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Comparative Validation of Monte Carlo Codes for Conversion of IRT MEPhI Research Reactor to LEU Fuel[1]

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ABSTRACT

In the framework of the conversion feasibility studies for 2.5 MW pool type research reactor IRT MEPhI of the National Research Nuclear University MEPhI the detailed neutronic core analysis using different Monte Carlo codes was performed. In order to validate the obtained results the comparison of these codes on some test problems calculation was carried out. The test problems for IRT-type reactor with tube-type low enriched uranium (LEU, 19.7 w/o, U-9%Mo) fuel and oxide high enriched uranium (HEU, 90 w/o) fuel were developed. The static cases and the depletion problem were examined. The calculations have been performed using continuous energy Monte Carlo codes: MCNP (+MCREB for burnup calculation) and MCU-PTR. The impact of cross-section libraries used for a particular problem on the calculated results was investigated. Calculated results for IRT MEPhI operational core with HEU fuel and fresh and operational core with LEU fuel are also presented.

1. Introduction

The present work is connected with the conversion analysis of the IRT MEPhI research reactor at the National Research Nuclear University MEPhI. IRT MEPhI is 2.5 MW pool type research reactor. For feasibility studies of the IRT MEPhI reactor conversion tube-type fuel assembly IRT-3M with U9%Mo-Al fuel (19.7 w/o) was chosen as a LEU fuel [1].The analysis sufficient to determine that conversion from HEU to LEU fuel is technically feasible was performed.
In the framework of the conversion feasibility studies the detailed neutronic core analysis using the Monte Carlo codes MCNP [2] (with MCREB [3] for burnup calculation) and MCU-PTR [4]

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was performed. In order to validate the obtained results the comparison of these codes on some test problems calculation was carried out. The test problems for IRT-type reactor with U-Mo LEU fuel and oxide HEU were developed. Real geometry of fuel assembly was considered. Core configuration was simplified. The static cases and the depletion problem were examined. The next step was to perform the calculations of the reference HEU and LEU cores of IRT MEPhI.

2. Models and codes

2.1. MCU-PTR

MCU-PTR code [4] was used for steady state neutronic calculation and for the burnup calculation. MCU-PTR is the code for pool and tank type research reactors calculation.
In calculation with MCU-PTR it is possible to use either the constants of the ACE/MCU library or the BNAB/MCU library in the fast energy region. ACE/MCU is the library of cross sections of neutron interaction with nuclei in the epithermal energy region in a pointwise representation obtained from ENDF/B-VII.0 files and other sources. BNAB/MCU is expanded and modified version of the BNAB-93 26-group system of constants.
In present work two variants of MCU-PTR calculations were examined:
- using BNAB/MCU library for energy region E>4.65 eV (ACE/MCU library is not used);
- using ACE/MCU library for energy region 100 keV<E<20 MeV and BNAB/MCU library for energy region 2.15 eV <E<100 keV).

For energy region E<2.15 eV or E<4.65 eV in both variants the same continuous-energy neutron interaction data were used. MCU-PTR calculations were performed at NRNU MEPhI.

2.2. MCNP and MCREB

MCNP code with ENDF/B-VII based cross section libraries was used for steady state neutronic calculation of the test problems. The calculations with previous versions of ENDF/B were also performed. The Monte Carlo burnup analyses are performed using the MCREB code (the linkage between REBUS-PC and MCNP codes) [3].
MCNP calculations with ENDF/B-VII based cross-section libraries and calculations by MCREB code were performed at ANL. MCNP calculations with ENDF/B-VI and ENDF/B-V based cross section libraries were performed at NRNU MEPhI.

3. Test problem calculation

3.1. Input data

The cross-sectional view of IRT-3M fuel assembly (FA) with LEU fuel is shown in Fig. 1. 6-tube FA consists of 6 co-axial fuel tubes with control rod (CR) channel in the center. The dimensions of 6-tube FA are shown in Table 1. Outer and inner dimensions of fuel tube (S1, S2), outer and inner radii of rounded corners (R and r) are presented. The first tube is the outer tube.

