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VENUS-2 Experimental Benchmark Analysis with MCU-REA

Project Manager

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A Russian Contribution to the Fissile Materials Disposition Program

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ABSTRACT

The VENUS critical facility is a zero power reactor located at SCK-CEN, Mol, Belgium, which for the VENUS-2 experiment utilized a mixed-oxide core with near-weapons-grade plutonium. In addition to the VENUS-2 Core, additional computational variants based on each type of fuel cycle VENUS-2 core (3.3 wt. % UO_2, 4.0 wt. % UO_2, and 2.0/2.7 wt. % MOX) were also calculated. The VENUS-2 critical configuration and cell variants have been calculated with MCU-REA, which is a continuous energy Monte Carlo code system developed at Russian Research Center "Kurchatov Institute" and is used extensively in the Fissile Materials Disposition Program. The calculations resulted in a k_{eff} of 0.99652 ± 0.00025 and relative pin powers within 2% for UO_2 pins and 3% for MOX pins of the experimental values.

1. INTRODUCTION

Since 1999 Russia specialists from the Russian Research Center “Kurchatov Institute” (RRC-KI) have participated in TFRPD (Task Force on Reactor Based Plutonium Disposition) NEA/OECD experts group. The purpose of this group is to facilitate the exchange expertise and data among its international members that can aid in the disposition of plutonium. Currently, the TFRPD is performing a benchmark exercise involving the VENUS-2[1] experiment. The VENUS critical facility is a zero power reactor located at SCK-CEN, Mol, Belgium and utilized a mixed-oxide core with near-weapons-grade plutonium. In addition to the VENUS-2 Core, additional computational variants based on each type of fuel cycle VENUS-2 core (3.3 wt. % UO_2, 4.0 wt. % UO_2, and 2.0/2.7 wt. % MOX) were also calculated.

In this report MCU-REA[2] results as well as comparison of MCU-REA results with other codes and with experiment data are presented. The MCU-REA code is a continuous energy Monte Carlo code system developed at RRC-KI and is used extensively in the Fissile Materials Disposition Program. Additional details regarding the MCU-REA code are provided in Appendix A.

2. VENUS-2 CRITICAL FACILITY CALCULATION BY MCU CODE

2.1 GEOMETRY

The 2-D model, shown in Fig. 1, is based on the benchmark specification provided in the document prepared by the OECD/NEA entitled: “BLIND BENCHMARK ON THE VENUS-2 MOX CORE MEASUREMENTS, NEA/SEN/ NSC/WPPR (99)2” without any approximation except of the neutron pad. The neutron pad outer radius was taken as 65.073 cm instead of value in the benchmark specification. This approximation does not influence on the criticality and fission rate distribution. Core criticality calculation was performed with vertical buckling value 2.4E-03 cm^{-2}, as provided in the specifications.

