Test case for VVER-1000 complex modeling using MCU and ATHLET

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Abstract. The correct modeling of processes occurring in the fuel core of the reactor is very important. In the design and operation of nuclear reactors it is necessary to cover the entire range of reactor physics. Very often the calculations are carried out within the framework of only one domain, for example, in the framework of structural analysis, neutronics (NT) or thermal hydraulics (TH). However, this is not always correct, as the impact of related physical processes occurring simultaneously, could be significant. Therefore it is recommended to spend the coupled calculations. The paper provides test case for the coupled neutronics-thermal hydraulics calculation of VVER-1000 using the precise neutron code MCU and system engineering code ATHLET. The model is based on the fuel assembly (type 2M). Test case for calculation of power distribution, fuel and coolant temperature, coolant density, etc. has been developed. It is assumed that the test case will be used for simulation of VVER-1000 reactor and in the calculation using other programs, for example, for codes cross-verification. The detailed description of the codes (MCU, ATHLET), geometry and material composition of the model and an iterative calculation scheme is given in the paper. Script in PERL language was written to couple the codes.

1. Introduction
For a long period of time simulation of nuclear reactors was carried out by means of simple mathematical models. This was mostly due to the low level of development of computer technology. However, it was enough to create a sustainable nuclear industry. Since then, methods of calculation and handy tools have changed a lot. Due to the growth of computer performance we can obtain closer to reality results. Today we see a trend to a more detailed description of simulated systems and growing complexity of calculation schemes. Modeling is gradually coming to an absolutely new level.

Nowadays scientists understand that the feedback of related physical processes occurring simultaneously could be significant. There are a number of issues, which could be solved only in the complex modeling. Coupled calculations could be done either on the basis of one calculation program, using simple physical models (BIPR, DYN3D, NESTLE), or by coupling the codes intended to simulate the processes described in different areas of physics (MCU, MCNP, ATHLET, ANSYS, etc.). Such kind
of coupling was performed before for different types of reactors [1-3]. In this paper is given description of the test case for coupled calculation of VVER-1000 using MCU and ATHLET codes.

2. Codes features

2.1. MCU

MCU (Monte Carlo Universal) - is a neutron code based on the Monte Carlo method, which allows to simulate the transport of neutrons, gamma rays and electrons of different energies. The code takes into account the effects of the continuous changes in the particle energy, as well as continuous or step-energy dependence of the cross-sections. The accuracy is determined primarily by used libraries of evaluated nuclear data. MCU allows to calculate the real geometry and material composition of the complex media at various temperatures. It contains cross-sections conversion modules in the thermal and resolved resonance region, depending on the temperature of the material (using the Breit-Wigner or Adler-Adler formalisms). It can be used for multi-processor calculations (MPI technology) [4].

2.2 ATHLET.

Thermal hydraulic system code ATHLET (Analysis of Thermal-Hydraulics of LEaks and Transients) developed in Gesellschaft für Anlagen-und Reaktorsicherheit (GRS mbH) and was originally intended for the analysis of the entire spectrum of leak cases and transients in LWR reactors (PWR and BWR). However, experience has shown that code could be fully used for the Russian VVER reactors. It should be noted that at present this code is approved in Russia for use in the analysis of the safety of reactors with water coolant.

ATHLET consists of several modules that allow to describe the various phenomena in the behavior of light water reactors: thermal hydraulic module (TFD), heat transfer and heat conduction unit (HECU), neutron-kinetic unit (NEUKIN) to describe the point and the one-dimensional kinetics, module for operation of the equipment (GCSM) and a module for the numerical integration (FEBE), implements a fully implicit scheme. Other independent modules (e.g., three-dimensional neutron kinetics, describe the behavior of containment, etc.) can be connected through the main interface.

The major is TFD module that is based on the use of five equations (equations of conservation of mass and energy for the liquid and vapor phase and the general equation for the angular momentum mixture drift flow) or six equations (equations of conservation of mass, energy, and pulse for the liquid and vapor in the description of the two-fluid model) with a wide range of closure ratios. In addition, the module allows to simulate the behavior of non-condensable gases, nitrogen dissolution and describe the boron transport in system. Reactor coolant system is modeled by a compound of basic thermodynamic objects (TFO), the detailed modeling is limited only by the possibility of computing - the amount of memory (RAM) and processor frequency. In addition, in TFD module it is possible for specific description of transverse coolant flow connected in parallel system [5].

