Development of VVER-1000 pin cell thermal-hydraulic model for MCU/FlowVision coupled calculations

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Abstract. The thermal-hydraulic model for the coupled neutronic and thermal-hydraulic calculations based on the VVER-1000 reactor pin cell is developed. Mesh convergence study is provided with detailed description. Special attention is paid to the impact of turbulence models on the results of calculations. Good agreement with reference calculations with the use of ATLET system thermal-hydraulic code is shown.

1. Introduction
Due to the growth of computer performance we can obtain results closer to reality. This is possible because of a more detailed description of the simulated systems and the complications of the calculation schemes.

When designing and operating nuclear reactors, it is necessary to cover the entire spectrum of reactor physics tasks. This requires to integrate calculations within various physics, such as neutronics or thermal-hydraulics. This can be done by combining codes designed to model the processes described by different areas of physics (MCU, FlowVision).

In this work, we attempted to develop a thermal-hydraulic model for coupled calculations by the precise neutron transport code MCU and CFD code FlowVision. A test case was developed to calculate reactor characteristics, which can be used in calculations with other programs, for example, for the purpose of cross-verification.

2. Models and codes
MCU (Monte Carlo Universal) is a neutron transport code based on the Monte Carlo method [1], the FlowVision software package is designed for numerical simulation of three-dimensional fluid and gas flows [2].

The model for the coupled neutronic and thermal-hydraulic calculations is based on the fuel pin of the VVER-1000 reactor.

The pin cell of the reactor is used as a model (figure 1). There is a gas cavity inside the fuel rod where helium is placed under a 20 atm (2.027 MPa) pressure. Helium also fills the central channel and the gap between the cladding and the fuel. Boric acid is not taken into account, all thermophysical properties of water are given for pure water. Only fuel part is considered, fuel rod end plugs are not taken into account. At the boundaries between the subdomains, the conditions of conjugate heat transfer are specified. At the lateral boundaries, symmetry conditions are specified. The mass velocity
at the inlet of the cell is \(2276.64 \text{ [kg / (m}^2 \text{s)}\)], the initial temperature is \(290 \degree \text{C}\) and the pressure is 16.2 MPa.

![Diagram](image1)

**Figure 1.** Geometrical characteristics of the thermal-hydraulic model of the VVER-1000 pin cell (mm).

For the FlowVision calculation we decided to consider the simplified cell sector of 4 degrees, formed as follows: all subregions except water remain the same, and the external radius of the subregion with water is to have the area of the resulting annular cross-section equal to the area of the original hexagonal cross-section (figure 2).

![Diagram](image2)

**Figure 2.** Geometry for the study.

Materials with corresponding thermophysical properties are specified in each of the subregions, which depend on pressure and temperature for water and on temperature for other materials.

The standard \(k-\varepsilon\) model of turbulence is used in water, the volumetric heat source obtained from the first iteration of the neutron-physical code MCU is set inside the subdomain with fuel, the motion of helium in the gap is taken into account.

At the outer boundary of the subregion with water, the boundary condition of symmetry is specified, as well as at the lateral boundaries of the sector. Thermal insulation is specified at all available end borders, except for the inlet and outlet. The mass velocity is specified at the inlet, the pressure is at the outlet, and the conditions of the conjugate heat exchange are specified at all boundaries between the subdomains.

It is required to calculate the axial temperature distributions of the fuel, cladding, coolant and density of the coolant for exchanging with MCU. The required parameters need to be averaged over the volume of each axial layer, so the values obtained were averaged over the volume of 12 cylinders created in FlowVision.

The calculation was performed with the standard settings of the Solver on a personal computer with a 2.53 GHz processor and 3 GB of RAM.
3. Mesh convergence study

The computational mesh was designed to be two-dimensional during any adaptation. This was made by creating a non-computational domain far from the sector and taking it into account when automatically generating a mesh. The mesh was especially refined in the area with water near the wall and in areas with a cladding and a gap.

First of all, the dependence of the results on the mesh refinement near the surface of the rod in water was studied. Calculations were carried out with five different meshes in the area with water, shown in figure 4 and described in table 1.

The meshes differed in levels of adaptation — the discretization levels of the initial mesh. The first level of adaptation means dividing the initial cell in half in all directions. The second level divides the initial cell by 4, etc. An example of dividing the mesh near the surface of the rod to the third level is shown in Figure 3.

![Figure 3. Levels of adaptation of the computational grid - the first, second and third.](image)

| Case No. | Number of radial cells |
|----------|------------------------|
|          | 0 level | 1 level | 2 level | 3 level |
| 1        | 12      | 0       | 0       | 0       |
| 2        | 8       | 8       | 0       | 0       |
| 3        | 8       | 4       | 8       | 0       |
| 4        | 9       | 2       | 4       | 8       |
| 5        | 5       | 8       | 8       | 8       |

The results of the mesh convergence study in the region with water are presented in figures 5 – 11. The axial distribution of the fuel temperature does not change depending on the mesh refinement except for the case No. 5, which differs from all other cases. In this case is the smallest mesh in the water.
Figure 4. Meshes for the mesh convergence study in the area with water.

