## METHODICAL UNCERTAINTY OF PRECISE CRITICALITY CALCULATIONS FOR A LEAD-COOLED FAST REACTOR

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Abstract. Criticality calculations for the BFS-1 test facility with a lead coolant were performed using MCU-BR, a Monte-Carlo code, to verify some evaluated neutron data files for fast spectra. These data files are RUSFOND, ENDF/B-VII.1, JEFF-3.2, JENDL-4.0, CENDL-3.1 and some combined data. Continuous energy treatment (ACE format) was used. Critical assemblies include pellets consisting of fissionable materials, lead, stainless steel and others. The average  $K_{eff}$  evaluation for each critical assembly was obtained. The standard deviation for  $K_{eff}$  with various data files is in an interval from 0.1% to 0.4% with a probability of 0.55 to 0.82, and the average  $K_{eff}$  evaluation is 0.14% with a probability of 0.73.

Key Words: MCU-BR, neutronic calculations, precision code.

#### Introduction

A precision code, MCU-BR, is used for neutronic calculations of a lead-cooled fast reactor [1-4].

The code is designed to model neutron and photon transport processes by Monte-Carlo method based on estimated neutron data in 3D-geometry systems with regard for changes in the nuclide composition of materials as the result of interactions with neutrons.

The constants for MCU-BR are provided by the MDBBR50 databank consisting of a set of sections (libraries) that can be used in calculations with different particles and different submodules of the composite physical module. The databank's neutron libraries are based predominantly on data from ROSFOND files [5] and support calculations in the neutron energy interval from 0 to 20 MeV. A program, NJOY [6] (version NJOY.393), was used to prepare library files in the ACE format.

Computational modeling of experiments at the BFS critical facility makes it possible to assess the effects of the neutron data uncertainty on the calculation results. To this end, the BFS [7] critical assemblies have been calculated with different file libraries of evaluated neutron data (FOND). As is the case with parameters of the MCU-BR analytical models, all parameters of analytical models in these calculations remain invariable.

In international practice, neutronic calculations are based on various libraries of evaluated neutron data developed by expert teams in countries developing nuclear power.

To calculate 11 BFS-1 critical assemblies, this study, along with the MDBBR50 library, uses neutron cross-sections in the ACE format prepared based on the following FOND libraries: ROSFOND, ENDF/B-7.1 [8], JEFF-3.2 [9], JENDL-4.0 [10], CENDL-3.1 [11].

#### Brief description of critical assemblies

Assemblies have been considered with uranium, plutonium and uranium-plutonium fuels, including with uranium nitride and lead-containing pellets for the lead-cooled reactor core simulation. Effective multiplication factor,  $K_{eff}$ , is used as the base functional for the computational analysis.

**The BFS-61** assembly is an experiment series of three critical configurations with a heterogeneous configuration of plutonium (95%  $^{239}$ Pu), depleted uranium, graphite and lead. The load for each assembly type is shown in Table I.

TABLE I– NUMBER OF DIFFERENT TUBE TYPES IN THE CRITICAL-STATE	
ASSEMBLY.	
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Tube type	BFS-61-0	BFS-61-1	BFS-61-2				
Core	277	289	346				
Sheathed lead	66	54	-				
Bare lead	246	246	-				
Steel	222	-	-				
Depleted uranium dioxide	$\geq$ 3 outer rows	$\geq$ 5 outer rows	$\geq$ 8 outer rows				
Average neutron spectrum energy, $\text{keV}^*$	172	189	210				
* - a calculated parameter characterizing the neutron spectrum "hardness"							

**The BFS-77** assembly is an experiment series of two critical configurations with a heterogeneous composition of plutonium (95%  $^{239}$ Pu), uranium (90%  $^{235}$ U), depleted uranium, graphite and lead. The load for each assembly type is shown in Table II.

TABLE II – NUMBER OF DIFFERENT TUBE TYPES IN THE CRITICAL-STATE ASSEMBLY.

Tube type	<b>BFS-77-1</b>	BFS-77-1a
Core	217	217
Driver region	176	178
Depleted uranium dioxide	812	812
Average neutron spectrum energy, keV	163	163

**The BFS-77-1a** configuration differs from that of BFS-77-1 in that the upper lead cavity's lower cell in 19 central rods was replaced for 5 natural boron carbide slugs, while two rods were added to the driver region periphery to keep the assembly critical.

**The BFS-85** assembly is a model of a lead-cooled fast reactor core with uranium fuel and lead-bismuth or lead inserts at the core center and a lead-bismuth reflector. The assemblies were used to study the properties of lead and the lead-bismuth alloy.

