

About Calculation of Axial Diffusion Coefficient in Nuclear Reactors Cells

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In this paper method for calculation of axial diffusion coefficient is developed. Purpose of this development is to analyze the significance of influence of neutron group spectrum of 2-dimensional problem into the value of axial leakage. To reach this purpose a way for calculation of direction probabilities in 2-D geometry has been suggested. Algorithm and code have been created on the base of this way. The code has been verified with the balance equation of the modeling problem.

The results obtained show that if the influence of heterogeneous structure of the neutron flux spectrum on the current along Z-axis is taken into account then for VVER-type cell the coefficient of axial diffusion is changed in fast group (~2%) and in thermal group (~15%). This discrepancy can lead to the multiplication factor discrepancy about 200-300 pcm. This difference can influence on the neutron leakage in the area closed to reactor reflector. Code VEPS-A can be recommended to estimate the fine effects of axial diffusion coefficients calculations in reactor cell.

KEYWORDS: *axial diffusion, direction probabilities, neutron group structure, reactor cell, closed grid, boundary conditions*

1. Introduction

Axial leakage in nuclear reactor cells with axial symmetry is defined with the coefficient of axial diffusion D^z (it is supposed Z is the axial cell direction)[1,2]. In the most cell codes (WIMS,[3],for example) Benoist leakage method [4] is used for D^z calculation analysis. In previous formulation of this method neutron phase density $f(\vec{r}, \vec{\Omega})$ is supposed as uniform and isotropic so the neutron flux spectrum of 2-D problem doesn't influence to the axial leakage and so the calculation analysis method of D^z is enough simple. But this assumption needs verification for complicate structure of modern nuclear reactors especially in the closed grids (as VVER-type reactor). There are a lot of works (Ex. [5]) that have developed Benoist leakage method since 1960 year and this assumption has been analyzed. A short comparison of different formulae for diffusion coefficient is given in [6] with inclusion of this value in the structure of finite-difference SHM-equations. In this paper method based on the works [1,2] is developed. This method supposes the division of the variables: z variable along axial direction and (x,y) variables in the plane, so axial diffusion coefficient is defined with direction probabilities P_{ij}^{zg} and group neutron spectrum of plane problem. To estimate the significance of the approximation is mentioned above, algorithm and code have been created. The results have been obtained with this code are compared with available ones.

2. Method for Calculation Analysis of Axial Diffusion Coefficient in Nuclear Reactor Cell

2.1 Definition of Axial Multigroup Diffusion Coefficient

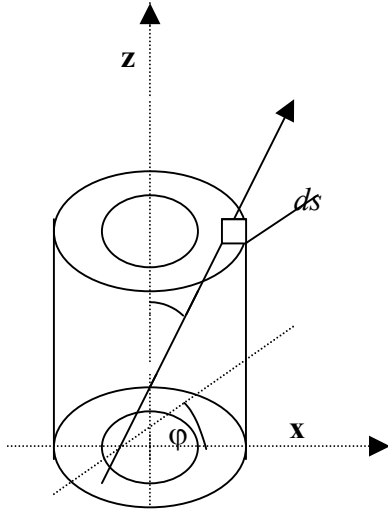


Fig.1. Calculation of the current along Z-axis

The integral expression for current with continual energy dependence is considered as the basic initial stage of calculation method (see fig.1) [1]

$$I(\bar{r}, E)ds = \left[\int d\bar{r}' \int dE' K(E', \bar{r}, \bar{r}') (\sigma^s(\bar{r}', E' \rightarrow E) \Phi(\bar{r}', E') + Q(\bar{r}', E)) \cos\theta \right] ds \quad (1)$$

Here the following designations are used:

$$Q(\bar{r}', E) = \chi(E) \nu \sigma^f(\bar{r}, E) \Phi(\bar{r}, E) \quad (2)$$

ν – average fission neutron number

$\sigma^f(\bar{r}, E)$ - fission cross section

$\chi(E)$ - fission neutron spectrum;

