System of coordinated calculation benchmarks for a fast reactor with sodium coolant in closed fuel cycle

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Abstract. System of benchmarks of the class "tests" with prototype for neutron-physical calculations of the BNtype reactors with nitride uranium-plutonium fuel is presented. The system includes benchmarks for models: cell, fuel assembly with end elements, active core, protection of the reactor installation. The system is intended for verification of the codes including constant support, methods and algorithms of calculation, scenarios of operation in closed fuel cycle. World experience of creation of the calculation benchmarks was used for the development of this system. Cases of analysis of nonlinear deformations of the active core and transition of the reactor to the equilibrium mode of operation are included. Formulation of test cases was based on the following principles: conformance of the benchmark model with the range of studied effects, founded rejection of unnecessary detail in models and material compositions, uniform information for construction of geometric models and the agreed size. System combines 6 types of benchmarks. The results of benchmark calculations made by the authors using codes CONSYST (ABBN-RF), MCU, JARFR, MMK, SCALE are presented.

Key Words: BN-1200, closed fuel cycle, benchmarks development.

1. Introduction

Test cases in the field of neutron-physical and thermal-hydraulic calculations can be presented in several categories depending on the way of defining the geometry and cross sections and/or composition, applications and information sources (this is not the only possible method of classification):

1. Mathematical test. Computational (mathematical) test with specified coefficients to solve equations that have no real prototype.

2. Mathematical test with Prototype. Computational test with the real reactor prototype, with full original data, allowing to obtain relatively accurate solution (all necessary macro- and microscopic cross sections and constants are specified).

3. Prototype-Operational test. Test with real reactor prototype but without values of the constants. Densities of the materials approximately correspond to the real compositions. Some other features can also be simplified in comparison with the prototype.

4. Operational test. Test, which models a real reactor without values of the constants. Sometimes these tests are called design or operational tests. The density of materials and/or other data accurately correspond to any real condition of the simulated reactor. Values of

calculated functionals in such tests are based, as a rule, on experimental data and are used for validation of programs. Tests of this type are sometimes not intended for public distribution, especially in the case of large efforts spent on evaluation of the experimental data, as well as in cases there are potential buyers.

Nowadays computational tests are intended to replace experimental tests because of high cost of experiments. Unfortunately, the number of test cases on fast reactors is small, some of them could be found in [1-4].

At present, scientists continue to work on the various concepts of BN-1200 reactor. Developed benchmarks are focused on the concept and design of high power reactors with sodium coolant, uranium-plutonium nitride fuel, and high values of fuel burnup. Typical features of these reactors are increased diameter of the active core and its considerable flattening. Fuel assemblies (FA) have large size of fuel elements and therefore increased fuel volume fraction with the respect to the core volume. Specific feature of these concepts is abandonment of application of separate zones of fuel reproduction in radial and axial directions. In order to flatten power release, fuel assemblies with increased diameter are used in the peripheral rows of the active core. Starting loading with the same fuel isotopic composition throughout the whole reactor is considered.

It is intended to reuse irradiated fuel in the reactor after cooling and processing. The secondary fuel is formed from uranium and plutonium extracted from irradiated fuel assemblies with account of fixed losses during processing. Burnt fuel mass is compensated by depleted uranium and, if necessary, plutonium with the isotopic composition of the starting loading of the reactor.

The following base principles were applied in the development of the system of coordinated calculation benchmarks:

- Separation on the basis of the size of simulated system,
- Denial of excessive details in models and structures,
- Compatibility of the benchmark model to the range of studied effects,
- Uniform information for building of geometric models and the agreed size,
- Universal information about material compositions, including irradiated fuel.

2. System of coordinated calculation benchmarks

System of benchmarks presented in this work belongs to computational tests with one of the projects of BN-1200 reactor as a prototype. The system includes benchmarks consistent by geometric and material parameters simulating different geometric elements of the reactor: fuel element, fuel assembly, active core, active core with the environment. Consistent transition from simple geometry to more complex one allows to identify the causes of discrepancies in the results on early stage of cross-verification of codes.

