Codes of New Generation Developed for Breakthrough Project

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Abstract. Within the «Breakthrough» project and the Federal Target Program "Nuclear power technologies of a new generation for 2010 – 2015 and for the future till 2020", a system of codes of new generation is being developed which provides validation of operation and safety characteristics for designing NPP with sodium, lead and lead-bismuth coolants, and closed nuclear fuel cycle. Usage of the developing codes by design-and-engineering and operating organizations provides a reduction of uncertainties through multi-scale modeling, based on a mechanical approach of model development, a more precise geometrical representation of modeling objects and self-consistent integrated analysis of nuclear reactors and the fuel cycle. Simulation objects include fast nuclear reactors with sodium coolant (BN-600, BN-800, BN-1200, MBIR), lead coolant (BREST-OD-300, BR-1200), lead-bismuth coolant (SVBR-100), and objects of the fuel cycle. This paper presents a review of developing codes, their current state of development and validation.

Key Words: safety, computational codes, nuclear plant, heavy liquid metal.

1 Introduction

The successful development of nuclear energy requires a transition to a new technological platform which uses fast nuclear reactors and closed nuclear fuel cycle. To solve this problem in the Russian Federation, the Federal Target Program "Nuclear Power Technologies of the New Generation, 2010–2015 up to 2020", was initiated, in which project «Breakthrough» was implemented [1]. The main advantages of nuclear technology using fast neutrons are substantial growth of efficiency of nuclear fuel using through applying depleted uranium, transition to closed nuclear fuel cycle, reducing the amount of generated spent nuclear fuel and radioactive waste, and providing radiation equivalence in radioactive waste disposal.

Within the scope of «Breakthrough» project, technical projects of innovative nuclear reactors BREST-OD-300 and BN-1200 have been developed, which assume usage of the mixed nitride uranium-plutonium fuel, and a project of near-station closed fuel cycle has been developed also. A high level of safety of the developed projects can be confirmed with the results of numerical simulations. This paper is about computational tools, developed for the support of designing and engineering objects of project «Breakthrough».

For the development of the corresponding computational tools in project «Breakthrough», a sub-project was created called «Codes of New Generation» [2]. The result of the sub-project should be a set of certified codes of new generation, belonging to the Russian Federation. A set of codes to be developed was composed by the main consumers – chief designers and scientific coordinators of the basic sub-projects of «Breakthrough» project (projects «BREST-OD-300», «BN-1200» et al.).

At the beginning of development, there were a certain set of codes in Russia designed for modeling of certain processes and phenomena at NPP with a fast reactor facility. FASO's institutions had developed certain improved models, and there was widespread use of foreign software tools. Codes of new generation should combine both commonly used engineer's methods, which are validated by large amounts of experimental data, and modern achievements in the field of physical models and numerical methods, which together with substantially increased computer productivity allow the implementation of improved methods of numerical modeling (for instance, calculations with the usage of DNS, quantum-mechanical codes) in the practice of safety justification for the checking of separate design solutions and obtaining parameters of engineering (empirical) models.

This paper provides the information on the set of codes of new generation and the current state of their development/validation/certification.

2 Set of the Developed Codes of New Generation

Table 1 shows the current state of development of codes of new generation within «Breakthrough» project at the beginning of 2017.

TABLE I: STATUS OF THE SYSTEM OF CODES OF NEW GENERATION DEVELOPMENT AT THE BEGINNING OF 2017.

Code	Comment	Development status
CRISS 5.3	Code for probabilistic safety analysis	Validated, certificated
BERKUT	Fuel rod code	Validated, first version submitted for certification
Neutron-physical codes		
MCU-FR	Neutron-physical code based on the Monte-Carlo method	Validation in progress
ODETTA	Neutron-physical code based on the kinetic approximation and on the methods of finite elements and discrete ordinates for the calculation of the reactor shielding	Validated, submitted for certification
CORNER	Neutron-physical code based on the kinetic approximation and on the method of finite differences	Validation in progress
NDP-ACE	Software for nuclear data processing	Being developed
Thermo-hydraulic codes		
HYDRA-IBRAE/LM/V1	System thermo-hydraulic code	Validated, submitted for certification
LOGOS	RANS CFD code	Validated, submitted for certification
CONV-3D	DNS CFD code	Validated, submitted for certification
KUPOL-BR	Modeling of the propagation of heat and mass transfer in the system of rooms of NPPs	Validation in progress
Codes for analysis of fission products transport in the environment		

