

COMPLEX MODELING OF VVER-1000 USING MCU-ATHLET-FLOWVISION

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Key words: Monte-Carlo, Coupled Problems, Multiphysics Problems, Engineering Computer Modeling, Iteration scheme, Power oscillations

Abstract. Nowadays modelling of physical processes is very spread in all fields of physics. It is possible because of high capacity of computing powers and capability of parallel computing. We can observe a trend to more detailed description of simulated systems and growth of calculation schemes complexity. Scientists understand that the feedback of related physical processes occurring simultaneously could have significant impact on the results of modelling and should be solved in the scope of multiphysics. That kind of problems exists in reactor physics. It is vital to perform complex modelling of processes occurring in a fuel core of a nuclear reactor, especially during the design of the next generation nuclear power plants. It is not possible to justify safety of the power reactor without complex calculations. In this paper, we proposed a test case for precise coupled neutronics-thermal hydraulics calculation of VVER-1000 reactor using MCU, ATHLET and FLOWVISION codes. MCU is a general-purpose stochastic neutron-physical code based on the Monte-Carlo method and characterized by large time of calculation, as well as CFD codes. Because of that system code ATHLET was used as a fast thermal hydraulic solver in the iterative scheme. In the end of the calculation we propose to use CFD code FLOWVISION in order to enhance the precision and verify CFD model for the further complication of the geometry. The obtained results showed oscillations of power and fuel temperature profiles. Detailed discussion is given in the article. It is assumed that the test case will be used for simulation of VVER-1000 reactor in accident-related regimes and for codes cross-verification. The obtained experience and developed coupling program (PERL script) will be used to create coupled schemes for complex modelling of generation IV nuclear reactors involving different computer codes.

1 INTRODUCTION

It is currently impossible to imagine modern engineering and construction of nuclear power installation without preliminary mathematical modeling. Analysis and research of various processes and phenomena occurring in the reactors is substantially simplified. Until recently, the process of nuclear installations modeling was limited to simple mathematical models, but with the rapid development of computer technology, it became possible to describe the simulated systems more accurately and complicate the calculation schemes.

Nuclear reactor in operation is a complex system of interacting processes. It is a very difficult issue to compile complex mathematical model describing a nuclear reactor as an integral object. In addition, often, the contribution of different processes is disregarded to some extent, so only one subject area is covered in the research, such as strength analysis, neutron-physical or thermal-hydraulic calculations. However, this is not always correct, because the feedback of related physical processes occurring simultaneously could be significant. There are a number of issues, which could be solved only in the scope of complex modeling. Coupled calculations could be done either on the basis of one calculation program, using simple physical models (BIPR, DYN3D, NESTLE, COMSOL, LOGOS), or by coupling the codes intended to simulate the processes described in different areas of physics (MCU, ATHLET, ANSYS, FlowVision). Such kind of coupling was performed before for different types of reactors [1, 2, 3].

This work is the first step in the validation of the computation scheme to simulate the steady state of the fuel rod of the reactor VVER-1000 with the neutron-physical code MCU [4] and the system code ATHLET [5]. As a simulated model was fuel assembly type TVS-2M No. 111 of the second unit of Rostov NPP.

At present, there are many software packages using various neutron codes and the system code ATHLET for modeling transient processes and emergency operation modes in reactor installations, but they all have a rather complex internal connection structure, which requires not only the creation of additional communication units, but also refinements in the control program, inside the ATHLET. To solve the stationary problem it was decided to build a relationship between the codes in order to be practically limited to using only the external communication between the codes through the input data to them, without making any changes to the internal structure of the codes. This scheme for detailed analysis of fuel assembly parameters using MCU and CFD code FlowVision [6].

At this stage, the neutron and thermal-hydraulic models of the TVS-2M of the reactor VVER-1000 were developed and the issue with the external module for coupling MCU and ATHLET was solved.

2 CODES FEATURES

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) [7]. MCU is certified in Russia for calculations of various types of reactors including VVER-1000.

To accelerate the calculation, the library for water was prepared in advance with cross-sections in the thermal region, taking into account molecular effects, the temperature range is 559 K-610 K with 0.5 K step.