The BFS-85 assembly core was composed of uranium dioxide pellets with an enrichment of 36 %, metallic uranium with an enrichment of 90 % and sodium; axially, the core was surrounded by the upper and the lower end shields formed by depleted uranium and sodium pellets. Above the upper end shield there was a gas space that models the gas space formed by sodium pellets and empty steel boxes, and there was a steel shielding layer formed by chromium steel and sodium pellets above the transition region. For the transition from the BFS-85-1 assembly to the BFS-85-2 assembly with the same composition of the core fuel rods as in the BFS-85-1 assembly, the central Pb-Bi insert was replaced for the Pb central insert.

A description of the BFS-85 assembly critical load is given in Table III, except some of the additional rods with a minor effect on criticality.

Tube type	BFS-85-1	BFS-85-2
Core	112	113
Core rods	19 (Pb-Bi)	19 (Pb)
Pb-Bi side shield	308	307
Depleted uranium dioxide	818	818
Average neutron spectrum energy, keV	205	205

TABLE III – NUMBER OF DIFFERENT TUBE TYPES IN THE CRITICAL-STATE ASSEMBLY.

**The BFS-95** assembly is a model of a lead-cooled fast reactor core. The critical assembly core has 2 regions: there is a low enrichment region at the center with uranium-plutonium fuel in 217 fuel rods (97 at the center with high-background plutonium – 11 %  $^{240}$ Pu, and 120 with low-background plutonium – 4 %  $^{240}$ Pu), surrounded by 139 fuel rods of the driver region (DR) in which uranium fuel is used. The BFS-95-2 assembly is a modification of BFS-95-1 with high-background plutonium replaced for low-background plutonium in its central part. A description of the BFS-95-1 and BFS-95-2 critical loads is given in Table IV, except some of the additional rods with a minor effect on criticality.

TABLE IV – NUMBER OF DIFFERENT TUBE TYPES IN THE CRITICAL-STATE ASSEMBLY.

Tube type	BFS-95-1	BFS-95-2
Core		
Low enrichment region	217	217
Driver region	139	134
Composite shield		
Pb	420	425
UO <sub>2</sub>	210	210
B <sub>4</sub> C	108	108
Average neutron spectrum energy, keV	155	153

**The BFS-113** assembly is a model of a lead-cooled fast reactor core with nitride fuel. The BFS-113-1A configuration is a test reactor model consisting of two subregions: a central subregion with oxide uranium-plutonium fuel and a driver one with oxide uranium fuel. The central subregion uses slugs of metallic low-background plutonium, depleted uranium dioxide, metallic uranium dioxide and lead. Metallic uranium (90% <sup>235</sup>U), depleted uranium dioxide and lead slugs are used in the driver subregion.

The BFS-113-1B critical assembly core consists of three subregions: a central subregion with nitride and oxide uranium-plutonium fuel, a middle subregion with oxide uranium-plutonium fuel and a driver subregion with oxide uranium fuel (the channels contain metallic plutonium and uranium).

Metallic low-background plutonium, depleted uranium nitride, depleted uranium dioxide and lead slugs are used in the central subregion. Metallic low-background plutonium, depleted uranium dioxide, metallic depleted uranium and lead slugs are used in the middle subregion. Metallic uranium (90% <sup>235</sup>U), depleted uranium dioxide and lead slugs are used in the driver subregion.

A description of the BFS-113-1A and BFS-113-1B critical loads is given in Table V, except some of the additional rods with a minor effect in criticality.

Tube type	BFS-113-1A	BFS-113-1B
Central subregion	217	91
Middle subregion	-	126
Driver subregion	206	211
Lead reflector	496	491
Average neutron spectrum energy, keV	144	142

TABLE V – NUMBER OF DIFFERENT TUBE TYPES IN THE CRITICAL-STATE ASSEMBLY.

### **Calculation results**

Experimental values of  $K_{eff}$  and calculation results based on different FOND libraries, as well as deviations of calculation data from experimental data are given in Tables VI and VII.

Assembly	Fuel	Experiment	MDBBR50	ROSFOND	<b>ENDF/B-7.1</b>	<b>JEFF-3.2</b>	JENDL-4.0	CENDL-3.1
BFS 61-0		1.0003	1.0018	0.9988	0.9977	0.9972	1.0034	1.0035
BFS 61-1	U-Pu	1.0004	1.0005	0.9975	0.9964	0.9960	1.0018	1.0016
BFS 61-2		1.0004	0.9980	0.9960	0.9951	0.9946	1.0004	0.9999
BFS 77-1	II Du	1.0004	1.0002	1.0019	1.0004	1.0022	0.9977	1.0023
BFS 77-1a	U-ru	1.0010	1.0003	1.0022	1.0006	1.0024	0.9979	1.0026
BFS 85-1	I	1.0007	0.9980	0.9971	1.0003	1.0046	0.9947	0.9924
BFS 85-2	U	1.0021	1.0001	0.9995	1.0020	1.0061	0.9964	0.9947
BFS 95-1	I Du	1.0004	1.0016	1.0021	1.0000	1.0004	0.9983	1.0036
BFS 95-2	U-ru	1.0004	1.0004	1.0010	0.9990	0.9994	0.9975	1.0026
BFS-113-1A	U-Pu	1.0006	1.0007	1.0017	0.9995	1.0004	0.9985	1.0026
BFS-113-1B	U-N, U-Pu	1.0011	1.0007	1.0015	0.9994	0.9999	0.9984	1.0021