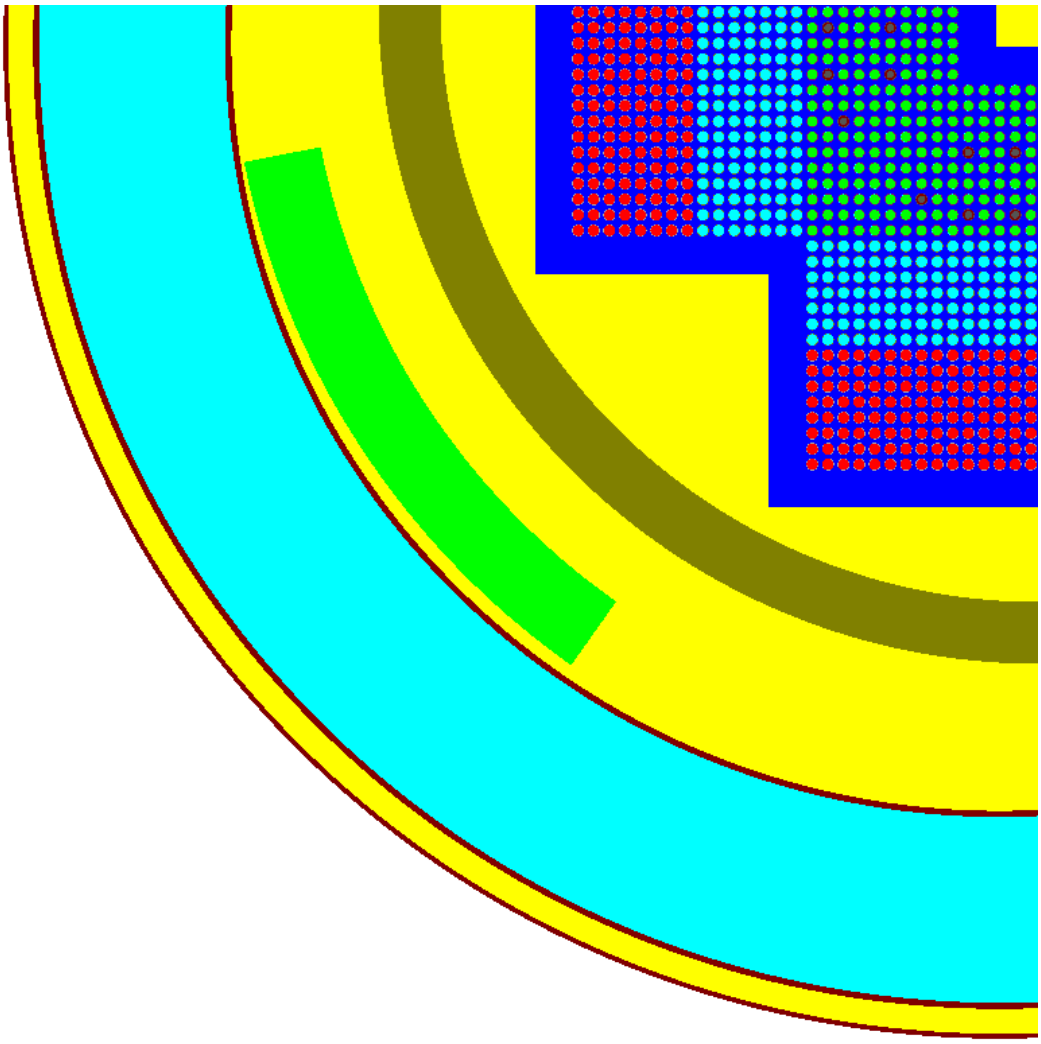

Fig. 2.1. MCU-REA 2-D model of the VENUS-2 experiment.

2.2. STATISTICAL UNCERTAINTIES

The number of particle histories and the associated standard deviations for the calculations are presented in Table 1. The number of histories performed result in sufficiently small statistical uncertainties for benchmarking purposes.

Table 2.1. Statistical uncertainties for core and cell calculations

	Core Calculation	Cell Calculations
Neutron histories	10,000,000	1,000,000
Uncertainty[a] for k_∞	0.00025	0.0007
Uncertainty[a] for fission rates in fuel rod	0.8%–1.2%	0.1%

[a]One standard deviation.

2.3 CROSS SECTION REPRESENTATION

The MCU-REA code has various cross section models that can be used for different elements and nuclides. Table 2 provides the detailed information about the cross section representation for each nuclide in the VENUS-2 model. Note that in this table the parameters MODS, BLOC and EMAX are defined as follows:

MODS - denotes the model of calculation of scattering cross-section in the thermal energy region:

- MODS=G – gas model;
- MODS=T – heavy gas model;
- MODS=H2O – model name if the cross-sections are calculated considering chemical bonds, when S(α,β) treatment is used; ENDF phonon spectrum of hydrogen in water.

BLOK - consideration of resonance effects:

- BLOK=0 – resonance effects not considered
- BLOK=1 – blocking in group's average (through f-factor)
- BLOK=2 – all resonances are considered in subgroup approximation
- BLOK=4 – calculation by resonance parameters from LIPAR at E<EMAX and in subgroup approximation at E>EMAX, EMAX – the upper energy boundary for calculation by resonance parameters.