It is also important to use a model of a monatomic gas in materials containing hydrogen and oxygen that do not form a water molecule. In our model hydrogen and oxygen are present in the cladding material. Otherwise, the MCU program will prepare cross-sections for water in the thermal region despite the fact that it is not there. The average time for calculation of one state (64 cores) was 55 minutes. The maximum statistical error in the local power value does not exceed 4.6% (taking into account three standard deviations in the value of the statistical error of the fission reaction rate).

Thermal hydraulic system code ATHLET (Analysis of Thermal-Hydraulics of LEaks and Transients) developed in Gesellschaft für Anlagen- und Reaktorsicherheit (GRS mbH) was originally intended for the analysis of the entire spectrum of crash conditions cases and transients in reactor installations, mainly with a water coolant, in conjunction with various three-dimensional neutron-physical programs to calculate the spatial distribution of energy release and also, with varying levels of approximation, the spatial distribution of the parameters of the coolant in the core of the reactor (right up to the assemblies). It is widely used in various types of calculations.

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.

Features of hydrodynamic code ATHLET for improved assessment, developed in GRS (Germany) and aimed at the analysis of transient and accidental conditions in reactor facilities, mostly water-cooled ones, in conjunction with a variety of three-dimensional neutron physics program (to calculate the spatial power density field distribution and spatial distribution of the coolant parameters in the reactor core up to pin-by-pin), are

widely used in different types of calculations.

Coupling the ATHLET with a neutron physics program DIN3D [8] was a pilot project. Recently during analysis of the international standard problem Kalinin-3 [9] the following complexes have been applied: ATHLET/BIPR-VVER [10], equipped with a neutron kinetic code developed by the NRC Kurchatov Institute, the coupled complex ATHLET-KIKO3D [11], developed in cooperation with Central Research Institute of Physics (Hungary). We must also mention the calculations concerning the software ATHLET-PARCS [12], applying the neutron-physics code, developed by the USA.

It is necessary to note that all the above coupled codes possess complex internal structure of links, demanding additional blocks of connection but also the further development and completion of the software ATHLET.

Taking into consideration the coupling of ATHLET with MCU code, it is possible

- 1) to calculate only the steady-state and
- 2) try to build the interconnection between the codes through entry data without changing the internal structure of the codes.

If we consider the coupling of the MCU code and CFD code (FLOWVISION) designed for three-dimension thermo-hydraulic calculations, the issues are becoming even more complex even in the steady-state with application of only external codes connection.

This is determined mostly by the time consumption of codes operation and the necessity of the iteration procedure caused by the coolant parameters feedback, influencing the distribution of the neutron flux in the model under study.

The research considers the algorithm of reducing the number of iterations for the external connection of the MCU code and CFD code.

The goal is to determine the stationary distribution of the neutron flux in the system with the fixed power of coolant (flow, pressure, temperature) as the entry condition.

The essence of the algorithm is as follows. In the first stage our project, there is only information exchange in the entry data between coupled codes ATHLET and MCU. The calculation of the parameters (of the coolant and the fuel) in the ATHLET was conducted for the averaged through the cross-section geometry of the examined structure. For example, during pin-by-pin analysis of the distribution within assembly there were used averaged control volumes through the cross-section of the assembly.

The data retrieved from ATHLET are converted via a certain software into the necessary set of data for the MCU code, which corrects the distribution of the power density in averaged volumes, and then using a special software, converts this distribution into the entry data for the ATHLET.

It is needed to note that the beginning of the iteration process can be on the conditions of a zero power, and every other iteration can lead to increasing of the power to the required value.

The whole algorithm can be constructed in such a way that ATHLET solves nonstationary problem to obtain stationary parameters at every iteration and further transfers all the necessary data to MCU, capable of solving the stationary problem.

