u_j^- - u_i^+)} - e^{-(u_j^- - u_i^-)} - e^{-(u_j^+ - u_i^+)} + e^{-\varepsilon}(1 - u_j^+ + u_i^- + \varepsilon)\right], \qquad u_j^- - u_i^- < \varepsilon, u_j^+ - u_i^+ < \varepsilon < u_j^+ - u_i^-; \varepsilon < u_j^- - u_i^+$$

Reaction rates and neutron balance

For every isotope k in every region l with nuclear concentration c_{kl}, capture, fission and multiplication rates are to be calculated:

$$C_{kl}^{i} = V\sigma_k c_{kl} \sum_{j=1}^{i} \Phi_k^j \sigma_{cl}^j;$$
$$F_{kl}^{i} = V_k c_{kl} \sum_{j=1}^{i} \Phi_k^j \sigma_{fl}^j; \qquad (3.1b.7)$$
$$\nu F_{kl}^{i} = V_k c_{kl} \sum_{j=1}^{i} \Phi_k^j (\nu\sigma)_{fl}^j;$$

and the current along energy axis:

$$\varepsilon_k^i = V_k \sum_{l\le j\le i} \sum_{m>i} \Sigma_k^{j\to m} \Phi_k^j; \qquad (3.1b.8)$$

their total values for the cell:

$$C^i, F^i, \nu F^i, \varepsilon^i \qquad (3.1b.9)$$

and total current of neutrons (from the first group to the given energy, defined by lower boundary of group i) across the cell boundary: J^i.

For all the groups below the lower boundary of fission spectrum the next balance equation is valid:

$$C^i + F^i + \varepsilon^i + J^i = 1; \qquad (3.1b.10)$$

(the sum in the left part of above equation can be different from 1 due to (n,2n) reactions).

For zero current across the cell boundary full number of neutrons reactions by capture and fission is equal to unity:

$$C + F \ (+J) = 1. \qquad (3.1b.11)$$

and by definition multiplication factor in both cases (zero or non zero current across boundary) is equal:

$$k_{eff} = \nu F; \qquad (3.1b.12)$$
$$k_{eff} = k_\infty$$

- infinite multiplication factor if the current J across cell boundary is equal zero.

c) thermal neutrons
(thermalization problem)

Space -energy distribution of thermal neutrons (for example in the energy interval from 0 to 0.465 eV or 1 eV) in a reactor cell depends on up and down scattering of neutrons by chemically bounded nucleus. Some models for scattering of neutrons can be used.
Space-energy distribution of thermal neutrons in a multi-region cylindrical reactor cell is the solution of the equation:

$$\Sigma_t(v,r) = 2\pi \int_0^R r'\,dr'\,S(r'|r,v) \qquad (3.1c.1)$$

$$P(r'|r,v)$$

$$(r',v) = \int_0^{v_{max}} dv'\,\Phi(v',r')\Sigma_s(v'|v,r') + \qquad (3.1c.2)$$

$$+S^F(v,r')$$

v -relative neutron velocity, v_{max} -its upper boundary, r - radial coordinate, R - cell radius
$P(r'|r,v)$ - space kernel normalized to 1:

$$2\pi \int_0^R rdr\,P(r'|r,v)=1 \qquad (3.1c.3)$$

$\Sigma_s(v'|v,r)$ – - scattering cross-section with the normalization

$$\int_0^{v_{max}} dv\Sigma_s(v'|v,r) = \Sigma_s(v',r) \qquad (3.1c.4)$$

S (v,r) - external source due to slowing down of epithermal neutrons.
Piece-wise representation of equation.
For M groups and N radial rings piece-wise representation of equations is as follows:

$$\varphi(l,j) = \sum_{i=1}^{N} S(i,l)P(i|j,l)$$

$$(i,l) = \sum_{m=1}^{M} \varphi(m,i)H(m|l,i) +$$

$$+S(l,i)$$

$$\varphi(l,j) = \Sigma_t(l,j)\Phi(l,j)\Delta v_l \Delta r_j \qquad (3.1c.5)$$

$\varphi(l,j)$ - collision density

$$H(m|l,i) = \Sigma_s(m|l,i) / \Sigma_t(m,i);$$

$$\Sigma_s(m|l,i) = (1/\Delta v_m) \int_{\Delta v_l} dv \int_{\Delta v_m} dv'\,\Sigma_s(v'|v,r_i) \qquad (3.1c.6)$$

-scattering matrix with normalization:

$$\sum_{l=1}^{M} \Sigma_s(m|l,i) = \Sigma_s(m|i);$$

$$s(l,i) = \Delta r_i \int_{\Delta v_i} dvs(v,r_i); \qquad (3.1c.7)$$

- external source due to slowed-down neutrons.

$H(m|l,i)$ – the probability of scattering to group l for a neutron having a collision in group m.

Scattering matrices

Next models are used for scattering cross-sections:
1. diagonal
2. free gas
3. Brown-Saint-Johns
4. Nelkin
5. Koppel-Yong
All the models obey detailed equilibrium condition with (M(v) - Maxvelian spectrum):

$$M(v)\sigma_s(v|v') = M(v')\sigma_s(v'|v);$$
$$M(v) = (2v^3 / v_T^4)\exp(-v^2 / v_T^2), \qquad (3.1c.8)$$
$$v_T^2 = T / 293;$$

so that calculations are to be done only for indices $m \le l$.

1. *Diagonal model*

(applicable for heavy elements without transition of neutrons from group to group)

$$\sigma_s(m|l) = \sigma_s(m)\delta_{ml} \qquad (3.1c.9)$$

δ_{ml} – Kronecker delta-function

2. *Free gas model*

Chemical binds are neglected. The formulas are as follows:

$$\sigma_s(v'|v) = \sigma_s^0\theta^2 m(v / v'^2)[\mathrm{derf}(\beta\theta v - \beta\varsigma$$
$$\mathrm{derf}(\beta\theta v + \beta\varsigma v', -\beta\theta v' - \beta\varsigma v)], v' > v$$

$$\sigma_s(v) = \sigma_s^0\{(1/\sqrt{\pi}\beta v)\exp(-\beta^2 v^2) +$$
$$(1 + 1/(2\beta^2 v^2))[1 - \exp(-\beta^2 v^2)\cdot \qquad (3.1c.10)$$
$$\mathrm{erf1}(\beta v)]\};$$
$$\sigma_s^0 = \lim_{v\to\infty}\sigma_s(v);$$

m- atomic mass of scattering nucleus;

$$\theta=(m+1)/(2m),\ \varsigma=(m-1)/2m;\ \beta^2 = mT_0/T;\ T_0\ T=293\ K, \qquad (3.1c.11)$$

T - media temperature,

$$\begin{aligned}&\mathrm{derf}(x,y) = \mathrm{sign}(x) - \exp(-x^2)\cdot\\&[\mathrm{erf1}(x) + \mathrm{erf1}(y)];\\&\mathrm{erf1}:\\&\mathrm{erf}(x) = 1 - \exp(-x^2)\mathrm{erf1}(x), x \geq 0\end{aligned} \qquad (3.1c.12)$$

erf - probability function.

3.Brown-Sent-Johnce model

In the center of mass system the scattering cross-section is as follows:

$\sigma_s(v_r) = \sigma_s^0 + B\exp(-Kv_r^2)$;
v_r - relative neutron velocity, B,K - empirical constants.
The next expression is used for scattering cross-section

$$\begin{aligned}&{}_s(v,v') = \sigma_s^{FG}(v,v') + B\theta m(v / v'^2)\times\\&(\tau^3/(1+m(1-\tau^2))\exp(-k\tau^2 v'^2)\times\\&\mathrm{derf}(\beta\theta' v - \beta\zeta' v', \beta\theta' v' - \beta\zeta' v) +\\&\mathrm{derf}(\beta\theta' v + \beta\zeta' v', -\beta\theta' v' - \beta\zeta' v)], v' > v\end{aligned} \qquad (3.1c.13)$$

$$\begin{aligned}&\sigma_s(v) = \sigma_s^{FG}(v) + B\tau^3\{(\tau/\pi^{1/2}\,\beta v)\exp(-\beta^2v^2) + (\tau^2 + 1/(2\beta^2v^2))\times\\&[\exp(-k\tau^2v^2) - \exp(-\beta^2v^2)\mathrm{erf1}(\tau\beta v)]\};\quad \tau^2 = \beta^2/(\beta^2+K);\\&\theta' = \theta/\tau;\quad \zeta' = \tau\zeta - (1-\tau^2)\theta/\tau;\end{aligned} \qquad (3.1c.14)$$

4. Nelkin model

Based on quantum-mechanic model for H_2O by Nelkin, parameters for D_2O - by Honeck, simplified version of the next model.

5.Koppel-Yong model

Double - differential cross-section is calculated as follows:

$$\sigma_s(E' \to E, \mu) = (\sigma_b/4\pi)(E/E')^{1/2}\int dv f(v^2), \qquad (3.1c.15)$$

where

$$f(v^2) = (1/(4\pi\lambda\xi E''))^{1/2}\sum_{m=0}^{2}(1/m)(\xi/\alpha)^m \sum_{n=-\infty}^{\infty} I_n(\xi/B)\times$$
$$\exp[-\xi/A + n\omega/2kT - (E - E' + n\omega + m\alpha/\beta + \lambda\xi)^2/4\lambda\xi E''] \qquad (3.1c.16)$$

$\sigma_b = \sigma_s^0(m+1)^2/m^2$- scattering cross-section of a binded nuclei, μ– mean cosines of scattering in a laboratory system of coordinates
$\xi = E' + E - 2\mu(E'E)^{1/2}$ - square of momentum change, E eV; $I_n(x)$ - Bessel function.

For $|E' - E| \leq E_1$:

$\lambda = \lambda_T$,
$E'' = kT$, T - media temperature K,

$$A = [\lambda_1/\omega_1 + \lambda_2/\omega_2 + \lambda_3/\omega_3 + (\lambda_r/\omega_r)\mathrm{cth}(\omega_r/2kT)]^{-1}; \qquad (3.1c.17)$$

$B = (\lambda_r/\omega_r)\mathrm{sh}(\omega_r/2kT)$, $\omega = \omega_r$, $\beta = 1/\lambda_1$, $\alpha/\beta = \omega_1$;

For $|E'-E|>E_1$:

$\lambda=\lambda_T+\lambda_r$; $E''=(\lambda_t kT+\lambda_r E_r)/\lambda$, $E_r''=\omega_r\{1/[\exp(\omega_r/kT)-1]+1/2\}$,(3.1c.18)
$A=[\lambda_2/\omega_2+\lambda_3/\omega_3+(\lambda_1/\omega_1)\mathrm{cth}(\omega_1/2kT)]^{-1}$; $B=(\lambda_1/\omega_1)\mathrm{sh}(\omega_1/2kT)$,
$\omega=\omega_1$, $\beta=1/(\lambda_2+\lambda_3)$, $\alpha/\beta=\omega_2=\omega_3$;

λ_r, $\lambda_{1,2,3}$ - the weights of rotation and 3 oscillations.
The weights of rotation and oscillations depend on the angle ν:
$\lambda_{r,1}=(3/2)\lambda^0_{r,1}(1-\nu^2)$, $\lambda_{2,3}=3\lambda^0_{2,3}\nu^2$. (3.1c.19)
For Nelkin model summation is used instead of integration with mean values
$\lambda_i=\lambda^0_i$, i=r,1,2,3.
The next parameters are recommended for H and D
in H_2O and D_2O

	λ_t	λ_{tr}	$\lambda_1=\lambda_2=\lambda_3$	ω_r	ω_1	$\omega_2=\omega_3$	E_1	$\sigma_{b,\,barn}$
H	0.0556	0.4310	0.1712	0.060	0.205	0.480	0.320	81.6
D	0.0500	0.2433	0.0689	0.050	0.150	0.350	0.250	7.54

On the basis of formula for scattering cross-section next moments are calculated:
$\sigma^l_s=(E'\to E)=(4\pi/2)\int_{-1}^{1} d\mu\mu^l\sigma(E'\to E,\mu)$, $\sigma^l_s(\nu'|\nu)=2\nu\sigma^l_s(\nu'^2\to\nu^2)$, l=0,1. (3.1c.20)

with the change of variables:

$E\to E/0.0253=\nu$, $\omega\to\omega/0.0253$, $\kappa T\to T/293$.

Next calculations must be fulfilled:

Gauss summation formula are used for μ, ν integrations:

$$(1/2)\int_{-1}^{1} g(\mu)d\mu\approx\sum_{k=1}^{15} W_k^{(15)}g(\mu_k) \qquad (3.1c.21)$$

$$\int_{-1}^{1} f(\nu^2)d\nu=2\int_0^1 f(\nu^2)d\nu=2\sum_{k=1}^{5} W_k^{(5)}f(\nu_k) \qquad (3.1c.22)$$

For Nelkin model

$$\int_{-1}^{1} f(\nu^2)d\nu=2\,f((\nu^2)'); \quad (\nu^2)'=\int_0^1 \nu^2 d\nu=1/3 \qquad (3.1c.23)$$

Bessel function can be calculated by Stegan Abramovich algorithm with initial parameters:

$I_{k+1}=0$, $I_k=\delta$, k=13, $\delta=10^{-37}$.

For $x<2\times10^{-5}$ the first term of series expansion $I_n(x)=(x/2)^n/n!$ can be taken.

Source

The source due to slowing down of neutrons scattered on the nuclides with atomic mass A:

$$s^F(v)= \int_{v_{max}} dv'\Phi^F(v')\sigma^F_s(v' \mid v),$$

$\Phi^F(v)=2/v$ - Fermi flux, (3.1c.24)

$$\sigma^F_s(v' \mid v)= \begin{cases} (2v\sigma^0_s/v'^2(1-\alpha^2)), & (v\le v'\le v/\alpha); \quad \alpha=(A-1)/(A+1); \\ 0 & (v'<v,\ v'>v/\alpha) \end{cases} \quad (3.1c.25)$$

Number of neutrons coming to group l is equal:

$$s^F(l) = \int_{v_l-\Delta v_l/2}^{v_l+\Delta v_l/2} dv s^F(v)$$

or after integration:

$$s^F(l)=\sigma^0_s(2/(1-\alpha^2))\times [\frac{\bar{v}_l \Delta \bar{v}_l}{v^2_{max}} - \alpha^2 \ln(1+(\Delta v_l / (v_l - \Delta \bar{v}_l / 2)) \quad (3.1c.26)$$

For $v_l + \Delta v_l / 2 \le \alpha v_{max}$: $s(l) = 0$

Iterations

The dimension of the problem is M×N with the (M×N)(M×N) matrix structure as M (N×N.) matrices multiplied by N (M×M) matrices.
2 stage iteration procedure with sequential averaging over space and over energy is applied for the solution of equations:

$$S(i',g)=\sum_{g'}^{G} \tilde{\Phi}(g',i')H(g'|g,i') + s^F(g,i'); \quad \tilde{\Phi}_{n+1}(g,i) = \sum_{i'=1}^{I} s(i',g)P(i'|i,g) \quad (3.1c.27)$$

i=1,....I - I - number of layers; g=1,....G ; G - number of groups;

Spectral normalisation

At the 1st step S(i,g) is excluded

$$\tilde{\Phi}(g,i) = \sum_{i'=1}^{I}[\sum_{g'=1}^{G} \tilde{\Phi}(g',i')H(g'|g,i') + s^F(g,i')]P(i'|i,g) \quad (3.1c.28)$$

Summing and using next notation we obtain:

$$\sum_i \tilde{\Phi}(g,i) = \Phi(g); \sum_i s^F(g,i) = s_\Phi(g); \quad (3.1c.29)$$

$$\tilde{\Phi}(g) = \sum_{i'=1}^{I}[\sum_{g'=1}^{G} \tilde{\Phi}(g',i')H(g'|g,i') + s^F(g,i') \ ]$$

Changing the order of summation we get:

$$\tilde{\Phi}(g) = \sum[\sum_{g'=1}^{G} \tilde{\Phi}(g')[(1/\Phi(g')\sum_{i'} \tilde{\Phi}(g'|gH(g'|g,i') \quad] + s_F(g) \quad (3.1c.30)$$

The solution of above equation is used for spectrum renormalization by a multiplier

$$a(l) = \Phi_0(l) / \Phi(l)$$

$$a(l) = \sum_m a(m)H(m|l) + F(l)$$

$$H(m|l) = \frac{1}{\Phi(l)} \sum_j \Phi(m,j)H(m|l,j)$$

$$F = S(l) / \Phi(l)$$

$$\Phi(l) = \sum_j \Phi(l,j)$$

corrected

$$\Phi(l,j) \rightarrow \Phi(l,j)a(l) \qquad (3.1c.31)$$

Space normalisation

Define $P(i|j) = (1/S(j)) \sum_l S(i,l)P(i|j,l)\Sigma_s(l,j)/\Sigma_t(l,j)$ (3.1c.32)

Define b(j) as the ratio below; excluding $\Phi(l,j)$ and taking a sum over l we get next formulas for space correction:

$b(j)=S_0(j)./S(j)$; $b(j)=\sum_i b(i)\,P(i|j) + F(j)$; $F(j)=S_s(j)/S(j)$;

$S_s(j) =\sum_l S^F(l,j)$; $S(j)= \sum_l S(j,l)$; $S(j,l)\rightarrow b(j)S(j,l)$

The procedure for renormalization is applied usually after 3-5 simple iterations.

d)Resonance absorption

A special subdivision of energy scale allows an effective direct treatment of resonances for prescribed nuclides (in this case twin isotopes can be introduced instead of basic isotopes). Subdivision of lethargy scale in a given lethargy interval

(u_0, u_n)

corresponds to a uniform division of F - image

$$F(u) = F(u)+\Delta, \quad \Delta=F(u_n)/n; \quad u = \ln E/E_0 \qquad (3.1d.1)$$

where function ($F(u_0)=0$) :

$$F(u)=\sum_{ij} \sqrt{z_{ij}\sqrt{\Gamma_{ij}/2E_{ij}}}\,(\mathrm{arctg}x_{ij}^{max}-\mathrm{arctg}x_{ij}); \qquad (3.1d.2)$$

$$z_{ij}=y_{ij}/\sqrt{1+y_{ij}}\ ;\ y_{ij}=c_i\,\sigma^r_{ij}l_i\ ;\ x_{ij} = 2(E-E_{ij})/\Gamma_{ij}\,z_{ij}; \qquad (3.1d.3)$$

roughly estimates absorption by all resonance nuclides present ; c_i- nuclear concentration of isotope i having resonance parameters in the given lethargy interval, l_i - estimated mean chord for isotope i; E_{ij} - energy of the center of resonance j for isotope j; σ^r_{ij} - capture cross-section at the center of resonance ; Γ_{ij} - resonance widths.

This procedure provides accumulation of lethargy points near the centers of resonances. As a result only a few lethargy intervals (5-7) are needed to describe absorption by a given resonance with a reasonable accuracy.

The cross-section for a single resonance is determined by Breight-Wigner formula:

$$\sigma_0 = 2.608 \cdot 10^6((A+1)/A)^2 g\Gamma_n/\Gamma;$$
$$\sigma_t = \sigma_0\psi(x,\vartheta) + (\sigma_0\sigma_p g\Gamma_n/\Gamma)^{1/2}\chi(x,\vartheta) + \sigma_p; \qquad (3.1d.4)$$
$$\sigma_\gamma = \sigma_0(\Gamma_\gamma/\Gamma)(E_0/E)^{1/2}\psi(x,\vartheta),$$

where A- atomic mass, $x=(2/\Gamma)(E-E_0)$, σ_p- potential scattering cross-section;

$$\theta^2 = 29015A\Gamma^2/(E_0(eV)T(°K)); \qquad (3.1d.5)$$

The functions ψ, χ for Doppler broadening are calculated as the solution of the set of differential equations:

$$d\psi(x,\theta)/dx = (\theta^2/4)\chi(x,\theta) - (\theta^2/2)x\psi(x,\theta); \qquad d\chi(x,\theta)/dx = \theta^2(1-\psi(x,\theta)) - (\theta^2/2)x\chi(x,\theta); \qquad (3.1d.6)$$

with the initial conditions:

$$\psi(0,\theta) = (\sqrt{\pi}/2)\theta\exp(\theta^2/4)\mathrm{erfc}(\theta/2)$$
$$\chi(0,\theta) = 0, \qquad (3.1d.7)$$
$$\mathrm{erfc}(z) = (2/\sqrt{\pi})\int_z^\infty \exp(-z^2)du$$

Effective resonance levels technique can be used as well for description of resonance absorption with reasonable accuracy. A set of parameters

$$(E, \Gamma_n, \Gamma\gamma, L, \sigma); \qquad (3.1d.8)$$

L - Doppler-broadening parameter divider (see below), σ - constant (background) capture cross-section in the group where this resonance lays, makes it possible to describe resonance absorption by a single resonance level instead of tens or hundreds of resonances in a given lethargy interval. The theory is based on a pre calculation of resonance absorption by initial set of resonances and by effective one in some simple homogeneous model, and the fact that an approximate equivalency exists between resonance absorption in homogeneous and heterogeneous systems.

Effective resonance levels

In narrow resonance approximation resonance absorption by a single level is defined by an expression

$$\Gamma_\gamma\sqrt{\Gamma_n/\Gamma_\gamma} \qquad (3.1d.9)$$

and by n levels with the same widths by

$$n\Gamma_\gamma\sqrt{\Gamma_n/\Gamma_\gamma} = n\Gamma_\gamma\sqrt{n\Gamma_n/(n\Gamma_\gamma)} \qquad (3.1d.10)$$

If we define one resonance with width n time larger it is expected that the absorption by n resonances can be approximately described by one resonance with increased widths. Effective resonance level is defined as a resonance that approximately describes resonance absorption by some fixed set of resonances. This is important for numerous high energy levels of uranium , for example (hundreds of resonances). The goal is - to substitute in calculations resonance absorption by many resonances for resonance absorption by few effective resonances.

There exist an approximate equivalence relation that describes resonance absorption in a heterogeneous media by resonance absorption in a homogeneous media and the last depends on the set P of 2 main parameters - dilution cross-section s and the temperature of media T, P={s,T}. The homogeneous model is used for the construction of effective levels, though after they their determination they are used for heterogeneous media.
The theory of intermediate resonances (defined by parameter λ) is used for this approach.

In an intermediate resonance theory resonance absorption by a single level is determined by a resonance integral:

$$I_\lambda = r\gamma_\lambda J_\lambda \qquad (3.1d.11)$$

where

$$r = \sigma_0 \Gamma_\gamma / E;$$
$$\sigma_0 = 2,608 \bullet 10^6[(A+1)/A]^2 \Gamma_n / (\Gamma E); \qquad (3.1d.12)$$
$$\gamma_\lambda = (s + \lambda \sigma_\rho[(\Gamma_\gamma + \lambda\Gamma_n)];$$

$$J_\lambda = \int_{-\infty}^{\infty} f_\lambda(\theta,\varepsilon,x)dx; \qquad f_\lambda = \psi(\Theta,x)[\gamma_\lambda + \psi(\Theta,x) + \xi_\lambda\chi(\Theta,x)]; \qquad (3.1d.13)$$

$$\varepsilon = [\sigma_p\Gamma_n / (\sigma_0\Gamma)]^{1/2},$$
$$\xi_\lambda = \varepsilon\lambda\Gamma / (\Gamma_\gamma + \lambda\Gamma_n) \qquad (3.1d.14)$$

Doppler broadening functions may be defined as real and imaginary parts of probability integral:

$$\psi = \frac{\sqrt{\pi}}{2}\Theta \,\mathrm{Re}\,\omega[\frac{1}{2}\Theta(x+i)]; \qquad \omega(z) = \exp(-z^2)[1 + (2i/\sqrt{\pi})\int_0^z \exp(t^2)dt] \qquad (3.1d.15)$$
$$\chi = \frac{\sqrt{\pi}}{2}\Theta \,\mathrm{Im}\,\omega[\frac{1}{2}\Theta(x+i)];$$

Parameter λ is determined as a solution of transcendental equation:

$$\lambda + (1/z_\lambda)\mathrm{arctg}z_\lambda = 1, \qquad z_\lambda = \pi\delta L_\lambda / (2M_\lambda^2); \qquad \delta = 8EA/[(A+1)^2\Gamma]; \qquad (3.1d.16)$$

$$L_\lambda = \int_{-\infty} \varphi_\lambda^2 dx \quad ; \quad M_\lambda = \int_{-\infty} \varphi_\lambda \, dx; \quad \varphi_\lambda = \psi / (\gamma_\lambda + \psi). \qquad (3.1d.17)$$

Let a set of pairs of $P_k = \{s_k, t_k\}$ parameters is fixed; U - the set of parameters of the effective resonance level (L - a divider in equation for Doppler-broadening function, E - energy of the center of resonance, A atomic mass). For every P_k resonance integral of effective resonance can be defined:

$$\begin{array}{ll} & \{P_k\}, k = 1, \ldots, K \\ \Theta = \Gamma / (L\Delta)), & U = \{E, \Gamma_n, \Gamma_\gamma, L\} \\ \Delta = 2\sqrt{ET/A} & I_k(U) \\ & P_k \end{array} \qquad (3.1d.18)$$

$I_k = \sum_{m=1}^{M} I_k^m$ - resonance integrals of a chosen fixed set of M resonaces, also depending on P_k can be calculated.

Take a function

$$\mathcal{J}(U) = \sum_{k=1}^{K} \{f_k^2(U) + F_k^2(U)\} + A(E/E_0 - 1)^4 + B(I_\infty(U)/I_\infty(U) - 1)^2 \qquad (3.1d.19)$$

$$f_k(U) = (I_{eff}(S_k, T_1; U) - I_{eff}(S_k, T_2; U)) / (I(S_k, T_1) - I(S_k, T_2)) - 1; \qquad (3.1d.20)$$

$$F_k(U) = I(S_k, T_1) / I_{eff}(S_k, T_1; U) - 1 \qquad (3.1d.21)$$

and put a requirement:

$$\mathcal{J} \underset{\{U\}}{\rightarrow} \min \qquad (3.1d.22)$$

The solution of this minimization problem gives the set of parameters of effective resonance level.

For nonresolved region of energies (11, 12, 13 groups of Abag'ans system) mean distance between s-levels for U238 was assumed to be D_0 =20.9 eV , between p-resonances D_1=7.2 eV . Radiation width was taken to be equal Γ_γ = 0.0235eV.

To generate resonance parameters in nonresolved region Porter-Thomas distribution was taken for neutron widths defined by the parameters:

Γ_n^0

Γ_n^1 $\qquad x = \Gamma_n^0 / \overline{\Gamma}_n^0;$

$n = 1$ $\qquad y = \Gamma_n^1 / \overline{\Gamma}_n^1$

and

$n = 2$

$$\begin{array}{ll} P(x)dx = P_1(x)dx; & P(y)dy = P_2(y)dy; \\ P_1(x) = \exp(-x/2)/\sqrt{2\pi x}; & P_2(y) = \exp(-y); \end{array} \qquad (3.1d.23)$$

For determination of mean values of Γ_n^0, Γ_n^1 next values of strength functions were used:

$_0 = 1,2 \cdot 10^{-4}$,

$_1 = 1,2 \cdot 10^{-4}$

$_0 = < g\Gamma_n^o >$;

$_1 = < g\Gamma_n^1 > / < 3D_1 >$

The parameters of effective resonances determined by the procedure described above are given in the table 3.1d.1

Table 3.d.1. Effective resonance levels parameters for U238

Group number	E,eV	Γ,eV	Γ,eV	L	σ, barn
11	15062.8	254.7	14.36	102.15	0.2347
12	7532.9	136.9	7.007	73.74	0.1996
13	3499.3	49.34	2.308	42.7	0.0546
14	1874.4	1.902	1.6136	14.18	0.2921
15	694.48	0.5008	0.4027	10.1	0.3138
16	342.51	0.1415	0.1564	5.95	0.2779
17	150.23	0.5055	0.0794	4.45	0.00056

3.2 One-velocity heterogeneous parameters of a reactor channel or a cell
a) monopole

Extrapolated length of a channel by definition is related to parameter Λ as follows:

$$\Gamma = N_{as}(\rho)/(l\partial N_{as}(\rho)/\partial\rho) = \rho/(l\Lambda) \qquad (3.2a.1)$$

Suppose a multilayer cylindrical channel is surrounded by an infinite moderator. At distances of the order of several mean free paths from channel surface the solution can be written as:

$$N_{as}(r) = A[I_0(\kappa r) + uK_0(\kappa r)] \qquad (3.2a.2)$$

u - a parameter (response coefficient) is related to Λ and Γ by equation:

$$\Lambda = a/\Gamma = y[I_1(y) - uK_1(y)]/[I_0(y) + uK_0(y)] \qquad (3.2a.3)$$

The equation for neutron flux can be written in a form:

$$H N = H_0 N + (H - H_0)N = 0;\ H = 1 - \ell \qquad (3.2a.4)$$

where ℓ - operator of one -velocity integral transport equation and H_0 is related to the system with no channel (infinite moderator)

If

$$G_{as}(\mathbf{r},\mathbf{r}_0) = a(c,\ell)\, K_0(\kappa |\mathbf{r}-\mathbf{r}_0|) \qquad (3.2a.5)$$

- asymptotic part of Green function for moderator

$H_0\, G(\mathbf{r},\mathbf{r}_0)= \delta(\mathbf{r}-\mathbf{r}_0)$ (3.2a.6)

asymptotic solution can be written as (after application of addition theorem for Bessel functions):

$N_{as}(r) = a(c,\ell)\, K_0(\kappa r)\int I_0(\kappa r_0)(H_0 - H)N dr_0$ (3.2a.7)

Comparing (3.2a.2) and (3.2a.7) we get next expression for response coefficient:

$u=(a(c,\ell)/A)\int I_0(\kappa r_0)(\ell - \ell_0)N\, dr_0=$ (3.2a.8)

$=(a(c,\ell)/A)\int (\ell - \ell_0)^+ I_0 N(r_1)\, dr_1$

Therefore the solution should be integrated over channel volume and in its vicinity of the order of several mean free paths (function $(\ell - \ell_0)^+ I_0$ exponentially decreases at several mean free paths) with the weight function:

$W(r)=[\Sigma(r)\int K(\mathbf{r},\mathbf{r}_0) - \Sigma_{mod}\int K_0(\mathbf{r},\mathbf{r}_0)]\, I_0(\kappa r_0) dr_0$ (3.2a.9)

For u next expression can be used [24]:

$u= a(c,\ell)/A)\int I_0(\kappa r_0)[Q(r_0)+(\ell - \ell_0) N^{(1)}]\, dr_0$ (3.2a.10)

Parameter u is zero if the properties of the channel are the same as of moderator. as it follows from equality (3.2a.10). The result of application of operator $(\ell - \ell_0)$ on N or $(\ell - \ell_0)^+$ on I_0 can by expressed by collision probabilities P_{ij}.

For a cell of finite radius the calculations are as follows. Let the channel is surrounded by a thick layer of moderator.

The solution is presented as follows:

$N(r)= N^{(0)}(r)+ N^{(1)}(r)$ (3.2a.11)

where

$N^{(0)}(r)=I_0(r)$ (3.2a.12)

- a fixed regular part of solution extended into the channel volume.

The equation for $N^{(1)}$ is next:

$N^{(1)}(r)= \ell\, N^{(1)}(r)+Q;\ Q=(\ell - \ell_0)N^{(0)}$ (3.2a.13)

ℓ and ℓ_0 are defined now for finite cell. At large distances the solution can be written as:

$N_{as}^{(1)}(r)=uK_0(\kappa r) +A[I_0(\kappa r) +uK_0(\kappa r)]=$ (3.2a.14)

$=A[I_0(\kappa r)+(I_1(\kappa R)/K_1(\kappa R))K_0(\kappa r)]$

the first term is due to fixed regular part of solution. the second depend on finite dimensions of reactor cell. The last equality follows from boundary condition: the current is equal zero. Coefficient A can be found from the requirement of the best adjustment of the solution to its asymptotic part. Then:

$$u = A(I_1(\kappa R)/K_1(\kappa R))/(1+A) \qquad (3.2a.15)$$

The results of calculations of $\Gamma(a)$, $a=\rho/l$ for absorbing rod , $c=\Sigma_s/\Sigma=0.9$, by the method described above (*) in comparison with approximate formula
(Kavenoky A. -Nucl. Sci. and Engng.,.1978. v.65. p.514) :

$$\Gamma(a) = \frac{0,7104a^2 + 0,6939a + 0,01147}{a^2 + 0,5416a + 0,0086} \qquad (3.2a.16)$$

having the accuracy about 0.01% are given the table 3.2a.1 .

Table 3.2a.1. Response parameter u and boundary condition Γ for absorbing rods.

–K -Kavenoky, * present calculation, δΓ/ Γ % -difference

a	u	Γ –K	Γ *	δΓ/ Γ %
0.1	-0.05781	1.38556	1.39790	0.89
0.2	-0.10988	1.29505	1.30461	0.74
0.3	-0.15974	1.22836	1.23675	0.68
0.5	-0.25921	1.13360	1.13951	0.52
0.7	-0.36445	1.06851	1.07204	0.33
1.0	-0.54463	1.00158	1.00251	0.09
2.0	-1.55752	0.89206	0.89258	0.06
3.0	-4.09100	0.84595	0.84795	0.15
5.0	-30.2026	0.80625	0.80816	0.36
8.0	-664.035	0.78355	0.78760	0.52

b) Axial dipole

Consider one-velocity problem.
For an axially uniform reactor of finite height H the variables can be separated as follows:

$$N(\mathbf{r}) = \exp(i\alpha z)N(x,y) \qquad (3.2b.1)$$

$\alpha=\pi/H$
In this case parameter Λ can be presented in a form:

$$\Lambda = \Lambda^0 + \alpha^2\Lambda^z \qquad (3.2b.2)$$

In diffusion approximation the neutron flux in a uniform cylindrical rod is equal

$$N(r) = AI_0(\kappa_i r);\ \kappa_i^2 = 1/L_i^2 + \alpha^2 \qquad (3.2b.3)$$

By definition (i -channel, e- moderator)

$$\Lambda = (\rho\partial N_e(\rho)/\partial\rho)/\ N_e(\rho) = (D_i/D_e)\rho(\partial N_i(\rho)/\partial\rho)/\ N_i(\rho) = D_i\rho^2\kappa_i^2/(2D_eQ) \qquad (3.2b.4)$$

$$Q = I_0(\kappa_i\rho)/(2\,\kappa_i\rho\, I_1(\kappa_i\rho)) \qquad (3.2b.5)$$

so that for Λ^0, Λ^z the next expressions are derived:

$\Lambda^0=\rho^2\Sigma_{ai}/2D_eQ$; (3.2b.6)
$\Lambda^z=\rho^2\omega/2Q$; $\omega=D_i/D_e$

ω - a parameter - axial polarizability of the channel describing neutron migration in axial direction.

b)Neutron migration area

Consider a uniform lattice of channels.
For a reactor of finite height H the variable of axial dependence for source Q and flux N are separated ($\alpha=\pi/H$) :

$Q(r)=q(\rho)\exp(i\alpha z)$; $N(r)=N(\rho, \alpha^2)\exp(iaz)$;

Next expression for neutron flux can be written:

$N= \ell(\Sigma_sN+q)\exp(-i\alpha(z-z'))]$ (3.2b.7)

Suppose:

$N(\rho,\alpha^2)=N_0(\rho)-(1/2)\alpha^2N_1(\rho)$. (3.2b.8)

Taking the expansion of exponential function up to α^2, the next equations can be derived:

$N_0=\ell(\Sigma_sN+q)$ (3.2b.9)

$N_1=\ell\Sigma_s N_1+\ell (z-z")^2(\Sigma_sN_0+q)$

The probability to escape leakage P_z can be defined as the ratio of neutrons absorbed in the reactor of finite height to the number of neutrons absorbed in a reactor of infinite height:

$P_z=\int N(\rho,\alpha^2)\Sigma_a(\rho)d\rho / \int N_0(\rho)\Sigma_a(\rho)d\rho=$
$=1-(\alpha^2/2)\int N_1(\rho)\Sigma_a(\rho)d\rho / \int N_0(\rho)\Sigma_a(\rho)d\rho$ (3.2b.10)

Assuming

$P_z=1/(1+\alpha^2L_z^2)$ (3.2b.11)

the next expression can be written for L_z^2:

$L_z^2=\int N_1(\rho)\Sigma_a(\rho)d\rho /(2\int N_0(\rho)\Sigma_a(\rho)d\rho)$ (3.2b.12)

Multiplying (3.2b.9) by $\Sigma(\rho)$ and taking the integral over all the volume we obtain:

$\int N_1(\rho)\Sigma_a(\rho)d\rho=\int drd\rho"S(r)K(r, \rho")(z-z")^2$ (3.2b.1)
$[\Sigma_s(\rho")N_0(\rho")+q(\rho")]$

so that

$$L_z^2=\int l^2_z(\rho)[\Sigma_s(\rho)N_0(\rho)+q(\rho)]/(2\int N_0(\rho)\Sigma_a(\rho)d\rho) \qquad (3.2b.13)$$

$$l^2_z(\rho)=\int \Sigma(\rho)\mu_z^2 R^2 \exp(-\Sigma R)\, dR/(4\pi R^2) \qquad (3.2b.14)$$

projection of mean square path of neutrons on z-axis, taken with the weight - neutron emission $\Sigma_s N_0+q$.
In homogeneous media

$$l^2_z=(2/3)\, l^2;\quad q=\Sigma_a N_0 \qquad (3.2b.15)$$

$$L^2_z=1/3\ \Sigma_a\,. \qquad (3.2b.16)$$

Subdividing the cell by thin layers, the expression for the square of diffusion length is written as a double sum

$$L^2_z \sim (1/2)\Sigma\ \Sigma P^z_{ij}\,(\Sigma_s N_0+q)_j / <\Sigma_a N_0 V>, \qquad (3.2b.17)$$

$$<\Sigma_a N_0 V> = \int_{V_{cell}} \Sigma_a(\rho)\, N(\rho)\, d\rho \qquad (3.2b.18)$$

depending on modified collision probabilities P^z_{ij}

Behrens formula [25] (for a cell with an empty cylindrical channel) is derived as follows:

$$L_z^2 = (1/2)\, P_2^z\ (\Sigma_{s2} N_2 + q)/(\Sigma_{a2} N_2 V_2) \qquad (3.2b.19)$$

$$=(1/2)\, P_2^z\ \Sigma_2/(\Sigma_{a2} V_2)$$

Neutron flux is supposed to be constant in the moderator and balance relation was used:

$q=\Sigma_{a2}N_2$.