### TABLE VI - RESULTS OF K<sub>EFF</sub> CALCULATIONS BASED ON MCU-BR USING DIFFERENT FOND LIBRARIES.

## TABLE VII – DEVIATIONS OF CALCULATED K<sub>EFF</sub> VALUES FROM EXPERIMENTAL VALUES.

Agaomhly			MAV	A				
Assembly	MDBBR50	ROSFOND	ENDF/B-7.1	<b>JEFF-3.2</b>	JENDL-4.0	CENDL-3.1	MAA	Average
BFS 61-0	145	-155	-264	-306	312	320	320	250
BFS 61-1	5	-286	-396	-444	144	124	444	233
BFS 61-2	-241	-441	-530	-585	-2	-48	585	308
BFS 77-1	-20	147	0	183	-270	187	270	135
BFS 77-1a	-74	124	-45	144	-315	162	315	144
BFS 85-1	-266	-357	-44	394	-599	-835	835	416
BFS 85-2	-204	-261	-10	401	-573	-742	742	365
BFS 95-1	115	173	-41	-3	-208	319	319	143
BFS 95-2	-2	60	-143	-97	-294	221	294	136
BFS-113-1A	12	114	-106	-17	-207	201	207	110
BFS-113-1B	-36	39	-171	-117	-269	103	269	123
MAX	266	441	530	585	599	835		
Average	102	196	159	245	290	297		

The following uncertainty estimates are presented for the calculations of 11 BFS-1 critical assemblies based on MCU-BR with different FOND libraries: root-mean-square (RMSD) and maximum deviations of calculation data from experimental values, and average and maximum absolute deviations of  $K_{eff}$  (pcm) (Table VIII).

FOND	MDBBR50	ROSFOND	<b>ENDF/B-7.1</b>	<b>JEFF-3.2</b>	JENDL-4.0	CENDL-3.1				
RMSD ( $\sigma$ ),	0.14	0.23	0.23	0.31	0.33	0.39				
% ΔK/K										
Max. dev., %	0.27	0.44	0.53	0.58	0.60	0.83				
$\Delta K/K$										
Average	102	196	159	245	290	297				
absolute										
deviations,										
pcm										

TABLE VIII – UNCERTAINTY OF K<sub>EFF</sub> CALCULATIONS FOR THE BFS CRITICAL ASSEMBLIES WITH DIFFERENT FOND LIBRARIES.

## Conclusions

Based on the considered set of 11 critical assemblies, the minimum calculation uncertainty was obtained using the MDBBR50 library with the minimum values for all analyzed options being as follows: an RMSD of 0.14 %  $\Delta$ K/K, the maximum deviation of 0.27 %  $\Delta$ K/K, and the average absolute K<sub>eff</sub> deviation from the experimental data of 102 pcm. The maximum deviation is approximately 2 times as great as the RMSD.

The average calculated value of  $K_{eff}$  obtained using MCU-BR with MDBBR50 for the 11 critical states is 1.0002, the average experimental value of  $K_{eff}$  is equal to 1.0007, and the average deviation of calculation data from experimental values is minus 50 pcm (-0.0005).

The library prepared based on ROSFOND files shows the following post-MDBBR50 uncertainties: an RMSD of 0.23 %  $\Delta$ K/K, the maximum deviation of 0.44 %  $\Delta$ K/K, and the average absolute K<sub>eff</sub> deviation from the experimental data of 196 pcm.

Calculations based on ROSFOND files show an RMSD increase of 0.09 %  $\Delta$ K/K (by 1.6 times), while the maximum uncertainty of calculated K<sub>eff</sub> increases by 0.2 %  $\Delta$ K/K (by 1.6 times). The observed uncertainty growth has been caused by an increase in the constant uncertainty. ENDF/B-7.1 files show uncertainties close to those obtained based on ROSFOND files.

JEFF-3.2, JENDL-4.0 and CENDL-3.1 files show a greater increase in the calculation uncertainty since the RMSD increases by 0.17 %, 0.19 % and 0.24 %  $\Delta$ K/K, and the maximum calculation uncertainty increases by 0.31 %, 0.33 % and 0.56 %  $\Delta$ K/K.

The calculation uncertainty Keff was analyzed separately for each assembly.