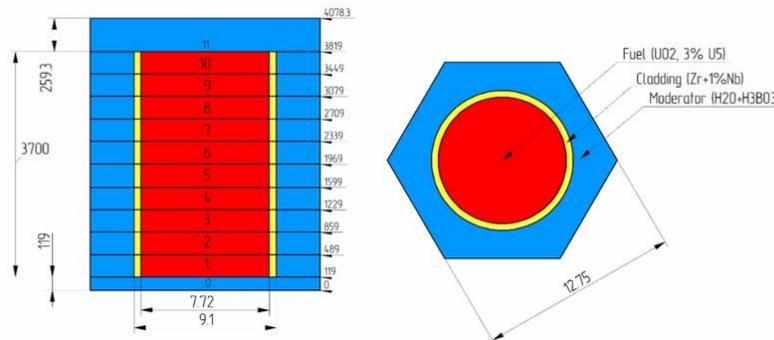


Figure 1: Fuel rod nodalization of VVER-1000 (mm)

On the conditions of a required power level there will be a shift to the detailed distribution of the parameters with the application of the coupled MCU and CFD codes, using averaged values (derived in the coupled ATHLET and MCU) as the initial parameters.

The transition from the coupled ATHLET–MCU to the coupled MCU–CFD using as an intermediate coupled MCU–sub channel code [13] will possibly provide a better approximation for the final result of the coupled MCU–CFD.

3 DESCRIPTION OF THE CALCULATION SCHEME

A detailed description of the calculation scheme is presented in work [14], initial conditions have been specified in accordance with [15].

The primary intent of this paper was to analyze the convergence of the calculation scheme, used for modeling the stationary state of the fuel assembly of the reactor VVER–1000 and create an external module for data exchange between the MCU and ATHLET. The scheme of coupled calculation was developed in such a way to maximally correspond to the state of TVS–2M No.111 of the second unit of Rostov NPP on the date 31.05.2010. The selected state is the most similar to the state of the test case. The following criteria were used to select the state:

1. The coincidence of dimensions.
2. The coincidence of material compositions (low enrichment and burnup, absence of burnable absorbers).
3. The coincidence of initial conditions (maintenance of stationary state operation of the reactor for several days).

The neutron model is an elemental cell of the reactor, consisting of the fuel part of rod and water moderator. During the calculation, the model is divided into 12 axial layers (see Fig. 1).

Simplified fuel assembly using the real geometry, represents a channel with a fuel structure is a thermo–hydraulic model. The nodalization is similar to the neutron model.

The external module is used to connect the calculation codes, written in cross–platform

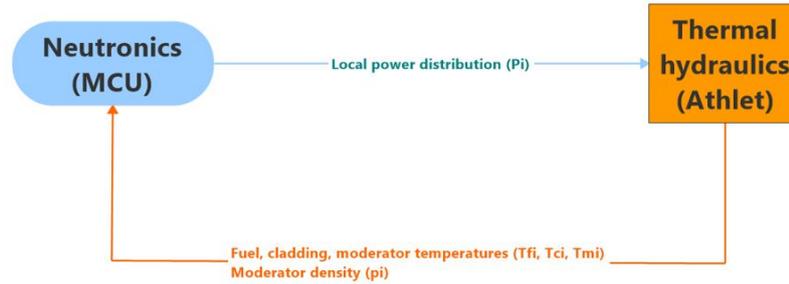


Figure 2: Coupling scheme

script language PERL. The most important features of PERL are the ability to quickly process data arrays, short code length, simplicity of implementation.

The calculation was made as follows (see Fig. 2). At the fuel assembly input, coolant parameters were maintained constant: flow rate, temperature, pressure, boric acid concentration. The first axial distribution of the coolant and fuel parameters was obtained with the zero power level using the ATHLET.

On the basis of the obtained data, the initial power distribution was constructed by MCU.

Further, it was two possible ways to solve the problem.

The initial power distribution received by the MCU was transferred to the ATHLET and was used immediately to calculate parameters at nominal power. In that case, the solution to the problem of obtaining a stationary axial distribution of the coolant and fuel elements was carried out through a nonstationary solution with ATHLET (from the previous state with zero power level), as a fact it was used the relaxation method. After receiving a new steady-state distribution of coolant and fuel rod parameters they were passed to the MCU, where it was taken into account during the calculation of the new power density distribution. The next iteration (data in ATHLET) was carried if there is no compliance of the convergence parameters, where as a parameter to monitor the convergence was selected:

$$dX_i = \frac{X_i - X_{i-1}}{X_i} \quad (1)$$

Where X_i is the local characteristic at the i -th iteration, X_{i-1} is the local characteristic at the $(i-1)$ iteration. The exit from the iterative scheme is carried out at the values dX_i , presented in Table 1.

