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Research Article

Nuclear data uncertainty on generation IV fast reactors criticality calculations analysis comparison*

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Abstract

The new calculation code capabilities are applied in the current work as well as important fast reactor criticality parameters uncertainty assessment articles' results based on different nuclear data libraries and covariance matrices. A comparative analysis of uncertainty estimations related to neutron reactions is presented for lead-cooled reactor models and sodium-cooled reactor models. For the models of advanced BN and BR fast reactors with three fuel types (UO_2, MOX, MNUP), the multiplication factor uncertainty calculations are performed using 252-group covariance matrices based on ENDF/B-VII.1 library via the SCALE 6.2.4 code system. The main nuclear data uncertainty contributors in the multiplication factor are determined. Recommendations are formulated for improving the cross sections accuracy for several nuclides in order to provide more reliable results of fast reactor criticality calculations. Lead-cooled reactors have no operational history compared to light-water and sodium-cooled reactors. The experimental data insufficiency calls in the question about reliability of the simulation results and requires a comprehensive initial data uncertainty analysis for the neutron transport simulation. The obtained results support the idea that lead- and sodium-cooled reactors have close nuclear data sensitivity using one and the same computation tools, nuclear data libraries and fuel compositions. This makes it possible to use the accumulated data of benchmarks for sodium-cooled reactors in the safety determination of lead-cooled reactors.

Keywords

Fast reactors, Generation IV, covariance matrices, sensitivity coefficient, nuclear data uncertainty, SCALE, MNUP, MOX

Introduction

Generation IV International Forum has identified and selected six nuclear power systems for further investigations and development making world's future energy demand supply possible. Sodium-cooled fast reactors are one of the most extensively studied and advanced considered commercial-size reactor concepts, greatly supported by industries and research institutions. For large-scale two-component nuclear power system (fast reactors with a closed nuclear fuel cycle), it is so far theoretically proven and computationally and experimentally attested that such three conceptual requirements as core BR close to unity, lead coolant and high-density mixed nitride uranium-plutonium (MNUP) fuel allow improving the safety of nuclear reactors notably (Adamov et al. 2022). Increased safety properties of lead (lead-bismuth), including relative chemical inertness, capability to retaining

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hazardous radionuclides, such as iodine and cesium, and high boiling temperature, contributes to the selection of lead-cooled reactor as an economically competitive Generation IV reactor. However, lead-cooled reactors do not have a comparably considerable operation experience as light water and sodium-cooled reactors do. It is stated in Trottier et al. 2018; Trivedi et al. 2020; Castelluccio et al. 2021; Romojaro et al. 2021, that insufficient experimental data calls in the question about reliability of computational simulation results and requires a comprehensive initial data uncertainty analysis for the neutron transport simulation. Propagating these uncertainties gives a better notion of their influence on the reactor core performance and makes it possible to estimate the design safety limits. Based on the results obtained, the paper supports the statement that the nuclear data sensitivity is close to both lead- and sodium-cooled reactors with analogous fuel compositions using one and the same computational tools and nuclear data libraries. This allows us to use the accumulated benchmarks of sodium-cooled reactors to prove the lead-cooled reactor safety.

Russia has the world's most highest level experience in developing and operating sodium-cooled fast reactors. During the initial stage of the BN technology development and adoption process, the use of oxide fuel, due to its maturity in terms of application in thermal reactors, was a reasonable decision. However, high-density fuel types on the account of their physical properties have obvious advantages in fast reactors. This is the reason why all countries, developing innovative fast-neutron reactors, are considering transition from oxide to high-density fuel types, though Russian and the international experience in using nitride fuel is not enough for predicting reliably the represented fuel elements serviceability working at the BN and BR reactor parameters.

The initial data uncertainties together with the obtained results uncertainties are an integral part of the studies aiming to demonstrate the reactor facilities nuclear safety. Analyzing innovative fast reactor models with mixed uranium-plutonium fuel, the cumulative nuclear data uncertainty contribution to the multiplication factor k_{eff} calculation without taking into account integral experiments is ± 1.5–1.9% [6]. Besides, it is noted in the Manturov et al. 2022 paper that the uncertainty may be decreased to ± 0.4–0.6% as a result of the compensative effect of the uncertainty correlations of evaluated quantities at different neutron energies and reaction channels.

