Conference Paper

Using the Scale Software for Critical Analysis

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Abstract

This article shows the experience of using the SCALE software package (hereinafter SCALE) to analyze the criticality of critical benchmark experiments. This experience was obtained during the familiarization of SCALE for research purposes on the basis of the Department of Nuclear Physics and Technologies (DNPaT) of the IATE MEPhI. Test calculations of the effective multiplication factor (K_{eff}) critical assemblies with different parameters was produced, research different method of calculate multigroup constants.

Keywords: SCALE, benchmark experiment, effective multiplication factor.

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1. INTRODUCTION

Calculation and evaluation K_{eff} of systems with fissile materials are integral components of scientific and design work in the development of nuclear facilities. Without knowledge of the value of the K_{eff} and its dependence on various system parameters, it is impossible to substantiate nuclear safety at the development stage, as well as the safe handling of nuclear facilities in the process of operation.

In the software part the transport codes are significant, which calculate K_{eff}, using various methods for solving the neutron transport equation: spherical harmonics, discrete ordinates, Monte Carlo. Combining the transport code with the isotope composition change code, we can calculate K_{eff} for a changing system (campaign). This transport codes are the basic elements of control modules that can search for critical parameters of the system under study, or - calculate the sensitivity coefficients of K_{eff} of system and its error.

To date, a large number of programs have been developed and tested, with the help of which it is possible to calculate K_{eff} of all possible research reactor systems.Among them, programs MCU (Kurchatov Institute), TDMCC (VNIIEF), TRIGEX (IPPE), MCNP (Los Alamos), SCALE (Oak Ridge), Serpent (Finland), etc.

At present, the DNPaT for calculating criticality mainly uses the program Serpent, because of its free distribution for research purposes. Currently, there is also the possibility of making calculations using a software package SCALE, obtained from NEA DATA BANK.

2. DESCRIPTION OF THE SCALE SOFTWARE AND THE TEST MODEL

SCALE is designed to obtain reliable calculation results K_{eff} of various geometric models with a short preparation time of input files and processing of output files [1]. This was achieved by creating additional interface applications (for example, Fulcrum in the latest versions), which are the user's workplace. In addition to a conventional text editor, there are error debugger, that occur during writing an input file (invalid keywords, links to materials and geometry) and a color renderer of a geometric model in this application. The main feature of these functions is their real-time mode.

The tasks for which SCALE can be used are listed in Table 1.

Table 1: Task classes solved in SCALE-6.2.1 [1].

№	Analysis area	Module
1	Criticality Safety	CSAS5 / CSAS6 STARBUCS Sourcer
2	Reactor physics	TRITON Polaris
3	Radiation shielding	MAVRIC
4	Activation, depletion and decay	ORIGEN ORIGAMI
5	Sensitivity analysis	TSUNAMI Sampler
6	Material specification and Cross section processing	XSProc
7	Radiation transport	KENO-V.a / VI XSDRNPM, NEWT
8	Libraries	XSProc Material Library Libraries of cross sections ENDF/B-VII.0 / VII.1 ORIGEN Library

Numbers 1 through 5 are control modules, 6 and 7 are modules or codes that prepare materials and cross sections and solve the transport equation.

Since this work analyzes the criticality, the CSAS5 module will be used as a manager, the KENO-V.a code for the Monte Carlo transport solution and the XSProc module for materials processing and cross section preparation, the ENDF/B-VII.1 librarie will be the source of the nuclear data.

Separately it is necessary to say about additional calculation parameters that significantly affect the results. Among them: the number of generations of neutrons (GEN) and the number of neutrons in the generation (NPG).

The assembly of the benchmark critical experiment was chosen as the calculation model, which was described in detail in [2].

The model is a sphere of alpha-plutonium with a water reflector, the geometric sizes and material description of which is presented in Table 2.

Table 2: Description of the calculation model.

