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Research Article

Comparison of the calculation accuracy of the neutronic characteristics of a heavy liquid metal cooled fast reactor model using various evaluated neutron data libraries*

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Abstract

The paper analyses the neutron data and covariance matrixes, which are crucial for the computational prediction of neutronic characteristics of fast neutron reactors with uranium-plutonium fuel and currently available in the state-of-the-art versions of evaluated nuclear data libraries: ENDF/B-VIII, JENDL-5, TENDL 2021, JEFF 4T1. The newly obtained covariance data are compared to the data that was presented in the Russian evaluated nuclear data library BROND 3.1. A simplified model of a fast neutron reactor with mixed dense nitride uranium-plutonium fuel and heavy liquid metal coolant was used to calculate the spread in neutronic performance values and their uncertainties due to neutron data using different evaluated nuclear data libraries for the following characteristics: effective multiplication factor, effective delayed neutron fraction, Doppler reactivity coefficient, breeding ratio and gain, reactivity margin for fuel burnup and other fuel burnup characteristics. It has been observed that, on the whole, the uncertainties of the reactor functionals have decreased when estimated using state-of-the-art versions of evaluated neutron data libraries, compared to previous releases of those libraries. The paper also examines changes in target accuracies for predicting the main neutronic characteristics of fast neutron reactors over the past decades, as well as evaluates the requirements for neutron data uncertainties to achieve the recently declared target accuracies. The main findings of this study are presented in two aspects: first, in terms of the effects evaluated neutron data from different libraries have on the accuracy of calculations for the key neutronic characteristics of fast reactors; and second, in terms of the potential for improving the accuracy of predicted neutronic characteristics of fast reactors by considering the results of reactor physics measurements.

Keywords

evaluated neutron data, uncertainties, covariance matrices, fast neutron reactor, sensitivity coefficient, uncertainty, data assimilation

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Introduction

Estimating the uncertainty and accuracy of computational predictions regarding the neutronic performance of nuclear reactors, radiation protection, and external fuel cycle technologies necessitates data on the uncertainties associated with the interactions of neutrons and material nuclei. The current state of knowledge regarding neutron data and their uncertainties is represented in various national libraries of evaluated neutron data for general applications: BROND 3.1 (Russian Federation, 2016), ENDF/B-VIII (USA, 2018), JENDL-5 (Japan, 2021), JEFF 3.3 and JEFF 4T1 (European Union, 2017, 2022 test version), and TENDL 2021 (IAEA, 2021). In the context of designing fast neutron reactors, evaluated neutron data play a crucial role in determining the accuracy of computational predictions for key reactor neutronic characteristics. These characteristics are essential for optimizing reactor core layouts, nuclear fuel refueling strategies, and the parameters of external fuel cycle technologies.

For several decades, working groups of the OECD's Nuclear Energy Agency (NEA), in collaboration with the Nuclear Data Section of the International Atomic Energy Agency (IAEA), have been engaged in analyzing and assessing the impact of uncertainties in neutron data on the accuracy of computational predictions for the neutronic performance of Generation IV nuclear reactors (WPEC Subgroup 46). The ultimate goal of this analysis is to establish both the achieved and target accuracies for computational predictions of reactor neutronic characteristics, as well as to identify priorities for updating neutron data. This updating is crucial for enhancing the accuracy and reliability of computational predictions for the performance of innovative facilities under design (Cabellos et al. 2023).

The increasing demands for cost-effectiveness and safety in the design of Generation IV reactor systems necessitate periodic revisions of both the target accuracy for computational predictions of essential neutronic characteristics and the required accuracy of neutron data. These revisions aim to make accuracy requirements more stringent and are informed by the accumulation of experimental information, as well as the development of computational models, methods, and tools. The target and achieved accuracies for calculating key neutronic performance data related to fast reactors are summarized in Table 1. The "current state" reflects the results of generalizing estimates obtained from the OECD NEA working groups.

Using a simplified model of a heavy liquid metal-cooled fast reactor (LFR) with nitride uranium-plutonium fuel, key neutronic characteristics have been calculated based on the current versions of evaluated neutron data libraries. These characteristics include the effective multiplication factor (k_{eff}), Doppler reactivity factor ($\Delta\rho_D$), burnup reactivity margin ($\Delta\rho_{burn}$), effective fraction of delayed neutrons (β_{eff}), breeding ratio (BR), and other fuel burnup characteristics. Additionally, the nuclear data uncertainty has been estimated based on the results of integrated measurements from the BFS-61 critical assemblies (DICE, IDAT), which possess similar neutronic properties. The ONIX code (Andrianov et al. 2023a, 2023b) was utilized to solve the inverse problem of defining the requirements for cross-sections of neutron interactions with actinide nuclei. This analysis assumes that the neutron data should ensure a target accuracy for the effective multiplication factor (k_{eff}) calculation of the considered LFR model at a level no greater than 0.2%.

