

Codes of new generation for safety justification of power units with a closed nuclear fuel cycle developed for the “PRORYV” project

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Academic editor: Andrei Rineiski ♦ **Received** 25 May 2020 ♦ **Accepted** 5 October 2020 ♦ **Published** 6 November 2020

Citation: Bolshov LA, Strizhov VF, Mosunova NA (2020) Codes of new generation for safety justification of power units with a closed nuclear fuel cycle developed for the “PRORYV” project. Nuclear Energy and Technology 6(3): 203–214. <https://doi.org/10.3897/nucet.6.54710>

Abstract

The article describes the status of development of codes of new generation for the “PRORYV” Project by the end of 2019: twenty-five commercial-grade software products to justify design solutions and safety of power units with fast neutron reactors and liquid metal coolant (sodium and lead) in a closed nuclear fuel cycle. The developed system of codes is multi-physical and multi-scale that allows performing both calculations of the whole installations and high precision calculations of their individual elements. The developed codes offer unique features. Twelve developed codes have already been certified by Rostekhnadzor, and six more have been submitted for certification. In addition to creating the software products, a large-scale work is being carried out to conduct experimental studies for code validation that meet modern requirements imposed by the codes: unique measurement techniques have been created; experimental data on flow characteristics of heavy liquid metal coolant (HLMC) in a fuel assembly simulator have been obtained, as well as of “gas-HLMC” interphase interaction after inert gas injection in HLMC and characteristics of heat exchange between the inert gas and HLMC. The results are already used for validation of system and CFD codes used in the “PRORYV” Project.

Keywords

code of new generation, “PRORYV” Project, code validation, MNUP fuel, EUCLID/V2 code, BERKUT-U code

Abbreviations

AHE	Air Heat Exchanger	DPA	Displacement Per Atom
CFD	Computational Fluid Dynamics	ECCS	Emergency Core Cooling System
CNFC	Closed Nuclear Fuel Cycle	FA	Fuel Assembly
CPS	Control and Protection System	FIMA	Fissions per Initial heavy Metal Atom
CTS	Carbothermic Synthesis	FR	Fast Reactor
DNS	Direct Numerical Simulation	FP	Fission Products
		HLMC	Heavy Liquid Metal Coolant
		IHX	Intermediate Heat eXchanger

MCP-1	Main Circulation Pump of the primary coolant system
MCP-2	Main Circulation Pump of the secondary coolant system
MNUP fuel	Mixed Nitride Uranium-Plutonium fuel
MOX fuel	Mixed Oxide Uranium-Plutonium fuel
NPP	Nuclear Power Plant
RANS	Reynolds-Averaged Navier-Stokes equations
RC	Reactor Core
RI	Reactor Installation
Rostekhnadzor	Federal Environmental, Industrial and Nuclear Supervision Service of Russia
RW	Radioactive Waste
SG	Steam Generator
TRL	Technology Readiness Levels

1. Introduction

One of unique projects being successfully realized in the Russian Federation is the “PRORYV” Project, aimed at developing power complexes with FRs in a closed nuclear fuel cycle. Due to a competently built system of scientific and technical management, consolidation of highly qualified result-motivated and wide-profile specialists, the availability of a unique experimental base, a stable funding, significant results were achieved in a short period of time: a technology for the production of MNUP fuel was created and experimental studies were performed that confirmed its efficiency; designs of FRs with lead (BREST-OD-300) and sodium (BN-1200) coolants have been developed; construction of pilot-demonstration facilities of a power unit with BREST-OD-300 and CNFC has been started.

Due to the project innovative nature, it would be impossible to obtain such results without using the potential and achievements in the field of mathematical modeling. This article covers the “Codes of new generation” subproject of the “PRORYV” Project and software products¹ developed within it. The “code of new generation” means commercial-grade software with the following characteristics:

- based on the state-of-the-art level of theoretical knowledge and experimental data on physical processes and phenomena;
- uses efficient numerical algorithms;
- written in accordance with the up-to-date requirements of programming language standards and adapted to state-of-the-art computer technology;
- has a friendly user interface;
- equipped with a full package of documentation (user guide, programmer guide, reference manual);
- has automatic interface with CAD data².

¹ In the article, the phrases “code of new generation”, “software product” and “software” are synonymous.

² For multidimensional codes.

General information on “Codes of new generation” project is briefly presented in (Bol’shov et al. 2016; Strizhov et al. 2017). The purpose of this article is to acquaint the NUCET Journal readers with the latest achievements in this field.

2. The list and status of the codes of new generation development by the end of 2019

The work on the “Codes of new generation” project started in 2010. At this time, the need was recognized to develop a system of broad-scoped software products. Likewise with other large-scale projects, the first years were spent for the development of technical specifications and detailed technical requirements. The large-scale development of the software products began in 2012.

First, the task was set to develop 17 codes; by 2019 their number had increased to 25, which was associated with an awareness of the possibilities and advantages of using state-of-the-art software systems.

The general information about the designation and development status of the codes of new generation is presented in the Table 1, including their Technology Readiness Levels (TRL).

Compared to earlier publications (Bol’shov et al. 2016; Strizhov et al. 2017), significant progress should be noted in expanding the applicability areas of codes, the status of their validation and certification in Rostekhnadzor. In addition, the codes of new generation package includes the codes for modeling of the installations of the closed nuclear fuel cycle, including 3D multi-component thermohydraulic models, the development of which was started in 2019.

The information about some of the most interesting models in the opinion of the article authors, included in the codes in 2018-2019, as well as the validation results is represented in the Section 3. Detailed information can be found in individual publications, which are referenced in this article.