Parameter	Value
Radius of the plutonium sphere, cm	4.1217
Radius of the water sphere, cm	29.5217
The density of plutonium, g/cm^3	19.74
Isotopic distribution of plutonium	94.5% Pu239, 5.18% Pu240, 0.3% Pu241, 0.02% Pu242
Density of water, g/cm^3	1.00
Isotopic distribution of water	natural distribution

3. CALCULATION RESULTS

At the first stage of the model's test calculations, a comparison was made K_{eff} obtained with the default settings and - specified in the Handbook [2]. At the same time, one library was used: 252-group ENDF/B-VII.1. The results are listed in Table 3 and Figure 1.

Table 3: comparison of the results of the first stage of calculations with benchmarks values (*default parameters GEN = 203, NPG = 1000, *centrm*; **parameters specified in Handbook GEN = 305, NPG = 1500, *centrm*).

№	1	2	3	4	5	6
Used code and library	KENO* (252-Group ENDF/B-VII.1)	KENO** (252-Group ENDF/B-VII.1)	KENO (Hansen-Roach)	KENO (27-Group ENDF/B-IV)	MCNP (CE ENDF/B-V)	Idealized benchmark-model K_{eff}
$K_{eff} \pm \Delta K/K$	1.0025 ±0.0022	1.0003 ±0.0013	1.0009 ±0.0016	1.0016 ±0.0013	0.9993 ±0.0011	1.0000 ±0.0010

The results of calculations coincided with the benchmark value K_{eff} within the confidence intervals for all options. The decrease in the error in the second option, compared with the first one, is due to an increase in the number of neutrons generations.

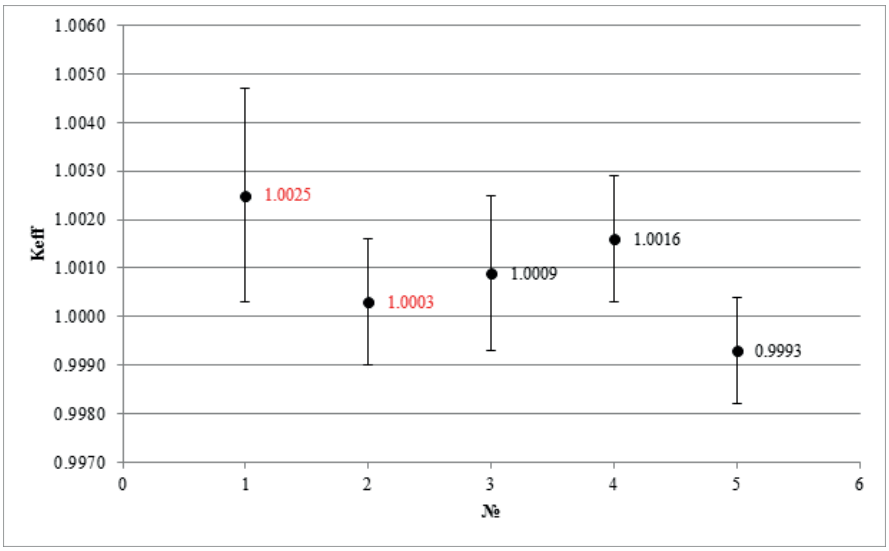

Figure 1: The results of the first stage of calculations and the values presented in the Handbook.

At the second stage, the values of K_{eff} were compared obtained using different SCALE libraries with different values of GEN and NPG parameters.

Used multigroup libraries:

- «v7.1-252» - ENDF/B-VII.1 252-group neutron library;
- «v7.1-200n47g» - ENDF/B-VII.1 200 neutron/47 gamma library;
- «v7.1-56» - ENDF/B-VII.1 56-group neutron library;
- «v7.1-28n19g» - ENDF/B-VII.1 28 neutron/19 gamma library.

For the first set of parameters, the coincidence of the results with the benchmark value is observed only for 3 libraries. In this case, a large difference of value K_{eff} for the 28-group energy partition and benchmark value was observed.