$\sigma^s(\bar{r}, E' \rightarrow E)$ - differential scattering cross section

Subdivision of the energy area into multi-group intervals gives the multi-group approximation:

$$I^g(\bar{r})ds = \left[\int d\bar{r}' \frac{e^{-\tau_g(\bar{r}, \bar{r}')}}{4\pi |\bar{r} - \bar{r}'|^2} \left(\sum_{g'} \sigma_{g' \rightarrow g}(\bar{r}') \Phi^{g'}(\bar{r}') + Q^g(\bar{r}') \right) \cos\theta \right] ds \quad (3)$$

$$Q^g(\bar{r}) = \chi_g \sum_{g'=1}^G \Phi^{g'}(\bar{r}) (\nu \sigma^f)^{g'}(\bar{r}) \quad (4)$$

$$I^g(\bar{r}) = \int_{E_{g(i-1)}}^{E_g} dEI(\bar{r}, E) \quad (5)$$

Approximation of this method is the diffusion approximation along Z ; in other words $\Phi^g(\bar{r})$ is slowly changed function within neutron free path along Z . Then one can use Taylor expansion along Z -axis and to take into account only two first terms; and k is supposed the same for all groups:

$$\Phi^g(x, y, z) = \Phi^{0g}(x, y) + kz\Phi^g(x, y) \quad (6)$$

It is not difficult to prove that $\Phi^{0g}(x, y) = \Phi^g(x, y)$ is neutron flux spectrum for plane problem. So the expression for the current along Z axis in the group "g" is becoming as following:

$$I^g(\bar{r})ds = \left\{ \int_V d\bar{r}' \frac{e^{-\tau_g(\bar{r}, \bar{r}')}}{4\pi|\bar{r} - \bar{r}'|^2} \left[\sum_{g'} \sigma_{g' \rightarrow g}(\bar{r}')\Phi^{g'}(x', y') + Q^g(x', y') \right] |\bar{r} - \bar{r}'| \cos^2 \theta \right\} ds \quad (7)$$

So the definition of the multi-group axial diffusion coefficient is as following:

$$D^g = \frac{\bar{I}^g(\bar{r})}{\bar{\Phi}^g(\bar{r})} ; \quad (8)$$

here $\bar{I}^g(\bar{r})$ means neutron current along Z in group "g" averaged over the cell; and $\bar{\Phi}^g(\bar{r})$ means neutron flux in group "g" averaged over the cell. To calculate the averaged current subdivision of the cell into a set of uniform zones is used and neutron flux as well the current are supposed to be constant within every zone. Then the following equation is coming

$$I_i^g V_i = \sum_{j=1}^N \left[\sum_{g'=1}^G \Phi_j^{g'} \sigma_{g' \rightarrow g} + Q_j^g \right] P_{ij}^{zg} \quad (9)$$

$$P_{ij}^{zg} = \int_{V_i} d\bar{r}' \int_{V_j} d\bar{r}'' \frac{e^{-\tau_g(\bar{r}, \bar{r}'')} \cos^2 \theta}{4\pi|\bar{r} - \bar{r}''|} \quad (10)$$

This coefficients P_{ij}^{zg} are called as "direction probabilities" and they are differed than the same coefficients in Benoist leakage method.

2.2 Calculation of the Direction Probabilities in 2D Geometry.

Calculation of the current in the group "g" (9) is defined by calculation of the coefficients- the direction probabilities (10)

Calculation of the P_{ij}^{zg} coefficients in 2-D geometry is the procedure of number integration over 2 parameters. This procedure is carried out with using of transformation of the Cartesian

coordinate system because of the calculations are more convenient in the system that is connected with neutron flight direction:

$$(x, y, z, x', y', z') \Rightarrow (\varphi, x_\varphi, x'_\varphi, y_\varphi, z, z') \text{ (see fig.1)}$$