Code	Comment	Development status
ROM	Evaluation of the radiation condition during atmospheric transport	Validated, submitted for certification
ROUZ	Code for calculation of the radiation conditions on the industrial site	Validated, submitted for certification
Sibilla	Calculation of irradiation along water pathways	Validated, certificated
GeRa/V1	Safety validation of the disposal of all types of prepared radioactive wastes	Validated, submitted for certification
Integral codes		
SOCRAT-BN/V1 SOCRAT-BN/V2	Comprehensive analysis of normal operating conditions, normal operation failure, accidents, including severe accidents, of NPPs with sodium coolant and oxide fuel	Validated, certificated Validated, submitted for certification
EUCLID/V1 EUCLID/V2	Comprehensive analysis of normal operating conditions, normal operation failure, accidents, including severe accidents, of NPPs with sodium, lead, or lead-bismuth coolant with oxide or mixed nitride uranium-plutonium fuel	Validated, submitted for certification Validation in progress
Codes for modeling processes in closed nuclear fuel cycle		
VIZART	Code for a calculation of the balance of materials and isotopic flows in a closed nuclear fuel cycle	Validation in progress
KOD TP	Code for simulating the operation of the technological scheme	Validation in progress

Brief description of codes from table 1 is shown below.

3 Code for Probabilistic Safety Analysis CRISS 5.3

Computational code CRISS 5.3 (JSC “Afrikantov OKBM”) is designed for conducting computations within the framework of probabilistic safety assessment of nuclear power plants and other nuclear facilities. Evaluation of the reliability of systems and probability safety analysis of NF is carried out using an analysis of failure trees, and event trees. Detailed information is presented in [3].

The V&V matrix for computational code CRISS 5.3 includes analytical and cross-verification tasks. A comparative analysis of results obtained by analytical formulas and software CRISS 5.3 had been conducted, as well as cross-verification of the CRISS 5.3 software with the Russian certified code CRISS 5.1 and Swedish code Risk Spectrum Professional, which confirmed not only the validity of the implemented algorithms in the code, but also its high performance in comparison with similar software.

4 Neutronic Codes: MCU-FR, CORNER, ODETTA

Within the framework of the project «Codes of New Generation» computational codes had been developed which allow modeling of neutron-physical processes in different approximations: in S_n approximation – CORNER code [4] based on the finite differences method and ODETTA code [4] based on the finite elements method; MCU-FR code [5]which utilizes the Monte-Carlo method.

CORNER code (IBRAE RAN) is designed to calculate the spatial and energy distribution of the neutron flux and its functionals, including tasks with cavities, large gradients of neutron field and problems with a high degree of attenuation of radiation. An improved quasi-static approximation had been implemented for the analysis of non-stationary processes. The code allows conducting calculations in a three-dimensional hexagonal geometry as well as in the combined geometry (to account for heterogeneous features of a specific computational model). Weighted Diamond Difference (WDD) and nodal schemes were implemented to approximate the spatial dependence.

Validation of the code was performed using experiments at the BFS, JOYO reactor facility, KNK-II benchmark-model reactor, calculations of the reactors BN-800 and BN-1200, critical assemblies BFS-44, BFS-56, BFS-58-1 and many others. The results of validation calculations give evidence of good quality modeling of such parameters as K_{eff}, efficiency of the control rods, and the sodium void reactivity effect.

The first version of the ODETTA code (IBRAE RAN, IPM RAN) was developed and submitted to the certification at the beginning of 2017. It is designed to calculate the neutron and photon fields in the shielding of fast nuclear reactor facilities.