By the second set of parameters, an attempt was made to improve the enhancement of calculation results for the remaining libraries, by simply increasing the number of neutron generations. The results are listed in Table 4 and Figure 2.

Table 4: Second stage of calculations comparing libraries (*first set of parameters GEN = 305, NPG = 1500, *centrm*; **second set of parameters GEN = 2000, NPG = 1500, *centrm*).

№	1	2	3	4	5
Library	v7.1-252n	v7.1-200n47g	v7.1-56	v7.1-28n19g	Idealized benchmark-model K_{eff}
K_{eff}* ±ΔK/K	1.0003 ±0.0013	1.0002 ±0.0013	0.9986 ±0.0014	1.0046 ±0.0013	1.0000 ±0.0010
K_{eff}** ±ΔK/K	0.9990 ±0.0005	1.0005 ±0.0005	0.9982 ±0.0006	1.0044 ±0.0005	1.0000 ±0.0010

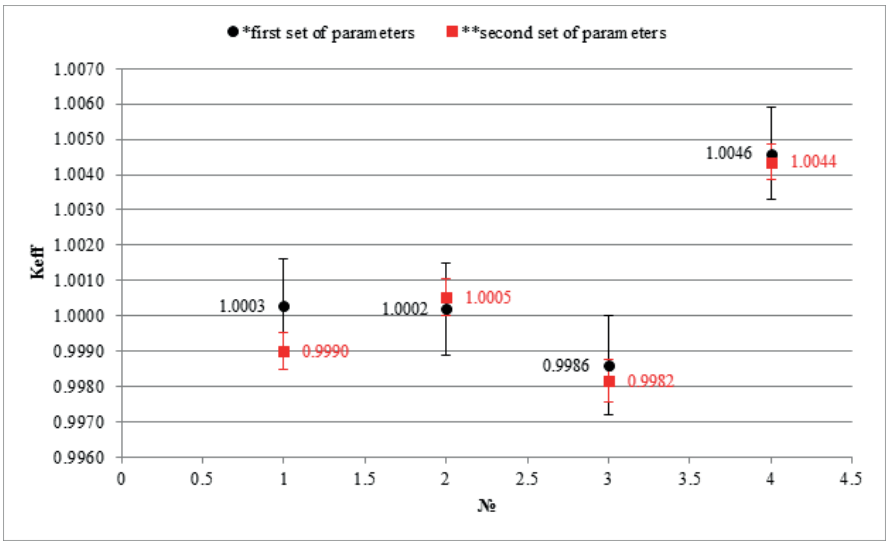

Figure 2: Comparison of calculation results for different libraries for two sets of parameters.

As expected, an increase in the number of neutrons generations led to an improvement in the enhancement of the results and a decrease in the error of K_{eff}.

The effect of the method of calculating multigroup constants on the value K_{eff} was studied. SCALE allows to calculate multigroup constants in two ways:

- The solution of the deceleration equation on the detailed energy scale with the subsequent convolution of the cross sections with the obtained neutron fluxes (abbreviated name of the method is *centrm*);
- Use the dilution cross section and Bondarenko factors to calculate the blocked constants (abbreviated name of the method is *bonami*).

Other GEN and NPG parameter values remained the same as in the second stage of calculations. The results for the two methods of preparation are presented in Table 5 and in Figure 3.

Table 5: The third stage of calculations comparing the libraries (*method *centrm*, **method *bonami*).

№	1	2	3	4	5
Library	v7.1-252n	v7.1-200n47g	v7.1-56	v7.1-28n19g	Idealized benchmark-model K_{eff}
K_{eff}* ±ΔK/K	0.9990 ±0.0005	1.0005 ±0.0005	0.9982 ±0.0006	1.0044 ±0.0005	1.0000 ±0.0010
K_{eff}** ±ΔK/K	1.0000 ±0.0006	1.0006 ±0.0006	0.9966 ±0.0005	0.9992 ±0.0006	1.0000 ±0.0010

A comparison of the microscopic scattering cross sections for the first zone consisting of a mixture of plutonium isotopes was made.