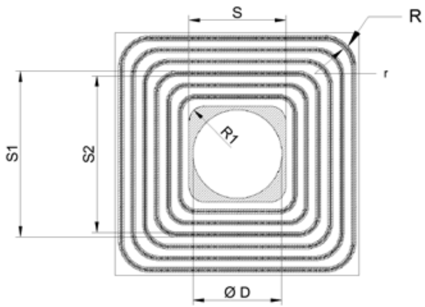


Table 1.
FA dimensions, cm

Tube #	S1	S2	R	r
1	6.94	6.66	0.92	0.78
2	6.25	5.97	0.84	0.7
3	5.56	5.28	0.76	0.62
4	4.87	4.59	0.68	0.54
5	4.18	3.9	0.6	0.46
6	3.49	3.21	0.52	0.38

Fig. 1. FA geometry

Outer dimensions of IRT-3M FA with HEU fuel are the same as the dimensions of FA with LEU fuel except for radii of rounded corners (R=r=0.4 cm for all tubes). In Table 2 the data about 6-tube FA IRT-3M with LEU and HEU fuel used in the study are presented.

Table 2. LEU and HEU FA parameters

Parameter	LEU	HEU
U density, g/cc	5.4	1.07
^{235}U mass in FA, g	355.1	263.7
Enrichment, %	19.7	90
Fuel composition	(U-Mo)-Al	UO_2-Al
Mo weight fraction in U-Mo	0.09	-
Meat thickness, cm	0.05	0.04
Clad thickness, cm	0.045	0.05
Clad material	Al	
Meat length, cm	58	58

The core consists of 48 cells (6x8 positions) for FA and reflector blocks. There is water between FA (reflector blocks) and in the cells without FA or reflector blocks. Core height is 58 cm. Water reflector thickness is 3x7.15 cm in X-Y direction and 29 cm in axial direction. There is vacuum boundary condition (BC) at external border. 1/4 of described system is considered in test problems: 1/2 in horizontal plane and 1/2 in axial direction. There are reflection boundary conditions at symmetry axes. Top and bottom reflector is water. Control rod consists of absorber rod in the clad of stainless steel. The core with 12 FA is presented in Fig.2.

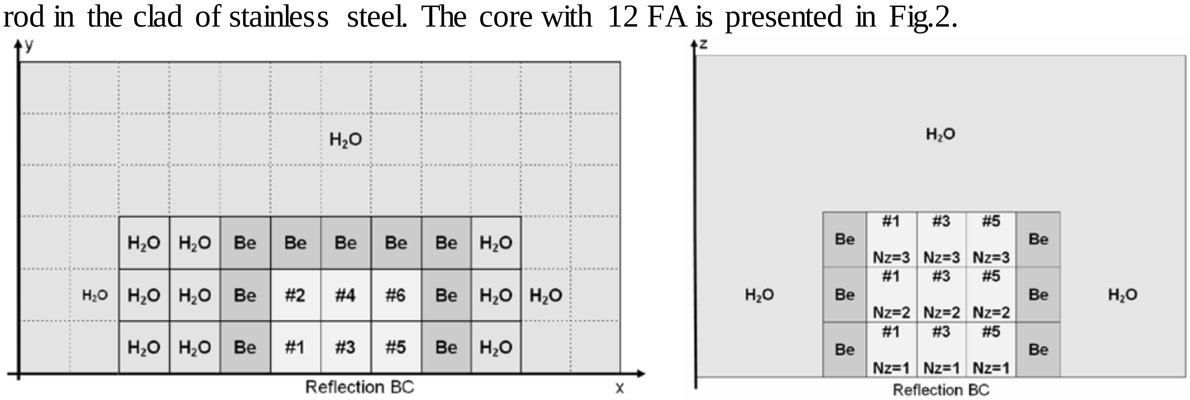
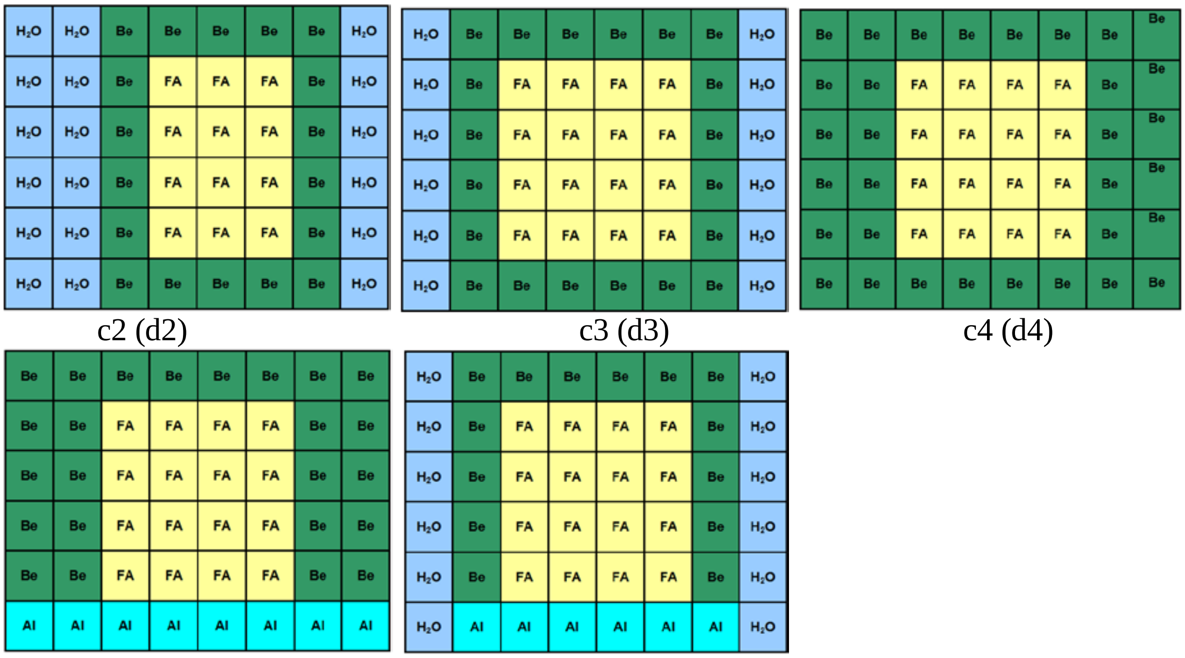