The formula for modified collision probability in this case is written as follows:

$$P_z^2 = (2/3)\, V_2 l_2^2 - V_2(c_1^{12} b_1^{11} + c_2^{12} b_2^{11}) \qquad (3.2b.20)$$

Taking account of the expression for Bickley functions for the limit $l_1 \to \infty$ we get

$$Ki_n(z) = Ki_n(0) - zKi_{n-1}(0) + (z^2/2)Ki_{n-2}(0) + o(z^2)\,; \qquad (3.2b.21)$$

$Ki_1(0)=\pi/2$; $Ki_2(0)=1$; $Ki_3(0)=\pi/4$; $Ki_4(0)=2/3$

$b_1^{11}=(V_1/3l_1)(1-2\rho/l_1)$; $b_2^{11}=(V_1/3)(4\rho/l_1-1)$

and finally Behrens formula is obtained:

$$L_z^2=[\,1+2p\,(1+\rho/l)],\ p=V_{hole}/V_{moder}\,. \qquad (3.2b.22)$$

Axial polarisability coefficient

A closed functional expression can be derived for axial coefficient of polarisability.
Suppose L_z^2 is determined by above formula.
Find Λ^z in the boundary condition

$$\rho dN/d\rho = (\Lambda^0 + \alpha_z^2 \Lambda^z)\, N, \qquad (3.2b.23)$$

Take integral of the both parts of diffusion equation

$$(-D\Delta + \Sigma_a)\, N = q;\ 2\pi D\rho d/d\rho + (D\alpha_z^2 + \Sigma_a)\, N_{mod} V_{mod} = q\, V_{mod} \qquad (3.2b.24)$$

or $2\pi D\,(\Lambda^0 + \alpha_z^2 \Lambda^z)\, N(\rho) + (D\alpha_z^2 + \Sigma_a)\, N_{mod} V_{mod} = q\, V_{mod}$

By definition of neutron leakage escape probability

$$1 + \alpha_z^2 L_z^2 = q\, V_{mod} / (2\pi D\Lambda^0 N(\rho) + \Sigma_{a\,mod} N_{mod} V_{mod}) \qquad (3.2b.25)$$

$$\Lambda^z = [\Lambda^0 + \frac{V_{mod}}{2\pi L_{mod}^2}\varsigma] L_z^2 - V_{mod}\varsigma / 2\pi; \qquad (3.2b.26)$$
$$= N_{mod} / N(\rho).$$

$$L_z^2 = (D_{mod} / \overline{\Sigma}_{a,cell})(1 + p\varsigma_0^{-1})^{-1}(1 + p\varsigma_0^{-1}) \qquad (3.2b.27)$$
$$p = V_{chan} / V_{mod};\ \varsigma_0 = \overline{N}_{mod} / N_{chan};$$

$$\Lambda^z = (\rho^2/2)(N_{chan} / N(\rho))\omega \qquad (3.2b.28)$$

A closed functional expression for ω is derived as follows. In the expression for L_z^2

$$\int \Sigma_a N_o d\rho = 2\pi D N_0 [\Lambda^0 + V_{mod}/(2\pi L^2{}_{mod})\xi] \qquad (3.2b.29)$$

consequently

$$\Lambda^z = (1/2\pi N_0(\rho))[3/2 \int l_z^2(\rho)/l_{mod}(\Sigma_s N_0 + q)d\rho - \int_{V_{mod}} N_0(\rho)d\rho] \qquad (3.2b.30)$$

But

$$\int_{V_{mod}} \Sigma(\rho) N_0(\rho) d\rho = \int_{V_{mod}} [\Sigma_s(\rho) N_0(\rho) + q(\rho)] d\rho \qquad (3.2b.31)$$

and the last term in (3.2b.30) can be written as:

$$\int_{V_{mod}} N(\rho) d\rho = l_{mod} [\int_{V_{mod}} (\Sigma_s N_0 + q) d\rho - \int_{V_{mod}} \Sigma(\rho)\, N(\rho) d\rho] \qquad (3.2b.32)$$

Thus the functional expression for ω is as follows:

$$\Lambda^z=(1/2\pi N_0(\rho))[\int_{Vcell}((3/2)l_z(\rho)/l_{mod}-l_{mod})(\Sigma_s N_0+q)d\rho+\int_{V_{mod}} l_{mod}\Sigma(\rho)\,N_0(\rho)d\rho]$$

(3.2b.33)

At the distances of the order of several mean free paths from channel surface

$$(3/2)l_z^2(\rho)\rightarrow l_{mod}^2 \qquad (3.2b.34)$$

so the first integral is taken over channel volume and in some vicinity around, the second - over channel volume only.

The first term is zero if total cross-section in channel is the same as in moderator ; if the c channel properties are the same as moderator properties then:

$$\Lambda^z=V_{chan}/2\pi,\ \omega=1. \qquad (3.2b.35)$$

3.2 c) Radial dipole

Suppose a multilayer channel is placed in an infinite moderator [5]. In one-velocity theory radial polarisability coefficient gives the relation between regular and singular parts of solution:

$$N(\mathbf{r}) = [I_1(\kappa r)+u^1K_1(\kappa r)]A\cos\varphi;\ u^1=-\kappa^2\rho^2\beta/2 \qquad (3.2c.1)$$

In the case of small absorption in the moderator:

$$N(\mathbf{r}) = (r-\rho^2\beta/r)A\cos\varphi \qquad (3.2c.2)$$

Suppose the regular part of solution is extended into channel and try to find the solution of integral equation in the next form:

$$(x+N^{(1)})=L(x+N^{(1)}) \qquad (3.2c.3)$$

Function x is the solution of the equation:

$$x=L_0(x) \qquad (3.2c.4)$$

so that regular part is presented as a source in the equation:

$$N^{(1)} = LN^{(1)} + Q; Q \equiv (L - L_0)x \qquad (3.2c.5)$$

Function Q(r) exponentially decreases at large distances from the channel and $N^{(1)}$ asymptotically behaves as:

$N^{(1)} \sim \cos\varphi/r$.

Divide the channel into thin layers. Multiplying the equation (3.2c.5) by $2\Sigma_{si}x/V_i$ and taking integrals over volumes V_i and assuming by definition:

$$\Sigma_s N^{(1)} = [F(r) / r]\cos\varphi \equiv [F(r) / r^2]x, \qquad (3.2c.6)$$

we derive the next equation for F:

$$F_i = \frac{\Sigma_{si}}{\Sigma_i V_i} S_j P_{ij}^1 F_j + Q_i, \qquad (3.2c.7)$$

with matrix elements:

$$P_{ij}^1 = (\Sigma_i/2\pi)\int\int \mathbf{dr dr'}(xx'/(R^2 r'^2)\exp(-s);\ R = |\mathbf{r}-\mathbf{r'}| \qquad (3.2c.8)$$

and the source term:

$$Q_i = (2\Sigma_{si}/V_i)\sum_j \int\int \mathbf{dr dr'}(xx'/(R^2 r'^2)(\exp(-s)\Sigma_{si} - \exp(-s_0)\Sigma_s)/(4\pi R^2) \qquad (3.2c.8)$$

(s - optical length, s_0 -optical length for the case when all the space is occupied my moderator)

Calculation of modified "probabilities"

Taking account of the relation

$$x = x' + \rho\cos(\omega + \varphi') = x' + \rho(\cos\omega\cos\varphi' - \sin\omega\sin\varphi' \rightarrow$$

$$\rightarrow x' + (x'/r')\rho\cos\omega$$

we can present the probability as a sum of two terms:

$$P^1_{ij} = P_{ij} + P_{ij}' \qquad (3.2c.10)$$

$$P_{ij} = (\Sigma_i/4\pi)\int_{V_i}\int_{V_j} \mathbf{dr dr'}\exp(-s)/R^2 \qquad (3.2c.11)$$

$$P_{ij}' = (\Sigma_i/4\pi)\int_{V_i}\int_{V_j} \mathbf{dr dr'}(x'^2/r'^3)\, R\mu_r \exp(-s)/R^2 \qquad (3.2c.12)$$

Above next relation was used:

$$\int_{V_j} x'^2/r'^2\, \mathbf{dr'} = (1/2)\int \mathbf{dr} \qquad (3.2c.14)$$

P_{ij} is proportional to the traditional collision probability

By definition of P'_{ij}
μ_r - is the projection of the direction neutron movement
to vector **r'** in the plane (x,y) (Fig. 3.3):

$\mu_r = \sin\vartheta\cos\omega$,

ω- the angle between projection of vector

R = r - r' and **r'**
If the center of coordinates is taken at point **r'** , the volume element is:

$$d\mathbf{r} = R^2 dR d\mu \qquad (3.2c.15)$$

$(d\mu = \sin\vartheta d\vartheta d\omega)$
Taking integrals over R,θ and φ' the next expression for P'_{ij} can be derived:

$$P'_{ij} = (1/\Sigma_i)\oint_{\Pi_i} (\mu_{x,y} d\Pi)\cos\omega/\rho[Ki_3(L)+\rho\Sigma_i Ki_2(L)] \int_{\Delta_i} dr' \qquad (3.2c.16)$$

The integral is taken over the boundary of layer i in the plane (x,y) :
$d\Pi = \mathbf{n}_i \Pi$ the element of arc with inward orientation along unit normal vector $\mathbf{n}_i$; $\mu_{x,y}$ - projection of vector $(\mathbf{r}-\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$ on the plane (x,y)

$\mu_{x,y} = d\Pi/\rho = \pm d\omega$

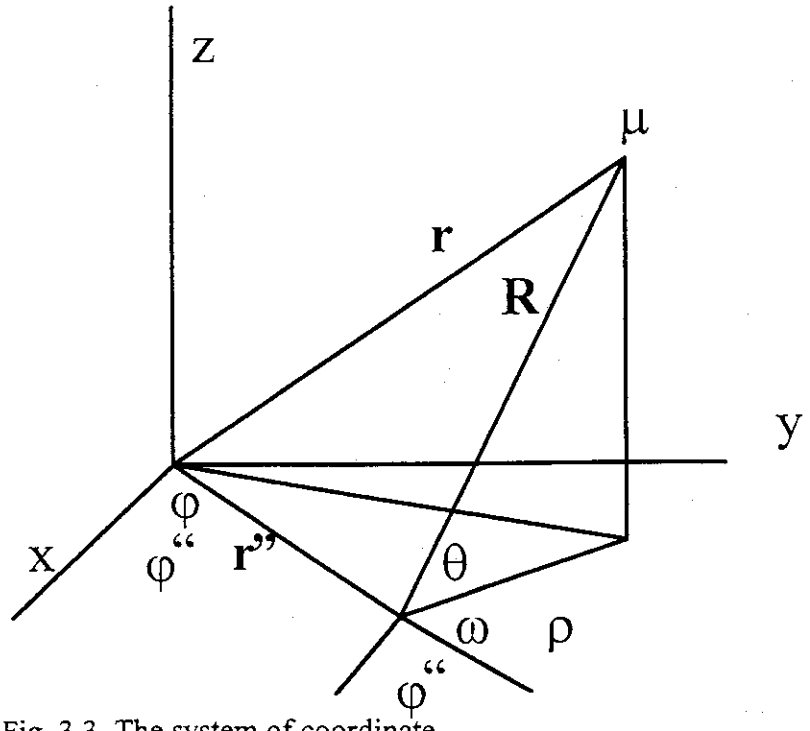


Fig. 3.3 The system of coordinate

The sign ± depends on mutual orientation of vectors $\mu_{x,y}$ and $\mathbf{n}_i$ and coincides with the sign of scalar product $(\mu_{x,y}\,\mathbf{n}_i)$.

For P_{ij} a similar expression can be written

$$P_{ij}=\oint_{\Pi_i}((\mu_{x,y}d\Pi)/\rho)_i Ki_2(L)]\int_{\Delta_i} r'\,dr' \qquad (3.2c.17)$$

but in this case more simple expression exist.

The source.

The part due to L_0 is easily calculated as follows:

$$Q_i''=(-2\Sigma_{si}/V_i)\sum_j \int\int \mathbf{dr}\mathbf{dr}'(xx')(\exp(-s)\Sigma/(4\pi R^2)= -(1/2)\Sigma_{si}(\rho_{i-1}^2+\rho_i^2) \qquad (3.2c.18)$$

The other part is next:

$$Q_i'=(2\Sigma_{si}/V_i)\sum_j \int_{V_i}\int_{V_j} \mathbf{dr}\mathbf{dr}'(xx')(\exp(-s)\Sigma_{sj}/(4\pi R^2)$$

First the integral by $\mathbf{dr}'$ is taken with the center of coordinates at point $\mathbf{r}$:

$$d\mathbf{r}' = R^2 dR d\mu,$$

$$x' = x + \rho\cos(\omega+\varphi) \rightarrow x + \rho\cos\omega\cos\varphi;$$

$$\mu = (\mathbf{r}'-\mathbf{r})/|\mathbf{r}'-\mathbf{r}|.$$

The result of calculations are given by the expression:

$$Q_{ij}=(\Sigma_{si}/V_i)\int_{\Delta_i} r^3 dr \oint_{\Pi_i}((\mu_{x,y}d\Pi)/\rho)[(\Sigma_{si}/\Sigma_i)\,Ki_2(L)(1+\rho\cos\omega/r)+(\Sigma_{sj}/\Sigma_j^2)Ki_3(L)\cos\omega/r]+ \qquad (3.2c.19)$$

$$(\Sigma_{sj}/2)(\Sigma_{si}/\Sigma_i-1)(\rho_{i-1}^2+\rho_i^2)+Q'''_{ij}$$

The last term takes account of diagonal terms of Q'_{ij}.

Full source in the layer i is the sum over all layers and can be written after the change of order of summation as follows:

$$Q_i = \frac{\Sigma_{si}}{V_i}\sum_j[(a_{j+1}-a_j)A_{ij}+(b_{j+1}-b_j)B_{ij}]m^j_{j+1}+ \qquad (3.2c.20)$$

$$+\frac{1}{2}\Sigma_{si}\left(\frac{\Sigma_{si}}{\Sigma_i}-1\right)(\rho_{i-1}^2+\rho_i^2).$$

The values in (3.2c.20) are defined by next expressions:

$$a_j=\Sigma_{sj}/\Sigma_j;\ b_j=a_j/\Sigma_j;\ m^j_{j+1}=\mathrm{sgn}(\mu_{x,y}\mathbf{n}^j_{j+1}) \qquad (3.2c.21)$$

$$A_{ij}=\int_{\Delta_i} r^3 dr \oint_{\Pi_i} d\omega\, Ki_2(L)(1+\rho\cos\omega/r)$$

$$B_{ij}=\int_{\Delta_i} r^2 dr \oint_{\Pi_i} d\omega\, Ki_3(L)\cos\omega$$

Π_j is the boundary of radius ρ_j.

The sum depends on thedifferences $a_{j+1}-a_j$ and $b_{j+1}-b_j$ that are zero if the properties of neighbor layers coincide - that is the sum is taken over boundaries of layers with different

physical properties and the sum is taken to the last boundary of channel. For the layer in the moderator the last term in (3.2c.20) is zero and the other terms exponentially decrease at distances of the order of several mean free paths from the channel boundary.

Coefficient of polarisability

In accordance with asymptotic presentation (3.2c.2) and definition (3.2c.6) the limit of F(r) at infinity must be a constant value and is related to β as follows:

$$\beta = -(1/\rho^2) \lim_{r\to\infty}(F(r)/\Sigma) \qquad (3.2c.22)$$

The other approach is to calculate the current of some field g_x, defined below [26].
Multiplying integro-differencial equation for neutron flux (space-angle distribution):

$$\mu\nabla N(\mathbf{r},\mu)+\Sigma(\mathbf{r})\, N(\mathbf{r},\mu) = \Sigma(\mathbf{r})\int N(\mathbf{r},\mu)d\mu + S(\mathbf{r},\mu) \qquad (3.2c.23)$$

by $x\Sigma + \mu_x$ (the regular solution of adjoint integro-differencial equation) and taking integral over angles, the next conservation equation can be derived for $\mathbf{g}_x$

$$\mathrm{div}g_x + (\Sigma(\mathbf{r}) - \Sigma) j_x + x\Sigma_a(\mathbf{r})\Sigma N(\mathbf{r}) = S_x + x\Sigma S_0; \qquad (3.2c.24)$$

$$(g_x)_i = \Sigma x j_i + \int \mu_x\mu_i N(\mathbf{r},\mu)d\mu \qquad (3.2c.24)$$

The dependence on the difference in channel and moderator properties exists inside the channel. In the moderator a conservation low can be written in the next form:

$$\mathrm{div}g_x \quad 0. \qquad (3.2c.25)$$

If we take two surfaces - one - the surface of the channel , the other - at some far distance from the channel boundary and take integral over the volume between these two surfaces the next expression can be derived for β as an integral over channel boundary:

$$\beta = (3/2\pi\rho^2) \oint g_x d\pi \qquad (3.2c.26)$$

with inward orientation of dπ on channel boundary. The calculations give the next expression for β:

$$\beta = (3/2\pi\rho^2) \oint_{\Pi_i} ((\mu_{x,y}d\pi)/\rho) \int_{\Delta_i} dr'(r'F_j + r'^3)\,[Ki_2(L)\Sigma(1+\rho\cos\omega/r') + Ki3(L)\cos\omega/r'] \qquad (3.2c.27)$$

Since the function F reaches a constant limit at infinity it is possible to choose some number J of layers and in the final layer to suppose an equality

$$F_{j+1} = F_j \qquad (3.2c.28)$$

Then the system of equations for F becomes closed:

$$F_i = \frac{\Sigma_{si}}{\Sigma_i V_i} \sum_{j=1}^{j+1} P_{ij}^1 F_j + Q_i; F_{j+1} = F_j, i = 1,\ldots,J \qquad (3.2c.29)$$

For empty channel an interpolation formula by Carter -Jarvis exists
(Carter C., Jarvis R.J. Reactor Sci. and Technol.., 1961, v.15, p.76)

$$\beta_e = (1/2 + a)/(1 + a);\ a=\rho\Sigma \qquad (3.2c.30)$$

For black bodies the next result can be derived from balance equation (3.2c.26):

$$\beta_b = (3/4)(a - 3/4a)/(1 + 3a/4 + f(a)); \qquad (3.2c.31)$$

$$f(a) = (3a/\pi)\int_0^\infty dx Ki_3(ax)\mathrm{arctg}(x) \qquad (3.2c.32)$$

At limiting cases:

$$\beta_b \underset{a\to 0}{\to} -9/32a;\quad \beta_b \underset{a\to\infty}{\to} (1-2\lambda/a) \qquad (3.2c.33)$$

$\lambda=0.7104$

3.3 Few-group heterogeneous parameters of a reactor cell.

a) monopole (Λ - matrix)

Λ-matrix is defined as G×G matrix in a boundary condition at the cell surface of radius ρ, giving the relation between the current and the flux N

$$\rho dN/d\rho = \Lambda N \qquad (3.3a.1)$$

in a few group theory (G - number of groups) for heterogeneous reactor calculations.
Λ-matrix is calculated as follows.
Let in a cell of radius ρ a source of neutrons S is given. It has an energy distribution corresponding to fission neutron spectrum and some preliminary estimated space distribution. S source is normalized to unity.
Let

$N_0 = N^{(1)}$

be a few-group vector-flux on the cell boundary derived from multi-group calculation for the case of zero current across cell boundary:

$J^{(1)} = 0.$

Let N , J -are similar values obtained for G multigroup solutions of space-time problems with G non-zero linear independent currents across cell boundary $J^{(g)}$ and the same neutron source S, g=2,....,G+1.

A system of equations is valid for triangular Λ_2-matrix, depending on slowing down and neutron absorption:

$$\Lambda^{-1}J^{(g)} + N_0 = N^{(g)} \quad , g=2,...,G+1 \qquad (3.3a.2)$$

Let

$$K_i^{(g)} = \int_{\Delta u_i} \nu\Sigma_f\varphi^{(g)}(u,\mathbf{r})dudV \qquad (3.3a.3)$$

be the number of neutrons appearing in the cell due to fissions in group i for the problem number g. A similar system of equations is valid for the elements of matrix Q, that determines the influence of currents J on the values of integrals (3.3a.3). The relations

$$QJ^{(g)} + K_0 = K^{(g)} \quad , K_0 \equiv K^{(1)};\ \ g=2,...G+1; \qquad (3.3a.4)$$

describe fission sources Q due to currents $J^{(g)}$.
Summing the components of of vectors in equation (3.3a.4) we get an equality valid for any J (qJ - scalar product of vectors q and J):

$$qJ/(k-k_0)=1; \qquad (3.3a.5)$$
$$q_j=\sum_{i=1}^{G} Q_{ij};\ \ k=\sum_{i=1}^{G} K_i$$

The equality (3.3a.5) can be considered as balance relation - the currents at cell boundary must compensate the difference k_0 -1 in a critical reactor. Substituting (3.3a.5) as a multiplier at N_0 in (3.3a.5) the next expression is derived:

$$(N_0 \otimes q \sim \{N_{0i}qj\}):$$
$$N = [\Lambda_2^{-1} + N_0 \otimes q / (k - k_0)]J \qquad (3.3a.6)$$

In other words full Λ-matrix is determined by the next relation:

$$\Lambda^{-1} = \Lambda_2^{-1} + N_0 \otimes q / (k - k_0) \qquad (3.3a.7)$$
$$(k = 1)$$

-for critical reactor.

The expression (3.3a.7) can be transformed to exclude a possible singularity in the second term. Multiplying (3.3a.2) by Λ_2 and taking a scalar product with q we obtain:

$$qJ = q\Lambda_2 N / [1 + q\Lambda_2 N_0 / (k - k_0)]. \qquad (3.3a.8)$$

Substituting qJ in (3.3a.6) for the right part of (3.3a.8) we get the relation that determines the full Λ-matrix
($\otimes$ - means tensor product of two vectors):

$$\Lambda = \Lambda_1 + \Lambda_2 \ , \ \Lambda_1 = -\Lambda_2 N_0 \otimes q\Lambda_1 / (k_{ef} - \upsilon); \qquad (3.3a.9)$$

$$\upsilon = k_0 - q\Lambda_2 N_0 \qquad (3.3a.10)$$

It follows from the expression (3.3a.9) that for $k_{ef}=k_0$
N_0 is the eigenvalue for matrix Λ.

Response matrices U. Equivalence of U and Λ matrices.
An equivalent to Λ –matrix characteristic is a response matrix U . Few-group diffusion solution in the moderator
can be written as:

$$\begin{aligned} &N = IA + KB; \\ &I \equiv CI_0C^{-1}; \\ &K \equiv C K_0 C^{-1}, \end{aligned} \qquad (3.3a.11)$$

Vector J is equal :

$$\begin{aligned} &J = \alpha IA - \beta KB; \alpha \equiv CyI\, I_0^{-1} C^{-1}; \\ &\beta = Cy\, K_1 K_0^{-1} C^{-1}; \\ &y = \underset{g}{\mathrm{diag}}\{\kappa_g \rho\} \end{aligned} \qquad (3.3a.12)$$

Le N_0 be a solution due to the source defined for calculation of Λ–matrix with zero currents across cell boundary, W - a constant G-vector:

$$\begin{aligned} &N_0 = (I + KP)W; P = CI_1K_1^{-1}C^{-1}; \\ &n = N - N_0; \\ &A = K(J + \beta n); B = -I(J - \alpha n); \\ &U_2A = B; \\ &(I + U_2K)J = (I\alpha - U_2K\beta)n. \end{aligned} \qquad (3.3a.13)$$

Matrix U_2 is due to slowing-down and absorption of neutrons; Λ_2 is related to U_2 as following:

$$\Lambda_2 = (I\alpha - K\beta U_2)(I + KU_2)^{-1} \qquad (3.3a.14)$$

The components of triangular matrix
ρ obey the equation

$$\rho A^{(g)} + \chi_0 = \chi^{(g)}; g = 2, \ldots, G+1 \qquad (3.3a.15)$$

Taking a sum of all components of vectors in (3.3a.15) we find:

$$pA / (k - k_0) = 1; p_i = \sum_{j=1}^{i} \rho_{ji} \qquad (3.3a.16)$$

Re defining one of equations in (3.3a.13) we can write a relation

$$U_2A + B_0 = B, B_0 = I\alpha N_0 \qquad (3.3a.17)$$

Taking account of (3.3a.16) one obtains:

$$U_2 + B_0 \otimes p / (k - k_0)]A = B,$$
$$U = U_1 + U_2; U_1 = B_0 \otimes p / (k - k_0) \qquad (3.3a.18)$$

the relation between U and Λ being the same as the relation between U_2 and Λ_2. Due to (3.3a.13) A is equal:

$$a = K(1 + \beta\Lambda^{-1})J \qquad (3.3a.19)$$

and the relation between Q and ρ is given by the equality:

$$Q = \rho K(1+\beta\Lambda_2^{-1}). \qquad (3.3a.20)$$

Consequently the equivalency of Λ and U is proven.

b)Reaction rate matrices

A similar method is used for reaction rate R-matrices calculation (reaction of type x):
Let reaction rate due to Σ_x cross-section in the given
volume V_x is defined as

$$H_i^{(g)} \quad \int_{\Delta u_i V_x} {}_x \; {}^{(g)} du dV$$
$$\Sigma_x - \rightarrow$$
$$V_x - \rightarrow$$
$$(i = 1, \ldots, G)$$
$$\rho_x - \rightarrow$$

$P_{x,2}$ defines the contribution of neutron currents on a cell boundary to above integrals depending on slowing-down and absorption of neutrons and in this case the next system of equations can be written:

$$P_{x,2}J^{(g)} + H_0 = H^{(g)}; H_0 \equiv H^{(1)};$$
$$g = 2, \ldots, G + 1;$$
For full matrix (including fission reactions (3.3a.21)
the next expression is valid:
$$\rho_x = \rho_{x,2} + H_0 \otimes q\Lambda_2 / (k - \nu)$$

In the limiting case when effective multiplication factor
$k \rightarrow k_0$ $P \rightarrow H_0$
that is reaction rate is determined by vector H_0.

c) axial dipole

The solution of multigroup equations for a reactor cell of finite height H can be presented with separated variables:

$$\Phi = \Phi(r)e^{i\alpha z}; Q = Q(r)e^{i\alpha z}; r \equiv (x, y). \qquad (3c.1)$$

an additional term in Λ–matrix should be defined due to neutron migration in axial direction and all the values defining Λ–matrix are to be calculated accounting for the 1st order expansion by a parameter (H - reactor height):

$$\alpha^2 = \pi^2/H^2;$$
$$\Lambda \Rightarrow \Lambda + \alpha^2 \Lambda^z; \quad \Lambda_2 \Rightarrow \Lambda_2 + \alpha^2 \Lambda_2{}^z; \qquad (3.3c.2)$$
$$N_0 \Rightarrow N_0 + \alpha^2 N^z; \quad k \Rightarrow k + \alpha^2 k^z; \quad q \Rightarrow q + \alpha^2 q^z$$

If the cell is divided by M thin layers with volumes V_m, and in the infinite volume outside cell boundary it is supposed

$$\Sigma_{M+1} = \Sigma_{sM+1} = \Sigma_M$$

a system of equations based on collision probability method can be derived with matrix elements L_{mn}:

$$V\Phi = L(\alpha^2)(\Sigma_s\Phi + Q); V \equiv \underset{m}{diag}\{V_m\} \qquad (3.3c.3)$$

$$L_{mn} = T_{mn} - T_{m-1n} - T_{mn-1} + T_{m-1n-1}(m > n);$$
$$L_{mn} = L_{nm}; \qquad (3.3c.4)$$
$$L_{nn} = T_{nn} - 2T_{n-1n} + T_{n-1n-1} + (V_n/\alpha)\mathrm{arctg}(\alpha/\Sigma_n);$$

$$T_{mn} = R^-_{mn} + R^+_{mn};$$
$$R^{\pm}_{mn} = 2\int_0^{r_m} dt \int_0^{\pi/2} d\theta \exp[-(s_m \pm s_n)\sin\theta]\,(\alpha^2\cos^2\theta+\Sigma_m{}^2)^{-1}\,(\alpha^2\cos^2\theta+\Sigma_n{}^2)^{-1}\{\cos[B(x_m \pm x_n)](\Sigma_m \Sigma_n - \alpha^2\cos^2\theta) -$$
$$\sin[B(x_m \pm x_n)]\,\alpha\,(\Sigma_m + \Sigma_m)\},$$

where

$$x_m = \sqrt{r_m^2 + t^2}; B = \alpha\mathrm{ctg}\vartheta; \qquad (3.3c.5)$$
$$_m = \sum_{k(r_k > t)} \Sigma_k(\sqrt{r_m^2 - t^2} - \sqrt{r_{k-1}^2 + t^2}$$

If we neglect the terms of the order higher than α^2

$$\Phi = \Phi_0 + \alpha^2\Phi^z; Q = Q_0 + \alpha^2 Q^z; L = L_0 + \alpha^2 L^z$$

a system of the two equations can be derived:

$$V\Phi_0 = L_0(\Sigma_s\Phi_0 + Q_0);$$
$$V\Phi^z = L_0(\Sigma_s\Phi^z + Q^z) + L^z(\Sigma_s\Phi_0 + Q_0) \qquad (3.3c.6)$$

Matrix elements for L_0 and L^z are given in sections (3.1a). Boundary conditions on cell surface for Φ^z are derived as follows. The leakage of neutrons in axial direction for neutrons in the layer n with emission density

$$\Psi_{0n} = \Sigma_{sn}\Phi_{0n} + Q_{0n}; \qquad (3.3c.7)$$

can be presented as

$$J^z_{0,n} = \alpha^2 \sum_{m=1}^{M+1} L^z_{mn}\Sigma_m\Psi_{0n}, \qquad (3.3c.8)$$

In the external layer M+1 a compensating source of neutrons with the next intensity is assumed

$$Q^z_{M+1} = J^z_{0,M+1} / V_{M+1} \qquad (3.3c.9)$$

Taking account of normalization condition:

$$V_n = \sum_{m=1}^{M+1}\Sigma_m L_{0,mn} \qquad (3.3c.10)$$

next equations for M-vector fluxes are obtained:

$$V\Psi_0 = \Sigma_s L_0^{(\theta)}\Psi_0 + Q_0;$$
$$V\Psi^z = \Sigma_s L_0^{(\theta)}\Psi^z + \Sigma_s L^{(\theta)}\Psi_0 + Q^z. \qquad (3.3c.11)$$

Operators

$$L_0^{(\theta)} = L_0 + \theta L_0'; \; L^{z(\theta)} = L^z + \theta L^{z\prime}; \qquad (3.3c.12)$$
$$L_0'_{,mn} = L_{0,Nn} L_{0,mN}/S_0;$$
$$L^{z\prime}_{mn} = (L_{0,mN} L^z_{,Nn} + L_{0,Nn} L^z_{mN} - S^z/S_0)/S_0;$$
$$S = \sum_{n=1}^{M} \Sigma_n L_{nN}; \; N=M+1$$

can be derived from the next equation for M-vector -flux, if the terms of the order higher than α^2 are neglected:

$$V\Psi(\alpha^2) = \Sigma_s L^{(\theta)}(\alpha^2)\Psi + Q(\alpha^2);$$
$$L_{mn}(\alpha^2) = L_{mn}(\alpha^2) + \Theta L'_{mn}(\alpha^2);$$
$$L'_{mn}(\alpha^2) = L_{mN}(\alpha^2) L_{Nn}(\alpha^2) / S(\alpha^2);$$
$$(\alpha^2) = \sum_{m=1}^{M+1}\Sigma_m L_{mN}(\alpha^2);$$
$$N \equiv M+1$$

The current $\bar{J}_0$ for θ differing from 1 , and its axial component can be presented as the next sums (<I, -symbol of summation):

$$\bar{J}_0 = \langle I,(E-\Theta)\Sigma L'_0 \Psi_0\rangle;$$
$$\bar{J}_0^z = \langle I, V(\Sigma-\Sigma_s)\Phi^z - \Sigma[L^z + (\Theta-E)L^{z'}]\Psi_0\rangle \qquad (3.3c.13)$$

The equations for Λ^z now can be presented as follows:

$$(\bar{\Lambda}_2^z)^{-1}J^{(g)} + \Lambda_2^{-1}J^{z(g)} + N_0^{(z)} = N^{z(g)};$$

$$Q^z J^{(g)} + QJ^{z(g)} + K_0^{(z)} = K^{z(g)};\ (g=2,\ldots G); \qquad (3.3c.14)$$

$$K_i^{z(g)} = \int_{\Delta u_i} \nu\Sigma_f\Phi^{z(q)}dudV;$$

$$N_0^{(z)} = N^{z(1)};\ K_0^{(z)} = K^{z(1)};\ \bar{\Lambda}_2^z = -\Lambda_2(\Lambda_2^z)^{-1}\Lambda_2$$

Matrix elements for different currents at cell boundary are determined by the same collision probabilities (or modified "collision probabilities), the difference - only in parameter θ.

4. Methods of Solution of Heterogeneous Reactor Equations

4.1 *A method of solution of heterogrnrous reactor equations based on matrix transformations*

Heterogeneous reactor equation can be written is as follows:

$$N = (H\gamma_1 /\lambda - H\gamma_2) N ; \quad H = C\mathcal{J}C^{-1}; \quad \mathcal{J} = K + IF \qquad (4.1.1)$$

The norm of operator H can be estimated by a sum

$$\sigma_j = \sum_k K_0(\kappa_j | \mathbf{r}_l - \mathbf{r}_k |)$$

or approximately by the integral

$$\sigma_j = (2\pi/a^2)\int kdkK_0(\kappa_j k) = (2\pi/\kappa_j^2 a^2)$$

For a finite reactor with regular lattice the solution can be presented in as $\exp(i\alpha ka)N(r_k)$ and the above the sum is estimated by an equality

$$\sigma_j = 2\pi/[\kappa_j^2 a^2(1+\alpha^2 \kappa_j^{-2})] \qquad (4.1.2)$$

$$N = \begin{pmatrix} n_1 \\ n_2 \\ . \\ . \\ n_G \end{pmatrix}$$

has K-subvectors n_i as its components.