Overview of codes and the LFR model

The simplified cylindrical LFR model, utilizing lead coolant and nitride uranium-plutonium fuel, consists of a homogeneous mixture containing 33 wt. % uranium-plutonium fuel, 60 wt. % lead, and 7 wt. % iron. The volume fractions of these materials are comparable to those of the BFS-61 model and are surrounded by a reflector made up of 88 wt. % lead and 12 wt. % iron (Bychkov et al. 2024). The plutonium composition in the fuel is sourced from open

Table 1. Target and achieved accuracies in calculating neutronic performance of fast reactors

Parameter	Accuracies achieved (current state) (Castelluccio et al. 2022)	Target accuracies (40 years ago) (Manokhin and Usachev 1984)	Target accuracies (current state) (Castelluccio et al. 2022)
Effective multiplication factor, k_{eff}	~1%	1%	0.2–0.3%
Power peaking factor	2%	2%	1%
Core power density distribution	5–7%	–	2%
BG	0.05–0.06	–	0.02
BR	~ 1%	2%	0.5%
Reactivity change due to fuel burnup	3%	Δk	<1%
	0.5%	5%	0.3%Δk
Reactivity coefficients			
major effects	10%	10–15%	5%
minor effects	20%		10%
Doppler effect	3–5%		–
Control rod efficiency			
individual rods	10%	5%	5%
rod groups	20%	–	10%
Kinetic parameters	5–10%	–	2–5%
EoC nuclide concentrations			
Fuel nuclides	1–2%	10%	< 1%
Minor actinides	10–20%	30%	10%
Fission products (FP)	20%	20%	10%

literature, with the plutonium content assumed to be 13 wt. % and the concentration of ^{235}U in depleted uranium set at 0.2% (Balovnev et al. 2021). The core height is specified to be 110 cm, while the radius is determined based on criticality conditions. The thickness of both the end and side reflectors is selected to ensure that neutron escape from the core is consistent with that of the standard LFR model. The fuel life of 900 effective days (without refueling) has been calculated for operation at a rated thermal power level of 700 MW. During the computational simulation, no partial refueling mode was implemented, and the refueling interval duration was assumed to be 150 effective days, with a 30-day outage at the end of each refueling interval.

For the neutronic calculations, a precision code equipped with a built-in module for calculating variations in nuclide composition was employed. The NUCLEX and NUDAPS codes were utilized to estimate the neutronic performance uncertainties due to nuclear data uncertainties. These codes incorporate a functional approach to assess both nuclear data and technological uncertainties in the calculated characteristics, utilizing sensitivity coefficients and variant calculations based on the generation of random input data samples (Andrianov et al. 2022, 2023c).

Estimation of a priori uncertainties in LFR neutronic performance due to nuclear data uncertainties

Table 2 presents the ranges of values and uncertainties associated with nuclear data for the key neutronic characteristics (k_{eff}, $\Delta\rho_D$, $\Delta\rho_{burn}$, β_{eff}, BR and fuel burnup characteristics) of the LFR model under consideration. These were calculated using various evaluated neutron data libraries, including BROND 3.1, ENDF/B-VIII, JENDL-5, TENDL 2021, and JEFF 4T. Table 3 outlines the uncertainties related to the nuclear data for the LFR model's fuel composition at the end of cycle (EoC), estimated at 900 days using the NUCLEX code. This estimation is based on uncertainty data for one-group neutron cross-sections obtained from the NUDAPS system, which utilizes covariance data from different evaluated nuclear data libraries.

Overall, the values of the reactor functional uncertainties estimated using the considered library versions were lower than those derived from earlier versions (see Andrianova et al. 2014, for example). Notably, uncertainties in neutron cross-sections were documented in the 2010 and 2011 library versions in two sections: MF32 (uncertainties of resonance parameters) and MF33 (uncertainties of cross-sections for energies above 0.2 MeV). In the most recent library versions, data on uncertainties in the resonance region have been consolidated into the MF33 section, covering a large number of groups (approximately 1000). However, the MF32 section for ^{238}U, which was necessary for estimating uncertainties in resonance self-shielding and Doppler effects, has been removed from the nuclear data files. None of the analyzed libraries provide data on uncertainties for nitrogen neutron reaction cross-sections, with the exception of the JENDL-5 library, which includes covariance data for the (n, p) cross-section.

The estimates indicate a preserved spread of 0.7% between the k_{eff} values obtained from the ENDF/B-VIII and JEFF 4T libraries. The maximum spread across all analyzed libraries is 1%, which corresponds to the uncertainties associated with nuclear data estimated using the current versions of non-Russian evaluated nuclear data libraries, ranging from 0.84% to 0.95%. The k_{eff} uncertainty due to nuclear data uncertainties for the initial state, estimated using the BROND 3.1 library, is significantly higher at 1.5%, primarily attributed to uncertainties in the capture cross-section and inelastic neutron scattering on ^{238}U nuclei.