Fig. 2. Core diagram (#1÷#6 – FA numbers, Nz=1÷3 - axial layers numbers)

3.2 Results of the test problems calculation

3.2.1. Steady-state neutronic calculation

Core diagrams for the considered test problems are shown in Fig. 3. The case c2 represents initial LEU core of 12 FA after conversion. The case d4Al represents existing HEU core of 16 FA with beryllium and aluminum reflector. Xe-free cores with fresh FA are considered.



c2 (d2) c3 (d3) c4 (d4)

c4Al (d4Al) c3Al (d3Al)

FA – 6-tube fuel assembly, Be – beryllium block, Al – aluminum block, H_2O – water.

Fig. 3. Test problems core configuration
(c2, c3, c4, c3Al, c4Al – LEU, d2, d3, d4, d3Al, d4Al –HEU)

The results of K_{eff} calculation for 7 test problems (all rods withdrawn) by MCNP with ENDF/B-VII cross-section libraries and with the former ENDF/B-V,VI cross-section libraries as well as the results of MCU-PTR calculations with using BNAB/MCU library for energy region E>4.65 eV are presented in Table 3. The difference between MCNP/ENDF/B-VII results and the other results is also presented.

As Table 3 shows, for HEU cases using of ENDF/B-VI cross sections and previous version of ENDF/B for beryllium, aluminum and water in MCNP calculations gives the change in the K_{eff} values up to 0.2 %ΔK/K in comparison with calculations with ENDF/B-VII. For LEU cases this change is larger because of Mo presence.

The discrepancy between MCNP/ENDF/B-VII results and MCU-PTR with BNAB/MCU library results is slightly larger for the core configurations with Al blocks and also this discrepancy is different for LEU and HEU cores. The value of this discrepancy for every considered case is not very large but it is not a constant bias and there is a spread in the discrepancy of about 0.6%ΔK/K. That is if we consider the transition from the core d4Al to the core c2 the discrepancy between MCNP/ENDF/B-VII and MCU-PTR/BNAB/MCU in the prediction of excess reactivity change can be about 0.6%ΔK/K.

