TANDEM Program for Parallel Computing of Coupled Neutron-Physical and Thermal-Hydraulic Characteristics of Reactor Cores

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Abstract. *Full-scale physical computing of reactor lifetime includes three types of computations: computing of neutron-physical parameters of the core, computing how nuclide composition of fuel changes with time due to fuel burnup, and thermal-hydraulic computations. For solving the problems of ionizing radiation transfer using the Monte-Carlo method, RFNC-VNIITF has developed the constantly-improving PRIZMA program. The RISK module is used to calculate how nuclide composition of reactor fuel changes with time due to this fuel burnup. Different CFD programs for computing of thermal-hydraulic characteristics of different-type reactor cores are considered. All three types of computations are interrelated. The paper describes the technology used to provide parallel computing of coupled neutron-physical and thermal-hydraulic characteristics of different-type reactor cores with due regard to the core materials temperature-and-density feedback. Such coupled computations preformed for the cores of the BREST-type, VVER-1000, and VVER-1200 reactors demonstrate that the state-of-the-art computer systems can be used to compute thermal-hydraulic characteristics of reactors with the help of neutron-physical characteristics evaluated using the methods of statistical modeling.*

Key words

Neutron-physical characteristics, PRIZMA, thermal-hydraulic characteristics, CFD codes, parallel coupled computations, TANDEM.

1 Introduction

In the near future, the main problems facing atomic energy industry of the Russian Federation are to provide the high-level security of atomic power plants, as well as to maintain the achieved level of electric-power production and insure its follow-on increase. Different RF institutions conduct R&D activities aimed to develop and implement the up-to-date reactors with intrinsic security, in which severe accidents involving the damage of reactor core fuel are impossible [1].

The core (Fig.1, left) is the main part of nuclear reactor, in which nuclear fuel is concentrated and both the chain fission reaction, and the energy release occur. Nuclear fuel is generally placed inside the fuel elements, and there can be many tens of thousands of such elements inside the core. At the end of their lifetime, fuel elements are taken out, in full or in part, and replaced by the new ones. For ease of loading, the fuel elements are got together into separate bundles (several tens or hundreds of fuel elements in each bundle) that are called fuel assemblies (Fig.2, right).

Coolant, namely water, liquid metal, or carbon dioxide gas, is pumped through the core. This coolant flows around the fuel elements and takes away the heat released in these elements that is later converted into electric energy.

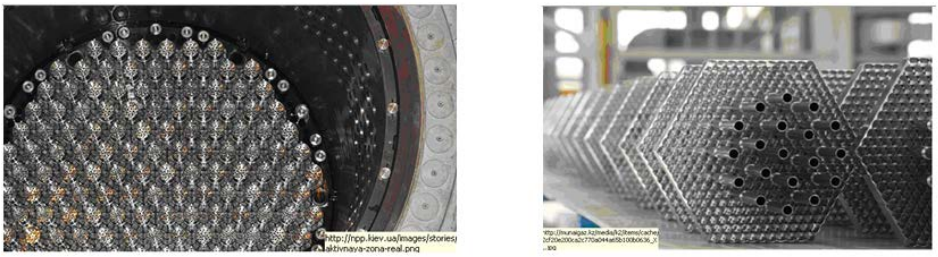

Fig. 1. Reactor core (left) and fuel assembly with a bundle of fuel elements (right).

2 Reactor lifetime computation

Full-scale physical computing of reactor lifetime includes three types of computations, namely:

- Computation of neutron-physical parameters of the core, which includes determination of the spatial, energy and angular distribution of density of gamma-neutron radiation flux in reactor at every instant, as well as evaluation of functionals (rates of different nuclear reactions) found based on this distribution in the course of solving conditionally critical problem for transfer equation;
- Computing how nuclide composition of reactor fuel changes with time due to fuel burnup;
- Computation of thermal-hydraulic characteristic of reactor core, which includes determination of spatial distribution of fuel temperature and density inside the fuel elements, as well as the temperature, density, and pressure of coolant and the coolant flux rate with due regard to possible deformation of fuel and jackets of these fuel elements under the effect of thermoelastic stresses.