Table 2.2. Cross section representation of the nuclides and elements in the MCU-REA VENUS-2 model

Material	MODS	BLOK	EMAX resonance boundary (eV)	Material	MODE	BLOK	EMAX resonance boundary (eV)
H	H2O	0	0	CO	T	2	21500
B-10	T	0	0	NI	T	2	0
B-11	G	2	0	ZR	T	2	10000
C[a]	G	2	0	MO	T	2	0
N	G	2	0	SN	T	0	0
O	G	2	0	U-234	T	4	465
NA	T	2	0	U-235	T	4	100
AL	T	2	0	U-236	T	4	1000
SI	T	2	0	U-238	T	4	2150
P	T	2	0	Pu-239	T	4	465
S	T	0	0	Pu-240	T	4	1000
K	T	2	0	Pu-241	T	4	100
CR	T	2	0	Pu-242	T	4	1000
MN	T	2	100000	Am-241	T	4	46.5
FE	T	2	0				

[a]Carbon calculation free gas model is used in pyrex zone.

3. MCU-REA CALCULATIONAL RESULTS

3.1 CELL CALCULATIONS

The MCU-REA results for the cell benchmark variants are given in Tables 3.1–3.5. Note that the pin dimensions are different for the 3.3 wt. % and 4.0 wt. % UO_2 cells resulting in the lower k_∞ for the 4.0 wt. % UO_2 cell.

Table 3.1. k_∞ values for cell calculations

Cell	k_∞
3.3 wt. % UO_2	1.4071
4.0 wt. % UO_2	1.3365
2.0/2.7 wt. % MOX	1.2549

Table 3.2. Energy integrated reaction rates in 2.0/2.7 wt. % MOX, 3.3 wt. % UO_2 and 4.0 wt. % UO_2 cells (reactions/cm^3/sec normalized to 1 fission neutron/sec)

Material	MOX cell (2.0/2.7 wt. %)		UO_2 cell (3.3 wt. %)		UO_2 cell (4.0 wt. %)	
	Absorption	Fission	Absorption	Fission	Absorption	Fission
U-234	8.596E-04	2.437E-05	1.932E-03	4.362E-05	2.025E-03	5.229E-05
U-235	1.742E-01	1.386E-01	6.582E-01	5.461E-01	6.270E-01	5.133E-01
U-236	3.257E-04	1.160E-05	3.995E-04	1.347E-05	6.394E-04	2.212E-05
U-238	2.404E-01	2.981E-02	2.697E-01	2.693E-02	2.772E-01	3.084E-02
Pu-239	4.239E-01	2.772E-01	-	-	-	-
Pu-240	8.348E-02	7.781E-04	-	-	-	-
Pu-241	1.731E-02	1.268E-02	-	-	-	-
Pu-242	9.605E-04	1.487E-05	-	-	-	-
Am-241	3.939E-04	5.112E-06	-	-	-	-
O	2.437E-03	0.000E+00	2.166E-03	0.000E+00	2.465E-03	0.000E+00
B-10	-	-	1.763E-05	0.000E+00	-	-
B-11	-	-	9.819E-11	0.000E+00	-	-
Total	9.441E-01	4.592E-01	9.324E-01	5.730E-01	9.093E-01	5.442E-01

Tables 3.3. Three group absorption and fission reaction rates in 2.0/2.7 wt. % MOX cell
(reactions/cm^3/sec normalized to 1 fission neutron/sec)

Material	Group 1 (E > 5 keV)		Group 2 (4 eV < E < 5 keV)		Group 3 (E < 4 eV)	
	Absorption	Fission	Absorption	Fission	Absorption	Fission
U-234	3.244E-05	2.279E-05	6.740E-04	6.400E-07	1.531E-04	9.403E-07
U-235	6.292E-03	5.317E-03	4.314E-02	2.749E-02	1.247E-01	1.058E-01
U-236	1.313E-05	7.804E-06	3.044E-04	3.691E-06	8.142E-06	1.040E-07
U-238	5.899E-02	2.981E-02	1.513E-01	0.000E+0	3.003E-02	0.000E+0
Pu-239	7.707E-03	6.835E-03	5.536E-02	3.182E-02	3.608E-01	2.386E-01
Pu-240	9.505E-04	7.317E-04	4.399E-03	3.059E-05	7.813E-02	1.576E-05
Pu-241	3.217E-04	2.909E-04	3.856E-03	2.819E-03	1.313E-02	9.572E-03
Pu-242	1.954E-05	1.461E-05	5.258E-05	1.824E-07	8.884E-04	7.197E-08
Am-241	6.379E-06	3.187E-06	4.905E-05	3.603E-07	3.384E-04	1.565E-06
O	2.431E-03	0.000E+0	4.538E-08	0.000E+0	6.026E-06	0.000E+0
Total	7.676E-02	4.304E-02	2.592E-01	6.217E-02	6.082E-01	3.540E-01