2.1.Benchmarks in 0-D and 1-D geometries

Benchmarks are designed to test constant support and modules of isotope kinetics. Neutronphysical characteristics of starting fuel downloads, their change during the irradiation, and compositions of irradiated fuel assemblies of BN-1200 reactor are determined. The cases are formulated both in homogeneous and heterogeneous statement for different types of plutonium isotopic composition in the fresh fuel. Equivalent cell of fuel assembly (FA) BN-1200 (figure 1). Simple geometry allows to study in detail the calculation of burnup, and also to compare models and approach at preparation of the constants, which were used in the various programs of the calculation.

Horizontal cross-section of FA of BN-1200 (figure 2). The model correctly takes into account the ratio of volume fractions of fuel, structural materials, and coolant in the core.

Vertical cross-section of FA of BN-1200 (figure 3). Multi-zone model takes into account the axial change of properties of fuel assemblies, structure elements (SE) above and below the core, end leakage from the reactor. Figure 3 presents the calculation model of FA, which takes into account the nonuniformity of change of the isotopic composition in the fuel zones 1-5. Calculations demonstrate that the chosen model allows predicting correctly multiplication properties of the entire reactor.



Figure 1. Equivalent cell of fuel assembly of BN-1200 reactor



Figure 2. Horizontal cross-section of FA calculation model



Figure 3. Vertical cross-section of FA calculation model

For all benchmarks, the history of FA irradiation is assigned the same: 6 in-core fuel lives - 330 days of operation at a given power, 30 day shutdown of the reactor. Recommended calculation steps in time: 3x10 + 6x50 days.

All the starting fuel compositions are made of mixed nitride fuel. It is recommended to control the content of nuclides ²³⁵U, ²³⁶U, ²³⁸U; ²³⁷Np, ²³⁸Pu, ²³⁹Pu, ²⁴⁰Pu, ²⁴¹Pu, ²⁴²Pu; ²⁴¹Am, ^{242m}Am, ²⁴³Am; ²⁴²Cm, ²⁴³Cm, ²⁴⁴Cm, ²⁴⁵Cm during fuel burnup.

2.2.Benchmarks in 3-D geometry

At simulation of active core of BN-1200 reactor, calculation model is formed from hexagonal cells with compositions corresponding to the assemblies of the reactor. Figure 4 shows scheme of FA loading for the calculation model of the benchmark. In the active core, seven types of cells of FA are radially selected for the differentiation of fuel compositions formed at the beginning of the cycle. Five axial layers with their compositions are vertically selected to account for the unequal fuel burnup in vertical direction of active core. Information about the composition of irradiated fuel assemblies in the active core is presented in two forms: concentration of the effective fission fragment and the composition of the loaded fuel and burnup.



Figure 4. Scheme of FA loading for calculation model of BN-1200 reactor

The following functionals are calculated: multiplication factor, efficiency of control rods, temperature Doppler Effect in the fuel and steel, density coefficients of reactivity for fuel and sodium, breeding ratio of fuel.

During an analysis of calculation results of these test cases, we can estimate a scale of impact of main sources of uncertainty on the accuracy of neutron-physical calculations. Special attention should be paid to the influence of the diffusion approximation, homogenization of fuel assemblies, and use of different complexes of constant support.

2.3.Benchmarks for simulations of operation modes in closed fuel cycle

We considered the following scenario of refueling. The lifetime of the reactor was supposed as 60 years with maximum fuel lifetime of 6 years. Average fuel burnup at maximum fuel lifetime was 100 MWd/kg. Time of cooling and reprocessing of irradiated fuel was 3 years. The time between refuelings was 1 year (1 in-core fuel life). 1/6 part of the irradiated fuel assemblies are

replaced in each refueling of the core. All fuel assemblies used in initial loading and in 1-8 refuelings have the same isotopic composition. After the 9th refueling (first fuel reprocessing), fuel assemblies have another compositions. In such a way, one cycle of FA is 9 in-core fuel lives. Reactor operation during more than 60 in-core fuel lives is analyzed in the paper.

