Generation of XS library for the reflector of VVER reactor core using Monte Carlo code Serpent

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Abstract. A physical model of the radial and axial reflector of VVER-1200-like reactor core has been developed. Five types of radial reflector with different material composition exist for the VVER reactor core and 1D and 2D models were developed for all of them. Axial top and bottom reflectors are described by the 1D model. A two-group XS library for diffusion code DYN3D has been generated for all types of reflectors by using Serpent 2 Monte Carlo code. Power distribution in the reactor core calculated in DYN3D is flattened in the core central region to more extent in the 2D model of the radial reflector than in its 1D model.

1. Introduction
Deterministic safety analysis of nuclear power plants is performed by using various reactor dynamics codes, such as DYN3D, BIPR, HEMERA, DIF3D, etc. Nodal reactor code DYN3D [1, 2], based on the solution of the transport equation in diffusion approximation is widely used for analysis of stationary and transient processes in the reactor core. A set of homogenized nuclear data (diffusion constants and group cross sections) is needed for each node to simulate neutron-physical processes in the reactor code. This data, called the XS library, can be prepared by using various spectral codes, such as Serpent [3], HELIOS, WIMS, TVS-M, some versions of the MCU and others. DYN3D deals with two-group diffusion coefficients and cross sections for fuel assemblies and the reflector.

A physical model of the reflector of VVER-1200-like reactor core has been developed for XS-generation library. Five types of radial and two types of axial reflectors with different material composition exist for the VVER reactor core [4]. A part of data available for VVER-1200 [5, 6] is used for calculation, the other data was taken from [7, 8] for VVER-1000.

2. Models of reflectors
The XS library of the reflector in the full core model is defined by the following characteristics, which are calculated in the two-group approximation:
• diffusion coefficient (D₁₂);
• group-removal cross section (Σ_{rem₁₂});
• group-transfer cross section (Σ_{S₁₂});

The library for DYN3D [1] contains these two-group constants for each reflector type depending on the following parameters:
• coolant temperature (T_m);
• boron acid concentration in the coolant (C_b);
coolant density \( (\gamma_m) \).

The dependence of the two-group diffusion coefficients and cross sections on these parameters in DYN3D is parameterized by the following form [1]:

\[
\Sigma = \Sigma_0 \left[ 1 + C_{R1} (\gamma_m - \gamma_{m0}) \right] * \\
\left[ 1 + C_{C1} (C_b \gamma_m - C_{b0} \gamma_{m0}) \right] * \\
\left[ 1 + C_{Tm} \left( \frac{1}{(T_m)^{1/2}} - \frac{1}{(T_{m0})^{1/2}} \right) \right]
\]

where \( \Sigma \) and \( \Sigma_0 \) are the actual and reference quantities of interest (cross sections or diffusion coefficients), \( C_{R1}, C_{R2}, C_{C1}, C_{C2}, C_{Tm} \) are parameterization coefficients. The quantities \( \gamma_m, C_b, T_m \) and \( \gamma_{m0}, C_{b0}, T_{m0} \) are parameters of the actual and reference states, respectively. The above-mentioned parameterization coefficients correspond to the DYN3D library in format \text{iwqs=2} \ [1].

Neutron production and energy production cross sections, and the data related to poisoning (yields of iodine, xenon and promethium, absorption cross section of xenon and samarium) as well as fuel temperature and burnup dependence are not included into this XS library since the reflector does not contain fissile materials.

Models for all types of radial reflector can be developed for the XS library generation in two different approaches: 1D and 2D models. The 2D model consists of hexagonal cells of radial reflector and one, two or three fuel assemblies.

A more simplified model for the radial reflector required less computing time in the 1D model composed of square cells and consisting of two fuel assemblies and homogeneous cells of the reflector and the surrounding region. Rectangular outer boundaries are used in both models. Black boundary conditions (BC) are used on the outer boundary in the 2D model, while the 1D model is calculated with black BC in one direction and reflective BC in another direction [9, 10] (see figure 3 and figure 4).

The radial reflector of the VVER reactor core can be modeled by one or more layers in radial direction. A three-layer structure of the reflector is shown in figure 1 for 60º symmetry sector of the core. It includes the corresponding part of the buffle, core barrel, coolant and the reactor vessel.

Taking into account 60º symmetry of the core and design features of the buffle, five types of radial reflector cells with different material composition for VVER reactor core can be constructed [4].