Here φ is the angle between the neutron flux projection and X axis; y_φ is the distance between neutron flux projection and the coordinate point “zero”; x_φ, y_φ are the coordinates of the point (\vec{r}, \vec{r}') in the system turned around the initial coordinate system by φ -angle. In these coordinates the coefficients are transformed as following way

$$\int_{V_i} d\vec{r} \int_{V_j} d\vec{r}' = \int d\varphi dy_\varphi dx_\varphi dz dz' |x_\varphi - x'_\varphi|; \quad (11)$$

$$\tau_g(\vec{r}' - \vec{r}) = \tau_g(z, x_\varphi, x'_\varphi, \varphi, y_\varphi) / \sin\theta; \quad (12)$$

here θ is the angle between the Z -axis and neutron flux direction; $\tau_g(z, x_\varphi, x'_\varphi, \varphi, y_\varphi)$ is optical thickness in the plane (x, y) . As result after the change of the coordinate system following relations are true:

$$\frac{z - z'}{x_\varphi - x'_\varphi} = ctg\theta \quad (13)$$

$$dz' = (x_\varphi - x'_\varphi) \left(-\frac{1}{\sin^2\theta} \right) d\theta \quad (14)$$

$$|\vec{r} - \vec{r}'| = |x_\varphi - x'_\varphi| \sqrt{1 + ctg^2\theta} \quad (15)$$

In these coordinates the expression for direction probabilities is coming as following:

$$P_{ij}^{zg} = \frac{-1}{4\pi} \int dz \int d\varphi dy_\varphi \int_0^\pi d\theta \frac{\cos^2\theta}{\sin\theta} \int_{x_\varphi^-}^{x_\varphi^+} dx_\varphi \int_{x'_\varphi^-}^{x'_\varphi^+} dx'_\varphi (x_\varphi - x'_\varphi) e^{-\tau_g(z, x_\varphi, x'_\varphi, \varphi, y_\varphi) / \sin\theta} \quad (16)$$

Here the values $x_\varphi^-, x_\varphi^+, x'_\varphi^-, x'_\varphi^+$ are the boundary cross points of the cell zones with neutron flux direction (see fig.2)

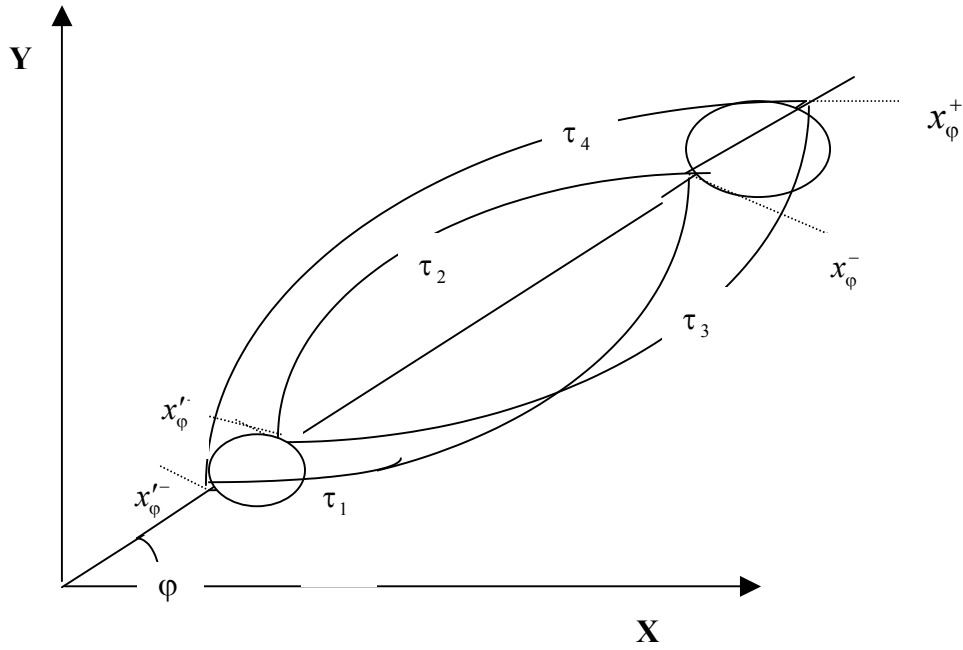


Fig.2 . Optical distances along neutron flight direction between two cell zones in the plane (x,y) . (For calculation of the direction probabilities.)