Suppose linear relations exist between n_i and n_G:

$$n_i = U_i n_G \qquad (4.1.5)$$

$$N = U n_G$$

$$U = \begin{pmatrix} U_1 \\ U_2 \\ . \\ U_{G-1} \\ 1 \end{pmatrix} \qquad (4.1.6)$$

$$TU n_G = (\gamma_1/\lambda - \gamma_2) U n_G \qquad (4.1.7)$$

The first row is used for determination of unknown value n_G:

$$T_{11}U_1 n_G = \sum_j (\gamma_1)_{1j}(U_j / \lambda) n_G \qquad (4.1.8)$$

$$n_j = (H_1 / \lambda) n_G$$

The other relations consider as the requirment for U-components determination (j=2, ...G):

$$(T+\gamma_2)_{21}U_1 + \ldots+(T+\gamma_2)_{2,G-1}U_{G-1}= -(T+\gamma_2)_{2,G}$$
$$(T+\gamma_2)_{G1}U_1 + \ldots+(T+\gamma_2)_{G,G-1}U_{G-1}= -(T+\gamma_2)_{G,G} \quad (4.1.9)$$

For G=2:

$$(T_{21}+\gamma_{2,21})U_1 = -(T_{22}+\gamma_{2,22})$$
$$U_1 = -(T_{21}+\gamma_{2,21})^{-1}(T_{22}+\gamma_{2,22}) \quad (4.1.10)$$

$$T=C\mathcal{J}C^{-1}=$$
$$=\begin{pmatrix} \mathcal{J}_1^{-1} & 0 \\ c_{21}(\mathcal{J}_1^{-1}-\mathcal{J}_2^{-1}) & \mathcal{J}_2^{-1} \end{pmatrix} \quad (4.1.11)$$

so that H_1 is as follows:

$$H_1 =U_1^{-1}\mathcal{J}_1U_1\,\gamma_{1,11} +(1+\mathcal{J}_2\,\gamma_{2,22})^{-1}[c_{21}(\mathcal{J}_1-\mathcal{J}_2)-\gamma_{2,21}]\,\gamma_{1,12} \quad (4.1.12)$$

For small channels with no absorption and fissions in epithermal region

$$H_1 = (1+\mathcal{J}_2\,\gamma_{2,22})^{-1}[c_{21}(\mathcal{J}_1-\mathcal{J}_2)]\,\gamma_{1,12} \quad (4.1.13)$$

The properties of operator $(1+\mathcal{J}_2\,\gamma_{2,22})^{-1}$ become clear from the next homogeneous analogy. Consider two Green functions in a homogeneous media with absorption macroscopic cross-section

$$\Sigma_a= \Sigma_{a1}+\Sigma_{a2}$$
$$(-\Delta+\Sigma_a/D)G(\mathbf{r},\mathbf{r}_0) = \delta(\mathbf{r}-\mathbf{r}_0)/D$$
$$(-\Delta+\Sigma_{a1}/D)G_1(\mathbf{r},\mathbf{r}_0) = \delta(\mathbf{r}-\mathbf{r}_0)/D \quad (4.1.14)$$

The solution of the equation with an arbitrary source S:

$$(-\Delta+\Sigma_a/D)N=S/D \quad (4.1.15)$$

can be written in a form:

$$N(\mathbf{r}) = \int G(\mathbf{r},\mathbf{r}_0)\,S(\mathbf{r}_0)\,d\mathbf{r}_0 \quad (4.1.16)$$

or , transforming the equation (4.1.15)

$$(-\Delta+\Sigma_{a1}/D)N=S/D-N\Sigma_{a2}/D$$

in the following form:

$$N(\mathbf{r}) = \int G_1(\mathbf{r},\mathbf{r}_0)\,S(\mathbf{r}_0)\,d\mathbf{r}_0-\Sigma_{a2}\int G_1(\mathbf{r},\mathbf{r}_0)\,N(\mathbf{r}_0)\,d\mathbf{r}_0$$

Define operator:

$$A_1(\cdot)\equiv\int G_1(\mathbf{r},\mathbf{r}_0)\,(\cdot)\,d\mathbf{r}_0$$

then

$$N = (1+A_1\Sigma_{a2})^{-1}A_1S \qquad (4.1.17)$$

So that we have next decomposition of Green function G by means of Green function G_1

$$G(\mathbf{r},\mathbf{r}_0)=G_1(\mathbf{r},\mathbf{r}_0) - \int G_1(\mathbf{r},\mathbf{r}_1)\, G_1(\mathbf{r}_1,\mathbf{r}_0)\, d\mathbf{r}_1\, \Sigma_{a2} + (-1)^k \int G_1(\mathbf{r},\mathbf{r}_1)\, G_1(\mathbf{r}_1,\mathbf{r}_2)\ldots G_1(\mathbf{r}_k,\mathbf{r}_0) d\mathbf{r}_k\, \Sigma_{a2}^k + \ldots \qquad (4.1.18)$$

Thus we have a decomposition

$$A=(1+A_1\Sigma_{a2})^{-1}A_1 \qquad (4.1.19)$$

In a similiar way operator

$$(1+\mathcal{J}_2\,\gamma_{2,22})^{-1}\,\mathcal{J}_2$$

presents a Green function in a heterogeneous media, with $\mathcal{J}_2$ presenting Green function in the moderator.

In 3-group approximation matrices U_1 and U_2 are calculated as follows:

$$U_1=(W_{32}W_{22}^{-1}\,W_{21}-W_{31})^{-1}(W_{33}W_{32}W_{22}^{-1}\,\gamma_{23});$$
$$U_2= -W_{22}^{-1}\,(\,\gamma_{23}W_{21}U_1), \qquad (4.1.20)$$
$$W_{ij} = T_{ij}+\gamma_{2,ij} \qquad (4.1.21)$$

and matrices T - from the relations:

$$S_i \equiv T_{ii} = \mathcal{J}_i^{-1} \quad , I=1,2,3; \quad T_{21} = c_{21}(S_1 - S_2); \quad T_{32} = c_{32}(S_2 - S_3);$$
$$T_{31} = c_{31}(S_1 - S_3)+c_{21}c_{32}(S_3 - S_2); \qquad (4.1.22)$$

For large arguments and large indices the expressions

$$I_{v-n}(\chi_j r_k)I_{v-m}(\chi_j r_l)\frac{K_v(\chi_j R)}{I_v(\chi_j R)},$$

n, m = 0, 1,
with asymptotic behaviar:

$$I_{v-n}(z) \approx \exp(z)/\sqrt{2\pi z};$$
$$K_v(z_0) \approx \sqrt{\pi/2z_0}\,\exp(-z_0)$$

are to be calculated. In this case instead of Bessel functions their products by exponential functions should be calculated and after that exponential multipliers depending on $z-z_0$ be applied.

A method of simple iterations may be used for the solution of equation for n_G:

$$n_G^{(n+1)} = H_1\, n_G^{(n)}; \quad \lambda^{(n+1)} = \varphi(n_G^{(n+1)})/\varphi(n_G^{(n)}) \qquad (4.1.23)$$

φ - a linear functional.
Iterations are finished if the next condition is fulfilled:

$$\delta^{(k)} \equiv \max_1 \left| n_{G,1}^{(k+1)} - n_{G,1}^{(k)} \right| \le \varepsilon \qquad (4.1.24)$$

ε- a chosen small value.

4.2 *Application of group-theoretical analysis for reduction of problem dimension*

Symmetry in the reactor can be used for the reduction of problem dimension.
First transform the heterogeneous equation as following:

$$(1+CKC^{-1}\gamma_2)N=[C(K+IF)C^{-1}\gamma_1/\lambda-CIFC^{-1}\gamma_2]N \quad (4.2.1)$$

$$U=(1+CKC^{-1})\gamma_2);\ N^*=UN;\ \gamma^*=\gamma U^{-1} \quad (4.2.2)$$

$$N^*=[C(K+IF)C^{-1}\gamma^*_1/k - CIFC^{-1}\gamma^*_2]N \quad (4.2.3)$$

In the above equation matrix F is the full matrix (with zero diagonal elements) and it depends only on **l** and **k** channels positions, while γ- matrices depend on the properties of a **k** channel. Consider a cylindrical reactor with different channels placed in a regular lattice, so that under group transformations
$(g\subset\mathcal{b})$,
this lattice superimposes with itself. Let $\mathcal{b}=C_{Mv}$ (M=4, square lattice)
Consider a channel with the number **l**, and all the channels with the numbers:
$\{gl\}=\{l, \sigma_1 l, cl, c,\sigma_1 l, ...\}$,
Consider also **k** channel and all the channels: $\{gk\}=\{k, \sigma_1 k, ck, c\sigma_1 k, ...\}$.
If independently $g_1, g_2\subset\mathcal{b}$ then we have 2Mx2M=64 matrix elements:
$F(g_1 l, g_2 k)$, $g_1, g_2 \in \mathcal{b}$
But due to symmetry (Fig. 4.1)
$F(cl, ck) = F(l,k)$ and this is fulfilled for all $g\subset\mathcal{b}$ $F(gl, gk) = F(l,k)$
Therefore:
$F(g_1 l, g_2 k) = F(l, g_1^{-1}g_2 k)$, $g = g_1^{-1}g_2\subset\mathcal{b}$ and for determination of all the elements $F(g_1 l, g_2 k)$ it is enough to calculate the elements: $F(l, gk)$, $g \in \mathcal{b}$.
The number of these elements is 2M=8
Let there is some symmetry in channels properties, for example for **k** and c^2**k** the properties are the same.
Let H is a subgroup with the elements $\{h\}=\{e, c^2\}$. Take elements $g \in \mathcal{b}$ and consider a set of elements $gH=\{g, gc^2\}$.
Then group $\mathcal{b}$ is splitted into left cosets - conjugacy classes with no intersections (factor space of $\mathcal{b}$ by H): $\mathcal{b}/H=\{g_1H, g_2H,...\}$.
Let x,y,... are the points of this space. Matrix elements now depend on the pairs of these points F(x,y). For the example above these poits are $X \ni x_1=\{l, c^2 l\}$; $x_2=\{\sigma_1 l, c^2\sigma_1 l\}$; $x_3=\{cl, c^3 l\}$; $x_4=\{c\sigma_1 l, c^3\sigma_1 l\}$and the same for Y, so that matrix element are to be determined as follows:
$F(x_1, y_1)=F(l,k) + F(l, c^2 k)$ and so on.
To find matrix elements for x, y; $x \in X$ and $y \in Y$
it is necessary to take the sum:

$$\sum_h F(l, hk), h \in H$$

In a more complicated case , for example dipole approximation more detailed group-theoretical analysis is needed. Consider again $\mathcal{b}=C_{Mv}$ (Fig.4.2);

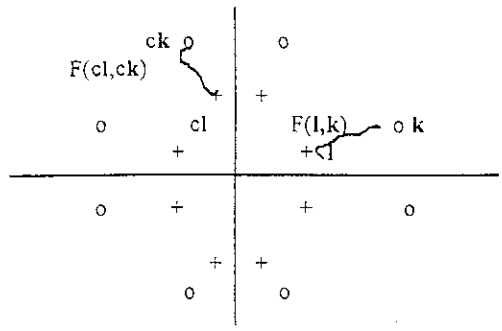


Fig. 4.1. Matrix elements for pairs of channels after group transformation

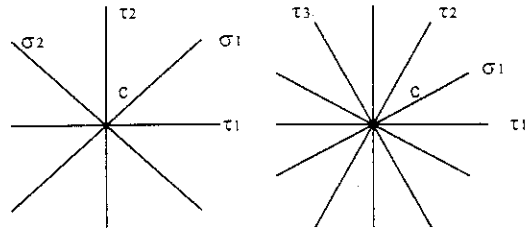


Fig. 4.2. Symmetry elements for groups C_{4v}, C_{6v}

The main relations in this group are (τ_1 -reflection relative to x-axis etc.):

$c^k c^l = c^{(k+l) \mathrm{mod} M}$; $c\tau_j = \sigma_j$; $\tau_j^2 = e$; $\sigma_j^2 = e$;
$\tau_2 = c\tau_j c^{-1}$ i=1,2(3). (4.2.4)

Let x be some node of lattice and gx its image. The set X={gx},g $\in$ $\mathcal{b}$ is a $\mathcal{b}$-orbite, or a uniform space, so that the set of all the nodes is splitted into orbites. The set h$\in$H$\in$$\mathcal{b}$, {h:hx=x} is a subgroup, - a stationary subgroup of point x, and uniform space is isomorphic to factor- space $\mathcal{b}$/H. For example, if the channel position is on x-axis, then stationary subgroup is $H=Z_\tau$, $Z_\tau=\{e,\tau_1\}$. For the channel in the center of coordinate $H=\mathcal{b}$.

Fig.4.3 shows different uniform spaces.

For a fixed point x_0 and for all the elements x$\in$X choose an element s(x)$\in$$\mathcal{b}$, so that
$s(x)x_0 = x$ (4.2.5)
that is a unique correspondence is stated between elements

$X \ni x \quad \leftarrow \rightarrow s(x) \in \mathcal{b}$ (4.2.6)
then for each element g there exist unique decomposition
$g = s(x)h(g)$ (4.2.7)
that is *cross-section* s(x) in $\mathcal{b}$ has a unique correspongence with x$\in$X, and function $h^{-1}(g)$ gives a projection g$\rightarrow$X (Fig. 4.4.)

For example for uniform space X_2 a cross section can be chosen as follows (Fig. 4.5.) :
$x_1 \leftarrow \rightarrow e$; $x_2 \leftarrow \rightarrow c\tau_1$; $x_3 \leftarrow \rightarrow c^2$; $x_4 \leftarrow \rightarrow c^3$
For the given cross-section the element σ_2 can be presented as follows:

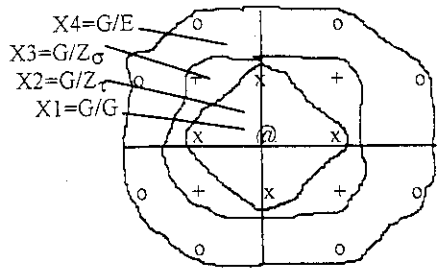
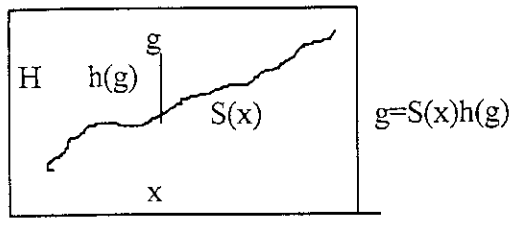


Fig. 4.3. Orbits in a reactor with square lattice



X=G/H

Fig. 4.4. Decomposition of group over uniform space X

$\sigma_2=c\tau_2=cc\tau_1c^{-1}=c^3\tau_1=s(x_4)\tau_1$; $h(\sigma^2)=\tau_1$

Suppose on X a space of functions $f(x)\in L(x)$ is given with the image in a linear space L_1 and these functions are transformed due to some representation of group H:

$h \rightarrow U(h)$; $h_1h_2 \rightarrow U(h_1h_2)=U(h_1)U(h_2)$

A *representation* of group $\mathcal{b}$ *induced* by U(h) is defined by equalities:

$$[T(g)f](x) = U^{-1}(h)f(g^{-1}x) \qquad (4.2.8)$$

with h determined from the relation:

$$g^{-1}s(x) = s(g^{-1}x)h \qquad (4.2.9)$$

that is the image is the value of f in the point $g^{-1}x$, transformed by U(h) with h determined by (4.2.9) (Fig. 4.6.)

Another equivalent realization of induced representation - in the space of functions on $\mathcal{b}$, but not on X : $\varphi(g)\in l(\mathcal{b})$. This subspace is determined by the following properties:

$$l(\mathcal{b})=\{\varphi(g) : (gh) = U^{-1}(h)\varphi(g)\} \qquad (4.2.10)$$

Projection operator from $L(\mathcal{b})$ to l(g) is:

$$P : L(\mathcal{b}) \rightarrow l(\mathcal{b}),\ P = \sum_{h\in H} U(h)\varphi(gh) / \dim H$$

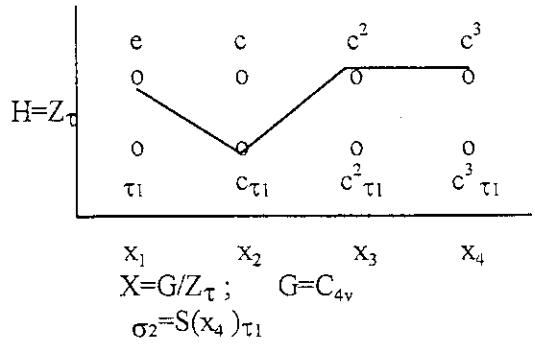


Fig. 4.5. An example of cross-section for X_2 space

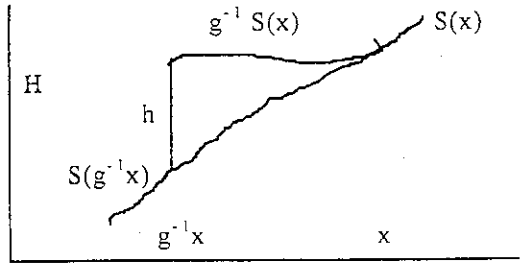


Fig. 4.6. Description of induced representation

The induced representation is given by a relation:

$$[T(g_1)\varphi](g) = \varphi(g_1^{-1}g) \qquad (4.2.11)$$

with the values of φ determined by their values on s(x) and U(h).
Suppose two orbites are given : X and Y and a linear operator C from L(X) to L(Y):

$$C:\varphi(y) = \sum_{x\in X} c(y,x) f(x) \qquad (4.2.12)$$

with two representations T_1 and T_2 induced correspondingly by
$U_1(h_1)$, $h_1 \in H_1$; $U(h_2)$, $h_2 \in H_2$;

Operator C is called a binding operator if the next diagram is commutative:

$$\begin{array}{ccc} & C & \\ L(x) & \longrightarrow & L(y) \\ \Big| & & \Big| \\ T_2(g) \downarrow & & \downarrow T_1(g) \\ & C & \\ L(x) & \longrightarrow & L(y) \end{array}$$

Binding operators present a class of operators

$$L(X) \xrightarrow{C} L(Y),$$

that is invariant relative to $\mathfrak{b}$:

$$c(gy,gx)= U_1(h_1)\, c(y,x)U_2^{-1}(h_2); \qquad (4.2.13)$$
$$gs(y)=s(gy)(h_1); \quad gs(x) = s(gx)h_2.$$

In the equivalent representation for the functions on the group $\mathfrak{b}$ in the spaces $l_1(\mathfrak{b})$ and $l_2(\mathfrak{b})$, the binding operator is given by the next relations:

$$\varphi(g_1) = \sum_{g_2} \Phi(g_1^{-1} g_2) f(g_2); \qquad (4.2.14)$$
$$\Phi(h_1 g h_2) = U_1^{-1}(h_1)\Phi(g)\, U_2(h_2),$$

In other words matrix elements are given by a function $\Phi(g)$ that is constant on double factor spaces $H_1\backslash\mathfrak{b}/H_2$ (and changing only by U-operators). It follows that the dimension of C-space is determined by the number of double conjugacy classes or: by the number of H_1 orbits in X or the number of H_2 -orbits in Y. In any case this dimension is lower than dimension of the group $\mathfrak{b}$. The order of space of arbitrary linear operators from L(X) to L(Y) is equal dimX×dimY, if L_1 is one-dimensional.

For example (Fig.4.7.),

$H_1=Z_\tau \times C_2$; $H_2=Z_\sigma \times C_2$; $X=\mathfrak{b}/H_2$; $Y=\mathfrak{b}/H_1$

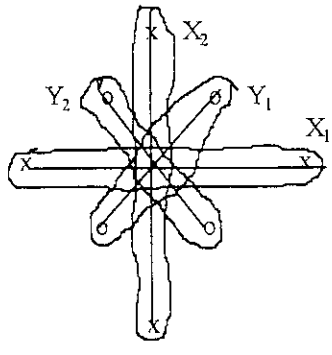


Fig. 4.7. Determination of the dimension of the space of binding operators

The space of H_1 -orbits in X consists of one orbit, coincident with all the space $X:\{x_1,\sigma_1 x_1\}=\{x_1,x_2\}=X$, that is the dimension of binding operators is equal unity, so that only one matrix element should be determined (in monopole case).
Dipolar part is a two-dimensional vector , that is the space L_1 is two-dimensional. It can be decomposed into two one-dimensional spaces.

Consider an orbit: $X=\mathcal{H}/E$. Suppose a vector field is given on X, that is the space of functions with its images in E_2. For a transform $x\to gx$ function f is transformed in the following way:

$$[T(g)f](x)=V(g)f(g^{-1}x). \qquad (4.2.15)$$

$V(g)$ - some transformation $E_2\to E_2$.
Take a decomposition of f in the basis $\mathbf{n}$, τ;
$\mathbf{n}$ is a unit vector with the direction from cymmerty center to point x and τ - a unit vector ortogonal to $\mathbf{n}$. Then

$$[T(g)(f_n\mathbf{n}_x+f_\tau\tau_x)](x) = V(g)[f_n(g^{-1}x)\mathbf{n}_{g^{-1}x}+f_\tau(g^{-1}x)\tau_{g^{-1}x}].$$

But

$$V(g)\mathbf{n}_{g^{-1}x}=\mathbf{n}_x \quad V(g)\tau_{g^{-1}x}=\mathbf{n}\tau_{g^{-1}x}=J(g)\tau_x$$

with

$$J(g)=\begin{cases} 1 & g\in H_c \\ -1 & g\notin H \end{cases} \qquad J(g_1g_2)=J(g_1)\,J(g_2). \qquad (4.2.16)$$

where H_c is a maximal subgroup with generator c, so that $\mathcal{H}=H_c\oplus\tau H_c$;
and vector-field is decomposed to two one-dimensional components:

$$[T(g)f_n](x)=f_n(g^{-1}x);$$
$$[T(g)f_\tau](x)=J(g)f_\tau(g^{-1}x). \qquad (4.2.17)$$

The construction of induced representations for f_τ can be described as follows.
Suppose we have a fixed point and a cross-section:

$$x=s(x)x_0; \quad x \leftarrow\!\!\!\rightarrow s(x)$$

Instead of $f_\tau(x)$ consider $\varphi_\tau(x)=J(s(x))f_\tau(x)$, with an operator multiplier on X

$$B(x)\equiv J(s(x)) \qquad (4.2.18)$$

The transformation of φ_τ is given by the next expression :

$$[T(g)\,\varphi_\tau](x) = \varphi_\tau(g^{-1}x). \qquad (4.2.19)$$

If $X=\mathcal{H}/H$, then

$$[T(g)\,\varphi_\tau](x) = U^{-1}(h)\,\varphi_\tau(g^{-1}x)\ ;\ g^{-1}s(x)=s(g^{-1}x)h. \qquad (4.2.20)$$

An arbitrary function f_τ transforms in a following way:

$$[T(g)f_\tau](x) = B^{-1}(x)\, U^{-1}(h)\, B(g^{-1}x)\, f_\tau(g^{-1}x)\,; \qquad (4.2.21)$$

If we accept for H including Z_σ or Z_τ , to choose cross-sections with no change of the orientation:

$(X = \mathcal{b}/Z_\sigma\,,\ x_k \leftrightarrow c^k$ or $x_k \leftrightarrow c^k\,\sigma_1)$, then $B^{-1}(x)\, B(g^{-1}x) = J(s(x)J(s(g^{-1}x)) = 1.$

If $H=C_{M_1}$, $\quad 1 \le M_1 \le M$,
$B^{-1}(x)\, B(g^{-1}x) = J(g).$ $\qquad (4.2.22)$

Binding operator has a characteristic property

$$c(gy,gx)=B_1^{-1}(gy)\, U_1(h_1)\, B_1(y)c(y,x)\, U_2^{-1}(h_2)B_2(gx)$$

$$B_1^{-1}(gy)\, B_1(y) = \begin{cases} J(g), & \text{if } H_1=C_{M_1}, \\ 1, & \text{if } H_1 \text{ includes } Z_\sigma \text{ or } Z_\tau \end{cases} \qquad (4.2.23)$$

In the following J (g) is supposed to be unity for monopole or normal dipole component and as determined above for tangential component.

Suppose a reactor loading has a symmetry of group R and some set of cnannel centers is defined - a uniform space $X=\mathcal{b}/H$. This space is decomposed to R-orbits -space X_R

$$\mathbf{X}_R=\omega_1 \cup \omega_2 \cup \ldots = R \setminus \mathcal{b} / H, \qquad (4.2.24)$$

If for example $H=Z_\tau$ and $R=Z_\sigma$,

$\mathbf{X}_R=\omega_1 \cup \omega_2$; $x_k \leftrightarrow c^k x_0$; $\omega_1=\{x_0, x_1\}$ $\omega_2=\{x_2, x_3\}$.

Is $\mathbf{X}_R$ a uniform $\mathcal{b}$-space? In this case not (Fig.4.8): $cx = x \in \omega_1$, $cx = x \in \omega_2$;
that is one element of $\omega 1$ after transformation lays in $\omega 1$ the other in ω_2.
$\mathbf{X}_R$ is a uniform space if R is a normal subgroup:

$$X_R = R \setminus \mathcal{b} \ / H = \mathcal{b}/RH. \qquad (4.2.25)$$

If for example $R=\{c^{2k}\}$; $k=0,1$; $H=Z_\tau$. Then $\mathbf{X}_R=\omega_1 \cup \omega_2$; $\omega_1=\{x_0, x_2\}$ $\omega_2=\{x_1, x_3\}$.
The elements g do next transformations on $\mathbf{X}_R$
c: $\omega_1 \leftrightarrow \omega_2$; σ_1: $\omega_1 \leftrightarrow \omega_2$; τ_1 : $\omega_1 \leftrightarrow \omega_1$, $\omega_2 \leftrightarrow \omega_2$;
that is ω_1 , ω_2 transform to each other. Therefore instead of R for symmetry group a maximal-normal subgroup is to be taken in this group.
For example if loading symmetry correspond to Z_τ then maximal normal subgroup is E, so that reactor is to be considered as fully non symmetric (in loading).
So if we take as symmetry group only normal subgroups, then binding operators dimension is determined by the number of H_1 orbits in X_R or the numbers of H_2 -orbits in Y_R , that is by the number of double classes :

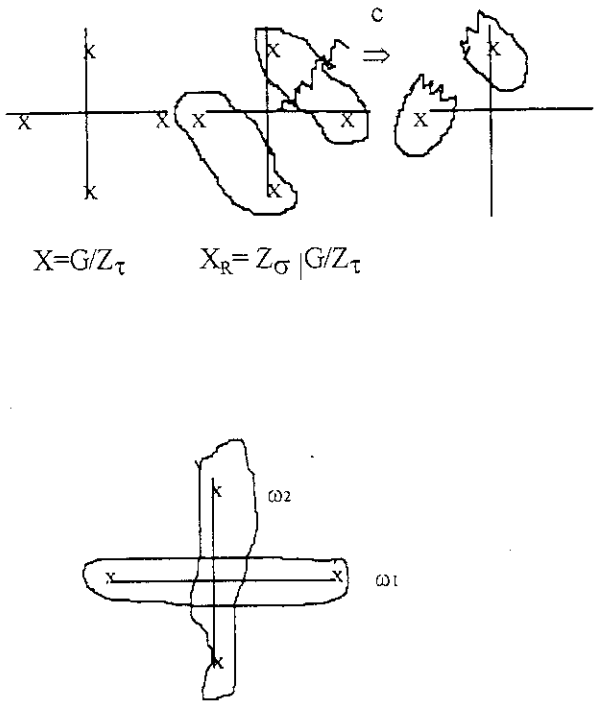


Fig. 4.8. The example of X_R being not a uniform space (above) and uniform space (below)

$$RH_1 \backslash \mathcal{b} /RH_2 = H_1 \backslash \mathcal{b} /RH_2 = RH_1 \backslash \mathcal{b} /H_2 \qquad (4.2.26)$$

Thus for symmetry group R the procedure is as follows. All channels are divided into $\mathcal{b}$-orbits $X=\{gx\}$, $g\in\mathcal{b}$.
So all the space of channels positions is a unification $X_1 \cup X_2$ .... Inside X_i an arbitrary element is taken x_i and an R-orbit is determined:
$\{rx_i\}$, $r\in R$; so that X_i is decomposed into R-orbits:

$$X_i \rightarrow X_{R_i} = \omega^i{}_1 \cup \omega^i{}_2 \ ... = \mathcal{b} /RH$$

The task is : to determine the dimensions of spaces of binding operators
$L(X_{R_i}) \rightarrow L(Y_{R_j})$,
that is the numbers of independent matrix elements; to indicate the pairs of indices for application of these matrix elements and the way they are transformed for different pairs of indices.
Suppose

$$R=\{c^{nk}\} = C_{M/n}, \text{ n divides M.} \qquad (4.2.27)$$

Below are the calculations for different pairs of spaces H1 , H2 are presented :

1. $H_1, H_2 = E$; $\mathbf{X}_R = \mathcal{b} / R$; $\mathbf{Y}_R = \mathcal{b} /R$.

Take a cross-section

$s(x_{l+nk})=c^l \sigma^k_1$ (l=0,...,n-1; k=0,1); $\sigma_1 \equiv \sigma$ (4.2.28)

and correspondingly a cross-section for elements:

$y_{\alpha+n\beta} \in Y_R (\alpha = 0,1,\ldots, n-1; \beta = 0,1);$
Binding operator is given by a formula:

$$c(y_0, x_{l+nk}) \approx \Phi(c^l \sigma^k) \equiv \Phi_{l+nk} \quad (4.2.29)$$

The next set of transformations is applied:

$g = c^\alpha \sigma^\beta,$
$gs(y_0) = c^\alpha \sigma^\beta e = s(y_{\alpha+n\beta});$
$gs(x_{l=nk}) = c^\alpha \sigma^\beta c^l \sigma^k = c^{\alpha+(-1)\beta l} \sigma^{\beta+k} =$
$= s(gx_{l+nk}) = c^\nu \sigma^\xi = s(x_{\gamma+n\xi}),$
that is

$$\alpha = (\gamma - (-1)\ l) \bmod n; \quad (4.2.30)$$
$$= (\xi - k) \bmod 2.$$

Thus matrix element $\Phi(c^l \sigma^k) \equiv \Phi_{l+nk}$ gives the relations of functions in points $x_{\gamma+n\xi}$ and $y_{\alpha+n\beta}$, with the relations between indices given by (4.2.30), the number of matrix elements equals 2n.

2.
$H_1 = E; H_2 = Z_\sigma = \{e, \sigma_1\}; X_R = \mathfrak{V} / RH_2 \ni x_i;$
$s(x_1) = c^1;$ (4.2.31)
$c(y_0, x_1) = \Phi(c^1) \equiv \Phi_1;$
$l = 0,\ldots, n-1;$
$gs(x_l)=c^\alpha \sigma^\beta c^l = c^{\alpha+(-1)^{\beta_l}} \sigma^\beta = s(gx_l)h_2;$ $s(gx_l) = c^\nu = c^{\alpha+(-1)^{\beta_l}};$ $h_2 = \sigma^\beta$

Thus n matrix elements give the relations between points x_γ, $y_{\alpha+n\beta}$, where

$\alpha=(\gamma-(-1)^\beta l) \bmod n,$ $h_2 = \sigma^\beta$

3. $H_1=E;$ $H_2=Z_\tau=\{e,\tau_1\};$ $\tau_1=c^{-1}\sigma_1;$ $X_R \supset x_l;$ $s(x_l)=c^l;$
$gs(x_l)=c^\alpha \sigma^\beta c^l = c^{\alpha+(-1)^{\beta_l+\beta}} \tau^\beta = s(gx_l)h_2;$ it follows that
$s(gx_l)=c^\gamma == c^{\alpha+(-1)^{\beta_l+\beta}};$ $h_2=\tau^\beta$ and Φ_l, $y_{\alpha+n\beta}$ x_γ have relations between indices:

$\alpha = (\gamma - (-1)^{\beta} l - \beta) \mathrm{mod} n, h_2 = \tau^{\beta}$

4. $H_1 = Z_\tau; H_2 = Z_\sigma;$

$s(x_l) = c^l; s(y_\alpha) = c^\alpha$

Since $\tau_1\sigma_1=c^{-1}$;

(4.2.32)

$\Phi(c^{l-1}) = \Phi(\tau_1\sigma_1 c^l) = \Phi(\tau_1 c^{-l}\sigma_1) =$

$= U_1(\tau_1)\Phi(c^{-l})U_2(\sigma_1)$

and binding operator is enough to calculate for points: c^l ; l=0,...,[(n+1)/2].

For

$s = c^\alpha \sigma^\chi$

$gs(y_0) = c^\alpha \sigma^\chi = c^{\alpha+\chi}\tau^\chi,$

$s(g\,y_0) = s(y_{\alpha+\chi}) = c^{\alpha+\chi};$

$h_1 = \tau^\chi;$

$gs(x_l)=c^\alpha \sigma^\chi c^l = c^{\alpha+(-1)^\chi l}\sigma^\chi = s(gx_l)h_2;$ $s(gx_l)=c^\gamma = c^{\alpha+(-1)^\chi l}$; $h_2=\sigma^\chi$;

consequently

Φ_l; l= 0,...[(n+1)/2]; x_γ, γ=0,..,n-1; y_α=0,...,n-1

$\alpha = (\gamma - (-1)^\chi l + \chi) \mathrm{mod}\, n;$

$h_1 = \tau^\chi; h_2 = \sigma^\chi; \chi = 0, 1.$

The results of all calculations are presented in the table below:
in the first row - the relations between indices of elements $x_{\gamma+n\xi}$, $y_{\alpha+n\beta}$ and Φ_{l+nk}, next row - the elements h_i, for representations $U_i(h_i)$ and finally the dimensions of Y_R, X_R and of the space of binding operators.

Table 4.2.1

	E	Z_σ	Z_τ	$\mathcal{Y}$
E	$\alpha=(\gamma-(-1)^\beta l) \mathrm{mod} n$ $\beta=(\xi-k) \mathrm{mod} 2$ 2n, 2n, 2n	$\alpha=(\gamma-(-1)^\xi l) \mathrm{mod} n$ $h_1=\sigma^\xi$ n, 2n, n	$\alpha=(\gamma-(-1)^\xi l+\xi) \mathrm{mod} n$ $h_1=\tau^\xi$ n, 2n, n	$h_1=c^\gamma\sigma^\xi$ 1, 2n, 1
Z_σ	$\alpha=(\gamma-(-1)^\beta l) \mathrm{mod} n$ $h_2=\sigma^\beta$ 2n, n, n	$\alpha=(\gamma-l) \mathrm{mod} n$ n, n, n	$\alpha=(\gamma-(-1)^\chi l+\chi) \mathrm{mod} n$ $(\chi=o,1)$ $h_1=\tau^\chi$ $h_2=\sigma^\chi$ n, n, [(n+1)/2]+1	 $h_1=c^\gamma$ 1, n, 1
Z_τ	$\alpha=(\gamma-(-1)^\beta l-\beta) \mathrm{mod} n$ $h_2=\tau^\beta$ 2n, n, n	$\alpha=(\gamma-(-1)^\chi l-\chi) \mathrm{mod} n$ $(\chi=o,1)$ $h_1=\sigma^\chi$ $h_2=\tau^\chi$ n, n, [(n+1)/2]+1	$\alpha=(\gamma-l) \mathrm{mod} n$ n, n, n	 $h_1=c^\gamma$ 1, n, 1
$\mathcal{Y}$	$h_2=c^\alpha\sigma^\beta$ 2n,1,1	$h_2=c^\alpha$ n, 1, 1	$h_2=c^\alpha$ n, 1, 1	 1, 1, 1

For symmetry group including reflection

$R = \{c^{nk}\sigma^{m}\}, m = 0, 1$ (4.2.33)

$\alpha = (\gamma - l) \bmod n$ (4.2.34)

If one of the spaces is

H_1

$H_2 = Z_\tau$

then the space of operators -one dimensional.

