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FEATURES OF CALCULATION OF TEMPERATURE REACTIVITY COEFFICIENT IN THE GT-MHR REACTOR

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ABSTRACT

Ensuring of negative reactivity temperature coefficient in all normal operation modes and at accidents is one of the most important goals when analyzing the nuclear reactor safety.

The world tendencies for improving of nuclear safety, economic realities demanding the nuclear power facilities to be more efficient, decreasing of excessive conservatism at reactor developments impose more strict requirements for neutronics calculation validation. First of all it supposes improving of calculation technologies with use of modern computer codes and nuclear data libraries which is especially important in absence of representative experimental data for considered characteristics. The report analyzes two problems:

- specific features of use of precision codes such as MONTEBURNS-MCNP5 for investigating of reactivity temperature coefficient of the GT-MHR with plutonium fuel;
- specific features of use of nuclear data libraries with pointwise neutron energy presentation, formed on the basis of estimated nuclear data files.

The report presents results of reactivity temperature coefficient analysis for various mock-ups simulating the reactor core structure.

The report evaluates allowable level of fuel burnup in the reactor, when reactivity temperature coefficient is negative.

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INTRODUCTION

When the fuel on the basis of pure plutonium use in reactor core the computational substantiation of behaviour of temperature reactivity coefficient depending on depth of fuel burn-up and temperature at absence of experimental data becomes dominant problem at reactor safety assessment. The comparison of results of isothermal temperature coefficient in GT-MHR reactor when using different Monte-Carlo codes (MCU [1], MCNP [2]) shows that the difference may reach 40 % for the same mock-ups.

In the end of burnup cycle for the temperature range from 700 K to 900 K which define the inlet coolant temperature at "hot" startup mode the temperature reactivity coefficient can be positive and it has certainly negative values when power and average temperature are increasing. So the range of temperatures from 700 till 900 K is the subject for analysis in this report. Besides, practically, it is very important to determine allowable burnup, when reactivity temperature coefficient would be negative for the states, corresponding to "hot" startup mode in the reactor.

For main isotopes Figure 1 shows the behavior of capture cross sections at neutron energy range, corresponding the maximum of the GT-MHR reactor spectrum, as well as variation of the neutron spectrum for given range of temperatures. These dependencies show that not only main plutonium isotopes (Pu-239, 241, 240) and erbium (Er-167 as burnable poison in the reactor core with pure plutonium for captures interlocking in fissile nuclides) but minor isotopes (Am-241, Cm-244), whose cross-sections have considerable resonances in the energy range of temperature-dependent neutron spectrum may influence reactivity temperature coefficient. Preliminary analysis (Figure 2) of fuel isotopic composition for fuel cell burnup when using the nuclear data libraries being formed from JENDL3.3 and ENDF-B/5,6 (further we indicate them as LIB-JEND and LIB-B56, respectively), show that the difference in Pu239, Pu240, Er167 concentrations may reach 10 % and more at high burnups.

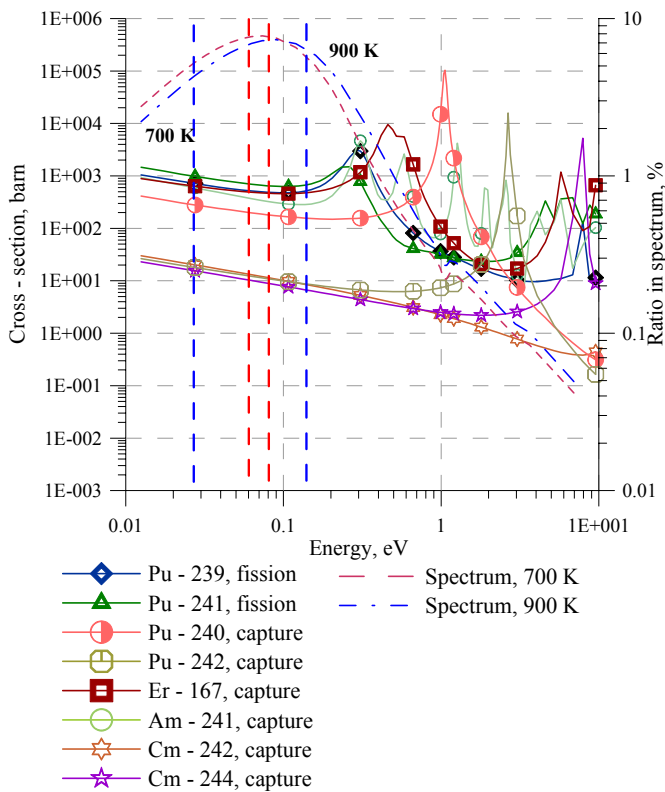


Figure 1. Variation of capture cross sections for main isotopes in the GT-MHR reactor spectrum