This paper analyzes the influence of nuclear data uncertainties in lead-cooled (Table 1) and sodium-cooled (Table 2) reactor models. The listed data have been supplemented with own calculations of BR-1200 and BN-1200 reactor models with three fuel types (UO2, MOX and MNUP). In the BR and BN calculations, the sensitivity analysis was provided using the TSUNAMI sequence of the SCALE 6.2.4 code (Bostelmann et al. 2022). The k_{eff} uncertainty was estimated and quantitatively investigated using the SAMS module applied in the TSUNAMI sequence. The results were compared to identify the potential needs for updating the nuclear data. Own calculations were undertaken to identify the nuclides and reactions that have the greatest effect on the BR and BN neutronic performance.

Table 1. Analyzed lead-cooled fast reactors

Reactor	Nuclear data library	Reference
SEALER	JEFF-3.1, ENDF/B-VII.1	Trottier et al. 2018
ALFRED	JEFF-3.3, ENDF/B-VIII.0	Romojaro and Alvarez-Velarde 2020
	ENDF/B-VII.0, ENDF/B-VII.1	Romojaro et al. 2017a
	ENDF/B-VIII.0	Castelluccio et al. 2021
DLFR	ENDF/B-VII.0	Trivedi et al. 2020
MYRRHA	JEFF-3.1.2, ENDF/B-VII.0, ENDF/B-VII.1	Romojaro et al. 2017b
	JEFF-3.3, ENDF/B-VIII.0	Romojaro et al. 2021

Table 2. Analyzed sodium-cooled fast reactors

Reactor	Nuclear data library	Reference
EBR-II	ENDF/B-VII.1, ENDF/B-VIII.0	Bostelmann et al. 2021
BN-600	ENDF/B-VII.1, ENDF/B-VIII.0	Ma et al. 2021
JOYO	ENDF/B-VII.1	Wan et al. 2020
ASTRID	ENDF/B-VII.1	Griseri et al. 2017
B & BR	ENDF/B-VII.0, ENDF/B-VII.1	Vu and Hartanto 2021
ZPPR-9	ENDF/B-VII.0	Zheng et al. 2018
ESFR	JEFF-3.3, ENDF/B-VIII.0	Romojaro et al. 2021

Observed fast reactors features

The following four models of lead-cooled reactors have been selected for the comparative analysis.

SEALER (Trottier et al. 2018) is a modular reactor with 19.9% enriched UO_2 fuel. The electric power is 3 to 10 MW. The reactor core life is 10 to 30 years (full power operation without refuelling).

ALFRED (Romojaro et al. 2017a; Romojaro and Alvarez-Velarde 2020; Castelluccio et al. 2021) is a small-size reactor, its core is divided in two zones (internal and external) with different plutonium contents (20.5% in the external zone) for power field flattening. The electric power is 125 MW and the maximum fuel burnup is 100 MW·day/kg. Each year, 1/5 of the core is unloaded and replaced with fresh fuel.

DLFR (Trivedi et al. 2020) is a medium-size reactor, its core includes two uranium enrichment zones (17.5% in the external zone). The electric power is 450 MW. The refuelling scenarios are at the development stage.

MYRRHA (Romojaro et al. 2017b; Romojaro et al. 2021) is a small-size reactor capable to operate both in a subcritical state when using a linear 600 MeV proton accelerator and in a critical mode (as a lead-bismuth-cooled fast-neutron reactor). The electric power is 57 MW. Different fuel compositions are considered.

Seven sodium-cooled reactor models have been taken for the comparative analysis.

EBR-II (Bostelmann et al. 2021) is a 20 MW(e) demonstration reactor, consisting of three regions (core, inner and outer shield). Fuel elements are fuelled with enriched uranium metal (67%) and it is chosen stainless-steel cladding.

BN-600 (Ma et al. 2021) is a 600 MW(e) commercial reactor using enriched UO_2 fuel since the start of the operation. The paper considers the results of a benchmark calculation with MOX fuel with a 20% plutonium content.

JOYO (Wan et al. 2020) is an experimental reactor using MOX fuel which comprises 23% enriched uranium and 17.7% plutonium. The fissionable plutonium isotopes content is 80.4%. The thermal power is 140 MW.

ASTRID (Griseri et al. 2017) is a commercial reactor with core comprising two fuel subzones. It is considered as an MA burner. The fuel consists of about 70% depleted uranium, 20% to 22% plutonium, and about 10% MAs. The electric power is 500 MW.