Table 3. Comparison of MCNP (ENDF/B-VII, ENDF/B-VI,V) and MCU-PTR (BNAB/MCU library) calculation results (standard deviation <0.0003)

Case	MCNP/ ENDF/B-VII	MCU-PTR/BNAB/MCU		MCNP/ENDF/B-VI,V[a]	
		K_{eff}	Difference, %ΔK/K	K_{eff}	Difference, %ΔK/K,
c2	1.1615	1.16028	-0.09	1.1585	-0.22
c4Al	1.1904	1.1944 (1.1924)[b]	0.28 (0.14)	1.1852	-0.37
d2	1.1933	1.1965	0.22	1.1930	-0.02
d3	1.2513	1.2550	0.24	1.2503	-0.06
d3Al	1.2061	1.2118	0.39	1.2053	-0.06
d4	1.2731	1.2783	0.32	1.2724	-0.04
d4Al	1.2248	1.2326	0.52	1.2223	-0.16

[a] - for the case MCNP/ENDF/B-VI,V cross sections data 1001.62c, 8016.62c, 4009.62c, 92235.66c, 92238.66c, 13027.50c, 42000.50c, lwtr.01t, be.01t were used.
[b] - Mo as a set of isotopes, in the other cases Mo is Mo-nat.

To extend the inter-code and inter-library comparison for the selected core configurations (c2, c4Al and d4Al) some additional investigations were performed. The case of c2 core with two central rods fully inserted is also considered (case c2r). The results of K_{eff} calculation for 3 test problems (all rods withdrawn, except for the case c2r) using MCNP with several cross-section libraries and MCU-PTR are presented in Table 4. MCU-PTR calculations were performed with using either BNAB/MCU library for energy region E>4.65 eV or with using ACE/MCU library for energy region 100 keV<E<20 MeV and BNAB/MCU library for energy region 2.15 eV <E<100 keV. For the inter-library comparison we substituted a single ENDF/B-VII nuclide with other library in MCNP calculations and assessed the change in the K_{eff} values.

It can be observed from the Table 4 that MCU-PTR with ACE/MCU library results give better agreement with MCNP/ENDF/B-VII calculations than MCU-PTR with BNAB/MCU library results. The spread in the discrepancy is 0.24%ΔK/K for the cases with all rods withdrawn. The discrepancy with MCNP/ENDF/B-VII in control rod (CR) worth defined as a difference between the reactivity of cases c2 and c2r is +2.2% (relative) and -3.1% for MCU-PTR with BNAB/MCU results and MCU-PTR with ACE/MCU results respectively.

It was also shown that cross sections for Be-9 and Mo give the main contribution to the difference in K_{eff} between MCNP/ENDF/B-VII results s and the results for previous version of ENDF/B.

Table 4. Comparison of MCNP (ENDF/B-VII, ENDF/B-VI,V) and MCU-PTR (BNAB/MCU, ACE/MCU) (standard deviation <0.0003)

Code	Libraries (except for)	K_{eff} (difference, %ΔK/K)			
		c4Al	d4Al	c2	c2r
MCNP	ENDF/B-VII	1.1904 (-)	1.2248 (-)	1.1615 (-)	1.0836 (-)
MCNP	ENDF/B-VII, (42000.66c)			1.1599 (-0.12)	1.0821 (-0.13)
MCNP	ENDF/B-VII, (Be-ENDF/B-VI)				1.0857 (0.18)
MCNP	ENDF/B-VI [a]	1.1872 (-0.23)	1.2250 (0.01)	1.1590 (-0.19)	
MCU-PTR	ACE/MCU	1.1879 (-0.18)	1.2253 (0.03)	1.1587 (-0.21)	1.0796 (-0.34)
MCU-PTR	BNAB/MCU	1.1944 (0.28)	1.2326 (0.52)	1.1603 (-0.09)	1.0848 (0.10)

[a] - for the case MCNP/ENDF/B-VI cross sections data 001.62c, 4009.62c, 8016.62c, 13027.62c, 42000.66c, 92235.66c, 92238.66c, be.60t, lwtr.60t were used.

3.2.2. Burnup calculation

The first burnup cycle for the reactor core of 12 LEU FA (Fig.2) was calculated. At the first time step Xe-free core with fresh FA is considered. For fresh core the composition of all fuel zones is the same. Two CR are fully inserted: in FA#3 and in the FA symmetrical to it. The reactor operation at full power is calculated. Integral energy generation of the core during the first cycle is 20000 MWh (333.3 full power days). Reactor power is 2.5 MW. To reduce the number of materials for burnup calculation, one quarter of real core with symmetry boundary conditions were calculated and therefore the power of 625 kW was intended in calculation. It is assumed that in horizontal plane all fuel tubes of one FA have the same burnup (they burn as one material). There are 3 burnup layers in axial direction. CR position does not change during the burnup process. ^{10}B in the control rods does not burn. Beryllium poisoning is not considered.