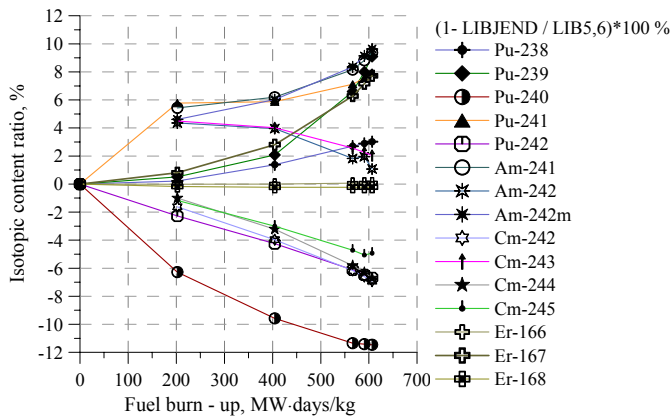


Figure 2. Differences of burnups for main isotopes in LIB-JEND (JENDL3.3) and LIB-B56 (ENDFB5, 6) libraries

These facts are the reason for detailed error analysis at reactivity temperature coefficient calculation and the results of this analysis are given in the present report.

Analysis was performed when using MONTEBURNS - MCNP5 - ORIGEN2 [3], [2], [4] with LIB-JEND and LIB-B56 libraries.

The following reactor mock-ups were considered during investigations are:

1. fuel block unit cell without cavity for control rod with detailed geometry description and heterogeneous fuel particle representation, boundary conditions – reflection of neutrons at all surfaces;
2. fuel block column with reflector blocks at the butt-ends, boundary conditions – reflection in radial direction and leakage in axial directions;
3. 3D reactor model with detailed geometry, boundary conditions – leakage at all surfaces.

1. BRIEF DESCRIPTION OF INVESTIGATED REACTOR AND ITS COMPONENTS

GT-MHR reactor and its fuel composition (Figure 3) are considered, their base characteristics are given in Table 1 [5]

Table 1. Main characteristics of GT-MHR type reactor

Characteristic	Value
Total thermal power of the reactor, MW	600
Coolant temperature at the reactor inlet/outlet, °C	490 / 850
Geometrical parameters of the core:	
- equivalent inner/outer diameter of the core, m	2.96/4.84
- core height, m	8.00
- outer reflector diameter, m	7.00
- end reflector thickness, m	0.80
Number of fuel blocks in the core	1020
Geometrical parameters of prismatic fuel blocks:	
- height, m	0.80
- size across flats, m	0.36
Characteristics of fuel and Er compacts:	
- diameter, mm	12.5
- height, mm	50.0
Pu loading into compact, g	~ 0.24
Number of fuel particles in fuel compact	~ 6420
Er _{nat} loading into compact, g	2.1
Number of burnable poison particles in Er compact	~ 4250
Characteristics of coated fuel particles,	
- kernel diameter, μm / material/ density, g/cm ³	200/PuO _{1.7} /10.0
- 1 st layer thickness, μm / material/ density	100 / PyC / 1.0
- 2 nd layer thickness, μm / material/ density	35 / PyC / 1.8
- 3 rd layer thickness, μm / material/ density	35 / SiC / 3.2
- 4 th layer thickness, μm / material/ density	40 / PyC / 1.8

Two states – the beginning and the end of fuel cycle – are considered in this report, they are characterized by fuel block loading scheme with three burnup histories:

Number of fuel layer along height										
1	2	3	4	5	6	7	8	9	10	
2/3	0	2/3	1/3	1/3	1/3	1/3	2/3	0	2/3	after refueling
(3/3)	1/3	(3/3)	2/3	2/3	2/3	2/3	(3/3)	1/3	(3/3)	before refueling

where 0 – fresh fuel, 1/3 – fuel burnt for 1/3, 2/3 – fuel burnt for 2/3, 3/3 – unloaded fuel (burnup ~ 605 MW-day/kg).