The variation in estimates for one-group cross-sections of neutron interactions with actinide nuclei is notably

Table 2. Spread in values and uncertainties in key neutronic characteristics of the LFR model due to nuclear data uncertainties from different evaluated neutron data libraries

Parameter	Library: BROND 3.1 (BR), ENDF/B-VIII (EN), JENDL-5 (JL), TENDL 2021 (TL), JEFF 4T (JF)					Variation in uncertainties, %	Spread in values *, %
	BR	EN	JF	JL	TL		
Relative uncertainty, %							
k_{eff} (BoC, cold)**	1.53	0.89	0.98	0.85	0.98	0.85–1.53 ****	1.43
k_{eff} (BoC, hot)***	1.52	0.9	0.96	0.85	0.97	0.85–1.52	1.67
k_{eff} (EoC)	1.83	0.99	1.09	0.95	1.09	0.99–1.83	1.02
$\Delta\rho_D$, pcm	1.65	1.97	2.05	1.68	2.05	1.68–2.05	– 22
$\Delta\rho_{burn}$, pcm	125	49	68	54	68	49–125	– 88
BR	1.95	0.83	0.96	0.81	0.95	0.81–1.95	1.64
B, %	0.95	0.78	0.71	0.66	0.71	0.66–0.95	0.72

* Spread in values = (max–min)/min;
** Initial composition, temperature of all materials is 300 K;
*** Initial composition, Fe and Pb temperature is 600 K, fuel temperature is 1100 K;
**** Minimum – maximum value of uncertainties due to nuclear data;
B_{HM} = 59.46 (GW day/tHM);
B – calculations with a fixed thermal power;
Reactivities are presented in 1 pcm (per cent mille) = $\rho \times 10^5$;
Stationary calculations were for 10^7 statistics;
for β_{eff} (BoC and EoC), the variation in values is 19%;
BoC/EoC (beginning/end of cycle) – initial state and end of cycle.

Table 3. Nuclear data uncertainties for fuel composition at end of cycle (900 days) for the LFR model

Nuclide	Library: BROND 3.1 (BR), ENDF/B-VIII (EN), JENDL-5 (JL), TENDL 2021 (TL), JEFF 4T (JF) (δn_{EOC},%)					Spread in uncertainties, %	
	BR	EN	JF	JL	TL	min	max
^{234}U	3	2	4	3	4	2	4
^{235}U	0.8	0.8	1.5	0.4	1.5	0.4	1.5
^{236}U	5	4	7	2	7	2	7
^{238}U	0.3	0.1	0.1	0.1	0.1	0.1	0.1
^{237}Np	2	2	2	1.3	4	1.3	4
^{238}Pu	4	1.2	7	4	7	1.2	7
^{239}Pu	2.0	0.9	0.8	0.8	0.8	0.8	0.9
^{240}Pu	1.3	1.6	2.7	1.3	2.6	1.3	3
^{241}Pu	3	2	14	4	14	2	14
^{242}Pu	1.0	1.2	1.4	1.3	1.4	1.0	1.4
^{241}Am	3	1.1	6	2	6	1.1	6
^{242m}Am	6	4	8	5	34	4	34
^{243}Am	7	4	9	10	5	4	10
^{242}Cm	6	2	8	5	8	2	8
^{243}Cm	20	23	30	23	62	20	62
^{244}Cm	8	6	13	14	8	6	14
^{245}Cm	19	25	17	28	14	14	28

high, exceeding 50% for the capture cross-sections of Am and Cm. Nonetheless, this variation is comparable to the uncertainties employed in the latest versions of non-Russian evaluated nuclear data libraries. The uncertainties presented in the BROND 3.1 library appear to be underestimated for several minor actinides.

As the core temperature increases, there are no changes in the uncertainties associated with neutron cross-sections, nor are there changes in uncertainties related to the dilution cross-section. Previously, information on the uncertainties of the self-shielding effect was included in the MF32 section, which, as mentioned earlier, has been excluded from the current versions of non-Russian evaluated nuclear data libraries. Consequently, the reactor functional uncertainties in both cold and hot states will remain the same. The spectral component of uncertainty for one-group neutron cross-sections of actinides is minimal, not exceeding 0.3% for capture cross-sections and 0.1% for fission cross-sections.

There is a notable variation in the data on delayed neutrons across non-Russian evaluated nuclear data libraries, with the maximum spread in the β_{eff} value reaching 19%. The statistical uncertainty of the Monte Carlo calculation is approximately $2\sigma \sim 9\%$, highlighting the necessity of adjusting the uncertainty for this parameter through integrated measurements. The minimum values of β_{eff} for both the initial state and at the end of the cycle (900 days) correspond to the calculations from the JENDL library.

Although the overall values of reactor functional uncertainties estimated using updated library versions have decreased compared to those derived from earlier versions, the uncertainties in reactor functionals due to nuclear data remain higher than what is required by reactor facility design engineers. This underscores the need for a thorough assessment of the accuracy of computational predictions for reactor performance. Such assessments should take into account a coupled analysis of accumulated experimental data from measurements conducted at critical assemblies (k_{eff}, β_{eff}, reactivity effects, spectral indices, etc.) as well as from research and power reactors, particularly focusing on post-irradiation experiments.

Estimated accuracy of neutronic performance calculations for the LFR

The estimated accuracy of computational simulations for neutronic processes is informed by the results of reactor physics experiments (Usachev and Bobkov 1980). Publicly accessible data regarding these reactor physics experiments can be found in the OECD NEA's international handbooks on evaluated criticality benchmark experiments (ICSBEP) and evaluated reactor physics benchmark experiments (IRPhE) (DICE, IDAT). An analysis of the information and data derived from measurements at various critical assemblies leads to the conclusion that the BFS-61 critical assembly is the closest match to the LFR model under consideration.