3. Summary of some new models of the codes of new generation and the results of their validation in 2018-2019

3.1. Improved (mechanistic) fuel code BERKUT-U

The advanced fuel code BERKUT-U is designed to calculate the thermo-mechanical behavior and justify the operability of single fuel rod with an oxide (uranium dioxide and MOX) and nitride (uranium mononitride and MNUP) pellet fuel, with a gas gap or a liquid metal gap, in normal and abnormal operation modes of advanced FRs with liquid metal coolant.

Table 1. The development status of the codes of new generation by the end of 2019.

Code name	Brief description	Development status	TRL level	References
Probabilistic safety assessment				
CRISS 5.3	Code for probabilistic safety assessment	Validated, certified	9	Abramov et al. 2016
Fuel rod behavior				
BERKUT*	Code for analysis of fuel rod behavior in normal and abnormal operation modes, engineering version	Validated, certified	9	Veprev et al. 2018, 2020
BERKUT-U*	Code for analysis of fuel rod behavior in normal and abnormal operation modes, advanced (mechanistic) version	Validated, in the process of certification	8	Boldyrev et al. 2020
Neutronics				
MCU-FR***	Neutronic code based on the Monte-Carlo method	Validated, in the process of certification	8	Kalugin et al. 2015; Gurevich et al. 2016
ODETTA**	Neutronic code for shielding calculations based on the S_n method and the finite element method	Validated, certified	9	Belousov et al. 2018
CORNER***	Neutronic code based on the S_n method and the finite difference method	Validated, in the process of certification	8	Bereznev et al. 2015
DOLCE VITA***	Neutronic code based on diffusion approximation	Validated, in the process of certification	8	Seleznev et al. 2018a
BPSD***	Nuclide kinetics code, for calculation of activity and residual decay heat	Validated, in the process of certification	8	Seleznev et al. 2018b
COMPLEX	System of codes for the radiation safety justification of a FRs installation and fuel cycle facilities	Under development	5	Belov et al. 2019
Thermohydraulics				
HYDRA-IBRAE/LM/V1*	System (channel) thermal-hydraulic code	Validated, certified	9	Alipchenkov et al. 2016; Mosunova et al. 2020
LOGOS	RANS CFD code	Validated, filed for certification	8	Kozelkov et al. 2016
CONV-3D	DNS CFD code	Validated, certified	9	Chudanov et al. 2017, 2020
CONV-3D/TwoPhase	DNS CFD code expanded to two-phase simulations	Under development	3	Chudanov et al. 2016, 2019
KUPOL-BR	Code for modeling heat and mass transfer processes in reactor containment building	Validated, in the process of certification	8	Vitushkina et al. 2006
Fission products transport				
ROM*	Code for assessing the radiation situation outside the NPP site	Validated, certified	9	Dzama et al. 2019a
ROUZ	Code for assessing the on-site NPP radiation situation taking into account the 3D built-up environment	Validated, certified	9	Dzama et al. 2019b
Sybilla	Code for modeling of radioactivity migration in reservoirs	Validated, certified	9	Krylov et al. 2016
GeRa/V1	Code to assess the safety of radioactive waste disposal	Validated, certified	9	Kapyrin et al. 2015; Novikov et al. 2020
Multiphysics codes				
SOCRAT-BN/V1	Comprehensive analysis of normal and abnormal operation modes, including severe accidents, for NPPs RI with sodium coolant and oxide fuel	Validated, certified	9	Usov et al. 2012
SOCRAT-BN/V2		Validated, certified	9	
EUCLID/V1	Comprehensive analysis of normal and abnormal operation modes, including accidents, for NPPs RI with sodium, lead and lead-bismuth coolant and fuel rods with oxide or nitride fuel	Validated, certified	9	Mosunova 2018; Alipchenkov et al. 2018
EUCLID/V2		Partially validated	5	
Models of closed nuclear fuel cycle processes and installations				
VIZART	Code to simulate the balance of materials and nuclide flows in the CNFC	Partially validated	8	Shmidt et al. 2017
TP CODE	Code to simulate the work of technological schemes	Partially validated	8	Goryunov et al. 2018
Precision computational models for the CNFC facilities	Precise calculation models for the CNFC facilities	Under development	3	–

* above the code name means that this code is included in the multiphysics EUCLID code as a module;

** above the code name means that this code is included in the COMPLEX code system.

A distinctive feature of the code is the presence of a mechanistic fuel behavior module, the prototype of which was the MFPR/R fuel code (Veshchunov et al. 2006; Veshchunov et al. 2007), simulating the behavior of oxide fuel in thermal reactors under normal and emergency conditions. The fuel behavior module of the BERKUT-U code includes four basic macromodels: (1) breeding process and FP radioactive decay; (2) the evolution of the fuel microstructure and FP intragranular transport; (3) the formation of intergranular porosity, intergranular transport and FP release into open porosity; (4) thermodynamics of burnt fuel, the formation of FP chemical compounds and their distribution over phase states. The evolution of the fuel microstructure, the formation of FP gas and conden-

sed phases and FP transport are modeled, which makes possible to predict the fuel swelling and FP release under fuel rod cladding and, consequently, the change of the fuel thermo-physical characteristics, pressure and thermal conductivity of gas gap as fuel burns out, and in the case of depressurization – the FP amount injected in the coolant.