Table 3.4. Three group absorption and fission reaction rates in 3.3 wt. % UO_2 cell
(reactions/cm^3/sec normalized to 1 fission neutron/sec)

Material	Group 1 (E > 5 keV)		Group 2 (4 eV < E < 5 keV)		Group 3 (E < 4 eV)	
	Absorption	Fission	Absorption	Fission	Absorption	Fission
U-234	5.351E-05	3.773E-05	1.105E-03	1.057E-06	7.729E-04	4.830E-06
U-235	9.390E-03	7.943E-03	6.588E-02	4.199E-02	5.829E-01	4.961E-01
U-236	1.468E-05	8.794E-06	3.603E-04	4.361E-06	2.452E-05	3.161E-07
U-238	5.287E-02	2.693E-02	1.416E-01	0.000E+0	7.520E-02	0.000E+0
O	2.150E-03	0.000E+0	4.333E-08	0.000E+0	1.553E-05	0.000E+0
B-10	3.458E-08	0.000E+0	6.548E-07	0.000E+0	1.694E-05	0.000E+0
B-11	2.862E-12	0.000E+0	2.930E-12	0.000E+0	9.240E-11	0.000E+0
Total	6.448E-02	3.492E-02	2.090E-01	4.199E-02	6.590E-01	4.961E-01

Table 3.5. Three group absorption and fission reaction rates in 4.0 wt. % UO_2 cell
(reactions/cm^3/sec normalized to 1 fission neutron/sec)

Material	Group 1 (E > 5 keV)		Group 2 (4 eV < E < 5 keV)		Group 3 (E < 4 eV)	
	Absorption	Fission	Absorption	Fission	Absorption	Fission
U-234	6.759E-05	4.721E-05	1.349E-03	1.302E-06	6.081E-04	3.776E-06
U-235	1.369E-02	1.156E-02	9.147E-02	5.853E-02	5.218E-01	4.432E-01
U-236	2.489E-05	1.465E-05	5.872E-04	7.117E-06	2.731E-05	3.510E-07
U-238	6.191E-02	3.084E-02	1.581E-01	0.000E+0	5.716E-02	0.000E+0
O	2.453E-03	0.000E+0	4.879E-08	0.000E+0	1.172E-05	0.000E+0
Total	7.815E-02	4.246E-02	2.515E-01	5.854E-02	5.796E-01	4.432E-01

3.2 CORE CALCULATIONS

The VENUS-2 core calculation with MCU resulted in a k_{eff} of 0.99652 ± 0.00025. The corresponding fission rate distribution is given in Table 3.6.

