Calculation of the numerical benchmark NURISP based on the complex MRNK + KEDR-D

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Abstract. The Kurchatov Institute developed the MRNK software package that provides the solution of the nonstationary neutron transfer equation based on the multipoint kinetics method. Currently, work is underway to improve the MRNK software package - connecting feedback on the thermophysical properties of reactor materials. To determine the thermophysical parameters, the KEDR-D program is used - a modified version of the stationary three-dimensional KEDR program for calculating non-stationary processes. The task was set to verify the MRNK + KEDR-D complex based on published data for the international numerical benchmark NURISP. The report presents the stages of achieving the goal (calculation of the stationary state of the core and comparison with the reference data; investigation of fast transient process and comparison with reference data.) In this paper, the data obtained for the MRNK + KEDR-D complex are compared with the data obtained for the Tripoli4-SubChanFlow and DYN3D-FLICA, DYN3D-SubChanFlow complexes. When calculating the steady state of the active zone, the results are in excellent agreement with the results obtained on foreign complexes. Discrepancies in temperature of the fuel and coolant, density of the coolant and distribution of energy release over the height of the assembly are minimal. When calculating the fast transient process (removal of control rods in the central fuel assembly in 0.1 s), the results are consistent with the reference data satisfactorily. There are discrepancies in the area of the greatest impacts of feedback. A comparison was made of the dependence of the temperature of the fuel and the coolant, the power change over time.

1. Introduction

Computing technology is developing rapidly in the present. This allows the use of the Monte Carlo method more widely. In particular the method is used for modeling of neutron-physical processes. The main area of application of the programs based on this method is the modeling of processes in systems with a complex structure and highly heterogeneous material composition.

The well-known MCU [1] application package is one of the developments based on the Monte Carlo method. Many programs were created on the basis of MCUs, designed to calculate the stationary processes for various reactors. MCU continues to evolve, including for simulation of non-stationary processes.

The MRNK code was developed at the Kurchatov Institute. It solves the non-stationary neutron transport equation with multipoint kinetics method [2]. The MRNK code works in conjunction with a custom module written for the MCU program. The module is used to determine Monte Carlo exchange coefficients in stationary calculations.
At the present time MRNK code is actively improving. The KEDR-D code is connected to MRNK code to take in account the thermal-hydraulic feedback [3]. The calculation of the transients is carried out under the control of a shell program MRNK + KEDR-D. The shell program controls the calculation and ensures the exchange of data between codes. As part of the work, the task of verification was set based on published data for the boron dilution benchmark NURISP [4].

The NURISP benchmark is based on the PWR MOX / UO$_2$ benchmark. It is a simplified version because the core model is smaller — 9 fuel assemblies are used instead of 193. The benchmark consists of two calculations: stationary calculation with feedbacks; non-stationary calculation - simulation of power acceleration with the introduction of a large positive reactivity.

The MRNK + KEDR-D shell program has been already tested on the PWR MOX / UO$_2$ benchmark data [5]. However, the calculation of this benchmark is highly demanding of computing resources. Moreover, the analysis of huge arrays of output data is a laborious process. Therefore, the choice of the NURISP benchmark looks more preferable for conducting multiple research calculations and analyzing their results.

The following data are presented in paper:

1. The results of stationary state calculation with using the MCU and KEDR codes for the core operating at full power. The purpose of this calculation is a preliminary verification of the models created for neutron-physical and thermal-hydraulic programs.
2. Calculation of the transient process - extracting the absorbing rods from the core, using the MRNK + KEDR-D shell program.
3. Comparison with the results of the calculation by other codes.

This work has been carried out using computing resources of the federal collective usage center Complex for Simulation and Data Processing for Mega-science Facilities at NRC “Kurchatov Institute” (ministry subvention under agreement RFMEFI62117X0016), http://ckp.nrcki.ru/.

2. Description of the benchmark NURISP
The current section describes the boron dilution benchmark NURISP [4]. The computational model is a core composed of nine fuel assemblies without jackets, which are washed by light-water coolant (figure 1). The fuel assembly is surrounded by a layer of water reflector. Axial reflectors are missing – the vacuum boundary conditions are set.

![Figure 1. The scheme of core model.](image)
All nine fuel assemblies are conditionally combined into two types. Eight fuel assemblies of the first type contain MOX fuel. One central fuel assembly of the second type contains uranium-dioxide (UO$_2$) fuel. A fuel assembly consists of inner elements, such as fuel pins, absorption rods, guide tubes and etc. They are arranged in a 17 × 17 square grid. Fuel differs in composition and enrichment within the fuel assemblies. Control rods with an absorber are only present in an assembly with UO$_2$ fuel. The height of each fuel assembly is 366 cm.