B & BR (Vu and Hartanto 2021) is a modular reactor with UO_2 fuel, enriched to 12.32%. The electric power is 400 MW. The reactor core life is up to 50 years (full power operation without refuelling).

ZPPR-9 (Zheng et al. 2018) is a zero-power reactor using MOX fuel with a 17.7% plutonium content.

ESFR (Romojaro et al. 2021) is a commercial-size reactor with two subzones core with different fuel section heights in the fuel rods. There is a MOX fuel used with a 14.6% and 17% plutonium content in the subzones. The electric power is 1500 MW.

Codes and methodologies

The sensitivity and uncertainty calculations were performed in the software suite SCALE 6.2.4. In particular, the package was used to test the developed new-generation codes for fast reactor neutronic calculations (Ternovykh et al. 2017; Ternovykh and Bogdanova 2020; Tikhomirov et al. 2021). System code SCALE involves several control sequences for neutronic calculations and nuclear safety analysis, it has been developed and evolved by Oak Ridge National Laboratory. It combines modules for criticality calculation, radiation shielding and nuclide kinetics, sensitivity and uncertainty analysis and other problems. A Monte Carlo transport code, KENO-VI, is used to support calculations in a 3D geometry. The neutron transport simulation can be performed both in a multi-group approximation and with continuous representation of cross-sections by energy. TSUNAMI is a sensitivity and uncertainty analysis module. The TSUNAMI module uses the forward and adjoint neutron transport solutions, obtained by a KENO-VI calculation, using SAMS to compute sensitivities via first order perturbation theory. Sensitivity calculations together with the ENDF/B-VII.1 covariance data can be used to estimate the uncertainty of k_{eff} or other functionals.

Analysis of observed and scale calculated reactor results

Increased reactor safety requirements call for improving the characteristics prediction accuracy of the fast reactors both in operation and under design. One of the key objectives is to refine the available and develop new, more advanced software tools and databases to support neutronic calculations, estimate the existing uncertainties and work out recommendations for reducing them (Manturov et al. 2022).

Sensitivity analysis of observed fast reactors

There is a comparative analysis of the k_{eff} sensitivity coefficients using different nuclear data libraries in the observed fast reactors presented.

Fig. 1 presents the k_{eff} sensitivity coefficients to the seven most important nuclides and reactions for the investigated reactor models with MOX fuel. The k_{eff} sensitivity coefficients for MYRRHA, using two different libraries (JEFF-3.3 and ENDF/B-VII.0), are close to the k_{eff} sensitivity coefficients for ALFRED. When comparing ZPPR-9 and ESFR sodium-cooled reactors with MYRRHA lead-cooled reactor, with similar libraries used (ENDF/B-VII.0 and JEFF-3.3), it is noted that the sensitivity coefficients have close values. The sensitivity coefficient differences are explained mainly by the ESFR design features (fertile

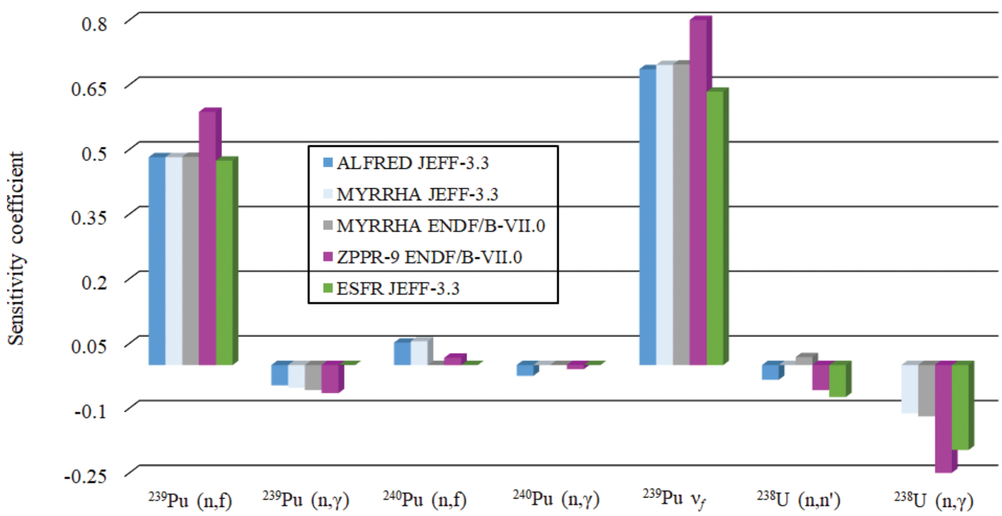

Figure 1. Top 7 integrated k_{eff} sensitivity coefficients for reactors with MOX fuel.

blankets) and a smaller plutonium content rather than by different coolants used in the reactors.