When developing the fuel module as part of the BERKUT-U fuel code, it was taken into account that most of processes in oxide fuel are common for thermal and fast neutron reactors, so that the corresponding particular models developed earlier for thermal reactors can also be used for calculations of FRs. Moreover, the functional form of code models is also mainly suitable for describing processes in nitride fuel, since they have similar physics with

oxide fuel. However, the microscopic parameters of models for oxide and nitride fuels often differ greatly, and for nitride fuel, these parameters are usually poorly known or not determined at all. To identify them, the experimental data obtained from the studies of nitride fuel after its irradiation in a reactor have been used, as well as the results of atomistic modeling (Veshchunov et al. 2015; Tarasov and Polovnikov 2017; Starikov et al. 2017). In addition, new models were developed or existing ones were improved to describe thermochemical processes in nitride fuel, capture of gaseous fission products by technological porosity, helium diffusion, and also impurities (oxygen, carbon) with the formation of secondary oxide and carbide phases.

By mid-2019, the models for nitride fuel were validated on the results of post-reactor studies of BORA-BORA fuel rods irradiated in the BOR-60 reactor, KETVS-1, 2, 3, 6, 7 and ETVS-4, 5 experimental assemblies irradiated in the BN-600 RI. These studies provided experimental data concerning the behavior of fission products in the fuel, their release into the fuel-cladding gap, the mechanical state of the fuel pellets and the fuel element as a whole. In particular, for MNUP fuel, the content of plutonium varied from 10 to 60%, maximum burn-up – from 3.5 to 12%, and damaging doses – from 20 to 70 DPA, maximum temperatures – from 1100 to 1700 °C.

The results show that the BERKUT-U calculation code allows describing the entire existing experimental data array on the fission products release and the mechanical state of the fuel with a fairly good accuracy. The change in the size of fuel pellets is calculated with an accuracy of 1–2%, the fuel swelling – on average 30–40%, the swelling rate – 30%, and the release of gaseous fission products – 30–50%. These results can be considered satisfactory taking into account the uncertainties of the experimental measurements. Unlike engineering techniques, the BERKUT-U code allows predicting the isotopic and molecular-phase compositions of irradiated fuel, as well as obtaining axial and radial distributions of porosity, actinides and fission products.

Examples of such results are presented in Figures 1 and 2. The fuel rod with mixed uranium-plutonium nitride fuel ($U_{0.55}Pu_{0.45}N$) without a central hole and with a helium gas gap of the BORA-BORA experiments irradiated in the BOR-60 fast reactor was considered. The maximum burn-up for this fuel rod was equal to 9.4% FIMA (Rogozkin et al. 2013). The calculated and experimental distributions of porosity (Fig. 1) and fission products (Fig. 2), Cs and Mo, along the pellet radius in the central part of a fuel rod are shown. In Figure 1, the NM variant is the calculation for the case of the nominal sizes of the fuel pellets; the CT variant corresponds to a reduced diameter within the technological tolerance (0.1 mm). The reduction of porosity in Figure 1 is caused by the reduction of temperature of the fuel pellets with pellets radius.

Currently, the consolidation and analysis of the results of the BERKUT-U code validation is being completed. At the end of 2019, the code was submitted for certification to Rostechndzor.

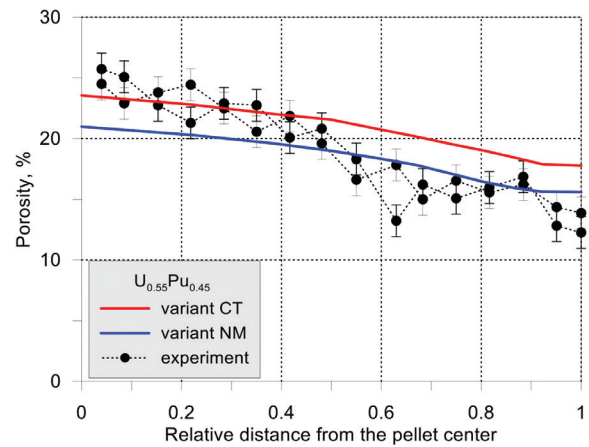


Figure 1. Radial porosity distribution in $U_{0.55}Pu_{0.45}N$ fuel pellets from the middle of fuel rod, BORA-BORA experiments.

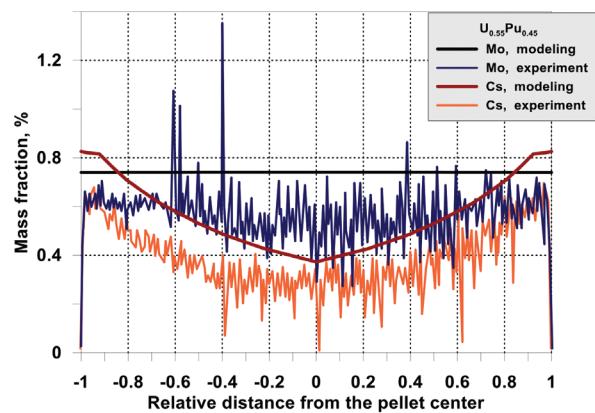


Figure 2. Radial distribution of Cs and Mo in $U_{0.55}Pu_{0.45}N$ fuel pellets from the middle of fuel rod, BORA-BORA experiments.

3.2. Two-phase CFD CONV-3D/TwoPhase code

The direct numerical simulation of Navier-Stokes equations expanded for a two-phase medium is realized in the CONV-3D/TwoPhase code. The interphase heat- and mass-transfer using the equations of state like stiffened and Noble-Abel ones are taken into account. The HLLC-solver (Harten-Lax-van-Leer-Contact) and the two-step predictor-corrector of the MUSCL algorithm (Monotonic Upwind Scheme for Conservation Laws) are realized in the module (Chudanov et al. 2019). The CFD module is adapted to massive supercomputers and is scalable in a wide range of dimensions of computational grids.