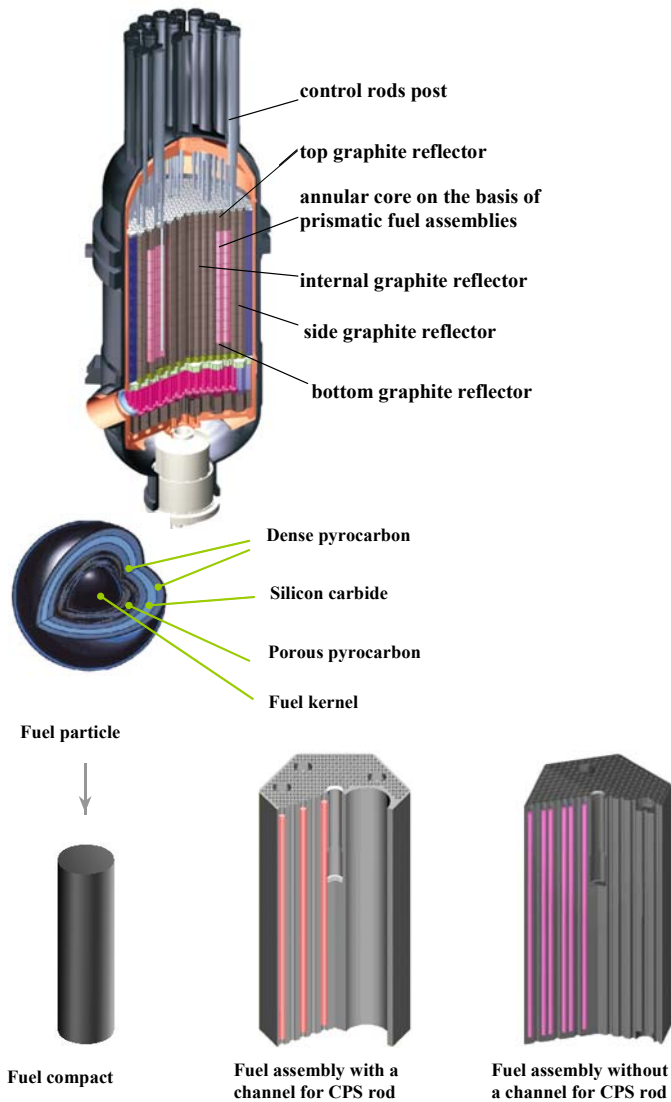


Figure 3. GT-MHR type reactor and fuel composition

2. SPECIFIC FEATURES OF USE MONTEBURNS-MCNP5-ORIGEN2 FOR ANALYSIS OF REACTIVITY TEMPERATURE COEFFICIENTS

Precision neutronics calculations are not only precision codes, which allow direct simulation of neutron trajectories in complicated heterogeneous structure by Monte-Carlo method, using specialized nuclear data libraries formed at given parameters (temperature, accuracy, etc) for definite reactor systems but also particular technology of calculations [6].

Calculation techniques and Nuclear data base (as the set of nuclear libraries of different type) are the main components of any computer code. For some codes the nuclear data libraries are the part of this code so calculation techniques and the nuclear data base are considered as self-coordinated components. When forming nuclear data base independently from codes the obligatory preliminary calculations are required for coordinating Nuclear data - Computer codes - Mock-up models. Such coordination is based on sensitivity analysis of calculated neutronic characteristics to parameters of calculations and nuclear data, as well as multi-version calculations analyses for appropriate simplified systems.

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Because of objective quantitative shortage of representative experimental data for new reactor systems the problem of precision calculations reliability and results validation becomes dominant for key calculations stages.

Specific features of MONTEBURNS-MCNP-ORIGEN use for investigation of reactivity temperature coefficient are:

- detailed description of reactor design (geometry);
- detailed description of fuel block and fuel compact design with fuel particles, which are described in the form of regular structure in analyses;
- calculation of continuous neutron moderation spectrum within the energy range from 0 to 20 MeV in approximation of pointwise nuclear data presentation;
- calculation of multiplication factors on the basis of direct simulation of neutron trajectories by Monte-Carlo method;
- generation of single-group micro-cross sections averaged in calculated system spectrum to use them in ORIGEN2 at fuel burnups calculation and using of obtained fuel compositions for evaluating of multiplication factors for various fuel life periods and various temperatures.