Three critical configurations of BFS-61, composed of heterogeneous reactor materials (plutonium, depleted uranium, graphite, and lead), were employed in a series of measurements aimed at studying the neutronic performance of a lead-cooled reactor facility. These measurements focused on critical parameters, reactivity coefficients, and ratios of fission and capture reaction rates for various materials, including structural and fuel materials as well as minor actinides. The BFS-61 assemblies featured a standard core layout but differed in the composition of the side reflector: BFS-61-0 had a three-layer side reflector made of lead, steel, and depleted uranium dioxide; BFS-61-1 utilized a double-layer reflector of lead and depleted uranium dioxide; and BFS-61-2 incorporated a bottom-layer reflector of depleted uranium dioxide.

The uncertainties in posterior reactor functionals, attributed to nuclear data uncertainties (with the results of integral measurements considered), were estimated using the ONIX code (Andrianov et al. 2023b). Prior estimates – defined in this paper as the uncertainties in neutronic functionals arising from the variability in neutron-nuclei interaction characteristics derived from evaluated nuclear data files –a re contrasted with posterior estimates. The uncertainties in posterior reactor functionals incorporate the results of integrated measurements taken at critical assemblies with neutronic properties similar to those of the target facilities. Fig. 1 illustrates both prior and posterior estimates for reactor functional uncertainties related to nuclear data uncertainties, as well as the variance in calculated values obtained from different sets of evaluated neutron data.

The figure demonstrates that adjusting neutron constants within their uncertainty limits can effectively reduce discrepancies between calculations and experimental results for the integrated experiments considered. Consequently, this adjustment leads to a decrease in both the uncertainties of reactor functionals due to nuclear data uncertainties for target systems and the spread among values derived from various evaluated neutron data libraries.

