New neutronic calculation codes based on discrete ordinates method using methods of finite differences and finite elements

Bereznev V.P.[1], Belousov V.I.[1], Grushin N.A.[1], Seleznev E.F.[1], Sychugova E.P.[1]

[1]Nuclear Safety Institute of the Russian Academy of Sciences (IBRAE RAN), Moscow, Russia

E-mail contact of main author: bvp@ibrae.ac.ru

Abstract. CORNER and ODETTA codes for neutrons and photons transport based on discrete ordinates using finite differences and finite elements methods have been developed as a part of the new generation codes for the construction and validation of the perspective FBR safety. Modern CONSYST software is used for the preparation of the macroscopic cross sections. Both eigenvalue (k_{eff}) and fixed source problems can be solved, including joint calculations of neutrons and gamma rays. The principal application is solving transport problems with deep penetration. OpenMP technology is applied for parallel computing. The CORNER code allows calculations in three-dimensional hexagonal and combined geometry (to account for the heterogeneous features of the computational model). Weighted Diamond Difference and nodal schemes are used to approximate the spatial dependence. The calculations have been performed for models of BN-800 and BN-1200 reactors, and for BFS critical assemblies. ODETTA code uses discontinuous linear finite element method on unstructured tetrahedral meshes, based on the selected CAD model with Salome and Gmsh programs. Space rebalance method and δ-process are used to speed up the inner and outer iterations respectively. Results of code validation against safety experiments ASPIS and EURACOS from SINBAD database and cross-verification on a test model of the reactor BN-1200 are presented.

Key Words: radiation safety, neutron transport calculation, discrete ordinate method, finite elements method

1. Introduction

Industry codes for neutrons and photons transport based on discrete ordinates (S_n) using methods of finite differences and finite elements have been developed to achieve the goals of the Development Project of fast breeder reactors (FBR). It's a part of the new generation codes for the construction and validation of the security perspective FBR, the design of nuclear power plants, the creation of technologies and Closed Nuclear Fuel Cycle (CNFC).

Developed codes (CORNER [1] and ODETTA [2]) significantly expand the scope of S_n approximation in design practice and the safety of Nuclear Power Plant (NPP) and CNFC facilities in the case of the calculating neutron and photon radiation transport with high attenuation in safety regions, verification nuclear and radiation safety in the handling of nuclear materials and radioactive waste at all stages of the fuel cycle in a reasonable time calculations thus expanding the range of tasks within acceptable errors of calculation modeling compared to the existing design codes.

2. Codes description

2.1. Calculation code CORNER

Calculation code CORNER is based on S_n discrete ordinates method and P_m scattering cross-section approximation and is designed for precise deterministic neutrons and photons calculations of FBR and its safety.

Calculations can be carried out in a three-dimensional hexagonal geometry and in combined geometry to account for the heterogeneous features of the computational model. Weighted Diamond Difference and nodal schemes have been applied to approximate the spatial dependence.

The energy dependence is represented by multigroup approximation. Modern CONSYST software is used for the preparation of the macroscopic cross sections.

The angular variable is discretized by introduction of the angular quadrature sets. The CORNER code supports Level Symmetric (LQ_N) and Legendre-Chebyshev (P_N-T_N) quadrature sets.

An iterative solution process is used, including external iterations for the fission source and internal iterations for the scattering source. It provided a way out of an iterative process, both in terms of accuracy, and the number of iterations.

The CORNER code is developed in the Fortran language and has a modular structure. Its key modules are:

- module for the preparation of neutron constants in the ANISN format;
- geometric module containing a description of the core's loading map and fuel assembly types, including their axial meshing and material composition;
- module for preparing angular quadrature sets;
- an input data module containing the parameters of the approximation used and the control parameters;
- neutronic calculation module and a calculation data processing module.

OpenMP technology is applied for parallel computing.