To calculate the direction probabilities (16) the integration over x_ϕ, x_ϕ' is carried out with analytical way because of

$$\tau_g(z, x_\phi, x_\phi', \phi, y_\phi) = [\sigma''(x_\phi^+ - x_\phi') + \sigma\tilde{t} + \sigma'(x_\phi - x_\phi^-)] / \sin\theta \quad (17)$$

σ'' designates the total neutron cross section of zone neutron is left out;
 σ' designates the total neutron cross section of zone neutron is coming in
 $\sigma\tilde{t}$ designates the optical distance between these two zones
Also it is true that

$$x_\phi = \sin\theta \frac{\partial\tau_g}{\partial\sigma'} \quad \text{and} \quad x_\phi' = -\sin\theta \frac{\partial\tau_g}{\partial\sigma''} \quad (18)$$

The integration over θ is carried out with tabulation and interpolation of combination of Bickley-function [7]:

$$Ki_n(\tau) = \int_0^{\pi/2} e^{-\tau/\sin\theta} \sin^{n-1} \theta d\theta \quad (19)$$

Thus the expressions for the integration values along Z-axis are coming as following

$$\begin{aligned} & \int d\theta \frac{\cos^2 \theta}{\sin \theta} \int_{x_\phi^-}^{x_\phi^+} dx_\phi \int_{x_\phi^-}^{x_\phi^+} dx_\phi' x_\phi e^{-\tau_g(z, x_\phi, x_\phi', y_\phi) / \sin \theta} = \\ & = \frac{1}{\sigma' \sigma''} \left[x_\phi^- (K\tilde{i}_2(\tau_2) - K\tilde{i}_2(\tau_4)) - x_\phi^+ (K\tilde{i}_2(\tau_1) - K\tilde{i}_2(\tau_3)) \right] - \\ & - \frac{1}{\sigma' (\sigma'')^2} \left[K\tilde{i}_3(\tau_1) - K\tilde{i}_3(\tau_3) - (K\tilde{i}_3(\tau_2) - K\tilde{i}_3(\tau_4)) \right] \end{aligned} \quad (20)$$

$$\begin{aligned}
& \int d\theta \frac{\cos^2 \theta}{\sin \theta} \int_{x_\varphi^-}^{x_\varphi^+} dx_\varphi \int_{x_\varphi'^-}^{x_\varphi'^+} dx_\varphi' x_\varphi' e^{-\tau_g(z, x_\varphi, x_\varphi', \varphi, y_\varphi)/\sin \theta} = \\
& = \frac{1}{\sigma' \sigma''} [x'^+ (K\tilde{i}_2(\tau_1) - K\tilde{i}_2(\tau_2)) + x'^- (K\tilde{i}_2(\tau_3) - K\tilde{i}_2(\tau_4))] - \\
& - \frac{1}{\sigma'' (\sigma')^2} [K\tilde{i}_3(\tau_1) - K\tilde{i}_3(\tau_3) - K\tilde{i}_3(\tau_2) + K\tilde{i}_3(\tau_4)]
\end{aligned} \tag{21}$$

There is the designation here:

$$K\tilde{i}_n(x) \equiv Ki_n(x) - Ki_{n-2}(x); \tag{22}$$

$\tau_1, \tau_2, \tau_3, \tau_4$ are the optical distances between intersection points of neutron flight direction with zones boundary when φ, y_φ are constant (see fig.2). These expressions are true for the direction probabilities P_{ij}^{zg} when $i \neq j$. For the diagonal elements of the direction probabilities matrix the expressions for calculation are as following:

$$\begin{aligned}
& \int d\theta \frac{\cos^2 \theta}{\sin \theta} \int_{x_\varphi^-}^{x_\varphi^+} dx_\varphi' \int_{x_\varphi'^-}^{x_\varphi'^+} x_\varphi' e^{-\tau_g(z, x_\varphi, x_\varphi', \varphi, y_\varphi)/\sin \theta} = \\
& = \frac{1}{(\sigma')^2} x_\varphi^+ [K\tilde{i}_2(\tau) - K\tilde{i}_2(0)] + \frac{1}{\sigma'} K\tilde{i}_1(0) \frac{(x_\varphi^+)^2 - (x_\varphi^-)^2}{2} - \\
& - \frac{1}{(\sigma')^3} [K\tilde{i}_3(0) - K\tilde{i}_3(\tau)] + \frac{1}{(\sigma')^2} K\tilde{i}_2(0) (x_\varphi^+ - x_\varphi^-);
\end{aligned} \tag{23}$$

$$\begin{aligned}
& \int d\theta \frac{\cos^2 \theta}{\sin \theta} \int_{x_\varphi^-}^{x_\varphi^+} dx_\varphi \int_{x_\varphi'^-}^{x_\varphi'^+} dx_\varphi' x_\varphi' e^{-\tau_g(z, x_\varphi, x_\varphi', \varphi, y_\varphi)/\sin \theta} = \\
& = \frac{1}{(\sigma^e)^2} x_\varphi^- K\tilde{i}_2(\tau) + \frac{1}{(\sigma')^3} [K\tilde{i}_3(0) - K\tilde{i}_3(\tau)] - \\
& - \frac{1}{(\sigma')^2} x_\varphi^+ K\tilde{i}_2(0) + \frac{1}{(\sigma')^2} K\tilde{i}_1(0) \frac{(x_\varphi^+)^2 - (x_\varphi^-)^2}{2}
\end{aligned} \tag{24}$$

In this expressions integration is carried out within one and the same zone; thus there is one pair of the intersection points of neutron direction and the boundary of the zone. The designate τ is the optical distance within the zone.

2.3 Balance Relation for the Direction Probabilities

The balance relations are true for direction probabilities P_{ij}^{zg} . They are coming from balance equations for infinite uniform medium

$$\sum_i P_{i \rightarrow j}^{zg} + P_{s \rightarrow j}^{zg} = \int_{V_j} d\vec{r} \int_{V_\infty} d\vec{r}' \frac{e^{-\tau(\vec{r}, \vec{r}')} \cos^2 \theta}{4\pi |\vec{r} - \vec{r}'|^2} \quad (25)$$

In this equation the relation between the integration way over the surface around the finite volume and the integration way over all space is used. In the spherical coordinates:

$$d\vec{r}' = |\vec{r} - \vec{r}'|^2 \sin \theta d\rho d\theta d\phi; \quad (26)$$

so the integration over all space is carried out in spherical coordinates:

$$\begin{aligned} & \int_{V_i} d\vec{r} \int_{V_\infty} d\vec{r}' \frac{|\vec{r} - \vec{r}'| e^{-\rho\sigma} \rho \cos^2 \theta d\rho d\theta d\phi}{4\pi |\vec{r} - \vec{r}'|^2} = \\ & = \frac{1}{4\pi} \int_{V_i} d\vec{r} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin \theta \cos^2 \theta \int_0^\infty d\rho \rho e^{-\rho\sigma} = \frac{V_i}{3\sigma^2} \end{aligned} \quad (27)$$

So the balance relation for direction probabilities that can use to verify code results is as following:

$$\sum_i P_{i \rightarrow j}^{zg} + P_{s \rightarrow j}^{zg} = \frac{V_i}{3\sigma^2} \quad (28)$$

