VVER-1000 pin cell benchmark for coupled neutronics/thermal-hydraulics calculations: preliminary results

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Abstract. There is a need for verification of coupled neutronics/thermal-hydraulics calculation schemes. For this, we propose to use the benchmark based on the pin cell of VVER-1000 reactor. This paper gives a detailed description of the benchmark as well as the results of calculations obtained by MCU/ATHLET and MCU/FLOWVISION coupled codes. We also proposed a new convergence criterion, and showed that some power levels lead to the iterative instability of coupled solution. To enhance the stability one could use stochastic method.

1. Introduction

Coupling of precise neutron transport and thermal-hydraulic codes is becoming widely used to improve the accuracy of the calculations of characteristics of nuclear reactors. Examples of the implementation of such coupled schemes are MCNP/COBRA-TF [1], MCNP/SUBCHANFLOW [2], SERPENT/RELAP 5 [3]. Some precise programs include a thermal-hydraulic module (MC21 [4], MCU6 [5]). However, one of the main drawbacks of precise coupled calculations is the long calculation time. For this reason, such coupled calculations are mainly used for verification of calculations carried out by deterministic programs, or for scientific research.

In the development of coupled programs, it becomes necessary to verify the obtained results. For these purposes, verification of calculation results using benchmarks can be performed. At the initial stage, it is reasonable to use simple benchmarks, because it saves the time when searching for errors. Unfortunately, there are not so many such benchmarks (for example, [6,7]).

The purpose of this work was to develop a coupled benchmark based on the previously proposed test problem for coupled calculations of VVER-1000 pin cell [8], and to obtain preliminary results of the calculations. This paper provides data necessary for the development of neutron transport (for Monte-Carlo codes) and thermal-hydraulic (for system and CFD codes) models, the results of the benchmark coupled solutions obtained with MCU/ATHLET and MCU/FLOWVISION coupled codes. A new convergence criterion is proposed. It is shown that some power levels could lead to sustained oscillations of coupled solution.
2. Codes

2.1. MCU
MCU (Monte Carlo Universal) is a Monte Carlo code, which was developed at the National Research Center “Kurchatov Institute” (Russia) [9]. It could be used for simulation of neutron, gamma ray and electron transport in 3D geometry with analog or weight Monte Carlo methods. MCU supports multi-processor interface (MPI), uses point-wise cross-section libraries and contains cross-section conversion sub-modules. Cross-sections in the thermal energy region are generated using phonon spectra, in resolved resonance region with Breit-Wigner, Adler-Adler or Reich-Moore formalisms, in unresolved resonance region using Bondarenko f-factors or sub-group parameters.

There are some examples of MCU coupling with thermal-hydraulic codes [10,11]. Some versions of MCU include Thermo-Physical Analysis module (TPA) for thermal-hydraulic calculations [12].

In this work we used MCU-PTR code [13]. Thermal cross-section libraries were prepared in advance with 4 K temperature step. In the fast energy region, we used point-wise cross-sections based on ENDF/B-VII.0, in unresolved and resolved resonance regions – sub-group BNAB/MCU and LIPAR libraries, correspondingly.

2.2. ATHLET
The ATHLET thermo-hydraulic system code (Analysis of THERmal-hydraulics of LEaks and Transients) [14] was developed in Gesellschaft für Anlagen- und Reaktorsicherheit (GRS mbH). Experience of long-term work with ATHLET has shown that it can be used for Russian VVER and RBMK type reactors. The ATHLET code is certified in Russia for use in safety analysis of VVER reactors [15].

ATHLET consists of several basic modules that allow describing various phenomena in thermal hydraulic systems: Thermo-Fluid dynamics module (TFD), Heat Conduction and Heat Transfer module (HECU), Neutron Kinetics module (NEUKIN) for describing point and one-dimensional kinetics, Control and Balance of Plant module for describing equipment during operation (GCSM) and a fully implicit numerical integration module (FEBE). Other independent modules can be connected via the main interface.

The TFD module is based on the use of five equations for one-fluid model (the general equation for the moment of motion of the mixture with the drift flow) and six equations for two-fluid model. In addition to light water, the module allows calculations with other coolants, such as: heavy water, liquid metals (lead, lead-bismuth, sodium), gases (helium). It is possible to simulate the behavior of non-condensable gases (air, nitrogen, argon, hydrogen, helium, oxygen, user gas — when the user specifies its properties), dissolving nitrogen and describing boron transport in systems with light and heavy water.