The non-continuous linear finite element method on unstructured tetrahedral grids, construction of which is based on the selected CAD model, was implemented in the ODETTA code. Validation of the code against experiments on shielding (installation of ASPIS and EURACOS SINBAD database) proved a high accuracy of calculations of the radiation conditions of operations of nuclear facilities.

Code MCU-FR (NRC "Kurchatov Institute") [5] is a continuation of the development of MCU line of codes and is designed to model using Monte-Carlo method processes of separate and joint transport of neutron, gamma rays and charged particles (electrons and positrons) in fast nuclear facilities and objects of closed nuclear fuel cycle. Validation of MCU-FR code performed on experiments, including experiments from the International Criticality Safety Benchmark Evaluation Project (ICSBEP), experiments carried out on the BN-350 reactor, as well as experiments on the BFS, the BN-600 reactor and the reactor JOYO.

5 Hydrodynamic Codes: HYDRA-IBRAE/LM/V1, LOGOS, CONV-3D

Thermo-hydraulic calculations are playing important role in designing nuclear facilities with liquid metal coolant. Several software tools are developed in the project "Codes of New Generation", allowing modeling of the processes in the core and in the loops of the nuclear facility with a different level of detail:

- System (channel) thermo-hydraulic code HYDRA-IBRAE/LM/V1 (IBRAE RAN, JSC "OKBM "Afrikantov", JSC “NIKIET") [6] designed for a computation analysis of non-stationary thermo-hydraulic processes in the loops of liquid metal cooled reactors in normal operating conditions, normal operation failure and in case of accidents. Code allows to model behavior of sodium, lead, lead-bismuth, and water coolants. The two-phase flow (vapor and liquid) is modelled in two-phase fluid approximation.

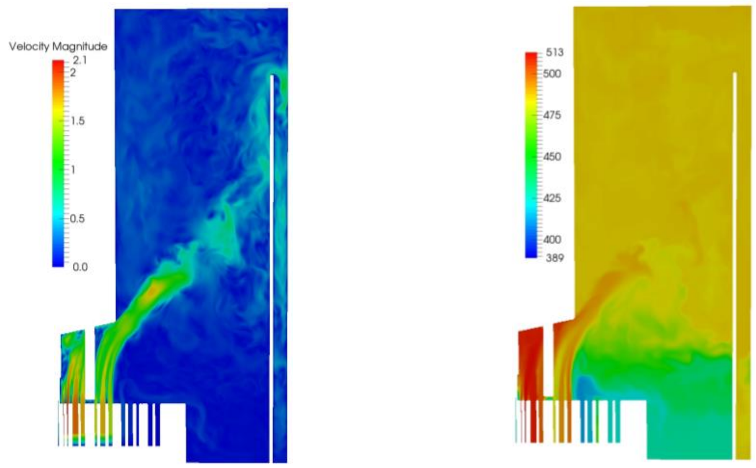
Furthermore, the code allows to model thermo-hydraulic processes carrying out in case of steam generator tube rupture (in quasi three-phase approximation), and air heat-exchangers. Correlations, that are implemented in the code, validated on a wide range of experimental data, received as in Russia (SPRUT (JSC "IPPE"), VTI (JSC "NPO CKTI), nuclear facility BOR-60 and BN-600, and others), as well as abroad (the HELIOS (South Korea), LIFUS-5 (Italy), SIENA (Japan), KNS (Germany), THORS (USA) and others) on lead, lead-bismuth, and water coolants. Implemented in the code technology allows to add and conduct calculations for user-defined coolants from the data base (for instance for the glycerin). Validation of the results showed satisfactory precision of calculated parameters such as temperature of the coolant, pressure, steam and gas concentration;

