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Abstract. For the computational support of innovative projects it is necessary to use high-fidelity codes, which must be verified and validated. In Russia, MCU and SERPENT codes are widely used. The MCU code was previously chosen as the 'Proryv' project code. Both of these codes are used for calculation of fast reactors, although they are certified for thermal reactors. Therefore, there is a need to show how accurately they allow calculating the characteristics of fast reactors. For cross-verification of these codes, the main characteristics of the benchmark of BN-600 reactor with a hybrid core were calculated: neutron multiplication factors, reactivity coefficients, distribution of energy release over zones, reaction rates. The values of the neutron multiplication factors for various states of the model obtained with the MCU-PTR are systematically higher than the values obtained with the SERPENT 2 (for majority of the states by 0.4%). The values of the reactivity coefficients have the same sign, however, difference between both codes can reach 160% and if compared with the benchmark – 181%. For the majority of reactivity coefficients this compares with the distribution of the results presented in the benchmark. The MCU results are closer to the benchmark than the Serpent ones.

1. Introduction

Since the launch of the world's first nuclear power reactor in 1954 in Obninsk, great experience has been accumulated in the operation and design of nuclear reactors (more than 18 000 reactor-years). New designs of nuclear installations have appeared, and the characteristics of existing ones have undergone significant changes. Today around the world there are about 450 operating units and more than 50 are under construction [1]. According to IAEA forecasts, by 2050 the amount of electricity generated by nuclear power plants may increase by about 2 times [2]. However, long-term sustainable development of nuclear power is unlikely without closing the nuclear fuel cycle using fast reactors (due to limited uranium resources) and putting into operation modern nuclear facilities with increased safety. To address these problems, projects such as "INPRO" [3], the Generation IV reactor forum [4], and "Proryv" [5] were created.

Today, Rosatom Corporation is conducting R&D of new fast spectrum nuclear reactors BR-1200 and BN-1200 ("Proryv" project), which are planned to be used to close the nuclear fuel cycle in Russia. For the computational support of these innovative projects, it is necessary to use not only modern

engineering codes, but also precision codes (like in [6]), which must be verified and validated using computational and experimental benchmarks of fast reactors.

This article is devoted to cross-verification of the MCU-PTR and Serpent 2 Monte Carlo codes using the benchmark of the BN-600 reactor with a hybrid core. The benchmark, created in the period from 1999 to 2005, was intended for cross-verification of diffusion and transport computer codes and did not touch Monte Carlo codes. There are several works that describe the results of calculating some of the characteristics of this benchmark using the MCNP [7] (before the publication of the IAEA technical report [8]) and MCNPx [9, 10] (after the report was released).

For cross-verification of the Monte Carlo codes MCU-PTR and Serpent 2, using the BN-600 benchmark with a hybrid core, the main neutron characteristics were calculated: k_{eff}, reactivity coefficients, distribution of energy release over zones, neutron fission and absorption reaction rates. The values obtained by the Monte Carlo codes were compared with the values obtained using the transport codes and presented in the benchmark description.

2. Codes features

MCU (Monte Carlo Universal) is a software used for simulating the processes of neutron and gamma transport with use of the Monte Carlo method. MCU was created and maintained by the Kurchatov Institute [11]. Serpent is a similar code developed by VTT (Finland) [12].

The main difference between Serpent and MCU is in the approach for modeling of neutron-physical processes. In Serpent, simulations are performed with a single physics module that uses continuous-energy cross section libraries of evaluated nuclear data. The physical module of MCU consists of three parts:

1. FARION, designed to simulate the interaction of neutrons with matter in the energy range of fast neutrons (from 20 MeV to 100 KeV), continuous-energy cross section libraries are used; in terms of operation algorithms it is identical to the physical module of Serpent, but it can be enabled or disabled in the program settings.
2. FIMBROEN, designed to simulate the interaction of neutrons with matter in the epithermal energy range (from 20 MeV to 2 eV).
3. FIMTOEN, used in the energy range of neutron thermalization. The difference in physical modules results in the use of different evaluated nuclear data libraries. Serpent uses continuous-energy cross section library (in this work ENDF/B-VII.0). In MCU is a combined library based on ENDF/B-VII.0, BNAB-93, LIPAR, 301-group MULTIC - MCU.