The complete calculation of the benchmark consists of two stages. At the first stage, the stationary state of the core at hot full power (HFP) conditions is calculated with completely removed absorbing rods. The parameters of the HFP are presented in the table 1.

**Table 1.** Hot state of the core at full power.

| №  | Characteristic               | Value | unit of measurement |
|----|------------------------------|-------|---------------------|
| 1  | Core power                  | 100   | MW                  |
| 2  | Mass flow rate (core)       | 739.08| kg / s              |
| 3  | Mass flow rate (Fuel Ass.)  | 82.12 | kg / s              |
| 4  | Core Outlet pressure        | 15.4  | MPa                 |
| 5  | Coolant inlet temperature   | 560   | K                   |
| 6  | Boron concentration         | 200   | mg                  |
| 7  | Insertion depth control rods| 0     | cm                  |

After verifying the prepared models, the transient calculation can be performed. The transient process is a complete extraction of the rods in the central fuel assembly at a constant speed in a time of 0.1 s. Such a change in the properties of the system leads to an increase in the reactivity of the core beyond the effective fraction of delayed neutrons. This leads to a rapid acceleration of power on prompt neutrons.

The transient calculation consists of two steps. The first step of transient calculation is the determination of critical boron at the hot zero power (HZP) conditions. The HZP parameters differ from the parameters of the previous stage (HFP) - the control rods are induced by 232.433 cm and the initial power output is reduced to 1 W. After that, at second step, the calculation of the transient process is carried out.

The verification of results is carried out on the basis of the reference data calculated by neutronic codes Dynamic Tripoli 4 [7] and DYN3D [8]. In the Dynamic Tripoli 4 code the direct Monte Carlo method for modeling of neutron kinetics is used, and the DYN3D program is based on a two-group diffusive method. For accounting of feedback the thermal-hydraulic SubChanFlow [9] and FLICA codes were connected to neutronic codes.

**3. Brief description of used codes**

The MCU and KEDR programs were used to calculate the steady-state state of the core, taking into account feedbacks on the thermophysical properties of materials. Their interaction was carried out according to the iterative scheme described later in the current paper. The MLE generator was used to prepare the model for the MCU program. Pre-created software modules were used for conversion of input and output data.

**3.1 MCU**

The MCU program is designed to simulate neutron transfer processes using analog and non-analog Monte Carlo methods [10]. The program works on the basis of estimated nuclear data in systems with
three-dimensional geometry, taking into account changes in the isotopic composition of materials. The program allows solving a neutron transport equation (criticality problem) with modeling of neutron transport.

### 3.2 MLE

The NURISP benchmark model was created on the basis of the MLE (MCU Language Expander) software module, specially designed to reduce the complexity of the following tasks: preparing the input data for the MCU model; assignment of a grid for partitioning geometric regions into subregions; processing the calculation results. The program has an input data language similar to the MCU language. Additional operators are introduced for dividing of geometric regions.

### 3.3 KEDR, KEDR-D

The KEDR program is designed to solve the stationary problem of heat transfer in fuel assemblies with a regular arrangement of fuel pins. The canal (cell-by-cell) method is used to determine the thermal-hydraulic parameters. The heat transfer problem is written by following equations:

- One-dimensional equations of conservation of mass, momentum and energy for a homogeneous steam-water mixture and hydraulic cells.
- Two-dimensional heat equation for fuel rods.
- Conditions for coupling at the fuel-water boundary.

The solution of the above equations is carried out on the basis of a finite-difference scheme. [3]

The KERD-D program was created on the basis of the KEDR program and is used to solve the non-stationary conjugate heat exchange. The heat transfer problem is modeled on the basis of the same equations as in KEDR, recorded in non-stationary form.

### 3.4 MRNK

MRNK (Multi-Region Neutron Kinetics) is a code under development. It is used to solve the nonstationary neutron transport equation by the multipoint kinetics method. The MRNK software package works in conjunction with a custom REC module [6] written for an MCU program. The module is designed to calculate the exchange coefficients.

### 3.5 MRNK + KEDR-D shell program

MRNK code is connected with the KEDR-D code for the calculation of non-stationary processes, taking into account feedback on the thermal-physical properties.