Figure 5. Axial distribution of the fuel temperature.

The axial distribution of the cladding temperature practically does not change depending on the mesh refinement in water, but the results of each subsequent variant fluctuate around the results for initial case (No.1) with increasing deviation.
The axial distribution of the water temperature does not change depending on the mesh refinement except for the case No. 5, which results slightly differ from all other results.

The radial distribution of the fuel temperature in the central section does not change depending on the mesh refinement in water area.
The radial distribution of the cladding temperature in the central section noticeably change depending on the mesh refinement in water area. The results of cases No.4 and 5 are almost the same.

The radial distribution of the water temperature and velocity in the central section noticeably change depending on the mesh refinement in water. The results of cases No.4 and 5 are almost the same.
Figure 10. Radial distribution of the water temperature in the central section.

Figure 11. Radial distribution of the water velocity in the central section.

Table 2 presents the results of the mesh convergence study in the region with water. It contains the temperature values in the axial layers with the largest deviation among all cases, the temperatures and velocities at the points in the model cross section with the maximum deviation among all cases.
Table 2. Change in parameters after the transition from larger to smaller mesh.

| №   | $T_{\text{fuel}}^5$ | $T_{\text{clad}}^5$ | $T_{\text{coolant}}^5$ | $T_{\text{fuel}}^{\text{min}}$ | $T_{\text{clad}}^{\text{min}}$ | $T_{\text{coolant}}^{\text{max}}$ | $v_{\text{max}}$ |
|-----|---------------------|---------------------|------------------------|-------------------------------|-------------------------------|-------------------------------|---------------|
| 1   | 747.150             | 336.139             | 318.195                | 573.789                       | 329.615                       | 313.630                       | 4.470         |
| 2   | 747.324             | 336.328             | 318.201                | 573.950                       | 328.119                       | 314.921                       | 4.069         |
|     | (+0.023%)           | (+0.056%)           | (+0.002%)              | (+0.028%)                     | (-0.454%)                     | (+0.412%)                     | (-8.971%)     |
| 3   | 746.775             | 335.823             | 318.215                | 573.455                       | 326.690                       | 318.038                       | 2.924         |
|     | (-0.073%)           | (-0.150%)           | (+0.004%)              | (-0.086%)                     | (-0.436%)                     | (+0.990%)                     | (-28.14%)     |
| 4   | 747.553             | 336.573             | 318.208                | 574.067                       | 326.938                       | 319.161                       | 2.664         |
|     | (+0.104%)           | (+0.223%)           | (-0.002%)              | (+0.107%)                     | (+0.076%)                     | (+0.353%)                     | (-8.892%)     |
| 5   | 729.783             | 335.555             | 317.863                | 574.071                       | 326.942                       | 319.166                       | 2.664         |
|     | (-2.377%)           | (-0.302%)           | (-0.108%)              | (+0.001%)                     | (+0.001%)                     | (+0.002%)                     | (0%)          |

From the obtained figures, we can conclude that the optimal mesh refinement in the water is in the case No. 4 and that the radial temperature and velocity distributions are the most informative in this respect, because the mesh was discretized in this direction.

Then, the dependence of the results on mesh refinement inside the fuel rod was investigated. Calculations were carried out with five different meshes, which are shown in figure 12 and described in table 3.

Table 3. Meshes for the mesh convergence study inside fuel rod.

| Case No. | Adaptation levels by subdomains |
|----------|---------------------------------|
|          | Central hole | Fuel | Gap | Cladding |
| 1        | 0            | 0    | 0   | 0        |
| 6        | 0            | 0    | 0   | 1        |
| 7        | 0            | 0    | 3   | 1        |
| 8        | 1            | 0    | 3   | 1        |
| 9        | 1            | 0    | 3   | 2        |
| 10       | 1            | 1    | 3   | 2        |

Figure 12. Meshes for the mesh convergence study inside fuel rod.

The results of the mesh convergence study in the region inside the rod are presented in figures 13–19.
The axial distribution of the fuel temperature depending on the mesh refinement inside the fuel rod does not change except for the case No.1.

The axial distribution of the cladding temperature is almost the same in the cases No. 1, 6, 7 and in the cases No. 9, 10. The axial distribution of the water temperature is almost the same in all cases.
Figure 15. Axial distribution of the water temperature.

Figure 16. Radial distribution of the fuel temperature in the central section.

The radial distribution of the fuel temperature in the central section does not change except for the case No. 1, the same as for axial distribution of the fuel temperature.
Figure 17. Radial distribution of the cladding temperature in the central section.