At the end of the first burnup cycle 4 fresh FA were added to the core and the second burnup cycle for the reactor core of 16 LEU FA was calculated. The parameters of the second cycle was the same as for the first cycle.

Fig. 4 presents the results of multiplication factor calculation by two codes: MCREB code (with ENDF/B-VII libraries, except for 42000.66c) and MCU-PTR with BNAB/MCU library. The depletion step for time > 33 days was as follows: MCREB – 16.66 days, MCU-PTR – as shown in Fig. 4 (66.7 days and 83.3 days). MCREB calculation accounted for 45 actinides and fission products and also a lumped fission product. MCU-PTR calculation accounted for 47 actinides and fission products and other isotopes were calculated with lumped fission product cross sections.

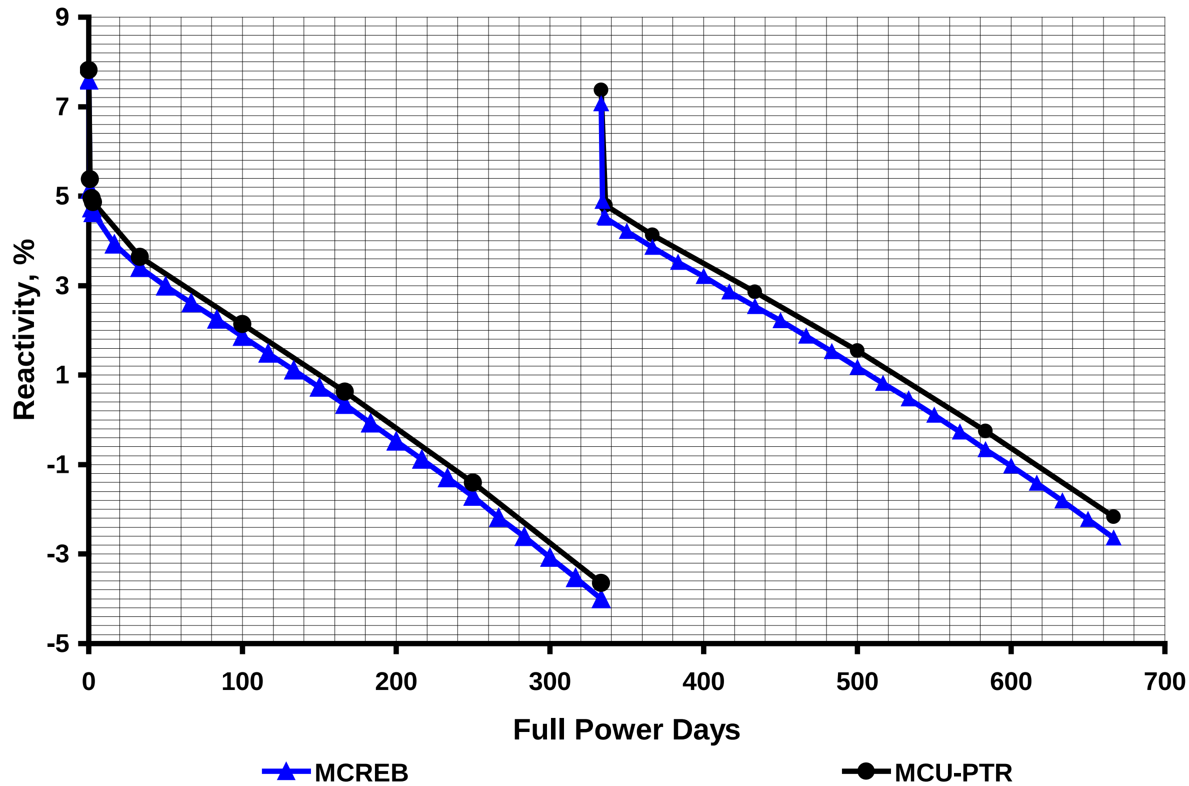


Fig. 4. Reactivity vs. time calculated using MCREB and MCU-PTR

There is a bias of ~0.3 %ΔK/K between MCU-PTR and MCREB at the beginning of the first cycle. As shown above it is concerned with using of different cross-section libraries. Up to the end of the second cycle the bias increases to 0.2%.