By the middle of 2019, a method for obtaining more accurate coefficient values was developed for the Noble-Abel state equations, which is based on experimental dependencies on the saturation line (temperature dependencies of gas and liquid enthalpy, inverse density of gas and liquid, saturation pressure) and applying the least square method. Based on the solution of a transcendental equation, the numerical temperature dependence of pressure is determined from the condition that the Gibbs potentials of the gas and liquid phases are equal. An adaptation of a two-phase module was carried out taking into

account mass transfer and more accurate values of the coefficients for stiffened and Noble-Abel state equation in simulating sodium coolant flows.

The two-phase model development has been continued using the method of a priori estimates, allowing carrying out calculations with lower computational costs, without additional iterative procedures. Work on the model extension for the case of a three-component medium, for example, lead-water-vapor and other possible three-component media, has been started.

3.3. The EUCLID/V2 multiphysics code for justifying the safety of NPPs with fast neutron reactors

3.3.1. Brief information

The EUCLID/V2³ code is designed to analyze and justify the safety of NPPs with fast neutron reactors with liquid metal coolants in the normal and abnormal operation modes, including accidents, severe ones as well (Usov et al. 2018a, 2018b; Butov et al. 2019a, 2019b). It is based on the first version of the code EUCLID/V1 (detailed information about which can be found in (Mosunova 2018; Alipchenkov et al. 2018)) and includes all of its models.

The following modules work together as part of the EUCLID/V2 calculation code, providing multi-physical consistent simulation of different processes and phenomena:

- thermohydraulic (HYDRA-IBRAE/LM), which includes a module of the FP transport and behavior, the corrosion and activation in the RI primary circuit and gas system (AEROSOL-LM), a module of solid impurity transport in the RI primary circuit with heavy liquid metal coolant (OXID), a module of tritium migration in the coolant of the first, second, and third (if available) circuits (TRITIUM);
- sub-channel module (CELSIST) for two-dimensional modeling of coolant flow in fuel assemblies;
- neutron diffusion and transport modules (DN3D and CORNER, respectively), modules for burn-up (BPSD) and decay heat (OSTB) calculation;
- fuel rod module (BERKUT and BERKUT-U) with models for calculating sources of fission products in a core in the event of fuel rod cladding failure, intended for numerical simulation of behavior and calculation of operability of nitride and oxide fuel rods;
- module for calculating the disruption of fast reactor fuel rods and other core structures (SAFR). The module implements a multicomponent one- and three-dimensional models for calculations of the movement and heat exchange of components of disrupted fuel rods and fuel assemblies in the core and upper mixing chamber of liquid-metal cooled reactor. To calculate the movement of components, the laws of conservation of mass, energy and momentum are used, as well as the equation for the sum of volume fractions of the compo-

nents. The module also allows calculation of the movement of the formed cladding and fuel melt by gravity, friction with the gas flow and wall friction;

- module of mass transfer and FP behaviour in NPP compartments (KUPOL-BR or HYDRA-IBRAE/LM);
- module for assessing the radiation situation outside the NPP site (ROM).

The SMART/LM integration shell provides a consistent calculation by all modules.

3.3.2. Improvement and development of individual models

The main model improvement and development areas of the EUCLID/V2 multiphysics code in 2018-2019 include:

- development of a model which describes the transport of steam-water formations in the circuits of reactor installations with a heavy liquid-metal coolant, taking into account their size distribution;
- development of a nitride fuel dissociation model and its implementation into the code;
- improvement of the diffusion neutronic module for correct simulation of core disruption (the values of diffusion coefficients were corrected to take into account the collapse of materials during core disruption, the cross sections change due to materials flowing down during fuel rod melt was considered, etc.);
- turbine model development and integration into the code.

More detailed information about some of the models is given below.

In 2019, the model for transport of vapor-gas formations (bubbles) was added to the system thermal-hydraulic module HYDRA-IBRAE/LM of the EUCLID/V2 code, taking into account the evolution of their size distribution. It should be noted that the description of the particle size of the dispersed phase (droplets, bubbles, vapor agglomerates) is a key point in models of two-phase media. The traditional approach used in system thermal-hydraulic codes is to determine the size of the dispersed phase from empirical correlations with instantaneous adjustment to changes in the thermal-hydraulic parameters of the carrier flow. In reality, the zone, in which a more complex than instantaneous approach is needed, can be significant (up to several meters, it depends on the flow parameters), which can be essential when analyzing, for example, the transport process of steam formations in the circuits of reactor installations with a heavy liquid-metal coolant.

The evolution of the bubble size distribution can be described more precisely by a volumetric interfacial area transport equation (Yao and Morel 2004). To solve the transport equation for the particle size distribution, the method of fractions (groups) is used in the HYDRA-IBRAE/LM module. In this method, the set of particles is subdivided into a number of fractions (groups or classes) depending on particle size and it is assumed that there can be

³ V2 in the code name means “version 2”.

an exchange of particles between different fractions as a result of phase transitions, coagulation, fragmentation and other processes.

The experimental data on which validation of the developed models could be performed are now practically absent in the available literature. Therefore, a comparison of the calculation with the analytical solution was performed. For comparison, the article results (Gelbard and Seinfeld 1978) were used. In this work, it was obtained that with the initial distribution and the constant coagulation nucleus β_0 , the solution is represented as

$$n(t) = \frac{4N_0}{v_0(N_0\beta_0 t + 2)^2} \text{Exp} \left[-\frac{2v/v_0}{N_0\beta_0 t + 2} \right] \quad (1)$$

where N_0 and v_0 – parameters; β_0 – size-independent portion of coalescence kernel; t – time; v – bubble volume.

The simulation results in comparison with solution (1) from the work (Gelbard and Seinfeld 1978) are presented in Figure 3.