A common conclusion for lead- and sodium-cooled reactors with MOX fuel is that greater k_{eff} sensitivity is shown to ν_f and ^{239}Pu fission. We should note that these reactions with highest sensitivity coefficients usually do lead to the largest uncertainties with different used libraries in the reactor calculations.

Analysis of k_{eff} nuclear data uncertainties

The k_{eff} nuclear data uncertainties introduced by their major contributors in the different libraries used in ALFRED reactor calculations are provided in Table 3. The biggest contributors to the k_{eff} uncertainties are the uncertainties of ^{239}Pu ν_f and ^{238}U (n,n′) when ENDF/B-VII.0 library is used, the cross-section uncertainties of ^{238}U (n,n′) and ^{239}Pu (n,γ) when ENDF/B-VII.1 library is used, the cross-section uncertainties of ^{240}Pu (n,f) and ^{240}Pu (n,γ) when JEFF-3.3 library is used, and cross-section uncertainties of ^{238}U (n,f) and ^{239}Pu (n,γ) when ENDF/B-VIII.0 library is used. It is to be noted that a re-estimation of cross-sections in ENDF/B-VIII.0 library have led to the k_{eff} uncertainties caused by the cross-section uncertainties of ^{240}Pu (n,f) and ^{240}Pu (n, γ), regarding the cross-correlations between ^{240}Pu (n,γ) and ^{240}Pu (n,γ), reduced by a factor of 10, and the uncertainties caused by the ^{239}Pu (n,f) and ^{239}Pu (n,γ) reactions increased by a factor of over 1.5 as compared with JEFF-3.3 calculations. When ENDF/B-VII.0 library is used for the calculations, the uncertainties of ^{239}Pu ν_f and ^{238}U (n,n′) are the biggest contributors in contrast to the other libraries where their values are several times smaller. The covariance matrix of ENDF/B-VII.1 library have the smallest k_{eff} uncertainty caused by the uncertainty of ^{239}Pu ν_f, as compared to the other libraries. The total uncertainty in k_{eff} does not exceed 0.8% when ENDF/B-VIII.0 and JEFF-3.3 libraries are used.

Table 3. k_{eff} nuclear data uncertainties in different libraries in ALFRED, %

Covariance	JEFF-3.3	ENDF/B-VIII.0	ENDF/B-VII.1	ENDF/B-VII.0
^{240}Pu (n,f) - ^{240}Pu (n,f)	0.52	-	-	-
^{240}Pu (n,f) - ^{240}Pu (n,γ)	-0.42	-	-	-
^{239}Pu ν_f - ^{239}Pu ν_f	0.32	0.19	0.06	0.7
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.3	0.58	0.2	0.2
^{238}U (n,n‘) - ^{238}U (n,n‘)	0.23	0.13	0.54	0.53
^{239}Pu (n, γ) - ^{239}Pu (n, γ)	0.14	0.21	0.25	0.27
Total uncertainty	0.79	0.75	-	-

The k_{eff} nuclear data uncertainties introduced by their major contributors in the different libraries used in the MYRRHA reactor calculations are provided in Table 4. The same conclusions can be made as well as for ALFRED reactor due to the close characteristics of the two reactors. When JENDL-4.0 m library is used, the major contributors to the k_{eff} nuclear data uncertainty are the cross-section uncertainties of ^{239}Pu (n,f) and ^{239}Pu (n,γ). The smallest uncertainties are found in JENDL-4.0 m data, as compared to the other libraries, except the ^{239}Pu (n,f) uncertainty value in ENDF/B-VII.0. The total uncertainty is equal to 0.96% when ENDF/B-VII.0 library is used, 0.77% when ENDF/B-VIII.0 and JEFF-3.3 libraries are used, and 0.55% when JENDL-4.0 m library is used.