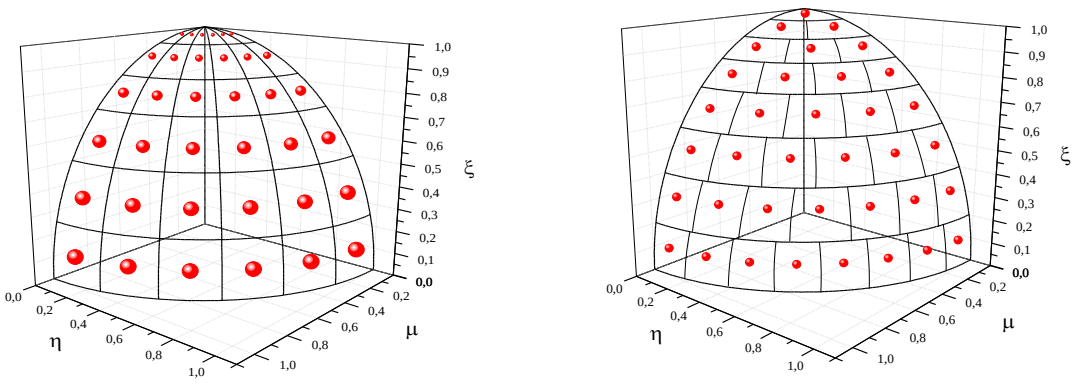
The CORNER code and its individual modules tested to FBR models: BN-600, BN-800, BN-1200 for stationary and transient problems.

2.2. Calculation code ODETTA

ODETTA [1] transport code developed for solving the stationary multigroup neutron and gamma rays transport equation using discrete ordinates method and discontinuous linear finite element method on unstructured tetrahedral meshes.

Space rebalance method [3] and δ-process [4] are used to speed up the inner and outer iterations respectively. The anisotropic scattering represented by the expansion in the series of associated Legendre functions of arbitrary order. Two types of quadrature sets can be used: triangular (ESN Carlson quadrature with equal weights) and square (Chebyshev-Legendre quadrature) (Figure 1).

Three types of boundary conditions for the incoming values of the angular fluxes are defined: the first type is vacuum (i.e. set to zero incoming flows at the external borders of the computational domain), the second type is the reflection conditions and the third type is a given non-zero input flux.



a b

FIG. 1. Types of quadrature sets used in ODETTA code (a – ES_8 Carlson, b – CL_6 Chebyshev-Legendre)

Dynamic allocation of memory in conjunction with the algorithm parallelization by the angular directions is implemented in ODETTA code.

ODETTA code operates on Microsoft Windows systems, including Windows XP 32/64, Windows Vista 32/64; Windows 7 32/64, Windows 8 32/64; on single-processor computers with single-core or multi-core processors.

Technical equipment must satisfy the following system requirements: CPU is compatible with the x64 architecture, with a 1 GHz or higher (recommended Processor: Intel Core 2, Core I3, I5, I7; Intel Xeon E3, E5, E7); amount of RAM 2 GB or more; available amount of disk space at least 100 MB.

ODETTA code can be easily adapted to any type of modern computers with Windows operating systems, Linux and Unix. Machine-dependent additional structural possibilities kept strictly localized and are not included in the routines that perform basic computing functions.

Computation time depends on the problem type (fixed source calculation, k-eigenvalue calculation etc.) and the mesh size (number of nodes, number of the angular directions, number of energy groups etc.) and can vary from several minutes to several days.

ODETTA uses unstructured tetrahedral meshes, built on the corresponding CAD-model. One of the advantages of such mesh is the possibility of detailed description of complex geometries. Another advantage is possibility of building a larger mesh in areas where properties do not change significantly, and thus reducing the computation cost.

SALOME program [5] is used for the construction of unstructured tetrahedral meshes. CAD-model is imported in SALOME and checked for defects. The parameters of computational mesh is specified by the user. The next step is to analyze the constructed mesh and its characteristics. At the last stage the mesh is exported to an external file. From SALOME mesh imported in binary format *.med. Using this format can save the names of parts contained in the CAD-model. It's not possible to run the binary file directly, so it is converted into a format *.msh using mesh generator Gmsh. In this format, grid data is presented in a text file in ASCII format.