To our knowledge, a model of this type is not included in some well-known and widely used codes-analogous such as RELAP5-3D, ATHLET, ASTEC-Na (RELAP5-3D Code Manual 2012a, 2012b; Palazzo et al. 2013; Zhou et al. 2013; Flores et al. 2016; Bandini et al. 2018; Forgione et al. 2019; Narcisi et al. 2019; Shen et al. 2019 and many others). Similar models are available only in some CFD codes.

In 2019, a model for calculating the nitride fuel dissociation was integrated into the fuel rod destruction module of the EUCLID/V2 multiphysics code. The most important for the dissociation modeling is to determine the rate of mass loss due to release of nitrogen and uranium vapor according to the equation

$$(U_{1-x}Pu_x)N(c) = U_{1-x}(l) + Pu_x(l) + 0,5N_2(g) \quad (2)$$

The rate of mass loss is calculated by the ratios:

$$\Delta m_{(Pu_x, U_{1-x})N} = -2 \cdot \frac{M_{(Pu_x, U_{1-x})N}}{M_{N_2}} j_{N_2} S \cdot \Delta t \quad (3)$$

$$\Delta m_U = 2 \cdot \frac{(1-x)M_U}{M_{N_2}} j_{N_2} S \cdot \Delta t - j_U S \cdot \Delta t \quad (4)$$

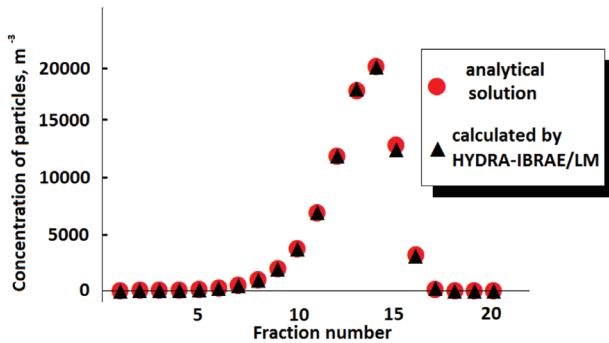


Figure 3. The results of simulation by the HYDRA-IBRAE/LM module of the EUCLID/V2 code in comparison with the solution (1).

$$\Delta m_{Pu} = 2 \cdot \frac{x \cdot M_{Pu}}{M_{N_2}} j_{N_2} S \cdot \Delta t - j_{Pu} S \cdot \Delta t \quad (5)$$

where j_{N_2} , j_U , j_{Pu} – the mass flows of nitrogen, uranium and plutonium from the fuel surface; x – plutonium mass fraction; M_{N_2} , M_{Pu} , M_U , $M_{(Pu_x, U_{1-x})N}$ – molar mass of nitrogen, Pu, U and MNUP fuel, respectively; S – fuel surface where the process of dissociation occurs; Δt – time step; Δm_U , Δm_{Pu} , $\Delta m_{(Pu_x, U_{1-x})N}$ – changes of total masses of U, Pu and MNUP fuel due to dissociation process respectively.

To our knowledge, this process is not modelled in codes such as SIMMER-III/IV, SOCRAT-BN (Usov et al. 2012; Cheng et al. 2015; Li et al. 2017).

3.3.3. Validation on the results of experimental regimes of the BN-800 RI

In 2015, the fourth power unit of the Beloyarsk NPP (RI BN-800 with sodium coolant) achieved its first criticality successfully, after that the first start took place. Then pilot operation of the unit was carried out. At that time, the tests of the RI main technical characteristics in stationary and transient modes at different power levels up to the nominal one were carried out. At present, the EUCLID/V2 multiphysics code is validated on the data obtained on the BN-800 in the following modes:

- shutdown of one of the three operating loops when the reactor is operating at a power level of $\sim 100\% N_{nom}$;
- cooldown of the reactor by ECCS from the initial power level of $\sim 50\% N_{nom}$;
- power unit shutdown;
- power unit start-up, where N_{nom} is the nominal reactor power.

The neutronics and thermohydraulic computational models of the BN-800 core, a thermal-hydraulic model of the coolant circulation circuits, including the upper mixing chamber, intermediate heat exchangers, drain chambers of intermediate heat exchangers, main circulation pumps, pressure pipe lines, pressure chamber, pipe lines of the secondary circuit, sodium buffer tank, main circulation pumps of the secondary circuit, steam generators and other equipment, as well as fuel rod models for fuel assemblies of various types are developed.

To evaluate the uncertainties and sensitivity of main RI parameters calculated using the EUCLID/V2 code, some parameters affecting the simulation results in a most significant way were determined based on previously validation calculations of experiments accounting for some individual phenomena (Table 2). The ranges of data variation were selected based on the experimental uncertainties of relevant measurements. The uncertainties of empirical correlations used in the calculations were determined in accordance with available literature data or expert estimates.

To perform the uncertainty and sensitivity analysis of the results 200 calculations have been carried out.

Figure 4 shows a comparison of the results of multivariate calculations obtained using EUCLID/V2 code with the experimental values of integral power of the BN-800 RI in the mode of “Shutdown of one of the three operating loops when the reactor is operating at a power level of $\sim 100\% N_{nom}$ ”. The intervals of calculated data are shown by blue shading. It can be seen that the deviation of the average calculated values from the experimental average ones does not exceed 5%.

Figure 5 shows the EUCLID/V2 calculated values of sodium temperature in the primary loop at the IHX inlet of the BN-800 RI in the mode “Cooldown of the reactor by ECCS from the initial power level of $\sim 50\% N_{nom}$ ” in comparison with the experiment. The intervals of calculated data are shown by blue shading. The experimental uncertainties are shown by vertical bars. The maximum absolute deviation does not exceed 10 K.

