## MCU Code Precision Calculation of a Full-Scale VVER-1000 Model Considering Feedbacks

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**Abstract** - The paper dwells on the three problems. The first problem is development and verification of a full-scale VVER-1000 model with detailed description of geometry and material composition. Verification of VVER-1000 model was performed based on the simulation of start-up physics tests using the MCU code and on the comparison of the calculated values with the measured ones. The second problem is implementation of precision neutron-physical calculations of VVER-1000 reactor conditions at nominal power considering thermal-hydraulic feedbacks. The feedbacks on coolant density, coolant temperature, fuel temperature, and the xenon feedback were taken into account by means of the thermophysical module TPA connected to MCU. The TPA module had been developed within the framework of the MCU Project for use in the stationary condition calculations of 3D full-scale fuel assembly models with feedbacks and burnup.

# I. INTRODUCTION

A lot of attention is given to the stages of analysis and verification of safety in the process of design and commissioning of nuclear power plants. These stages include:

- calculations of neutron-physical characteristics which are important for safety using design codes;
- safety analysis;
- experimental validation of some neutron-physical characteristics, which are important for safety.

The first two stages are carried out during the NPP design, the third stage is carried out during start-up physics tests.

Unfortunately, the experimental validation of neutronphysical characteristics is limited by the technological, metrological and time frames. Therefore, a small number of measurements of the most important safety parameters are carried out during the commissioning of a NPP. In case of the adequate agreement between calculated neutron-physical characteristics and measured data, it can be concluded that:

- fuel composition in the core corresponds to the calculated ones;
- the reactor model used at the design calculations describes the real core with good precision;
- design codes will simulate the processes which take place in the core during the further operation of NPP with sufficient precision.

If the measurements on the existing NPP are difficult or impossible, the precision codes are used to verify the accuracy of design codes. Furthermore, the results of neutron-physical calculation of a full-scale reactor core by precision code are especially useful for analysis of perspective fuel cycle for which there is no operating experience.

In the past few years, there is a stable trend to attract the precision Monte Carlo codes to calculate the neutronphysical characteristics of the full-scale reactor cores considering thermal-hydraulic feedbacks. Examples of such codes include: MC21 v.6 [1], BGCore system (MCNP/THERMO) [2], MCB/FLUENT [3], Serpent 2/CFD codes (OpenFOAM) [4], and others.

# **II. DESCRIPTION OF THE ACTUAL WORK**

The work is carried out in three stages.

The first stage is a development and verification of a full-scale VVER-1000 model with a detailed description of the geometry and material composition. The VVER-1000 is a pressurised water reactor developed in Russia [5]. Power output is 1000 MWe.

The second stage is the implementation of precision neutron-physical calculations of a VVER-1000 reactor condition at a nominal power considering feedbacks.

The third stage is the calculations of 3D full-scale fuel assembly models with feedbacks and burnup.

# 1. The first stage: development and verification of a fullscale VVER-1000 model

A computer model specifying the considered system is a prerequisite for precision Monte Carlo codes calculations.

The computer model of VVER-1000 has been developed over the past few years [6, 7] using the design documentation of the fuel assemblies and the reactor facility: reports, blueprints, explanatory notes, and technical validations. Study of the effect of detail in describing some structural elements of fuel assembly (top nozzle, bottom nozzle and spacer grids) on the basic neutron-physical characteristics of the reactor core was preliminarily carried out [8].

The computer model consists of the geometry and material description of the following elements, beginning from the center: 163 fuel assemblies forming the core; a baffle; a reactor pit; a reactor vessel; and some elements of beyond vessel space.

In a fuel assembly model development, the special attention was given to the accurate specification of the

geometry and material description of fuel and control rods, spacer and mixing grids, thimble tubes, bottom and top nozzles. The model of a fuel rod consists of a cladding, fuel pellets, a spring lock, and top and bottom end-pieces.

The chemical isotopic composition of all materials used in computer model is described in detail. Information about the chemical isotopic composition of steels, alloys and other structural materials is taken from the relevant state standards, technical specifications or design documentation.

The 2D images of the computer model are shown in Fig. 1 and Fig. 2.