In the MCU, the dependence of the cross sections on the temperature in the resonance energy range can be calculated in three ways – nuclides are divided into three types:

1. Resonance, for which the cross sections in the region of allowed resonances are calculated in a pointwise representation using the Breit-Wigner, Adler-Adler, Reich-Moore formalisms (depending on the MCU settings), and in the region of unresolved resonances, the cross sections are calculated using the subgroup parameters of the BNAB-93 or MULTIC-301. If the subgroup parameters are absent, the Bondarenko f-factors are used.
2. Subgroup, for which the cross sections over the entire resonance region are calculated using the subgroup method based on the BNAB-93 and MULTIC-301 libraries, in the absence of subgroup data in the libraries, the cross sections are calculated using Bondarenko f-factors.
3. Group, in which the resonant self-shielding of the cross sections is either not taken into account, or taken into account using f-factors, which depend on the temperature and the dilution cross section.

Differences in approaches to modeling neutron transport in Serpent and MCU are the object of research, and in our case, cross-verification of these codes can show the appropriateness of using a complex physical MCU module or the absence of any advantages of MCU over Serpent.

3. Description of the model

The calculations were carried out for a three-dimensional model of the HEX-Z type [8]. It has 1/6 rotational symmetry and consists of an inner zone with an enrichment of 17% 235U (LEZ, figure 1) with three groups of CPS elements of the compensation system (SHR) and one group of CPS elements for emergency protection (SCR), a zone with 21 enrichment % 235U (MEZ), a zone with MOX fuel with 21.3% plutonium (MOX), of which 93.8% is 239Pu, and an outer zone with 26% enrichment of 235U (HEZ). The fuel zones are surrounded by depleted uranium (LB, UB) blankets. On the outside, the core is surrounded by two steel protection zones (SSA1, SSA2) and a reflector.

The model built for the MCU and SERPENT calculations is slightly different from the one given in the benchmark description. This is due to the fact that the benchmark was created for calculating with deterministic codes and some features cannot be taken into account in the Monte Carlo calculation. That is why fission products were not taken into account when simulating with Monte Carlo codes, since they are specified in the benchmark as an effective fission fragment FP39, which is an option for deterministic codes.

20.0	Axial reflector												
24.7		UB		UB	SCR	UB		UB	UB	UB			
5.5	SHR		SHR				SHR						
52.2		LEZ1		LEZ2	Follower + rod tail	LEZ3		MEZ	MOX	HEZ	SSA1	SSA2	Radial reflector
52.2	Follower + rod tail	LEZ1	Follower + rod tail	LEZ2	Follower	LEZ3	Follower + rod tail	MEZ	MOX	HEZ			
5.5													
29.7		LB		LB		LB		LB	LB	LB			
20.0	Axial reflector												
(cm)	5.2	36.8	1.8	5.8	1.6	18.9	2.25	10.38	13.5	9.48	9.48	25.43	50.0

Figure 1. Axial section of the model of the hybrid core of the BN-600 reactor [8].

The calculation results for the unperturbed state given in the benchmark were obtained at the temperature of fuel isotopes equal to 1500 K, temperature of other isotopes equal to 1200 K, and coolant temperature – 600 K. However, in our calculations using the Serpent and MCU codes, the temperature of all materials containing fuel isotopes is 1500 K, since the MCU does not have the ability to set different temperatures for the isotopes that make up one geometric zone. Thus, in our models, all materials have a temperature of 1500 K, except for materials No. 26-35 (see the benchmark description), the temperature of which is 600 K.

4. Description of the calculated functionals

Cross-verification of the SERPENT and MCU codes is based on the calculation of the main functionals that demonstrate the features of the physical modules and the databases of evaluated nuclear data used by them.

The main calculated functional is criticality. In Serpent, k_{eff} is calculated by 4 methods:

- analog;
- implicit;
- by points of collisions;

- by points of absorption.

The MCU uses three methods:

- by points of collisions;
- by points of absorption;
- along the path length of neutrons.

The methods for collision and absorption points in SERPENT and MCU are similar. Therefore, for cross-verification, we used k_{eff} values calculated from absorption points.

However, the calculation of k_{eff} by itself can tell little about the features of the databases of estimated nuclear data and the physical modules of the codes. To obtain a more detailed picture, it is necessary to calculate the functionals derived from k_{eff}, which depend on the spectrum of neutrons, their leakage from the reactor, and also on the temperature of the materials. These features can be illustrated by the example of calculating the reactivity coefficients described in table 1. The description indicates the changes made to the model in comparison with the unperturbed state.