The reactivity temperature coefficient is calculated as difference of multiplication factors at T_1 and T_2 temperatures

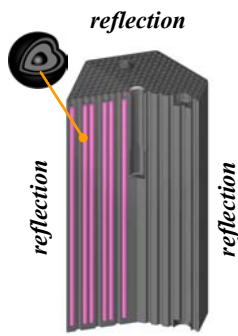
$$\frac{dK}{KdT} = \frac{1}{T_2 - T_1} \frac{K(T_2) - K(T_1)}{K(T_2)K(T_1)}$$

The LIB-B56 (ENDF/B5,6) and LIB-JEND (JENDL3.3) libraries can result in some differences for burnup of Pu-239, Pu-241, Er-167 and other isotopes (Figure 2), which may become the important ones at high burnups and result in changing of reactivity temperature coefficient sign. So while fixing of burnups for Pu-239 it is possible to determine the ultimate burnup when further irradiation in reactor may result in positive value of reactivity temperature coefficient, that is inadmissible from point of view of regulatory safety requirements. The considered mock-ups of the reactor core and its components (at analysis of temperature reactivity coefficients) are given in Figure 4.

In all performed analyses of K_{eff} by MCNP5 the statistics amount to 6 – 15 millions of neutron histories.

1 model

Fuel block without rod cavity



- heterogeneous setting of fuel kernel and its coatings
- homogenization of burnable poison inside the compact
- detailed geometry of fuel block
- boundary conditions – reflection at all surfaces

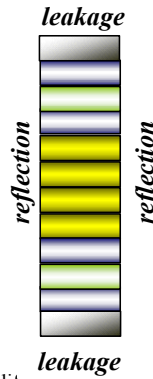
2 model

Fuel block column with reflector blocks at the butt-ends

Number of layer	Beginning of cycle	End of cycle
1	2/3	3/3
2	0	1/3
3	2/3	3/3
4	1/3	2/3
5	1/3	2/3
6	1/3	2/3
7	1/3	2/3
8	2/3	3/3
9	0	1/3
10	2/3	3/3

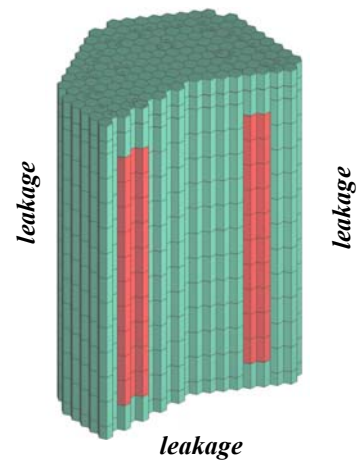
- 0 – fresh fuel
- 1/3 – fuel irradiated in reactor for 1/3 of core life
- 2/3 – fuel irradiated in reactor for 2/3 of core life
- 3/3 – fuel irradiated in reactor for 3/3 of core life

- heterogeneous setting of fuel kernel and its coatings
- homogenization of burnable poison inside the compact
- detailed geometry of fuel block
- concentrations for discrete states of life are obtained at fuel block burnup stage
- boundary conditions – reflection in radial direction, leakage in axial direction



3 model

3D reactor model



- heterogeneous setting of fuel kernel and its coatings
- detailed setting of the core layout
- detailed setting of the core component design
- concentrations for discrete states of life are obtained at fuel block or column burnup stage

Figure 4. Mock-ups of the nuclear core and its components

3. ANALYSIS OF RESULTS

3.1 Influence of nuclear data libraries (LIB-JEND and LIB-B56) on temperature reactivity coefficient

The influence of nuclear data libraries on reactivity temperature coefficient was evaluated for the mock-up of fuel block for burnup of ~ 605 MW·day/kg. The temperature reactivity coefficient is calculated with concentrations of isotopes obtained at fuel block burnup when **using LIB-B56 library**. The temperature reactivity coefficient evaluated for temperatures in range from 700 to 900 K is practically zero when using **LIB-B56**. The reactivity coefficient amounts to +0.36·10⁻⁵ 1/K when using LIB-JEND and the difference of fuel block unit-cell multiplication factor amounts to ~ 0.3 % (**1.1261 for ENDF/B5,6 and 1.1234 for JENDL3.3**). Thus, use of different nuclear data libraries results in the considerable differences of reactivity temperature coefficient, whereas multiplication factor is calculated within error of less than 0.3 % of Δk/k

3.2. Influence of isotopic compositions on reactivity temperature coefficient at different burnups

Table 2 gives reactivity temperature coefficients for temperature range from 700 to 900 K, depending on burnup calculations when using **LIB-B56 and LIB-JEND** (the range of reactivity coefficient values are determined by static error).