2.3. FLOWVISION
The FlowVision software package is designed for numerical simulation of three-dimensional fluid and gas flows [16]. FlowVision is based on the numerical solution of three-dimensional stationary and non-stationary equations of fluid and gas dynamics, which include the conservation laws of mass, momentum (Navier-Stokes equations), the equation of state. FlowVision uses a finite-volume approach to approximate the equations of a mathematical model. Navier-Stokes equations are solved by splitting into physical processes (MAC projection method).

3. Benchmark specifications

3.1. Coupling scheme
The coupled neutronics/thermal-hydraulics calculation scheme is developed for the model of the standard fuel rod of VVER-1000 reactor with the modern generation of fuel assemblies of the TVS-2M type. The model is similar to the presented in [8], but taking into account the central hole and the helium gap.
The external iterative scheme is used for coupled calculations (figure 1). The transient process is simulated with the thermal-hydraulic code until stationary state is reached. The stationary state is considered at each iteration in the neutronics calculations.

The input values for the Monte Carlo code on each iteration are:
- \( T_f^i \) – fuel temperature [K];
- \( T_c^i \) – cladding temperature [K];
- \( T_m^i \) – moderator temperature [K];
- \( \rho m_i \) – moderator density [g/cm\(^3\)].

The calculated functionals are local power \( (P_i) \) and its error \( (\Delta P_i) \), which are calculated by the formulas from [10] considering one standard deviation for the fission reaction rates:

\[
P_k = P \sum_k \frac{R_f^k}{R_f}
\]

\[
\Delta P_k = \pm \left( \left( \frac{P \cdot \Delta R_f^k}{R_f} \right)^2 + \left( \frac{P \cdot R_f^k \cdot \Delta R_f^k}{R_f^2} \right)^2 \right)^{1/2}
\]

where \( P \) – power of entire system, \( \Delta R_f^k \) – statistical error of the total fission rate, calculated in k-layer, \( R_f = \sum R_f^k \) – cumulative total fission rate, \( \Delta R_f \) – statistical error of cumulative fission rate.

The obtained values of the power distribution are transferred to the input file of the thermal-hydraulic code (with the PERL script) and the average values for the cell are calculated. These values are used on the next iteration as the input data for the neutron transport code.

![Neutronics](image1.png)

Figure 1. The iteration scheme of coupled calculations.

In this paper the new convergence criterion is proposed – power residual sum (PRS):

\[
R_S = \sum_j (P_i^j - P_{i-1}^j) \leq 2 \sum_j (\Delta P_i^j)
\]

where \( R_S \) – residual sum, \( i \) – iteration number, \( j \) – number of material cell.

3.2. MCU model

The neutron transport model is the VVER-1000 pin cell, which consists of the central hole, fuel part, helium gap, cladding and water moderator (figure 2). The model is divided into 10 axial layers and 1 radial layer. The following notation of calculation case is applied: Qn_Tm, where Q means power.
calculation with \( n \) radial layers, \( T \) means fuel temperature calculation with \( m \) radial layers (power density is the same). Mirror reflection of neutrons is present only on the lateral border of the model, at the ends is black border.

Before the obtaining of coupled solution, the multiplication factor should be set equal unity. It is reached by changing the boric acid concentration.

Compatibility of neutron and thermal-hydraulic models is achieved by setting a fixed temperature of the moderator at the entrance to the model (layer No. 0). The neutron model does not take into account changes in the density of the fuel, helium and cladding. The average energy per one fission is assumed constant and the same for the both uranium isotopes. Description of materials and parameters of the model is given in tables 1-2.

![Figure 2. Geometrical characteristics of the neutron transport model of VVER-1000 pin cell (mm).](image)