Figure 1. 60º sector of reflector for the VVER reactor core.
The correct boundary conditions for the neutron flux at the outer boundary of the reflector can be obtained by taking into account the surrounding (S) materials of the reflector region.

To cover all components of the surrounding region, two square layers of homogeneous surrounding are used in the 1D model (figure 3) of the radial reflector, while one hexagonal layer of heterogeneous surrounding is applied in the 2D model (figure 2).

The central cell of the reflector 2D model underlined in figure 2 is under consideration (for which the few-group cross section is calculated). Three FAs serve as a source of neutrons in r_type1 reflector while r_type2 needs only one FA and two FAs are used for other type of the radial reflector.

![Figure 2. Five types of the 2D models of the radial reflector in Serpent.](image)

Few-group constants for radial reflector are calculated by considering detailed geometry of all components (reflector, surrounding and fuel assembly). The above mentioned 2D model is rather accurate but needs considerable computing time.

To reduce the time of calculation, the 1D model for radial reflector was developed (see figure 3). Symmetry of the model reflects the specifics of boundary conditions (BC) for the system “reflector + neutron source (one or several FA)” available in Serpent. Each compartment of the system is presented as a square region. The boundary conditions in the 1D model are “black” in the direction of the reflector and reflective in the FA direction. The symbols RS_1 and RS_2 correspond to the first and second layers of the radial surroundings representing of homogenized regions with different water/steel ratio.

![Figure 3. 1D model for each of five types of the radial reflector in Serpent.](image)

The 1D model usually used for axial reflector is shown in figure 4. It is presented as an inhomogeneous three layer structure with different material composition in each layer [7]. The
composition of each layer was calculated from the data of the FA design of VVER-1200 [6]. To simplify the 1D model for top and bottom axial reflectors the three layer structure was homogenized into one layer. The symbols AS’s in both sides of figure 4 correspond to the layer of homogenized axial surroundings.

Figure 4. 1D models of the axial reflector in Serpent.

3. Generation of two-group XS library for reflector

The quantities of interest were determined by using Serpent 2 spectral code. The reference values of the parameters for calculation of two-group constants were the following: \( T_f= T_m= 574 \) K, \( \gamma_m= 0.726098 \) g/cm\(^3\), \( C_b= 0 \) g/kg. The values of the coolant temperature, coolant density and boron acid concentration in the coolant used for calculation are presented in table 1 where different values of the parameters are in bold.

| parameter | \( T_{mod}, \) K | \( T_{fuel}, \) K | \( \gamma_{mod}, \) g/cm\(^3\) | \( C_b, \) g/kg |
|-----------|-----------------|-----------------|-----------------|-----------------|
| \( \gamma_{mod} \) | 574 | 574 | 0.5 | 0.0 |
| \( \gamma_{mod} \) | 574 | 574 | 0.6 | 0.0 |
| \( \gamma_{mod} \) | 574 | 574 | 0.8 | 0.0 |
| \( \gamma_{mod} \) | 574 | 574 | 0.9 | 0.0 |
| \( C_b \) | 574 | 574 | 0.726098 | 8.015 |
| \( C_b \) | 574 | 574 | 0.726098 | 16.03 |
| \( C_b \) | 574 | 574 | 0.726098 | 27.48 |
| \( C_b \) | 574 | 574 | 0.726098 | 40.075 |
| \( T_{mod} \) | 533 | 533 | 0.726098 | 0.0 |
| \( T_{mod} \) | 553 | 553 | 0.726098 | 0.0 |
| \( T_{mod} \) | 596 | 596 | 0.726098 | 0.0 |
| \( T_{mod} \) | 619 | 619 | 0.726098 | 0.0 |

Two-group constants for five types of radial and two types of axial (top and bottom) reflector in the 2D and 1D models calculated for the reference parameters are presented in table 2.