The programs based on the Monte-Carlo method are used for precision computations of neutron-physical parameters of reactor core. Due to their capability to practically precisely simulate the geometry of 3D systems having complex heterogeneous structure, the error in computations performed with the help of these programs depends mainly on the quality of nuclear data libraries that are used [2]. This method has an additional advantage, i.e. high-level paralleling of computational process when using up-to-date multiprocessor complexes. For solving the problems of ionizing radiation transfer using the Monte-Carlo method, RFNC-VNIITF has developed the constantly-improving PRIZMA program [3,4]. The RISK module is used to calculate how nuclide composition of reactor fuel changes with time due to its burnup [5]. Fig.2 shows combinatorial 3D model of theVVER-1000 reactor core, which is used in the PRIZMA program computations.

Both the PRIZMA and the RISK programs are written in C++ language; they operate under the control of Linux operational system. In parallel mode, the MPI library is used.

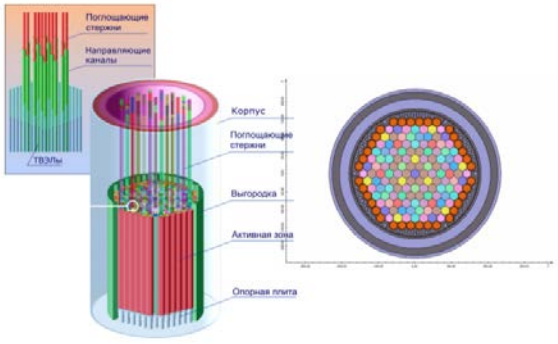

Fig. 2. Combinatorial 3D model of VVER-1000 reactor core.

The PRIZMA program computes neutron-physical parameters of reactor core using the data on spatial temperature distribution (Fig.3), as well as the data on coolant density, which are obtained by computing the thermal-hydraulic characteristics. In thermal-hydraulic computations the energy release considered as a thermal load is determined for each fuel element in the fuel assembly, and depends on the core height and the fuel element radius. Radiation energy release is computed using the PRIZMA program.

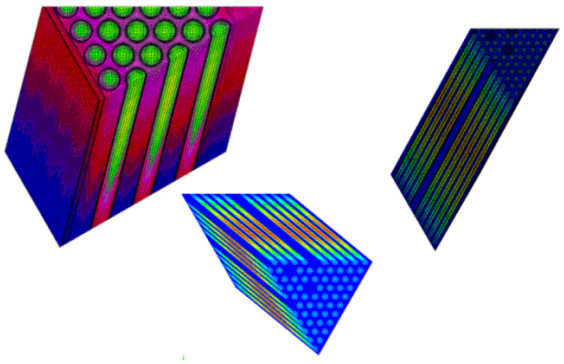

Fig. 3. Spatial distribution of temperature in the fuel assemblies for different types of reactors.

Nowadays, there are a lot of programs with different capabilities allowing for computation of thermal-hydraulic characteristics of reactor core. All these programs use mesh methods for solving partial differential equations, i.e. the finite-difference method or the finite-element method.

The following programs were considered for computation of thermal-hydraulic characteristics of reactor core:

- The CONV 3D program developed at IBRAE, RAS [6];
- The open integrated platform OpenFOAM used for numerical simulation of continuum mechanics problems [7].

Thermal-hydraulic computations were performed both in uniprocessing, and in parallel mode.

All three types of computations are interrelated. This means that there is a feedback between the changes in neutron-physical, thermal-hydraulic characteristics of reactor core and nuclide composition of fuel. Thus, spatial distributions of neutron flux density, together with energy release distribution related thereto, depend on both the fuel nuclide composition, and the coolant temperature and density distribution. In its turn, the temperature distribution in reactor core is determined by the energy release distribution in this core and the coolant speed. At that, even if reactor power is kept at a constant level, during reactor lifetime, these distributions undergo changes both due to the fact that the burnup of fissional nuclides in the fuel is ununiform throughout the core, and due to the movement of elements that control nuclear reactivity.

3 Technology for coupled computations

In this connection, there emerged a need to develop a technology that would allow for coupled computations of the neutron-physical and thermal-hydraulic characteristics of different-type reactor cores for with due regard to the core materials temperature-and-density feedback.

For the purpose of data exchange between the CFD programs and the PRIZMA program, the coupling program module called TANDEM module was developed; which operates in the distributed mode. The coupling module is written in C# language and has several modes. In some modes, this module simultaneously process data for all the fuel assemblies; in other modes, it performs this operation only for a particular fuel assembly. This permits the data exchange between the distributed computations of thermal-hydraulic characteristics and parallel computations of neutron-physical characteristics. Besides, while preparing data for transfer, the coupling module can save information (if specified in the input data) on the calculated temperatures and densities in files having special formats for the purpose of further processing and plotting.