Table 1. Calculated functionals.

No.	Functional	State	Comment
1	k_{eff}	Unperturbed	In Serpent and MCU, the temperature of all materials with fuel is 1500K, the rest is 600K
2	Fuel Doppler coefficient	T (materials with fuel) = 2100 K	Fuel consists of 235U, 236U, 238U, 239Pu, 240Pu, 241Pu, 242Pu, 16O.
3	Sodium density coefficient	ρNa'=0.99*ρNa	Sodium desity changed in all cells by 1%
4	Sodium density coefficient	ρNa'=0.97*ρNa	Sodium desity changed in all cells by 3%
5	Steel density coefficient	ρsteel'=0.99*ρsteel	Reactivity coefficient for steel density is calculated with steel density change in all zones by 1% and 3%. The steel contains Fe, Cr, Ni and Mo.
6	Steel density coefficient	ρsteel'=0.97*ρsteel	
7	Fuel density coefficient	ρfuel'=0.99*ρfuel	Reactivity coefficient for fuel density was calculated with fuel density change by 1%. The fuel consists of 235U, 236U, 238U, 239Pu, 240Pu, 241Pu, 242Pu, 16O.
8	Absorber density coefficient	ρabs'=0.99*ρabs	Reactivity coefficient for absorber density was calculated with density change by 1% and 3%. Absorber consists of 10B, 11B and C.
9	Absorber density coefficient	ρabs'=0.97*ρabs	
10	Axial expansion coefficient	Raxial'=1.01*Raxial	Calculated with the expansion of the entire model in the axial direction by 1%. The masses of the isotopes with the exception of sodium are conserved (ρ' =ρ/1.01, h'=h*1.01).
11	Radial expansion coefficient	Rrad'=1.01*Rrad	Calculated with the expansion of the entire model in the radial direction by 1%. The masses of the isotopes with the exception of sodium are conserved (ρ' =ρ/1.01, R'=R*1.01).
12	Effective delayed neutron fractions	Unperturbed	[pcm]
13	Prompt neutron lifetime	Unperturbed	[10^{-7}*s]
14	Neutron leakage	Unperturbed	Normalized per one fission neutron

5. Results cross-verification

For cross-verification of the MCU-PTR and SERPENT 2 codes, we calculated a part of the parameters from the benchmark. The differences between the calculated effective multiplication factors using Serpent 2 and MCU-PTR codes do not exceed 0.63% (table 2). It can be observed that the effective multiplication factors obtained with the MCU are systematically higher by at least 0.4% than those obtained with the SERPENT (figure 2).

Table 2. Calculated k_{eff} for various states of the model.

State No.	SERPENT		MCU		(MCU-SER)/MCU
	k_{eff}	σ	k_{eff}	σ	difference
1	1.019800	0.000010	1.023960	0.000008	0.41%
2	1.015600	0.000007	1.022030	0.000021	0.63%
3	1.019770	0.000007	1.023900	0.000006	0.40%
4	1.019620	0.000007	1.023780	0.000015	0.41%
5	1.019770	0.000007	1.024010	0.000006	0.41%
6	1.019940	0.000007	1.024080	0.000015	0.40%
7	1.019670	0.000007	1.020320	0.000015	0.06%
8	1.020080	0.000007	1.024230	0.000016	0.41%
9	1.020900	0.000350	1.024730	0.000016	0.37%
10	1.018000	0.000007	1.022410	0.000010	0.43%
11	1.014820	0.000007	1.018990	0.000015	0.41%