Fig. 1. Vertical section of VVER-1000 computer model.



Fig. 2. Horizontal section of VVER-1000 computer model.

It should be noted that the development of VVER-1000 computer model with the detailed description of geometry and material composition is complex and extremely laborious work. The input data file of VVER-1000 computer model contains about 1 million lines and has a size greater than 100 MB. The computer model is created using the KASKAD-MCU [9] interface.

The KASKAD-MCU interface is designed for automated creation of MCU [10] input file using interface library and some data obtained by means of KASKAD software package: fuel-loading pattern, control rods position, the distributions of fuel temperature and coolant parameters, etc. The interface library contains the information about the geometry and material composition of the fuel assembly and reactor facility in the form of prototype files. The KASKAD software package is typically used to design VVER fuel cycles [11]. The KASKAD-MCU interface significantly reduces the MCU calculation time by automated creation of input file, postprocessing of results, and use of the KASKAD thermophysical parameters as the initial approximation in the iterative process of taking feedbacks into account.

The complexity of the model development leads to the need of a thorough verification of the match between the computer model (geometry, material composition, etc.) and the real core.

Precision calculations of start-up physics tests using the MCU code allow comparing the measured values with the calculated ones and confirm the correctness of the computer model. In case of coincidence of these results within the limits of calculated and experimental errors, the MCU code can be used to carry out a numerical experiment. The purpose of the numerical experiment is to obtain the credible values of the important reactor safety characteristics, for which measurement is difficult or impossible. The examples of such characteristics are the pin-by-pin power density, the efficiency of control rods in the working conditions, the efficiency of control rods in the cold conditions, the efficiency multiplication factor  $k_{eff}$  for cold subcritical conditions and others.

Precision simulation of start-up physics tests for the unit 3 of Rostov NPP was carried out using the MCU code for quality test and verification of the VVER-1000 computer model. All calculations were performed by means of the HPC2 cluster. The HPC2 cluster is a multiprocessor computer cluster for parallel computing, part of the computational resources of the NRC "Kurchatov Institute" [12]. More than a hundred various reactor conditions were calculated using the MCU code. From 8 to 1000 CPU cores were used and from 80 million to 130 billion neutron stories were simulated to calculate each reactor condition.

Precision calculations of the following neutron physical characteristics were carried out:  $k_{eff}$  and the boric acid concentration in coolant for all critical conditions of the core, the efficiency of single control rods, the integral and differential efficiency of the rod cluster control assembly groups, the efficiency of the emergency protection and the reactivity coefficients.

Fig. 3 shows, as an example,  $k_{eff}$  values calculated by the MCU code.



Fig. 3.  $k_{eff}$  values for all critical conditions of the core.

The comparison of the calculated neutron-physical characteristics with the measured values was carried out. From the comparison, it can be concluded that there are slight differences in the values, which do not exceed the sum in quadrature of the experimental and the calculated (statistical) errors.

To sum up, the VVER-1000 model describes the real reactor core with good precision. The model can be used for precision neutron-physical calculations of a VVER-1000 reactor conditions to full power considering feedbacks.

# 2. The TPA module

The TPA module is the thermophysical module connected to MCU. The TPA module has been developed within the framework of the MCU Project to be used in the calculation of the stationary condition of VVER at non-zero power. TPA module is designed for iterative accounting of reactivity effects: feedback of the coolant density and coolant temperature, feedback of the fuel temperature, xenon feedback.

# A. Feedback on the coolant density and the coolant temperature

There are two options in TPA module to calculate the coolant parameters: integrated SC-1 code and the model of an isolated channel. The SC-1 code is based on the use of the 3D cellular method [13]. The cross section of the reactor core is divided into cells. Eight cells are used to describe a fuel assembly, see Fig. 4. Cells interact with each other by means of turbulent and convective cross mixing of the coolant. In the model of an isolated channel, coolant mixing between the fuel assemblies is not taken into account, and the coolant pressure is considered constant over the height of the core. At a constant pressure, the enthalpy H change of the coolant is equal to the quantity of received heat:

$$\Delta H_z = \frac{\int_0^z q(z)dz}{G} \tag{1}$$

where q(z) is the high-altitude distribution of the channel power, *G* is the coolant flow.