- CFD code LOGOS (VNIIEF) with RANS models of turbulence designed to calculate flows of the coolant, including mixturing of different temperature streams, natural and forced convection, as well as heat exchange with solid elements of the equipment of fast nuclear reactor facility. Calculations are carried out in the three-dimensional setting with numerical integration of Navier-Stokes equations using the control volume method. Coolant is assumed to be a single phase, one component fluid. Code is validated on the representative set of experimental data, received on nuclear facilities BN-600 and MONJU, installations for the study of mixturing of different temperature flows of heavy liquid coolant in IT SO RAN, test facility of Institute of Continuous Media Mechanics, TEFLU facility (Germany) and others [7]. According to obtaining results, the estimated error of calculation of pressure drop, velocity of the flow, and temperature is not higher than 15%;
- DNS code CONV-3D (IBRAE RAN) [7, 8] designed for calculation stationary and non-stationary laminar and turbulent flows of the coolant, as well as heat exchange with solid elements of the equipment of fast reactors during forced convection, caused by temperature inhomogeneity and/or volumetric heat generation, including mixing of flows with different temperatures. Calculations are carried out in the three-dimensional setting with numerical integration Naiver-Stokes system of equations for an incompressible fluid. Method of finite volumes is used for the numerical integration, based on irregular Cartesian mesh and fictitious domain method. Implicit time difference scheme of first and second order is used for solving the corresponding system of difference equations.

  Validation base for codes LOGOS and CONV-3D is the same. According to results of validation, code CONV-3D has higher accuracy, but taking significant computational resources [7]. Figure 1 presents results of calculation of velocity (a) and temperature (b) fields for the upper plenum of reactor facility MONJU [9] with sodium coolant obtained with the code CONV-3D. The direction of flow and range of the calculated velocity and temperature values have satisfactorily agreement with the experimental data.

6 BERKUT Fuel Rod Code

The code BERKUT (IBRAE RAN) [10] is designed for multi-scale mechanistic modelling and justification of operability and safety of fuel rods with different types of fuel (uranium dioxide, mixed oxide fuel, mixed nitride uranium-plutonium fuel) for the perspective cores of fast nuclear reactors with liquid metal coolants (sodium, lead, lead-bismuth) under normal and emergency conditions, during transients and accidents.



a) *b)*

FIG. 1. Velocity (a) and temperature (b) fields of sodium coolant in the upper plenum of reactor facility MONJU, obtained by the code CONV-3D.

The code provides self-consistent description of the thermomechanical state, heat and mass transfer processes occuring in the fuel rod, evolution of fuel microstructure. The temperature distribution and stress-strain state of the cladding and pellets are modeled together with damage accumulation, isotopic, molecular and phase composition of the fission products, their generation, transport and release into the gap, fuel swelling.

The validation of the code is performed on the experiments on irradiated fuel rods with oxide and mixed nitride uranium-plutonium fuel in nuclear facilities BN-600, BOR-60, PHENIX, confirmed a satisfactory quality of modeling of composition and quantity of fission products, released in the gas gap, the temperatures of the fuel and the cladding, and the value of fuel swelling irreversible deformations of the cladding and others parameters.

7 Codes for Simulation of Fission Products Transport in the environment: ROM, ROUZ, SIBYLLA, GeRa/V1

Computational code SIBYLLA (IBRAE RAN) [11] is designed for the calculation of parameters of radiological situation, formed in the surface of freshwater objects that are actually or potentially affected by nuclear facilities:

– the content of radioactive substances in water, sediment;

– doses for the population, formed due to the different types of water consumption, including drinking water.

Code allows for modelling radiological situations in the water bodies during normal operating conditions of the nuclear facilities, or during normal operation failure and accidents.

The code is based on the numerical solution of the equations of transport and dispersion of radionuclides in the water, taking into account their interaction with sediments and suspended particles in the water. The V&V matrix includes: measurements of the quantity of radioactive substances in water and sediments of lakes Svyatoe, Esthwaite and Windermere; data measurement of the quantity of ^{137}Cs in the water of the river Plava; data measurements of the quantity of ^{239}Np in the water of the river Tom; data measurements of the quantity of ^{137}Cs and ^{239,240}Pu in the river Techa; data measurement of the quantity of ^{90}Sr in the water of Lake Tygish; data measurement of the quantity of ^{137}Cs in bottom sediments of the Kiev reservoir.

Validation results showed that in 95% of cases the difference between calculated and measured data does not exceed 3 times.

