A stable algorithm for calculating one-group diffusion coefficient in a multi-zone cylindrical cell by the surface pseudo-sources method

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Abstract. In the surface harmonics method, designed to solve the neutron transport equation of in the core of a nuclear reactor, the distribution function is decomposed by trial functions. The first trial function is the absorption and division matrix. It is responsible for the main processes (absorption and fission) that occur inside the nuclear reactor cell. The second trial function is the diffusion coefficient matrix. It is associated with the processes of neutron flow from one cell to another. It is usually calculated in the $P_2$ and $P_4$ approximations of the spherical harmonics method and by the surface pseudo-sources method. In close lattices with high absorption of $P_2$ and $P_4$ approximations may not be enough, and the surface pseudo-sources method proves to be unstable in the calculation of multi-zone cylindrical cells. This work is dedicated to the development of stable one-group calculation of the diffusion coefficient by the surface pseudo-sources method first, by eliminating the divergent integrals, and secondly, the modification of the algorithm of matrix factorization for calculating one-group neutron transport equation. Developed program DICOF may use in the complexes of WIMS-SH and SVL for stable calculation of the diffusion coefficients matrix for calculation of the VVER and RBMK reactors.

1. Introduction

In the surface harmonics method [1], designed to solve the neutron transport equation of in the core of a nuclear reactor, the distribution function is decomposed by trial functions. The first trial function is the absorption and division matrix. It is responsible for the main processes (absorption and fission) that occur inside the nuclear reactor cell. For its calculation it is convenient to use the surface pseudo-sources method for cylindrical [2] and cluster [3] cells of nuclear reactors. The second trial function is the diffusion coefficient matrix. It is associated with the processes of neutron flow from one cell to another. It is usually calculated in the $P_2$ and $P_4$ approximations of the spherical harmonics method and by the surface pseudo-sources method [4]. In close lattices with high absorption of $P_2$ and $P_4$ approximations may not be enough, and the surface pseudo-sources method proves to be unstable in the calculation of multi-zone cylindrical cells [4-7]. This work is dedicated to the development of stable one-group calculation of the diffusion coefficient by the surface pseudo-sources method first, by eliminating the divergent integrals by analogy with the work [3], and secondly, the modification of the algorithm of matrix factorization for calculating one group neutron transport equation. Developed program DICOF may use in the complexes WIMS-SH [8] and SVL [9] for stable calculation of the diffusion coefficients matrix for calculation of the VVER and RBMK reactors.
2. The surface pseudo-sources method in the \( G_1^P \) - approximation

The surface pseudo-sources method refers to integral methods, as well as the method of the first collision probabilities. In the surface pseudo-sources method, the neutron distribution function within the zone of a multi-zone two-dimensional cylindrical cell has the following form:

\[
\Psi^t(r, \Omega) = \int S^z \int dV' \int G^t(r, \Omega') G^s(r, \Omega, \Omega') \frac{d\Omega'}{\Omega} + \int S^z \int dV' \int g^t(r, \Omega') G^s(r, \Omega, \Omega') dr'd\Omega' \tag{1}
\]

where \( S^z \) - the neutron source in the zone \( z \); \( g^t(r, \Omega') \) - the surface pseudo-source in zone \( z \), it is antisymmetric, i.e. \( g^s(r, \Omega) = -g^s(r, -\Omega) \); \( G^s(r, \Omega, \Omega') \) - the Green's function in an infinite homogeneous medium with \( z \)-zone material.

To decompose various functions in the surface pseudo-sources method, the spherical functions \([10]\) are used:

\[
Y^m_n(\Omega) = P^m_{m,n}(\cos \theta) \cos m\varphi
\]

where \( P^m_{m,n}(\cos \theta) = \frac{(n-m)!}{(n+m)!} \left( \frac{1}{2} \right)^{\frac{1}{2}} \frac{\sin^m \theta}{\sin \theta} \sin \theta \]

here \( P^m_{m,n}(\cos \theta) \) - the Legendre polynomial \([11]\).