The script for bash standard interpreter of Linux system was developed for coupled computations. This script represents a multistage process that allow us to start up the programs for coupled computations both in parallel mode, and in distributed mode using computational servers. The program start-up is described independently for each program. The script includes the start-up parameters checkout, the preparation of files and directories that are needed for computations, and the control of return codes for programs that are started up. Standard output of errors of all commands started up using the script is redirected either to the standard output of script errors, or to special files. In case any of the programs returns the code corresponding to the error, the error massage is displayed and the entire complex is shut down.

Coupled computations represent an iterative process (Fig. 4). After each iteration, the coupling module decides whether to complete computations based on the data on mesh node temperatures obtained during the current and previous iterations. The temperature difference in the appropriate mesh nodes is estimated; and if this difference is less than that specified in the input data of the coupling module, the computations are considered to be completed.

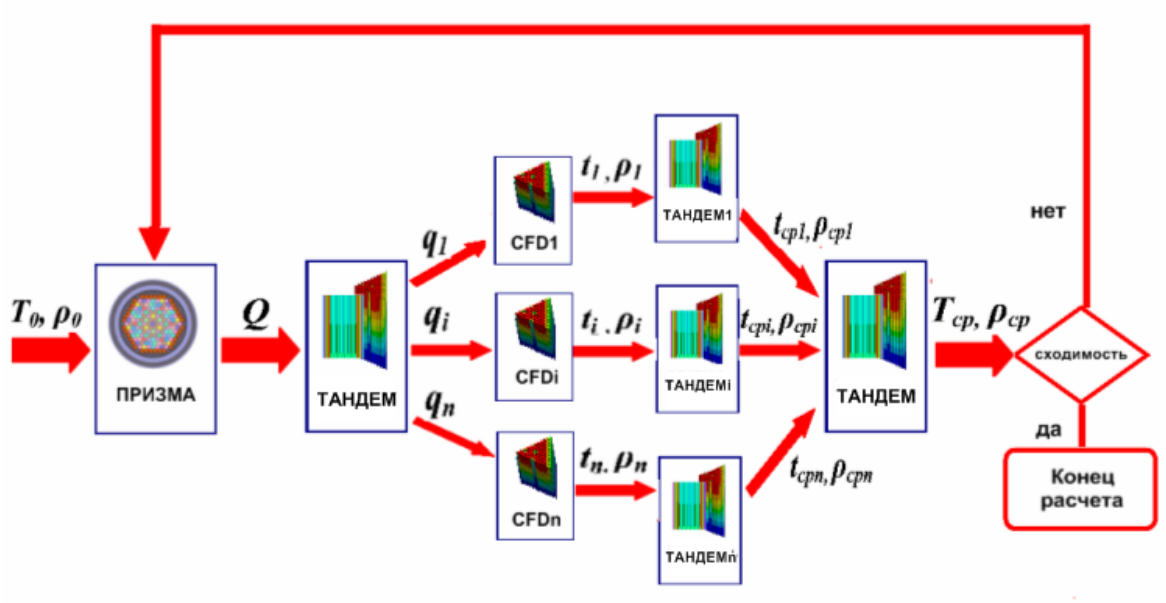

Fig. 4. Schematic representation of coupled computations technology.

When developing technology for coupled computations, first of all, we have to take into account the fact that input data are specified differently in the PRIZMA program and in the programs for thermal-hydraulic computations.

Thus, the PRIZMA program describes the full-scale 3D reactor model including the core, the fuel assembly support, and the space above this core. The model is described by combinatorial set-theoretical method in PRIZMA format (Fig.5).

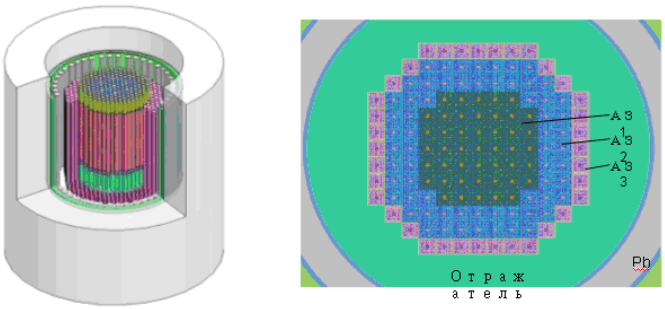

Fig. 5. Combinatorial 3D model of the BREST reactor core.