Set of 12 numbers for each tetrahedron is required for using mesh in ODETTA codes: numbers of 4 vertices, numbers of 4 neighboring tetrahedrons, the types of boundary conditions on the 4 faces of the tetrahedron. In addition, the list of correspondence between the tetrahedrons and the number of the physical areas in which they are located is required.

CONSYST-RF [6] software with ABBN-RF [6] multigroup library is used as a main cross section preparation system but other libraries with AMPX format can be used for calculations.

Figure 2 shows a block diagram for ODETTA code. In addition to the computational mesh user generates a configuration file. In this file, the type of boundary conditions, the type of problem (k-eigenvalue problem, fixed source problem), the type and order of the quadrature set are defined. It is necessary to prepare the additional file for fixed source to solve the corresponding problem. If the source parameters are known a priori, the user generates the source file by using the implemented module. It is possible to calculate k-eigenvalue and as a result, to obtain the neutron source distribution.

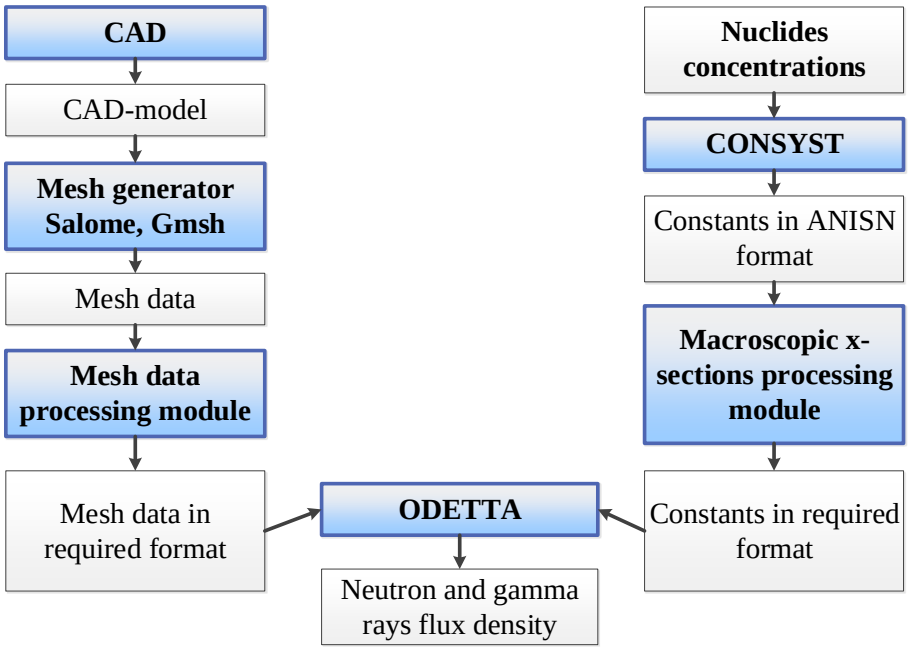


FIG. 2. Structure of ODETTA code.

Multigroup calculations require using of big size data (hundreds of gigabytes to several terabytes). Obviously, the volume of memory (RAM) for such data may be insufficient, so this problem was proposed to solve as the use of more disk space memory (ROM) for the individual arrays.

To implement the proposed solutions MassiveFile module was created in Fortran-90, which includes mfArray class (Massive File Array). This class allows storing an array of data on disk as a file. Array file size is determined by the size of the available space. Creating and removing array file implemented by the constructor and destructor of the class. Default destructor saves the data set file on the disk. Access to an array of file is made through the corresponding read and write operations. Thus, the read operation implements the retrieval of data at the specified index from a file into an array, located in RAM. Similarly, the write operation is implemented for storing data in an array of the ROM-RAM file array. It is allowed to rename and copy the file array.