Equating on the zone boundaries of the cell the neutron distribution function \( \Psi^t(r, \Omega) \), we obtain integral equations for surface pseudo-sources. Applying to their solution the Galerkin’s method with respect to the spatial functions \( \cos \alpha \) and \( \sin \alpha \) (\( p \leq P \)) and spherical harmonics \( Y^m_n(\Omega) \) (\( m \leq N \), \( n \leq N \)), we obtain an algebraic system of equations for the angular moments of surface pseudo-sources in the cell. To solve this problem, we use a matrix factorization method that is resistant to rounding and approximation errors. Having determined the surface pseudo-sources, we calculate the neutron fluxes and currents at the boundaries of the zones. Then the neutron fluxes average over the zones are calculated from the balance equations. It should be noted that Green's cylindrical functions for an infinite medium in one- and two-dimensional media are constructed from regular and singular cylindrical elementary solutions of the transport equation in the sense of the Case \([12, 13]\). Regular and singular cylindrical elementary solutions of the transport equation for arbitrary geometry are constructed from of plane elementary solutions of the transport equation.

Calculated instability was observed in 69 - group calculations of two-dimensional cylindrical cells (see, for example, \([3]\)). In the \( G_1^P \) -approximation of the surface pseudo-sources method the angular moments of the sine components of the neutron distribution function (\( \Psi_{1s}, \Psi_{2s}, \Psi_{3s} \) and \( \Psi_{3s} \)) for the two angular moments of the sine components of the surface pseudo-sources \( g_{1s}, g_{2s}, g_{3s} \) are equated at the boundaries of the cylindrical zones. It turned out that the reason for such instability is the presence of divergent integrals in the sine components \( \Psi_{1s}, \Psi_{2s} \) and \( \Psi_{3s} \) for the sine components of surface pseudo-sources \( g_{1s}, g_{2s}, g_{3s} \).
\[
G_{\kappa\nu}^{\text{new}} \left( r / r' \right) = \left\{ \begin{array}{ll}
G_{\kappa\nu}^{\text{in}} & r / r' + \\
\sum_{l=1,3} A_{\nu l} \Phi_{m l}^{\nu} r / r' \int \frac{1}{vN} \frac{F_{m l}^{\nu}}{v / l} dv \ldots r' \leq r
\end{array} \right.
\]

where \( G_{\kappa\nu}^{\text{new}}, r / r' \) – part of the moments of the Green's function without diverging characteristics, and the hatched parts are the angular moments of the sine component of the surface pseudo-sources, no hatched – to the angular moments of the sine component of the distribution function.

It turned out that integrals in this formula diverge only with \( l=1 \) with singularity \( 1 / v \) when \( v \) tends to 0. To eliminate this divergence, it is proposed to take the sum of the following angular moments of the spatial sine components of the neutron distribution function \( 0,12 \Psi_{1l} + 0.08(6)^{1/2} \Psi_{3l} \), which is achieved by summing the corresponding two lines with the corresponding coefficients. As a result, the following matrix element is obtained:

\[
0.12G_{1l}^{211l}(r_j / r_j) + 0.08(6)^{1/2}G_{1l}^{231l}(r_j / r_j) = (2)
\]

Substituting explicit expressions of the moments of the Green's function, we obtain an integral

\[
\int \frac{A_{\nu l} \Phi_{m l}^{\nu} r / r' \int \frac{1}{vN} \frac{F_{m l}^{\nu}}{v / l} dv}{v^2 / 2} = \frac{3}{80} 2 \left[ 9(1-5v^2)/x^2 - 4v^2 \right] K_2(x) + (6 - 23v^2 / x) / xK_3(x)
\]

Let's determine whether there is any feature in the integral (3) or not. To do this, we substitute the functions into the integral:

\[
A_{\nu l} \Phi_{m l}^{\nu} r / r' \int \frac{1}{vN} \frac{F_{m l}^{\nu}}{v / l} dv = 0.5(1 - v^2) \right]^{1/2} \Phi_{m l}^{\nu}(x) = -0.25 I_1(x) - I_0(x) \quad x = r / v
\]

where \( I_0(x) \approx 2\pi x^{-1/2} e^{-x} \quad K_0(x) \approx \left( \frac{\pi}{2x} \right) e^{-x} \) when \( v \to 0 \).