Axial distributions of the main thermo-hydraulic parameters obtained from the calculation of TVS-2M steady-state are at the Fig. 3-7.

The convergence parameters of the obtained results at the nominal power level dont correspond to the criterion exit from the iterative scheme. The power and temperature profile oscillations begin. They could be caused by a set of effects that take place in the nuclear reactor:

Table 1: The value of exit parameters of iterative process

Parameter	dXi
Keff	<0.1 %
Pi	<1.0 %
TFi	<0.5 %
TCi	<0.5 %
TMi	<0.5 %
pi	<0.5 %

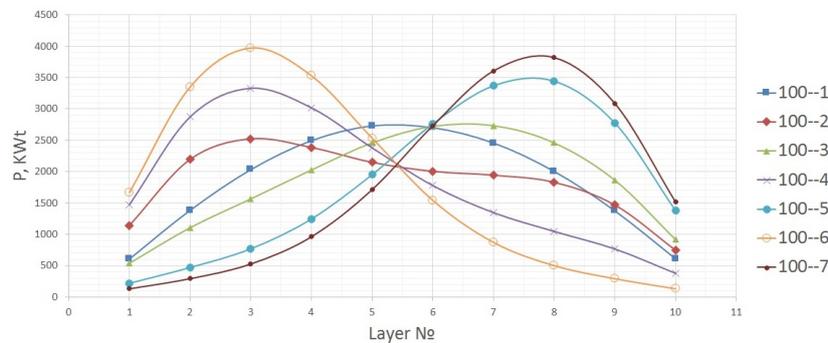


Figure 3: Power distribution (In Power-Iteration format)

- displacement of the power profile maximum to the core bottom, due to the presence of the moderator density profile and the negativity of the reactivity coefficient for the coolant temperature (appears at iteration 100-2);
- fuel temperature feedback (Doppler effect), which causes a decrease in the local power with the increase of temperature and vice versa (appears at the iteration of 100-3);
- displacement of the maximum rate of the fission reaction (and hence the power profile) to the center of the fuel rod due to the effects of leakage at the rod sides.

Also, the presence of a statistical error in calculation of the fission reaction rates may lead to the occurrence of oscillations.

Based on the obtained data, it was decided to gradually increase the power level from 0 to 100% in steps of 10% to improve the convergence of scheme. Preliminary calculations show that this approach allows to find a stable solution up to 40% of the power from the nominal level, however, with a further power jump to 100%, oscillations still arise.

Thus, according to the results, a new problem was state: to find the optimal step of the power level changing for the solution to a coupled problem (no oscillations arise, or they quickly decay) and optimizing the iterative scheme.