3. Description of the test case

This chapter provides a description of the VVER-1000 reactor model for coupled neutron and thermal hydraulic calculation for MCU and ATHLET codes. The model is based on the fuel assemblies type 2M. Name of the test case is C2M5W.

The codes have their own features, therefore, in order to simplify the calculation, two models of the reactor have been developed. The first model represents the neutron characteristics of the reactor, and the second - thermal hydraulic. The detailed description is given next.

3.1. Model for the neutron calculation

The neutron model is an elemental cell of the reactor, consisting of the fuel part put into water moderator (Figure 1). During the calculation, the model is divided into 12 axial layers (10 layers in the fuel part and 2 in inlet and outlet moderator). Mirror reflection of neutrons is present only on the lateral border
of the model, at the ends is black border. The effective neutron multiplication factor \( K_{\text{eff}} \) should be equal unity and it is changed by boric acid concentration. Compatibility of NT and TH models is achieved by specifying a fixed inlet temperature to the cell (290 °C in layer \( N=0 \)). Neutron model does not account changes in fuel and cladding density, average energy per fission is considered to be constant, the same for both uranium isotopes. Description of the initial materials and the model parameters is given in Table 1. The fuel has a porosity of 95%, the central hole and the gap between the cladding and the fuel is not considered. Nominal power is equal to 19.6319 MW (average power of the fuel assembly) [6].

![Image of VVER-1000 neutron model](image)

**Figure 1.** Neutron model of VVER-1000 (mm).

### Table 1. Characteristics of materials for MCU first iteration [6-11].

| Material          | Composition (mass fractions)                                      | \( \rho, \text{ g/cm}^3 \) |
|-------------------|-------------------------------------------------------------------|-------------------------------|
| UO\(_2\), 1.6 % \(^{235}\)U | \(^{235}\)U – 1.4104 %, \(^{238}\)U – 86.7411 %, O – 11.8484 % | 9.445                         |
| \(^{90}\)Zr, 1% \(^{93}\)Nb (\(\Theta\)-110) | 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% | 6.550                         |
| 7g (H\(_3\)BO\(_3\)) /kg (H\(_2\)O) | H – 11.1577 %, O – 88.7455 %, B10 – 0.0178482 %, B11 – 0.0789902 % | 0.7136                         |

### 3.2. Model for the thermal hydraulic calculation

Simplified fuel assembly is used as a TH model, which is a channel with a heat-generating structure. Real geometric dimensions are considered. Layering is the same as for the neutron calculation. Materials of rod endings are not considered. The channel simulates fuel assembly from the top of the bottom support plate to the top of the fuel rod stopper. Fuel assembly contains 312 fuel rods, 18 guide channels and a central channel (Figure 2). All the required dimensions are given in Table 2.

The heated part is located at a distance from 0.119 to 3.819 from the top of the bottom support plate. Entering flow rate is 100 kg / s. The initial temperature is 290 °C. Inlet pressure is 162·10^5 Pa. Table 1
gives the main characteristics of the model materials. It should be noted that the code does not consider the impact of boron on the moderator properties.

![Figure 2. Layout of VVER fuel assembly](image)

**Table 2.** The geometry of TVS-2M fuel assembly [6].

| Element title               | The distance between closer elements (mm) | The distance from the origin (mm) |
|-----------------------------|--------------------------------------------|----------------------------------|
| Top of rods stopper         | 5                                          | 4078.3                           |
| Top of reflection shield    | 4070                                       | 4070                             |
| Top of upper spacer grid    | 40                                         | 4073.3                           |
| Bottom of upper spacer grid | 214.3                                      | 4033.3                           |
| Top of heated rod part      | 3700                                       | 3819                             |
| Bottom of heated rod part   | 10.7                                       | 119                              |
| Top of lower spacer grid    | 16                                         | 108.3                            |
| Bottom of lower spacer grid | 92.3                                       | 92.3                             |
| Top of lower support plate  | 0.0                                        | 0.0                              |

### 3.2 Iterative scheme

The aim of this work is to create a test case, reflecting the physics of a real facility, which will be further used to determine the characteristics of the VVER-1000 reactor.

The iterative scheme is shown on Figure 3. The external iterative scheme is used, where transients are considered separately by each code. In fact, the transients are modeled only in TH code. Description of the calculated values and the iterative scheme is given below.
Figure 3. Iterative scheme for coupled calculation.