The result is \( 9/(160r^2) \) without singularities. The previous transformation was applied to the matrix elements associated with \( g_{1l} \). Similar transformations are done for matrix element \( g_{3l} \) by formula (2).

Thus, the feature of type \( 1 / v \) at \( v \to 0 \) is eliminated. Here the divergences in the first and second angular moments of formula (2) were compensated. Thus eliminating the features, we come to an incomplete system of algebraic equations - the number of unknowns is greater than the number of equations per unit. Here we can go two ways. We can add the following equation for the angular momentum of a sine component \( \Psi_{4l} \) whose all members are without singularities. We can go and by the other way. Note that the expression (2) is an equalization of the angular moments of the sine component on the boundaries of the zones from the expression \( \left( \Phi_{m l}^{\nu} \right)^2 \Psi'(r, \Omega) \), which are natural boundary conditions for the surface pseudo-sources method [14]. Then the missing equation can be a combination of two divergent equations: \( \Psi_{3l} \) and \( \Psi_{5l} \). In the present work the first way is realized.
3. An alternative method of matrix factorization

Let us consider the scheme of matrix factorization method different from the one that was implemented in [5]. Since we have two components: cos and sine, we first get rid of the sine component, and then of the cos at each step of the forward motion of the matrix factorization method.

We write the matrix equation after equating the sine components of the angular moments of the neutron distribution functions at the boundary of 1 and 2 zones as

\[ A^{sc}_{1} g^{c}_{1} + A^{ss}_{1} g^{s}_{1} + B^{s}_{11} (S^{c}_{1}, S^{s}_{1}) = A^{sc}_{23} g^{c}_{23} + A^{ss}_{23} g^{s}_{23} + B^{s}_{22} (S^{c}_{2}, S^{s}_{2}) \]  

(4)

where

\[ A^{sc}_{1} = \left[ G_{nm}^{sc} (r_{1} / r_{1}^{*}) \right], \quad A^{ss}_{1} = \left[ G_{nm}^{ss} (r_{1} / r_{1}^{*}) \right] \]

\[ A^{sc}_{23} = \left[ G_{nm}^{sc} (r_{2} / r_{2}^{*}), G_{nm}^{ss} (r_{2} / r_{2}^{*}) \right], \quad A^{ss}_{23} = \left[ G_{nm}^{ss} (r_{2} / r_{2}^{*}), G_{nm}^{ss} (r_{2} / r_{2}^{*}) \right] \]

\[ B^{s}_{11} = [S^{s}_{11}, S^{s}_{11}] \quad B^{s}_{22} = [S^{s}_{22}, S^{s}_{22}] \quad g^{s}_{1} = [g^{s}_{n1}, g^{s}_{n1}] \quad g^{s}_{23} = [g^{s}_{n23}, g^{s}_{n23}] \]

Equation (4) can be written as

\[ A^{sc}_{12} g^{c}_{12} = -A^{sc}_{1} g^{c}_{1} + A^{sc}_{23} g^{c}_{23} + A^{sc}_{23} g^{c}_{23} - B^{s}_{11} (S^{c}_{1}, S^{s}_{1}) + B^{s}_{22} (S^{c}_{2}, S^{s}_{2}) \]

(5)

Solving equation (5), we obtain

\[ g^{c}_{12} = -A^{ss}_{12} g^{s}_{1} + A^{sc}_{23} g^{c}_{23} + A^{ss}_{23} g^{s}_{23} \]

(6)