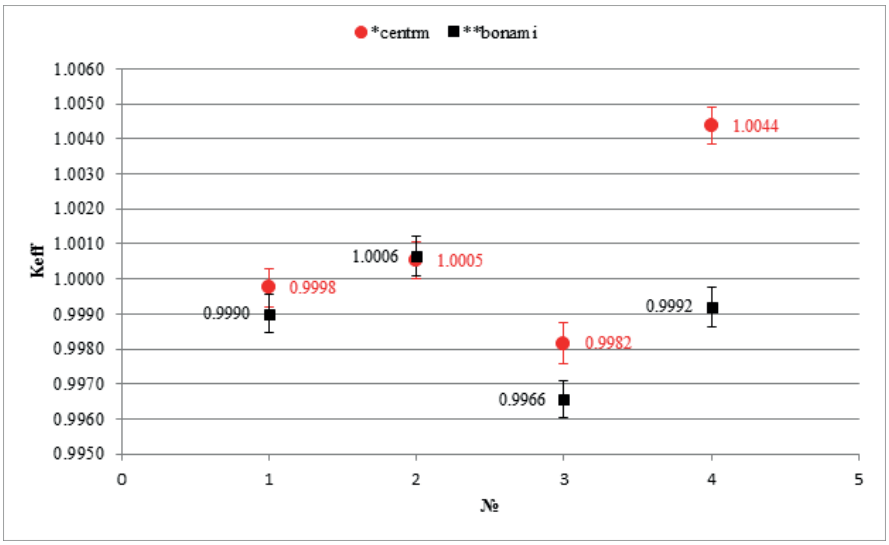

Figure 3: Comparison of calculation results for different libraries for two methods of calculate multigroup constants.

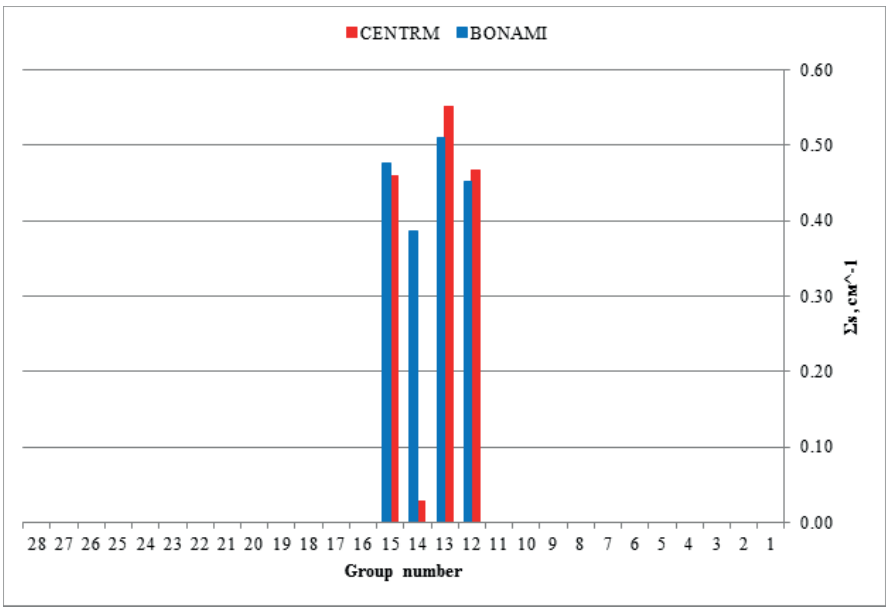

Figure 4: Macroscopic scattering cross sections for 12-15th groups obtained with two methods.

The macroscopic scattering and absorption cross sections in the resonance energy region (12-15 groups corresponding to energies from 5 to 103 eV) are given below (Figure 4).

As can be seen from the graph in Figure 4, for groups with 12th to 15th, significant differences are observed in macroscopic scattering cross sections. This is especially noticeable for the 14th group (5.00 - 10.68 eV), in which the resonance with peak energy completely included $E = 7.8$.