2.4 Boundary conditions for direction probabilities

For axial leakage problem in reactor cell a formulation of boundary conditions has to take into account periodical structure of reactor core. Approximation of the cylindrical equivalent cell boundary (instead real cell boundary) and “white” boundary condition instead real mirror reflection condition is usually used to obtain the convenient formulae. It is shown in [8] how to calculate direction probabilities if this approximation is true. Also possible significance of this approximation in VVER-type cell is analyzed. So formula for direction probabilities (10) if approximation of “white” boundary conditions is taken into account is transformed as following:

$$\left(P_{ij}^{zg} \right)^* = P_{ij}^{zg} \frac{P_{is}^{zg} \times P_{sj}^{zg}}{1 - P_{ss}^{zg}} \quad (29)$$

here it is the designations:

$$P_{is}^{zg} = \int_{V_i} d\vec{r}' \int_S d\vec{r} \frac{e^{-\tau_g(\vec{r}, \vec{r}')} \cos^2 \theta}{4\pi |\vec{r} - \vec{r}'|}; \quad (30)$$

$$P_{sj}^{zg} = \int_S d\vec{r}' \int_{V_j} d\vec{r} \frac{e^{-\tau_g(\vec{r}', \vec{r})} \cos^2 \theta}{4\pi |\vec{r} - \vec{r}'|} \quad (31)$$

$$P_{ss}^{zg} = \int_S d\vec{r}' \int_S d\vec{r} \frac{e^{-\tau_g(\vec{r}', \vec{r})} \cos^2 \theta}{4\pi |\vec{r} - \vec{r}'|^2} \quad (32)$$

$\int_S d\vec{r}$ designates integration over surface cell boundary.

3. Brief Description of Algorithm and Code for Axial Leakage Calculation in Reactor Cell

So method for the problem of axial leakage calculation has been described. In this method axial diffusion coefficient is defined with direction probabilities (29) and 2-dimensional neutron flux distribution. It has been shown that calculation of these coefficients comes to 2-D number integration over the cell:

$$P_{ij}^{zg} = \iint P_{ij}^{zg}(\varphi, y_\varphi) d\varphi dy_\varphi \quad (33)$$

The integrated function is transformed to linear combinations of trigonometric function φ with Bickley functions [8] of different orders from the following arguments: “optical” distances along neutron fly direction projection on the (x,y) plane from intersection of this projection with neutron birth zone boundary to the intersection of this projection with the neutron registration zone boundary. To provide the integration over 2-dimensional cell area the uniform distributed sequences [9] are used. The coordinates of the mesh points (and the number of trajectories) are defined with using of Korobov generator of quasi random numbers. To use these sequences it is needed to change the integration variables in Eq. (33):

$$\varphi = \varphi(\gamma_1, \gamma_2); \quad y_\varphi = y_\varphi(\gamma_1, \gamma_2) \quad (34)$$

These variables are coordinates of the points in the unit cube and the following relation is true:

$$\frac{dy_\varphi d\varphi}{2\pi S_j} = d\gamma_1 d\gamma_2 \quad (35)$$

After this change of variables the integrals (33) are calculated over the unit cube with the use of the standard integration formula: if $\chi(n)$ is the value of the sub-integral function in the mesh point number n , then the integral value is the averaged arithmetic value $\chi(n)$ over all mesh points. The coordinates of the mesh points are defined with using of “uniformly” distributed sequences. It has been shown [9] that using of these sequences provides a high integration convergence order ($\approx \frac{1}{N^{1-\varepsilon}}$) (ε is small). The universal module of combinatorial geometry SCG-5 [10] is used to describe the geometry of calculation cell. Neutron data library of WIMS-code and it's module PINCELL for generation of multigroup cross sections is used as input data. 2-Dimensional distribution of neutron flux over the cell is as input data too. This distribution is calculated with neutron transport multigroup code GEFCOP [11]. This code uses the same cross section library, the same geometrical module SCG-5 and General First Collision Probabilities Method.