Table 3.6. VENUS-2 calculated core fission rate distribution
(normalization mid-plane average = 1, normalized over all 640 pins in the ¼ core)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
1	0.443	0.530	0.607	0.680	0.736	0.812	0.894	1.092	1.045	1.193	1.267	1.332	1.359	1.430	1.535	1.246	1.223	1.391	1.396	1.365	1.260	1.312	1.342	1.249	1.034
2	0.445	0.526	0.597	0.681	0.738	0.815	0.906	1.089	1.044	1.172	1.268	1.330	1.373	1.439	1.495	1.198	0.000	1.311	1.379	1.284	0.000	1.284	1.336	1.250	1.042
3	0.433	0.525	0.601	0.666	0.733	0.815	0.922	1.075	1.028	1.174	1.240	1.321	1.375	1.413	1.511	1.232	1.262	1.370	1.395	1.381	1.283	1.345	1.358	1.267	1.031
4	0.439	0.512	0.589	0.657	0.724	0.788	0.897	1.061	1.035	1.150	1.245	1.303	1.360	1.437	1.510	1.237	1.253	1.363	1.406	1.380	1.294	1.362	1.384	1.316	1.063
5	0.417	0.518	0.564	0.635	0.711	0.789	0.872	1.035	1.015	1.150	1.214	1.284	1.354	1.412	1.505	1.187	0.000	1.297	1.377	1.336	0.000	1.327	1.392	1.331	1.132
6	0.404	0.498	0.557	0.621	0.689	0.767	0.851	1.007	0.990	1.120	1.211	1.276	1.348	1.397	1.513	1.240	1.241	1.338	1.407	1.403	1.347	1.420	1.463	1.414	1.304
7	0.395	0.476	0.542	0.619	0.678	0.744	0.824	0.991	0.958	1.097	1.175	1.253	1.323	1.393	1.495	1.275	1.299	1.280	1.391	1.433	1.458	1.461	1.473	1.455	
8	0.391	0.453	0.525	0.591	0.668	0.719	0.806	0.950	0.944	1.070	1.164	1.224	1.305	1.363	1.485	1.263	1.248	0.000	1.352	1.443	1.478	1.511	1.493		
9	0.364	0.430	0.494	0.572	0.627	0.693	0.773	0.934	0.903	1.028	1.103	1.191	1.262	1.333	1.474	1.244	1.323	1.302	1.408	1.495	1.510	1.517			
10	0.350	0.411	0.477	0.530	0.596	0.660	0.734	0.896	0.865	0.982	1.086	1.145	1.219	1.313	1.448	1.252	1.365	1.409	1.452	1.469	1.509				
11	0.329	0.388	0.448	0.508	0.573	0.622	0.693	0.830	0.814	0.951	1.046	1.113	1.173	1.253	1.393	1.209	1.346	1.393	1.433	1.467					
12	0.301	0.361	0.421	0.471	0.517	0.570	0.652	0.781	0.767	0.887	0.969	1.065	1.124	1.200	1.356	1.193	1.316	1.371	1.424						
13	0.283	0.336	0.380	0.429	0.484	0.530	0.612	0.726	0.699	0.824	0.912	0.975	1.035	1.142	1.279	1.123	1.263	1.314							
14	0.250	0.311	0.353	0.395	0.437	0.500	0.536	0.666	0.630	0.746	0.817	0.869	0.962	1.037	1.202	1.057	1.179								
15	0.223	0.259	0.298	0.337	0.371	0.424	0.477	0.562	0.539	0.613	0.668	0.718	0.767	0.846	0.985	0.922									

4. COMPARISONS WITH EXPERIMENT AND OTHER CALCULATIONS

Twelve solutions were submitted and the agreement is generally satisfactory [3]. The results are summarized as follows:

Average K_{eff} over 12 solutions	0.99758±0.0045
Average K_{eff} over transport calculations (5)	0.99750±0.0044
Average K_{eff} over Monte-Carlo calculations (7)	0.99983±0.0037
Power(fission rate) distribution	5% deviation in the UO_2 regions 10% deviation in the MOX region.

Figures 4.1 and 4.2 show results of MCU calculations and experiments for horizontal and diagonal rows. Tables 4.1 and 4.2 present comparisons of k_∞ and k_{eff} values obtained from Monte Carlo core and cell calculations.

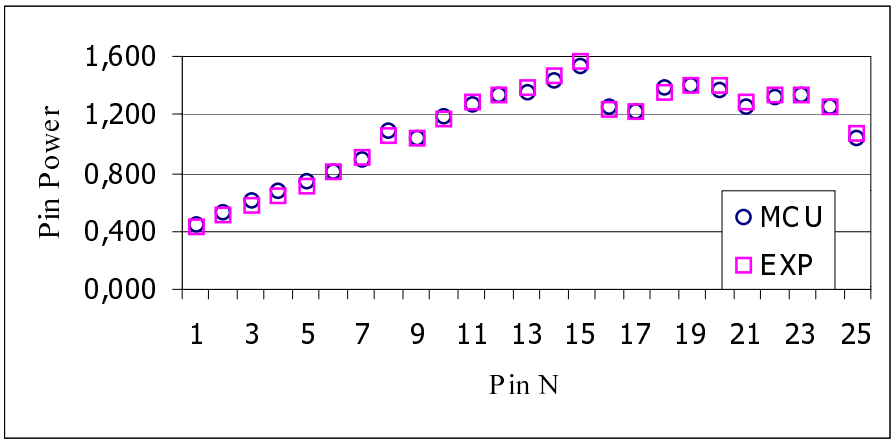

Fig. 4.1. Comparison of pin Power Distribution in the horizontal row.