A feature of the preparation of dilution cross sections is the fact that the deceleration equation is replaced by an approximation with a constant scattering cross section,

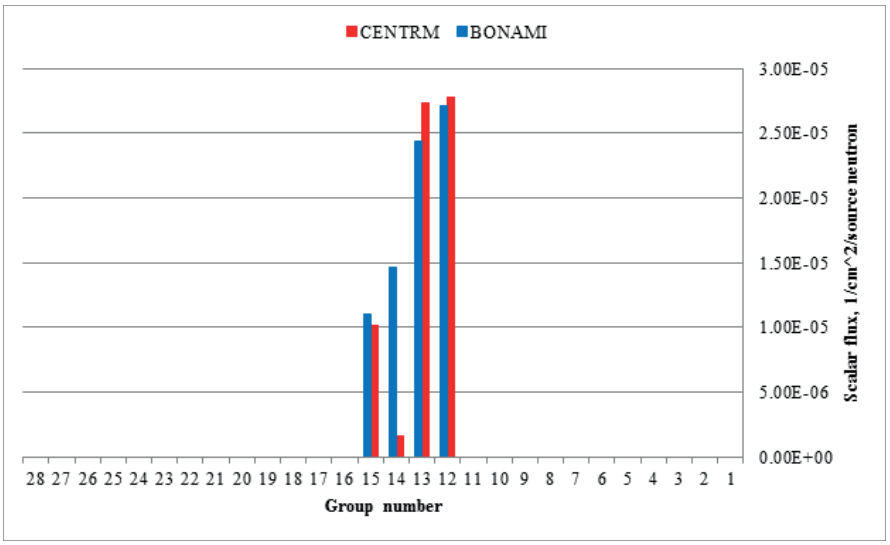

Figure 5: Scalar neutrons fluxes for 12-15th groups obtained with two methods.

which leads to a significant increase in the neutron flux (Figure 5) density in this group ($1,5 \cdot 10^{-5}$ against $1,6 \cdot 10^{-6}$ in relative units). For systems with a resonant neutron spectrum this can lead to a noticeable distortion of the values of K_{inf}.

4. CONCLUSION

In the course of this work, a scrutiny of the structure of SCALE and the functional links between the various modules was made and the preparation of input files was mastered. Having a user-friendly application makes it much easier and, as a consequence, accelerates the preparation of input files: the syntax of geometric and material parameters is intuitive, and the debugger and visualizer save time to search for errors.

To verify the reliability of the results, a test calculation of simple model of the reference experiment was carried out for various quantities of model neutrons, used libraries, and methods for preparing blocked cross sections:

- increase in the number of neutrons generations to GEN=2000 and the number of neutrons per generation to NPG=1500 reduces the error for all used libraries to values not exceeding $\delta = 0.06\%$;
- increase in the number of neutrons generations to GEN=2000 and the number of neutrons per generation to NPG=1500 allows to obtain results for the libraries «v7.1-252n», «v7.1-200n47g», which within the confidence intervals converge with the benchmark value. The relative difference between the calculated and benchmark values was: $\delta_{252} = 0.10\%$, $\delta_{200} = 0.05\%$, $\delta_{56} = 0.18\%$, $\delta_{28} = 0.43\%$; the maximum relative difference between the calculated values was: $\delta_{56/28} = 0.50\%$

- relative difference macroscopic scattering cross sections obtained with two methods was for 14^{th} group $\delta_{14} = 1242.20\%$.

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[1] Rearden B.T., Jessee M.A.. SCALE Code System. / Oak Ridge National Laboratory, Oak Ridge, 2016.

[2] Roger W. Brewer. BENCHMARK CRITICAL EXPERIMENT OF A WATER REFLECTED ALPHA-PHASE PLUTONIUM SPHERE / Los Alamos National Laboratory, Los Alamos, 1995.