4. Calculation Results

4.1 Uniform Infinite Medium

To obtain verification results the modeling problem of uniform infinite medium was considered. Calculations were carried out in one group. The cell was divided into 5 zones and the cross section was supposed to be closed to graphite cross section in thermal group. The balance relation (28) was used. These results are given in table 1

Table 1 Direction probabilities for infinite uniform medium

Zone number	1	2	3	4	5
$1/3\sigma^2$	5.846	32.336	66.043	11.260	64.960
$\sum_i P_{ij}^{zg} + P_{s \rightarrow j}^{zg}$	5.847	32.331	66.053	11.252	64.946

4.2 Comparison of Calculation Analysis of the Axial Diffusion Coefficients for VVER-Type Cell.

Comparison calculation analysis of axial leakage for the VVER-type cell have been carried out. WIMS-code and VEPS-A code have been used. 20 group subdivision was used. The group cross sections were the same for both codes and generated from WIMS nuclear data library. The results were multigroup axial diffusion coefficients that were averaged over flux spectrum into two groups as fast group diffusion coefficient and thermal group diffusion coefficient. These coefficients were obtained with both codes (WIMS and VEPS-A) and compared. The cell parameters are given in table 2. The comparison results for axial diffusion coefficients are given in table 3.

Table 2. Geometrical and material parameters of the equivalent cylindrical cell.

	Fuel		Clad		Moderator	
Radius, cm.	0.413		0.474		is changed	
Nuclear densities	235-U	8.255 E-04	Zr	4.259 E-02	H	6.671E-02
	238-U	2.210 E-02	Hf	6.597E-06	O	3.336E-02
	O	4.586 E-02	Nb	4.225E-04		

Table 3. Group axial diffusion coefficients for VVER-type cell obtained with different codes

Group number	1	2	3	4	5	6	7	8	9	10	11	12
WIMS-code	2.154	0.860	0.574	0.622	0.554	0.487	0.421	0.397	0.366	0.345	0.280	0.263
VEPS-A-code	2.181	0.868	0.625	0.653	0.595	0.541	0.472	0.454	0.430	0.375	0.329	0.311
Descrep. %	0.9	0.9	9.2	4.6	7.0	10.4	11.6	13.8	16.5	18.0	16.7	17.8

Table3. Group axial diffusion coefficients for VVER-type cell obtained with different codes (continue)

Group number	13	14	15	16	17	18	19	20	Averag. over fast	Averag. over thermal	Averag. over all
WIMS-code	0.246	0.227	0.209	0.194	0.178	0.162	0.145	0.113	1.1575	0.299	1.026
VEPS-A code	0.292	0.268	0.246	0.227	0.207	0.186	1.164	0.127	1.1831	0.3451	1.054
Descrip. %	17.7	17.5	17.1	16.4	15.1	14.7	13.1	12.4	2.0	15.0	3.0

4.3 Comparison of Calculation Analysis Results of Axial Diffusion Coefficients for RBMK-Type Cell

Also axial leakage coefficients have been analyzed for RBMK –type reactor cell. For this purpose also both WIMS-code and VEPS-A code were used. RBMK-type reactor cell is the cluster with lay of graphite width of 4,6 cm. Group cross sections for such cell were generated with two ways: PERSEUS-option (variant of cluster homogenization) and PIJ+PERSEUS-option (variant of cluster geometry). Also 20-group subdivision was used and the results were averaged into 2 groups

Table 4 Comparison of calculation results of the coefficients of axial diffusion for RBMK-Type Cell

Group Number	WIMS, ARIADNE	VEPS-A cylindr.	VEPS-A cluster
1	1.1647	1.1641	1.1636
2	0.7595	0.7608	0.76547

5. Conclusions

In conclusion, the following items must be submitted

- The results obtained show that if the influence of heterogeneous structure of the neutron flux spectrum on the current along Z-axis is taken into account then for VVER-type cell the coefficient of axial diffusion is changed in fast group (~2%) and in thermal group (~15% This discrepancy can lead to the multiplication factor discrepancy about 200-300 pcm.
- This difference can influence on the neutron leakage in the area closed to the axial reflector of the nuclear reactor.
- Code VEPS-A can be recommended to use for the estimation of fine effects of axial diffusion coefficients calculations analysis in reactor cell.

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