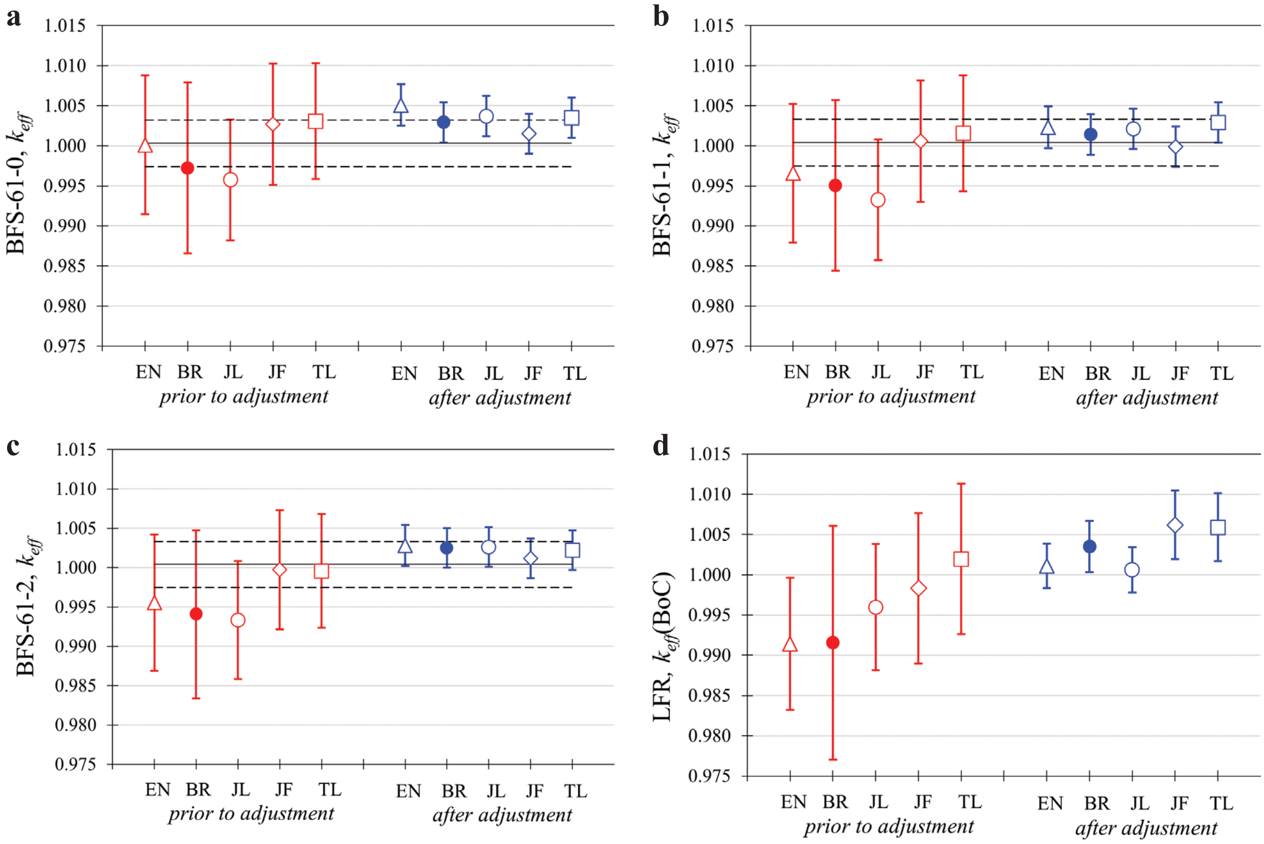

Figure 1. Values of k_{eff} prior to (red) and after (blue) adjustments of neutron data for experiments **a.** BFS-61-0; **b.** BFS-61-1; **c.** BFS-61-2, and **d.** the LFR model based on BROND 3.1 (BR), ENDF/B-VIII (EN), JENDL-5 (JL), TENDL 2021 (TL) and JEFF 4T (JF) libraries (– experimental values of k_{eff}, – – – measurement uncertainties ± 1 σ).

The adjustment of nuclear constants results in reduced discrepancies between calculations and experimental data, as well as smaller calculation uncertainties. This adjustment leads to a shift in the neutronic performance values and their associated uncertainties for the LFR model under consideration. Prior to the adjustment, the spread in nuclear constants for the k_{eff} calculations of the BFS-61-0 experiments ranged from 0.6% to 0.8%. In contrast, the spread in the k_{eff} calculations (beginning of cycle, cold) for the LFR model was approximately 1%. After the adjustment, this spread decreased to 0.2% to 0.4% for the BFS-61 and to 0.6% for the LFR model, respectively.

Furthermore, the uncertainties in k_{eff} due to nuclear data uncertainties were significantly reduced following the adjustment: for BFS-61, they decreased from 0.8%–0.9% to 0.25%, while for the LFR model, the uncertainties diminished from 0.8%–1.5% to a range of 0.3%–0.4%. It is noteworthy that different neutron data libraries exhibit negligible differences in terms of quality, as they generally yield similar discrepancies between calculations and experiments, as well as comparable calculation uncertainties.

Tables 4, 5 present data on the estimated posterior uncertainties for criticality—taking into account the results of integrated measurements—at both the beginning and end of the cycle. Additionally, they include the fuel composition uncertainties calculated for different libraries at the end of the cycle, as applied to the LFR model under consideration.

Table 4. A priori and posterior uncertainties of $k_{eff\ BoC}$ and $k_{eff\ EoC}$ for the LFR model due to nuclear data uncertainties

Parameter	Library: BROND 3.1 3.1 (BR), ENDF/B-VIII (EN), JENDL-5 (JL), TENDL 2021 (TL) и JEFF 4T (JF)					Spread in values*, %	
	BR	EN	JF	JL	TL	min	max
Prior to adjustment							
$\delta k_{eff\ BoC}$ (δσ) ,%	1.53	0.89	0.98	0.85	0.98	0.85	1.53
$\delta k_{eff\ EoC}$ (δσ) ,%	1.45	0.89	0.96	0.84	0.96	0.84	1.45
δk_{eff} (δn_{EoC}),%	1.12	0.44	0.52	0.44	0.52	0.44	1.12
$\delta k_{eff\ EoC}$,%*	1.83	0.99	1.09	0.95	1.09	0.95	1.83
After adjustment							
$\delta k_{eff\ BoC}$ (δσ) ,%	0.32	0.28	0.42	0.28	0.42	0.28	0.42
$\delta k_{eff\ EoC}$ (δσ) ,%	0.35	0.31	0.45	0.32	0.45	0.31	0.45
δk_{eff} (δn_{EoC}),%	0.79	0.35	0.48	0.35	0.47	0.35	0.79
$\delta k_{eff\ EoC}$,%	0.85	0.45	0.64	0.45	0.63	0.45	0.85

* Total value is equal to the square root of the sum of squares for components $\delta k_{eff\ EoC}$ (δσ) and δk_{eff}(δn_{EoC}).

Required and achieved uncertainties in evaluated neutron data

Since the 1970s, the need to update neutron data for fast reactor calculations has evolved, driven by the increasing demand for greater accuracy in computational predictions of key reactor characteristics. Early studies (Usachev and Bobkov 1980) assessed both the achieved and required accuracies of neutron data, establishing these based on the

Table 5. Posterior uncertainties in EoC fuel composition for the LFR model due to nuclear data uncertainties

Nuclide	Library: BROND 3.1 (BR), ENDF/B-VIII (EN), JENDL-5 (JL), TENDL 2021 (TL) и JEFF 4T (JF) (δn_{EoC},%)					Spread in values, %	
	BR	EN	JF	JL	TL	min	max
^{234}U	3	2	4	3	4	2	4
^{235}U	0.8	0.8	1.4	0.4	1.5	0.4	1.5
^{236}U	5	4	7	2	7	2	7
^{238}U	0.23	0.09	0.10	0.09	0.10	0.1	0.2
^{237}Np	2	2	2	1.3	4	1.3	4
^{238}Pu	4	1.2	7	4	7	1.2	7
^{239}Pu	1.5	0.7	0.7	0.7	0.7	0.7	1.5
^{240}Pu	1.2	1.4	3	1.2	2	1.2	3
^{241}Pu	3	2	13	4	13	2	13
^{242}Pu	1.0	1.2	1.4	1.3	1.4	1.0	1.4
^{241}Am	3	1.1	6	2	6	1.1	6
^{242m}Am	6	4	8	5	34	4	34
^{243}Am	7	4	9	10	5	4	10
^{242}Cm	6	2	8	5	8	2	8
^{243}Cm	20	23	30	23	62	20	62
^{244}Cm	8	6	13	14	8	6	14
^{245}Cm	19	25	17	28	14	14	28

conditions necessary to meet target accuracies for calculating the BR and k_{eff}, set at 2% and 1%, respectively, for sodium-cooled fast reactors utilizing uranium-plutonium oxide fuel (see Table 1).