Table 2. Reactivity temperature coefficients depending on burnups

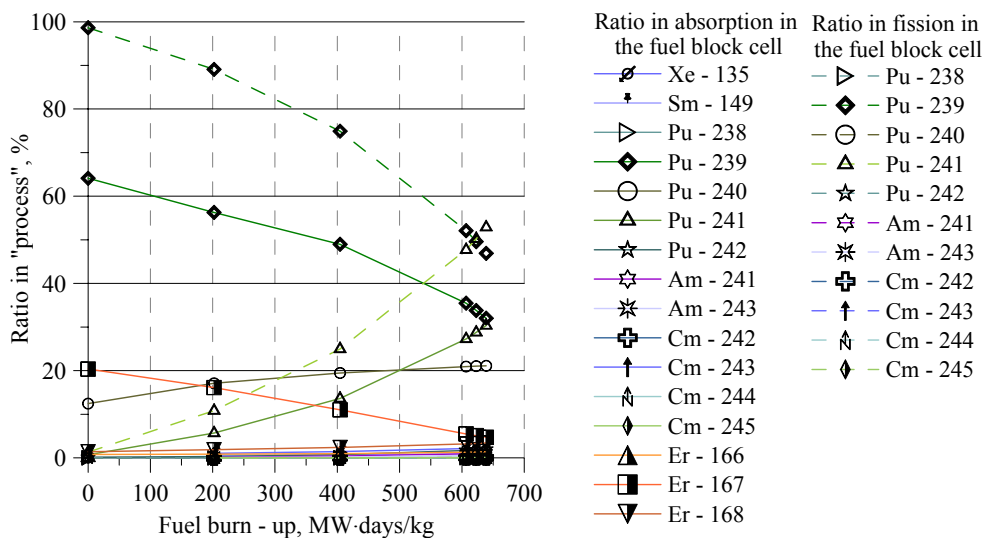
Fuel burnup, MW·day/kg	Pu-239 burnup, % (JENDL 3.3)	Reactivity coefficient, 10 ⁻⁵ 1/K (JENDL 3.3)	Pu-239 burnup, % (ENDF/B-5,6)	Reactivity coefficient, 10 ⁻⁵ 1/K (ENDF/B-5,6)
560	86	(-1.26)-(-0.71)	-	-
590	88	(-0.24)-(+0.080)	-	-
605	90	(+0.85)-(+1.17)	89	(-0.026)-(+0.019)
620	-	-	90	(+0.38)-(+0.68)

The results in Table 2 show that reactivity coefficient is negative at fuel burnups up to 605 MW·day/kg and it is positive at higher burnups. The critical point corresponds to Pu-239 burnup of ~ 90 % *. At burnup analysis when using LIB-JEND and LIB-B56 there is burnup uncertainty of about 15 MW·day/kg, when temperature coefficient changes the sign.

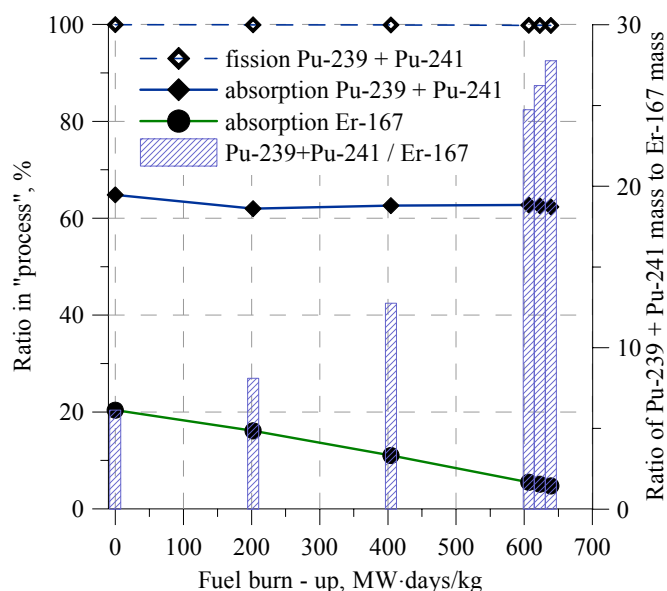
* Typical isotopic content for plutonium fresh and burnout fuel was presented in [7].