The groups that are not normal subgroups: n=4 for square lattice; n=3 or 6 for hexagonal lattice intis case maximal normal divider $\{c^{nk}\}$ is considered as symmetry group in R. For central channel dipolar flux is two dimensional and transforms according to representation with the next basic matrices for σ_1 and c:

$U(\sigma_1)=\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$;

$U(c)=\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ for square lattice;

$U(c)=\begin{bmatrix} 0 & -1 \\ 1 & 1 \end{bmatrix}$ for haxagonale lattice

If

$\mathbf{Y}_R = G / G$

$x_{\gamma+n\xi} \in \mathbf{X}_R$, $h_l = c^{\gamma}\sigma_l^{\xi}$

$c(y_0, gx_0) = U_l(c^{\gamma}\sigma_l^{\xi}) \times \Phi(l)\, J^{(2)}(g)$

Matrix U_l can be expressed by U(c) and $U(\sigma)$:

$U_l(c^{\nu}\sigma_l^{\xi}) = (U(c))^{\nu} U(\sigma^{\beta})$

If

$X_R=\mathcal{b}/\mathcal{b}$; then $h_2=c^{\alpha}\sigma^{\beta}$; $c(gy_0,x_0)=J^{(1)}(g)\Phi(l)U_2^{-1}(c^{\alpha}\sigma^{\beta}{}_1)$ (4.2.36)

$U_2^{-1}(c^{\alpha}\sigma_l^{\beta}) = U(\sigma^{\beta})(U(c))^{-\alpha}$ (4.2.37)

Calculation of matrix elements

At initial spaces of functions L(y), L(x), $Y=\mathcal{b}/H_1$, $X=\mathcal{b}/H_2$ an arbitrary linear operator can be presented as:

$$\varphi(y) = \sum_{x \in G/H_2} c(y, x) f(x)$$

If the lodaing in reactor corresponds to symmetry group R and the basis in L(x) is taken so that

$$f(rx) \quad V(r)f(x) \tag{4.2.38}$$

X-space is splitted to R--cosets ω_i, so that

$$\varphi(y) = \sum_{\omega \in G/RH_2} \sum_{r \in R} c(y, rx) V(r) f(x) \tag{4.2.39}$$

and in each ω a representative x is chosen. If R includes a subgroup R_0, stationary for x, then

$$\sum_{r \in R} \rightarrow \sum_{r \in R/R_0},$$

and it must be $f(x) = V(r_0)f(x), r_0 \in R_0$

The last equatity is valid if and only if

$$f(x) = P_x f(x);$$

$$P_x = \frac{1}{N_0} \sum_{r_0 \in R_0} V(r_0)$$

- projection operator on functions which are constunt relative to $V(r_0)$. Similarly an operator R_y can be defined and both operators can be included in the matrix element

$$P_y \sum_{r \in R/R_0} c(y, rx) V(r) P_x \tag{4.2.40}$$

For example if the function F(x) is transfored corresponding to the rule:
$V(e)=1$, $V(\sigma)=-1$,
and the point x is a stationary point:
σ: $\sigma x = x$ $\quad \sigma \in R_0 \subset R$

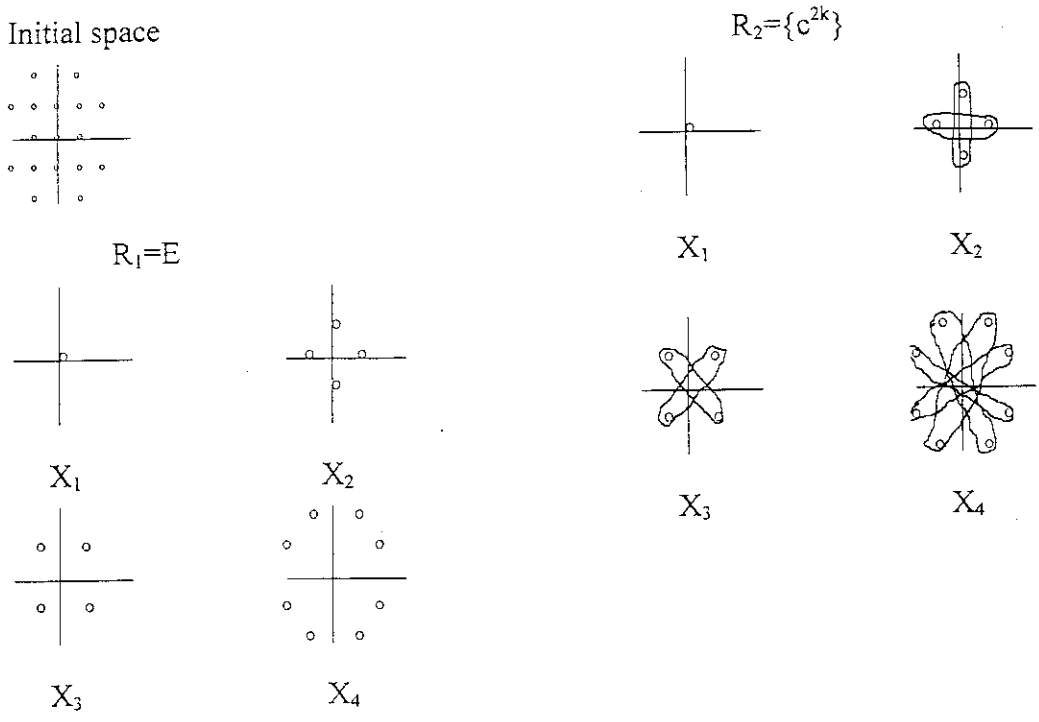
Then
$P_x = [V(e) + V(\sigma)]/2 = (1-1)/2 = 0$
so that matrix element is equal zero.
For example consider a reactor having 17 channels (see Fig. 4.9). For monopole approximation the exist 17× 17 matrix elements. The order of the spaces of binding operators $L(X_i) \rightarrow L(X_j)$ for the case of symmetry absence $R_1=E$ and for symmetry groups $R_2=\{c^{2k}\}$ and
$R_3=\{c^{2k}\sigma^j\}$ is shown in table 4.2.2 .

Table 4.2.2 Parameters for different symmetries

$X_j \setminus X_i$	X_1	X_2	X_3	X_4
X_1	1,1,1	1,1,1	1,1,1	1,1,1
X_2	1,1,1	3,2,2	2,1,1	4,2,1
X_3	1,1,1	2,1,1	3,2,2	4,2,2
X_4	1,1,1	4,2,1	4,2,2	8,4,2

4.3 An iterative method of solution of heterogeneous reactor equation based on line by line multiplications.

Contrary to the method based on matrix transformations the operator of equation (2.2) is no longer positive, on the contrary it has a structure of a difference of two operators with big norm. The next approach can be used to transform it to an operator with some property of positivity.



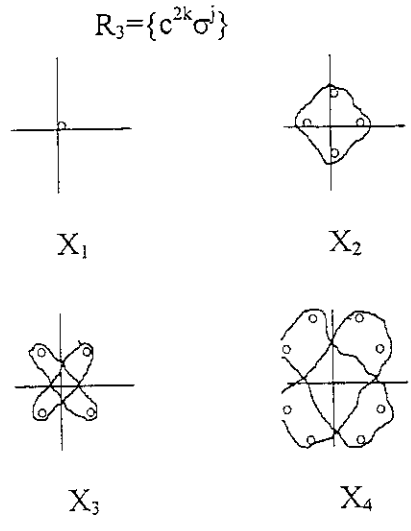


Fig. 4.9. Reactor with different symmerties

$$N=H(\lambda_0)N \tag{4.3.1}$$
$$H(\lambda_0) = H_1 / \lambda_0 - H_2 \tag{4.3.2}$$

Define functional φ_k and suppose a positivity properties are fulfilled for H_1 and H_2 operators:

$$\varphi_k(N) = n_{G,k} \tag{4.3.3}$$

$$N > 0 \rightarrow \varphi_k(H_{1,2} N) > 0$$

Corresponding to equation define operator

$$T(\bullet) \equiv \{ H_1 / \min_k [\varphi_k(H_1 \bullet) / \varphi_k((E+H_2) \bullet)] - H_2 \} (\bullet) \tag{4.3.4}$$

Non linear operator T has positivity property:

$$N > 0 \rightarrow \varphi_k(T(N)) > 0 \quad \text{for any } \mathbf{k} \tag{4.3.5}$$

since

$$\varphi_l(T(N)) = \varphi_l(H_1 N) \max_k [\varphi_k((E+H_2)N) / \varphi_k(H_1 N) - \tag{4.3.6}$$
$$-\varphi_l(H_2 N) / \varphi_l(H_1 N)] > 0$$

Besides it is a uniform operator ,

$$T(tN) = tT(N) \tag{4.3.7}$$

so that it is defined on a compact space so that it must have a stationary positive point - the solution of equation:

$$N^* = T(N^*), \varphi_k(N^*) > 0 \tag{4.3.8}$$

The iteration procedure is defined as follows

$$\lambda^{(n+1)} = \min_k [\varphi_k(H_1 N^{(n)}) / \varphi_k((E+H_2) N^{(n)})]$$
$$N^{(n+1)} = [H_1 / \lambda^{(n+1)} - H_2) N^{(n)} + \omega_n N^{(n)} \tag{4.3.9}$$

Parameter ω_n can be used for shift of operator spectrum.
Spectral radius of operator

$$(H_1/\lambda^{(n+1)} - H_2) \rightarrow 1 \quad \text{for } n \rightarrow \infty.$$

4.4 A method of solution of heterogeneous reactor equation in difference form

A nonlinear procedure is used for the solution of heterogeneous reactor equation:

$$PN = Q\gamma(K_{eff})N \quad \Rightarrow \qquad (4.4.1)$$

$$(P+S)N^{j,n} = Q\delta\gamma N^{j,n} + (1/\lambda^{j,n})\{Q[\gamma(K_{eff}^{j-1}) - \delta\gamma] + S\}N^{j,n-}$$

$$\lambda^{j,n} \to \lambda^{j};\ N^{j,n} \to N^{j}$$

$$(4.4.2)$$

$$K_{eff}^{j} = K_{eff}^{j} + (\lambda^{j} - 1)/(\partial\lambda^{j-1}/\partial K_{eff});$$

$$\partial\lambda^{j}/\partial K_{eff} = -(\lambda^{j} - \lambda^{j-1})/(K_{eff}^{j}\text{eff} - K_{eff}^{j-1})$$

$$K_{eff}^{j} \to K_{eff};\ N^{j} \to N$$

j- number in cycle of outer iteration, n- number of outer iteration; $\lambda^{j,n}$ - flow value of main egenvalue with fixed K_{eff}.

For iteration acceleration S-matrix is introduced and for separation of stable solution - triangular matrix

$$\delta\gamma = -I_0\, C^{-1}\delta\Lambda C I_0 \qquad (4.4.3)$$

$\delta\Lambda$ - lower triangular matrix with no diagonal elements
not depending on **k** and m. Negative values S of S-operator usually increase the distance between the main and the second eigenvalues.

To provide convergence of inner iterations the elements of matrix S must meet the requirement

$S \geq a\xi$

Outer iterations

The iteration procedure for λ determination (with K_{eff} fixed) can be rewritten as follows:

$$N^{n+1} = (1/\lambda^{n+1})\, HN^{n};\ H=(P+S-Q\delta\gamma)^{-1}\,[Q(\gamma(K_{eff}) - \delta\gamma)+\delta]$$

$$\lambda = l(HN^{n})/l(N^{n}) \to \lambda;\ N^{n} \to N \qquad (4.4.4)$$

$l(\psi)$ - a linear functional:

$$l(\psi) = (1/K)\sum_{k}\sum_{m=1}^{[\frac{M+1}{2}]} (1/(2\mu-1))\psi_{G,2m-1,k} \qquad (4.4.5)$$

For outer iterations the Chebyshev's acceleration procedure may be used:

$$\psi^{n+1} = HN^{n} - (\tau_{n+1} - \delta)\, N^{n}$$

$$N^{n+1} = \psi^{n+1}/l(\psi^{n+1});$$

$$\lambda^{n+1} = l(\psi^{n+1}) + \tau_{n+1} - \delta \qquad (4.4.6)$$

δ – parameter of operator spectrum shift

τ - parameter for iterations determined by the expression:

$\tau_n = ((\lambda_1 + \delta)/2)(1+\cos\pi\theta_n)$
λ_2 - estimate for second egenvalue
θ - an ordered numerical sequence inside interval [0,1]:

$$\theta \quad \{3/4,1/4,7/12,.....5/36\} \qquad (4.4.7)$$

composed of 18 elements and optimal at n=2,6,18.
Spectrum shift parameter usually is taken inside interval
$\delta \subset (2,6)$
Negative elements of S increase the distance between the main and second eigenvalue.

Inner iterations:

The solution of nonuniform linear eqution for each group g and each axial mode m is found by the symmetric successive over- relaxation method with the change of direction in step by step iterations.

$$A_{gm}\varphi_{gm} = q_{gm}$$
$$A_{gm} = P_{gm} + S_g; \qquad (4.4.8)$$
$$q_{gm} = Q\{\sum_{g'=1}^{G}\sum_{m'=1}^{M}[\gamma(K_{ef}) - \delta\gamma]^{gg'}_{mm'} N^{n-1}_{g'm'} + \sum_{g'=1}^{g-1}\delta\gamma^{gg}_{m}\varphi_{g'm}\} + S_g N^{n-1}_{gm}$$

Successive over- relaxation method for inner iterations
For a reactor with square lattice the next procedure is applied:

$$\varphi^{n}_{i,j} = (1-\omega)\varphi^{n-1}_{i,j} + (\omega/p)(\varphi^{n}_{i-1,j} + \varphi^{n}_{i,j-1} + \varphi^{n-1}_{i+1,j} + \varphi^{n-1}_{i,j+1} + q_{i,j});$$
$$i, j\uparrow; \qquad (4.4.9)$$
$$\varphi^{n+1}_{i,j} = (1-\omega)\varphi^{n}_{i,j} + (\omega/p)(\varphi^{n+1}_{i+1,j} + \varphi^{n+1}_{i,j+1} + \varphi^{n}_{i-1,j} + \varphi^{n}_{i,j-1} + q_{i,j});$$
$$i, j\downarrow;$$

ω - iteration parameter, determined from the relation:

$$\omega = 2/(1+\sqrt{1-\mu^2}) \qquad (4.4.10)$$

μ - spectral radius of a matrix A with elements divided by diagonal elements;
An analytical estimate of μ is next:

$$\mu(\text{square}) = (4/(P_0+S))(1 - \sin^2\frac{\pi}{2(N_x+1/(1-b))} - \sin^2\frac{\pi}{2(N_y+1/(1-b))});$$
$$\mu(\text{hex}) = (6/(P_0+S))(1 - 2\sin^2\frac{\pi}{2(N_x+1/(1-b))}) \qquad (4.4.11)$$

for square and hexagonal lattices correspondingly;
N_x, N_y - maximum number of channels in opposite directions along x and - axises.
The number of inner iterations can be estimated from the relation:

$$N = C\ln(1/\varepsilon)/\ln((1/(\omega-1)) \qquad (4.4.12)$$

C -an empirical constant (taken to be 2),
ε - a given accuracy of inner iterations.

Subcritical reactor with external sources

A heterogeneous reactor equation for a subcritical system with external sources q

$$N=CF(\gamma N+q) \qquad (4.4.13)$$

$q=I_0 C^{-1}S$; S external source term, can be written in a difference form

$$PN=Q(\gamma N+q);\ Q=P(I^{-1}K-D)+R; \qquad (4.4.14)$$

For an axially uniform system γ-matrix is m-diagonal (m=1,...M) and the system of equations decomposes into M independent equations, so that for a nonuniform source the result is the sum of M independent solutions.
For a weak axial dependence of γ-matrices the problem can be decomposed to a M_1 (<M) - dimensional problem and M-M_1 one-dimensional problems.

Numerical method:

The next outer iteration procedure is used

$$P N^n = Q[\delta\gamma\, N^n + (\gamma-\delta\gamma)\, N^{n-1} + q\,] \qquad (4.4.15)$$

Two-term Chebyshev method is used for
Acceleration of iterations:

$$N^n = (1-\tau_n) N^{n-1} + \tau_n (H N^{n-1} + f)$$

$$H = (P - Q\delta\gamma)^{-1} Q(\gamma-\delta\gamma); \qquad (4.4.16)$$

$f = (P - Q\delta\gamma)^{-1} Qq$
τ_n – acceleration parameter
Number of iterations grows as
$(1-\lambda_1)^{-1/2}$
λ_1
- main eigenvalue of operator H, equal 1 for critical reactor.
For weakly subcritical system with

$$1-\lambda_1 << 1-\lambda_2 \qquad (4.4.17)$$

(λ_2 -second eigenvalue) the next two - stage procedure can be applied for the choice of τ_n. At the 1st stage τ_n are chosen on the basis of uniform suppression of error inside the interval:

$\lambda \in [\lambda_{min}, \lambda_2\,]$

$\tau_n =$ (4.4.18)

$= 2/(b+a+(b-a)\cos\pi\theta_n)$

a and b - lower and upper boundaries of operator I - H
$(a = 1-\lambda_2, b = 1-\lambda_{min})$
θ_n – a numerical sequence inside interval [0,1]
- the same as used above for critical reactor calculations.

The main eigenvalue is calculated until the difference in λ becomes less than a given accuracy ε_F:

$$\lambda_1^n = 1 - 1/\tau_{n-1} + \Delta N^n / \Delta N^{n-1}$$

$$\Delta N^n = (1/K)\sum_k \sum_m (1/m)(N^n_{gmk} - N^{n-1}_{gmk}) \qquad (4.4.19)$$

$$|\lambda_1^{na} - \lambda_1^{n\,0-1}| \le \varepsilon_F$$

ε_F – agivenvalue

At the second stage the error for the main eigenfunction is suppressed and is flattened for other egenfunctions..

Take

$$\tau_{n_0+1} = \frac{1}{a_0}; \quad a_0 = 1-\lambda_1^{n_0} \qquad (4.4.20)$$

If the system of eigenfunctions is full, then the norm of error
$\varepsilon^n = N^n - N$
after n_1 iterations of second stage satisfy an unequality:

$$\left\|\varepsilon^{n_0+n_1}\right\| \le \max_{\lambda\in[a,b]} P_{n_1}(\lambda) \left\|\varepsilon^{n_0}\right\|$$

$$P_{n_1}(\lambda) = (1-\lambda/q_0)\prod_{n=n_0+2}^{n_0+n_1}(1-\tau_n\lambda) \qquad (4.4.21)$$

The parameters τ (n=n+2,...,n+n) are found from a condition that the value $\max_{[a,b]} P(\lambda)$ is minimal

For n_1=2 this problem is solved analitically:

$$\tau_{n0+2} = \begin{cases} [2b-3a_0+2\sqrt{2}\,(b-a_0)]/(4b^2-4a_0b-a_0^2); & c>0 \\ (a+b-2a_0)/(a^2+b^2-a_0(a+b)); & c<0 \end{cases} \qquad (4.4.22)$$

$$c = b-a-(a-a_0)\sqrt{2}$$

c - the point of function $P(\lambda)=(1-\lambda/a_0)(1-\tau_{n0+1}\lambda)$ extremum.
For c>0 this point is inside [a,b]
for c<0 outside [a,b]

If after 2nd stage the accuracy is not obtained the 1st stage is repeates and so on.
Calculation is finished if the following unequalities are satisfied (ε - given accuracy):

$$\frac{\ell_1[(H\quad 1)N\quad q]}{(1-\lambda_1^{n_0})L_2(N^n)} \le \varepsilon \qquad (4.4.23)$$

$$\ell_1(\psi) = (1/K)\sum_k \sum_{m=1}^{\left[\frac{M+1}{2}\right]} \frac{1}{2m-1}\psi_{g,2m-1,k}$$

$$\ell_2(\psi) = (1/K)\left|\sum_k \sum_{m=1}^{\left[\frac{M+1}{2}\right]} \frac{1}{2m-1}\psi_{g,2m-1,k}\right|$$

A rough estimate of λ_2 is possible , and some times it is enough to take it zero.
The experience of calculations has shown that for $\lambda_1 > 0.9$ two-stage procedure leads to saving in running time 3 times and more.

5. Space-time Reactor Calculations

5.1 Space-time kinetics in a reactor cell

Let channel volume is divided by L regions, I_l - number of isotopes in region l;

$$I=I_1+I_2+....I_L \qquad (5.1.1)$$

- full set of indices for isotopes in these volumes; (i=1, ...I).
Let ρ be a set of isotope concentrations in these volumes: $\rho=\{\rho_i\}$; G -number of groups in multigroup calculations of neutron space-energy distribution in the cell.

R^K means a linear vector-space of dimension K.
The following system of equations describes destruction and build-up of isotopes concentrations:

$$d\rho(t)/dt = \omega(t)[<\varphi(t),yF>_G \rho + <\varphi,(t)C>_G \rho] + \Lambda\rho; \qquad (5.1.2)$$

where
φ is vector-flux; yF - matrix of fission cross-sections and production due to fissions (y - yields of fission products; F -fissions); C - matrix of capture cross-sections; Λ - matrix of decay constants for corresponding pairs of nuclides;
$<\ ,\ >_G$ means scalar product of values depending of group index g=1,..., G;

$$\rho \in R^I; \varphi \in R^{L\times G}; yF \in R^I \times R^{I\times G};$$
$$C \in R^I \times R^{I\times G}; \Lambda \in R^I \times R^I; \qquad (5.1.3)$$
$$<\varphi, yF>_G, <\varphi, C>_G \in R^I \times R^I;$$

The equations are normalized to W - power production in an axial layer of the cell of unit height:

$$\omega=W/(e,<\varphi,F>_G\rho), \qquad (5.1.4)$$

$$dWt/dt=\omega[e,<\varphi,F>_G\rho],\ Wt\in R^L \qquad (5.1.5)$$

e - power released in fissions of corresponding isotopes;
Wt = burn-up in the layer of unity height.
It should be mentioned that yF, C and Λ are sparse matrices , diagonal relative to region index l and connecting isotopes only in a given volume:

yF- fissile isotopes and fission products ;
C - connecting isotopes (by neutron captures) with atomic masses differing by 1;
Λ - connecting isotopes with charges of nuclei differing by 1 or 2 and atomic numbers differing by 0 or 4 depending on the type of decay (β or α).

In the same way reactions (n,2n), n(3n) and so on can be included;
As soon as initial state

$$\rho(0)=\rho_0 \qquad (5.1.6)$$

is given all the connections between isotopes which are incorporated in the library must be included in the equations (5.1.2).
The time interval is divided by points $(t_0, t_1, \ldots, T)$ and for every time point a multigroup space-energy neutron distribution problem is solved. The last is the most time-consuming procedure. The cross-sections in (5.1.2) are derived from the results of these calculations as reaction rates divided by mean fluxes and nuclides concentrations in corresponding volumes.

To increase the time intervals within between re calculations for the solution of cell space-energy problems within (t_0, T) the next procedure can be accepted.

It is supposed that reaction rate r for some isotope i in some volume can be separated to thermal and epithermal parts :

$$r_i = r_{i,th} + r_{i,epi}; \qquad (5.1.7)$$

The slowing down source of neutrons entering thermal group is equal to the number of thermal neutrons absorbed in the cell. Usually removal cross-section in the cell is a weakly changing value with burn up. In this case slowing down current across upper energy boundary of thermal neutrons (the source of thermal neutrons) is close to constant value and mean flux in the channel is inversely proportional to the mean value of macroscopic absorption cross-section, so that within a given time interval the next dependence can be supposed:

$$r_{i,th}(t) = (A_i / \Sigma_a(t)) + B_i; \qquad (5.1.8)$$

where A_i and B_i are determined by reaction rate values at initial and final points of a given interval.

For resonance absorbing nuclides the next time dependence of $R_{i,epi}$ (t) is assumed:

$$r_{i,epi}(t)=a_i + b_i/\sqrt{\rho_i(t)} \qquad (5.1.9)$$

with a_i and b_i determined at the boundary points of given time interval (t_j, t_{j+1}) . Then the solution of differential equations is repeated.

5.2 *Burn-up calculations including control rod movements and refueling*

A method of simulation of 3D-space time kinetic of a reactor including burn-up of fuel assemblies, reloading of fuel, control rod movements, change of reactor power Xe poisoning and transiens, reactivity control by a solution of an absorber in moderator (boric acid) - is presented below. Heterogeneous reactor equations in a difference form are used for neutron flux description in a reactor. Some thermohydraulic models can be included for simulation general neutron termohydraulic process. Control rods movements can be used for automatic holding criticality of a reactor.

It is supposed that time interval is subdivided by fixed points and power dependence on time is a given function.

Isotopic composition for each part of a fuel assembly or an absorbing rod is supposed to depend on one or two parameters - burn up, or fluence, specific power, one of the "main" nuclides concentrations and so on. It is supposed that channel characteristics are pre calculated as function of these parameters and stored in some arrays.

Axially non-uniform channels are supposed to be placed in the nodes of square or hexagonal lattice,
boundary conditions on channel surfaces of radii ρ_k are given in the next form:

$$\rho\partial N/\partial\rho = \Lambda(z,S)N(z) - \Lambda_z(z,S)\partial^2 N(z)/\partial z^2 \qquad (5.2.1)$$

N - G×K - vector-flux (G - number of groups, K - number of channels including moderator cells);
ρ – k-diagonal matrix of radii, Λ – is composed of G×G matrices for every channel.
The state vector includes the next values:

$$S = (B(t),X(T),T(t),U(t)) \qquad (5.2.2)$$

$B= (B^1,B^2)$ - burn up, X- Xe concentrations,
T - temperature and density of coolant, U - criticality parameter (control rods depths , Boric acid concentration or k_{eff})

Neutron flux in the moderator is supposed to obey next equations :

$$-\Delta N^g(r,z,t) + \xi_g N^g(r,z,t) = \xi_{g-1} N^{g-1}(r,z,t);\ g=1,...,G \qquad (5.2.3)$$

G-number of groups, $\xi=1/\tau$ $(g<G)$; $\xi_G=1/L^2$

After finite Furie expansion

$$N^g(\mathbf{r},z)=\sum_{m=1}^{M} N^g_m(\mathbf{r})\ \sin\alpha mz,\ \alpha=\pi/H \qquad (5.2.4)$$

H -reactor height, heterogeneous reactor equation in a difference form can be written as:

$$PN=Q\,\gamma(S)N \qquad (5.2.5)$$

N - M×G×K - vector-flux,
P end Q - difference operators defined in section 2.
$\gamma(S)$ - depends (linearly) on Λ matrix (axial expansion)

B and X are given values, T and U depend on the solution N . So the above equation is a nonlinear one.

Next iteration procedure is considered:

$$PN^n = (1/\lambda^n)\, Q\gamma(S^{n-1})N^n \qquad (5.2.6)$$

$N^n \rightarrow N \quad S^n \rightarrow S; \quad \lambda^n \rightarrow 1$

N^n and λ^n are main eigenfunction and eigenvalue of linear equation (5.2.6);

$$S^n = (B, X^n, T^n, U^n)$$

$$X^n = X \text{ or } X^n = X(N^n)$$
$$U^n = U^{n-1} + (\lambda^n - 1)/\partial\lambda^{n-1}/\partial U;$$
$$\partial\lambda^n/\partial U = -(\lambda^n - \lambda^{n-1})/(U^n - U^{n-1}); \qquad (5.2.7)$$
$$T^n = T(N^{n-1}) + \beta(T(N^n) - T(N^{n-1})); \quad 0 < \beta < 1$$

Nonlinear iteration process is reduced to a successive eigensolutions of linear equations. Parameter β is introduced to provide stability of iteration procedure for the case of a strong negative thermohydraulic feedback .(calculation of boiling water reactor with strong feed back caused oscillations of solution and stability was achieved at β=0.25)

Burnup calculation
Let **k** channel is divided by L_k layers
Normalizing constants can be determined as follows:

$$A_F(t) = \sum_k \int_0^H W_k(z, B_k)\, N_k(z,t)dz \qquad (5.2.8)$$

i=1,2; (in this case i=1 is related to fuel burnup, i=2- to absorbers depletion) . The change of burn-up or other parameter describing the dependence on time within a given time interval obeys the equation:

$$\partial B_k^i(z,t) / \partial t = C_B P_t A_k^i(z,B,t)/A_F(t); \quad B_k^i(z,0) = B_0(z);$$

$$A_k^i(z, B_k, t) = \alpha_k^i(z, B_k)\, N_k(z,t) \qquad (5.2.9)$$

The values of W and α - are composed of power and reaction rate G-vectors for each axial layer of channels (cells);

$C_B = 1/E_f$ (E_f - energy release per fission) if B -the amount of fissile material per unit height of channel, α_k^i - reaction rate vector.
For a time interval (t_j, t_{j+1})

$$B^{j+1} = B^j + C_B P_t A^j / A j_F (t_{j+1} - t_j); \quad B^0 = B_0 \qquad (5.2.10)$$
j=0,1,2,...;

(the indices **k** -number of channel, l_k - number of layer in channel **k**, I , -are omitted);

$$A_j^{ij} = \alpha^i (B^j) N^j \qquad (5.2.11)$$
$$A_F^j = \sum_{k,l} W_{kl}^T (B^j_{kl}) N^j_{kl} \Delta z_l$$
$$N^j = 1/\alpha \Delta z_l \sum_m (1/m) N^j_m (\cos \alpha m z_{l-1} - \cos \alpha m z_l);$$
$$\Delta z_l = z_l - z_{l-1}$$

5.3 *Transients with xenon poisoning*

With fixed burnup I, X - I and Xe concentrations (**k** -vectors) obey the next nonstationary equations:

$$\partial I(z,t)/\partial t = y_I P(z,t) - \lambda_I I(z,t) \qquad (5.3.1)$$
$$\partial X(z,t)/\partial t = y_X P(z,t) + \lambda_I I(z,t) - (\lambda_X + A^X(z,B)) X(z,t)$$

with

$$P(z,t) = C_X P_t(t) W(z,B) N(z,t)/A_F(t) \qquad (5.3.2)$$
$$A_X(z,t) = P_t(t)\, \alpha^X N(z,B)/A_F(t)$$

$P_t(t)$ - prescribed power behavior, y_I , y_X – I and Xe yields; λ_I, λ_X -decay constants for I, X. $C_X = 1/S_F E_f$ (if I, X describe mean concentration in channels); S_F- cross-section area of fuel

At the beginning I and Xe are supposed to have stationary initial values:

$$I(z,t_0) = y_I P(z,t_0)/\lambda_I \qquad (5.3.3)$$
$$X(z,t_0) = ((y_X + y_I) P(z,t_0))/(\lambda_x + A^X(z,B))$$

Analytical solution of above equations , at the supposition of a constant P is as follows (now within a time interval corresponding to time scale splitting for description of Xe transient process):

$$I^{i+1} = D^{Ii} \exp(-\lambda_I \Delta t_{i+1}) + y_I P^i/\lambda; \qquad (5.3.4)$$

$$X^{i+1} = (D^{Ii}/(S^{Xi} - \lambda_I)) \exp(-\lambda_I \Delta t_{i+1}) + D^{Xi} \exp(-S^{Xi} \Delta t_{i+1}) + (y_X + y_I) P^i / S^{xi};$$

$$D^{Ii} = I^i - y_I P^i/\lambda_I ; \; D^{Xi} = X^i - (y_X + y_I) P^i / S^{xi} - D^{Ii} \lambda_I / (S^{xi} - \lambda_I)$$

$$I^0 = y_I P^0/\lambda_I; \; X^0 = (y_X + y_I) P^0 / S^{x0}$$

$i = 0,1,2,...$; ($l = 1,2,...,L_k$ - numbers of layers were omitted)

$$S^{xi} = \lambda_x + A^{xi}; \; A^{xi} = P^i_t \alpha^{x\,T} (B^i) N^i / A^i_F ; \; P^i = C_x P^i_t W^T (B^i) N^i / A^i_F ; \; A^i_F = \sum_{k,l} W^T (B^i) N^i \Delta Z_l;$$
$$N^i_{kl} = 1/(\alpha \Delta z_l) \sum (1/m) N^i_{mkl} (\cos \alpha m z_{l-1} - \cos \alpha m z_l); \; \Delta z_l = z_l - z_{l-1}. \qquad (5.3.5)$$

5.4 Three-dimensional simulation of transients in a heterogeneous reactor with delayed and prompt neutrons.

Non-stationary equations and non-stationary boundary conditions, accounting for a difference in neutron spectrum of prompt and delayed neutrons are applied for simulation of 3D -space -time transients. The solution is presented as a product of a 3D function as a solution of 3D stationary equation by a function describing point kinetic of mean values in the reactor. 3D solutions of heterogeneous reactor equations for critical reactor and sub critical system with external source are used for process simulation.
Consider a heterogeneous reactor with nonuniform channels in a hexagonal or square lattice. Few-group time dependent equations in the moderator can be written as follows:

$$(1/v_g D_g)\,(\partial N^g(r,z,t)/\partial t - \Delta N^g(r,z,t) + \xi_g N^g(r,z,t) = \xi_{g-1} N^{g-1}(r,z,t);\ g=1,\ldots,G \qquad (5.4.1)$$

G- number of groups, $\xi_g=1/\tau_g$ $(g<G)$, $\xi_G=1/L^2$;
τ_g, L^2 ; v_g ; D_g - age , square of neutron diffusion in thermal (G) group, neutron velocity in group g, diffusion coefficient.
Non-stationary boundary conditions on channel surfaces can be presented as:

$$\rho\,(\partial N(z,t)/\partial\rho = \Lambda^p(z,t)N(z,t) - S^d(z,t)B(z,t). \qquad (5.4.2)$$

$$B(z,t) = \Sigma\lambda_j C_j(z,t), \qquad (5.4.3)$$

- the rate of decay of precursors (supposed J groups)

$C_j(z,t)$ - concentrations of precursors of delayed neutrons,
λ_j - their decay constants.
C_j are determined from the equations:

$$\partial C_j(z,t)/\partial t + \lambda_j C_j(z,t) = \beta_j(z)W(z,t)N(z,t). \qquad (5.4.4)$$

$\beta_j(z)$ - fractures of delayed neutrons

Operators Λ, ,S, W are determined by the next expressions:

$$\Lambda^p = \Lambda^p - \Lambda^p_z(\partial^2/\partial z^2) + \Lambda^p_t(\partial/\partial t); \qquad (5.4.5)$$
$$S^d = S^d - S^d_z(\partial^2/\partial z^2); \qquad (5.4.6)$$
$$W = \omega^p N(z,t) - \omega^p_z(\partial^2 N(z,.t)/\partial z^2).$$

Λ^p, Λ^p_z, Λ^p_t, ω^p, ω^p_z and S^d, S^d_z are determined for prompt and delayed neutrons.
The boundary conditions for a stationary state:

$$J = \Lambda N;$$
$$J \equiv \rho\,(\partial N/\partial\rho);\quad \Lambda = \Lambda_1 + \Lambda_2$$
$$\Lambda_1 = -S\omega;\quad S = \Lambda_2 N^0/(1-V) \qquad (5.4.7)$$
$$\omega = q\Lambda_2;\quad V = k^0 - q\Lambda_2 N^0$$

A system of equations in the cell is used for the determination of above parameters:
Stationary system of integral equations in the reactor cell-

$$\varphi^i(\mathbf{r})=\int K_i(\mathbf{r},\mathbf{r}')\,(\Sigma^i_s\varphi^i+Q^i)(\mathbf{r}')d\mathbf{r}' \qquad (5.4.8)$$

the source consist of two terms $Q=Q_s+Q_f$ -due to scattering of neutrons from upper groups (s) and due to fissions (f).
In a non-stationary case the system of equations becomes as follows:

$$\varphi^i(r,t)= \int K_i(\mathbf{r},\mathbf{r}')(\Sigma^i_s(v')\varphi^i(\mathbf{r}',t') +Q^i(\mathbf{r}',t')d\mathbf{r}' \qquad (5.4.9)$$
$$t'=t-(|\mathbf{r}-\mathbf{r}'|)/v_i$$