In these calculations, diagonalized matrices of neutron constant uncertainties were employed (solving a conditional nonlinear optimization problem) without directly considering the energy cross-correlations among cross-sections. As a result, the required accuracies of neutron data determined through this method may be regarded as overestimated. For instance, in reference Manokhin and Usachev 1984, the necessary uncertainties for the one-group fission cross-sections of ^{239}Pu and ^{241}Pu, which were estimated to ensure a k_{eff} uncertainty of 1%, were reported as 4% and 8%, respectively.

Later studies (Working Party 2008) demonstrated that directly accounting for energy cross-correlations among actinide neutron cross-sections – determined from actual experimental data – significantly improved the criticality uncertainty estimation for sodium-cooled fast reactors and lead-cooled fast reactors. This approach enabled a criticality calculation accuracy of 0.3% to 0.4%, even when the one-group fission cross-sections for ^{239}Pu and ^{241}Pu were set at 5% and 10%, respectively. This finding underscores the importance of accurately considering the correlation properties of neutron data uncertainties when estimating the target accuracies of reactor parameters.

Table 6 presents data on the currently achieved accuracies of one-group actinide neutron cross-sections (averaged with a neutron spectrum for the LFR model). These estimates are based on the latest versions of various non-Russian evaluated nuclear data libraries, including ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, and TENDL-2019, as well as the Russian BROND-3.1 library. Since the estimates for covariance matrices—and, consequently, for one-group neutron cross-sections – vary significantly, Table 6 provides both the average values of uncertainties and the range of values for one-group cross-sections calculated using the libraries in question. The required accuracies (see Table 6) were obtained by solving the inverse problem for determining target accuracies using the ONIX code, under the assumption that neutron constants must ensure a k_{eff} calculation accuracy for the LFR model of no more than 0.2% (Andrianov et al. 2023a, 2023b).

As shown in Table 6, the uncertainties of neutron cross-sections for the actinides most critical to the estimation of k_{eff} calculation accuracy for LFRs, identified as "required" in the 1984 study, have now been achieved thanks to advancements in experimental techniques and neutron data estimation. Consequently, the current a priori uncertainty for LFR k_{eff} – estimated based on covariance matrices of neutron data uncertainties without incorporating the results of integrated measurements – aligns with

Table 6. Achieved and required neutron data uncertainties for actinide nuclei

Nuclide	This study			Manokhin and Usachev 1984		This study			Manokhin and Usachev 1984	
	Mt = 102 (radiation capture cross-section)					Mt = 18 (fission cross-section)				
	1	2	required*	achieved	required	1	2	required	achieved	required
^{238}U	2	4	<0.5**	8	8	2	6	1	5	4
^{238}Pu	31	14	10	–	–	5	3	3	–	–
^{239}Pu	4	7	2	10	4	0.8	1.2	<0.5	4	4
^{240}Pu	12	8	<5	20		3	6	2	10	10
^{241}Pu	10	10			7	3	2	<3	8	5
^{242}Pu	7	17	<10	50	15	3	5		30	30
^{242m}Am	44	17		30	20	24	6	5		
^{241}Am	6	11	5	15	15	4	8	3	15	15
^{242}Am	44	17	<10	30	30	24	6	<5	30	30
^{243}Am	8	26		50	20	4	5		50	50
^{243}Cm	40	56	<20	–	–	6	3		–	–
^{244}Cm	18	51				7	9			
^{245}Cm	33	34				3	3			
^{237}Np	10	10	<10	50	15	3	2	<3	10	10
FP	12	–		30				–		

1 – Average uncertainty value for ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, TENDL-2019 and BROND-3.1 libraries, 2 – Spread in values of one-group cross-sections for ENDF/B-VIII.0, JEFF-3.3, JENDL-4.0, TENDL-2019 and BROND-3.1 libraries, * – required accuracy obtained from the $\delta k_{eff}(\delta n_{EoC})<0.2\%$ condition, ** – provided there are correlations between different reactions (rounded).

the 1984 target uncertainty of approximately 1%. However, given that the presently required k_{eff} calculation accuracy for LFRs utilizing uranium-plutonium fuel is around 0.2% to 0.3%, the achieved accuracies in neutron data cannot be regarded as being sufficient.

Discussion of results

The key observations regarding the current study can be summarized from two perspectives: 1) the effects of evaluated neutron data from different libraries on the accuracy of calculating key neutronic characteristics of LFRs, and 2) the potential for improving the accuracy of computational predictions for LFR neutronic performance by incorporating integrated measurement results.