Figure 5 presents the scheme of refueling of the reactor core (in 60° symmetry). Elements 0 are technological channels in the reactor core and assemblies of the reactor radiation protection. Elements 1-6 are groups of FA reloaded in the core at the same time. The selected clusters show repeated elements in different radial zones of the core. It is possible to solve the task of simulation of the reactor operation in closed fuel cycle using a cluster model of FA.



Figure 5. Examples of selection of calculation clusters of FA in the core.

To obtain the isotopic composition and the multiplying characteristics of FA during all time of reactor operation, calculations of 7 cycles of FA consisting of 9 in-core fuel lives are required. Reprocessing of irradiated fuel is modeled in the following way. All fission products and all isotopes except for uranium and plutonium are removed from the fuel. Masses of uranium and plutonium isotopes used in the next cycle of FA are determined with account of the parameters of the loss of uranium ε_U and plutonium ε_{Pu} during the processing. Mass of plutonium in the fuel after processing is equal to the initial loading of the reactor. The isotopic composition of plutonium feed is the same as in the starting loading. The mass of feeding uranium is determined by the condition of preservation of equivalent fuel density.

For fuel compositions included in benchmarks, there are intervals of increase and decrease of reactivity during irradiation. This feature allows to compensate mutually the reactivity change in the reactor under partial reloading of FA. Figure 6 presents the results of calculation of the multiplication factor of fuel assembly versus the time of reactor operation in the refuelling mode for different plutonium compositions.



Figure 6. Multiplication factor of fuel assembly versus the time of reactor operation in the refuelling mode for different plutonium compositions.

Test characteristics in benchmarks of this group are required feed of fuel and isotopic compositions of irradiated FA for reactor operation in a closed fuel cycle. Characteristics of fuel assemblies after 1-7 reprocessing are shown in Table 1. Negative values of plutonium feed mean excessive production of plutonium in the considered fuel cycle.

| Ν | $M_{ m U}$ | $M_{ m Pu}$ | X ₂₃₈ | X239 | X240 | <i>X</i> ₂₄₁ | X242 |
|---|------------|-------------|------------------|------|------|-------------------------|------|
| 1 | 110.4 | -3.5 | 1.3 | 65.0 | 25.0 | 3.9 | 4.7 |
| 2 | 111.7 | -5.7 | 0.7 | 65.1 | 27.1 | 3.2 | 3.9 |
| 3 | 112.1 | -6.3 | 0.5 | 64.8 | 28.3 | 3.2 | 3.3 |
| 4 | 112.3 | -6.5 | 0.4 | 64.5 | 28.9 | 3.2 | 2.9 |
| 5 | 112.3 | -6.6 | 0.4 | 64.4 | 29.3 | 3.3 | 2.6 |
| 6 | 112.3 | -6.7 | 0.4 | 64.4 | 29.5 | 3.3 | 2.4 |
| 7 | 112.3 | -6.7 | 0.4 | 64.3 | 29.7 | 3.3 | 2.3 |

Table 1. Feed by Uranium and Plutonium (M, g/kg), isotopic composition (X, %) after reprocessing with number N

2.4.Benchmarks in 2-D geometry for estimation of effects of geometry deformation

Benchmarks are intended to model the deformation of the geometry of the core of BN-1200 reactor. Basic forms of deformation (Figure 7) and form of deformation of expansion or compression (Figure 8) are considered for calculations. Changes of neutron-physical characteristics for starting loading of reactor fuel are estimated.