Suppose:

$$Q^i_f(\mathbf{r},t) =Q^i_f(\mathbf{r},t_0)\exp(\theta t) \qquad (5.4.10)$$

t_0 - some fixed time point

Assume

$$\varphi^i(\mathbf{r},t) =\varphi^i(\mathbf{r},t_0)\exp(\theta t) \Rightarrow$$
$$\varphi^i(r,t)= \int K^i{}_\theta(\mathbf{r},\mathbf{r}')[\Sigma^i_s(\mathbf{r}')\varphi^i(\mathbf{r}',t) +Q^i(\mathbf{r}',t)]d\mathbf{r}' \qquad (5.4.11)$$

with the next difference

$$\Sigma^i_t \Rightarrow \Sigma^i_t +\theta/v_i \quad \text{in the kernel } K^i$$

Let (at the supposition that θ/v_i is small)
Λ_θ be presented as a linear function of θ:

$$\Lambda_\theta = \Lambda + \theta\,\Lambda_t \qquad (5.4.12)$$

Λ_t can be derived from the equation (5.4.12), while Λ_θ may be calculated with a 1/v absorber of small concentration included uniformly in the cell:

$$\Lambda_t = (\Lambda_\theta - \Lambda)/\theta_0 \quad \theta_0=\Sigma_{a0}v_0 \qquad (5.4.13)$$

Σ_{a0} - absorption cross-section of 1/v absorber at some velocity v_0.
Now

$$J(t) = \Lambda_\theta N(t) \qquad (5.4.14)$$

and due to the dependence

$$\partial N(t)/\partial t =\theta N(t) \qquad (5.4.15)$$

the next non-stationary equation is derived:

$$J(t) = \Lambda N(t) + \Lambda_t\,\partial N(t)/\partial t \qquad (5.4.16)$$

The last expression is valid for an arbitrary superposition:

$$Q^{i}_{f}(\mathbf{r},t) = \sum_{n} q_{n}(\mathbf{r})\exp(\theta_{n}t) + \int q(\mathbf{r},t)\exp(\theta t)d\theta \qquad (5.4.17)$$

Let us take into account delayed neutrons.
Since ωN -is the rate of fissions, present it as

$$\omega N \Rightarrow (1-\beta)\omega N + B \qquad (5.4.18)$$

B- the source due to delayed neutrons by the decay of precursors..
Parameters Λ_2, q, N^0, k^0 depend on source Q spectrum.
Since the spectrum for delayed neutrons is different from fission spectrum, additional calculations for this different spectrum are necessary. Thus next expression can be used for Λ_1:

$$\Lambda_1 N \Rightarrow (1-\beta)\Lambda^{p}_{1}N - S^{d}B; \qquad (5.4.19)$$

p - prompt; d - delayed neutrons; β – total fraction of delayed neutrons.
Non-stationary boundary conditions can be written now as follows:

$$dN = \Lambda_k^{p}(z,t)N_k(z,t) - \Lambda_{z,k}^{p}(z,t)[\partial^2 N_k(z,t)/\partial z^2] + \Lambda_{t,k}^{p}(z,t)[\partial N_k(z,t)/\partial t] - S_k^{d}(z,t)B_k(z,t) +$$

$$+ S^{d}_{z,k}(z,t)[\partial^2 B_k(z,t)/\partial z^2]; \quad dN \equiv \rho_k \partial N/\partial\rho\,|_{\rho=\rho_k} \qquad (5.4.20)$$

where

$$\Lambda^{p} = \Lambda^{p}_{2} + (1-\beta)\Lambda^{p}_{1}; \quad \Lambda^{p}_{1} = -S^{p}\omega^{p}; \quad \omega^{p} = q^{p}\Lambda^{p}_{2}; \quad S^{p,d} = -\Lambda_2^{p,d}N^{0p,d}/(1-\nu^{p,d});$$

$$\nu^{p,d} = k^{0p,d} - q^{p,d}\Lambda_2^{p,d}N^{0p,d} \qquad (5.4.21)$$

$C_{j,k}$ - the amount of precursors for group j;j=1,...,J ; J - number of groups of delayed neutrons.
Then

$$B_k(z,t) = \sum_{j}^{J} \lambda_j C_{j,k}(z,t) \qquad (5.4.22)$$

The concentrations of precursors C are defined from the next system of equations:

$$[\partial C_{j,k}(z,t)/\partial t] + \lambda_j C_{j,k}(z,t) = \beta_j W_k(z,t);$$

$$W_k(z,t) = \omega_k^{p}(z,t)N_k(z,t) - \omega_{z,k}[\partial^2 N_k(z,t)/\partial z^2], \qquad (5.4.23)$$

β_j - fraction of delayed neutrons for group j.
The initial conditions taking account of stationary state at initial moment can be written as follows:

$$-\Delta N^{g}_{o} + \xi_g N^{g}_{o} = \xi_{g-1}N_0^{g-1}; \quad g = 1,...,G \qquad (5.4.24)$$

$$\rho_k \partial N_{0,k}/\partial\rho_k = \Lambda_{0,k}N_{0,k} - \Lambda_{0z,k}\partial^2 N_{0,k}/\partial z^2; \quad \Lambda_{0k} = \Lambda^{p}_{2,0k} - [(1-\beta)S_{0,k}^{p} + \beta S_{0,k}^{d}]\,\omega_{0,k}^{p};$$

$$C_{0,jk} = (\beta_j/\lambda_j)[\omega_{0,k}^{p}N_{0,k} - \omega_{0z,k}^{p}\partial^2 N_{0,k}/\partial z^2]; \quad j = 1,...\,J$$

The system of above equations with boundary conditions and initial conditions presents a closed system of equations for non-stationary dynamic process in a reactor.

Method of solution

Time interval is devided by subintervals and neutron flux is presented as a product:

$$N^g(\mathbf{r},z,t) = P(t)\Phi^g(\mathbf{r},z,t), \qquad (5.4.25)$$

P(t) - amplitude coefficient; $\Phi^g(\mathbf{r},z,t)$ - form - function , weakly dependent on time.
Finite Furie expansion is used for flux and precursors concentrations presentetion:

$$\Phi^g(\mathbf{r},z,t) = \sum_n \psi^g{}_n(\mathbf{r}, t)\sin\alpha nz\ ; \qquad (5.4.26)$$

$$C_{jk}(z,t) = \sum_n C^n{}_{jk}(t)\sin\alpha nz$$

($\alpha=\pi/H$) sin αmz - axial modes. Next system of equations can be derived in the moderator:

$$(1/v_gD_g)\,(\partial\psi^g{}_m/\partial t-\Delta\,\psi^g{}_m+\kappa^2{}_{gm}\psi^g{}_m=\xi_{g-1}\psi^{g-1}{}_m; \qquad (5.4.27)$$

$$\kappa^2{}_{gm}=\xi_g+(1/v_gD_gP)(dP/dt)+\alpha^2m^2;\ \ g=1,...,G;\ m=1,....M;$$

with boundary conditions:

$$d\Psi = \Lambda^*\Psi - S^*\,B^*; \qquad (5.4.28)$$

$$B^*(t) = \sum_j^J \lambda_j\,C_j(t),$$

Ψ consists of G-vectors Ψ_{km} ; components of Λ^* -matrices and vector S^* are as follows:

$$\Lambda^*{}_{k\,mn}(t) = (2\alpha/\pi)\int_0^H [\Lambda^p{}_k(z,t) +\alpha^2n^2\,\Lambda^p{}_{z,k}(z,t)+[1/P(t)](dP(t)/dt)\Lambda^p{}_{t,k}(z,t)]\sin\alpha mz\sin\alpha nz\,dz;$$

$$S_{k\,mn}(t) = (2\alpha/\pi P(t))\int_0^H [S^d{}_k(z,t) +\alpha^2n^2\,S^d{}_{z,k}(z,t)]\ \sin\alpha\ mz\ \sin\alpha\ nz\ dz \qquad (5.4.29)$$

C_j -components obey the equations:

$$\partial C^m{}_{j,k}/\partial t +\lambda_jC^m{}_{j,k} = P(t)(\beta_jW^m)^*; \qquad (5.4.30)$$

$$(\beta_jW^m{}_k(t))^* = (2\alpha/\pi)\sum_{n=1}^M\int_0^H \beta_j(z)[\omega^p{}_k(z)+\alpha^2n^2\,\omega_{z,k}(z)]\ \psi_{kn}(t)\sin\alpha\ mz\ \sin\alpha n\ z\ dz.$$

Applying Furie expansion for initial moment $t=t_0$, we get:

$$-\Delta\,\psi^g{}_{0,m} + \xi_g+\alpha^2m^2)\psi^g{}_{0,m}=\xi_{g-1}\psi^{g-1}{}_{0,m}\ ;\ g=1,...,G;$$

$$d\,\Psi_0 = \Lambda^*{}_0\Psi_0\,; \qquad (5.4.31)$$

$$\Lambda_{0,k}{}^{mn} = (2\alpha/\pi)\int_0^H [\Lambda_{0,k}(z) +\alpha^2n^2\,\Lambda_{0z,k}(z)]\ \sin\alpha\ mz\ \sin\alpha\ nz\ dz$$

For determination of P(t) consider an adjoint equation:

$$-\Delta \psi^{g+}_{0,m} + (\xi_g + \alpha^2 m^2)\psi^{g+}_{0,m} = \xi_g (\psi^{g+1})^{+}_{0,m}; \qquad (5.4.32)$$

$$d\,\Psi_0^{+} = \Lambda^{*}{}_0^{+}\,\Psi_0^{+},$$

$\Lambda^{*}{}_0^{+}$ - transpose of $\Lambda^{*}{}_0$.

Multiplying equations (5.4.27) by $\psi^{g+}_{0,m}$ and equations (5.4.32) by $\psi^{g}_{0,m}$, subtracting, summing by g and by m , taking integrals over **r** and taking account of Gauss-Ostrogradsky theorem we can derive the next equation for P in the interval Δt:

$$dP(t)/dt = (\rho^{*}(t) - \beta^{*})/l \times P(t) + \sum_j \lambda_j C_j^{*}(t) \qquad (5.4.33)$$

$$\rho^{*} = \Psi_0^{+T}[\Lambda^{*}{}_0 - \Lambda^{*}(t)]\Psi/x;\ \mathbf{C}^{*}_j = \Psi_0^{+T}\mathbf{S}^{*}\mathbf{C}^{*}/(xl)$$

$$\beta^{*}_j = \Psi_0^{+T}\mathbf{S}^{*}\beta^{*}\mathbf{W}^{*}/x;\ \beta^{*} = \sum_j \beta^{*}_j;$$

$$l = \Psi_0^{+T}\Lambda_t^{*p}\Psi/x;\quad x = \Psi_0^{+T}\Lambda_1^{*p}{}_1\Psi.$$

$\beta_j{}^{*}\mathbf{W}^{*}$- vector consisting of components $(\beta_j W_k^{m})^{*}$; $\Lambda^{*p}{}_t$, $\Lambda^{*p}{}_1$- Furie expansions of Λ - matrices; ρ^{*}, β^{*}_j, C_j^{*}, l - have an evident physical meaning; x - parameter of normalization. For derivation of above equations the next condition was used:

$$d(\Psi_0^{+T}\Lambda^{p}_t\Psi)/dt = 0 \qquad (5.4.34)$$

Multiplying (5.4.30) by S^{*} and taking a supposition that it does not depend on time within a fixed time interval , multiplying by Ψ_0^{+} and taking sum over g, m, **k** we get an equation:

$$dC_j^{*}(t)/dt = (\beta_j/l)P(t) - \lambda_j C_j^{*}(t);\ j = 1,\ldots J \qquad (5.4.35)$$

The system of equations (5.4.34), (5.4.35) is a point-like system of differencial equations with the initial conditions:

$$P(t_0) = P_0;\ \rho^{*}(t_0) = 0;\ C^{*}_j(t_0) = \beta^{*}_j(t_0)P_0/(l(t_0)\lambda_j),\ j = 1,\ldots,J. \qquad (5.4.36)$$

Adiabatic approximation
The sources of prompt and delayed neutrons are united and time derivatives in (5.4.27) are supposed to be zero. For each time point the equations for criticality are calculated. For point approximation form-function is calculated only for initial state.
Quasi-static approximation
Takes account of space-time dependence of delayed neutrons precursors. The first term in equation (5.4.27) is supposed to be zero. P(t) and its derivative is determined from point kinetic equation. In this case form-function is calculated by the method of solution of heterogeneous reactor equation with external source. In a given time interval the value $\alpha_0 = 1/P(dP/dt)$ in (5.4.27) is supposed to be constant and is estimated from a previous time interval. For the initial moment it is estimated as a value $\alpha_0 = \rho_0/l_0$.

6. Perturbation Theory and Optimization

6.1 General formulation

The problem of optimization of reactor characteristics generally can be formulated as follows [5]. Consider a reactor in a steady state. Two types of variables can be defined:
1) u - a set of free parameters ("controls")
(nuclide densities, channel sizes, control rod depths etc.)

$$u \in U \qquad (6.1.1)$$

2) vector-flux N - the solution of the equation:

$$H(u,\lambda)N=0;\ H(u,\lambda)=H_1(u)/\lambda-H_2(u) \qquad (6.1.2)$$

H depends on u and its positive solution exists for a maximal positive eigenvalue λ.
Physical parameters (mean power output, critical mass etc.) are given by functionals

$$F(u,N) \qquad (6.1.3)$$

Consider a perturbation of parameters:

$$u \rightarrow u+v$$

Variation of parameters leads to a variation of flux $N \rightarrow N+n$ and a variation of functional

$$F(N,u) \rightarrow F(N+n,u+v) \qquad (6.1.4)$$

The aim of perturbation theory is to present variation of functional with the accuracy in linear terms as depending only on free value v, but not n , that depend on v in a complicated manner , since the equation (6.1.2) must be now valid for N+n, u+v:

$$F(N+n,u+v)= F(N,u)+g(N,u)v +o(||v||) \qquad (6.1.5)$$

so that g(N,u) operates only on the free variable v, but not on unknown value n.
By definition g(N,u) is the gragient of functional.
Consider a Lagrange function:

$$L_0(N^+,N,u)\equiv\langle N^+,H_2(u)N\rangle/\langle N^+,H_1(u)N\rangle \qquad (6.1.6)$$

$\langle\ \rangle$ means scalar product for all the independent variables (space, energy).
Let N_0 , N_0^+ be the solutions of reciprocal adjoint equations with he same eigenvalue:

$$HN_0=0;\ H^+N_0^+=0, \qquad (6.1.7)$$

The value of L_0 with N_0^+, N_0 is an inverse value of λ :

$$L_0(N_0^+,N_0,u)=1/\lambda. \qquad (6.1.8)$$

For a functional of the type

$$F(N,u)=P(N,u)/\ Q(N,u);\ P(N,u)=\langle I,\ p(N,u)\rangle; \qquad (6.1.9)$$

$$Q(N,u)=\langle I,q\ (N,u)\rangle$$

introduce lagrange function:

$$L_F(N^+,N,u)=[<N^+,H(u)N>+P(N,u)]/Q(N,u) \qquad (6.1.10)$$

L_F is equal F if N is the solution of equation:
$HN_0=0$
Let N^+ be the solution of the equation (index N means derivative by N)

$$H^+N^+=-p_N+Fq_N\equiv -F_N \qquad (6.1.11)$$

Then the variation of L_F does not depend on n, n^+, under the variation
$u\rightarrow u+v$, $N\rightarrow N+n$, $N^+\rightarrow N^++n^+$

That is gradient of functional F is equal:

$$g_F=[(N^+,H_uN_0)+p_u-Fq_u]/Q \qquad (6.1.12)$$

the brackets (,) mean scalar product relative to energy variable; index u - derivative by u.
The independence of functional variation on the variation of $1/\lambda$ is provided by the requirement

$$<N^+,H_1N>=0 \qquad (6.1.13)$$

that always can be fulfilled since N^+ allows an additional term:

$$N^+\longleftrightarrow N^++AN_0^+ \qquad (6.1.14)$$

and

$$<N_0^+,H_1N_0>\neq 0;\ \text{since}\ \lambda\neq 0. \qquad (6.1.15)$$

The gradient of functional $1/\lambda$ is given by the expression

$$\delta L_0=g_\lambda v;\ g_\lambda=<N_0^+,H_uN_0>/<N_0^+,H_1N_0> \qquad (6.1.16)$$

It is essential for linear perturbation theory to be able to find the solution of nonuniform equation for N^+ , provided operator $H^+(u)$ has a nontrivial solution of uniform equation:
$H^+(u)N_0^+=0$.
The solution exists if and only if the source term is orthogonal to N

$$<N_0,\ -p_N+Fq_N>=0 \qquad (6.1.17)$$

This condition is fulfilled due to definition of F.

The problem of optimization is formulated as follows.
Let a set of physical restrictions is given in the form

$$u\in -U$$
$$a_0\le F_0\equiv 1/\lambda\le b_0;\ a_j\le F_j\le b_j,\ j=1,\ldots \qquad (6.1.18)$$

Find a maximal value of functional F

$$F_J\rightarrow \max \qquad (6.1.19)$$

if N obey the equation (6.1.2).

The simplest functionals do not depend on N explicitly, in this case their gradients do not depend on N .
On the contrary functional of the type:

$$\max p(N,u)/Q \qquad (6.1.20)$$

(flattening factor) gives rise to a set of functionals for "hot" points.
Suppose some u is taken as an initial value and the gradients of functionals are calculated.
The solution of linear programming problem

$$a_j-F_j \le g_jv \le b_j-F_j,\ j=0,...,J-1, \qquad (6.1.21)$$
$$g_Jv\rightarrow\max,\ (u+v)\subset U$$

allows to improve the solution $u\rightarrow u+v$
(some restrictions are to be applied to v from the requirements that linear approximation for functional variations be valid).
The iteration procedure is defined for step by step variations of v (n=0, ...)
until linear programming problem has only zero solution (with a prescribed accuracy).
For the functional of the type

$$\max p(N,u)/Q$$

a set of K functionals corresponding to "hot" points is introduced with the restrictions:

$$g_J^kv+w\le F_J-F_J^k,\ k=1,...K \qquad (6.1.21)$$

and max value

$$w\rightarrow\max$$

is to be found.

At the initial stage, while some of the restrictions are violated some types of "punishing" functions are introduced, bringing the functionals to their boundaries.

Formulation of optimization problem for heterogeneous equations in difference form

The above theory is applicable to the solution of optimization problem governed by heterogeneous reactor equation [5,22)]

$$N = H(\gamma_1/\lambda - \gamma_2)N; \quad H = CFC^{-1}; \quad F = K + IF \qquad (6.1.22)$$

that can be presented in difference form as follows:

$$\begin{aligned} &HN=0;\ H=H_2-(1/\lambda)H_1;\\ &H_1=(PI^{-1}K+R)\gamma_1(u);\ H_2=PW(u)+R\gamma_2(u),\\ &\gamma_1(u)=-IC^{-1}\Lambda_1(u);\\ &\gamma_2(u)=-IC^{-1}\Lambda_2(u)+\partial IC^{-1};\\ &W(u)=I^{-1}(C^{-1}+K\gamma_2(u)). \end{aligned} \qquad (6.1.23)$$

The lattice and moderator properties are supposed to be fixed, the properties of channels can be varied by changing the "control" function u; $\Lambda(u)$ are supposed to be pre calculated with u-dependence presented for example by polinomials.
Adjoint operators can be written as follows:

$$\begin{aligned} &H_1^+=\gamma_1^+(u)(I^{-1}KP^+ + R^+);\\ &H_2^+=W^+(u)P^+ + \gamma_2^+(u)R^+. \end{aligned} \qquad (6.1.24)$$

symbol + means transpose relative to energy (group) index.
P^+ and R^+ are the same as P, R (except for the central channel if a symmetric problem is considered).
The derivative is written as:

$$H_u = (PI^{-1}K+R)IC^{-1}\Lambda_u;\ \Lambda_u = (1/\lambda)\Lambda_{1,u} - \Lambda_{2,u}, \qquad (6.1.25)$$

so that F gradients depend on the values

$$(N_j^+, H_u N_0) = ((I^{-1}KP^+ + R^+)N_j^+, IC^{-1}\Lambda_u N_0) \qquad (6.1.26)$$

Uniform adjoint equation for N_0^+ is solved by the same method as the equation for N_0 (for eigenvalue a more exact expression now can be used - functional L_0).
Non-uniform equation is solved as follows (starting from group G)

$$\begin{aligned} &\varphi^{m+1}=(1-\omega_{m+1})\varphi^m + \omega_{m+1}(T^+\varphi^m/\lambda + Q);\\ &T^+=(H_2^+)^{-1}H_1^+;\ Q=-(H_2^+)^{-1}(W^+)^{-1}F_{jN}.\\ &\varphi^0=0;\ \varphi^m \to N_j^+. \end{aligned} \qquad (6.1.27)$$

The eigenvalue is fixed and the inverse of H_2^+ is taken by the next iteration procedure:

$$A_g^+\psi_g = q_g;\ A_g^+ \equiv P_g^+ + \gamma^*_{2,gg}R_g^+;\ \gamma^* = \gamma W^{-1}; \qquad (6.1.28)$$

$q_g=\sum\gamma^*_{1,g'g}(\Gamma^{-1}KP^+ + R^+)_{g'}\varphi_{g'}^m + f_g - \sum_{g'=g+1} \gamma^*_{2,g'g}R^+_{g'}\psi_{g'}$; $f_g = -(W^+)^{-1}F_{jN}$

(g=G, G-1,...1)

The component N_0^+ can be excluded at the end of iterations by the condition:

$$\langle N_j^+, H_1 N_0 \rangle = 0. \qquad (6.1.29)$$

The convergence of iteration procedure is provided by next: in a subspace orthogonal to N_0^+ the spectrum of operator T^+/λ lays inside the circle of radius unity(λ– maximal eigenvalue) so that T^+/λ is a compressing operator:

$$(1/\lambda^2)\langle T^+\varphi, T^+\varphi\rangle \le (\lambda_1^2/\lambda^2)\langle\varphi,\varphi\rangle < \langle\varphi,\varphi\rangle, \qquad (6.1.30)$$

Consequently the difference between N_j^+ and its value at iteration m

$$\delta^m \equiv \varphi^m - N_j^+ \qquad (6.1.31)$$

obeys an equation

$$\delta^{m+1} = (1/\lambda)T^+\delta^m \qquad (6.1.32)$$

and due to (6.1.30) $\delta^m \to 0$ if $m\to\infty$.

6.2 Minimal critical mass

The problem of minimum critical mass is formulated as follows. Consider a cylindrical heterogeneous reactor with axially uniform channels placed in a regular lattice (hexagonal lattice was considered). The core is surrounded by radial reflector . The properties of reactors and the results of the solution of optimisation problem are given in table 6.1.

1 case

Fission and absorbing properties of channels are supposed to depend linearly on fissile material concentration. No absorption of epithermal neutrons is supposed.
The solution of this problem for one-dimensional homogeneous case is known and has been derived by Goertzel: optimal control should provide flat thermal flux in the core.
The solution of the problem stated above is similar: thermal neutron flux on all the channel surfaces with nonzero control (fuel concentration) occurred to be constant (table 6.2).

2 case

It is supposed that epithermal absorption exists and the Λ_{22} in 3-group approximation describing epithermal absorption is non-zero and is proportional to $\sqrt{U}$, simulating resonance absorption with self-shielding. The solution appeared to be typical for the case of resonance absorption: in some of the channels fuel concentration appeared to become zero (Fig. 6.1, table 6.3) so that in optimal solution a lattice changed to provide higher probability for neutrons to escape resonance absorption.

Table 6.1 Minimal critical mass problem;
Case 1 - no epithermal capture of neutrons,
Case 2-with epithermal capture of neutrons.

	Case 1	Case 2
Number of groups	2	3
Reactor radius, m	2.2	2.2
Pitch, m (hexagonal lattice)	0.28	0.20
Neutron age, cm^2	120	40;80
Square of diffusion length, cm^2	5500	5500
Number of fuel channels	199	379
Channel radius,cm	6.4	6.4
Λ–matrix	0;-0.95711U	0;0;-1.0426U
	0; 0.9U	0;0.05$U^{1/2}$; 0;
		0;0;0.9U
Critical mass		
initial	199	379
minimal	110.67	38.04

Table 6.2. Case 1. Optimal fuel concentration (upper values) and thermal flux (lower values)
(initially U=1. for all fuel channels)

												0 0.37		
									0.20 1.00		0 0.75		0 0.34	
						1.16 1.00		0.66 1.00		0.14 1.00		0 0.67		0 0.25
			1.99 1.00		1.59 1.00		1.08 1.00		0.54 1.00		0 0.98		0 0.50	
2.32 1.00		2.21 1.00		1.89 1.00		1.41 1.00		0.86 1.00		0.30 1.00		0 0.77		0 0.30

Table 6.3 Case 2 . Optimal fuel concentrations (upper values)
and thermal flux (lower values);
(initially U=1. for all fuel channels)

							0.47 0.59	
					0.62 0.64	0.54 0.59		
			0.71 0.73	0.66 0.68			0.51 0.57	0.41 0.51
	0.74 0.78	0.72 0.75			0.64 0.66	0.57 0.61		

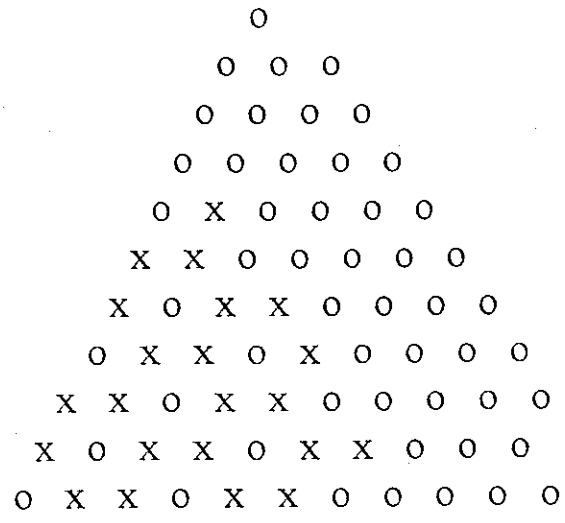


Fig 6.1. Minimal critical mass; case 2
(with epithermal capture of neutrons);
o - fuel concentration zero in optimal solution;
x - fuel concentration non zero.

6.3 Optimal power distribution flattening by control rods movements

The next problem is considered:
for a given set of control rods find its positions giving the best flattening of power distribution in the reactor.

Optimization problems usually are effectively solved by the method of sequential linearizing (reducing of initial nonlinear problem to a sequence of linear optimization problems). Yet due to high nonlinearity of the problem under consideration relative to control rod positions an alternative approach to the solution of neutron power flattening by control rods is applied. The method is based on the change of variables - control rod positions to reactivities inserted by control rods movements (this approach was used in the work: Afanasiev A.M. "Optima"-computer code for optimal power ditribution in a reactor", Preprint ITEP (Russ.), N 112, Moscow, 1982 and applied by Malofeev V.M (3D power flattening in a heterogeneous reactor, Report ITEP(Russ.), N 804, Moscow, 1992) to heterogeneous reactor. It can be expected that the dependence of power distribution due to changes of reactivities caused by control rods movements is close to linear.
Suppose that 3D flux distribution obeys the steady state heterogeneous equation in a difference form:

$$T\varphi=0;\ T=P-Q\gamma(u);\ \gamma(u)=\gamma_1(K_{eff})+\gamma_2(u); \qquad (6.3.1)$$

φ - M×G×K vector, representing the flux taken as a finite Furie expansion with M axial modes,
G-number of groups,
K-number of channels
u- I-vector of control rod positions, chosen for
flattening of power distribution (I - the number of control rods),
P and Q - difference operators

The equation for power normalization is as follows:

$$Pw=<W,N> \qquad (6.3.2)$$

Pw - reactor power
W- vector of power coefficients
N - G-K vector flux (recovered from φ).
Optimal state (pointed out by *) can be supposed to be reached after variations:

$$u^*=u+\delta u;\ \varphi^*=\varphi+\delta\varphi;\ \gamma^*=\gamma+\delta\gamma. \qquad (6.3.3)$$

Take the reactivities $\rho=\{\rho_i\}$, i=1,...I, caused by control rods positions changes, as new independent variables instead of u.
Due to criticality condition the next sum is to be zero:

$$\sum_{i=1}^{I}\rho_i=0; \qquad (6.3.4)$$

Let

$\rho_i = -(\varphi^+, Q\delta\gamma_2(u,\delta u_i)\varphi^*)$; $\delta\gamma_2(u,\delta u_i) \equiv \gamma_2(u+\delta u_i) - \gamma_2(u)$ (6.3.5)

δu_i- vector with i-th nonzero component, φ^+- the solution of adjoint equation:

$T^+\varphi^+ = 0$; $T^+ = P + \gamma^+(u)Q^+$; $\gamma^+ = \gamma^+_1(K_{eff}) + \gamma^+_2(u)$ (6.3.6)

with normalization condition:

$(\varphi^+, Q\gamma_1\varphi) = 1$ (6.3.7)

Symbol $^+$ means transpose.
Critical condition does not require that δu, $\delta\varphi$, $\delta\gamma$ be small values.
φ^* is related to φ by an equality:

$$\varphi^* = \varphi + \sum_{i=1}^{I} \rho_i \psi_k^i; \quad (6.3.8)$$

provided ψ^i are the solutions of the equations:

$T\psi^i = q^i$, i=1,2...I.

$q^i = Q\gamma_1\varphi - (Q\delta\gamma_2(u,\delta u_i)\varphi^*)/(\varphi^+, Q\delta\gamma_2(u,\delta u_i)\varphi^*)$ (6.3.9)

Due to normalization condition for power:
$\langle W, n\rangle = 0$ (6.3.10)

n^i is related to ψ^i in the same way as N^i to φ^I.
Since an arbitrary term constN can be added to ψ^i, the latter can be chosen from the relation

$n^i \Rightarrow n^i - ((W, n^i)/Pw)N$ (6.3.11)

so that condition (6.3.10) is fulfilled.
The equations (6.3.4)-(6.3.11) are exact relations between φ^* and φ provided critical condition is fulfilled. But the solution depends on the unknown value φ^*.
Suppose an approximate relation exists:

$\delta\gamma_2(u,\delta u_i)\varphi^* \approx c_i\delta\gamma_2(u,\delta u_i)\varphi$ (6.3.12)

c_i - unknown constant multipliers.
This condition is exact in 2D case or if $\delta\gamma_2$ depends only on thermal neutrons absorption
In 3D case the above relation is rather exact if neutron flux distribution across control rod is changed weakly (but amplitude can change strongly).
Since δu_i is not known an additional supposition is assumed

$\delta\gamma_2(u,\delta u_i) \approx c_i^* \gamma_{2u}^i(u)$ (6.3.13)

with γ_{2u}^i defined as a derivative of γ_2 by u_i, c_i^* - constant multiplier.
For the case of one variable depending on u_i in $\delta\gamma_2(u,\delta u_i)$ the above relation is exact.
Under the above suppositions:

$$q^i = Q\gamma_1\varphi - (Q\gamma_{2u}^i(u)\varphi)/(\varphi^+, Q\gamma_{2u}^i\varphi) \qquad (6.3.14)$$

Iteration procedure :

The iteration procedure is determined as follows.
For n th iteration suppose φ^n be an n-th approximation to φ^*:

$$\varphi_k^n = \varphi_k + \sum_{i=1}^{I} \rho_i^n \psi_k^i; \quad \varphi_k^0 = \varphi_k; \qquad (6.3.15)$$

ρ_i^n - n-th approximation to ρ_i as the solution of the next linear programming problem:

$$\sum_{i=1}^{I} \rho_i^n = 0;$$
$$\omega^n + \sum_{i=1}^{I} \alpha_{ki}\rho_i^n \le P_{max} - P_k; \quad \mathbf{k} \subset K^n; \qquad (6.3.16)$$
$$\rho_i^{n-} \le \rho_i^n \le \rho_i^{n+}; \quad i=1, \ldots I;$$
$$\omega^n \Rightarrow \max$$

By definition:

$$\rho_i^{n+} = -(\varphi^+, Q\delta\gamma_2(u, u_i^+ - u_i)\varphi^n); \qquad (6.3.17)$$
$$\rho_i^{n-} = -(\varphi^+, Q\delta\gamma_2(u, u_i^- - u_i)\varphi^n);$$

$$\alpha_{ki} = \langle W_k, n^i \rangle; \qquad (6.3.18)$$

and u^+, u^- are maximal and minimal control rods positions;
K^n - the number of potentially "hot" channels . The problem (6.3.16)-(6.3.18) is being solved until φ (see(6.3.15)) does not converge to φ^*, and $\rho^n \to \rho$.
Vector δu is determined as a solution of transcendental equations:

$$\rho_i + (\varphi^+, Q\delta\gamma_2(u, \delta u_i)\varphi^*) = 0; \quad i=1,\ldots I \qquad (6.3.19)$$

A new stationary distribution is re calculated with new values u*.
If a necessary flattening of power distribution is not reached, the iteration procedure is repeated.

The experience:

2D calculation (1 axial mode) needs 1 cycle of iterations; exact solution for 3D case is usually obtained after 2 cycles of iterations.

7. Computer Code's Descriptions

The methods of heterogeneous reactor theory presented in lectures 1-6 has been used for the development of computer codes.
The limitations of initial heterogeneous reactor theory were overcome by a transformation of heterogeneous reactor equations to a *difference* form and by the development of a *consistent theory* for the characteristics of reactor channel or a cell based on detailed space-energy calculations of a cell. These two main points created the basis for the development of effective computer codes from codes for detailed space-energy calculations of a reactor cell (with a simulation of time process) to 3D space-time reactor codes for simulation of slow processes and fast transients.

The system of computer codes was tested by comparisons with calculations by other methods (Monte-Carlo, WIMS) and by comparisons with the results of critical experiments in heavy-water critical assemblies and graphite-moderated, light water-cooled critical assemblies (RBMK type). The work on verification of the system of computer codes is continued now.

Computer codes are widely used for the analysis of physical properties of reactors of different types - heavy-water gas cooled , modular heavy-water moderated, heavy water cooled, research reactors with high flux, graphite-moderated, gas cooled (RBMK).

7.1 Reactor cell calculations - steady state and space-time kinetics

Computer code
Name: TRIFON[23)]
Computer: IBM/PC; VAX.
Physical problem solved: calculation of detailed space-energy neutron distribution in a multi-region reactor cell (with fast, intermediate or thermal spectrum); simulation of time-dependent nuclear chain transformations in a reactor cell.
Thus generally the solution depends on 3 variables: space - energy -time.

Method of solution[6,7,13,14)]:
Neutron transport in every group is evaluated by *collision probability* method (see 3.1) in multiregion *cylindrical geometry* and in *cluster geometry*, by and by S_n *-method in R-Z geometry*. The system of neutron transport equations is solved for space-energy distribution of neutrons. The source of neutrons in every group in epithermal region consists of two parts: due to neutrons scattered from upper groups; due to fissions corresponding to fission spectrum with the normalization of space energy distribution to unity. Space distribution of neutrons born by fission is estimated according to a pre-calculated distribution of fissions by thermal neutrons. This is a weak supposition since in a cell of small dimensions fast neutrons have large mean free paths, the solution weakly depends on their space distribution and can be improved by iteration procedure.

Energy distribution is based on multi-group approximation. The library may have an arbitrary fixed group structure (now 26 groups library is used with the upper energy 10.5 Mev).

A *special subdivision of energy scale* allows an effective *direct treatment of resonances* for prescribed nuclei (in this case twin isotope has a prefix RZ). Subdivision of lethargy scale in a given lethargy interval (u_0 , u_n) corresponds to uniform division of F - image

$$F(u) = F(u)+\Delta, \quad \Delta=F(u_n)/n; \quad u = \ln E/E_0$$

where function ($F(u_0)=0$): F(u) roughly estimates absorption by all resonance nuclei present. This procedure provides accumulation of lethargy points near the centers of resonances. As a result only a few lethargy intervals (5-7) are needed to describe absorption by a given resonance.