1. Effects of evaluated neutron data from different libraries on calculation accuracy of key neutronic characteristics for LFRs

All analyzed libraries of evaluated neutron data contain the necessary information for estimating the uncertainty of the initial load criticality of LFRs in the cold state. However, no single library provides a comprehensive set of data on uncertainties required to estimate the uncertainty for a potentially complete set of stationary neutronic functionals, such as the Doppler reactivity coefficient and the effective fraction of delayed neutrons. For example, all libraries lack the MF32 section necessary to estimate uncertainties related to resonance self-shielding and Doppler effects for ^{238}U. Only the JENDL library includes covariance matrices (MF section = 31) for the average number of prompt and delayed neutrons emitted per fission event (MT = 452, 455, 456) for ^{239}Pu, which is a major contributor to the β_{eff} uncertainty in LFRs with uranium-plutonium fuel.

When estimating the uncertainty of point kinetics parameters, none of the analyzed libraries include covariance data on the decay constants for precursor nuclei of delayed neutrons (λ_i) or the yield fractions of delayed neutrons (β_i). Similarly, for nuclide kinetics problems, there is no complete set of data on neutron data uncertainties; the libraries provide only uncertainty data (without correlations) for decay constants and yields of fission products. There is also no data available for estimating the uncertainty of branching factors, as covariance data for isomer formation cross-sections are absent. Among the libraries considered, only TENDL provides all the necessary data for estimating the uncertainty of neutron cross-sections for all fission products, while other libraries offer limited lists of fission products with available covariance data.

In the absence of the required covariance data in these libraries, the variation in estimates for respective characteristics, using neutron data from different libraries, can serve as a ersatz approach for estimating the uncertainties due to nuclear data in the calculation of the most critical neutronic characteristics of LFRs. Significant spreads have been observed in the values of one-group neutron cross-sections for minor actinides, with spreads exceeding 50% for the capture cross-section of Am and Cm, and uncertainties differing by several times when averaged with the LFR neutron spectrum.

The calculations and uncertainty estimates reveal that the ENDF, JENDL, JEFF, and TENDL libraries produce similar results. This can be attributed to the fact that the neutron cross-sections in the fast energy region and the resonance parameters for key fuel nuclides (^{235}U, ^{238}U, and ^{239}Pu) are consistent across these library groups.

The a priori criticality uncertainty values for the starting load (cold state), as estimated using non-Russian evaluated nuclear data libraries, range from 0.9% to 1%, while the value from the BROND 3.1 library is 1.5%. For criticality uncertainty values at the end of the cycle (900 days), the estimates using non-Russian libraries vary from 0.9% to 1.2%, with the BROND 3.1 value being 1.8%. The spreads in criticality values calculated using different libraries for all considered states are approximately 1% to 1.5%.

2. Possibilities for improving the accuracy of computational predictions for LFR neutronic performance by incorporating integral measurement results

Over the past 40 years, the accuracy of calculations for key LFR reactor characteristics has significantly improved, with average uncertainties reduced by approximately 50%. The accuracies achieved today align with the target values established several decades ago.

The estimates indicate that achieving a target calculation accuracy for k_{eff} of 0.2%, without incorporating integral experiments, necessitates a substantial reduction in neutron cross-section uncertainties – by a factor of 7 to 10. This level of reduction cannot always be achieved solely through numerous differential measurements (i.e., measurements of neutron cross-sections) due to the limitations of existing measurement methodologies and equipment. Currently, it is not feasible to significantly reduce the neutron cross-section uncertainties of key contributors to the uncertainties in neutronic characteristics, specifically ^{238}U and ^{239}Pu. Thus, integral experiments using uranium-plutonium fuel become increasingly important as the most realistic means to enhance the computational prediction accuracy for LFR neutronic performance.

A significant reduction in the uncertainty of neutronic performance calculations can be accomplished through the assimilation of experimental reactor physics data, which enables the integration of information from integral measurements conducted at critical assemblies. For instance, by incorporating the results from BFS-61 series critical experiments, the uncertainties in the criticality of the starting load (cold state) can be reduced from 1% to 0.5%, while uncertainties in criticality at the end of the cycle can be decreased from 1.2% to 0.6%. Concurrently, the spread in criticality values calculated using non-Russian evaluated nuclear data libraries is also halved, decreasing from 1.4% to 0.6%.

The uncertainty in criticality at the end of the cycle is significantly influenced by the uncertainty in the nuclide composition of heavy nuclei in irradiated fuel, which primarily stems from the uncertainties associated with one-group fission cross-sections and the capture of actinides. It is worth noting that the uncertainty of fission product yield and capture cross-sections does not substantially contribute to the criticality uncertainty at the end of the cycle.

Conclusions

Using a simplified model of a heavy liquid metal-cooled fast reactor (LFR) with dense uranium-plutonium fuel, an analysis was conducted to assess the effects of various evaluated neutron data libraries (ENDF/B-VIII, JENDL-5, TENDL-2021, JEFF-4T1, BROND-3.1) on the accuracy of calculating key neutronic characteristics. The results indicate that uncertainties in determining essential reactor functional – such as the effective multiplication factor, effective fraction of delayed neutrons, Doppler reactivity effect, breeding ratio, and burnup reactivity margin – have decreased compared to the results obtained with earlier versions of these libraries. This improvement highlights progress in neutron data evaluation.