Change of the sign at Pu-239 burnup of ~ 90 % can be explained by change of ratio between plutonium/erbium isotopes (Figure 5 a, b). The isotopes of Pu-239, Pu-241, Pu-240, Er-167 determine the fission/absorption correlations in the reactor system with pure plutonium fuel. Fission fraction of Pu-241 starts to exceed the fission fraction of Pu-239 (Figure 5 a) at burnups 605 MW-day/kg, whereas total fission fraction of Pu-239 and Pu-241 does not change (Figure 5 b) while the absorption fraction of Er-167 is decreasing, and absorption fraction of Pu-240 does not change. Therefore when the ratio of total mass of Pu-239 and Pu-241 to Er-167 mass is equal to ~ 25 (Figure 5 b), the reactivity temperature coefficient becomes positive.

Burnup value (605 MW-day/kg) for fuel block without reflector should be considered as ultimate one from point of view of requirements for reactivity temperature coefficient negativity.



5 a– Dependence of absorption and fission ratio of main isotopes



5 b – Correlation between plutonium and erbium isotopes for loading and fraction during interaction processes

Figure 5. Correlation between main plutonium, actinide and erbium isotopes

3.3. Analysis of significance of curium, americium and even-even plutonium isotopes

The results of fuel block burnup at use of **LIB-B56** and **LIB-JEND** libraries were taken as base ones at analysis of significance evaluation of even-even plutonium isotopes and some minor actinides for multiplication factor values and reactivity temperature coefficient. Change of reactivity temperature coefficient was analyzed for the temperatures ranging from 700 to 900 K at ~ 605 MW·day/kg burnup. Presented analysis results show that use of nuclear data of different libraries for indicated above isotopes may result in the considerable differences (practically double increase) in reactivity temperature coefficient evaluation. Obviously, these differences are determined by differences of nuclear data in high neutron energy region (Figure 6)

Thus, the obtained reactivity temperature coefficient value at use of **LIB-B56**, amounts to $(-2.62 \cdot 10^{-5})$ 1/K.

At replacement of the Pu-238, 240, 242 cross sections (**LIB-B56**) on those of **LIB-JEND** (library) with invariable isotope concentrations, the reactivity temperature coefficient is decreased almost in two times when remaining negative value $(-1.12 \cdot 10^{-5})$ 1/K. Multiplication factor is changed by less than 0.1 %.

At replacement of Am-241 cross sections (**LIB-B56**) on those of **LIB-JEND** (library) with invariable isotope concentrations, the reactivity temperature coefficient is close to zero value, and replacement of Am-243 nuclear data does not practically change the value and the sign of temperature coefficient. Multiplication factor is reduced by not more than 0.1 %.

The replacement of Cm-242, 243, 244 cross sections (**LIB-B56**) on those of **LIB-JEND** (library) with invariable isotope concentrations results in more negative significances of reactivity temperature coefficient $(-4.12 \cdot 10^{-5})$ 1/K. Multiplication factor is reduced by less than 0.1 %.

Obviously, these differences are determined by differences of nuclear data in high neutron energy region (Figure 6)

3.4. Sensitivity of reactivity temperature coefficient to computational techniques

Influence of burnable poison homogenization at temperature coefficient analysis. Reactivity temperature coefficient is equal to $+1.05 \cdot 10^{-5}$ 1/K in mock-up with homogenous Er in burnable poison compact when using **LIB-JEND** library for 605 MW·day/kg burnup and temperature range from 700 to 900 K. In the mock-up with heterogeneous model of burnable poison particles in the fuel compact the reactivity temperature coefficient is practically zero. Thus, consideration of real burnable poison arrangement results in more negative reactivity temperature coefficients due to differences in accounting of burnable poison particles self-shielding and behaviour of fuel and erbium isotopes as a function of burnup.

Influence of neutron leakage and graphite reflectors on temperature coefficient.