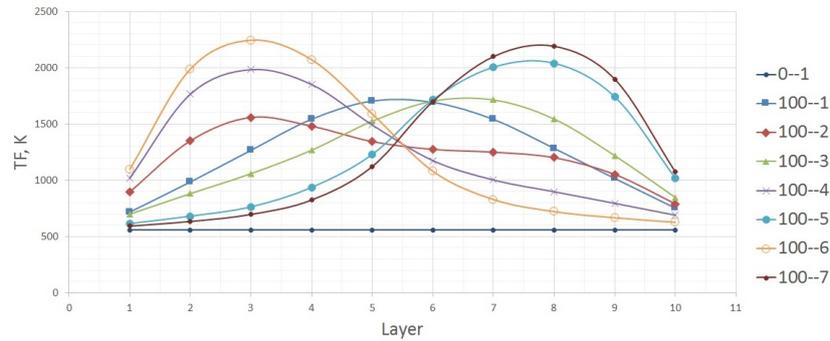


Figure 4: Fuel temperature distribution

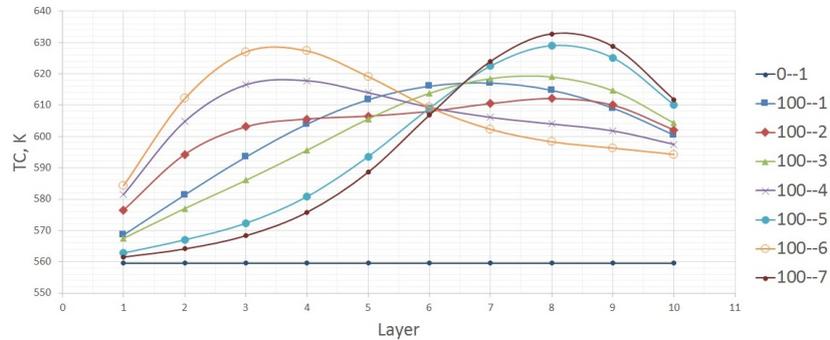


Figure 5: Cladding temperature distribution

4 CONCLUSIONS

This article presents results of the first step of the validation of the computation scheme to simulate the steady-state of the fuel rod of the reactor VVER-1000 with the neutron-physical code MCU, system code ATHLET and code FLOWVISION. As a result, the axial distributions of the main thermo-hydraulic parameters of the reactor VVER-1000 were obtained.

According to the results, it can be concluded that the solution of this problem with instantaneous setting of the nominal power level does not converge to a definite value (undamped oscillations appear). Preliminary calculation shows that a gradual increase in the power level by 10% gives a stable solution (at 40% of nominal power).

Consequently, it is necessary to determine the best step of the power increase value for the quick solution of the coupled simulation problem at nominal power.

5 ACKNOWLEDGEMENT

This work was supported by the MEPHI Academic Excellence Project (agreement with the Ministry of Education and Science of the Russian Federation of August 27, 2013, project no. 02.a03.21.0005).