The available validation results show that for the considered types of transients, the EUCLID/V2 code describes adequately the change in the integrated power as well as the thermohydraulic processes in the BN-800 type RI core and its cooling circuits, including air circuit cooling modes.

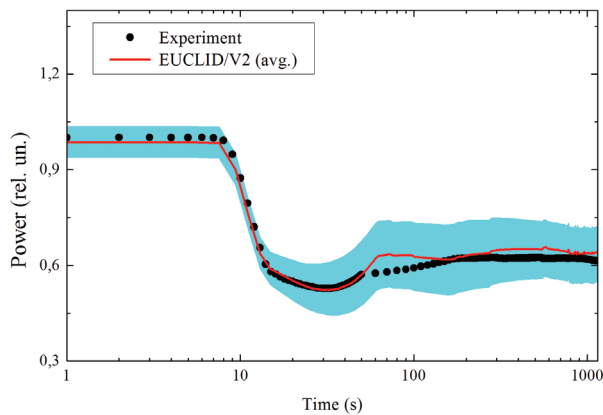


Figure 4. Change in the integral power of the BN-800 RI with time in the mode of “Shutdown of one of the three operating loops when the reactor is operating at a power level of $\sim 100\% N_{nom}$ ”; (the experimental uncertainty is about 1% and is not seen in the figure).

Table 2. Parameters and ranges of their variation.

Parameter	Variation range
Initial integrated RC power, MW	$\pm 5\%$
Residual power, MW	$\pm 25\%$
The frequency of MCP-1 rotation, rpm	± 3.75
The frequency of MCP-2 rotation, rpm	± 3.75
Feedwater flow rate in SG, kg/s	± 5.8
Speed of CPS rods, cm/s	$\pm 5\%$
Feedwater temperature in SG, $^{\circ}\text{C}$	± 3.5
Initial diameter of fuel pellets, mm	-0.15
Multiplier applied to the wall heat transfer closure relation in SG from the water side or in AHE from the air side, rel. units	$\pm 30\%$
Multiplier applied to the wall friction closure relation in SG from the water side or in AHE from the air side, rel. units	$\pm 30\%$
Multiplier applied to the interfacial friction closure relation in SG for water, rel. units	$\pm 30\%$
Multiplier applied to the wall heat transfer closure relation in RC, IHE and SG from the sodium side, rel. units	$\pm 20\%$
Multiplier applied to the wall friction closure relation in RC, IHE and SG from the sodium side, rel. units	$\pm 10\%$
Thermal conductivity of fuel, W/m/K	$\pm 20\%$
Thermal conductivity of the gas gap in the fuel rod, W/m/K	$\pm 10\%$

3.4. Computational models of the facilities of the closed nuclear fuel cycle

In 2019, the development of calculation models for the closed nuclear fuel cycle installations was started, allowing assessing the nuclear and radiation safety of installations and selecting their optimal technological parameters. A brief description of some of the models developed is given below. Based on the spatial and phase distribution of radionuclides in the installation elements obtained in the approximations described below, the calculation of nuclear safety is performed in an automated mode by MCU-FR code and calculation of radiation safety by the COMPLEX system of codes (see Table 1).

3.4.1. Model of the electrochemical dissolution of solid particles of plutonium and uranium oxides

In a closed nuclear fuel cycle, spent nuclear fuel is reprocessed to extract uranium and plutonium for further re-use as fuel for fast reactors.

An important step in the technology of the spent nuclear fuel (SNF) reprocessing is the operation of further dissolving the remainder of plutonium and uranium oxide solid particles ($U_xPu_yO_2$) after the completion of basic technological cycles of SNF reprocessing. Its distinguishing feature is the electrochemical catalytic conversion of plutonium dioxide PuO_2 from the insoluble solid phase to PuO_2^{2+} ions soluble in nitric acid HNO_3 solution. A computational model was developed describing:

- real three-dimensional geometry of the installation elements;
- three-dimensional picture of medium flow in the anode and cathode volumes (CFD);
- ion transfer to electrodes with a detailed resolution of the structure of the boundary layer near the electrodes;
- heat transfer for various elements of the installation;
- sources of heat generation due to electrolysis processes and decay of radionuclides;
- migration of ions through the membrane in the approximation of transport equations for a porous medium, taking into account the electric field gradient.

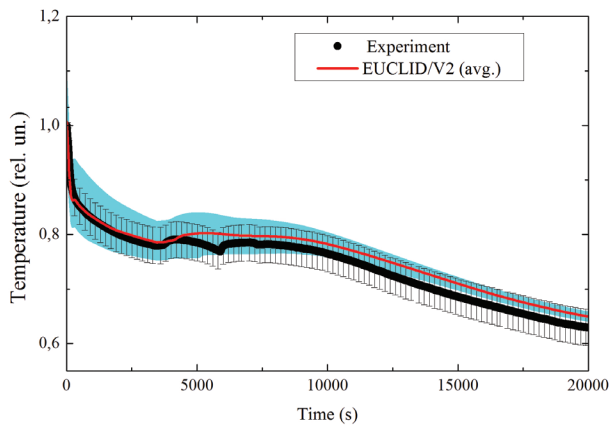


Figure 5. The change of sodium temperature in the primary loop with time at the IHX inlet of the BN-800 RI in the mode “Cooldown of the reactor by ECCS from the initial power level of $\sim 50\% N_{nom}$ ”

3.4.2. Model of membrane clarification

Upon the end of the cycle of electrochemical dissolution of solid particles of actinide oxides, the solution from the anode space with the remaining particles of the dispersed phase is sent to the control clarification apparatus for separating solid particles. The filtered solution containing the solid phase is delivered to a membrane filter, which contains several multichannel filtering ceramic elements that are hollow fibers coated with a membrane layer. The concentrate remains inside the channels of the filtering element, and outside the filtering element a solution is accumulated that is free from solid particles and insoluble impurities deposited in the membrane pores.