The minimum uncertainties have been obtained for the BFS-113-1A and BFS-113-1B assemblies, the average absolute deviations are respectively 110 pcm and 123 pcm, and the maximum deviations are 207 pcm and 269 pcm. The maximum differences have been obtained for BFS-85-1 and BFS-85-2. The uncertainties for BFS-77 and BFS-95 are 135 – 144 pcm for the average deviations and ~ 300 pcm for the maximum deviations.

The analysis results also show that MDBBR50 is the only of the libraries considered for each of the 11 assemblies with the  $K_{eff}$  calculation uncertainty smaller than the average uncertainty for all libraries.

Therefore, calculations done based on the MCU-BR code with the MDBBR50 library have the minimum calculation uncertainty  $K_{eff}$ . A comparison with the results obtained for other libraries makes it possible to determine the constant uncertainty for these libraries.

# References

- Dragunov Yu.G., Lemekhov V.V., Moiseyev A.V., Smirnov V.S. Lead-Cooled Fast-Neutron Reactor (BREST) // INPRO Dialog-Forum, IAEA HQ, Vienna, Austria, May 26-29 2015 p.32
- [2] *Dragunov Y.G., Lemekhov V.V., Smirnov V.S., Chernetsov N.G.* Technical Solutions and Development Stages for the BREST-OD-300 Reactor Unit // Atomic Energy. 2012. Vol. 113, Iss. 1., pp. 70-77.
- [3] Dragunov Y.G., Lemekhov V.V., Smirnov V.S. Fast Neutron Reactor with Lead Coolant (BREST) // Innovative Designs and Technologies of Nuclear Power», Third International Scientific Conference: reports, JSC «NIKIET», Moscow, Russia, 2014 -Vol.1. - pp. 94-102
- [4] Dragunov Yu.G., Lemekhov V.V., Moiseyev A.V., Smirnov V.S., Yarmolenko O.A. Detailed Design of the BREST-OD-300 Reactor Facility: Development Stages and Justification // Innovative Designs and Technologies of Nuclear Power, IV International Scientific Conference: reports, JSC «NIKIET», Moscow, Russia, 2016 - Vol.1.- pp. 21-30.
- [5] Encyclopedia of ROSFOND Neutron Data. IPPE, Obninsk, 2006.
- [6] *MacFarlane R.E. and Muir D.W.* The NJOY Nuclear Data Processing System. LA-12740, LANL, 1994.
- [7] Verification of the MCU-BR Code Based on the Results of Experiments at the BFS-1 Test Facility, «Innovations in Atomic Energy», Conference of Young Scientists (25-26 November 2015) JSC «NIKIET», Moscow, Russia, pp. 705-714.
- [8] Chadwick M.B, Herman M., Oblozinsky P., Dunn M.E., Danon Y., Kahler A.C., Smith D.L., Pritychenko B., Arbanas G., Arcilla R., Brewer R., Brown D.A., Capote R., Carlson A.D., Cho Y.S., Derrien H., Guber K., Hale G.M., Hoblit S., Holloway S., Johnson T.D., Kawano T., Kiedrowski B.C., Kim H., Kunieda S., Larson N.M., Leal L., Lestone J.P., Little R.C., McCutchan E.A., MacFarlane R.E., MacInnes M., Mattoon C.M., McKnight R.D., Mughabghab S.F., Nobre G.P.A., Palmiotti G., Palumbo A., Pigni M.T., Pronyaev V.G., Sayer R.O., Sonzogni A.A., Summers N.C., Talou P., Thompson I.J., Trkov A., Vogt R.L., van der Marck S.C., Wallner A., White M.C., Wiarda D., Young P.G. ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data. Nuclear Data Sheets, Volume 112, Issue 12, December 2011, Pages 2887-2996.
- [9] A. J. Koning, E. Bauge, C. J. Dean, E. Dupont, U. Fischer, R. A. Forrest, R. Jacqmin, H. Leeb, M. A. Kellett, R. W. Mills, C. Nordborg, M. Pescarini, Y. Rugama and P. Rullhusen. Status of the JEFF Nuclear Data Library, Journal of the Korean Physical Society, Vol. 59, No. 2, August 2011, pp. 1057-1062.
- [10] Shibata K., Iwamoto O., Nakagawa T., Iwamoto N., Ichihara A., Kunieda S., Chiba S., Furutaka K., Otuka N., Ohsawa T., Murata T., Matsunobu H., Zukeran A., Kamada S., Katakura J., JENDL-4.0: A New Library for Nuclear Science and Engineering, J. Nucl. Sci. Technol..48(1), 1-30 (2011).
- [11] Z. Ge, H. Yu, et al. The Updated Version of Chinese Evaluated Nuclear Data Library (CENDL-3.1) // Nuclear Engineering and Technology, 2010.