The cross-section for a single resonance is determined by Breight-Wigner formula: The functions ψ, χ for Doppler broadening are calculated as the solution of the set of differential equations:

Effective resonance levels technique can be used as well for description of resonance absorption with reasonable accuracy. A set of parameters (E, Γ_n , Γ_γ , L, σ); L - Doppler-broadening parameter divider, σ - constant capture cross-section in the group where this resonance lays, makes it possible to describe resonance absorption by a single resonance level instead of tens or hundreds of resonances in a given lethargy interval. The theory is based on pre calculation of resonance absorption by initial set of resonances and effective one in some simple homogeneous model, and the fact that an approximate equivalency exists between resonance absorption in homogeneous and heterogeneous systems.

If both energy intervals I and j lay in the basic library scale, scattering cross-sections are taken from this library; if at least one of these intervals is subdivided for resonance absorption description, then the model of scattering by free atoms is used with the probabilities $P^{j\leftarrow i}$ of elastic scattering from group i to group j.

Reaction rates and neutron balance

For every isotope k in every region l with nuclear concentration C_{kl}, capture, fission and multiplication rates up to a flow group j are calculated: C_{kl}^j, F_{kl}^j , νF_{kl}^j ,
and the current along energy axis ε_k^j:
their total values for the cell:
C^i, F^i, νF^i, ε^i and total current of neutrons (from the first group to the given energy, defined by lower boundary of group i) across the cell boundary: J^i.

For all the groups below the lower boundary of fission spectrum
the next balance equation is fulfilled:

$$C^i + F^i + \varepsilon^i + J^i = 1;$$

(the sum in the left part of above equation can be different from 1
due to (n,2n) reactions).

For zero current across the cell boundary full number of neutrons
reactions by capture and fission is equal to unity:

$$C + F \ (+J) = 1.$$

and by definition multiplication factor in both cases (zero or non zero current across boundary) is equal:

$$k_{eff} = \nu F;$$
$$k_{eff} = k_\infty$$

if the current J is equal zero.

The problem of space-energy distribution of neutron flux in the thermal region of energies is solved by subroutine TERMIT.
Time -dependent equations (see (5.1)) are solved for burn-up simulation.

Nuclear data included in the library:

- multi-group microscopic cross sections,
- parameters of resonances and effective resonances.
- scattering matrices for neutron thermalization and tables giving the dependence of absorption and fission cross-sections on energy.

The data for *chain transformations* (channels for capture, fissions, decay, (n,2n) reactions) are (and may be) included in the library.

Input data include only data for *geometry* and *isotope* (nuclear densities) *composition* (initial for the case of time simulation), *power* and *time points of burnup calculations*.

Special language has been developed for input data:

- for geometry and isotope composition,
- a set of *orders* (pointed by symbol *) to generate the library, to change the basic nuclear data (editor), to define the special regimes of calculations and for output data.

Output :

- space energy distribution of neutron flux (depending on time if necessary),
- reaction rates for nuclei in all physical regions, depending on energy (starting from the first , fast group)
- multiplication factor,
- few-group cross-sections,
- monopole and dipole (axial and radial) few-group Λ-matrices (3.3a; 3.3b),
- reaction rate R-vectors.

The latter data are used as an *input for 3-dimensional heterogeneous reactor codes* and stored in exchange files.

Programming language: FORTRAN-77.

Tests: comparisons were done with the results of calculations by Monte-Carlo methods for TRX, BETTIS, MIT reactor cells, for light-water cells NB, for RBMK cells.

Output data for heterogeneous parameters (Λ– matrices and reaction rates vectors) were used for investigation of critical assemblies experiments of heavy-water type and critical assemblies of RBMK type.

Status: a new version is under development to improve the structure of computer code and the system of input data and to extend it for the case of subcritical systems with an external source (for simulation of target/blanket accelerator-driven facilities)

Computer code
Name:TERMIT[16)]
Computer: IBM/PC; VAX.
*Physical problem solved:*T space -energy distribution of thermal neutrons (in the energy interval from 0 to 0.465 eV or 1 eV) in a reactor cell depending on up and down scattering of neutrons by chemically bounded nucleus.
Method of solution[15,16)].
Space-energy distribution of thermal neutrons in a multi-region cylindrical reactor cell is the solution of the multigroup system of neutron transport equations.
Piece-wise representation of space-energy dependent functions is used with M groups and N space regions.
Scattering matrices
are based on the models:1. diagonal, 2. free gas, 3. Brown-Saint-Johns, 4. Nelkin 5. Koppel-Yang.
Source
The source due to slowing down of neutrons scattered by the nuclides depends on the atomic mass A and scattering cross-sections of nuclides.
Iterations
The dimension of the problem is M×N with the (M×N)(M×N) matrix as a product of a system of N M× M "energy matrices" by a system of M N ×N "space" matrices.
Simple iteration procedure for the solution of this system of equations is combined with 2 stage iteration procedure with sequential averaging on space and energy.
The computer code is used now as a subroutine in computer code TRIFON.
The library for thermal neutron consists of a system COMBIB.EXE (FOR)-
to create temporary library from basic data COMBIB.DAT and COMBIB.DBF,
with the indication what elements are to be included and a system of constant cross -sections. Cross-section library can be changed by any FORTRAN editor
(for example Multi-Edit).
Input data include only data for *geometry* and *isotope* (nuclear densities) *composition* , scattering models and are included in the input of computer code TRIFON.
Some data are used by default.
To change the input data for neutron thermalization is possible by changing some parameters of arrays
(used as NAMES in TRIFON) : ITH, RTH
ITH(1) =0 uniform division of V-scale,
1 the centers of groups - in the array RTH, starting from RTH(2);
2 the boundaries of groups in array RTH;
ITH(2)= 0 standard scattering models;
1 models in array ITH, starting from ITH(10),
(models: 1 - diagonal, 2 - free gas, 3 - Brown-Saint-Johns, 4- Nelkin, 5 Koppel-Yang)
ITH(3) - number of groups
ITH(4) = 1 printing of spectrum in points
0 no print
ITH(5) - similar for zones
ITH(6) = 1 printing of flux averaged by spectrum,
0 no print
ITH(8) =1 transport cross-section

0 scattering cross-section
GROU(50) - number of groups (besides 26th) included in thermal region;
by default 1 :25, 26 groups of Abag'ans system are included in thermal region with upper energy of neutrons 0.465 eV; for value 2 the upper boundary of thermal region - in group 24 - 1 eV).
The order:
*NOTE can be use d to ignore thermalization ; in this case 1-group cross-sections from Abag'an system are used
Library data are in the file
COMBIB.DBF;
NOTE: The second names used for isotopes in TRIFON should be the same as the names in thermal part of library.
(For example U235 has two names: R5 and 92235 , the latter
is given in input files for COMBIB)
The isotopes that are to be included in the thermal part of library in TRIFON are to be given in file
COMBIB.DAT
(second names, in a sequence corresponding the sequence in COMBIB.DBF).
Execution
>run COMBIB
includes these isotopes in the library.
Output :
- space energy distribution of neutron flux (depending on time if necessary),
- reaction rates for nuclei in all physical regions, depending on energy are used for overall calculation in computer code TRIFON.

7.2 2D heterogeneous reactor calculations in monopole and dipole approximations

Computer code
Name:DISHER[5,17]
Computer: IBM/PC; VAX.

Physical problem solved: 2-dimensional flux, power or reaction rates distribution in a heterogeneous reactor of finite height with cylindrical outer boundary in monopole or dipole approximation (in this case with azimuthal dependence of flux on channel boundary).
Method of solution[5,6,17]:
the solution of few-group heterogeneous reactor equation in matrix form (see equation 1.4.12), 2-dimensional problem; dipole approximation; group-theoretical analysis based on consideration of symmetry groups C_{4v}, C_{6v} or their subgroups for square and hexagonal lattices correspondingly is used to decrease the dimension of problem table 4.2.1). The method of solution of heterogeneous matrix equations is based on an iteration procedure with line by line multiplications of matrix by vector-flux after preliminary transformation of the problem to a problem with an operator having some positivity properties (see lecture 4, (4.3.1)-(4.3.9)).
Input data include data on the lattice its loading by different types of channels, symmetry parameters; the characteristics of channels (few-group Λ-matrices, giving the relations between vector-flux and vector-current on channel or cell boundaries and reaction-rate vectors) are supposed to be calculated by computer code TRIFON and stored in some exchange files. The number of fuel assemblies or control rods - several hundreds.

Output includes effective multiplication factor K_{eff}, 2-dimensional distribution of neutron flux (including asimuthal dependence on channel boundaries in the case of dipole approximation), power (or reaction rates) distribution and the values that determine the balance of neutrons- numbers of fissions, neutron captures in channels and so on.

Programming language: FORTRAN-77.

7.3 3D heterogeneous reactor calculations based on a difference form of heterogeneous reactor equations in monopole and dipole approximations; subcritical systems with external sources

Computer code

Name: TRECD[18], *TRECS*[19]
Computer: IBM/PC; VAX.
Physical problem solved: 3-dimensional flux, power or reaction rates distribution in a heterogeneous reactor of finite height in monopole or dipole approximation. The channels are supposed to have non-uniform piece-wise properties in axial direction.
Method of solution[3,4,5,6, 18,19].
the solution of 3-dimensional heterogeneous reactor equations in difference form (see lecture 2, (2.6.8)-(2.6.11)), dipole (or monopole) approximation, for a reactor with square or hexagonal lattice (parameters of difference operators defined in 2.7). Axial dependence is presented as finite Furie-expansion of few-group vector-fluxes and Λ–matrices - characteristics of channels, giving the relations between vector-flux and vector-currents on channel or cell boundaries (including their axial and radial parts), as well as reaction rate vectors. The number of axial modes
M, the number of channels K and the number of types of channels T are limited by a relation $3K+2T(2M+1)< L$ (where L is of the order 20 000 and depends on the type of computer), for example calculations can be fulfilled for a reactor with 2000 channels , 100 types of channels and 10 axial modes.

The method of solution is based on Chebyshev acceleration procedure for outer iterations , and symmetric successive over-relaxation method for inner iterations (see 4.4).

Input data include data on the lattice its loading by different types of channels, the type of reactor lattice and so on. Channel characteristics (Λ–matrices, reaction-rate vectors) are supposed to be pre calculated by computer code TRIFON and stored in some exchange files.

The *output* includes effective multiplication factor K_{eff}, three-dimensional distribution of reaction rates (power distribution) and the values that determine the balance of neutrons-numbers of fissions, neutron captures in channels and so on.

Programming language: FORTRAN-77.

7.4 Simulation of 3D slow reactor processes with reloading of fuel, control rod movements, Xe poisoning.

Computer code

Name: BARS[20]
Computer: IBM/PC; VAX.
Physical problem solved: simulation of 3D-space time kinetic of a reactor including burn-up of fuel assemblies, reloading of fuel, control rod movements, change of reactor power, Xe poisoning and Xe transients, reactivity control by a solution of an absorber in moderator (boric acid). Axially non-uniform channels are supposed to be placed in the nodes of square or hexagonal lattice 0f 3D model of a reactor.
Method of solution[3,4,20]*:* heterogeneous reactor equations in a difference form are used for neutron flux description in a reactor. Some thermal-hydraulic models can be included for simulation general neutron termal-hydraulic process. Control rods movements can be used for automatic holding criticality of a reactor.
Time interval is subdivided by fixed points and power dependence on time is a given function.

Isotopic composition for each part of a fuel assembly or an absorbing rod is supposed to depend on one or two parameters - burn up, or fluence, specific power, one of the "main" nuclides concentrations and so on. It is supposed that channel characteristics, depending on a number of burn-up parameters and physical properties of channels (Λ–matrices, reaction rate vectors) are pre calculated as function of these parameters by computer code TRIFON and stored in some arrays.

The state vector includes the next values (see 5.2, 5.3):

$S = (B(t),X(T),T(t),U(t))$

$B= (B^1,B^2)$ - burn up, X- Xe concentrations,
T - temperature and density of coolant, U - criticality parameter (control rods depths , Boric acid concentration or *k*eff)
Non-linear problem is reduced to a sequence of linear problems to resolve the dependence of temperature and Xe-I concentrations on neutron flux:
Analytical solution of above equations for Xe and I concentrations are used for a given time interval end point. At fixed time points a decision can be taken for reloading of fuel assemblies and for power distribution flattening by changing the positions of control rods. Reactivity effects (for example void effect can be calculated at fixed time points by additional calculations with the change of some physical properties of channels). Some thermal-hydraulic models are included (for heavy water-cooled, gas cooled and boiling light-water cooled reactors).

Programming language: FORTRAN-77.

7.5 Simulation of 3D fast transients with the effects of prompt and delayed neutrons

Computer code
Name: DINAR[21]
Computer: IBM/PC; VAX.
Physical problem solved: three-dimensional simulation of time transients in a heterogeneous reactor with delayed and prompt neutrons.
Method of solution[3,4,21]: non-stationary equations and non-stationary boundary conditions, accounting for a difference in neutron spectrum of prompt and delayed neutrons are applied for simulation of 3D -space -time transients (see 5.4). The solution is presented as a product of a 3D function as a solution of 3D stationary equation by a function describing point kinetic of mean values in the reactor. 3D solutions of heterogeneous reactor equations for critical reactor and sub critical system with external source are used for process simulation.

Heterogeneous reactor equations in difference form are used for reactor steady-state calculations for a reactor with non-uniform channels in a hexagonal or square lattice. Few-group time dependent equations in the moderator include the term depending on fast transients that is included into point-like equation for overall power change simulation A system of equations in the cell is used for the determination of above parameters:
Time dependent boundary conditions depend on a "time"characteristic
Λ_t -matrix that can be calculated (by computer code TRIFON) with a 1/v absorber of small concentration included uniformly in the cell:
The system of equations include a set of equations for slowly varying function describing power (or flux distribution), a set of equations for delayed neutron precursors and point-like equation for fast varying function describing the change of reactor power . Steady-state

adjoint equations are used for formulation of point-like equations depending on generalized parameters: time of life of prompt neutrons, mean fractures of delayed neutrons, change of reactivity.

Adiabatic approximation

The sources of prompt and delayed neutrons are united and time derivatives For each time point the equations for criticality are calculated. For point approximation form-function is calculated only for initial state.

Quasi-static approximation

Takes account of space-time dependence of delayed neutrons precursors. P(t) and its derivative is determined from point kinetic equation. In this case form-function is calculated by the method of solution of heterogeneous reactor equation with external source. In a given time interval the value $\alpha_0=1/P(dP/dt)$ is supposed to be constant, is estimated from a previous time interval and is included in moderator characteristic for a given time interval.

Programming language: FORTRAN-77.

8. Numerical Results

8.1 Reactor cell calculations

Light water systems

As the first example the results of comparisons for light-water TRX cells are presented. Geometry and nuclear cell composition is presented in table .8.1.1; the results of calculations by computer code TRIFON(T) [27] and by method Monte-Carlo (MC) (Hardy J. Monte-Carlo analysis of TRX lattices with ENDF/B-3 data, Seminar on ^{238}U resonance capture, 1975, BNL-NCS-50541.) - in table .8.1.2.

Next example - for uranium-light water cells (Badalov A.F., Kononov, S.L., The results of Monte-Carlo calculations for light-water lattice cells with different moderator-fuel ratio. VANT (Russ.) , ser. PHTYAR, 1988, v.3, p. 24-29); the parameters of cells are presented in table .8.1.3. The results of calculations of conversion ratio (CRR)-absorption by ^{328}U/ absorption by ^{235}U and K_∞ - in table .8.1.4, reaction rates (normalized to 1 for total absorption) -in table .8.1.5. The comparison is given between TRIFON (T), WIMS and Monte-Carlo) results (computer code MCU -Liman G.F., Maiorov L.V. , Yudkevich M.S., A complex of MCU programms for the solution of neutron transport problems in nuclear reactors by Monte-Carlo method, VANT (Russ.) , ser. PHTYAR, 1985, v.7, p. 27-31).

Table .8.1.1 Composition of TRX cells

Region	ΔR, cm	Isotope concentr. (10^{24} cm^{-3})	ω
Fuel	0.4915	U235 0.0006253 U238 0.047205	
Gap	0.0127		
Clad	0.0711	Al 0.06025	
Moderator	0.181	H 0.06676 O 0.03338	1.00
	0.373	the same	2.35
	0.566	the same	4.02
	0.938	the same	8.11

Table .8.1.2 Reaction rates for TRX cells by TRIFON (T) and Monte-Carlo (MC); C -capture, F -fission, t-thermal neutrons, e- epithermal neutrons; ω -the ratio of moderator to fuel volumes; in brackets - statistical error (%) of MC method.

			ω			
			1.0	2.35	4.02	8.11
	F-e	T	0.05862	0.03863	0.02836	0.01893
		MC	0.05908(0.3)	0.03896(0.5)	0.02873(0.5)	0.01907(0.5)
^{238}U	C-e	T	0.3436	0.1969	0.1290	0.07030
		MC	0.3477(0.3)	0.1962(0.5)	0.1294(0.6)	0.07035(0.8)
	C-t	T	0.11295	0.1492	0.15575	0.1424
		MC	0.1125(0.2)	0.1488(0.1)	0.1548(0.1)	0.1409
	F-e	T	0.07093	0.03898	0.02511	0.01354
		MC	0.07044(0.3)	0.03865(0.4)	0.2501(0.5)	0.01357(0.5)
	F-t	T	0.29543	0.39920	0.42017	0.38626
		MC	0.29541(0.2)	0.40075(0.1)	0.42032(0.1)	0.38508(0.1)
^{235}U	C-e	T	0.03540	0.01950	0.01251	0.00666
		MC	0.03151(0.4)	0.01764(0.4)	0.01135(0.5)	0.00601(0.5)
	C-t	T	0.05126	0.06841	0.07166	0.06564
		MC	0.05187(0.2)	0.06919(0.1)	0.07209(0.1)	0.06573(0.1)
K_∞		T	1.0502	1.1676	1.1559	1.0194
		MC	1.0517	1.1732	1.1587	1.0185

Table .8.1.3 Composition (10^{-24} 1/cm^3) and dimensions for uran-water cells (Clad Zr 0.0425)

Parameter	**Variant**					
	1	**2**	**3**	**4**	**5**	**6**
Fuel	**UO_2**	**U**	**UO_2**	**U**	**UO_2**	**U**
Enrichment %	**3.9**	**2.0**	**5.9**	**3.0**	**7.9**	**4.0**
Fuel composition						
U-235	0.00085	0.00085	0.00128	0.00128	0.00165	0.00165
U-238	0.0205	0.0409	0.0200	0.0405	0.0197	0.0401
O	0.0426		0.0426		0.0426	
Cell radius, cm	**0.693**		**0.597**		**0.531**	
Fuel pin, rad. cm	**0.387**					
Pin in clad, cm	**0.455**					

Table .8.1.4. The results of calculations of conversion ratio (CRR) and K_∞ for uranium-water cells

Variant	TRIFON		WIMS		MCU	
	K_∞	CRR	K_∞	CRR	K_∞	CRR
1	1.449	0.318	1.451	0.311	1.458/.1/	0.317/.4/
2	1.274	0.556	1.282	0.542	1.278/.2/	0.560/.7/
3	1.417	0.372	1.425	0.358	1.421/.3/	0.370/.9/
4	1.239	0.640	1.256	0.607	1.241/.2/	0.643/.6/
5	1.293	0.484	1.314	0.449	1.301/.3/	0.473/1./
6	1.116	0.832	1.146	0.768	1.113/.4/	0.844/1.1/

Table .8.1.5. Reaction rates in uranium-water cells, C-capture, F -fission for ^{235}U and ^{238}U.

Var iant	Method	E> 1 eV				E< 1 eV		
		C5	F5	C8	F8	C5	F5	C8
1	TRIFON	0.0312	0.0595	0.1576	0.0228	0.0877	0.5124	0.0622
	MCU	0.0301/1	0.0605/1	0.1555/4	0.0230/1	0.0869/1	0.5084/8	0.0617/1
2	TRIFON	0.028	0.0546	0.2204	0.0390	0.0729	o.4261	0.1035
	MCU	0.0273/1	0.0556/1	0.2206/8	0.039/1	0.0722/2	0.422/1	0.1024/2
5	TRIFON	0.1074	0.2246	0.2900	0.0427	0.0448	0.2584	0.0173
	MCU	0.1071/5	0.2339/7	0.2824/14	0.0432/1	0.0430/3	0.2490/18	0.0168/1
6	TRIFON	0.0884	0.1898	0.3934	0.0662	0.0334	0.1931	0.0264
	MCU	0.0889/5	0.1973/8	0.3951/17	0.0663/2	0.0312/3	0.1806/18	0.0250/2

Next example -uranium-plutonium-water cells (Williams M.L. et.el., Analysis of thermal reactor benchmarks with design codes based on ENDF/B-V data. Nuclear Techn., 1985, vol. 71, p. 386-401). Composition of NB cells is presented in the table .8.1.6.

Table .8.1.6. Composition of NB cells (nuclear densities , 10^{24} cm^{-3}; h, s -hexagonale, square lattice; for NB-2 lattice some amount of B-10 was dissolved in moderator).

	Variant			
Parameter	**NB-1**	**NB-2**	**NB-4**	**NB-5**
Fuel	**UO2**	**U+Pu**	**UO2**	**U**
Fuel composition				
U-235	0.0003112	0.0001504	0.0006465	0.00069411
U-238	0.023127	0.02073	0.022559	0.021895
Pu-239		0.0003974		
Pu-240		0.00003344		
Pu-241		0.0000016		
O	0.046946	0.04401	0.04442	0.045047
Pitch, cm	**1.5557 (h)**	**2.210(s)**	**1.4605(s)**	**1.166(h)**
Fuel pin, rad., cm	**0.4864**	**0.6414**	**0.508**	**0.4675**
Pin in clad, rad., cm	**0.5735**	**0.7176**	**0.59474**	**0.529**
Clad comp.	**Al(0.04899)**	**Zr(0.04266)**	**Zr(0.04015)**	**Al(0.0473054)**

The results of calculations of K_∞, ρ_8 (the ratio of epithermal to thermal captures by ^{238}U) and conversion ratio CR (the ratio of ^{238}U captures to ^{235}U fissions) - in table .8.1.7

Table .8.1.7. The results of calculations of NB cells , in brackets / /- statistical error of Monte-Carlo method (last digits).

		TRIFON	WIMS	Monte-Carlo
NB-1	K_∞	1.1344	1.1254	1.1471/16/
	ρ_8	1.375	1.458	1.363/8/
	CR	0.804	0.829	0.798/3/
NB-2	K_∞	1.1734	1.1640	1.1748/23/
	ρ_8	2.526	2.372	2.612/15/
	CR	2.110	2.319	2.148/8/
NB-4	K_∞	1.3363	-	1.3424/35/
	ρ_8	2.666	-	2.654/16/
	CR	0.556	-	0.549/2/
NB-5	K_∞	1.1302	-	1.1456/17/
	ρ_8	8.452	-	8.503/68/
	CR	1.015	-	1.006/3/

Computer code TERMIT used as a subroutine in computer code TRIFON has been tested by comparison with THERMOS code results (Stammlerr R.J.J et.al.Neutron thermalization in reactor lattice cells: an NPY-project report, Vienna, 1966), composition of reactor cells was taken from the work by Stammler, the results of calculations are presented in the table .8.1.8.

Table .8.1.8 The ratio of neutron densities and neutron fluxes ξ_m , δ_m in moderator and fuel; the ratio of neutron densities and neutron fluxes ξ_c , δ_c in clad and fuel ; [*] - calculation by THERMOS code, TERMIT - by TERMIT code; ε –difference (%) in the results.

		N1	N2	N3	Y1	Y2	Y3
ξ_m	[*]	1.457	1.576	1.658	1.614	1.745	1.862
	TERMIT	1.438	1.547	1.629	1.598	1.717	1.825
	ε	-1.3	-1.8	-1.8	-1.0	-1.6	-2.0
δ_m	[*]	1.327	1.423	1.490	1.464	1.579	1.683
	TERMIT	1.314	1.400	1.468	1.451	1.556	1.654
	ε	-1.0	-1.6	-1.5	-0.9	-1.5	-1.7
ξ_c	[*]	1.178	1.180	1.181			
	TERMIT	1.172	1.173	1.173			
	ε	-0.5	-0.6	-0.7			
δ_c	[*]	1.132	1.136	1.137			
	TERMIT	1.128	1.131	1.132			
	ε	-0.4	-0.4	-0.4			

Heavy-water systems

An example of neutron flux dependence in a two-region heavy water cell with resonance absorprion by ^{238}U is shown in Fig 8.1

An example of calculations of heavy-water cells of a Modular heavy-water reactor (Bergelson B.R., Kiselev G,V., Chuvilo I.V., The modular heavy-water reactor (MHWR) as an energy source for nuclear thermal station and nuclear power station. ENS/ANS-Foratom Conference Transactions, v.II, p.816-820, 1990 (Lyon, France, Sept. 23-28)) with and without coolant by TRIFON code and MCU (Monte-Carlo) code are presented in table .8.1.10 (the cell composition - inner region with heavy water, Zr tube, coolant, two rows of fuel pins, two Zr tubes, heavy-water moderator) . Nuclear densities in fuel pins (material 1), clad and tubes (material 2), coolant (material 3) and moderator (material 4) are given in the table .8.1.9.

Table .8.1.9. Nuclear composition of materials for MHWR

Material	Nuclear densities, 10^{-24} 1/cm^3
1	U235 3.0787-4 U238 0.0233 O 0.047364
2	Zr 0.047364
3	like 4 or O 0.0001
4	O 0.033 D 0.066 H 0.0001339

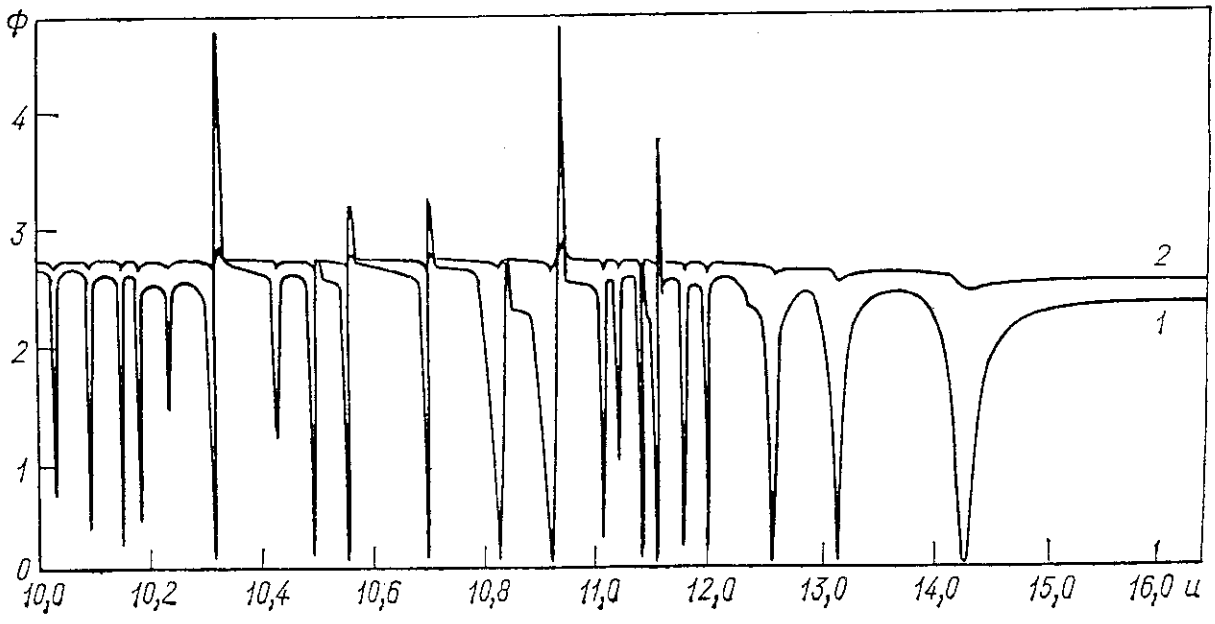


Fig 8.1 An example of neutron flux dependence on lethargy in fuel rod (1) and in heavy-water moderator (2) for a two-region cell with ^{238}U resonance absorption.

Table .8.1.10. Reaction rates and multiplication factor for Modular heavy-water reactor cell with coolant (D_2O) and without coolant (empty); T-TRIFON, M-C -MCU-cluster, M-H - MCU -homogenized (cylindrical geometry); statistical error by MCU - in brackets / /.

			C_8-epi	C_8-th	F_8 -epi
1 row	D_2O	T	0.04762	0.0715	0.00459
		M-C	0.0473/3/	0.0707/3/	0.0468/6/
		M-H	0.0488/5/	0.0696/3/	0.00458/5/
	Empty	T	0.0402	0.0746	0.00594
		M-C	0.0411/4/	0.0741/3/	0.00611/7/
		M-H	0.0418/4/	0.0730/3/	0.00594/7/
2 row	D_2O	T	0.0649	0.118	0.00670
		M-C	0.0648/6/	0.117/4/	0.00675/7/
		M-H	0.0661/6/	0.116/4/	0.00670/7/
	Empty	T	0.0613	0.118	0.00835
		M-C	0.0620/5/	0.116/5/	0.00853/9/
		M-H	0.0655/6/	0.115/4/	0.00844/9/
Total	D_2O	T	0.1125	0.190	0.0113
		M-C	0.1121	0.1874	0.0114
		M-H	0.1149	0.1860	0.0113
	Empty	T	0.1015	0.1920	0.0143
		M-C	0.1031	0.1899	0.0146
		M-H	0.1072	0.1883	0.0144
K_{eff}	D_2O	T	1.3141		
		M-C	1.3149/38/		
		M-H	1.3053/40/		
	Empty	T	1.3369		
		M-C	1.3378/40/		
		M-H	1.3279/38/		

Coolant removal effect $\delta K_\infty = K_\infty^{empty} / K_\infty^{D2O} - 1$:

T	M-C	M-H
0.01735	0.01740/42/	0.01730/42/

The cells of critical assemblies MIT

The dimensions and nuclear composition is presented in table 8.1.11. The results of calculations by computer code TRIFON[27] and by Monte-Carlo method (Rosenstein W., Thermal reactor lattice analysis using ENDF/B-IV data with Monte-Carlo resonance reaction rates, Nucl. Sci. & Engng., 1976, 59, p.337-349) -in table 8.1.12.

Table .8.1.11. Composition of MIT cells

Region	R, cm	Isotope concentr. (10^{24} cm^{-3})
Fuel	1.283	U235 0.0003441 U238 0.04745
Clad	1.354	Al 0.06049
Moderator		H 0.000185 D 0.06641 O 0.03321
Pitch (hex. lattice), cm		
MIT-1	11.43	
MIT-2	12.70	
MIT-3	14.605	

Table 8.1.12 The results of experiments (Exp), calculations by TRIFON (T) and by Monte-Carlo method (MC) for MIT cells; ρ_8 -the ratio of epithermal to thermal capture by ^{238}U, δ_{25} - the ratio of epithermal to thermal fissions by ^{235}U, δ_{28}- the ratio of ^{238}U to ^{235}U fissions, C -the ratio of captures of neutrons by ^{238}U to ^{235}U fissions. Experimental error is given below measured experimental values.