We write the matrix equation after equating the cos components of the angular moments of the neutron distribution functions at the boundary of 1 and 2 zones as follows

\[ A^{cc}_{1} g^{c}_{1} + A^{cs}_{1} g^{s}_{1} + B^{c}_{11} (S^{c}_{1}, S^{s}_{1}) = A^{cc}_{23} g^{c}_{23} + A^{cs}_{23} g^{s}_{23} + B^{c}_{22} (S^{c}_{2}, S^{s}_{2}) \]  

(7)

where

\[ A^{cc}_{1} = \left[ G_{nm}^{cc} (r_{1} / r_{1}^{*}) \right], \quad A^{cs}_{1} = \left[ G_{nm}^{cc} (r_{1} / r_{1}^{*}) \right] \]

\[ A^{cc}_{23} = \left[ G_{nm}^{cc} (r_{2} / r_{2}^{*}), G_{nm}^{cc} (r_{2} / r_{2}^{*}) \right], \quad A^{cs}_{23} = \left[ G_{nm}^{cc} (r_{2} / r_{2}^{*}), G_{nm}^{cc} (r_{2} / r_{2}^{*}) \right] \]

\[ B^{c}_{11} = [S^{c}_{11}, S^{c}_{11}] \quad B^{c}_{22} = [S^{c}_{22}, S^{c}_{22}] \quad g^{c}_{1} = [g^{c}_{n1}, g^{c}_{n1}] \]

Substituting in (7) the values of surface pseudo-sources from equation (6), after some simplifications we obtain

\[ A^{cc}_{1} g^{c}_{1} + A^{sc}_{1} g^{s}_{1} + B^{c}_{11} (S^{c}_{1}, S^{s}_{1}) = A^{cc}_{23} g^{c}_{23} + A^{sc}_{23} g^{s}_{23} + B^{c}_{22} (S^{c}_{2}, S^{s}_{2}) \]  

(8)

where

\[ A^{cc}_{1} = A^{cc}_{1} - A^{cs}_{12} A^{cs}_{12} \quad A^{cs}_{1} = A^{cs}_{1} + A^{cs}_{12} A^{cs}_{12} \]

\[ B^{c}_{11} = [S^{c}_{11}, S^{c}_{11}] \quad B^{c}_{22} = [S^{c}_{22}, S^{c}_{22}] \]

The equation (8) can be written as
\[
\tilde{A}_{12}^{sc} g_{12}^{\ast} - \tilde{A}_{3}^{sc} g_{3}^{\ast} + \tilde{A}_{2}^{sc} S_{1}^{\prime} + B_{22}^{s} (S_{1}^{\prime}, S_{2}^{\prime}, S_{2}^{\prime}) \]

where \(\tilde{A}_{12}^{sc} = \tilde{A}_{22}^{sc} \quad \tilde{A}_{3}^{sc} = \tilde{A}_{3}^{sc} \quad \tilde{A}_{2}^{sc} = \tilde{A}_{2}^{sc}\),

\[
B_{22}^{s} (S_{1}^{\prime}, S_{2}^{\prime}, S_{2}^{\prime}) = -\tilde{B}_{11}^{sc} (S_{1}^{\prime}, S_{1}^{\prime}) + \tilde{B}_{22}^{sc} (S_{2}^{\prime}, S_{2}^{\prime})
\]

Solving equation (9), we obtain

\[
g_{12}^{\ast} - \tilde{A}_{12}^{sc} g_{12}^{\ast} = \tilde{A}_{1}^{sc} g_{2}^{\ast} + \tilde{A}_{2}^{sc} g_{3}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{2}^{\prime}, S_{2}^{\prime})
\]

Equating the sine components of the angular moments of the neutron distribution function at the boundary of 2 and 3 zones, we obtain the following matrix-vector equation for the angular moments of surface pseudo-sources in the form

\[
A_{23}^{sc} = A_{23}^{sc} + A_{23}^{sc} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime}, S_{2}^{\prime}) = A_{23}^{sc} g_{12}^{\ast} + A_{23}^{sc} g_{12}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime}, S_{1}^{\prime})
\]