Table 4. k_{eff} nuclear data uncertainties in different libraries in MYRRHA, %

Covariance	JEFF-3.3	ENDF/B-VIII.0	JENDL-4.0 m	ENDF/B-VII.0
^{240}Pu (n,f) - ^{240}Pu (n,f)	0.54	-	-	-
^{240}Pu (n,f) - ^{240}Pu (n,γ)	-0.42	-	-	-
^{239}Pu ν_f - ^{239}Pu ν_f	0.32	0.19	0.11	0.7
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.3	0.55	0.27	0.19
^{238}U (n,n‘) - ^{238}U (n,n‘)	-	-	0.15	0.32
^{239}Pu (n, γ) - ^{239}Pu (n, γ)	0.15	0.23	0.19	0.27
Total uncertainty	0.77	0.77	0.55	0.96

The k_{eff} nuclear data uncertainties introduced by their major contributors in the different libraries used in BN-600 and ESFR reactors are provided in Table 5.

Table 5. k_{eff} nuclear data uncertainties in different libraries in ESFR and BN-600, %

Reactor	ESFR		BN-600	
Covariance	JEFF-3.3	ENDF/B-VIII.0		ENDF/B-VII.1
^{240}Pu (n,f) - ^{240}Pu (n,f)	0.59	-	0.01	0.01
^{238}U (n,γ) - ^{238}U (n,γ)	0.3	-	0.24	0.27
^{239}Pu χ - ^{239}Pu χ	0.46	0.22	-	0.24
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.31	0.55	0.71	0.25
^{238}U (n,n‘) - ^{238}U (n,n‘)	0.48	0.24	0.15	0.7
^{239}Pu (n, γ) - ^{239}Pu (n, γ)	-	0.25	0.28	0.29
Total uncertainty	1.05	0.8	0.88	0.9

The total BN-600 and ESFR uncertainties are close to each other. In BN-600, the uncertainty of ^{238}U (n,n′) is decreased from 0.7 to 0.15%. The uncertainty of ^{239}Pu (n,f) is increased from 0.25 to 0.7% when changing library from ENDF/B-VII.1 to ENDF/B-VIII.0. In ESFR, using ENDF/B-VIII.0 instead of JEFF-3.3, the uncertainty of ^{238}U (n,n′) changed from 0.48 to 0.24%, and the uncertainty of ^{239}Pu (n,f) changed from 0.31 to 0.55%. The total uncertainty, using ENDF/B-VIII.0, has the smallest value and the closest one for sodium- and lead-cooled reactors.

Analysis of the SCALE calculated reactor results

The BR-1200 and BN-1200 reactor models were calculated with three fuel types: uranium dioxide, MOX and MNUP fuel. The reactor calculations were performed using the TSUNAMI-3D module, the 252-group ENDF/B-VII.1 nuclear data library and 252-group covariance matrices were used. The k_{eff} calculation statistical error did not exceed 0.0001.

Fig. 2 presents the most important k_{eff} sensitivity coefficients for reactors with MOX and MNUP fuels. Coolant or fuel type difference does not lead to a great effect on the k_{eff} sensitivity coefficients. The sensitivity coefficients to ^{239}Pu reactions are a little smaller for BN compared to

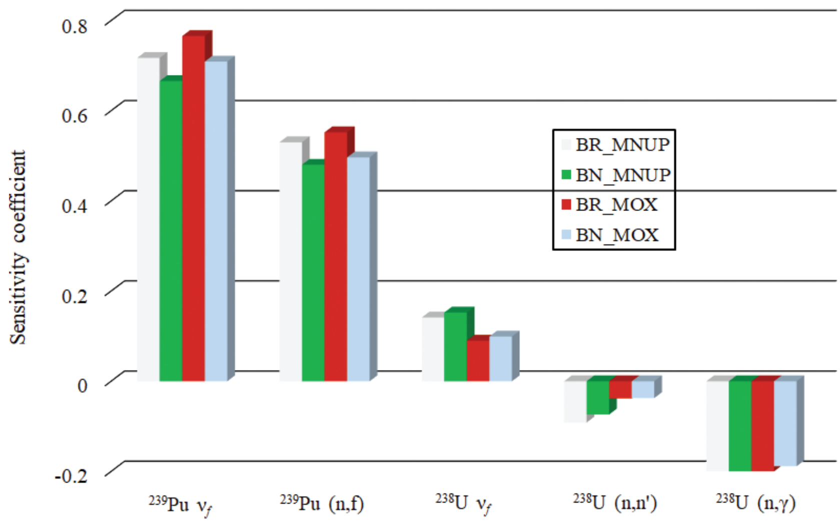

Figure 2. Top 5 integrated k_{eff} sensitivity coefficients for BR and BN reactors with MNUP and MOX fuel.