	MIT-1			MIT-2			MIT-3		
	T	MC	Exp	T	MC	Exp	T	MC	Exp
ρ_8	0.481	0.500	0.498 0.008	0.383	0.411	0.394 0.002	0.307	0.315	0.305 0.004
δ_{25}	0.0452	0.0462	0.0447 0.0019	0.0369	0.0376	0.031 0.003	0.0284	0.0284	0.0248 0.0010
δ_{28}	0.0588	0.0579	0.0597 0.0020	0.0568	0.0562	0.0596 0.0017	0.0552	0.0546	0.0583 0.0012
C	0.958	0.965	1.017 0.023	0.900	0.913	0.948 0.020	0.855	0.856	0.859 0.016

Light-water cooled graphite moderated cell (RBMK type)

The results of calculations light-water cooled graphite moderated cell by TRIFON and MCU are presented ion table 8.1.13 (TRIFON input-output see Appendix)

Table 8.1.13. TRIFON(T) and MCU(M) reaction rates and multiplication factor for RBMK cells (statistical error of MCU - in brackets / /).

			empty		water	
			epi-thermal	thermal	epi-thermal	thermal
U235	C	M	0.0239	0.0864	0.0153	0.0877
		T	0.0243	0.0879	0.0156	0.0886
	F	M	0.0587	0.501	0.0361	0.513
		T	0.0539	0.511	0.0342	0.518
U238	C	M	0.1469	0.1005	0.1072	0.101
		T	0.1454	0.1022	0.1087	0.102
	F	M	0.0185	-	0.0151	-
		T	0.0176	-	0.0145	-
K_{eff}		M	1.4147/43/		1.3790/45/	
		T	1.416		1.378	

Simulation of burn-up calculations in a reactor cell

The results of burn-up calculations for light-water cell by TRIFON code and comparison with experimental data (Gabeskiria V.Ya et.al. Atomic Energy (Russ.), 1978, 44, p.446; Stepanov A.V. et. al. , Atomic Energy (Russ.), 1980, 49, p.225) are presented in Fig. 8.2-8.8. Input data for TRIFON code are presented below (C ( ) - concentration , RZ means a twin isotope for resonance absorption calculation, NGRR - the sets of initial groups for lethargy scale subdivision, NSRE - numbers for subintervals for resonance absorption calculation, POWER - power Mwt/cm of cell height, TBURN includes time points in years)

```
* ASSIGN BN
ZONE 1:T=.2, NS=3
C(O)=0.04552,C(U5)=0.0006913,C(U8)=0.02207,C(RZU8)=0.02207
C(U6)=0.,C(RZU6) =0.,C(PU9) =0., C(PU0) =0.,C(RZPU0) =0.,C(PU1) =0.,C(PU2) =0.,
C(RZPU2) =0.,C(AM3) =0.,C(FP5) =0.,C(FP9) =0.,C(FP8)=0.,C(FP1)=0.,C(FP8)=0.,
C(ZEL1) =0.,C(ZEL2) =0.,C(ZEL3) =0.,C(XE) =0.
ZONE 2:T=.1, NS=3
' Initial composition the same as in ZONE 1
ZONE 3:T=.0775, NS=3
' Initial composition the same as in ZONE 1
ZONE 4:T=.0775, NS=1, C(ZR)=.0365
ZONE 5:T=.214, NS=5,C(H)=0.052,C(O)=0.026
ZONE 6:T=.018, NS=1,C(ZR)=0.0429
NGRR =17,17,18, 21,22,22,23,24,  NSRE=40,60,10,10
,NGROU=26,NGAUSS=7,NZONE=6, =1.204-4, TEMPER=718,718,718,578,533,533
TBURN=5,0,3,.17,3,.34,3,.793,5,1.7,10,3.4
*END*
```

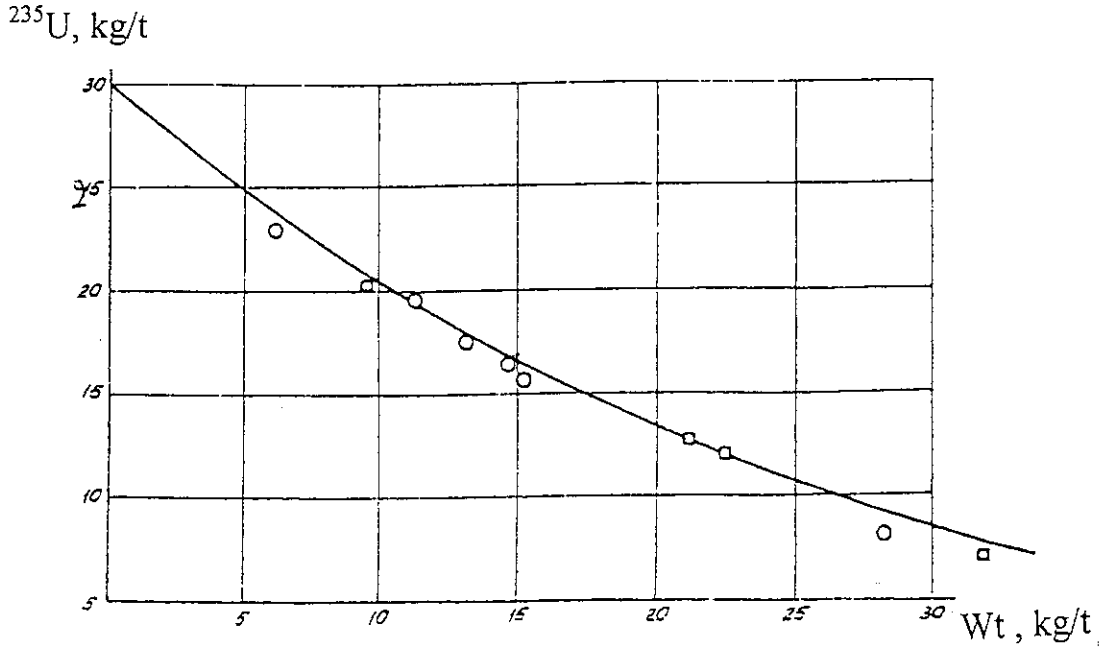


Fig. 8.2. The dependence of ^{235}U concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

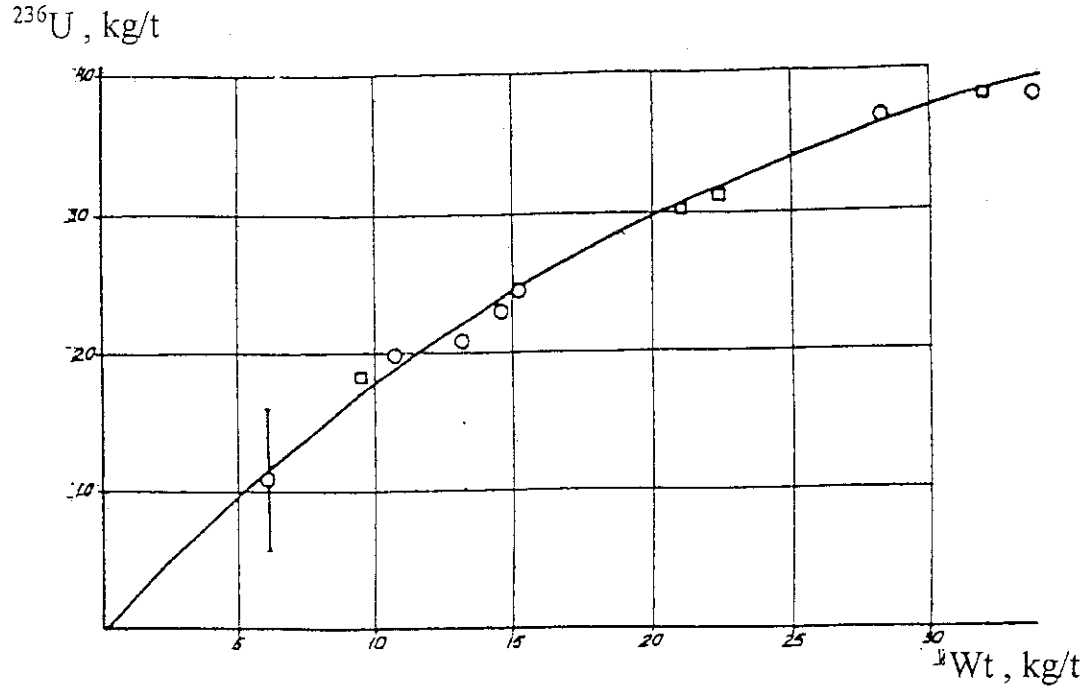


Fig. 8.3. The dependence of ^{236}U concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

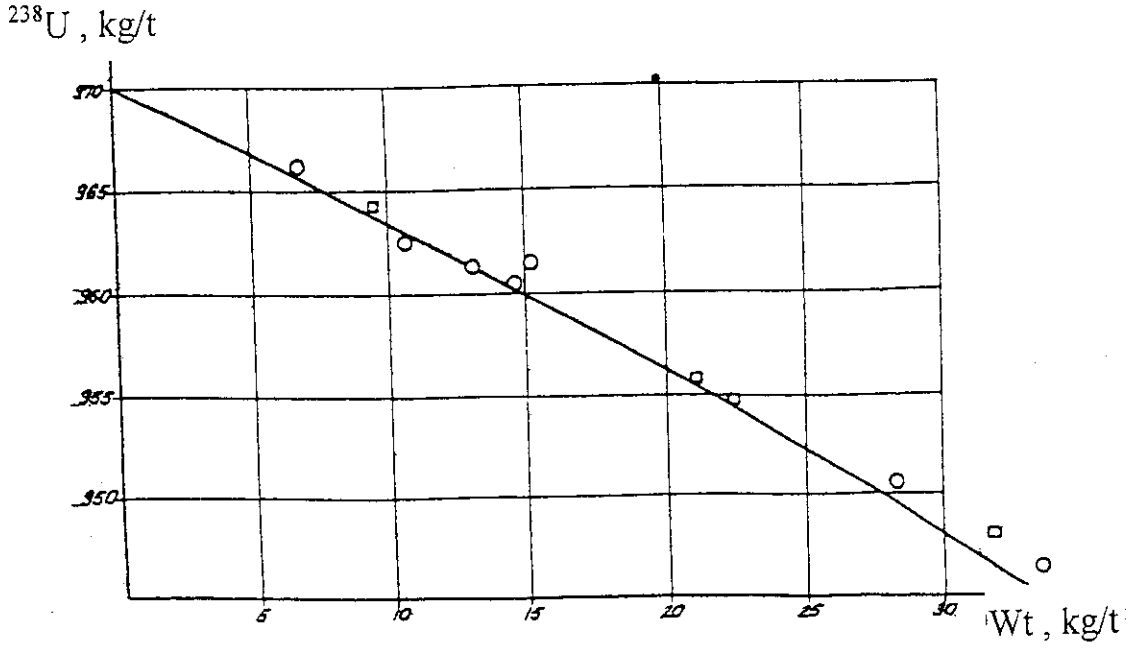


Fig. 8.4. The dependence of ^{238}U concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

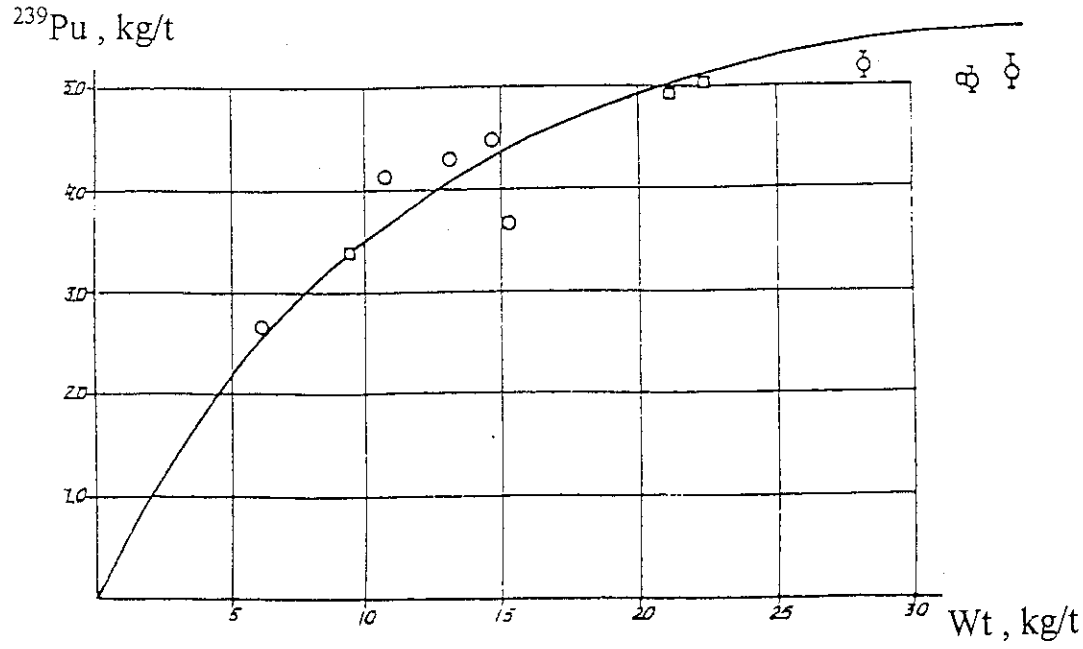


Fig. 8.5. The dependence of ^{239}Pu concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

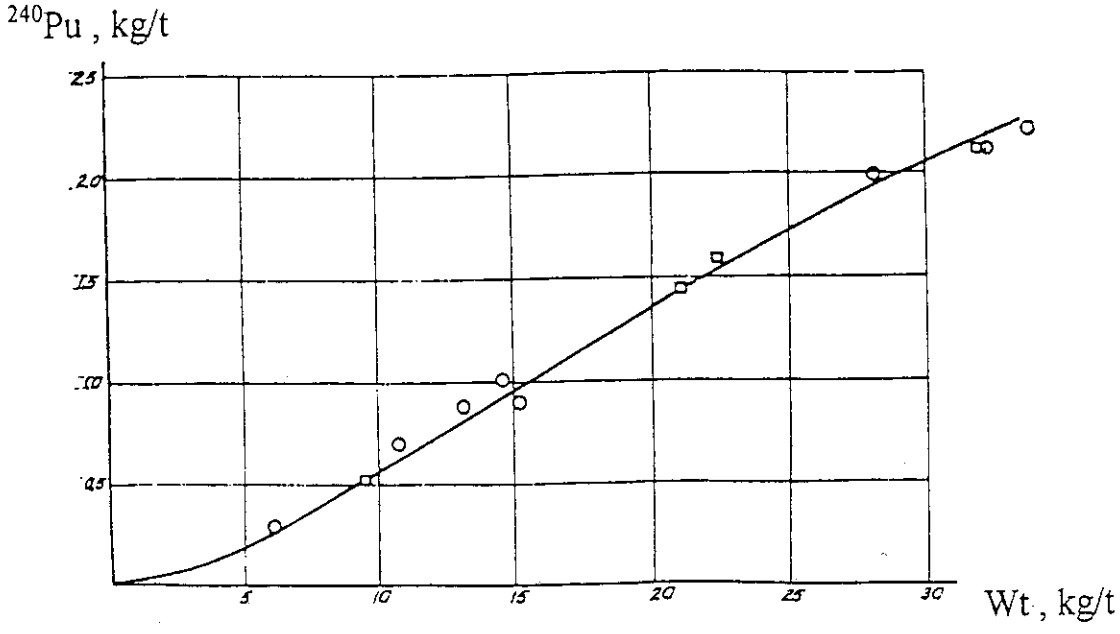


Fig. 8.6. The dependence of ^{240}Pu concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

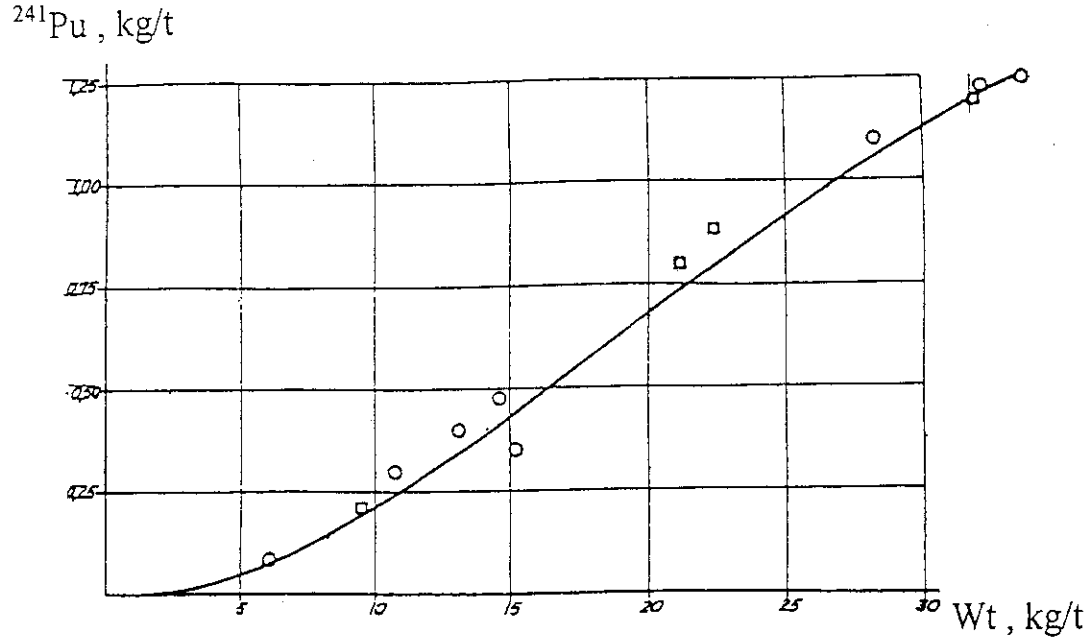


Fig. 8.7. The dependence of ^{241}Pu concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

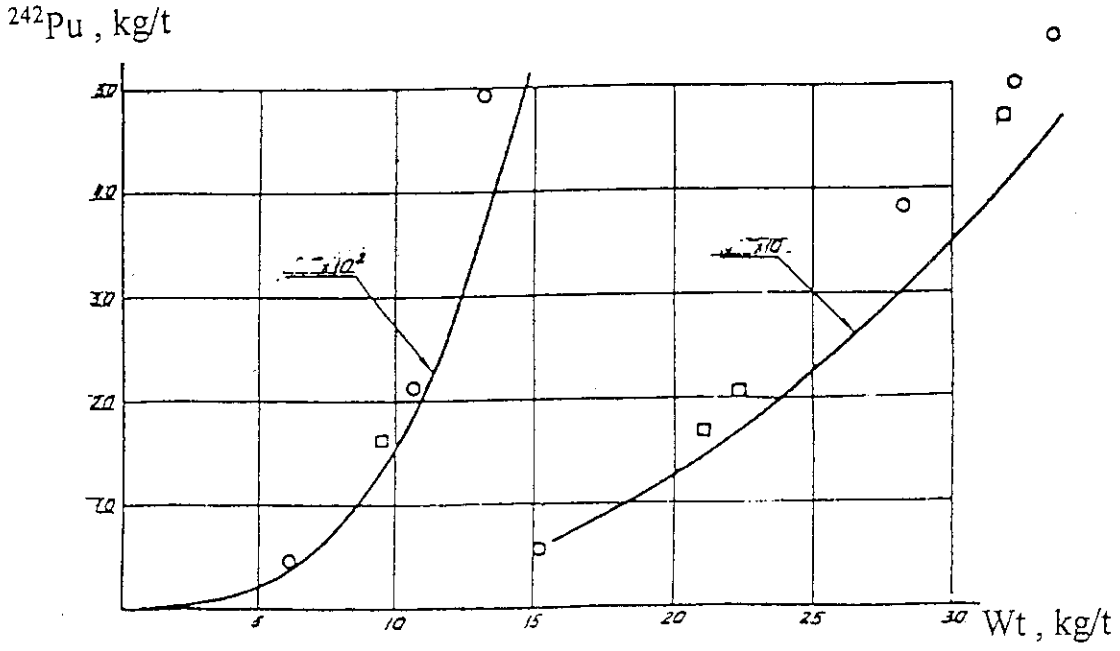


Fig. 8.8. The dependence of ^{242}Pu concentration (kg/t) on burnup Wt (kg/t fission products in a tone of heavy nuclides),
□, O - experimental data -Gabeskiria, Stepanov

One-velocity monopole parameters of channels

The results of calculations of responce parameter u and boundary condition Γ (lecture 3.2a) for 4-region channels are presented in table 8.1.14

Table 8.1.14. The resuls of calculations of parameters u and Γ in one-velocity theory for two 4-region channels; ΔR_i - layer thickness, cm, Σ_i , Σ_{si} - total and scattering macroscopic cross-sections.

N	Parameter	i					u	Γ
		1	2	3	4	Moder.		
1	ΔR_i	5.0	0.1	0.3	0.04		-0.2385	3.059
	Σ_i	0.2	0.09	3.0-5	0.09	0.4001		
	Σ_{si}	0.14	0.08	3.0-5	0.08	0.4000		
2	ΔR_i	2.5	0.4	0.3	0.3		-0.1830	2.922
	Σ_i	0.5	0.01	2.0	0.01	0.4001		
	Σ_{si}	0.25	0.01	1.98	0.01	0.4000		

One-velocity dipole parameters of channels

The results of calculations of polarisability coefficient for one region rods by P_1, P_2 approximations of spherical harmonics method, by balance method (Kochurov B.P., Calculation of dipole moment of a cylindrical rod, Atomic Energy (Russ.), 1965, v.19, N 6, p.530) and by the method, presented in lecture 3.2c (*)are given in table 8.1.15.

Table 8.1.15. Polarisability coefficient β for one region channels

a	Σ,cm^{-1}	Σ_s,cm^{-1}	P_1	P_2	Balance	*
1.0	10^{-5}	10^{-5}	-	-	0.7408	0.7373
0.1	10^{-5}	10^{-5}	-	-	0.5428	0.5394
1.0	20.0	0.01	-	-	0.0886	0.0836
0.1	50.0	0.01	-	-	-2.99	-2.89
1.0	0.15	0.15	0.7391	0.5469	0.5880	0.5857
1.0	0.15	0.075	0.7409	0.5545	0.5944	0.5909
1.0	0.15	0	0.7425	0.5621	0.6004	0.5958
1.0	0.5	0.5	0.3333	0.2914	0.2979	0.2976
1.0	0.5	0.25	0.3720	0.3287	0.3404	0.3375
1.0	0.5	0	0.4054	0.3510	0.3723	0.3667

The dependence of β on macroscopic absorption cross-section Σ_a and the dimension of gap Δ by present method (*)– and by method (B) used in the work :
Berna Ph., Comparison between Benoist and Selengut diffusion coefficientsin one-veloccity theory when absorbing media is present in the cell. -J.Nucl. Energy, 1973, v.27, p.663. - is presented in table 8.1.16.

Table 8.1.16 The dependence of β on macroscopic absorption cross-section Σ_a and the dimension of gap Δ; * – present method; B- Berna

Δ, cm		Σ_a, cm^{-1}			
		0.01	0.1	0.3	0.5
0	*	-0.2237	-0.1246	0.0088	0.0868
	B	-0.2189	-0.1232	0.0102	0.0867
3	*	0.5511	0.5695	0.5959	0.6124
	B	0.5514	0.5704	0.5972	0.6422

8.2 Comparison of calculations by direct equation solutions and solutions of equations in an approximate difference form

A comparison of the results of calculations by approximate 9-point scheme for difference equations (with parameters of difference operators from table 2.3.1) and by direct metod of solution of matrix equations is presented in table 8.2.1.

Next example - calculations for two graphite-moderator critical assemblies with fuel assemblies of RBMK type . The height of critical assemblies 408 cm, radius 295.5 cm ; pitch 25 cm for square lattice, 26.86 cm for hexagonal lattice, symmetry- 1/4 and 1/6 correspondingly, the fuel assemblies were placed in positions (measured by pitch distance in square and hexagonal lattice): 0 0, 1 0, 2 0, 1 1. The results of calculations in monopole approximation - power W, neutron flux N and K_{eff} by computer codes DISHER (matrix equation) and TRECD (difference equation, parameters of difference operators taken from section 2.7) are presented in table 8.2.2, in dipole approximation - in table 8.2.3. The difference between dipole and monopole approximations in K_{eff} is about 1% for square lattice and 0.7% for hexagonal lattice, in power and flux distribution - about 3-4%.
The error of difference equation solution relative to direct solution in W and monopole component of flux for square lattice is about 0.1% , for hexagonal lattice 3-4 times higher, the error in K_{eff} is 0.0005 for square, 0.0015 for hexagonal lattice; the error in dipole component of neutron flux N^1 is about 10 %.

Table 8.2.1. The main reactor characteristics and multiplication factor and flux difference between direct (computer code DISHER) and difference equation solution (computer code TRECD), for 9-point scheme in square lattice , with difference operator parameters taken from table 2.3.1 (lecture 2.3)

N	1	2	3
Numb. of groups	2	3	3
Reactor rad., m	650	500	105
Pitch, m	0.26	0.20	0.085
Neutron age, cm^2	100	40; 80	80; 40
Diffusion area, cm^2	10 000	5 000	10 000
Number of channels	(1)-55; (2)-2	(1)-124; (2)-20; (3)-77	(1)-124; (2)-97;
Channel radius, cm	(1)-5.7; (2)-2.9	(1)-5; (2)-3; (3)-5	(1)-3; (2)-3
δK_{eff}	$<10^{-4}$	$<10^{-4}$	2.5×10^{-4}
δ (Flux)	$<10^{-3}$	$<10^{-3}$	1.4×10^{-3}

Table 8.2.2. The results of calculations in monopole approximation by computer codes DISHER(D) and TRECD(T) , $\mathbf{k}(k_x,k_y)$- coordinates of channels

Lattice		square				hex.			
k		0 0	1 0	2 0	1 1	0 0	1 0	2 0	1 1
W	D	1.00	0.869	0.683	0.827	1.00	0.899	0.680	0.745
	T	1.00	0.897	0.683	0.827	1.00	0.898	0.679	0.745
N_1^0	D	1.242	1.064	0.556	0.815	1.176	1.049	0.614	0.745
	T	1.245	1.064	0.556	0.816	1.171	1.045	0.613	0.741
N_2^0	D	1.00	0.908	0.754	0.878	1.00	0.901	0.725	0.777
	T	1.00	0.909	0.754	0.879	1.00	0.900	0.723	0.776
K_{eff}	D	1.0042				1.0678			
	T	1.0043				1.0655			

Table 8.2.3. The results of calculations in dipole approximation by computer codes DISHER(D) and TRECD(T)

Lattice		square				hex.			
k		0 0	1 0	2 0	1 1	0 0	1 0	2 0	1 1
W	D	1.00	0.887	0.660	0.808	1.00	0.891	0.655	0.723
	T	1.00	0.887	0.661	0.808	1.00	0.891	0.655	0.724
N_1^0	D	1.253	1.064	0.541	0.806	1.181	1.046	0.597	0.729
	T	1.255	1.063	0.541	0.806	1.175	1.042	0.595	0.726
N_2^0	D	1.00	0.899	0.730	0.858	1.00	0.892	0.697	0.754
	T	1.00	0.909	0.730	0.859	1.00	0.892	0.697	0.754
$\|N_1^1\|$	D	0.00	0.206	0.314	0.381	0.00	0.140	0.319	0.310
	T	0.00	0.209	0.320	0.390	0.00	0.139	0.315	0.306
$\|N_2^1\|$	D	0.00	0.105	0.118	0.063	0.00	0.106	0.085	0.082
	T	0.00	0.111	0.107	0.070	0.00	0.113	0.084	0.086
K_{eff}	D	0.9941				1.0606			
	T	0.9946				1.0590			

8.3 Reaction rate distributions

Light - water critical assembly

The composition of uranium oxide- water, uranium - water cells (Kouts e.a. Physics of slightly enriched, normal water lattices (theory and experiment) , In: Proc. Second UN International Conf. on the Peaceful Uses of Atomic Energy. Geneva, 1958, v. 12, p.446-482) is presented in table 8.3.1.

Table 8.3.1. Composition of cells for uranium-water critical assembly (37 cells of the 1st type in the central region; 936 cells of 2nd type in outer region)

Type	Region	ΔR, cm	Isotope (10^{24} cm^{-3})
1	Fuel	0.486	U235 0.000305 U238 0.0232 O 0.047
	Clad	0.071	Al 0.0602
	Moderator	0.391	H 0.0666 O 0.0333
2	Fuel	0.490	U235 0.000615 U238 0.00474
	Clad	0.071	Al 0.0602
	Moderator	0.387	H 0.0666 O 0.0333

Reaction rates distributions (^{235}U detectors (fissions) and ^{238}U detectors (fissions)) - experimental and calculated by computer codes TRIFON and DISHER is shown in Fig 8.9. It should be noted the difference in fast flux distribution and ^{238}U fissions distribution; theoretical distribution of ^{238}U fissions(calculated on the basis of reaction rate vectors and heterogeneous equations solution for flux) is close to the experimental points.

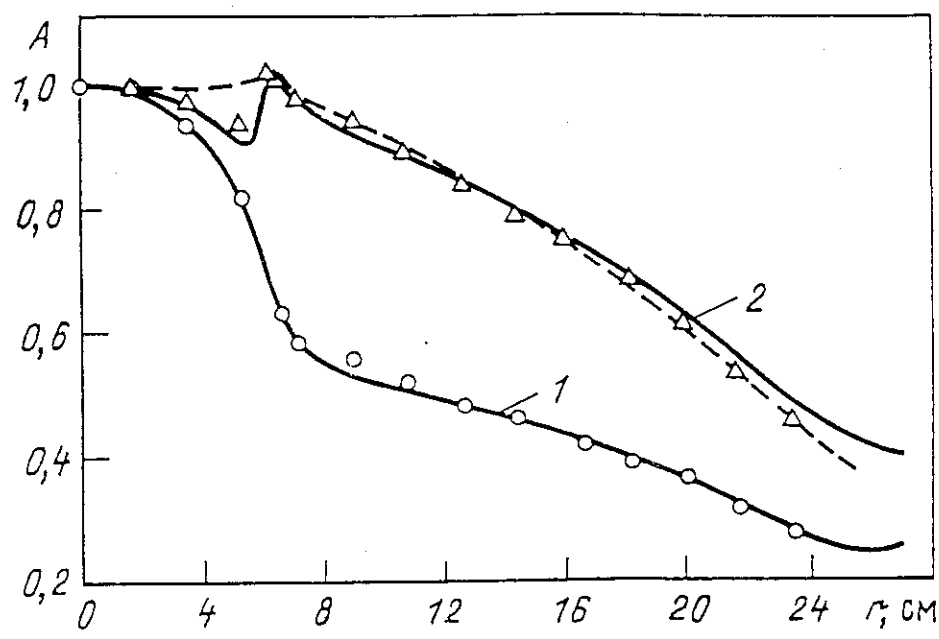


Fig. 8.9. Reaction rates distributions in a uranium-water critical assembly ; 1- ^{235}U detectors (fissions), 2- ^{238}U detectors (fissions) ; o, Δ – experiment, solid curves - calculation by computer code DISHER (solution of heterogeneous matrix equations) ,
- - - - -fast neutron flux.

RBMK critical assemblies

Examples of reaction rates distribution (Cu detectors) for 3 RBMK critical assemblies are shown below (upper values - calculation by TRIFON- TRECD, lower--experimental values , experimental error about 3%).

Ass. 5

			0.86 087	0.72 0.70
0.84 0.84	1.02 1.04	1.13 1.15	1.05 1.06	0.91 0.90
0.94 0.94	1.13 1.15	1.24 1.26	1.19 1.19	1.01 1.01
0.92 0.92	1.11 1.12	1.21 1.22	1.14 1.14	0.96 0.96
0.80 0.77	0.96 0.96	1.05 1.04	0.97 0.97	0.83 0.79

Ass. 7

	0.88 0.89	1.01 1.03	0.93 0.94	0.71 0.68
	1.11 1.11	1.25 1.27	1.13 1.13	
	1.12 1.13	1.26 1.27	1.10 1.10	
0.68 0.65	0.91 0.92	1.01 1.02	0.88 0.88	

Ass. 8

			0.77 -
0.90 0.89	1.03 1.05	1.05 1.06	0.92 0.91
1.01 1.02	1.18 1.18	1.18 1.20	1.03 1.06
0.99 1.02	1.17 1.18	1.18 1.18	1.01 1.03
0.87 0.84	1.02 1.02	1.02 1.03	0.90 0.89
0.66 -			

8.4 Critical experiments

An example of a representative set of critical experiments and its numerical analysis by heterogeneous reactor code calculations - for the model of a research reactor TWR-M. The experiments were cariied out in the period 20.12.1983 to 29.06.1984 in an experimental heavy-water facility "MAKET" in ITEP (Shvedov O.V., Kukushkin Yu. A. et.el., Experimental and Numerical studies of neutron-physics parameters of the model of TBR-M reactor on the facility "MAKET" Report ITEP N409, (Part 1 and 2), 1985) and included 85 critical experiments. The key physical parameters of critical assemblies are presented in the table 8.4.1.

Table 8.4.1 The key physical parameters of critical assemblies for the model of TWR-M reactor

Core, height, D_2O level, m			1.80 m
Fuel assemblies height			0.6355 m
Number of cylindrical tube fuel elements in a fuel asembly			6
Number of fuel assemblies (3 row with 6 assemblies in hexagonall lattice)			18
Inner diameter of a heavy-water vessel with a reflector			2.60 m
Hexagonal lattice pitch			0.11 m
Lattice pitch for fuel assemblies and SLR channels			0.0635 m
Fuel assembly outer diameter (6 th ring)			0.07 m
U-235 amount in fuel assembly	Relative.	Weight(g)	
	0.791	298.39	
	0.633	238.57	
	0.468	176.63	
Temperature			17.5 -: 23.0 grad.C

Steel tube was placed in the center of the core
Al tubes for control rods were placed in the reflector
near themaximum of neutron flux distribution.

The composition of critical assemblies was changed due to
- insertion or removal of Gd neutron absorbing pins in fuel assemblies (diam. 4 and 6 mm);
- filling with D_2O or removal of D_2O in SLR channels
- insertion of Cu tubes in the channels of SLR (diam. 6×0.5 mm or 6×1.0 mm);
- interchange of Al and steel control rods;
- the level of heavy water moderator (upper reflector)

The main part of theoretical values of K_{eff} lays in the limits

$$K_{eff} = 0.996 \pm 0.002;$$

6 experimental points - with GD absorbers near 1.005 ± 0.001

8.5 Calculation of states of Nuclear Power plant

An example of calculation by computer codes TRIFON and TRECD of some steady states of nuclear power plants with reactor cores of RBMK type , for Ignalina and Smolensk power stations are showm in table 8.5.1 and some reactivity effects - in the table 8.5.2.

Table 8.5.1 Multiplication factors for different NPP states

NPP		K_{eff}
Ignalina	**1. Basic state**	**1.0052**
	2. All contr. rods removed	**1.0330**
	3. All contr. rods completely inserted	**0.9537**
	4. Control rods in basoc state, coolant removed	**1.0227**
Smplensk	**1. Basic state**	0.9990
	2. All control rods removed	**1.0119**
	3. All control rods completely inserted	**0.9473**
	4. Control rods in basic state, coolant removed	**1.0304**

Table 8.5.2. Reactivity effects for NPP

Effect	Smolensk	Ignalina
Mean control rod worth	3.5×10^{-4}	4.6×10^{-4}
Coolant removal effect	0.0334	0.0175

8.6 Simulation of Xe poisoning 3D space - time process

An example of sumulation by computer code BARS (with cell parameters calculated by TRIFON as function of Xe, I concentrations) of Xe poisoning 3D space-time process for a heavy-water reactor , based on the work : S.V.Akimushkin, B.P.Kochurov, V.M.Malofeev, The studies of Xe stability of reactor TR-1000 PB, Report N805 (Russ.), ITEP, 1991. - is presented below.

Xe stability of heavy-water reactor TR-1000 PB at a constant level of power and without control rod influence on neutron flux distribution was studied. From a steady state the reactor was shut down for a 10 hour period of time and after that the reactor was put into operation at 100% power level. Re distribution of Xe concentration over reactor core during 10 hours period caused a redistribution of neutron flux, simulation of Xe process during 140 hours period of time showed the existance of stable periodic oscilations of neutron flux , I and Xe concentration in x-y plane with a period about 37 hours; no axial oscillations were discovered. The maximum of neutron flux in the periphery of reactor core moved a around with a period 37 hours. The oscillations of neutron flux in a channel (row 9, position 18) is shown in Fig. 8.10, Xe-I oscillations in the phase plane concentration I - concentration Xe - in Fig 8.11

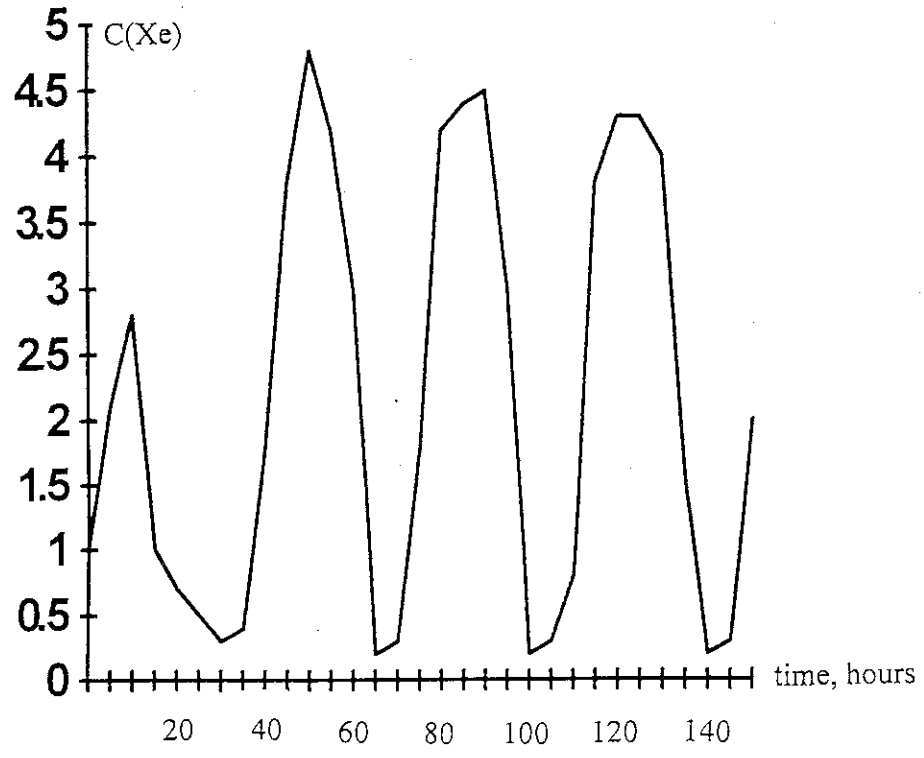


Fig 8.10. Time dependence of Xe concentration, 10^{15} cm^{-3}, in channel 9,18.

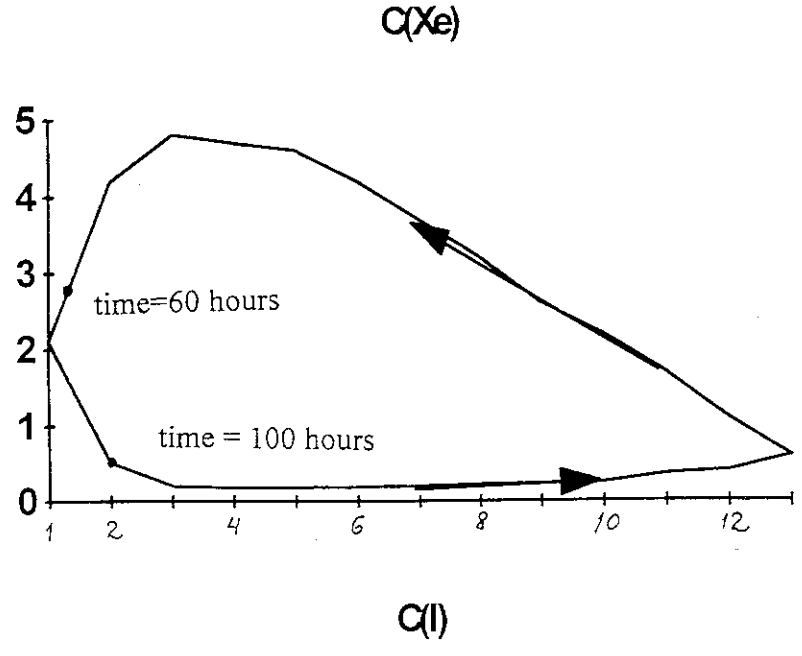


Fig 8.11. The dependence of Xe concentration C(Xe), 10^{15} cm^{-3}, on I concentration C(I), 10^{15} cm^{-3}, in channel 9, 18.

8.7 Simulation of fast transients on prompt and delayed neutrons

The model of reactor -heavy-water gas cooled , the main parameters are presented in table 8.6.1. The transients were caused by a chenge of control rods positions - some inserted , some removed .The results of calculations by computer code DINAR are presented in table 8.6.2.

Table 8.6.1 Reactor parameters for investigation of transients due to change of control rod positions (heavy-water, gas cooled reactor).