The input values for the MCU code are ($i = 0, 11$):
- $T_f^i$ – fuel temperature [°K],
- $T_c^i$ – cladding temperature [°K],
- $T_m^i$ – moderator temperature [°K],
- $\rho_i$ – moderator density [g/cm$^3$].

Calculated functionals (using MCU):
- $R_f^i$ – sum of fission reaction rates of $^{235}\text{U}$ and $^{238}\text{U}$ normalized per 1 fission neutron [%],
- $P_i$ – local power (i-layer) [KWt],
- $X_b^i$ – boric acid fraction [%].

It should be noted, that the local power distribution is calculated by the formula:

$$P_i = P \frac{R_f^i}{\sum_i R_f^i}$$ (1)

where $P$ - power of the entire system. This formula is valid, as the volume of fuel layers are the same, and $^{238}\text{U}$ fission rate is more than ten times smaller than $^{235}\text{U}$ fission rate. Local power calculation error obtained as the indirect calculation error:

$$\Delta P_i = \pm \left( \left( P \cdot \frac{\Delta R_f^i}{R_f} \right)^2 + \left( P \cdot R_f \cdot \frac{\Delta R_f}{R_f^2} \right)^2 \right)^{\frac{1}{2}}$$ (2)

where $\Delta R_f^i$ – error of total fission rate calculated in i-layer (equivalent to three standard deviations), $R_f = \sum_i R_f^i$ – cumulative total fission rate, $\Delta R_f$ – error of cumulative fission rate.

The distribution of local power $P_i$ [KWt] is transferred into the ATHLET input file, after that the averaged of all nodes parameters are calculated: $T_f^i$ [°C], $T_c^i$ [°C], $T_m^i$ [°C], $\rho_i$ [kg/m$^3$].

The convergence of the scheme is tested primarily on local power distribution and fuel temperatures, in addition on the effective neutron multiplication factor, coolant temperatures and densities. Iterative scheme ending parameter ($dX_i$):

$$dX_i = \frac{X_{i-1} - X_i}{X_{i-1}}$$ (3)
where $X_i$ - local characteristic in i-iteration, $X_{i-1}$ - local characteristic in (i-1) iteration. Deviation is considered relative to the previous iteration (i-1), because iterative process is aimed at specifying values. Values $dX_i$ leading to the exit from the iteration scheme are given in Table 3. Worth mentioning that all ending parameters depend on the power error ($\Delta P_i$) caused by Monte Carlo method error. Preliminary calculations show that the power error causes a variation of other parameters and the impact is higher for the higher power level.

Table 3. Values of the output parameters of the iterative scheme.

| Functional | $dX$ |
|------------|------|
| $K_{\text{eff}}$ | <0.1% |
| $P_i$ | <1% |
| $T_{f_i}$ | <0.5% |
| $T_{c_i}$ | <0.5% |
| $T_{m_i}$ | <0.5% |
| $\rho_i$ | <0.5% |

Coupled calculation scheme:
1. ATHLET: Calculation on a small power level (for example, 3% of nominal) $\Rightarrow$ $T_{f_i}$, $T_{c_i}$, $T_{m_i}$, $\rho_i$
2. MCU: Calculation for $K_{\text{eff}}=1$ by changing the boric acid fraction $\Rightarrow$ $X_{b_i}$
3. MCU: Fission reaction rates calculation $\Rightarrow$ $R_{f_i}$
4. Calculation of local power $\Rightarrow$ $P_i$
5. Transfer of $P_i$ in the ATHLET input file
6. ATHLET: Calculation of the temperature and density of the moderator $\Rightarrow$ $T_{f_i}$, $T_{c_i}$, $T_{m_i}$, $\rho_i$
7. Transfer of $T_{f_i}$, $T_{c_i}$, $T_{m_i}$, $\rho_i$ in the MCU input file
8. Return to step 1 (with the increase of power).

4. Conclusions
In this paper is given description of the test case for coupled calculation of VVER-1000 using MCU and ATHLET codes. Detailed iterative scheme is provided, the necessary accuracy of calculations by MCU is given. Iterative scheme ending parameter is discussed. The test case will be used for cross-verification of the coupled NT and TH codes, study of the convergence acceleration technics and calculation of VVER-1000.

Expected results of calculation, such as power distribution, fuel temperature, cladding temperature, coolant temperature and density distribution, must meet the criteria set by the iterative scheme ending parameter and meet the real characteristics of the existing power plant with VVER-1000 reactor. Data for the comparison of the results can be found in sources [8, 12].

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