The transition from enthalpy to temperature *T* and the transition from temperature to coolant density  $\gamma$  are made using tables of properties of water and steam *T*(*H*),  $\gamma(T,P)$ , where *P* is the coolant pressure in the core [14].

A comparative analysis of the SC-1 code and the isolated channel model was performed [15]. Study showed that approximation of the isolated channel leads to the methodological error  $\sigma \approx 0.5$  % in the calculation of functionals of power density.



Fig. 4. SC-1 cellular partition.

#### B. Feedback on the fuel temperature

There are two options in TPA module to calculate the fuel temperature: integrated TOPRA-s code [16] and a polynomial approximation. TOPRA-s code is intended for the express analysis of thermophysical parameters of VVER fuel rods during normal operation of the reactor. The solution of the thermophysical task in 1D r-geometry is based on analytical thermophysical correlations and physical models describing fundamental processes that occur in a fuel rod during its operation and influence the temperature field in it. When using a polynomial approximation, fuel temperature  $T_{fuel}$  is determined by the equation:

$$T_{fuel} = \left(T_c + \sum_{i=1}^{5} a_i W^i\right) \times \sum_{i=0}^{3} \beta_i B^i$$
(2)

where  $T_c$  is the coolant temperature around the fuel rod, W is the power density of a fuel element, B is the burnup of the fuel element,  $\alpha_i$  and  $\beta_i$  are the approximation coefficients.

## C. Xenon feedback

In the TPA module, the spatial distribution of the equilibrium concentration of <sup>135</sup>Xe nuclei  $\rho^{Xe}$  is determined for each fissile material by the formula:

$$\rho^{Xe} = \sum_{i} \frac{(\delta_{i}^{Xe} + \delta_{i}^{I}) \Sigma_{f}^{i} \Phi}{\lambda^{Xe} + \sigma_{c}^{Xe} \Phi}$$
(3)

where  $\delta$  is the nuclide fission yield,  $\Sigma_f$  is the macroscopic fission cross section,  $\Phi$  is the neutron flux,  $\lambda$  is the exponential decay constant,  $\sigma_c^{Xe}$  is the capture cross section. Summing over all fissile nuclides is performed.

# 3. The second stage: precision neutron-physical calculations of VVER-1000 reactor conditions at nominal power

Full-scale computer models of the VVER-1000 of the units 2 and 3 of Rostov NPP and the unit 3 of Tianwan NPP (China) with the first fuel-loading pattern were developed using KASKAD-MCU interface.

In the computer models, the core is divided uniformly into 60 layers along the height. The partitioning of the core signifies that the coolant materials are unique for each height layer of a fuel assembly and the fuel materials are unique for each height layer of a fuel rod. The total amount of fuel materials in models exceeds  $3 \times 10^6$  units. Such partitioning in the materials is necessary in order to calculate the feedbacks on the temperature and density of the coolant, fuel temperature, and equilibrium concentration of xenon in the calculation of the reactor condition at nominal power. Every fuel element at each height layer is segregated into a separate tally object, which makes it possible to evaluate different functionals in the height fragments of the fuel elements.

For each model, calculations of two reactor conditions with fresh fuel were performed using the MCU code: for the lowest controllable and nominal power levels. The TPA module connected to MCU was used to take feedbacks into account in the calculation of the reactor condition at nominal power. The feedback on the coolant density and the coolant temperature was taken into account in an approximation with 163 isolated channels (one channel – one fuel assembly), partitioned into 60 layers along the height in accordance with the partitioning of the core in the computer model. The feedbacks on the fuel temperature and xenon feedback were taken into account separately for each fuel material. The spatial distributions of coolant temperature, coolant density, fuel temperature, an equilibrium concentration of <sup>135</sup>Xe obtained by means of the KASKAD software package were used as the initial approximation in the iterative procedure to take feedbacks into account. Use of spatial distribution obtained by means of the KASKAD allowed reducing the number of iterations by half and therefore the total calculation time almost halved.