At the end of the calculation angular moments of the neutron and gamma rays flux are recorded in the archive file into groups of four vertices of each tetrahedron. Processing the results of the calculations is to compute a variety of functionals, which are specified by the user. At this point it is possible to calculate the following functional:

– neutron flux and gamma rays density of different energies;
– spectrum of neutrons and gamma rays;
– neutron flux density with energy above 0.1 MeV;
– the rate of gain in damaging dose to the elements of the pin, fuel assembly, reactor equipment, etc
– the distribution of neutron reaction speed on selected volumes, types of nuclides and reactions;
– the components of neutron balance integrally throughout the core, the subdomains, the isotopes, including the relative amount of the produced and absorbed neutrons, the number of fissions and the number of neutrons leaking;
– the energy (heat) in local volumes with the the axial and radial distributions on the core in a user-selected regions and sectors; and etc.

Computation of the functional at the given points of the spatial region is carried out by solution reconstruction in the tetrahedron calculated by linear interpolation at the vertices of the average values of the flux density. Since the point can be placed on the border of the two zones, user must specify the number of the zone, which belongs to this point and where output interpolation result is placed. Thus, it is possible to calculate the value of the total flux or the values of response functions along the length of the given line. In the future it is expected to define arrays of points on the plane. It is possible to output the spectrum values at given points.

3. Nuclear safety calculations with ODETTA

Within the code verification calculations experiments were conducted performed on plants ASPIS and EURACOS, which simulate reactor safety compositions of low carbon steel and stainless steel, and graphite (JANUS experiments Phase 1, IRON 88 and ISPRA Iron contain low carbon steel and stainless steel, an experiment Winfrith Graphite Benchmark contain graphite, JANUS experiments and Phase 8 ISPRA sodium had protective material sheet steel tanks and sodium). Descriptions of the experiments are taken from the SINBAD 2000 database [7]. The principle of the experiments: the output beam of neutrons from the reactor irradiates fuel plates in the converter, thereby forming a neutron source, distributed over the fission spectrum. Detectors are located in safety regions behind the converter along the central axis of the fuel to measure the rate of the reactions on their material (Figure 3).

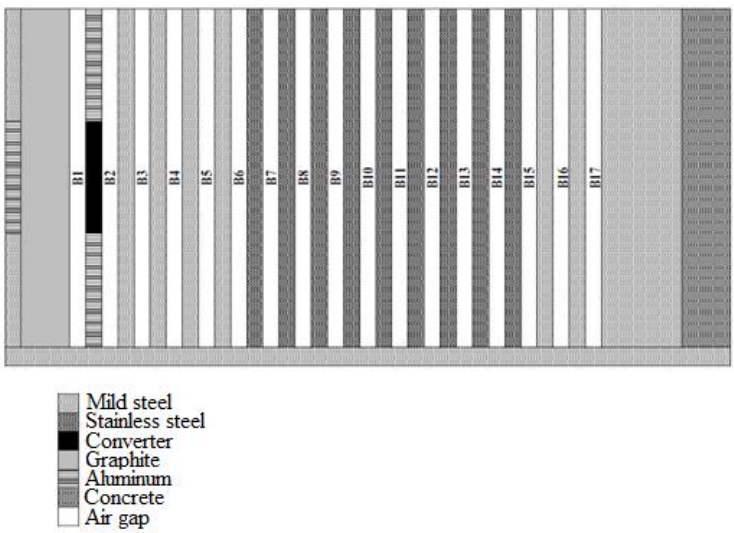


FIG. 3. JANUS Phase I scheme experiment

The results of calculations are presented for P_3 scattering approximation with S_{12} Chebyshev-Legendre angular quadrature, which consists of 288 discrete areas. In Table I, for example, the main characteristics of the spatial grid and neutron constants used in some experiments are presented.