Reactor height, m	5
radius	5
Pitch, m (hex. lattice)	0.43
Channel	
number	361
radius, cm	10
Fuel composition , 10^{24} cm^{-3}	U238 0.0089; U235 0.00004; Pu239 0.00002
Prompt neutron life time, s	0.0007
Delayed neutron fracture	0.0058

Table 8.6.2. Power dependence on time- transients due to jump insertion and removal of control rods ; A-adiabatic, Q-quasi-static, P - point approxomations.

	ρ/β	t=0,5 s			t=60 s		
		A	Q	P	A	Q	P
6	-0,25	0,7576	0,7575	0,7067	0,2478	0,2465	0,1809
18	-0,94	0,4512	0,4476	0,3762	0,0582	0,0570	0,0396
12	0.18	1.280	1.269	1.158	8.014	7.958	3.492
6	0,09	1,120	1,117	1,073	2,262	2,258	1,720
30*	-0,23	0,9758	0,7875	0,3327	0,3416	0,2766	0,0314
42**	0,18	1,501	1,296	0,597	8,490	7,135	0,105

* Inserted 6, removed 24 control rods;

** The same for 6 and 36 control rods.

A big difference can be observed between adiabatic, quasi-static and point approximations (see Lecture 5.4)

Conclusion

Some new approaches in the development of heterogeneous reactor theory has been presented in the course of 8 lectures given in JAERI in April-June 1994.

The limitations of initial heterogeneous reactor theory known as Galanine -Feinberg heterogeneous theory were overcome by *general formulation of few-group heterogeneous reactor equation in dipole approximation*, its transformation a *difference form* and by the development of a *consistent theory for the characteristics of reactor channel or a cell* based on detailed space-energy calculations of a cell. These main points created the basis for the development of effective computer codes from codes for detailed space-energy calculations of a reactor cell (with a simulation of time process) to 3D space-time reactor codes for simulation of slow processes and fast transients.

This work has been carried out in the Institute for Theoretical and Experimental Physics, Reactor Physics laboratory, starting approximately from 1975.

The main outlines of the theory (difference approach to the solution of heterogeneous reactor theory and the theory of boundary conditions on the surface of a reactor cell surface) were developed by B.P.Kochurov , the part for neutron migration with collaboration with A.Yu.Kvaratzheli, computer code TRIFON was written by B.P.Kochurov and A.Yu.Kvaratzheli [23] (with participation of A.Ya.Burmistrov at the initial stage), computer code TERMIT - by V.M.Michailov [15,16], computer code DISHER - by B.P.Kochurov[5,17], computer code TRECD - by V.M.Malofeev and S.E.Smirnov [19], computer code BARS - by V.M.Malofeev [20]. The method for the calculations of fast transients taking account of prompt and delayed neutrons and computer code DINAR - by A.V.Avvacumov and V.M.Malofeev [21].

The system of computer codes was tested by comparisons with calculations by other methods (Monte-Carlo, WIMS) and by comparisons with the results of critical experiments in heavy-water critical assemblies and graphite-moderated, light water-cooled critical assemblies (RBMK type). The work on verification of the system of computer codes is continued now.

Computer codes are widely used for the analysis of physical properties of reactors of different types - heavy-water gas cooled , modular heavy-water moderated, heavy water cooled, research reactors with high flux, graphite-moderated, gas cooled (RBMK). These codes can find applications for such kinds of reactors as CANDU, FUGEN, ATR. Additional studies are necessary to understand the possibility of application of these approaches and computer codes to light-water reactors.

The work for the extension of computer codes for subcritical systems (based on the modification of code for cell calculations for the case of extended subcritical systems with modified for this case collision probabilities (A.P.Knyazev) and heterogeneous reactor equations) and new versions for 3D -space time simulations is under development now.

Acknowledgments

I wish to express my acknowledgment to the members of Reactor Physics laboratory of ITEP for their participation in the development of methods and computer codes for heterogeneous reactor studies.

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Appendix. Input-output data for TRIFON code, RBMK-type reactor cells , 18 fuel pins, water-cooled, graphite-moderated, with and without water coolant.

```
                                VERSIO,  1.04 OT 16. 4.90
                                ITEP, MOSCOW, 1990.
*ASSIGN BN

 *NOPEN, file MVAX1$DUA0,[LAB321.KOCHUROV]FOR001.DAT;3
'****** test RBMK ****** EMPTY, multi-layer moderator *
 '                        multi-layer coolant air*
 *CLUS
 LB    13,18,1,0,1,100,10,-12
 NSUB  2/
 RAN   .75,0.91,2.29,2.41,3.79,4.,4.4,5.4043,6.5986,
              8.01889,9.70788,11.71643,14.105/
 NZR1  1,1/
 RAR1  0.59,.68/
 ROD1  2,6,1.6,0.,1.,2,12,2.994370061,.80233904,0./
 SQ2   0.,0.//
 'ITH(1)=2
 ITH(6)=0
 NGRR=11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,21,26,26
 NSRE=10,10,10,10,10,10,10,40
 GROU=11,17,24,26
 NGRO=26,NGAU=7,NZON=17,NCAN=11
 ZONE 1,RV=.75 ,NS=1,C(ZR)=.0322
 ZONE 2,RV=0.91 ,NS=1
C(O)=1.-4
 ZONE 3,RV=2.29 ,NS=1
 C(O)=1.-4
 ZONE 4,RV=.59 ,NS=1
 C(U5)=.0005465,C(U8)=.022022,C(RZU8)=.022022,C(O)=.045137
 ZONE 5,RV=.68 ,NS=1,C(ZR)=.0425
 ZONE 6,RV=2.41 ,NS=1
C(O)=1.-4
 ZONE 7,RV=3.79 ,NS=1
C(O)=1.-4
 ZONE 8,RV=.59 ,NS=1
 C(U5)=.0005465,C(U8)=.022022,C(RZU8)=.022022,C(O)=.045137
 ZONE 9,RV=.68 ,NS=1,C(ZR)=.0425
 ZONE 10,RV=4.0 ,NS=1
 C(O)=1.-4
 ZONE 11,RV=4.4 ,NS=1,C(ZR)=.0425
 ZONE 12,RV=5.4043 ,NS=1,C(C)=.0837
 ZONE 13,RV=6.5986 ,NS=1,C(C)=.0837
 ZONE 14,RV=8.01889 ,NS=1,C(C)=.0837
 ZONE 15,RV=9.70788 ,NS=1,C(C)=.0837
 ZONE 16,RV=11.71643 ,NS=1,C(C)=.0837
 ZONE 17,RV=14.105,NS=1,C(C)=.0837
 *END*

..... HORDA=  1.942
 CRSBL FOR U5 , HORD=  0.1941E+01 S=  0.9426E+03 TEMPER=  0.2930E+03 GROUPS,  11  23
 CRSBL FOR U8 , HORD=  0.1942E+01 S=  0.2338E+02 TEMPER=  0.2930E+03 GROUPS,  8  21
 CRSBL FOR ZR  , HORD=  0.1310E+01 S=  0.1839E+02 TEMPER=  0.2930E+03 GROUPS,  11  24
...FOR 126 GROUPS AND  34 GEOM. ZONES
 LENGTH of Scr.  BLOCK FOR SOURCES AND FLUX IS  4284 WORDS
   ----------------------------------------------------
```

group 1 ,from 1 to 11 10.50000 MEV 10.00000 KEV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J		
CELL	0.18001	0.00024	0.00020	0.00054	0.26578	0.26621	0.00846	0.00000	0.00000
CANAL	0.26310	0.00106	0.00092	0.00251	0.20727	0.20925	0.00278	0.00000	0.00000
ZONE 1	0.29553	0.00037	0.00000	0.00000	0.19226	0.19263	0.00050	0.00000	0.00000
ZONE 2	0.30204	0.00000	0.00000	0.00000	0.00033	0.00033	0.00000	0.00000	0.00000
ZONE 3	0.29900	0.00000	0.00000	0.00000	0.00033	0.00033	0.00000	0.00000	0.00000
ZONE 4	0.31387	0.00380	0.00376	0.01024	0.31603	0.32358	0.00187	0.00000	0.00000
ZONE 5	0.30347	0.00048	0.00000	0.00000	0.25156	0.25204	0.00064	0.00000	0.00000
ZONE 6	0.29751	0.00000	0.00000	0.00000	0.00033	0.00033	0.00000	0.00000	0.00000
ZONE 7	0.27742	0.00000	0.00000	0.00000	0.00033	0.00033	0.00000	0.00000	0.00000
ZONE 8	0.29794	0.00389	0.00372	0.01013	0.31855	0.32616	0.00198	0.00000	0.00000
ZONE 9	0.28372	0.00049	0.00000	0.00000	0.25430	0.25479	0.00069	0.00000	0.00000
ZONE 10	0.25552	0.00000	0.00000	0.00000	0.00034	0.00034	0.00000	0.00000	0.00000
ZONE 11	0.24607	0.00050	0.00000	0.00000	0.26288	0.26339	0.00079	0.00000	0.00000
ZONE 12	0.22370	0.00002	0.00000	0.00000	0.26685	0.26687	0.00751	0.00000	0.00000
ZONE 13	0.20056	0.00001	0.00000	0.00000	0.27282	0.27283	0.00837	0.00000	0.00000
ZONE 14	0.18217	0.00001	0.00000	0.00000	0.27781	0.27782	0.00919	0.00000	0.00000
ZONE 15	0.16780	0.00001	0.00000	0.00000	0.28185	0.28186	0.00992	0.00000	0.00000
ZONE 16	0.15793	0.00001	0.00000	0.00000	0.28464	0.28465	0.01047	0.00000	0.00000
ZONE 17	0.15648	0.00001	0.00000	0.00000	0.28389	0.28390	0.01053	0.00000	0.00000

BALANCE, C+F= 0.4876775E-01; C+F-1=-0.9512323E+00;
REMUV= 0.9514192E+00; C+F+REMUV-1= 0.1869202E-03

---

group 2 ,from 12 to 17 10.00000 KEV 100.00000 EV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J	
CELL	0.11823	0.00072	0.00016	0.00039	0.36241	0.36330	0.01200	0.00000
CANAL	0.11110	0.00522	0.00117	0.00282	0.29672	0.30310	0.00549	0.00000
ZONE 1	0.10723	0.00179	0.00000	0.00000	0.23842	0.24020	0.00087	0.00000
ZONE 2	0.10681	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001	0.00000
ZONE 3	0.10746	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001	0.00000
ZONE 4	0.10619	0.02082	0.00560	0.01356	0.48924	0.51567	0.00430	0.00000
ZONE 5	0.10707	0.00236	0.00000	0.00000	0.31476	0.31712	0.00115	0.00000
ZONE 6	0.10778	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001	0.00000
ZONE 7	0.11000	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001	0.00000
ZONE 8	0.10827	0.02385	0.00562	0.01361	0.50722	0.53670	0.00430	0.00000
ZONE 9	0.10954	0.00237	0.00000	0.00000	0.31456	0.31692	0.00115	0.00000
ZONE 10	0.11199	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001	0.00000
ZONE 11	0.11265	0.00238	0.00000	0.00000	0.31424	0.31662	0.00115	0.00000
ZONE 12	0.11463	0.00000	0.00000	0.00000	0.37291	0.37291	0.01256	0.00000
ZONE 13	0.11668	0.00000	0.00000	0.00000	0.37292	0.37292	0.01271	0.00000
ZONE 14	0.11820	0.00000	0.00000	0.00000	0.37292	0.37292	0.01287	0.00000
ZONE 15	0.11928	0.00000	0.00000	0.00000	0.37293	0.37293	0.01300	0.00000
ZONE 16	0.11997	0.00000	0.00000	0.00000	0.37293	0.37293	0.01310	0.00000
ZONE 17	0.12023	0.00000	0.00000	0.00000	0.37293	0.37293	0.01314	0.00000

BALANCE, C+F= 0.1139829E+00; C+F-1=-0.8860171E+00;
REMUV= 0.8866040E+00; C+F+REMUV-1= 0.5869865E-03

---

group 3 ,from 18 to 24 100.00000 EV 0.46500 EV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J
CELL	0.11872	0.00136	0.00050	0.00122	0.36029	0.36215	0.01009
CANAL	0.10153	0.01067	0.00401	0.00969	0.26669	0.28137	0.00505
ZONE 1	0.09457	0.00013	0.00000	0.00000	0.19759	0.19772	0.00081
ZONE 2	0.09359	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001
ZONE 3	0.09452	0.00000	0.00000	0.00000	0.00036	0.00036	0.00001
ZONE 4	0.09201	0.04651	0.02007	0.04858	0.39759	0.46417	0.00418
ZONE 5	0.09377	0.00017	0.00000	0.00000	0.26080	0.26097	0.00107

ZONE 6, 0.09499 0.00000 0.00000 0.00000 0.00036 0.00036 0.00001
ZONE 7, 0.09919 0.00000 0.00000 0.00000 0.00036 0.00036 0.00001
ZONE 8, 0.09561 0.05657 0.02009 0.04861 0.40165 0.47831 0.00414
ZONE 9, 0.09821 0.00017 0.00000 0.00000 0.26080 0.26096 0.00105
ZONE 10, 0.10321 0.00000 0.00000 0.00000 0.00036 0.00036 0.00001
ZONE 11, 0.10458 0.00016 0.00000 0.00000 0.26080 0.26096 0.00103
ZONE 12, 0.10862 0.00002 0.00000 0.00000 0.37373 0.37375 0.01112
ZONE 13, 0.11351 0.00002 0.00000 0.00000 0.37373 0.37375 0.01099
ZONE 14, 0.11760 0.00002 0.00000 0.00000 0.37373 0.37375 0.01089
ZONE 15, 0.12090 0.00002 0.00000 0.00000 0.37373 0.37375 0.01082
ZONE 16, 0.12325 0.00002 0.00000 0.00000 0.37373 0.37375 0.01078
ZONE 17, 0.12424 0.00002 0.00000 0.00000 0.37373 0.37375 0.01076
BALANCE, C+F= 0.2521915E+00; C+F-1=-0.7478085E+00;
REMUV= 0.7483930E+00; C+F+REMUV-1= 0.5844831E-03

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group 4 ,from 25 to 26 0.46500 EV 0.00000 EV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT
CELL	0.25353	0.00150	0.00322	0.00780	0.35219	0.35692
CANAL	0.16454	0.01375	0.03383	0.08188	0.26623	0.31382
ZONE 1	0.12766	0.00386	0.00000	0.00000	0.23486	0.23872
ZONE 2	0.12295	0.00000	0.00000	0.00000	0.00034	0.00034
ZONE 3	0.12785	0.00000	0.00000	0.00000	0.00034	0.00034
ZONE 4	0.11571	0.07279	0.19492	0.47170	0.33538	0.60309
ZONE 5	0.12405	0.00507	0.00000	0.00000	0.30997	0.31505
ZONE 6	0.13025	0.00000	0.00000	0.00000	0.00034	0.00034
ZONE 7	0.15152	0.00000	0.00000	0.00000	0.00034	0.00034
ZONE 8	0.13480	0.07619	0.20510	0.49634	0.33559	0.61689
ZONE 9	0.14645	0.00535	0.00000	0.00000	0.31017	0.31552
ZONE 10	0.17193	0.00000	0.00000	0.00000	0.00034	0.00034
ZONE 11	0.17963	0.00562	0.00000	0.00000	0.31037	0.31599
ZONE 12	0.20177	0.00020	0.00000	0.00000	0.36050	0.36070
ZONE 13	0.22689	0.00020	0.00000	0.00000	0.36088	0.36109
ZONE 14	0.24785	0.00021	0.00000	0.00000	0.36110	0.36130
ZONE 15	0.26479	0.00021	0.00000	0.00000	0.36122	0.36143
ZONE 16	0.27699	0.00021	0.00000	0.00000	0.36130	0.36151
ZONE 17	0.28195	0.00021	0.00000	0.00000	0.36133	0.36154

BALANCE, C+F= 0.1000583E+01; C+F-1= 0.5829334E-03;
REMUV= 0.0000000E+00; C+F+REMUV-1= 0.5829334E-03

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zones 17#groups 25 #integration nodes 7 #spectrum FISS.....#variant, 0 .....

* * ZONE	VOLUME	THERMAL FLUX	IZOTOPES NAME	COMP. CONC.	EPI- CAPTURE.	THERMAL FISSION.	THERMAL CAPTURE	THERMAL FISSION.
1	1.7671	0.1277	ZR	.3220E-01	.8709E-03	.0000E+00	.5518E-03	.0000E+00
2	0.8344	0.1230	O	.1000E-03	.1202E-08	.0000E+00	.7448E-07	.0000E+00
3	5.1572	0.1279	O	.1000E-03	.7842E-08	.0000E+00	.4539E-06	.0000E+00
4	6.5615	0.1157	U5	.5465E-03	.2550E-01	.1480E+00	.7891E-02	.1764E-01
			U8	.2202E-01	.2976E-01	.0000E+00	.9158E-02	.6123E-02
			RZU8	.2202E-01	.0000E+00	.0000E+00	.3307E-01	.0000E+00
			O	.4514E-01	.3969E-05	.0000E+00	.2909E-03	.0000E+00
5	2.1545	0.1241	ZR	.4250E-01	.1356E-02	.0000E+00	.8934E-03	.0000E+00
6	1.7719	0.1303	O	.1000E-03	.2755E-08	.0000E+00	.1567E-06	.0000E+00
7	9.4474	0.1515	O	.1000E-03	.1798E-07	.0000E+00	.7220E-06	.0000E+00
8	13.1231	0.1348	U5	.5465E-03	.6238E-01	.3628E+00	.1641E-01	.3629E-01
			U8	.2202E-01	.7239E-01	.0000E+00	.1801E-01	.1145E-01
			RZU8	.2202E-01	.0000E+00	.0000E+00	.8512E-01	.0000E+00
			O	.4514E-01	.9663E-05	.0000E+00	.5407E-03	.0000E+00
9	4.3090	0.1465	ZR	.4250E-01	.3374E-02	.0000E+00	.1783E-02	.0000E+00
10	5.1393	0.1719	O	.1000E-03	.1147E-07	.0000E+00	.3208E-06	.0000E+00
11	10.5558	0.1796	ZR	.4250E-01	.1066E-01	.0000E+00	.4314E-02	.0000E+00
12	30.9335	0.2018	C	.8370E-01	.1256E-02	.0000E+00	.1912E-03	.0000E+00
13	45.0349	0.2269	C	.8370E-01	.2094E-02	.0000E+00	.2420E-03	.0000E+00
14	65.2228	0.2479	C	.8370E-01	.3351E-02	.0000E+00	.3167E-03	.0000E+00
15	94.0604	0.2648	C	.8370E-01	.5203E-02	.0000E+00	.4257E-03	.0000E+00
16	135.1883	0.2770	C	.8370E-01	.7859E-02	.0000E+00	.5878E-03	.0000E+00
17	193.7619	0.2819	C	.8370E-01	.1149E-01	.0000E+00	.8835E-03	.0000E+00

full balance and mean concentrations of 6 isotopes,

			ZR	.1248E-02	.1626E-01	.0000E+00	.7542E-02	.0000E+00
			O	.1425E-02	.1367E-04	.0000E+00	.8333E-03	.0000E+00
			U5	.1721E-04	.8788E-01	.5108E+00	.2430E-01	.5394E-01
			U8	.6936E-03	.1022E+00	.0000E+00	.2717E-01	.1758E-01
			RZU8	.6936E-03	.0000E+00	.0000E+00	.1182E+00	.0000E+00
			C	.7556E-01	.3125E-01	.0000E+00	.2647E-02	.0000E+00

TRIFON K-INF, 1.41600, NU-AVERAGE, 2.43158.....

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*PRINT FULL
'****** test RBMK ****** H2O  , multi-layer moderator *
'                        multi-layer coolant   *
'
 *CLUS
 LB    13,18,1,0,1,100,10,-12
 NSUB  2/
 RAN   .75,0.91,2.29,2.41,3.79,4.,4.4,5.4043,6.5986,
                 8.01889,9.70788,11.71643,14.105/
 NZR1  1,1/
 RAR1  0.59,.68/
 ROD1  2,6,1.6,0.,1.,2,12,2.994370061,.80233904,0./
 SQ2   0.,0.//
 'ITH(1)=2
 ITH(6)=0
 NGRR=11,11,12,12,13,13,14,14,15,15,16,16,17,17,18,21,26,26
 NSRE=10,10,10,10,10,10,10,40
 GROU=11,17,24,26
 NGRO=26,NGAU=7,NZON=17,NCAN=11
 ZONE 1,RV=.75 ,NS=1,C(ZR)=.0322
 ZONE 2,RV=0.91 ,NS=1
 C(H)=.066,C(O)=.033
 ZONE 3,RV=2.29 ,NS=1
 C(H)=.066,C(O)=.033
 'C(O)=1.-4
 ZONE 4,RV=.59 ,NS=1
C(U5)=.0005465,C(U8)=.022022,C(RZU8)=.022022,C(O)=.045137
 ZONE 5,RV=.68 ,NS=1,C(ZR)=.0425
 ZONE 6,RV=2.41 ,NS=1
 C(H)=.066,C(O)=.033
 ZONE 7,RV=3.79 ,NS=1
 C(H)=.066,C(O)=.033
 ZONE 8,RV=.59 ,NS=1
C(U5)=.0005465,C(U8)=.022022,C(RZU8)=.022022,C(O)=.045137
 ZONE 9,RV=.68 ,NS=1,C(ZR)=.0425
 ZONE 10,RV=4.0 ,NS=1
 C(H)=.066,C(O)=.033
 ZONE 11,RV=4.4 ,NS=1,C(ZR)=.0425
 ZONE 12,RV=5.4043 ,NS=1,C(C)=.0837
 ZONE 13,RV=6.5986 ,NS=1,C(C)=.0837
 ZONE 14,RV=8.01889 ,NS=1,C(C)=.0837
 ZONE 15,RV=9.70788 ,NS=1,C(C)=.0837
 ZONE 16,RV=11.71643 ,NS=1,C(C)=.0837
 ZONE 17,RV=14.105,NS=1,C(C)=.0837
 *END*

..... HORDA=  1.222
CRSBL FOR U5 , HORD=  0.1221E+01 S=  0.1499E+04 TEMPER=  0.2930E+03 GROUPS,  11  23
CRSBL FOR U8 , HORD=  0.1222E+01 S=  0.3715E+02 TEMPER=  0.2930E+03 GROUPS,   8  21
CRSBL FOR ZR  , HORD=  0.6322E+00 S=  0.3809E+02 TEMPER=  0.2930E+03 GROUPS,  11  24
 ...FOR 126 GROUPS AND  34 GEOM. ZONES
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group 1 ,from 1 to 11 10.50000 MEV 10.00000 KEV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J		
CELL	, 0.11960	0.00023	0.00024	0.00065	0.27404	0.27450	0.01287	0.00004	0.00000
CANAL	, 0.17115	0.00105	0.00112	0.00308	0.27026	0.27243	0.02688	0.00021	0.00000
ZONE 1,	0.19597	0.00035	0.00000	0.00000	0.18396	0.18431	0.00041	0.00000	0.00000
ZONE 2,	0.20142	0.00013	0.00000	0.00000	0.26553	0.26566	0.08670	0.00074	0.00000
ZONE 3,	0.19268	0.00012	0.00000	0.00000	0.26830	0.26843	0.08985	0.00077	0.00000
ZONE 4,	0.21458	0.00350	0.00433	0.01189	0.30192	0.30975	0.00148	0.00000	0.00000
ZONE 5,	0.20168	0.00046	0.00000	0.00000	0.24018	0.24064	0.00052	0.00000	0.00000
ZONE 6,	0.19171	0.00013	0.00000	0.00000	0.26760	0.26772	0.08993	0.00077	0.00000
ZONE 7,	0.17633	0.00012	0.00000	0.00000	0.27369	0.27381	0.09703	0.00084	0.00000
ZONE 8,	0.20314	0.00357	0.00432	0.01184	0.30354	0.31143	0.00158	0.00000	0.00000
ZONE 9,	0.18659	0.00047	0.00000	0.00000	0.24254	0.24301	0.00057	0.00000	0.00000
ZONE 10,	0.15957	0.00010	0.00000	0.00000	0.28250	0.28261	0.10738	0.00093	0.00000
ZONE 11,	0.15454	0.00049	0.00000	0.00000	0.25372	0.25421	0.00071	0.00000	0.00000
ZONE 12,	0.14309	0.00002	0.00000	0.00000	0.25823	0.25825	0.00672	0.00000	0.00000
ZONE 13,	0.13032	0.00002	0.00000	0.00000	0.26489	0.26490	0.00756	0.00000	0.00000
ZONE 14,	0.11996	0.00001	0.00000	0.00000	0.27049	0.27050	0.00835	0.00000	0.00000
ZONE 15,	0.11179	0.00001	0.00000	0.00000	0.27504	0.27506	0.00905	0.00000	0.00000
ZONE 16,	0.10620	0.00001	0.00000	0.00000	0.27818	0.27819	0.00958	0.00000	0.00000
ZONE 17,	0.10572	0.00001	0.00000	0.00000	0.27749	0.27750	0.00964	0.00000	0.00000

BALANCE, C+F= 0.3488538E-01; C+F-1=-0.9651147E+00;
REMUV= 0.9652418E+00; C+F+REMUV-1= 0.1271963E-03

group 2 ,from 12 to 17 10.00000 KEV 100.00000 EV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J	
CELL	, 0.07042	0.00082	0.00016	0.00038	0.38113	0.38210	0.02093	0.00004
CANAL	, 0.06419	0.00610	0.00118	0.00285	0.43424	0.44152	0.07205	0.00027
ZONE 1,	0.06113	0.00212	0.00000	0.00000	0.23776	0.23988	0.00091	0.00000
ZONE 2,	0.06109	0.00012	0.00000	0.00000	0.55684	0.55696	0.27580	0.00113
ZONE 3,	0.06143	0.00012	0.00000	0.00000	0.55686	0.55698	0.27673	0.00113
ZONE 4,	0.06021	0.02597	0.00574	0.01390	0.51887	0.55058	0.00451	0.00000
ZONE 5,	0.06104	0.00281	0.00000	0.00000	0.31387	0.31668	0.00120	0.00000
ZONE 6,	0.06174	0.00012	0.00000	0.00000	0.55687	0.55699	0.27718	0.00114
ZONE 7,	0.06297	0.00012	0.00000	0.00000	0.55690	0.55702	0.27843	0.00114
ZONE 8,	0.06180	0.02736	0.00576	0.01394	0.52672	0.55984	0.00453	0.00000
ZONE 9,	0.06268	0.00281	0.00000	0.00000	0.31367	0.31649	0.00121	0.00000
ZONE 10,	0.06460	0.00012	0.00000	0.00000	0.55692	0.55704	0.27922	0.00115
ZONE 11,	0.06562	0.00281	0.00000	0.00000	0.31352	0.31633	0.00120	0.00000
ZONE 12,	0.06717	0.00000	0.00000	0.00000	0.37292	0.37292	0.01305	0.00000
ZONE 13,	0.06883	0.00000	0.00000	0.00000	0.37292	0.37292	0.01302	0.00000
ZONE 14,	0.07018	0.00000	0.00000	0.00000	0.37292	0.37292	0.01302	0.00000
ZONE 15,	0.07125	0.00000	0.00000	0.00000	0.37292	0.37292	0.01302	0.00000
ZONE 16,	0.07201	0.00000	0.00000	0.00000	0.37292	0.37292	0.01303	0.00000
ZONE 17,	0.07231	0.00000	0.00000	0.00000	0.37292	0.37292	0.01304	0.00000

BALANCE, C+F= 0.7780000E-01; C+F-1=-0.9222000E+00;
REMUV= 0.9227269E+00; C+F+REMUV-1= 0.5269051E-03

group 3 ,from 18 to 24 100.00000 EV 0.46500 EV

GROUPS CROSS SECTIONS..

	FLUX	CC	CF	CNF	CE	CT	C I-I+J
CELL	, 0.07360	0.00178	0.00052	0.00127	0.37729	0.37959	0.01776
CANAL	, 0.06513	0.01354	0.00403	0.00976	0.40109	0.41867	0.06295
ZONE 1,	0.06023	0.00014	0.00000	0.00000	0.19759	0.19773	0.00078
ZONE 2,	0.06017	0.00172	0.00000	0.00000	0.56541	0.56714	0.24439
ZONE 3,	0.06104	0.00172	0.00000	0.00000	0.56541	0.56713	0.24369
ZONE 4,	0.05797	0.06344	0.02047	0.04953	0.40289	0.48680	0.00411
ZONE 5,	0.05990	0.00019	0.00000	0.00000	0.26079	0.26098	0.00104

ZONE 6, 0.06174 0.00172 0.00000 0.00000 0.56541 0.56714 0.24420
ZONE 7, 0.06412 0.00172 0.00000 0.00000 0.56541 0.56713 0.24330
ZONE 8, 0.06078 0.06778 0.02047 0.04953 0.40428 0.49252 0.00410
ZONE 9, 0.06301 0.00019 0.00000 0.00000 0.26079 0.26098 0.00103
ZONE 10, 0.06694 0.00172 0.00000 0.00000 0.56541 0.56713 0.24207
ZONE 11, 0.06789 0.00019 0.00000 0.00000 0.26079 0.26098 0.00102
ZONE 12, 0.06952 0.00002 0.00000 0.00000 0.37373 0.37375 0.01107
ZONE 13, 0.07157 0.00002 0.00000 0.00000 0.37373 0.37375 0.01104
ZONE 14, 0.07331 0.00002 0.00000 0.00000 0.37373 0.37375 0.01102
ZONE 15, 0.07472 0.00002 0.00000 0.00000 0.37373 0.37375 0.01101
ZONE 16, 0.07573 0.00002 0.00000 0.00000 0.37373 0.37375 0.01100
ZONE 17, 0.07615 0.00002 0.00000 0.00000 0.37373 0.37375 0.01100
BALANCE, C+F= 0.1837328E+00; C+F-1=-0.8162672E+00;
REMUV= 0.8167810E+00; C+F+REMUV-1= 0.5137920E-03

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group 4 ,from 25 to 26 0.46500 EV 0.00000 EV

GROUPS CROSS SECTIONS..

FLUX CC CF CNF CE CT C I-I+J
CELL , 0.24634 0.00194 0.00337 0.00815 0.39790 0.40321
CANAL , 0.17047 0.01714 0.03314 0.08019 0.71631 0.76658
ZONE 1, 0.11124 0.00433 0.00000 0.00000 0.23523 0.23956
ZONE 2, 0.11262 0.01644 0.00000 0.00000 2.05527 2.07171
ZONE 3, 0.11832 0.01646 0.00000 0.00000 2.05695 2.07341
ZONE 4, 0.10050 0.07970 0.21559 0.52173 0.33575 0.63104
ZONE 5, 0.11042 0.00562 0.00000 0.00000 0.31040 0.31603
ZONE 6, 0.12902 0.01665 0.00000 0.00000 2.07380 2.09045
ZONE 7, 0.15060 0.01693 0.00000 0.00000 2.09911 2.11604
ZONE 8, 0.12838 0.08223 0.22325 0.54027 0.33584 0.64131
ZONE 9, 0.14155 0.00580 0.00000 0.00000 0.31053 0.31633
ZONE 10, 0.18758 0.01754 0.00000 0.00000 2.15454 2.17208
ZONE 11, 0.20511 0.00619 0.00000 0.00000 0.31081 0.31700
ZONE 12, 0.21880 0.00022 0.00000 0.00000 0.36176 0.36198
ZONE 13, 0.23394 0.00022 0.00000 0.00000 0.36182 0.36204
ZONE 14, 0.24663 0.00022 0.00000 0.00000 0.36186 0.36208
ZONE 15, 0.25692 0.00022 0.00000 0.00000 0.36189 0.36211
ZONE 16, 0.26433 0.00022 0.00000 0.00000 0.36191 0.36213
ZONE 17, 0.26737 0.00022 0.00000 0.00000 0.36192 0.36214
BALANCE, C+F= 0.1000517E+01; C+F-1= 0.5170107E-03;
REMUV= 0.0000000E+00; C+F+REMUV-1= 0.5170107E-03

* * ZONE	VOLUME	THERMAL FLUX	IZOTOPES NAME	COMP. CONC.	EPI- CAPTURE.	THERMAL FISSION.	THERMAL CAPTURE	THERMAL FISSION.
1	1.7671	0.1112	ZR	.3220E 01	.8517E-03	.0000E+00	.3665E-03	.0000E+00
2	0.8344	0.1126	H	.6600E-01	.1544E-02	.0000E-00	.9256E-04	.0000E+00
			O	.3300E- 01	.4140E-06	.0000E-00	.2139E-04	.0000E-00
3	5.1572	0.1183	H	.6600E- 01	.1004E-01	.0000E-00	.5794E-03	.0000E-00
			O	.3300E- 01	.2692E-05	.0000E-00	.1225E-03	.0000E-00
4	6.5615	0.1005	U5	.5465E- 03	.2436E-01	.1422E-00	.5066E-02	.1113E-01
			U8	.2202E- 01	.2819E-01	.0000E-00	.5725E-02	.5023E-02
			RZU8	.2202E- 01	.0000E-00	.0000E-00	.2828E-01	.0000E-00
			O	.4514E- 01	.3767E-05	.0000E-00	.2525E-03	.0000E-00
5	2.1545	0.1104	ZR	.4250E- 01	.1338E-02	.0000E-00	.5939E-03	.0000E-00
6	1.7719	0.1290	H	.6600E- 01	.3805E-02	.0000E-00	.2015E-03	.0000E-00
			O	.3300E- 01	.1020E-05	.0000E-00	.4264E-04	.0000E-00
7	9.4474	0.1506	H	.6600E- 01	.2409E-01	.0000E-00	.1113E-02	.0000E-00
			O	.3300E- 01	.6457E-05	.0000E-00	.1943E-03	.0000E-00
8	13.1231	0.1284	U5	.5465E- 03	.6428E-01	.3761E-00	.1057E-01	.2305E-01
			U8	.2202E- 01	.7424E-01	.0000E-00	.1131E-01	.9456E-02
			RZU8	.2202E- 01	.0000E-00	.0000E-00	.6341E-01	.0000E-00
			O	.4514E- 01	.9927E-05	.0000E-00	.4733E-03	.0000E-00
9	4.3090	0.1415	ZR	.4250E- 01	.3536E-02	.0000E-00	.1186E-02	.0000E-00
10	5.1393	0.1876	H	.6600E- 01	.1691E-01	.0000E-00	.6303E-03	.0000E-00
			O	.3300E- 01	.4532E-05	.0000E-00	.8594E-04	.0000E-00
11	10.5558	0.2051	ZR	.4250E- 01	.1341E-01	.0000E-00	.2876E-02	.0000E-00
12	30.9335	0.2188	C	.8370E- 01	.1474E-02	.0000E-00	.1446E-03	.0000E-00
13	45.0349	0.2339	C	.8370E- 01	.2302E-02	.0000E-00	.1786E-03	.0000E-00
14	65.2228	0.2466	C	.8370E- 01	.3525E-02	.0000E-00	.2284E-03	.0000E-00
15	94.0604	0.2569	C	.8370E- 01	.5307E-02	.0000E-00	.3008E-03	.0000E-00
16	135.1883	0.2643	C	.8370E- 01	.7859E-02	.0000E-00	.4095E-03	.0000E-00
17	193.7619	0.2674	C	.8370E- 01	.1140E-01	.0000E-00	.6210E-03	.0000E-00

full balance and mean concentrations of 7 isotopes,

			ZR	.1248E-02	.1914E-01	.0000E-00	.5022E-02	.0000E-00
			H	.2360E-02	.5638E-01	.0000E-00	.2617E-02	.0000E-00
			O	.2602E-02	.2881E-04	.0000E-00	.1193E-02	.0000E-00
			U5	.1721E-04	.8864E-01	.5183E-00	.1564E-01	.3418E-01
			U8	.6936E-03	.1024E-00	.0000E-00	.1703E-01	.1448E-01
			RZU8	.6936E-03	.0000E-00	.0000E-00	.9168E-01	.0000E-00
			C	.7556E-01	.3187E-01	.0000E-00	.1883E-02	.0000E-00

TRIFON K-INF, 1.37771, NU-AVERAGE, 2.43001.....