All calculations were performed by means of the HPC2 cluster. 1000 CPU cores were used. The calculation time for one condition (one iteration) equals approximately 4 h when modeling  $10^{10}$  neutron histories. Total calculation time is within the range of 1 to 2 days; it depends on fuel-loading pattern.

A comparative analysis of the critical boric-acid concentration in the coolant, three-dimensional power density, coolant temperature and density, fuel temperature, and equilibrium xenon concentration, all obtained with the MCU and BIPR-7A [17] codes, was performed for all calculations. The certified two-group diffusion code BIPR-7A, which is a part of the KASKAD software package, is the basic tool for designing and validating the safety of VVER fuel cycles, and for this reason it can serve as a good tool for making checks.

The primary neutron-physical characteristics performed with both codes are close to each other, see Table 1. The largest difference of the critical boric acid concentration  $C_B$ in the coolant, calculated with the MCU and BIPR-7A codes, equals 0.07 g/kg for the unit 2 of the Rostov NPP at nominal power. The average difference equals 0.05 g/kg, which is six times less than the certified error in the BIPR-7A calculation of critical boric acid concentration. The highest relative powers of a fuel assembly  $K_Q$  are also close. The maximum difference in the calculations equals 2.5 %, and the average difference is 1.4 %. The statistical error (one standard deviation) of the MCU calculation does not exceed 0.1 % for relative power value of a fuel assembly.

Table 1. The primary neutron-physical characteristics of the core obtained by means of the MCU and BIPR-7A codes

	Power			
Parameter	lowest controllable		nominal	
	MCU	BIPR-7A	MCU	BIPR-7A
unit 2, Rostov NPP				
$C_B$ , g/kg	6.9	7.0	4.6	4.7
$K_Q$	1.41	1.42	1.21	1.23
unit 3, Rostov NPP				
$C_B$ , g/kg	9.3	9.3	6.8	6.8
$K_Q$	1.42	1.43	1.23	1.24
unit 3, Tianwan NPP				
$C_B$ , g/kg	7.0	7.1	4.8	4.8
Ko	1.36	1.34	1.26	1.23

Fig. 5 and Fig. 6 show, as an example, pin-by-pin power density in the core of the unit 3 of Rostov NPP at nominal power obtained by means of the MCU code. The dark points in Fig. 6 are the fuel rods containing the gadolinium oxide.



Fig. 5. Pin-by-pin power density in a vertical section of the core.



Fig. 6. Pin-by-pin power density in a central layer of the core.

Nevertheless, the discrepancies between the relative powers of some fuel assemblies calculated by MCU and BIPR-7A are observed for some of the reactor conditions. The discrepancy reaches 6.3 %. In addition, in the MCU calculations of the reactor condition at nominal power the peak power density is observed to shift systematically upwards relative to the BIPR-7A calculations. The height distribution of the energy release in the reactor core of unit 3 of Rostov NPP is shown in Fig. 7. The small fluctuation of the height distribution of the energy release in the MCU calculation is due to the detailed description of the spacer grids in the model. As shown in [18], a dip of energy release in the region of the spacer grid location is caused by a local change in the uranium-water ratio.



Fig. 7. Height distribution of the energy release in the core for the reactor condition at the lowest controlled (a) and nominal (b) power obtained by means of the MCU (1) and the BIPR-7A (2) codes.

# 4. The third stage: calculations of 3D full-scale fuel assembly models with feedbacks and burnup

3D infinite lattice of VVER-1000 fuel assemblies (FA) was considered [19]. Two models with different type of fuel were made:

uranium fuel of 4.4 % enrichment;

 uranium-erbium fuel of 4.4 % enrichment with 1 % wt. of Er<sub>2</sub>O<sub>3</sub>.

All FA structural elements, including top and bottom nozzle, are described as detailed as possible. The 2D images of the FA computer model are shown in Fig. 8. At the external FA borders the following boundary conditions are set: black neutron absorption at FA top and bottom ends and translational symmetry at FA flat sides.



Fig. 8. Computer model of VVER-1000 fuel assembly

In the computer models, the core is divided uniformly into 30 layers along the height.

The TPA module connected to MCU was used to take feedbacks into account. Coolant temperature, coolant

density, fuel temperature, and equilibrium concentration of xenon in each height layer are determined iteratively.