TABLE I: THE MAIN CHARACTERISTICS OF THE SPATIAL MESH AND NEUTRON CONSTANTS

Model	The number of tetrahedrons	The number of nodes	The number of energy groups
Janus Phase I	2506067	428152	175
Winfrith Graphite Benchmark	1420595	249032	299 ABBN-RF

In these experiments, measurements were made on the threshold detectors. Reaction rates were measured: Au^{197} (n, γ) Au^{198}, S^{32} (n, p) P^{32}, In^{115} (n, n') In^{115m}, Rh^{103} (n, n') Rh^{103m}, Al^{24} (n, α) Na^{24}. Table II identifies the approximate reactions thresholds used in the experiment.

TABLE II: THRESHOLDS REACTIONS USED IN THE EXPERIMENTS

	^{27}Al (n,α) ^{24}Na	^{32}S (n,p) ^{32}P	^{115}In (n,n')^{115m}In	^{103}Rh (n,n')^{103m}Rh	$Au^{197}(n,\gamma)Au^{198}$
E≥, MeV	3,25	0,95	0,33	0,04	-

Figure 4 shows the calculated reaction rates relationship to the experimental data (C / E) for JANUS Phase 1 experiment with sulfur detectors. The calculations were performed on DORT program [8] (S_n finite-difference) and ODETTA (S_n finite element method) using a 175 group library [9], prepared on the files of evaluated nuclear data ENDF / B-6 Version 8.

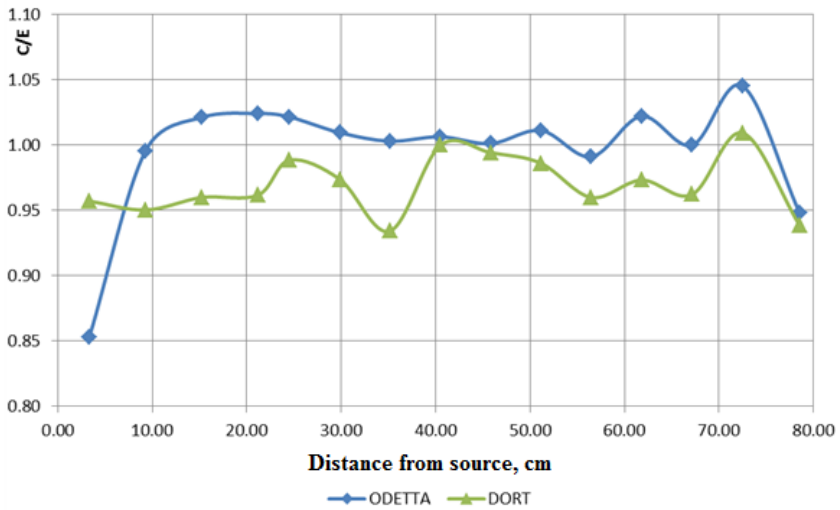


FIG. 4. The ratio of the calculated reaction rate to the experimental for sulfur (S) detector.

Consideration the angular dependence, i.e. namely the use of S_n approximation allowed to perform calculations with a voided core layers, and the program has successfully managed with such problem. Good agreement of numerical results with experimental data is received from the presented data.

Figure 6 shows the estimated rates of reactions to the experimental data for Winfrith Graphite Benchmark experiment [10] obtained under different programs, including DORT (of S_n in

finite differences) used the 175 group library, MCBEND (Monte Carlo) used DICE VI Data Library (100 groups), and the KATRIN (S_n in finite differences, rectangular geometry), CORNER (S_n in finite differences, hexagonal geometry) and ODETTA (S_n, finite element method) using ABBN-RF 299 group library.