Thermal-hydraulic computations consider only the reactor core. Fuel assembles of different configurations can be placed there. That is why several thermal models of fuel assemblies are constructed. At that, in case fuel assemblies are rotation-symmetric ones, the thermal model is constructed only for one symmetric part. The target meshes of finite elements are constructed based on model geometry (Fig.6). All the data prepared for each fuel assembly configuration are saved in appropriate catalogs both in text, and in binary format.

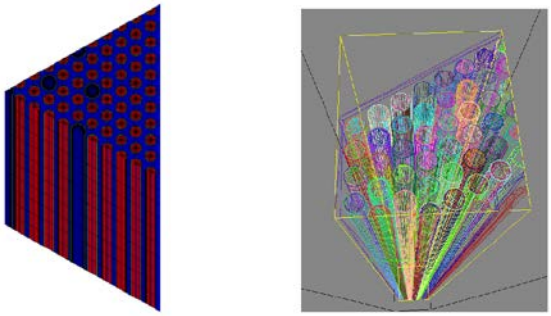

Fig. 6. Mesh models of 1/6 VVER-1000 reactor fuel assembly (left) and 1/4 BREST reactor fuel assembly (right).

Another feature of coupled computations is that the CFD codes compute temperature and density in the mesh nodes while the PRIZMA complex utilizes computations by Monte-Carlo method and thus, computational meshes are not used in this complex. For mesh data reception, the PRIZMA program has a capability to receive data from particular intervals along the height of computed model. Therefore, it was decided to divide reactor zone into the intervals ('layers') along its height and to exchange data computed for each layer. Thus, the average temperature and density for each fuel assembly in every layer is found using the temperature and density data calculated by thermal-hydraulic program; and these averaged data are transferred to the appropriate layers of the PRIZMA program regions. In a similar manner, after the energy release is computed using the PRIZMA code, all cells of the thermal-hydraulic program mesh, which are located in particular layer, are assigned the value of energy release from the appropriate PRIZMA layer. Data exchange is performed using files.

Besides, it should be taken into account that the PRIZMA program computations cover the entire core, while the thermal-hydraulic computations are performed in the distributed mode for each fuel assembly because at this moment they can't cover the entire reactor core since the mesh is too large in size.

Thus, correct computations require the programs that have coordinated description of geometric objects in the same system of coordinates. In the absence of this coordination (for example, the axial displacement of objects, another arrangement of coordinate axes), appropriate information is specified in the input data of the coupling module.

The TANDEM coupling module should coordinate the measurement units of physical quantities used in different programs, as well as should ensure the single-valued correspondence between the system parameter values (i.e. temperature, density, and specific power of energy release) calculated in the mesh nodes of thermal-hydraulic program and the parameter values computed in the system partition regions (whereto these nodes belong) using the program based on Monte-Carlo method.

All geometric objects in the PRIZMA program are located in appropriate regions. In order to bring to correspondence the geometric objects of both the CFD codes, and the PRIZMA program, the functions written in C++ were developed on the basis of *Geom* library (the PRIZMA program), which are used to determine whether the node from CFD code belongs to the reactor zone region of the PRIZMA program.

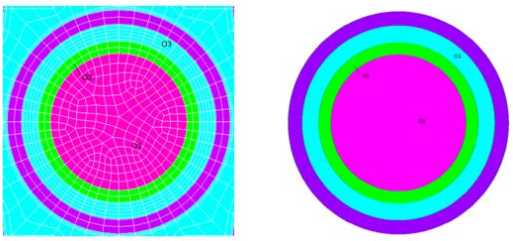

Fig. 7. Correspondence between the regions in channel specified in the CFD (left) and PRIZMA (right) programs.

4 Data transfer for coupled calculations

Data transfer for the coupled computations of the neutron-physical and thermal-hydraulic characteristics of different-type reactor cores taking into account the core material temperature-and-pressure feedback is performed on a step-by-step basis.

Stage I

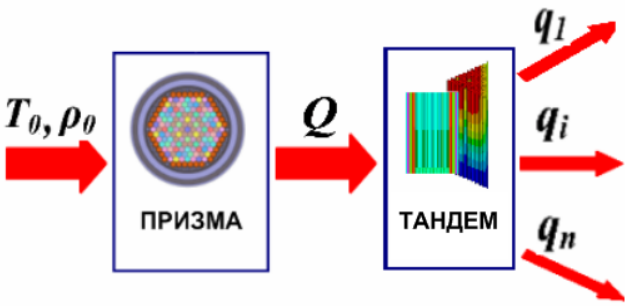

Fig. 8. Transfer of the energy release data.