The integration of programs is carried out under the control of the program shell, which ensures the launch of programs, control over calculations, data exchange, generation of options for the MCU-TR program, checking the convergence of parameters, processing results, etc. The shell is optimized for calculations on the supercomputer of the Research Center Kurchatov Institute.

### 4. The steady state calculation

#### 4.1 Description of MCU model

An MCU source data model was prepared in the MLE generator format for calculating the stationary state of the core in accordance with the benchmark description. The fuel region of each fuel rod was divided into 30 axial zones to calculate the spatial energy release. The domain of water coolant in each fuel assembly was divided also into 30 layers. The fuel temperature was considered to be the same within the axial fuel layer (a combination of 264 fuel zones in the altitude of the fuel assembly).

The result of the calculation is the distribution of energy release in the fuel zones and the value of the effective multiplication factor.

#### 4.2 Algorithm of stationary state calculation
The iterative calculation algorithm for MCU and KEDR programs is presented in figure 2 in the form of a block-scheme. The calculation begins with the preparation of a model of initial data for the MLE generator. After the variant is generated by the MCU program, the $K_{\text{eff}}$ and the power release ($W$) for the first iteration are determined. Next, the output data of the MCU is converted into the input data format of the KEDR program. In the calculation under the KEDR program, axial distributions are determined for each fuel assembly for the following parameters: fuel temperature ($T_{\text{fuel}}$), coolant temperature ($T_{\text{water}}$) and coolant density ($\rho_{\text{water}}$). After that, the convergence is verified for each parameter $K_{\text{eff}}$, $W$, $T_{\text{fuel}}$, $T_{\text{water}}$ and $\rho_{\text{water}}$. If the parameters are converged, then the calculation ends. Otherwise, the calculation of next iteration is carried out with the adjustment of the material composition in the initial data of the MLE program. Such a cycle is repeated until a stable solution is obtained, determined by the convergence in temperatures and power.

**Figure 2.** Algorithm of iterative calculation using MCU and KEDR programs.

4.3 Comparison with reference data

Reference data are used to verify the obtained data - the calculation results for the Tripoli4-SubChanFlow and DYN3D-FLICA. The effective multiplication factors and various distributions in the central channel are compared.

In MCU+KEDR-D calculation five iterations were provided to achieve stable results. According to the effective multiplication factor, the percentage deviation of the MCU-KEDR ($K_{\text{eff}} = 1.01949$) from
Tripoli4-SubChanFlow (\textit{K eff} = 1.018) is 0.62\%, and the MCU - KEDR from DYN3D-FLICA (\textit{K eff} = 1.0828) is 2.36\%.

Figure 3 shows the results of axial power distribution for central fuel assembly calculated by all three codes. It is clear that the greatest match for MCU-KEDR is achieved with the Tripoli4-SubChanFlow. At the peak of power distribution the deviation is 1.85\%.

**Figure 3.** Distributions of energy release in height, obtained by MCU-KEDR, Tripoli4-SubChanFlow and DYN3D-FLICA.

Comparison of coolant temperature axial distributions is shown in figure 4. As in the previous figure, we see that the results best fit with the Tripoli4-SubChanFlow. The maximum percentage deviation is achieved at a height of 67 cm - 0.27\%.

**Figure 4.** The temperature profile of the moderator in the central fuel assembly at hot full power by MCU-KEDR, Tripoli4-SubChanFlow and DYN3D-FLICA.
When comparing the results with the DYN3D-FLICA, the maximum percentage deviation is achieved at a height of 92 cm and takes the value of 0.77%.

The results of the calculation of the stationary state of the core are in good agreement with the reference data for the calculations given in the benchmark description. The best results coincide with a Tripoli4-SubChanFlow, in which neutron-physical processes are modeled based on the Monte Carlo method. Deviation from the results of this code is not significant.

Thus, according to the results obtained, it can be argued that the input data models for the MCU and KEDR programs were created correctly. Moreover, the iterative calculation algorithm for the MCU and KEDR programs was successfully verified using the benchmark data.

5. Calculation of the transient process

5.1 Results of preparing the model for non-stationary calculation
The transient process starts at HZP. The control rods were lowered by 232.433 cm. The critical boron concentration was obtained before the non-stationary calculation with MCU code. The concentration was determined using two previous iterations based on linear extrapolation.

The MRNK model was also tested. The initial state of the core was calculated using the MCU and MRNK programs. The graphs of the axial power distribution in the central channel are shown in figure 5. The calculation results are completely the same.