The ROM code (IBRAE RAN) [12] is designed to calculate the transport of released fission products and doses for population outside the industrial site of NPP or other nuclear facilities. The code implements the Lagrangian trajectory model of the spread of radionuclides in the atmosphere, which makes a statistically more realistic (less conservative) estimation of the radiation situation on large distances in comparison with Gaussian models. The code has the possibility of using real meteorological data series from recent years for the given object in assessing the impact of prolonged releases (duration of several days or more). It also allows avoiding excessive conservative assumptions about the weather situation. Along with a set of commonly used radioactive products for water reactors, the models of the rate of deposition of aerosols produced by sodium burning products and polonium, which expands the scope of code application to liquid metal cooled reactors, are implemented.

Validation of the code was performed on a series of mesoscale experiments on atmospheric dispersion of contaminants conducted in the 80s in KfK (Germany), in a number of experiments in other European laboratories, including calm-wind conditions, as well as full-scale industrial experiments with the release of large volumes of natural gas conducted by VNIIGAZ together with other organizations during 1970-1977. According to the results, the ROM code provides an unbiased estimate of surface impurity concentration. Peak magnitude is predicted quite accurately at all distances for all points in time, the deviation does not exceed 3 times with a probability of 90%.

Code ROUZ (IBRAE RAN) [13] is designed to model the spread of impurities in the atmosphere in a real three-dimensional geometry of the object, calculate dosages for different ways of exposure (from the cloud of arbitrary shape, from deposition by inhalation). Code ROUZ includes the module for calculating the three-dimensional wind velocity field based on the solution of the Navier-Stokes equations, module for the calculation of atmospheric turbulent advection-diffusion of impurities in the gas and aerosol form.

The ROUZ code uses the k-ε turbulence model, modified for taking into account the stratification of the atmosphere and the usage of boundary conditions for k and ε, which does not require refining of the computational grid near solid surface. Special models while simulating the atmospheric transport in industrial build-up for recovery parameters of the oncoming flow (atmospheric boundary layer based on limited information - class stability and wind speed and direction on the wind vane height), and three-dimensional digital representation of the objects reflecting the dimensions of buildings and installations and the relative distances between them are used.

Large-scale field experiments were involved for the validation of the code: in Oklahoma 2005 (US), MUST experiment (the Great Basin Desert, USA), as well as laboratory experiments on special installations SEDVAL and WOTAN (University of Hamburg, Germany). The validation matrix contains about 10,000 points for comparison. As a result of the code validation it is established that a deviation of the calculated wind speed components is less than 2 times relative to the measured values with a probability of 95%, and the deviation of the calculated impurity concentration from measured ones does not exceed 2 times with a probability of 78%.

The result of the calculation of the impurity concentration in Oklahoma for the experiment are shown in Figure 2.

Code GeRa/V1 (IBRAE RAN and INM RAS) is designed for the solution of problems of waste disposal generated in a closed nuclear fuel cycle, from the point of view of the possible migration of radionuclides in groundwaters [14]. The scope of application of the code is solving the problems of filtration and transport in geological environments based on different physical and chemical processes, including density and thermal convection, chemical reactions, radioactive decay, and others.

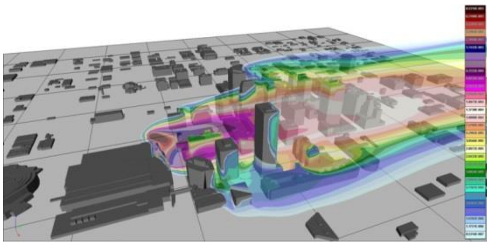


FIG. 2. The result of the calculation: Isosurfaces of volumetric concentration of the tracer experiment in Oklahoma.

Code GeRa/V1 is an integral code, allowing the carrying out of a full cycle of the calculation for safety assessment, starting from the creation of a geological model of the object and ending with the calculations of consumed water activity and doses for the population. V&V of models of saturated and unsaturated filtration, mass transfer and density convection, transfer with chemical interactions were carried out on a number of problems with analytical solutions and results of full-scale experiments. Besides the cross-verification of GeRa/V1 code with foreign codes FEFLOW, MODFLOW, MT3DMS, HYDRUS and others was performed.