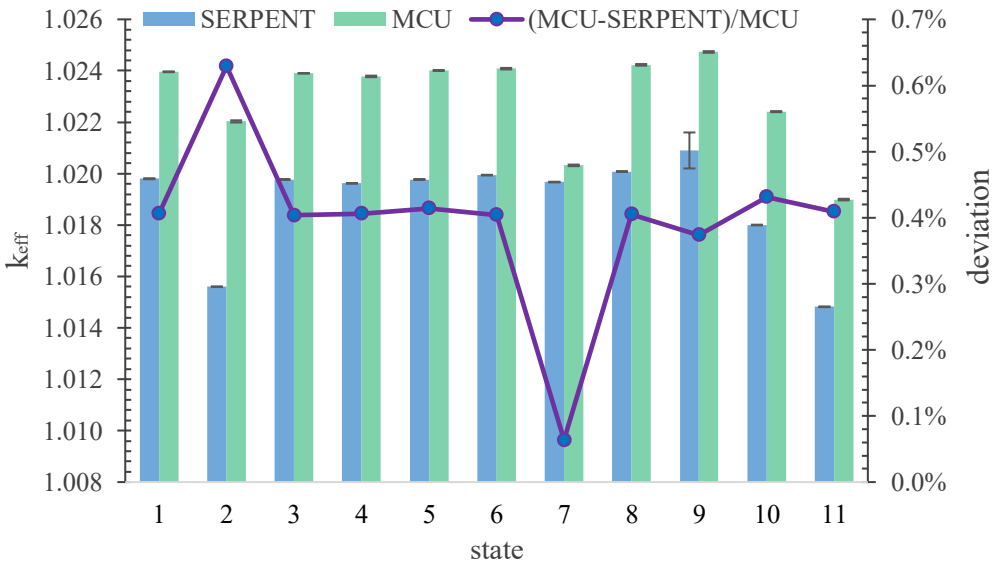

Figure 2. Calculated k_{eff} for different states of the model and their deviations (2σ error is shown).

The differences in the obtained values of the multiplication factors are most likely caused by the use of different libraries of cross-sections for the interaction of neutrons with matter. Two states deviate from the general trend - No. 2 and 7, which differ from the unperturbed state (No. 1) by the temperature and density of the fuel, respectively. Since these are the only states in which only the characteristics of the fuel change, it can be concluded that the deviations are caused by the difference in the cross-sections for the interaction of fuel isotopes.

The number of neutron histories was selected in such a way that the double standard deviation was one to two orders of magnitude less than the difference in the multiplication factors obtained using the two codes. For all calculations, 32 cores of the BASOV cluster (Intel Xeon CPU E5-2680 2.70GHz) were used. The time for calculating state No. 1 with MCU was 5.4 days, 7.7 billion particles were simulated. The calculation time for the same state using SERPENT was 2.6 days, 7.7 billion particles were simulated. The accuracy in the obtained value of the multiplication factor turned out to be similar, however, the calculation time for the SERPENT code is two times less than for the MCU.

The results of power distribution calculation in reactor core zones, obtained by MCU and SERPENT, are in good agreement with each other (table 3) - the deviations do not exceed fractions of a percent (maximum 0.23%). When compared with the results given in the benchmark, more significant deviations are observed - for the three central fuel zones less than 1% and for the high enrichment zone about 3.5%. It is noteworthy that the deviations are greatest for the outer reflector zones - about 11-13%. This may be due to the presence of the boundary condition of equality of the neutron flux to zero, which was used when calculating the benchmark using deterministic codes.

Table 3. Power distribution calculation results.

Mat	Zone	Bench	MCU	SERPENT	(Bench-MCU)/Bench	(Bench-SER)/Bench	(MCU-SER)/MCU
1,2	LEZ	42.60%	42.33%	42.27%	0.64%	0.77%	0.14%
3	MEZ	16.12%	16.10%	16.13%	0.13%	-0.03%	-0.19%
4	MOX	21.64%	21.67%	21.66%	-0.13%	-0.09%	0.05%
5	HEZ	17.19%	17.74%	17.78%	-3.23%	-3.45%	-0.23%
1÷5	Core	97.55%	97.84%	97.84%	-0.30%	-0.30%	0%
6÷15	LB	1.58%	1.40%	1.40%	11.21%	11.36%	0%
16÷25	UB	0.87%	0.76%	0.76%	12.93%	12.48%	0%

Table 4 shows the values of the reactivity coefficients, the effective fraction of delayed neutrons, the lifetime of prompt neutrons and their leakage. The results are compared with the average values calculated by transport codes (for reactivity coefficients) and by transport and diffusion codes (for other parameters). For the analysis, the maximum relative deviation of the value (among the deviations of the values obtained by the transport codes) from the average over all transport codes is used (the fourth column in table 3).