Previous results of reactivity temperature coefficient analysis were obtained for fuel block unit-cell model. Obviously, behavior of temperature coefficient in the core is characterized by more complicated processes, which depend on actual distribution of fuel isotopic composition over the core and the influence of reflectors. At the end of cycle (before refueling) the core is characterized by set of fuel blocks with average burnup of 200, 400 and 600 MW·day/kg.

In accordance with diagram given in Figure 4, actual distribution of fuel blocks for burnup shows that average fuel burnup in the GT-MHR reactor core at the end of fuel cycle is about 400 MW·day/kg.

Analysis of reactivity temperature coefficient of fuel column with actual distribution of fuel block burnup along its height show that reactivity temperature coefficient within temperature range of 700 – 900 K at the average burnup of 400 MW·day/kg amounts to $(-2.78 \cdot 10^{-5})$ 1/K. Analysis was performed using **LIB-JEND** library. The influence of upper and lower reflectors on reactivity temperature coefficient results in more positive significance for temperature coefficient instead of $(-3.17 \cdot 10^{-5})$ 1/K for temperature coefficient of the column without reflectors.

It shall be noted that value of temperature coefficient for fuel block model with the same average burnup of 400 MW·day/kg amounts to $(-3.34 \cdot 10^{-5})$ 1/K. Reactivity temperature coefficient can be represented in the form of two components: changes of K_{inf} and changes of neutron migration square:

$$\frac{1}{K_{eff}} \frac{dK_{eff}}{dT} \approx \frac{1}{K_{inf}} \frac{dK_{inf}}{dT} - \frac{1}{M^2} \frac{dM^2}{dT} (K_{inf} - 1),$$

where second member of expression is much less than the first one. As the migration square is increasing when increasing of temperature, then conservative evaluation of temperature coefficient is the first member of this expression, i.e. change of K_{inf} . It allows using temperature coefficient evaluation for fuel block cell as conservative evaluation, regarding the requirements of safety regulatory documents. Presence of reflectors in 3D calculation model of the core influence on calculated significances of reactivity temperature coefficient any more. Positive contribution of graphite reflectors to reactivity temperature coefficient when increasing the temperature results in positive significance of temperature coefficient of the reactor even at fuel burnup of 400 MW·day/kg. Isothermal reactivity temperature coefficient of the reactor designed for temperature range of 700 – 900 K, using **LIB-JEND**, amounts to $+0.77 \cdot 10^{-5}$ 1/K, using **LIB-B56** $+0.19 \cdot 10^{-5}$ 1/K. It shall be noted that reactivity temperature coefficient becomes negative and equals to $\sim (-1 \cdot 10^{-5})$ 1/K when temperature is changed only in the core fuel blocks (without change of reflector temperature).