8 Integrated Codes EUCLID/V1, SOCRAT-BN

In the safety analysis, together with an analysis of the individual processes is very important to use the integrated computer codes that allow a comprehensive analysis of the behavior of radiation hazardous objects under various conditions - from the normal to emergency conditions of operation, including accidents with core melting.

Two versions of the code had been developed - EUCLID/V1 and EUCLID/V2 (IBRAE RAN, JSC "OKBM "Afrikantov", JSC “NIKIET"). Code EUCLID/V1 [15] is designed for the numerical simulation of thermal-hydraulic, neutron-physical and thermo-mechanical processes in the fast nuclear reactors in the conditions of normal operation, design and beyond design basis accidents. The code allows calculating parameters such as temperature, flow, pressure and phase composition of the coolant, as well as temperatures of structural materials, fuel and fuel cladding, the neutron power, stresses, strains and displacement in the fuel pellets and fuel claddings.

The main modules are: HYDRA-IBRAE/LM/V1 (thermal hydraulics), DN3D (module for simulation of spatial diffusion neutron kinetics in conjunction with the module CORNER in the kinetic approximation), BERKUT (module for calculations of cladding stresses and strains, fission product release into the gap), BPS (burnout calculation module), OSTB (module for the calculation of decay heat).

The second version of EUCLID/V2 code allows calculating accidents with core melting and the release of radioactive fission products. In addition to the above listed modules of the first version, the following modules are added: SAFR (core melting and destruction), AEROSOL-LM (transport of fission products in the loops), KUPOL-BR (mass transfer in the rooms), ROM (transport of the fission products in the environment).

Validation base includes both experiments on separate phenomena’s (as described above for the each module) and integrated experiments on the nuclear facilities BN-600 and BOR-60.

Integral Code SOCRAT-BN (IBRAE RAN, JSC "OKBM "Afrikantov", SSC RF TRINITY) is designed for numerical modeling (in the engineering approach) of SFRs behavior under DBA and BDBA conditions from initial set of events up to release of FP to environment. Used engineering approach allows performing calculations in a relatively short period of time and with reasonable accuracy. Code was validated on the wide range of out-of-pile and in-pile experiments. Currently the development of SOCRAT-BN code is completed and it is applied for the safety assessments of SFR NPPs (BN-600, BN-800, BN-1200).

9 Code VIZART for a Calculation of the Balance of Materials and Isotopic Flows in a Closed Nuclear Fuel Cycle

The VIZART code (FSUE “RFNC-VNIITF”, JSC “VNIINM”) is designed for the simulation and optimization of the individual processes of the closed nuclear fuel cycle (reprocessing of spent nuclear fuel, re-fabrication of fuel, and radioactive waste management, including disposal), nuclear fuel cycle technologies and closed nuclear fuel cycle as a whole.

Technological schemes builder and a library of technological models of the VIZART code provides the flexibility to change the composition of the computational scheme and the parameters of technological processes, thereby increasing the number of options under consideration and reducing the time required for analysis and decision making.

The presence of specialized modules in the software complex allows calculating specific parameters of the radiochemical processes, such as maximum one-time content of nuclear materials in containers and devices, taking into account the evolution of the isotopic composition of the nuclear fuel components and therefore, a change in the chemical properties, radioactivity, and energy release characteristics. These calculations are used to estimate the effect of energy release of products on the operating temperature of the processes and the equipment, furthermore to determine the final shape and volume of radioactive products, as well as to support safety of nuclear technologies used.

10 Conclusion

Within the framework of the sub-project “Codes of the New Generation” of “Breakthrough” project the first stage of the development of system of codes with various degrees of complexity is being finalizing. The codes allow solving main tasks of safety justification of the NPP with fast reactors designed in Russia in frame of Federal Target Program “Nuclear power technologies of a new generation for 2010 – 2015 and for the future till 2020”. A set of codes include both standalone codes and integral (integrated) codes, which are built through the integration of individual components of a system of codes into a unified software package.

The system of codes allows the conducting of a consistent multi-physical and multiscale analysis of operating and emergency regimes, including conduction of PSA levels 1, 2 and 3.

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