There is a different agreement between the results obtained by the MCU and SERPENT codes when compared to the benchmark results. Deviations of functionals No. 1, 3, 4, 5, 6, 10 (MCU), 11, 12 from the mean values obtained by transport codes are within the maximum relative deviation of the parameter values obtained by transport codes. Deviations of parameters No. 2, 7 (Serpent), 8, 9 significantly exceed the limits of the maximum relative deviation of the values. Deviations of parameters No. 7 (MCU), 10 (Serpent), 13 do not greatly exceed the limits of the maximum relative deviation of values. It is noteworthy that the deviations from the benchmark obtained by Serpent, as a rule, exceed the deviations obtained from the MCU. It can also be noted that when calculating the materials density reactivity

coefficients, it is better to take a greater perturbation (not 1% but 3%), and then the value is closer to that obtained in the benchmark and coincides in sign.

Table 4. The results of reactivity coefficients and other functionals (deviation from the average benchmark results is indicated as a percentage under the value, in the form (Bench - Code)/Bench).

Func No.	Description	Bench mean (transport)	Max rel. dev. from the mean	SERPENT	MCU	(MCU – SER)/MCU
1	k_{eff}	1.01134	1.32%	1.0198 -0.84%	1.02396 -1.25%	0.41%
2	Fuel temperature reactivity coefficient (Doppler broadening)	-0.00679	12.51%	-0.01205 -77.47%	-0.00548 -19.29%	-119.89%
3	Sodium void reactivity effect (W_{Na}) 1%	0.00487	57.73%	0.00288 40.86%	0.00572 -17.45%	49.65%
4	Sodium void reactivity effect (W_{Na}) 3%			0.00577 -18.48%	0.00572 -17.45%	-0.87%
5	Steel density reactivity coefficient (W_{steel}) 1%	-0.0036	189.97%	0.0029 180.56%	-0.0048 -33.33%	160.42%
6	Steel density reactivity coefficient (W_{steel}) 3%			-0.0045 -25.00%	-0.0038 -5.56%	-18.42%
7	Fuel density reactivity coefficient (W_{fuel})	0.3427	1.22%	0.0125 96.35%	0.3484 -1.66%	96.41%
8	Absorber density reactivity coefficient (W_{abs}) 1%	-0.022	6.53%	-0.027 -22.73%	-0.026 15.38%	-3.85%
9	Absorber density reactivity coefficient (W_{abs}) 3%			-0.035 -59.09%	-0.025 -12.00%	-40.00%
10	Axial thermal expansion reactivity coefficient (R_{ax})	-0.1448	6.64%	-0.1734 -19.75%	-0.1481 -2.28%	-17.08%
11	Radial thermal expansion reactivity coefficient (R_{rad})	-0.473	2.64%	-0.481 -1.69%	-0.476 -0.63%	-1.05%
12	β_{eff},	590	3.01%	584 1.02%	576 2.37%	-1.39%
13	Λ, 10^{-5} c	4.409	6.32%	4.736 -7.42%	5.14 -16.58%	7.86%
14	Neutron leakage, as all reactions fraction	–	–	0.0924	0.0925	0.11%

The reasons for some significant deviations from the benchmark results are not clear and a set of additional calculations will be required. It is probably necessary to perform burnup calculations to determine the isotopic composition of the fuel in order to take into account the fission products. Another reason for this deviation may be the comparison of values obtained from codes based on different methods and using different cross-section libraries. The method of changing the cross-sections for the

required temperature is also important. Serpent uses 300 K step library and interpolates cross-sections between the points, while MCU calculates the cross-section for the desired temperature.

The values of the parameters obtained by the MCU and Serpent are closer to each other than to the values from the benchmark, although there are large deviations (functionals No. 2, 3, 5, 7, 9). The comparison also shows that it is better to use a larger perturbation when calculating the density reactivity coefficients (not 1% but 3%). As it was indicated above when comparing the multiplication factors, the greatest disagreement between the codes is obtained for the states in which the properties of the fuel are changed (No. 2, 7).

Tables 5 and 6 show the values of the fission and capture reaction rates integrated by the volume and energy. The sum of the values of the given reaction rates and neutron leakage gives 100%. For MCU, this value is slightly more than 100% by the magnitude of the secondary neutron production reactions (due to a different normalization).