Thermal-hydraulic computations use the radiation energy release determined with the help of the PRIZMA code as a thermal load. The PRIZMA code calculates energy release in each layer for each fuel assembly. A coupling module for all thermal model cells, wherein centers of these cells are found in a certain layer of each fuel assembly, specifies values of energy release from the appropriate layer (Fig.8). For this purpose, the energy-release rate density is calculated at the point in the *i-th* spatial element (layer) of the fuel assembly according to the formula:

$$q_i = \frac{W}{V_i}\frac{Q_i}{\sum_k Q_k},$$

where W – thermal power of the reactor, V_i- fuel amount in the i-th layer of a fuel assembly, Q_i – energy release for a fuel assembly in the i-th layer, $\sum Q_k$ - total energy release of the reactor over all fuel assemblies. Calculation is performed only for the layers with fuel assemblies. So, for all cells of each fuel assembly being in one layer, the energy-release rate density will be the same.

Stage II

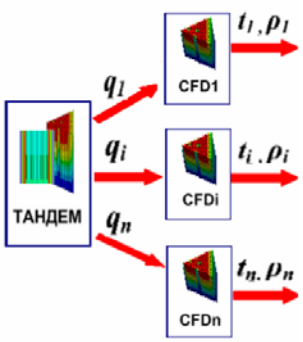

Fig. 9. Data transfer for the thermal-hydraulic calculations.

Thermal-hydraulic calculations are performed in the distributed mode for each fuel assembly (Fig.9). The coupling module makes catalogs whereto the data needed for the thermal-hydraulic calculations are entered. Here, location of different-configuration fuel assemblies in accordance with the specified cartogram of the reactor core is taken into account.

The number of catalogs depends on the number of fuel assemblies constituting the reactor core. The energy-release data calculated with the help of the PRIZMA code and converted by the coupling module are also entered in the appropriate catalogs. The temperature field of the design is determined based on the calculated energy release in the fuel. These computations are performed with the help of the selected thermal-hydraulic program and can go both in uniprocessing, and parallel modes.

Results of the thermal-hydraulic calculations (values of steady-state temperatures and densities in each node of the finite-element model with coordinates x, y, and z) for each fuel assembly in the text format are transferred into the coupling module that forms the temperature and density data for all regions and layers of a particular fuel assembly.

Stage III

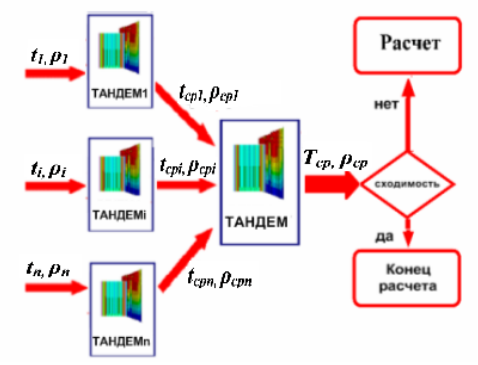

Fig. 10. Data transfer for the PRIZMA code calculations.

After the steady thermal-hydraulic state is calculated for all fuel assemblies using the CFD code, the coupling module performs the test for convergence. The temperature difference in appropriate mesh nodes is determined at the current and previous iterations of the coupled calculation. If this difference is less than that specified in the input data of the TANDEM program, the calculation is considered to be completed. Otherwise, the coupling module forms the input data to calculate the energy release by the PRIZMA code using the coolant temperature and density, both calculated by the CFD code (fig.10). The coupling module processes the temperature and density data in two stages.

At the first stage, the TANDEM program is started up in the distributed mode and processes the temperature and density data calculated for each individual fuel assembly. It coordinates description of geometrical objects of codes in the same system of coordinates.

For each layer in each PRIZMA region, the coupling module accumulates information on cells that are included in the given layer and belong to the CFD code model and also forms information on the coolant temperature and density for all regions and layers of a particular fuel assembly. All the values are converted into the system of units accepted in the PRIZMA code and the average temperature and density in the layer are calculated for each layer of each PRIZMA region according to formulas:

$$T_{cp} = \frac{\sum_{i=1}^{n} T_i P_i V_i}{\sum_{i=1}^{n} P_i V_i}, \quad P_{cp} = \frac{\sum_{i=1}^{n} P_i V_i}{\sum_{i=1}^{n} V_i},$$

where T_i – average temperature in the cell, P_i – average density in the cell, V_i – cell volume, n – number of cells belonging to the given layer of the given region.