The feedback of the coolant density and the coolant temperature was taken into account in an approximation with an isolated channel (one channel – one fuel assembly), partitioned into 30 layers along the height in accordance with the partitioning of the core in the computer model. Density of the coolant above and below the fuel is set in accordance with the data on coolant temperature of FA inlet and outlet and the pressure in the core.

The feedback on the fuel temperature was taken into account using TOPRA-s code. The feedback on the fuel temperature and xenon feedback were taken into account separately for each fuel material.

The burnup was calculated using the BURNUP module [20] connected to MCU. The FA burnup was modeled at the average power level and constant boron acid concentration (4.6 g/kg).

All calculations were performed by means of the HPC2 cluster. The following Monte Carlo simulation parameters were chosen:

- the number of neutron histories for one processor core is 1.5×10<sup>6</sup> (uranium fuel) and 2×10<sup>6</sup> (uraniumerbium fuel);
- the number of processor cores is 800 (uranium fuel) and 1000 (uranium-erbium fuel);
- the total number of neutron histories is  $1.2 \times 10^9$  (uranium fuel) and  $2 \times 10^9$  (uranium-erbium fuel).

Such an amount of simulated histories provides the  $k_{eff}$  statistical error  $\sigma$  of no more than 0.003 % for uranium fuel and 0.002 % for uranium-erbium fuel, the fission reaction rate statistical error for each layer of no more than 0.4 %. Calculation time for one condition is about 70 min for uranium fuel and 100 min for uranium-erbium fuel. Total calculation time is about 2 weeks.

A comparative analysis of effective multiplication factor, power density, burnup of materials, coolant temperature and density, fuel temperature, and equilibrium xenon concentration, all obtained with the MCU and BIPR-7A codes, was performed for all calculations.

The effective multiplication factor depending on the burnup time for uranium and uranium-erbium fuel obtained by MCU and BIPR-7A codes is shown in Fig. 9 and Fig. 10. Agreement in  $k_{eff}$  is fine, the maximum difference is 0.8 %.

The power height distributions obtained by means of BIPR-7A and MCU codes are practically the same. At alltime steps the difference between MCU and BIPR-7A does not exceed 7 % for both uranium and uranium-erbium fuel, with the exception of boundary points where the power density is very small.



Fig. 9. Effective multiplication factor depending on the burnup time for uranium fuel.



Fig. 10. Effective multiplication factor depending on the burnup time for uranium-erbium fuel.

# **III. CONCLUSIONS**

In summary, we demonstrated an ability to carry out the precision calculations of some neutron-physical characteristics that are important for the VVER-1000 safety. Precision neutron-physical calculation of a VVER-1000 reactor condition at non-zero power considering thermalhydraulic feedbacks can be carried out by means of the MCU code. Calculation of a full-scale fuel assembly with feedbacks and burnup can also be carried out. The TPA thermophysical module connected to MCU is used for iterative accounting of reactivity effects: feedback on the coolant density and coolant temperature, feedback on the fuel temperature, xenon feedback. The TPA module has been developed within the framework of the MCU Project.

The use of the MCU code for independent precision neutron-physical calculations of a full-scale core can be especially useful in the elaboration of the physical part of the perspective fuel cycle design which operating experience is absent.

The results obtained on the second and the third stages were used to verify the accuracy of some design codes and to fine-tune the boundary conditions of BIPR-7A code.