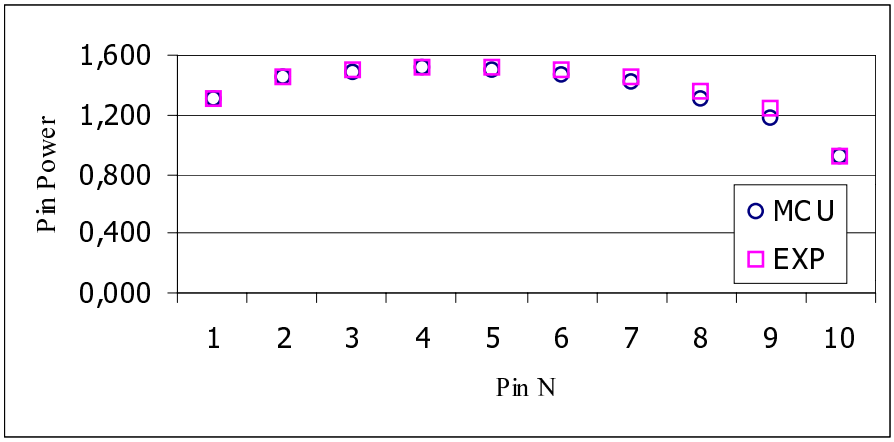

Fig. 4.2. Comparison of pin power distribution in the diagonal row.

Table 4.1. Comparison of k_∞ values from Monte Carlo cell calculations

Participant	Code/Method	UO_2 (3.3 wt. %)		UO_2 (4.0 wt. %)		MOX (2.0/2.7 wt. %)	
		k_∞	Dev. (%)	k_∞	Dev. (%)	k_∞	Dev. (%)
NEA+KAERI	MCNP-4B	1.4048	-0.22	1.3364	-0.22	1.2545	-0.28
JAERI	MVP	1.4112	0.23	1.3455	0.47	1.2631	0.41
RRC-KI	MCU	1.4071	-0.05	1.3365	-0.21	1.2549	-0.25
KFKI	MCNP-4B	1.4065	-0.10	1.3364	-0.21	1.2631	0.41
GRS	MCNP-4B (square cell)	1.4112	0.24	1.3437	0.33	1.2614	0.27
GRS	MCNP-4B (cyl. cell)	1.4095	0.12	1.3402	0.07	1.2543	-0.29
LJS-Jeraj	MCNP-4B	1.4048	-0.22	1.3361	-0.24	1.2547	-0.26
Average		1.4079		1.3393		1.2580	
St. dev.		0.0028		0.0040		0.0043	

Table 4.2. Comparison of core k_{eff} values from Monte Carlo core calculations

Participant	Code	k_{eff}	Dev. (%)	Data library
NEA+KAERI	MCNP-4B	1.00213(13)	0.21	ENDF/B-VI Rel.2
RRC-KI	MCU	0.99650(25)	-0.35	ENDF/B-VI, JENDL-3.2, BROND
KFKI	MCNP-4B	1.00050(26)	0.05	ENDF/B-VI, ENDF/B-V
GRS	MCNP-4B	1.00430(20)	0.43	JEF2.2, ENDF/B-VI, JENDL-3.1, BROND
IJS-Jeraj	MCNP-4B	0.99570(10)	-0.43	ENDF/B-VI, ENDL85

Table 4.3 presents averages of deviation (%) of the relative fission rate from the experimental value and associated standard deviations for each type of fuel cell in the VENUS-2 core.