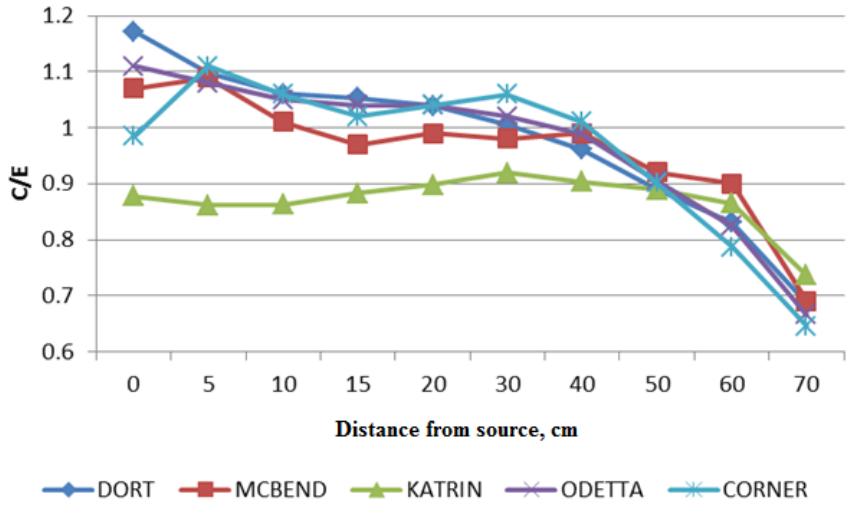


FIG. 5. The calculated reaction rate related to the experimental data for rhodium (Rh) detector obtained by the various programs.

As a result of comparison of calculations performed using ABBN-93 and ABBN-RF libraries, it was found that ABBN-RF library provides a more correct result than ABBN-93 (Figure 8).

Computational researches provided the range of calculation errors of neutron flux density and its dependent characteristics appearing in the Table 3. Errors are given based on experimental data errors.

TABLE III: RANGE ACCURACY FOR THE NEUTRON FLUX DENSITY

Characteristics	Materials	Total thickness	Range of errors
Total neutron flux density (E>0 eV)	Low Carbon Steel, stainless steel, sodium, graphite, aluminum, and boron carbide in various combinations	Up to 306 cm (455 cm considering air gaps)	10-35 %
Neutron flux density (E>0.1 MeV)			5-25 %
Neutron flux density (E>0.5 MeV)			5-20 %
Rate of receiving damaging dose			10-35 %
The rate of activation of reactor construction materials and technology environments			5-35 %
Radiation energy			5-35 %
Neutron and photon radiation dose rates			35 %

4. Critical assemblies calculations with CORNER

Critical assembly BFS-58-1 models sodium-cooled fast breeder reactor. The core of BFS-58-1 assembly includes the central low-enriched zone of MOX fuel and two peripheral zones of uranium loading with medium and high enrichment.

Sodium plenum is above the core, boron carbide is above the plenum, blanket of depleted uranium dioxide is under the core.

BFS-58-1 consists of steel tubes of 5.0 cm diameter, arranged in a hexagonal lattice with a pitch of 5.1 cm, in which pellets are stacked (fuel pellets, pellets simulating coolant and constructional materials pellets).

The core of the critical assembly BFS-58-1 contains cells with a plane structure. The structure of the fuel cells is shown in Figure 6.