BR. We should note that the sensitivity coefficients to ^{238}U are smaller than to ^{239}Pu, but the uncertainties for ^{238}U are larger than for ^{239}Pu.

Tables 6 and 7 present the k_{eff} uncertainties introduced by their major contributors in BR-1200 and BN-1200 reactors. The calculated uncertainties mainly agree with the Andrianova et al. 2014 results.

It is to be noted that the major contributor to the k_{eff} uncertainty in reactors with MOX fuel is ^{238}U (n,n′) and its value is about 0.6%. The major contributor for reactors with uranium fuel is ^{235}U (n,γ) with an uncertainty of 2%.

Table 6. k_{eff} nuclear data uncertainties in reactors with MNUP fuel, %

Covariance	BR-1200	BN-1200
^{238}U (n,n‘) - ^{238}U (n,n‘)	1.28	1.03
^{238}U (n,γ) - ^{238}U (n,γ)	0.32	0.31
^{239}Pu (n, γ) - ^{239}Pu (n, γ)	0.23	0.2
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.22	0.2
^{239}Pu χ - ^{239}Pu χ	0.22	0.18
^{238}U χ - ^{238}U χ	0.17	0.18
^{238}U ν_f - ^{238}U ν_f	0.17	0.18
^{239}Pu (n,n‘) - ^{239}Pu (n,n‘)	0.13	0.09
^{56}Fe (n,n‘) - ^{56}Fe (n,n‘)	0.12	0.12
^{207}Pb (n,n‘) - ^{207}Pb (n,n‘)	0.11	-
^{23}Na (n,n) - ^{23}Na (n,n)	-	0.1
Total uncertainty	1.45	1.21

Table 7. k_{eff} nuclear data uncertainties in reactors with MOX fuel, %

Covariance	BR-1200	BN-1200
^{238}U (n,n‘) - ^{238}U (n,n‘)	0.53	0.61
^{239}Pu (n, γ) - ^{239}Pu (n, γ)	0.31	0.25
^{238}U (n,γ) - ^{238}U (n,γ)	0.28	0.27
^{56}Fe (n,n) - ^{56}Fe (n,n)	0.23	0.08
^{239}Pu (n,f) - ^{239}Pu (n,f)	0.23	0.2
^{56}Fe (n, γ) - ^{56}Fe (n, γ)	0.17	0.2
^{239}Pu χ - ^{239}Pu χ	0.15	0.15
^{207}Pb (n,n‘) - ^{207}Pb (n,n‘)	0.13	-
^{56}Fe (n,n‘) - ^{56}Fe (n,n‘)	0.12	0.17
^{238}U ν_f - ^{238}U ν_f	0.11	0.12
Total uncertainty	0.85	0.86

The contribution of the structural material reactions to the k_{eff} uncertainty is about 0.2%, which agrees with the papers analyzed above.

For reactors with MNUP fuel, the BR and BN total uncertainties differ by 20% and are defined, basically, by differences in the uncertainties of ^{238}U (n,n′), which requires an additional analysis. In general, the comparison of the uncertainties shows that the lead- and sodium-cooled reactors have close nuclear data sensitivity using one and the same calculation tools, nuclear data libraries and fuel compositions.

Conclusions

The calculated results of the sensitivities and uncertainties for Generation IV sodium- and lead-cooled fast reactors have been analyzed. The SCALE code was used for BR-1200 and BN-1200 reactors with three fuel types to calculate the sensitivities and uncertainties for the multiplication factor due to nuclear data.

The major uncertainty contributors for multiplication factor have been identified. For MOX and MNUP fuel, these are uncertainties of inelastic scatter and capture cross-sections for ^{238}U, and, to a smaller extent, uncertainties of the capture and fission cross-sections and the fission neutron spectrum uncertainty for ^{239}Pu; for reactors with uranium fuel, these are the capture and fission cross-sections and the fission neutron spectrum uncertainty for ^{235}U.

The operation experience of lead-cooled reactors is not as comparably considerable as light water and sodium-cooled reactors one has to be. The experimental data insufficiency requires an in-depth analysis of the initial data uncertainty during modeling.

The obtained results confirm the statement that nuclear data sensitivity is close to both lead- and sodium-cooled reactors with analogous fuel compositions using one and the same computational tools and nuclear data libraries. This allows us to use the accumulated benchmarks of sodium-cooled reactors to prove the lead-cooled reactor safety.

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