#### REFERENCES

- D. GRIESHEIMER, D. GILL, B. NEASE, et al., "MC21 v.6.0 – a continuous-energy Monte Carlo particle transport code with integrated reactor feedback capabilities," *Proc. Joint Int. Conf. Supercomputing in Nuclear Applications and Monte Carlo 2013*, Paris, France, October 27–31, 2013.
- D. KOTLYAR, Y. SHAPOSHNIK, E. FRIDMAN, E. SHWAGERAUS, "Coupled neutronic thermo-hydraulic analysis of full PWR core with Monte-Carlo based BGCore system," *Nuclear Engineering and Design*, 241, 3777 (2011).
- I. KRÓLIKOWSKI, J. CETNAR, "Neutronic and thermal-hydraulic coupling for 3D reactor core modeling combining MCB and fluent," *NUKLEONIKA*, 60(3), 531 (2015).
- R. TUOMINEN, V. VALTAVIRTA, J. PELTOLA, J. LEPPÄNEN, "Coupling Serpent and OpenFOAM for Neutronics - CFD Multi-physics Calculations," *Proc. PHYSOR 2016*, Sun Valley, Idaho, May 1–6, 2016.
- H. BÖCK, "WWER/VVER (Soviet designed Pressurized Water Reactors)," *Vienna University of Technology*, Viena, Austria, September 28 (2011).
- V. DEMENT'EV, D. OLEINIK, "Monte Carlo Simulation of the Neutron Characteristics of VVER-1000 Core Using the MCU-PD Program and Comparison of the Results with Calculations by the BIPR-7A Program and Experimental Data," *Physics of Atomic Nuclei*, 74, 13, 1831 (2011).
- A. BIKEEV, M. KALUGIN, D. SHKAROVSKY, "Precision calculation using the MCU code of the energy release in the VVER-1000 core at nominal power taking feedbacks into account," *Atomic Energy*, 114, 5, 254 (2013).
- A. BIKEEV, S. MARIN, E. SUKHINO-KHOMENKO, "A comparison of the FA's models with the detailed and simplified description in the MCU code calculations," *Kerntechnik*, 78, 4, 330 (2013).

- A. BIKEEV, D. SHKAROVSKIY, M. KALUGIN, "The status of KASKAD-MCU interface," *First International Conference of the KASKAD Users Club*, Moscow, Russia, April 24-25, 2014.
- M. KALUGIN, D. OLEYNIK, D. SHKAROVSKY, "Overview of the MCU Monte Carlo Software Package," *Annals of Nuclear Energy*, 82, 54 (2015).
- M. LIZORKIN, P. GORDIENKO, M. KALUGIN, et al., "Development of codes and KASKAD complex," *Kerntechnik*, 80, 4, 314 (2015).
- 12. Multipurpose computer system of NRC "Kurchatov Institute", <u>http://computing.kiae.ru/</u>.
- L. KOBZAR, D. OLEKSYUK, Y. SEMCHENKOV, "Experimental and computational investigations of heat and mass transfer of intensifier grids," *Kerntechnik*, 80, 4, 349 (2015).
- W. WAGNER, H.-J. KRETZSCHMAR, International Steam Tables - Properties of Water and Steam based on the Industrial Formulation IAPWS-IF97, p. 389, Second edition, Springer, Berlin (2008).
- 15. A. BIKEEV, D. SHKAROVSKY, E. SUKHINO-KHOMENKO, "Results of precision calculations of three-dimensional power density in VVER-1000 core with feedbacks using MCU-PD code," 22nd Symposium of AER on VVER Reactor Physics and Reactor Safety, Průhonice, Czech Republic, October 1-5, 2012.
- 16. A. SCHEGLOV, V. PROSELKOV, "Code package to analyze behavior of the WWER-fuel rods in normal regimes of operation. TOPRA-s code," *Proc. of the Fourth International Conference «WWER Fuel Performance, Modelling and Experimental Support»*, Albena, Bulgaria, October 1–5, 2001.
- A. GOROKHOV, YU. DRAGUNOV, G. LUNIN, et al., Validation of the Neutron-Physical and Radiation Parts of VVER Designs, IKTs Akademkniga, Moscow (2004).
- S. GORODKOV, L. SHISHKOV, E. SUKHINO-KHOMENKO, "MCU calculation of spacing grid influence on FA's axial power distribution," 20th AER Symp. on VVER Reactor Physics and Reactor Safety, Espoo, Finland, September 20–24, 2010.
- S. ALESHIN, A. BIKEEV, S. BOLSHAGIN, et al., "Calculations of 3D full-scale VVER fuel assembly and core models using MCU and BIPR-7A codes," *Kerntechnik*, 80, 4, 326 (2015).
- 20. M. YUDKEVICH, "The BURNUP package of applied programs used for computing the isotopic composition of materials of an operating nuclear reactor", *Physics of Atomic Nuclei*, 75, 14, 1647 (2012).