### Table 1. Characteristics of the fuel pin of TVS-2M.

| Parameter                        | Value         |
|----------------------------------|---------------|
| Lattice spacing                  | 12.75 mm      |
| Height of fuel                   | 3700 mm       |
| Power of the model               | 58.99 kW (100%)|
| Inlet flow rate                  | 100 kg/sec    |
| Inlet temperature                | 290 °C        |
| Inlet pressure to the core       | 16.2 MPa      |
| Helium pressure                  | 2.027 MPa     |
| Outer diameter of the cladding   | 9.1 mm        |
| Inner diameter of the cladding   | 7.73 mm       |
| Outer diameter of the fuel pellet| 7.60 mm       |
| Diameter of the central hole     | 1.2 mm        |
Table 2. Composition of the materials of the model (the mass fraction of isotopes)

| Material | Density, g/cm$^3$ | Composition (mass fractions) |
|----------|------------------|-------------------------------|
| UO$_2$, 1.6 % $^{235}$U | 10.4 | $^{235}$U – 1.41%, $^{238}$U – 86.74%, O – 11.85 % |
| E-110 $^{[3]}$ | 6.55 | Zr – 98.8925 %, Nb – 1%, Fe – 0.015%, Ni – 0.007%, Al – 0.004%, Ti – 0.003%, C – 0.02%, Si – 0.004%, O – 0.05%, N – 0.003%, H – 0.0015% |
| H$_2$O, x% H$_3$BO$_3$ | 5.36 g/kg (for the state with 100% power) | – |

3.3. ATHLET model

Model for the calculations with ATHLET code has similar division into layers and dimensions as the neutron model (figure 3). There is no fuel rod end plugs and spacer grids, but the helium gap, the central hole and the gas collector (on top of the model) are taken into account. There could be different number of radial calculation points in the fuel (variants Q1_10, Q1_20). Properties of the materials are in tables 3 and 4. Properties of water and helium are taken from the built-in library.

![Figure 3. The scheme of the model for the thermal-hydraulic calculations by ATHLET](image)

HE.IN – thermal object with helium, internal gas volume in the center of the fuel pin
HV-CHA – thermal structure with fuel divided into three radial sections by energy release (in this work power density is the same)
HF.FC – thermal object with helium, gas volume between the fuel and the cladding
HE-BR – thermal object with helium, upper gas collector
H-CLAD – thermal structure with cladding
V-CHA – thermal object with coolant, cell with water around fuel pins

| T, °C | $C_{\text{clad}}$, J/kg/K | $\lambda_{\text{clad}}$, W/m/K | $\rho_{\text{clad}}$, kg/m$^3$ |
|------|-----------------|-----------------|----------------|
| 100  | 285.0           | 18.0            | 6550          |
| 200  | 301.0           | 19.3            |               |
| 300  | 322.0           | 20.1            |               |
| 400  | 343.0           | 20.5            |               |
| 500  | 368.0           | 20.9            |               |
| 600  | 398.0           | 21.8            |               |
| 700  | 448.0           | 22.9            |               |

| T, °C | $C_{\text{fuel}}$, J/kg/K | $\lambda_{\text{fuel}}$, W/m/K | $\rho_{\text{fuel}}$, kg/m$^3$ |
|------|-----------------|-----------------|----------------|
| 27   | 274.0           | 8.50            | 10400         |
| 227  | 291.0           | 6.70            |               |
| 527  | 305.0           | 5.40            |               |
| 627  | 315.0           | 4.40            |               |
| 827  | 318.0           | 3.75            |               |
| 1027 | 324.0           | 3.25            |               |
| 1227 | 328.0           | 2.80            |               |
| 1427 | 335.0           | 2.50            |               |
| 1627 | 347.0           | 2.40            |               |
| 1827 | 364.0           | 2.42            |               |
| 2027 | 390.0           | 2.44            |               |
| 2227 | 426.0           | 2.50            |               |
| 2427 | 470.0           | 2.65            |               |
| 2627 | 520.0           | 3.00            |               |
| 2827 | 394.0           | 3.50            |               |

3.4. FLOWVISION model

The pin cell of the reactor is used as a model (figure 4). There is a gas cavity inside the fuel rod where helium is placed under 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 thermo physical 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 [kg / (m$^2$-s)], the initial temperature is 290 °C and the pressure is 16.2 MPa.
Figure 4. Geometrical characteristics of the thermal-hydraulic model of 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 has the area of the resulting annular cross-section equal to the area of the original hexagonal cross-section (figure 5).

Figure 5. Geometry for the study.

Materials with corresponding thermo physical properties are specified in each sub region, which depend on pressure and temperature for water and on temperature for other materials.

The standard k-ε model of turbulence is used in water, the volumetric heat source obtained from the first iteration of the neutron transport 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 code. The required parameters are averaged over the volumes in each axial layer.