A distinctive feature of the filtered solution is the presence in the solution of liquid and solid high-level waste of SNF and ionic components. A feature of the membrane filtration process from the point of view of radiation safety is the accumulation of radioactive sediments on the surface of membrane fibers and filter walls.

The developed calculation model takes into account:

- three-dimensional hydrodynamics (CFD) of the solution flow with particles through the membrane and filter volume;
- kinetics of radioactive particles charging in nitrate electrolyte;
- possible heating of particles due to decay of radionuclides;
- thermal interaction of the dispersed and liquid phases;
- sedimentation and separation of particles from the surface of membrane channels, taking into account their charge;
- sediment formation taking into account spatial effects;
- variation in time of the sediment activity on the membrane.

3.4.3. Model of carbothermic synthesis of nitride fuel

Currently, the most promising option for the MNUP pellet production in industrial scale is the method of carbothermic synthesis (CTS), based on the reduction of mixed uranium-plutonium dioxide by carbon in nitrogen atmosphere.

The carbothermic synthesis reaction of (U,Pu)N is carried out with powder mixtures of uranium dioxide or uranium – plutonium, (U,Pu)O₂, and graphite. Synthesis occurs at temperatures of 1700–2000 K in nitrogen stream. At the last stage of the process, some amount of hydrogen is added to nitrogen atmosphere. The role of the nitrogen flow, especially of the N₂+H₂ mixture, consists, in particular, in removing gaseous compounds of carbon and oxygen (CO, CN, CH₄) from the reaction zone, thus ensuring a sufficiently low concentration of oxygen and carbon impurity in the final product, which is a critical point in the production of nitride fuel by the CTS method.

There are several factors that significantly affect the CTS efficiency and the final product characteristics: the size of the particles of original powder, the presence of impurities, the temperature-time mode, the volume and composition of gas flow in the chamber. The feature of the technological process from the point of view of radiation safety is the mass loss of samples and the accumulation of radioactive dust in the CTS chamber.

The developed mathematical model for the physico-chemical processes of the carbothermic synthesis of uranium and plutonium nitride powders is intended to describe the effect of process parameters — temperature, atmospheric composition, and others — on the characteristics of the products and, above all, on the concentration of impurities.

The developed calculation model takes into account:

- chemical reactions of oxygen substitution by carbon and nitrogen at the border of fuel and graphite with CO formation;
- chemical reactions of carbon substitution by nitrogen in the presence of hydrogen to form CH₄;
- diffusive transport of oxygen, nitrogen and carbon in the solid phase;
- mass transfer of N₂, H₂, CO, CH₄ in the gas phase.

The complex mathematical model includes the heat-transfer equation, the Navier-Stokes equations, and the convection-diffusion equation.

3.4.4. Model for sintering of nitride fuel pellets

The final step in the process of the MNUP fuel pelletizing is sintering of fuel pellets. At the preliminary stages, the UN or (U, Pu)N powder is produced, which is then pressed, resulting in an intermediate product with a density of $\sim 60\%$ having sufficient mechanical strength and the

required chemical composition. At the sintering stage, a part of the fuel main characteristics is formed, such as density, size and type of porosity, grain size, determining the fuel performance.

There are several factors that significantly affect the sintering efficiency of (U, Pu)N and the characteristics of the final product: the size and shape of the particles of the original powder, the initial porosity of the sample, the sintering temperature and time, and the atmosphere in the sintering chamber.

The developed computational model takes into account the following processes:

- fuel recrystallization by the mechanisms of normal grain growth and re-condensation;
- relaxation of intergranular porosity due to the diffused drain of vacancies and external thermo-mechanical stresses;
- thermochemical reactions, leading to a mass loss of the sample.

In the constructed computational model, three-dimensional heat transfer in a complex furnace design, mass transfer of the gas mixture in the working area, multi-component diffusion and reactions in fuel grains are described consistently.

4. Experiments to validate the codes of new generation

To validate the developed and being developed codes of new generation, it was necessary to create a database of evaluated available experimental data. For this, the analysis and evaluation of the results of experimental studies conducted prior to the start-up of the “PRORYV” Project were carried out. According to the analysis results, work programs for obtaining the missing experimental data were prepared. At the same time, validation of a number of high fidelity codes required experimental data obtained at a fundamentally new level with the measurement of local flow characteristics.

In this regard, a program of experimental studies of thermal-hydraulic and physicochemical processes is developed, and the studies are performed at JSC “NIKIET” (Moscow), JSC “SSC RF – IPPE” (Obninsk, Russia), IT SB RAS (Novosibirsk, Russia) and other organizations.

In particular, at the IT SB RAS a series of well-instrumented model experiments has been performed to study the heat transfer and thermohydraulic characteristics of a heavy liquid-metal coolant in the elements of a reactor installation, including the processes occurring during steam generator tube rupture of lead cooled reactor installation (Kashinsky et al. 2016; Lobanov et al. 2017; Kashinsky et al. 2018; Usov et al. 2018c).

Various outflow regimes (bubble, slug) when water vapor or gas is flowing out into a lead or Rose’s alloy coolants, modeling the steam generator tube rupture in fast reactors facilities, and the heat transfer between water vapor and lead coolant have been studied (Lobanov et al. 2017; Usov et al. 2018c). The lead temperature during experiments was about 400 °C, the Rose’s alloy – about 150 °C. The outflow of water vapor / gas occurred through the tubes with a diameter of 2 – 4 mm. In the different series of experiments, the pressure drop between the steam (gas) and the coolant and the time of the outflow of water vapor (gas) were changed. The evolution and size of steam or inert gas bubbles in lead were measured. The regimes of steam / gas outflow were found in which large pressure pulsations are formed in the channel. Also the data on lead temperature evolution were obtained in the experiments with outflow of “cold” water vapor or inert gas into the lead. The obtained experimental data were used to validate the calculation code HYDRA-IBRAE/LM (Usov et al. 2018c).