4. Reference cores calculation

In course of conversion analysis of IRT MEPhI to LEU fuel the calculations using MCNP with detail geometrical model of the core and reflector were used. For the calculation results validation the detailed geometrical model of the IRT MEPhI reactor with HEU and LEU fuel for the calculation using MCU-PTR code was developed. The geometrical model of the reactor for MCU-PTR is practically identical with corresponding model for MCNP (Fig. 5).

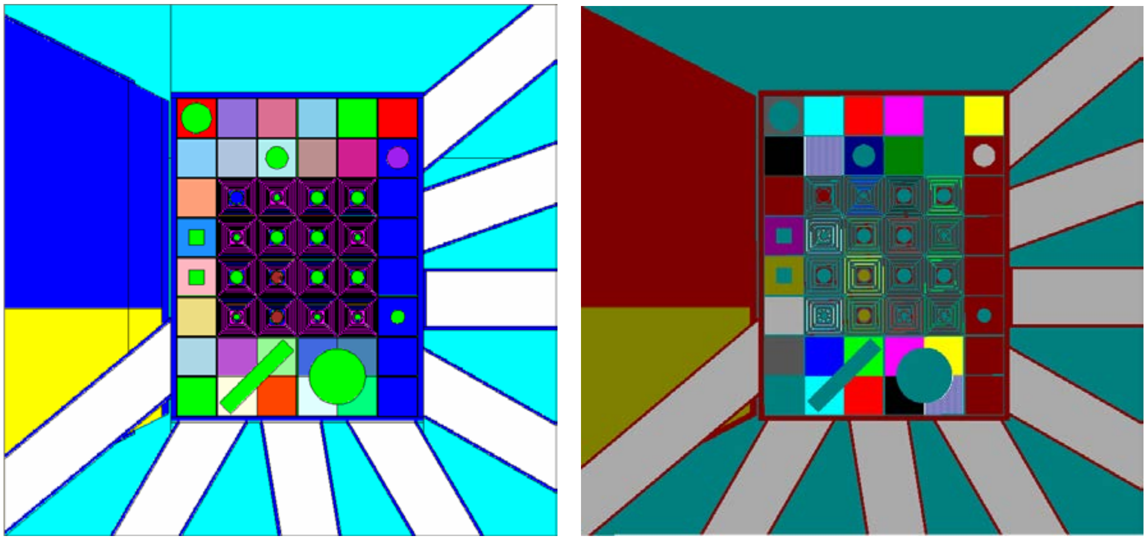


Fig.5. IRT MEPhI geometrical models: (a) – MCNP; (b) - MCU-PTR.

Calculation was performed for three reference cores. Current HEU core of 16 FA with current reflector, initial (fresh) LEU core of 12 FA and 8 fresh beryllium blocks and operational LEU core of 16 FA were selected as the reference cores. Table 6 presents 3 cases with different CR (automatic regulator and 3 shim rods) positions for the reference HEU and LEU cores. These data enables to estimate criticality, excess reactivity and shutdown margin.

Table 6. CR position for reference cores calculation (scram rods withdrawn)

Core	Case	CR position, mm			
		AR	KC-1	KC -2	KC -3
HEU operational	#1	250	0	0	393
	#2	0	0	0	0
	#3	580	580	580	580
LEU fresh	#1	250	0	180	580
	#2	0	0	0	0
	#3	580	580	580	580
LEU operational	#1	250	0	0	390
	#2	0	0	0	0
	#3	580	580	580	580

Table 7 presents the results of calculation of the reference cores using MCNP and MCU-PTR with different CR positions (case #1, #2, #3) described in Table 6. The calculations were performed with different cross section libraries. The difference between MCNP/ENDF/B-VII results and the other results for the case#1 is also presented. The calculations for Table 7 were performed with the same fuel isotopic composition for MCNP and MCU-PTR. For the operational core fuel isotopic composition was obtained on the basis of ^{235}U burnup distribution in the core and polynomial approximations of actinides and fission products concentrations (isotope concentration vs. ^{235}U burnup). These polynomial approximations were determined by burnup calculation of the cell using MCU-PTR code. ^{235}U burnup distribution was determined by burnup calculation of IRT MEPhI core using 3D diffusion code.