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

4. Comparison of the results

The coupled benchmark solutions were obtained using MCU/ATHLET and MCU/FlowVision codes for 100% of the power. The MCU/ATHLET calculations were carried out with different parameters: 10 and 20 radial layers in the fuel for heat transfer calculations using ATHLET code without using methods of acceleration of convergence; with 10 radial layers in the fuel for heat transfer calculations using the stochastic method [17].

Final power profiles for calculations with 10 and 20 radial layers without the use of convergence acceleration methods are presented in figure 6.

![Figure 6](image)

**Figure 6.** Comparison of power in coupled calculations using MCU/ATHLET with 10 and 20 radial layers in the fuel without using methods of convergence acceleration.

Since the coupled solution fluctuates depending on the iteration number, we took solutions with the minimum total relative difference $R_\Sigma$ among 30 iterations for comparison. For the Q1_T10 variant $R_\Sigma = 10\%$ (iteration 22, convergence criterion reached at 14th iteration), corresponds to a maximum local residual of 2%. For the Q1_T20, $R_\Sigma = 47\%$ (iteration 12, convergence criterion is not reached), corresponds to the maximum local residual of 6.9%. As it can be seen from the figure 6, the calculated power profiles are within the error range, therefore, for further comparison with other calculations, the Q1_T10 was chosen because of significantly lower value of $R_\Sigma$.

The coupled solution obtained using the stochastic method for the model with 10 radial layers by MCU/ATHLET converged in 4 iterations. However, to obtain a more accurate solution we calculated 20 iterations (maximum local residual is 0.1%). Final axial power profiles obtained by MCU/ATHLET for the Q1_T10 variant using stochastic method and without it are presented in figure 7.

As can be seen from the figure, the obtained power values coincide within the limits of statistical errors. In this case, the maximum power deviations reach 2.5% at the edges of the fuel rod, where the power is the smallest. This deviation behavior can be explained by the accumulation of smaller statistics during MCU calculations.
As a reference solution in this benchmark, a calculation using MCU/FlowVision was performed. The convergence criterion was reached on the 3rd iteration with maximum local residual of 1.5%. The use of precise neutron transport and CFD codes allows obtaining the most accurate solutions, however, the calculations are long.

The calculation time of one iteration by MCU/ATHLET without the use of convergence acceleration methods takes about 60 minutes, while the ATHLET calculation takes several seconds. Calculations with MCU code were performed on the MEPhI BASOV cluster using 64 cores and 128 million histories. MCU/ATHLET calculation using the stochastic method took a different amount of time at each iteration due to the different number of simulated neutron histories (from 60 to 120 minutes per iteration). The calculation time of one iteration with MCU/FlowVision takes 420 minutes (60 minutes by MCU on the BASOV cluster and 360 by FlowVision on a computer with a 2.53 GHz CPU (core i3) and 3 GB of RAM).

The axial deviations in the power between various calculations with MCU/ATHLET and MCU/FlowVision are presented in figure 8.

![Figure 7. Comparison of the final axial power profile obtained by MCU/ATHLET for the Q1-T10 variant using stochastic method and without it.](image-url)
Figure 8. Deviation in axial power between the results obtained by MCU/ATHLET and MCU/FlowVision.

As can be seen from the figure 8, the smallest deviations are for stochastic method. In this case the relative power differences do not exceed 1%.

The extended results of the calculations with MCU/ATHLET and MCU/FlowVision are presented in tables 5-7. ΔP values were obtained considering three standard deviations.

**Table 5.** The results of calculations with MCU/ATHLET (Q1_T10).

| Layer № | MCU/ATHLET, Q1_T10 |
|---------|---------------------|
|         | P, W | ΔP, W | Tf, K | Tc, K | Tm, K | ρm, g/cm³ |
| 0       | -    | -     | -     | -     | 563.2 | 0.7472    |
| 1       | 2450 | 105   | 697   | 578   | 564.5 | 0.7447    |
| 2       | 5179 | 196   | 852   | 595   | 567.4 | 0.7391    |
| 3       | 6942 | 202   | 965   | 609   | 571.2 | 0.7315    |
| 4       | 7818 | 167   | 1026  | 618   | 575.6 | 0.7226    |
| 5       | 8127 | 124   | 1050  | 626   | 580.2 | 0.7129    |
| 6       | 7979 | 133   | 1045  | 630   | 584.7 | 0.7029    |
| 7       | 7405 | 170   | 1012  | 632   | 588.9 | 0.6932    |
| 8       | 6320 | 196   | 947   | 629   | 592.3 | 0.6847    |
| 9       | 4600 | 176   | 844   | 621   | 594.8 | 0.6783    |
| 10      | 2170 | 94    | 712   | 608   | 595.9 | 0.6753    |
| 11      | -    | -     | -     | -     | 595.9 | 0.6753    |