![Power distribution, MW](image)

**Figure 5.** The power profile in the central fuel assembly calculation by MCU and MRNK

5.2 Analysis of the results
The power evolution, the change of rods immersion and the reactivity are presented in figure 6. On the graph, the reactivity is measured in relative units and was found by the formula (1):

$$\rho = \frac{K_{eff} - 1}{K_{eff}}.$$  \hspace{1cm} (1)
Figure 6. The results of the calculation of changes in the power of the core, the position of the rods, the reactivity in time according to the program MRNK + KEDR-D.

The power evolutions in time calculated by MRNK + KEDR-D, DYN3D-SubChanFlow, Tripoli4-SubChanFlow and DYN3D-FLICA are shown on figure 7. At the stage of increasing the power release, the graph obtained from the MRNK + KEDR-D program coincides with DYN3D-SubChanFlow. Further, the codes showed some differences in peak power. But after 0.1 seconds, the power change obtained from MRNK + KEDR-D coincides with the power behavior by DYN3D-FLICA.

Figure 7. Power change over time, obtained by MRNK + KEDR-D, DYN3D-SubChanFlow and Tripoli4-SubChanFlow.
6. Conclusion.
Thus, in the course of the work, the numerical NURISP Benchmark was calculated by the MCU-KEDR and MRNK-KEDR. The reference data was preliminary obtained with DYN3D-SubChanFlow, Tripoli4-SubChanFlow and DYN3D-FLICA codes and were used for comparison of results.

The results of the calculation for steady-state are in good agreement with reference results. The results best coincide with Tripoli4-SubChanFlow, in which neutron-physical processes are modeled via the Monte Carlo method. The deviations of results are not significant.

Thus, according to obtained e results, it can be argued that the input data models for the MCU and KEDR programs were created correctly. Moreover, the iterative calculation algorithm for the MCU and KEDR programs was successfully verified using the benchmark data.

The obtained results of the transient process are closest to the data obtained using the DYN3D-SubChanFlow programs. During the growth of power, the results coincide, but, with the inclusion of feedback, there are discrepancies in the region of the power peak. It can be explained by the difference in thermal-hydraulic programs.

References
[1] Alekseev N I, Bolsagin S N, Gomin E A, Gorodkov S S, Gurevich M I, Kalugin M A, Kulakov A S, Marin S V, Novoseltsev A P, Oleinik D S, Pryanichnikov A V, Sukhino-Khomenko E A, Shkarovsky D A and Yudkevich M S 2011 MCU-5 status problems of atomic science and engineering Ser: Phys. of Nucl. Reactors Issue 4 (Russia: Moscow) pp 4 – 23
[2] Ioannisian M V 2012 Calculation of coupling coefficients for the equations of multipoint kinetics Problems of Atomic Science and Engineering. Ser.: Physics of Nuclear Reactors Issue 1 pp 27-33
[3] Ioannisian M V and Zakirov C Yu 2017 Verification calculations of the test problem and benchmark PWR MOX / UO2 using the method of multipoint kinetics. Proceedings of the conference of young professionals “Innovations in nuclear power” pp 23-24
[4] Bart L S, Hoogenboom J E, Escalante J J and Espinoza V S 2015 Coupling of dynamic Monte Carlo with thermal-hydraulic feedback. Annals of Nuclear Energy 76 27–39
[5] Kozlowski T and Downar T J 2006 The PWR MOX/UO2 Core Transient Benchmark Final Report, NEA/NSC/D0C
[6] Ioannisian M V 2018 Determination of Neutron Flux by Multi-Point Kinetics Method Problems of Atomic Science and Engineering Ser.: Physics of Nuclear Reactors Issue 1 pp 10-23
[7] Trama J C, Petit O, Dumonteil E, Hugot F X, Lee Y K, Mazzolo A and Diop C 2007 Review of the TRIPOLI-4 Monte Carlo Code ICAPP 07 (France: Nice Acropolis)
[8] Grundmann U, Rohde U, and Siegfried M 2000 DYN3D – Three Dimensional Core Model for Steady-State and Transient Analysis of Thermal Reactors (USA: Pittsburgh) pp 7 – 11
[9] Vazquez M et al 2012 Coupled neutronics thermal-hydraulics analysis using Monte Carlo and sub-channel codes Nucl. Eng. and Design 250 pp 403–411
[10] Bell G J and Glesston S 1970 Nuclear reactor theory (USA) pp 44-6