Table 7. Results of calculation of criticality (#1), excess reactivity (#2) and shutdown margin (#3) using MCNP and MCU-PTR of the reference cores (the same fuel isotopic composition for MCNP and MCU-PTR, standard deviation <0.0002**)**

Core	Code	Cross section libraries	ρ, %ΔK/K			Δ, %ΔK/K
			#1	#2	#3	#1
HEU operational	MCNP	ENDF/B-VII	0.35	-	-	0
	MCNP	ENDF/B-VI	0.32	5.47	-12.14	-0.03
	MCU-PTR	BNAB/MCU	1.03	6.16	-11.41	0.69
	MCU-PTR	ACE/MCU	0.32	5.52	-12.18	**-0.02**
LEU fresh	MCNP	ENDF/B-VII	0.37	10.28	-5.35	0
	MCNP	ENDF/B-VI	0.09	10.02	-5.60	-0.28
	MCU-PTR	BNAB/MCU	0.86	10.73	-4.95	0.49
	MCU-PTR	ACE/MCU	0.18	10.11	-5.68	**-0.20**

For the reference cores with identical fuel isotopic composition for MCNP and MCU-PTR the difference between MCNP/ENDF/B-VII results and the MCU-PTR with ACE/MCU cross section libraries results is approximately the same as for the test problems d4al, c4Al (0÷-0.2%ΔK/K). The difference between MCNP/ENDF/B-VII results and the MCU-PTR with BNAB/MCU cross section libraries results increases to 0.2%ΔK/K in comparison with the test problems d4al, c4Al.

Table 8 presents the same results as the Table 7, but for MCNP/ENDF/B-VII calculation the other fuel isotopic composition was used. This isotopic composition was determined by burnup calculation of the reference core using MCREB code.

Table 8. Results of calculation of criticality (#1), excess reactivity (#2) and shutdown margin (#3) using MCNP and MCU-PTR of the reference cores (the different fuel isotopic composition for MCNP and MCU-PTR, standard deviation <0.0002**)**

Core	Code	Cross section libraries	Fuel composition	ρ, %ΔK/K			Δ, %ΔK/K
				#1	#2	#3	#1
HEU operational	MCNP	ENDF/B-VII	MCREB	-0.22	5.00	-12.76	0
	MCU-PTR	ACE/MCU	MCU-PTR	0.32	5.52	-12.18	**0.54**
	MCU-PTR	BNAB/MCU	MCU-PTR	1.03	6.16	-11.41	1.25
LEU operational	MCNP	ENDF/B-VII	MCREB	0.34	4.85	-10.71	0
	MCU-PTR	ACE/MCU	MCU-PTR	0.62	5.13	-10.48	**0.29**
	MCU-PTR	BNAB/MCU	MCU-PTR	1.22	5.67	-9.85	0.89

Using of fuel isotopic composition calculated with different codes leads to the increase of the difference in K_{eff} between MCNP/ENDF/B-VII results and MCU-PTR results to 0.5%ΔK/K.

5. Conclusions

Comparative validation of MCNP (+MCREB for burnup calculation) and MCU-PTR codes based on test problems calculation and IRT MEPhI reference cores calculation was performed.
The calculation of the set of test problems for IRT-type research reactor with tube-type LEU (U-Mo) and HEU fuel, light water moderator and beryllium reflector was performed using the three-dimensional continuous-energy Monte Carlo codes (MCNP and MCU-PTR). Effective multiplication factors in the core for the several loading patterns were used in the validation process of the physical model of the core and neutron cross section data from the ENDF/B-VI, ENDF/B-VII and MCU/ACE, MCU/BNAB libraries evaluation.
The discrepancy between MCNP/ENDF/B-VII results and MCU-PTR with BNAB/MCU library results is from -0.1%ΔK/K to 0.5%ΔK/K for HEU and LEU fuel. The discrepancy between MCNP/ENDF/B-VII results and MCU-PTR with BNAB/ACE library results is from 0%ΔK/K to 0.3%ΔK/K for HEU and LEU fuel. It was concluded that for the conversion analysis of IRT-type research reactor it is better to use MCU-PTR code with BNAB/ACE library from the point of view of better agreement with MCNP results.
A good agreement between MCREB and MCU-PTR results is observed for the test problem with burnup. The increase of the discrepancy between the codes in K_{eff} after the second burnup cycle with LEU fuel is ~0.2%ΔK/K.
For IRT MEPhI reference cores with identical fuel isotopic composition for MCNP and MCU-PTR the difference between MCNP/ENDF/B-VII calculated results and the MCU-PTR with ACE/MCU cross section libraries calculated results is approximately the same as for the test problems.
More works are needed in the future to complete validation investigations.

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