**Table 6.** The results of calculations with MCU/ATHLET (Q1_T10-ST).

| Layer № | MCU/ATHLET, Q1_T10-ST |
|---------|------------------------|
|         | P, W | Tf, K | Tc, K | Tm, K | ρm, g/cm³ |
| 0       | -    | -     | -     | 563.2 | 0.7472    |
| 1       | 2389 | 694   | 578   | 564.6 | 0.7445    |
| 2       | 5060 | 845   | 596   | 567.5 | 0.7388    |
| 3       | 6837 | 958   | 610   | 571.5 | 0.7309    |
| 4       | 7810 | 1025  | 620   | 576.0 | 0.7217    |
5 8181 1054 626 580.6 0.7119
6 8066 1050 630 585.1 0.7020
7 7487 1017 631 589.1 0.6926
8 6375 950 628 592.5 0.6843
9 4613 845 620 594.8 0.6782
10 2173 712 608 595.9 0.6753

Table 7. The results of calculations with MCU/FlowVision.

| Layer No | MCU/FlowVision | 
|----------|----------------|
|          | P, W | ΔP, W | Tf, K | Tc, K | Tm, K | ρm, g/cm³ |
| 0        | -    | -     | -     | -     | 563.2 | 0.7476    |
| 1        | 2372 | 70    | 691   | 573   | 563.9 | 0.7462    |
| 2        | 5043 | 128   | 840   | 586   | 566.2 | 0.7418    |
| 3        | 6841 | 132   | 951   | 596   | 569.7 | 0.7350    |
| 4        | 7819 | 110   | 1018  | 604   | 574.0 | 0.7263    |
| 5        | 8177 | 83    | 1046  | 610   | 578.5 | 0.7168    |
| 6        | 8049 | 84    | 1042  | 614   | 583.0 | 0.7069    |
| 7        | 7489 | 111   | 1009  | 616   | 587.2 | 0.6971    |
| 8        | 6388 | 134   | 942   | 615   | 590.8 | 0.6883    |
| 9        | 4635 | 114   | 843   | 611   | 593.6 | 0.6811    |
| 10       | 2178 | 60    | 728   | 605   | 595.4 | 0.6762    |
| 11       | -    | -     | -     | -     | 595.9 | 0.6749    |

The results of the calculations given in tables 5-7 allow to verify and compare the results of calculations for 2 types of coupled codes: precise neutron transport code + system thermal-hydraulic code and precise neutron transport code + CFD code. In the future, the results of calculations of this model using the remaining two types of coupled codes will also be obtained: deterministic neutron transport code + system thermal-hydraulic code (SKETCH/ATHLET) and deterministic neutron transport code + CFD code (SKETCH/FlowVision).

As part of this work, we calculated the model on 125% and 150% power level. However, the solutions obtained using both types of coupled codes do not converge. Axial power and temperature oscillations occur, which are caused by the fuel temperature feedback [10].

5. Conclusion
We proposed a benchmark for coupled neutron transport/thermal-hydraulic calculations of the VVER-1000 reactor pin cell. A detailed description of the data required for the development of calculation models for Monte Carlo, system and CFD codes, as well as the results of the benchmark solutions by MCU/ATHLET and MCU/FLOWVISION coupled codes are given.

The deviations in the local power values obtained with mentioned coupled codes do not exceed 1%, in fuel temperature - 2.2% (16 K), in coolant temperature - 0.4% (2.1 K, outlet temperature is the same), in cladding temperature - 2.6% (16 K), in coolant density - 0.7%. The increase of the power level leads to the sustained power oscillations, which are caused by the fuel temperature feedback. To stabilize the coupled solution stochastic method could be used.

We plan to expand this benchmark in the future in order to determine the influence of the model parameters, codes settings and coupling methods on the coupled solution and its oscillations. To address this issue, as well as to calculate the benchmark by different coupled codes, we are glad to invite other researchers.
Acknowledgments
This work was supported by Competitiveness Program of National Research Nuclear University MEPhI.
Authors express gratitude to Pazman Koppany for the useful discussions on the work and to the MEPhI BASOV cluster team for the help during calculations.

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