Substituting the variables \(g_{2}^{\ast}\) from (6) in (11), after some simplifications we obtain

\[
\tilde{A}_{12}^{sc} g_{12}^{\ast} + \tilde{A}_{23}^{sc} g_{12}^{\ast} + \tilde{A}_{3}^{sc} g_{3}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime}, S_{2}^{\prime}) = A_{23}^{sc} g_{12}^{\ast} + A_{23}^{sc} g_{12}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime})
\]

Substituting the variables \(g_{12}^{\ast}\) from (10) in (12), we obtain

\[
\tilde{A}_{12}^{sc} g_{12}^{\ast} + \tilde{A}_{23}^{sc} g_{12}^{\ast} + \tilde{A}_{3}^{sc} g_{3}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime}, S_{2}^{\prime}) = A_{23}^{sc} g_{12}^{\ast} + A_{23}^{sc} g_{12}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime})
\]

Simplifying equation (13), we write

\[
\tilde{A}_{23}^{sc} g_{23}^{\ast} + \tilde{A}_{23}^{sc} g_{23}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime}, S_{2}^{\prime}) = A_{23}^{sc} g_{12}^{\ast} + A_{23}^{sc} g_{12}^{\ast} + B_{22}^{s} (S_{1}^{\prime}, S_{1}^{\prime})
\]
\[
\hat{A}_{Z_{4}-2,2}^{c} = \hat{A}_{Z_{4}-2,2}^{c} + \hat{A}_{Z_{4}-4,2}^{c} = \hat{B}_{Z_{4}-2,2}^{c}(S_{1}^{c}, S_{r}^{c}, \ldots, S_{Z_{4}-1,2}^{c}, S_{Z_{4}-1,2}^{c}) =
\]
where matrices \( \hat{A}_{Z_{4}-2,2}^{c} \) and \( \hat{A}_{Z_{4}-4,2}^{c} \) are calculated by recurrent formulas (15) and (16) respectively; and matrix \( \hat{B}_{Z_{4}-2,2}^{c}(S_{1}^{c}, S_{r}^{c}, \ldots, S_{Z_{4}-1,2}^{c}, S_{Z_{4}-1,2}^{c}) \) - by formula (17).

In the last zone, to create an “isotropic” reflection of neutrons on the outer boundary of the cell, as this was done in the cylindrical symmetric case [15], we introduce two isotropic pseudo-sources located on the outer boundary of the cell. Then, having made transformations with equation (18) similar to (4)-(14), we obtain the following equation:

\[
\hat{A}_{\text{sink}}^{c} = g_{\text{sink}}^{c} + \hat{A}_{\text{sink}}^{c} = \hat{B}_{Z_{4}-2,2}^{c}(S_{1}^{c}, S_{r}^{c}, \ldots, S_{Z_{4}-1,2}^{c}, S_{Z_{4}-1,2}^{c}) = \text{tok}(S_{Z_{4}-2}^{c}, S_{Z_{4}-1}^{c})
\]

where \( \text{tok} = \frac{(\Omega k)T \cos \alpha}{(\Omega k)T \sin \alpha} \).

The last equation (19) contains the same number of equations and unknowns. Solving their similar to (4)-(10), we define an unknown vector \( g_{\text{sink}}^{c} \) : angular moments of an isotropic neutron source located at the last cell boundary. Then in the recursive formulas (6) and (11) we determine all the surface pseudo-sources. Thus, the inverse motion of the matrix factorization method is carried out. In result we defined the relationship of all surface pseudo-sources from all neutron sources in the cell in the form

\[
g = HS
\]

where \( g = g_{nm}^{c} \)

\[
S = \begin{pmatrix} S_{1}^{c}, S_{r}^{c} \\ \text{tok} \end{pmatrix}
\]

\( H \) - matrix of combinations of angular moments of Green's function.

4. Conclusion

So in this paper, two algorithms are written that should lead to a stable method for calculating the diffusion coefficient in a two-dimensional multi-zone cylindrical cell of a nuclear reactor.

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