At the second stage, all the data calculated at the first stage are combined and then converted into the PRIZMA code format to serve as the input data for the Monte-Carlo calculations of the radiation energy release.

The input data, needed for the coupling module to work in all modes, are specified in the control file *param.xml* in the XML format. Sections (tags) are formed and they contain the data on the unchangeable constants (number of fuel assemblies, temperature delta in degrees to test for convergence, power of the reactor or fuel assemblies in watts) and the data on the system geometry, as well as the catalog with files containing encoded syntactic rules to parse the on-entry lines of the PRIZMA program input data, and other control data.

5 Results of coupled calculations

RFNC-VNIITF performs coupled computing of the neutron-physical and thermal-hydraulic characteristics for the following reactor cores: VVER-1000, VVER -1200, and BREST-type. For the VVER-1000 reactor, this was the 656-processor computing with the OC Linux control. The complete computing process included 10 iterations and computation took about 120 hours astronomical time.

The neutron-physical characteristics were computed both in uniprocessing, and parallel modes. The thermal-hydraulic characteristics were computed in the distributed mode for 163 fuel assemblies. Each assembly was computed in the uniprocessing mode. The thermal-hydraulic computation takes 3 to 6 hours astronomical time depending on the thermal model configuration.

The fuel assembly of the VVER-1200 reactor has a non-symmetrical configuration and this results in the six-fold increase of the mesh volume if compared to the mesh thermal models of the VVER-1000 fuel assembly. This leads to approximately six-fold increase in the time needed for the thermal-hydraulic computation.

The CONV 3D program was used to calculate the thermal-hydraulic characteritics for one fuel assembly of the BREST reactor type. The code allows parallel computations on 256 processors.

Computation results can be presented in different ways: as fields of physical values, tables, cartograms, and plots (Fig. 10).

The computed average temperature of the coolant at the reactor outlet is in a good agreement with an appropriate performance characteristic for the steady-state mode of reactor operation. The maximum temperature of the fuel elements jackets is not higher than the maximum allowable value.

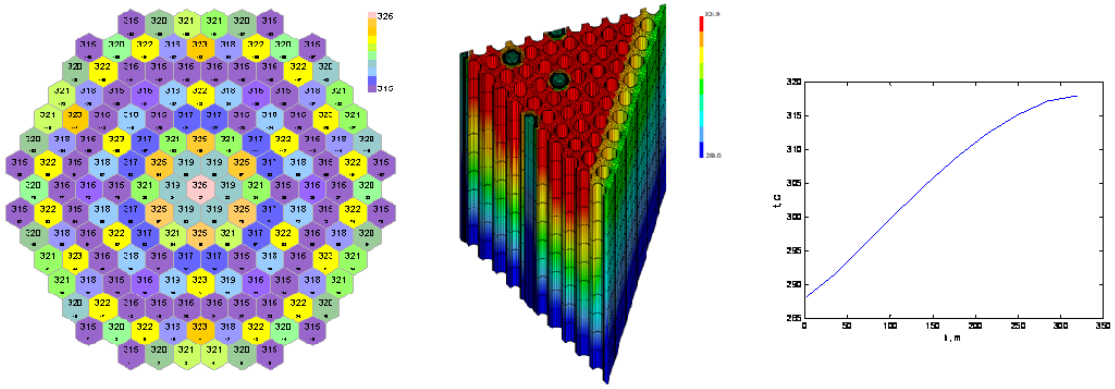

Fig. 10. Presentation of the VVER-1000 reactor core calculations: a cartogram of water temperatures (left), spatial distribution of water temperatures (center), and water temperature variation plot (right).

Our calculations demonstrated that state-of-the art computer systems can be used to calculate the thermal-hydraulic characteristics of reactors with the help of neutron-physical characteristics evaluated using the Monte-Carlo (statistical) modeling. At the same time, checking calculations outlined the way for further development of techniques.

At present, development of the method how to take into account the thermal flow transfer between neighboring fuel assemblies is currently underway. The thermal-hydraulic computation of an individual fuel assembly in the parallel mode as well as computation of the thermal-hydraulic characteristics of the entire reactor core are planned in the short term.

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