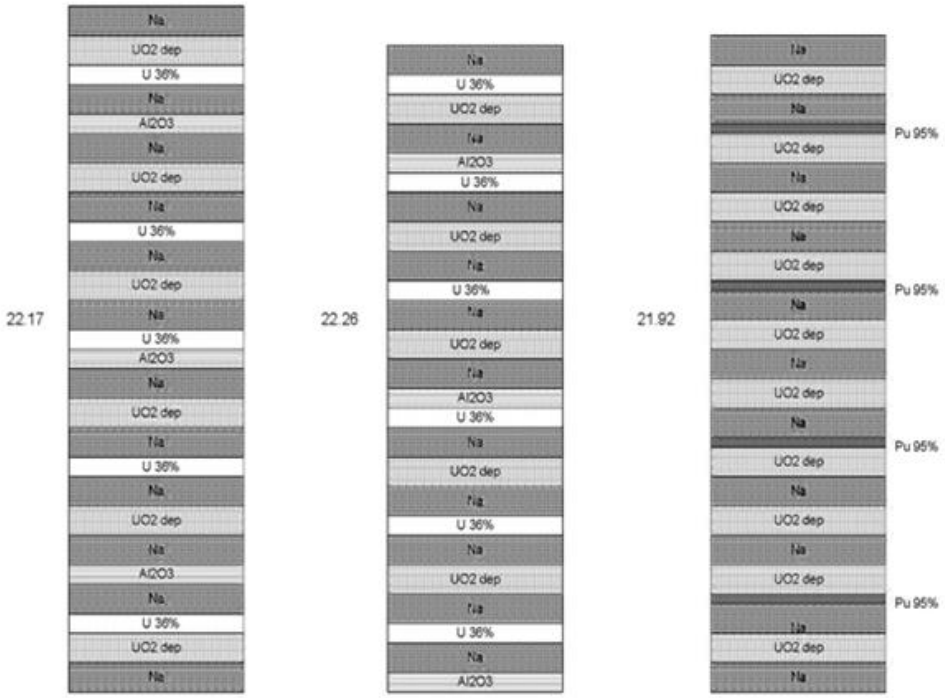


FIG. 6. Structure of the fuel cells.

CORNER can consider the heterogeneity of the fuel cells in the axial direction. Auxiliary problem is solved for each cell type to determine the neutron flux. The scheme of this problem is a set of plane layers that simulate pellets. Calculations of space-energy neutron flux distribution in the cell are performed. Further averaging of multigroup cross sections Σ_x^g of x type and fission neutron spectrum χ^g in the range of cells with the weight of neutron flux φ_k^g and volume V_k of pellets is performed.

$$\Sigma_x^g = \frac{\sum_k \Sigma_{x,k}^g \varphi_k^g V_k}{\sum_k \varphi_k^g V_k}, \quad \chi^g = \frac{\sum_k \chi_k^g V_k \sum_{g'} \nu\Sigma_{f,k}^{g'} \varphi_k^{g'}}{\sum_k V_k \sum_{g'} \nu\Sigma_{f,k}^{g'} \varphi_k^{g'}}.$$

Prepared macroscopic cross sections are used in the calculation of the critical assembly BFS-58-1. Effect of heterogeneity in the assessment of K_{eff} for different configurations of critical assembly is about 0.7%.
Calculations of critical assembly BFS-58-1 is carried out in a 26-group S_4P_1 approximation. The accuracy of the convergence of external and internal iterations was set equal to 10^{-5}.
Estimates of effective multiplication factor K_{eff} and sodium void effect reactivity (SVER) are made. Calculated value of SVER was estimated based on K_{eff} of two k-eigenvalue problems in which the coolant is present in the investigated region (k_1) and removed from the region (k_2):

$$SVER = \left(\frac{1}{k_1} - \frac{1}{k_2} \right) \cdot 10^5, \; pcm$$

Table IV describes the calculated states of BFS-58-1 for SVER evaluation.

TABLE IV: THE CALCULATED STATES OF BFS-58-1.

State	Sodium in core	Sodium in plenum	Changing the number of tubes on the periphery
1	+	+	
2a	–	+	
2b	–	+	– 5
3a	–	–	
3b	–	–	+ 58
4a	+	–	
4b	+	–	+ 5
5	+	+	

Comparison of calculations with experimental data for the SVER is given in Table V.

TABLE V: COMPARISON OF THE SVER.

Calculation	CORNER	Experiment
1 → 2a	112	105
2b → 3a	–648	–718
3b ← 4a	46	20
4b ← 5	–533	–624

The calculated values are in good agreement with the experimental data.

5. Conclusion

The results of the verification ODETTA code for nuclear safety show a good agreement between the calculated and experimental results in problems with steel and graphite. The range of deviations from the experimental values is from about 10% to regions adjacent to the source, and about 30% for regions distant from the source at a multiplicity of weakening total neutron flux of 1000 or more.

Critical assembly calculations show that the effects of heterogeneity are significant in the core so accounting BFS fuel pellets structure yielded good agreement with experimental data. In the analysis of experiments with voided sodium plenum kinetic effects play a major role, so using S_n method in the CORNER code allows to get a good accuracy.

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