The choice of core unit cells boundaries in surface harmonics method by the test tasks solving example

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Abstract. The surface harmonics method (SHM) is one of the approaches to neutronic reactor computation reasoning and developing method of homogenization. The symmetry of cells in the method of homogenization and in the SHM is still being used while equations deriving. The cells can be asymmetric in reality. The surface harmonics method allows us to obtain finite-difference equations for a heterogeneous reactor and for the reactor core with asymmetric cells. This allows one to check SHM recommendations on choosing boundaries of the unit cells of the reactor. The examples of test tasks with asymmetric cells are shown in this paper for substantiation of the unit cells boundaries choice for the reactor core.

1. Introduction

The symmetry of cells is used in derivation of the finite-difference equations for a heterogeneous reactor by surface harmonics method, in particular for ranking the trial functions depending on their importance. If neutron flux densities are expected to be equal at different faces of the cells in modulus from the symmetry of cells, the equations will become simpler. In reality, the cells can appear asymmetric (and they become asymmetric because of burnout process). The regularity of a mesh may also be disrupted in the reactor core for example in the gap between the PWR assemblies.

Therefore, in the paper [1] finite-difference equations for a heterogeneous reactor are derived without cells symmetry assumption. The trial functions were computed as a cell "response" to the single flux inflow (odd moment) of neutrons from a g-group from any cell edge.

The obtained finite-difference equations for a heterogeneous reactor (with irregular mesh and asymmetric cells) allow us to check the SHM thesis that the unit cells boundaries should be choose in moderator in order to describe the distribution of neutrons at the cell boundaries using less angular moments. The obtained equations possibilities for calculating the neutron distribution in the asymmetric cells system are used to demonstrate the boundaries choice influence on the calculation results in this paper. For simplicity one-dimensional one-group test tasks were used.

2. One-group one-dimensional test tasks

Test tasks are taken from [2]. In this paper test tasks were used in the method of homogenization to investigate the influence of different ways of diffusion coefficient calculating on the computing accuracy.

In the test tasks the problem was solved to get the eigenvalue for a one-dimensional reactor that is made up of different number of plates (5-75) with different sizes and properties (Figure 1) with the given one-group cross sections for fast sodium reactor.
The reference solution in the paper [2] was computed using the discrete ordinates method. In this paper the spherical harmonics method was used to obtain the reference solution. The spherical harmonics method was applied analytically for planar geometry with a minimum of VBA language coding for numerical results. In order to implement the vacuum boundary conditions in the SHM in the paper [3] the connection matrix has been obtained for odd and even angular moments of the neutron distribution at the edge with vacuum. The reference solution was computed to the \( P_{29} \)-approximation. This approximation would be sufficient for the convergence of the flux density in space (Figure 2).

The convergence of neutron flux angular distribution is not apparently achieved especially in sodium (Figure 3).
While receiving the numerical results it turned out more preferable to compute the trial functions with the same boundary conditions even in asymmetric cells and the flux inflow schemes (in the general case, of the odd angular moments of the neutron distribution) to be left in the ordered symmetry. In this case even angular moments on the right (the first) and left (the second) faces of one-dimensional asymmetric cell will be different. With this computation of trial functions the succession of finite-difference equations is obvious. It is also very important to have close affinity between the equations and finite-difference approximation of the diffusion equation.

Figure 3. Convergence of neutron flux angular distribution for U-Pu, U, Na.

It is not so important for the purpose of this paper, since it is enough that the trial functions inside the cell are computed to the same $P_{29}$-approximation as in the reference solution.

The resulting system of finite-difference equations in the case of asymmetric cells looks in this way:
(ψ^{1}_{k-1} + ψ^{2}_{k})^{-1} (Φ^{1}_{k-1}− T_k Φ^{1}_{k}) + (ψ^{1}_{k} + ψ^{2}_{k+1})^{-1} (T_{k+1} Φ^{1}_{k+1} − Φ^{1}_{k}) − Σ_k Φ^{1}_{k} = 0.

(1)

In the system of equations (1) lower index is the one of the cell and top index is the one of the cell face (visible from (1) that the values of even angular moments of "quasisymmetrical" \(\dot{\varphi}\) - functions and the "quasiasymmetrical" \(\psi\) - functions are different at different faces). \(\Phi^{1}_{k}\) is the vector close to the one of even moments of the neutron distribution at the first (right) face of the cell.

Since one-group case is considered in the test the matrix - coefficients of the equation (1) are composed of even neutron distribution moments at the face of the cell for different trial functions (with non-zero odd moments at the cell face). Matrix - \(T_k = (\dot{\varphi}^{2}_{k} − ψ^{2}_{k})(\dot{\varphi}^{1}_{k} − ψ^{1}_{k})^{-1}\) would be unit for symmetric cells. The role of the diffusion coefficient (coefficient matrix in the lattice) in the equation (1) has \(D_k = ψ^{−1}_{k}/2\), the role of the neutron absorption cross section (and neutron generation) has \(Σ_k = 2(\dot{\varphi}^{1}_{k} − ψ^{1}_{k})^{-1}\).

3. The results of test tasks solving

The method of surface harmonics advises us to choose cell boundaries in the places where the angular distribution of neutrons can be characterized by the small number of angular moments. The middles of zones should meet this condition. So the unit cell in the test task calculation was chosen with boundaries in the middle of uranium layer («Cell1» Figure 1). The cells at the edges of the system are half of the uranium layer. All cells in this case are symmetric. All sizes of cells are included into the trial functions, so the mesh irregularity is not important for the SHM. To investigate the effect of cells asymmetry on the calculation of eigenvalues (the neutron multiplication factor) and neutron flux density the face of the cell was shifted from the uranium layer center to some distance (both the left edge and the right one and the cell becomes asymmetric). In this case, uranium cells with different sizes remain at the edges of the system. The calculation results with 11 uranium layers are shown on the Figure 4.

![Figure 4](image)

**Figure 4.** Neutron flux density at the different boundary choice of unit cells.

The obtained results show that are the closer the chosen unit cells boundaries to the zone middle, the closer the obtained solution is to the reference one. It is interesting to note, that in the lowest approximations of SHM with “bad” choice of boundaries an asymmetric solution in symmetric task is possible (however, it is impossible to solve the problem with asymmetric cells using homogenization method). It is the result of the fact that neutron distribution inside a cell depends on the angular distribution of the neutrons flowing into the cell.
When choosing the unit cell boundaries in the middles of zones the problem can be solved arbitrarily selecting cells, for example with the cells which boundaries are located in the middle of plutonium and uranium layers (asymmetric cells, «Cell 2» on Figure 1). Results for system with these cells are shown on the Figure 5.

![Chart](chart.png)

**Figure 5.** Neutron flux density in the task with asymmetric cells. Comparing with the reference solution.

We have symmetric solution.

**Conclusion**
The test problem computations have shown the validity of the SHM recommendations on choosing boundaries of the core unit cells of a heterogeneous reactor. The importance of correct choice of the unit cell boundaries in the SHM is demonstrated in the SHM application to the asymmetric cells problems. The surface harmonic method is shown to be also applicable with asymmetric cells while following the SHM recommendations on selecting boundaries of the unit cells.

**References**

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