The radial distribution of the cladding temperature in the central section is practically the same in the cases No. 6 and 7, 9 and 10 as well as the axial distribution, but now it can be seen that the results in the case No. 1 are not completely the same as in the cases No. 6 and 7.

Figure 18. Radial distribution of the water temperature in the central section.
Figure 19. Radial distribution of the water velocity in the central section.

The results on the figures with the radial distribution of the water temperature and velocity in the central section behave in the same way as on the previous figures, but now cases No. 1, 6 and 7 are the same.

The results of the mesh convergence study inside the rod are presented in table 4.

Table 4. Change in parameters after the transition from larger to smaller mesh inside the rod.

|     | $T^\text{fuel}$ | $T^\text{clad}$ | $T^\text{coolant}$ | $T^\text{min}_\text{fuel}$ | $T^\text{min}_\text{clad}$ | $T^\text{max}_\text{coolant}$ | $T^\text{max}$ |
|-----|----------------|----------------|-------------------|-----------------------------|-----------------------------|-----------------------------|--------------|
| 1   | 747.150        | 336.139        | 306.107           | 573.789                     | 329.615                     | 313.630                     | 4.470        |
| 6   | 798.750        | 331.418        | 306.079           | 616.686                     | 323.399                     | 313.907                     | 3.783        |
| (+6.906%) | (-1.405%) | (-0.009%)     | (+7.476%)         | (-1.886%)                   | (+0.088%)                   | (-15.360%)                 |
| 7   | 745.822        | 331.444        | 306.071           | 558.432                     | 323.398                     | 313.908                     | 3.783        |
| (-6.626%) | (+0.008%) | (-0.003%)     | (-9.446%)         | (-0.001%)                   | (+0.0002%)                  | (-0.009%)                  |
| 8   | 745.814        | 331.444        | 306.082           | 558.432                     | 323.397                     | 313.908                     | 3.783        |
| 0.001% | (0%)           | (+0.004%)      | (0%)              | (0%)                        | (0%)                        | (0%)                        | (+0.009%)    |
| 9   | 748.716        | 334.212        | 306.156           | 560.638                     | 325.191                     | 316.561                     | 3.190        |
| (+0.389%) | (+0.835%) | (+0.024%)     | (+0.395%)         | (+0.555%)                   | (+0.845%)                   | (-15.70%)                  |
| 10  | 748.571        | 334.212        | 306.139           | 560.638                     | 325.191                     | 316.561                     | 3.190        |
| (-0.019%) | (0%)           | (-0.005%)      | (0%)              | (0%)                        | (0%)                        | (0%)                        | (+0.004%)    |

According to the graphs we can conclude:
1) The central hole does not need to be refined better than in the initial case No. 1, and the gap should be left with the third level of adaptation, according to the cases No. 1, 6, 7 and 8;
2) Comparing cases No. 9 and 10, the fuel should not be refined better than in the initial case.
3) From the comparison of cases No. 7 and 9, 1 and 6, and considering that the refinement of the central hole does not affect the results, it follows that it is impossible to make conclusions about the
sufficiency of the cladding refinement. Therefore, it is required to consider a variant similar to the case No. 7, but with third level of adaptation in the cladding.

4. Turbulence model selection
When creating the model a study of the dependence of the results on the turbulence model used was also conducted. The results of the comparison are presented in figures 20-22.

![Figure 20. Fuel temperature.](image)

![Figure 21. Cladding temperature.](image)
As can be seen from the graphs obtained the SST turbulence model is not suitable for this task, whereas the standard k-ε and k-ε FlowVision turbulence models show good agreement between the results.

5. Cross-verification
The results obtained using the described thermal-hydraulic model were compared with the results obtained using the ATHLET system thermal-hydraulic code the comparison results are presented in figures 23-25.
The thermal-hydraulic system code ATHLET (Analysis of Thermal-Hydraulics of LEaks and Transients) is used for various types of reactors, including Russian VVER-type reactors. ATHLET is certified in Russia for use in the safety analysis of water cooled reactors [4].

![Graph](image1)

**Figure 24.** Cladding temperature.

![Graph](image2)

**Figure 25.** Coolant temperature.

From the graphs obtained, one can see that the maximum deviation in temperatures is achieved in the center of the computational domain, both in height and in radius. This point is located at the maximum distance from all boundary conditions. However, all deviations do not exceed 3%.
6. Conclusion

The thermal-hydraulic model for the coupled calculations of the VVER-1000 reactor pin cell using MCU and FlowVision codes was developed in this work. The model was verified using ATHLET thermal-hydraulic code. Good agreement of the results is demonstrated. The coupled calculation test case is simulated using the neutron transport code MCU and thermal-hydraulic code FlowVision. The test case will be used for cross-verification of coupled neutron transport and thermal-hydraulic codes, research of convergence acceleration models for iterative schemes and calculations of the VVER-1000 reactor characteristics.

References

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