An analysis of the target calculation accuracy for LFR neutronic performance, as declared over the past decades, reveals the necessity for further enhancements in the accuracy of evaluated neutron data. This paper evaluates the requirements for neutron data accuracy needed to achieve the stated target accuracy.

To improve the accuracy of computational predictions for LFR neutronic performance, it is crucial to incorporate the results of integral measurements. This approach enables the validation and refinement of both computational models and evaluated neutron data libraries. Key factors in enhancing the reliability and safety of advanced LFR reactors include continued research in neutron data evaluation, upgrades to computational codes, and the execution of new, highly informative integral experiments.

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References

- Andrianov AA, Kuptsov IS, Osipova TA, Spiridonova AA, Andrianova ON, Utyanskaya TV (2022) Nuclear energy system modelling application package: functional overview and examples. Nuclear Energy and Technology 8(4): 289–295. https://doi.org/10.3897/nucet.8.97651
- Andrianov AA, Andrianova ON, Korovin YuA, Kuptsov IS, Spiridonova AA (2023a) A computer code for optimizing the neutronics model parameters based on results of reactor physics experiments. Nuclear Energy and Technology 9(4): 289–296. https://doi.org/10.3897/nucet.9.117198
- Andrianov AA, Andrianova ON, Korovin YuA, Kuptsov IS, Spiridonova AA (2023b) A computer code for optimizing the neutronic model parameters based on results of integral experiments. Izvestiya vuzov. Yadernaya energetika 2: 148–161. https://doi.org/10.26583/npe.2023.2.12 [in Russian]
- Andrianov AA, Andrianova ON, Golovko YuYe, Kuptsov IS, Lomakov GB, Spiridonova AA (2023c) Testing modern evaluations of neutron data accuracy in the problem of determining the accuracy of calculating neutronic characteristics of a fast reactor model with heavy liquid metal coolant. Manuscript deposited at VINITI, Deposition No. 14-V2023 24.05.2023. [in Russian]
- Andrianova ON, Golovko YuE, Zherdev GM, Zadornov DV, Koshcheev VN, Manturov GN, Peregudov AA, Tsibulya AM (2014) Testing covariance matrices of uncertainties in the BNAB data system. Izvestiya vuzov. Yadernaya energetika 2: 109–117. https://doi.org/10.26583/npe.2014.2.12 [in Russian]
- Balovnev AV, Davydov VK, Zhirnov AP, Moiseev AV, Soldatov EO (2021) Simulating the fuel cycle of a lead-cooled fast reactor. Nuclear Energy and Technology 8(1): 71–76. https://doi.org/10.3897/nucet.8.83062
- Bychkov SA, Varfolomeeva VA, Grushin NA, Ivanov IYe, Andrianova ON (2024) Nuclide kinetics problems solution using MNT-CUDA. Neutronic Problems of Nuclear Power: Abstracts of the Scientific and Technical Conference, May 28–31, 2024. Obninsk, 79–79. [in Russian]
- Cabellos O, Hursin M, Palmiotti P (2023) WPEC/SG46 Exercise on Target Accuracy Requirement. EPJ Web of Conferences 284: 14012 [4 pp.]. https://doi.org/10.1051/epjconf/202328414012
- Castelluccio DM, Grasso G, Lodi F, Peluso V (2022) Assessment of nuclear data target accuracy requirements for ALFRED. In Proc. of the Inter. Conf. on Phys. of Reactors 2022 (PHYSOR 2022), Pittsburgh, PA. May 15–20, 1085–1094. https://doi.org/10.13182/PHYSOR22-37572
- DICE. Database for ICSBEP (DICE). NEA/OECD Website. https://www.oecd-nea.org/dice/webstart/dice.jnlp [accessed Dec. 31, 2023]
- IAEA (2021) Official website of Evaluated Nuclear Data File (ENDF). https://www-nds.iaea.org/exfor/endf.htm [accessed Dec. 31, 2023]
- IDAT. International Reactor Physics Handbook Database and Analysis Tool (IDAT). NEA/OECD website. https://www.oecd-nea.org/idat/webstart/IDAT.jnlp [accessed Dec. 31, 2023]
- Manokhin VN, Usachev LN (1984) Nuclear data requirements for fast reactors. Atomic energy 57(4): 683–692. https://doi.org/10.1007/BF01123637
- Usachev LN, Bobkov YuG (1980) Perturbation theory and experiment planning in the problem of nuclear data for reactors. Moscow, Atomizdat Publ., 88–88. [in Russian]
- Working Party (2008) Uncertainty and target accuracy assessment for innovative systems using recent covariance data evaluations. A Report by the Working Party on International Evaluation Co-operation of the Nuclear Science Committee.
- WPEC Subgroup 46. Official website “Efficient and effective use of integral experiments for nuclear data validation”. https://www.oecd-nea.org/download/wpec/sg46/ [accessed Dec. 31, 2023]