Figure 7. Base forms of deformation of geometry



Figure 8. Form of deformation of expansion or compression

It is proposed to solve the case in r-z-geometry (Figure 9). Geometric case is based on 3-D model of the reactor with maximum preservation of neutron-physical parameters



Figure 9. Model of BN-1200 reactor in r-z geometry

2.5.Benchmarks for cases of protection

Benchmarks are intended to simulate the geometry of the environment of the active core of BN-1200 reactor. In the model (Figure 10) based on the prototype, we abandon unnecessary detail of design elements. Activation of coolant and the damaging dose in the specified design elements are determined in this case.



Figure 10. Model of BN-1200 reactor for cases of protection

3. Results of testing

3.1.Benchmarks in 0-D and 1-D geometries

The development of system of test cases allowed to begin cross-verification of programs of neutron-physical calculation used in the design of innovative reactor plants of new generation. This paragraph deals with the results of cross-verifications of engineering programs (JARFR and TRIGEX) [5] and programs that provide the solution of neutron transport equation by Monte-Carlo method (MCU, SCALE – MMK and TDMCC).

Calculation of test case No 1 are made for model of fuel element. They include significant number of different variants of initial loading. This item presents the results of one of them. The following functionals are compared: multiplication factor, isotopic composition of spent fuel, reaction rates, etc [6,7]. We compare results obtained by different programs with averaged value of calculations

| Program | MCU | SCALE - MMK | TDMCC | JARFR | TRIGEX |
|-----------------------------|-------|----------------|-------|-------|--------|
| Beginning of cycle | -0,45 | 0,18 | -0,53 | 0,3 | 0,49 |
| End of in-core fuel life | -0,51 | -0,01 | - | 0,4 | 0,12 |
| End of cycle | -0,29 | 0,34 | - | 0,09 | -0,14 |

Table 2. Deviation of calculated multiplication factor, $\Delta k/k$

As an example the Table 2 presents deviation of calculation results of multiplication factor calculated by different codes.

3.2.Benchmarks for modeling of operation in closed fuel cycle

In this item, results of benchmarks calculations by programs JARFR and SCALE-MMK are presented. The rate of transition to the equilibrium fuel composition for considered reprocessing conditions was determined for different starting isotopic compositions of plutonium, including compositions of irradiated fuel of different reactors and model composition with a high content of ²³⁹Pu (curve 5). Figure 11 presents a share of ²³⁹Pu in the fuel composition for considered compounds with the same proportion of the plutonium nitride in the fuel. Note that if the parameter of plutonium loss ε_{Pu} does not exceed 3%, then for all starting compositions of plutonium from power reactors, high power fast reactor with nitride fuel will require only the feed by depleted uranium and will not require plutonium feed during the whole reactor operation.



Figure 11. Part of ²³⁹Pu after fuel reprocessing for different start plutonium compositions.

Results of the performed variants of calculations allow to propose for testing starting fuel compositions having the properties of criticality of the reactor during the whole time of reactor operation and fast achievement of equilibrium fuel composition (Figure 12).



Figure 12. Multiplication factor of reactor versus the time of reactor operation in the refuelling mode for different plutonium compositions.

4. Conclusions

4.1.Codes of neutron-physical calculation

System of coordinated calculation benchmarks is developed with application of BN-1200 reactor with nitride fuel as prototype. The system is a sequence of benchmarks based on different geometric models: fuel element, fuel assembly, and the active core. This system was used in independent testing of programs for calculation of neutron-physical characteristics: engineering programs JARFR and TRIGEX, and codes MCU, TDMCC, and MMK based on Monte Carlo method.

The main calculated functionals involved in cross-verification of codes were multiplication factor, reactivity effects, and change of the isotopic composition of fuel during process of burnup, reactions rates, breeding ratio. Analysis of calculation results of test cases and their comparison allows to estimate the influence of the main sources of uncertainty on accuracy of neutron-physical calculations. Presented system of benchmarks can be used in the verification of programs for neutron-physical calculations, which are intended to be used in the design and operation of new generation reactors. The system is planned to be extended to include thermal-hydraulic test cases and test cases for integral codes.

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