Two-group parameter-dependent constants for the reflector were calculated according to the parameters values from table 1. The results of calculations are fitted according to the equation (1) to obtain the parameterization coefficients. As an example the calculated two-group constants depending on the boron acid concentration and results of their fitting are shown in figure 5 for the r_type5 radial reflector in the 1D model for the reference coolant density. The same for the top axial reflector is shown in figure 6. In both figures are shown the diffusion coefficients for the fast (\( D_1 \)) and thermal (\( D_2 \)) neutrons, group-removal cross sections (\( \Sigma_{rem1} \) and \( \Sigma_{rem2} \)) and group-transfer cross section (\( \Sigma_{S12} \)). In figure 5 and 6 arguments are \( C_b \gamma_m0.5 \) g\(^3\)/(kg cm\(^3\)), \( \gamma_m= 0.726098 \) g/cm\(^3\).
Table 2. Reference values of two-group diffusion coefficients and cross sections of the radial and axial reflector.

| Radial reflector          | D_1, cm | D_2, cm | Σ_{rem1}, cm⁻¹ | Σ_{rem2}, cm⁻¹ | Σ_{S12}, cm⁻¹ |
|---------------------------|---------|---------|----------------|----------------|--------------|
| r_type1                   | 1.05689 | 2.89315E-01 | 1.06416E-02 | 5.19650E-02 | 7.25384E-03 |
| r_type2                   | 1.02223 | 2.77912E-01 | 1.03660E-02 | 3.64028E-02 | 6.90553E-03 |
| r_type3                   | 1.04980 | 2.98462E-01 | 1.25117E-02 | 6.34928E-02 | 8.97670E-03 |
| r_type4                   | 1.06435 | 2.94033E-01 | 1.48532E-02 | 5.73539E-02 | 1.14607E-02 |
| r_type5                   | 1.07292 | 2.91831E-01 | 1.62414E-02 | 5.51828E-02 | 1.28671E-02 |

| 1D model                  |         |         |               |               |              |
|----------------------------|---------|---------|----------------|----------------|--------------|
| r_type1                   | 1.02548 | 3.33793E-01 | 1.29841E-02 | 9.98766E-02 | 8.89709E-03 |
| r_type2                   | 1.09480 | 3.18875E-01 | 2.09585E-02 | 8.52954E-02 | 1.74367E-02 |
| r_type3                   | 1.02912 | 3.32638E-01 | 1.38199E-02 | 9.87948E-02 | 9.75134E-03 |
| r_type4                   | 1.03598 | 3.30310E-01 | 1.55861E-02 | 9.54567E-02 | 1.16080E-02 |
| r_type5                   | 1.06443 | 3.24977E-01 | 1.83432E-02 | 9.05972E-02 | 1.45789E-02 |

| Axial reflector            |         |         |               |               |              |
|----------------------------|---------|---------|----------------|----------------|--------------|
| 1D model                   |         |         |               |               |              |
| a_top                      | 1.73119 | 2.99344E-01 | 3.59289E-02 | 1.17676E-02 | 3.51686E-02 |
| a_bottom                   | 1.33625 | 3.01945E-01 | 2.94695E-02 | 5.48096E-02 | 2.72188E-02 |

Figure 5. Dependence of two-group constants on the boron acid concentration and their fitting for the r_type5 radial reflector in the 1D model.

Figure 6. Dependence of two-group constants on the boron acid concentration and their fitting for the top axial reflector in the 1D model.
The similar plots were obtained for the XS dependence on the coolant temperature and coolant density for all types of the radial and axial reflectors. Fitting plots for all parameters of interest are in good agreement with the equation (1).

4. Calculation of normalized power distribution using DYN3D

A rough testing of the two-group constant library for the reflector was done in the reactor code DYN3D by using the fuel XS library in lwgs=2 format. The normalized power distribution in the core with using the XS library with and without constants for the reflector is presented in figure 7.

The first and the second values in the hexagonal cells in figure 7 are the sequence number of the cell and the normalized power distribution in the core without reflector XSs, respectively. The third value is the difference between the normalized power distributions in the model without reflector and with reflector (1D radial and 1D axial) XSs. The fourth value is the difference between the normalized power distributions in the model without reflector and with reflector (2D radial and 1D axial) XSs.

The data shown in figure 7 indicate that the normalized power distribution in the reactor core is flattened in the central region of the core better by using the 2D model of the radial reflector than the 1D model.

Figure 7. Power distribution in the reactor core model with and without reflector XSs.
5. Conclusion

A physical model of the radial and axial reflector of the VVER-1200-like reactor core has been developed. Five types of the radial reflector in the 1D and 2D models were developed. The axial top and bottom reflectors are described in the 1D model. The two-group XS library for the diffusion code DYN3D has been generated for all types of the reflectors by using Serpent 2 Monte Carlo code. A rough testing of the reflector library in DYN3D has shown that the normalized power distribution in the VVER-1200-like reactor core is flattened in the central region of the core better by using the 2D model of the radial reflector in comparison with the 1D model.

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