As can be seen, the fission and capture reaction rates differ within a few percent for significant fissile isotopes. The capture reaction rates for other significant isotopes are also in good agreement, with the exception of Cr and Mo, where the difference in values is about 10%.

Table 5. Total fission reaction rates (as a per cent of total, MT 18).

Nuclide	SERPENT		MCU		(MCU – SER)/MCU
	(n, f)	σ	(n, f)	σ	
U235	24.73%	0.02%	24.95%	0.003%	0.88%
U236	0.06%	1.17%	0.05%	0.004%	-20%
U238	4.26%	0.08%	4.18%	0.003%	-1.91%
Pu239	9.57%	0.01%	9.71%	0.004%	1.44%
Pu240	0.17%	0.14%	0.17%	0.006%	0%
Pu241	0.06%	0.17%	0.06%	0.006%	0%
Pu242	0.001%	4,35%	0.001%	0.008%	0%
Sum	38.84%	–	39.11%	–	0.7%

Table 6. Total capture reaction rates (as a per cent of total, MT 101).

Nuclide	SERPENT		MCU		(MCU – SER)/MCU
	(n, c)	σ	(n, c)	σ	
U235	7.00%	0.11%	6.85%	0.01%	-2.19%
U236	0.21%	0.47%	0.22%	0.01%	4.55%
U238	28.73%	0.01%	28.67%	0.00%	-0.21%
Pu239	2.37%	0.36%	2.44%	0.02%	2.87%
Pu240	0.18%	0.49%	0.18%	0.01%	0%
Pu241	0.01%	0.27%	0.01%	0.04%	0%
Pu242	0.001%	1.01%	0.001%	0.03%	0%
O	0.20%	0.38%	0.20%	0.01%	0%
Na	0.33%	0.18%	0.33%	0.00%	0%
Fe	5.38%	0.01%	5.38%	0.01%	0%
Cr	1.16%	0.01%	1.29%	0.01%	10.08%
Ni	0.94%	0.00%	0.95%	0.00%	1.05%
Mo	1.34%	0.04%	1.22%	0.01%	-9.84%
C	0.0002%	2.55%	0.0002%	0.16%	0%
B10	4.06%	0.13%	4.06%	0.01%	0%
B11	0.0002%	0.30%	0.0001%	0.06%	-100%
Sum	51.92%	-	51.80%	-	-0.23%

6. Conclusion

Verification and validation of computational codes are very important for design support of modern fast nuclear reactors. In this work, we carried out cross-verification of the MCU-PTR and Serpent 2 codes based on a set of parameters from the benchmark of BN-600 reactor with a hybrid core.

Some of the results obtained with the MCU show good agreement with the Serpent results, while others show large deviations. When compared with the results from the benchmark, there is a good agreement for the power distribution and part of the other functionals. The results obtained with the MCU are in better agreement with benchmark than those obtained with the Serpent.

Main conclusions:

- The effective multiplication factors obtained with MCU for different states of the model are systematically higher than those obtained with Serpent (by at least 0.4%).
- The calculation time for the Serpent is two times smaller than for the MCU.
- The deviations in the power distribution in all zones, between the MCU and Serpent, do not exceed 0.23%. The deviations from the benchmark results are higher – up to 0.77% for the three central fuel zones, about 3.5% for the high enrichment zone and 11-13% for the outer blanket zones.
- The deviations of the majority of reactivity coefficients from the average values obtained by the transport codes in the benchmark are within their maximum relative deviation from the mean. Some of the values significantly exceed the limits of the maximum relative deviation from the mean (by several times). The deviations received from Serpent calculations are generally higher than those obtained from the MCU.
- When calculating the reactivity coefficients for the density of materials, it is better to take a greater perturbation (not 1% but 3%), then the value is closer to that obtained in the benchmark and coincides in sign.
- The values obtained from the MCU and Serpent calculations are closer to each other than to the values from the benchmark, although there are large deviations for states with a change in fuel properties.
- The fission and capture reaction rates differ within a few percent for significant isotopes, with the exception of Cr and Mo, the difference in capture rates is about 10%.

The reasons for some significant deviations from the benchmark results are not clear and their identification will require additional calculations in which fission products should be taken into account and the same nuclear data libraries should be used. As well as the influence of the methods for cross-sections variation with the temperature should be investigated. However, when calculating the change in the isotopic composition of the fuel, certain uncertainties may arise, which will also affect the results.

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