Table 4.3. Relative fission rate average deviation (in percent) from the experimental value and associated standard deviations for each type of fuel

Participant	UO_2 (3.3 wt. %)		UO_2 (4.0 wt. %)		MOX (2.0/2.7 wt. %)	
	Average	St. Dev.	Average	St. Dev.	Average	St. Dev.
NEA	-2.42	1.51	-0.42	1.99	5.85	2.13
KAERI	-2.19	1.39	-0.37	1.88	4.92	2.10
ORNL	-0.60	1.53	-0.68	2.19	1.64	2.96
PSI	-2.65	1.56	-0.88	2.26	7.19	2.73
SCK	-2.37	1.51	-0.40	1.96	5.63	2.14
IJS-Trkov (JEF-2.2)	-2.36	2.00	-1.25	3.57	6.19	4.29
IJS-Trkov (ENDF/B-VI)	-2.36	1.96	-1.42	3.54	6.59	4.24
NEA+KAERI	-0.48	1.44	0.03	2.02	1.37	1.75
JAERY	-0.43	1.49	-0.95	1.80	3.15	2.09
KI	-0.54	1.65	-1.08	1.89	2.16	2.38
KFKI	-1.64	1.74	-0.99	2.25	6.66	2.32
GRS	-0.57	1.33	-1.05	1.77	3.33	2.05

5. CONCLUSIONS

The VENUS-2 Benchmark was calculated using the MCU-REA code. The MCU results show good agreement with experiment and other calculational results. A summary of the results are given in Table 5.1. The deviation of the MCU calculational k_{eff} value for the VENUS-2 critical facility is -0.35%.

As shown in Table 5.1, MCU-REA shows very good agreement with the experiment for the fission rate distribution. Maximum deviation for the pin fission rate does not exceed 0.5% for the UO_2 3.3% region, 1.9% for the UO_2 4.0% region and 2.2% for the MOX region.

Table 5.1. Summary of the MCU-REA deviations (%) from the cell calculation average and the VENUS-2 experiment

Functional	Variant	Deviation %	Deviation from
k_∞	Cell UO_2 (3.3 wt. %)	-0.05%	Calculation
	Cell UO_2 (4.0 wt. %)	-0.21%	average
	Cell MOX	-0.25%	
k_{eff}	VENUS-2 Core	-0.35%	Experiment
Relative Fission Rate	UO_2 3.3% region	-0.5%	Experiment
	UO_2 4.0% region	-1.9%	
	MOX region	2.2%	

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Appendix A

MCU-REA CODE INFORMATION

Appendix A. MCU-REA CODE INFORMATION

MCU-REA is a general-purpose continuous energy Monte Carlo code for solving the neutron transport problems with depletion. It is used with both pointwise and step function representations of cross sections. For neutron-nuclear interaction modeling the code includes:

- inelastic scattering laws from evaluated nuclear data files;
- cross section temperature dependence in unresolved resonance region with the subgroup approximation;
- Doppler broadening of resonance cross sections in resolved resonance region using infinite number of energy points;
- S(α,β) scattering law depending on temperature.

The geometry module of the code is the combination of the following approaches:

- combinatorial method, body technique, hierarchy description;
- Woodcock method;
- algorithm to model fuel elements with thousands of micro-spheres included in one fuel element.

The hierarchy geometry option permits one to describe full scale 3-D reactor model (VVER, PWR, BWR, RBMK, etc) using only 0.25 MB of RAM.

The change of isotopic composition of reactor materials is modeled with a burnup module that includes 39 actinides and 165 fission products.

The MCU-REA code was certified by the Russian regulator authority Gosatomnadzor (GAN) for neutronic calculations of VVER reactors.

More than 500 3D benchmark experiments published in the Handbook of International Criticality Safety Evaluation Benchmark Project and Russian literature have been calculated. The discrepancies between calculation and experiment results are within the experiment errors estimated. The full-scale 3-D models of the different reactors (transport, production, space, research, energy production, VVER and RBMK) are elaborated and used widely to estimate their parameters and to verify the design codes.

MCU data libraries is DLC/MCUDAT-2.1 based on:

- ENDF/B-VI; JENDL-3.2; BROND
- MCU group own evaluations and compilations:
    - LIPAR - parameters of the fully resolved resonances
    - BFS - phonon spectra library including the ENDF data
    - KORT - cross-sections for E=0.0253 eV, resonance integrals, etc.

The following data processing codes were used to obtain the cross-section data used:

- NJOY; GRUCON (IPPE, Russia)
- MCU group elaborations:
    - TERMAC - generation of the S(α,β) multigroup library;
    - STEN - generation of the S(α,β) pointwise library;
    - RAPAN - generation of the resonance cross sections;
    - SET OF MODULES for evaluating and analyzing the resonance parameters.

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