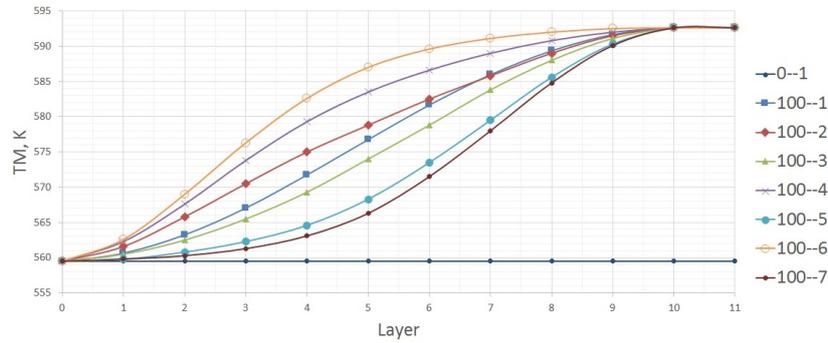


Figure 6: Coolant temperature distribution

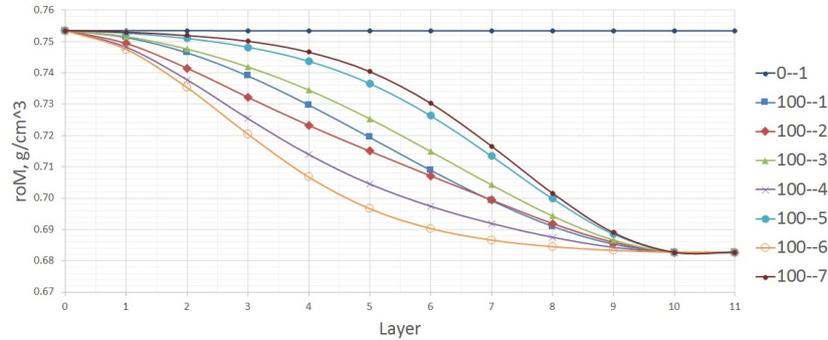


Figure 7: Coolant density distribution

REFERENCES

- [1] Sanchez, V. and Al-Hamry, A. Development of a coupling scheme between MCNP and COBRA-TF for the predictor of the pin power of a PWR fuel assembly. *Conf. on Math., Comp. Meth. & React. Phys. (M&C 2009)*, American Nuclear Society, Saratoga Springs, New York, (2009).
- [2] Ivanov, A., Sanchez, V and Imke, U. Development of a coupling scheme between MCNP5 and SUBCHANFLOW for the pin- and fuel assembly with simulation of LWR and Innovative Reactors. *Intern. Conf. on Math. and Comp. Meth. Applied to Nucl. Scienc. and Eng. (M&C 2011)*, American Nuclear Society, Rio de Janeiro, Brazil, (2011), ISBN 978-85-63688-00-2.
- [3] Waata, C.L., Shulenberg, T., Cheng, X., Starflinger, J. and Bernnat, W. Results of a coupled neutronics and thermal-hydraulics analysis of a HPLWR fuel assembly. *Proceedings of the American Nuclear Society. International Congress on Advances in Nuclear Power Plants ICAPP05*, (2005) 1:300-306.

- [4] Alekseev, N.I., Bolshagin, S.N., Homin, E.A and etc. Status MCU-5. *Questions of Atomic Science and Technology. Ser. Physics of nuclear reactors.* (2011) **14**:4–23.
- [5] Lerchl, G. and Austregesilo, H. ATHLET Mod2.2 Cycle A. *Users Manual*, GRS, (2009).
- [6] FlowVision Tutorial: Examples of typical tasks. Version 3.09.04. CAPVIDIA, Leuven, Belgium, (2014), p. 404.
- [7] Gurevich, M.I., and Shkarovsky, D.A. *Neutron transport calculation by the Monte-Carlo method on the MCU code.* Study guide NRNU MEPHI, (2012).
- [8] Grundmann, U., Lucas, D. and Rohde, U. Coupling of the thermohydraulic code ATHLET with the neutron kinetic core model DYN3D. *In: Proc. of Int. Conf. on Mathematics and Computations, Physics and Environmental Analysis*, Portland (USA), Vol. 1., (1995), pp. 257–263.
- [9] Tereshonok, V.A., Nikonov, S.P., Lizorkin, M.P., Velkov, K., Pautz, A. and Ivanov, K. *Kalinin -3 Coolant Transient Benchmark Switching-off of One of the Four Operating Main Circulation Pumps at Nominal Reactor Power*, OECD/NEA-DEC, (2008).
- [10] Nikonov, S., Pautz, A. and Velkov, K. Detailed modeling of KALININ-3 NPP VVER-1000 reactor pressure vessel by the coupled system code ATHLET/BIPR-VVER. *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C 2011)*, ISBN 978–85–63688–00–2, Rio de Janeiro, Brazil, May 8–12, (2011).
- [11] Panka, I., Hegyi, Gy., Marczy, Cs. and Keresztri, A. Uncertainties of the KIKO3D–ATHLET calculations using the KALININ-3 benchmark (phase II) data, *25th Symposium of AER on VVER Reactor Physics and Reactor Safety*, Hungary, Balatongyrk, Oct.13-16, (2015).
- [12] Pasichnyk, I., Nikonov, S., Zwermann, W. and Velkov, K. Coupled code analysis of uncertainty and sensitivity of Kalinin-3 benchmark, *25th Symposium of AER on VVER Reactor Physics and Reactor Safety*, Hungary, Balatongyrk, Oct.13-16, (2015).
- [13] Faghihi, F., Mirvakili, S.M., Safaei, S. and Bagheri, S. Neutronics and sub-channel thermal-hydraulics analysis of the Iranian VVER-1000 fuel bundle. *Progress in Nuclear Energy.* (2016) **87**:39–46.
- [14] Bahdanovich, R.B., Bogdanova, E.V., Gamtsemlidze, I.D., Nikonov, S.P. and Tikhomirov, G.V. Test case for VVER-1000 complex modeling using MCU and ATHLET. *IOP Conf. Series: Journal of Physics: Conf. Series.* (2017), 781.

- [15] Tereshonok, V.A., Ivchenkov, S.P., Nikonov, S.P., Pitilim, V.A., Sizov, R.A. and Shabunin, A.B. Offers of JSC VNIIAES according to the standard international problem for the reactor plant VVER-1000. All-Russian Scientific Research Institute for the Operation of Nuclear Power Plants (JSC VNIIAES), In. No17.1/33605 from 27.08.2015.