The experiments on mixing of liquid metal coolant flows at different temperatures in a T-junction were conducted (Kashinsky et al. 2016; Kashinsky et al. 2018). The T-junction consists of two pipes with internal diameters of 8 and 20 mm connected perpendicularly. The liquid metal coolant was a melt of Rose’s alloy (50 % bismuth, 25% lead, 25% tin). The temperature of the “hot” flow was about 150 °C, of the “cold” flow about 120 °C, flow rate ratios of the “hot” and “cold” flows were varied in the range between 0,02 and 0,63. The Reynolds numbers of the “cold” flow in the pipe were in the range 6500÷14500. As a result of the measurements, three-dimensional distributions of the average temperatures and temperature fluctuations were obtained both on the external surface of the T-junction and directly in the flow mixing area. Those data were used to validate RANS and DNS codes (LOGOS, CONV-3D, STAR-CCM+ and others).

In the experiments with a 7-rods model of a fuel assembly with spacer grids detailed data on the axial and azimuthal temperature distributions over the surface of the fuel rod simulators with nonuniform heating of one of the fuel rods, and the data on the impact of the spacer grids on the temperature field distribution on the surface of the fuel rod simulator were obtained (Kashinsky et al. 2018). The fuel assembly model consisted of 7 vertical rods with a diameter of 9 mm, arranged in a hexagonal pattern with a relative pitch between the rods equal to 1.4. The investigations were carried out at Reynolds number values 8000 and 14000 and the heat flux density 19.6 W/cm² using Rose’s alloy. An example of the typical axial sweep of the radial temperature distribution behind the spacer grid, when the peripheral simulator of the fuel element is heated, is shown in Figure 6. As one can see, a large irregularity of temperature distribution is observed. The experiments are conducted not only in the field of thermohydraulic. In the coming years, JSC “IRM” (Zarechniy, Russia) is planning to obtain reactor experimental

data and dependencies of the outflow kinetics of gaseous fission products released from the MNUP fuel required for setting the parameters of the models and validating the BERKUT-U fuel rod code. At the same time, tests of the MNUP fuel behavior after reactivity introduction will be conducted in the IGR reactor. The irradiation of experimental fuel assemblies and devices with MNUP fuel rods in the BN-600 and BOR-60 RI continues.

The obtained data are used for the validation of the multiphysics codes of new generation and the fuel rod codes.

Those are only some of the examples demonstrating that work on the code development is accompanied by the extensive program of experimental investigations.

Conclusion

In the “Codes of new generation” subproject of the “PRO-RYV” Project, the software was developed to justify the safety of the facilities being constructed, to understand the phenomenology of the processes, to optimize equipment and installations in general. High fidelity models and calculation codes based on them make possible to carry out predictive calculations in order to achieve optimal technical and economic indicators of the developed nuclear technologies.

A large effort on certification in Rostechnadzor of the developed software is being performed. At the same time, the principal novelty of the approaches underlying the creation of high precision software products requires changes in the accepted certification practice and the creation of an appropriate new infrastructure, including highly qualified experts for individual profiles, the agreement between the code developers and the regulator, formalized as the regulatory documents, on the necessary and sufficient experimental data and the limits of applicability of the corresponding tools, the formation of the “best practices” for the use of high fidelity codes at specific facilities.

Since the increasingly restrictive requirements are imposed on the safety justification of nuclear facilities,

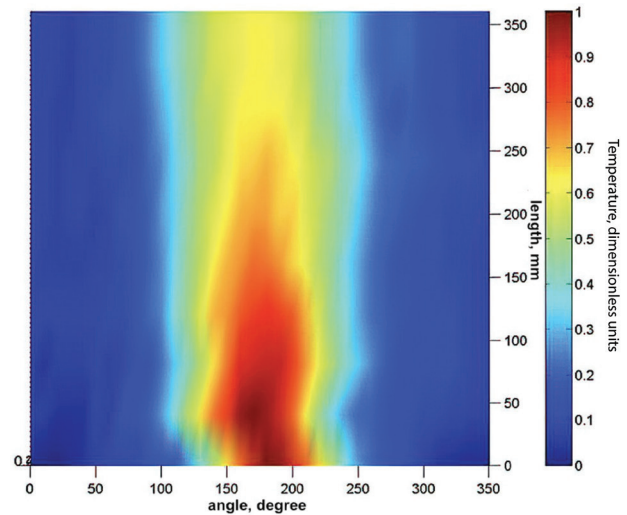


Figure 6. Typical axial sweep of the radial temperature distribution on the surface of the central fuel rod simulator behind the spacer grid. Rose’s alloy: $T = 150\text{ }^{\circ}\text{C}$, $Re = 8000$.

ties, in terms of detailed elaboration of models, many calculation codes in the nuclear industry are ahead of analogues that are available or are only planned to be developed in other industries. In this regard, the codes of new generation may be applied outside the nuclear industry, for example, to assess the effects of emissions from enterprises in other industries, to assess the impact on humans and the environment of facilities that pose a potential environmental hazard.

A program for the further development of codes of new generation has been outlined, including their validation on new experimental data, the creation of high precision models, and the introduction of the developed software into the practice of computational justification of nuclear facilities safety. To form a team of qualified users, it is planned to implement the developed software into higher educational institutions and hold annual user-training workshops.

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