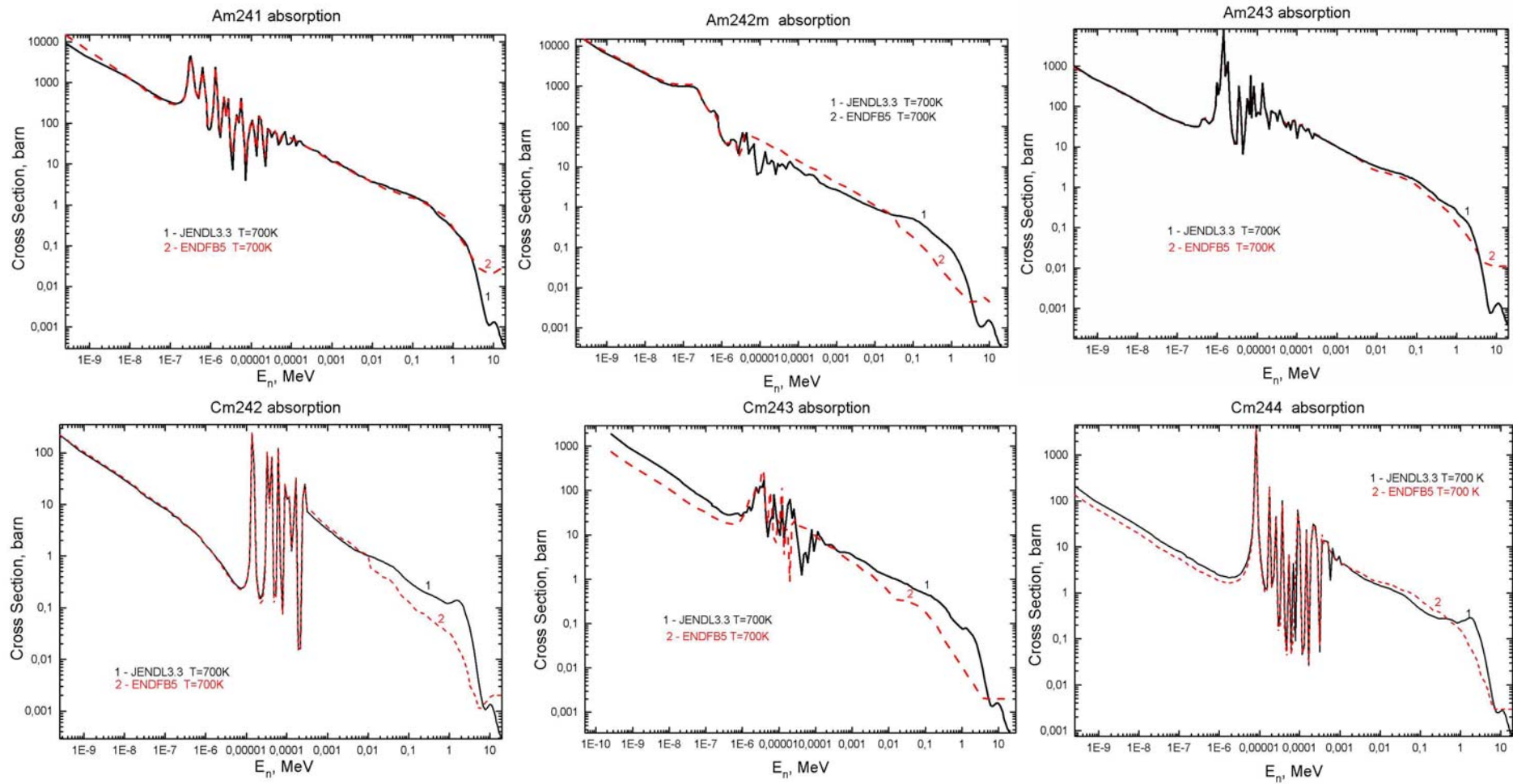


Figure 6. Behavior of radiation capture cross sections of americium and curium isotopes depending on nuclear data library

CONCLUSION

The comparisons of nuclear data libraries being formed from JENDL 3.3 and ENDF/B-5,6 for temperature reactivity coefficient analysis allows to conclude that use of JENDL3.3 is more conservative option for requirements of negativity for reactivity temperature coefficient. In these terms the use of JENDL 3.3 is more preferable during design analyses. The influence of main isotopes on reactivity temperature coefficient shows that the behavior of temperature coefficient at any burnups is determined by correlation of Pu-239 and Pu-241 mass to Er-167 mass in the core. If the ratio of Pu-239 plus Pu-241 masses to Er-167 one is more than ~ 20 , the reactivity temperature coefficient for temperature range from 700 to 900 K corresponding to "hot" reactor startup, becomes positive.

Influence of minor actinides, whose fraction is noticeable at high fuel burnups, on multiplication factor is inconsiderable. But the use of nuclear data from different libraries may result in considerable error in reactivity temperature coefficient analysis.

When calculating of temperature reactivity coefficient in reactor it was shown that temperature variations in reflectors may result in the positive temperature coefficient even for average burnup corresponding to the end of burnup cycle (before refueling) in reactor. When using different nuclear data libraries the differences in the coefficient values may be considerable (using JENDL3.3 amounts to $+ 0.77 \cdot 10^{-5}$ 1/K, using ENDF/B-5.6 $+ 0.19 \cdot 10^{-5}$ 1/K).

The results allow making condition when the reactivity temperature coefficient is remained negative for considered temperature region corresponding to "hot" reactor startup. So maximum fuel burnup shall not exceed ~ 590 MW-day/kg, and the average burnup in the core shall be less than 380 MW-day/kg with accounting of burnup distribution over fuel blocks in the reactor. Final conclusion about the preference use of nuclear constants as well as conclusion about the errors of temperature coefficients can be made only when using both precision calculations and experimental analysis.

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