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KRITZ-2 Experimental Benchmark Analysis with MCU-REA

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A Russian Contribution to the Fissile Materials Disposition Program

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ABSTRACT

The KRITZ-2 experiment has been adopted by the OECD/NEA Task Force on Reactor-Based Plutonium Disposition for use as a benchmark exercise. The KRITZ-2 experiment consists of three different core configurations (one with near-weapons-grade MOX) with critical conditions a 20°C and 245°C. The KRITZ-2 experiment has been calculated the MCU-REA code, which is a continuous energy Monte Carlo code system developed at the Russian Research Center—"Kurchatov Institute" and is used extensively in the Fissile Materials Disposition Program. The calculated results for k_{eff} and fission rate distributions are compared with the experimental data and results of other codes. The results are in good agreement with 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 studying the KRITZ-2 experiment for a common benchmark exercise. The KRITZ-2 experiment is particularly interesting because it was performed in such a manner as to obtain critical conditions a both room and elevated (245°C). The analysis of the KRITZ-2 experiment has been performed in RRC Kurchatov Institute. Good agreement of the experimental and calculational results has been obtained.

At the second TFRPD meeting (November 1999) it was decided that :

- First results from RF (RRC Kurchatov Institute) and USA should be analyzed. Specify data source. Adopt KRITZ-2 as TFRPD benchmark.
- Final specification should be prepared for calculation buy TFRPD members.

At the 3D TFRPD meeting (June 2000), after presentation of the results presented in this report, it was decided that:

- U.S. prepared specification should be distributed to all participants of the project.
- All participants should calculate the benchmark.

In this report MCU-REA[2,3] 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. MCU-REA MODEL OF THE KRITZ-2 CRITICAL FACILITY

2.1 KRITZ-2 SPECIFICATIONS

Three cores (2:1, 2:13, 2:19) at temperatures 20°C and 245°C were measured at the KRITZ-2 critical facility (see Ref. 1 and Figs. 2.1–2.6). Cores 2:1 and 2:13 contain only uranium pins, Core 2:19 contains only Mixed Oxide (MOX) pins. The MOX pins consist of vibro-compacted PuO_2UO_2 fuel with PuO_2 grain size of 25 μm. The specifications for KRITZ-2 are given in Tables 2.1–2.3 and were obtained from Ref. 1.

Table 2.1. KRITZ-2 fuel rod specifications (Ref. 1)

Fuel material parameter	UO_2	MOX
Fuel density (g/cm^3)	10.145	9.58
U-235 in U (wt. %)	1.86	0.16
PuO_2 in fuel (wt %)	-	1.50
Pu composition:		
Pu-239 (at. %)	-	91.41
Pu-240 (at. %)	-	7.83
Pu-241 (at. %)	-	0.73
Pu-242 (at. %)	-	0.03
Fuel diameter (mm)	10.58	9.45
Fuel length (mm)	3650	1232
Canning material	Zircaloy-2	Zircaloy-2
Canning thickness (mm)	0.74	?
Canning outer diameter (mm)	12.25	10.79

Table 2.2. KRITZ-2 experimentaluncertanities (Ref. 1)

Level measurements	1 or 2 mm (high temperature); 0.1 mm (room temperature)
Boron content	1 or 1.5 %
Temperature	1%
Radial fission rate distribution measurement:	1% (but may be higher)

Table 2.3. KRITZ-2 adjusted experimental results (Ref. 1)

Core	Rod Type	No. Rods	Pitch (mm)	dS/dW[a] (mm)	T (°C)	Boron (ppm)	B_z^2 (10^4 cm^{-2})	HK (mm)
2:1	U	44×44	14.85	81	20	217.9	14.75	652.8
					245	26.2	6.67	1015
2:13	U	40×40	16.35	113	20	451.9	8.04	959.7
					245	281.0	5.80	665.6
2:19	MOX	25×24	18.00	99	20	4.8	16.37	665.6
					245	5.2	7.15	1042

[a]dS is the distance from the bottom border of the bottom row of rods to the bottom border of the system. dW is the distance from the left border of the left row of rods to the left border of the system. They characterize the asymmetry of the position of the lattice in the moderator (see Figs. 1–6).

Table 2.4. Water properties used in the calculations (Ref. 4)

Temperature (°C)	Pressure (MPa)	Density (g/cm^3)	Condition
20	0.101325	0.998	Atmospheric pressure
245	3.6512	0.806	Saturation condition

2.2 CALCULATIONAL MODEL FOR KRITZ-2

The calculations were performed by means of the MCU-REA code, which is described in Appendix A. A two-dimensional (2D) calculational model was chosen for analysis. The model follows the specification given above and is limited to the inner part of the insert vessel. Calculations of a 3D model are planned for the future. B_z^2 buckling values were taken from the KRITZ-2 specifications. The boundary conditions are translation at the both top and bottom surfaces and black absorption at the other surfaces. The thickness of plutonium rod cladding was assumed to be 0.65 mm. U-234 was considered as 0.008 (wt% U-235)[1]. Thermal expansion was considered with coefficients: 7 x $10^{-6}/^{\circ}C$ for Zr, 11 x $10^{-6}/^{\circ}C$ for PuO_2 and UO_2 (from Ref. 1). Grids were not taken into account.

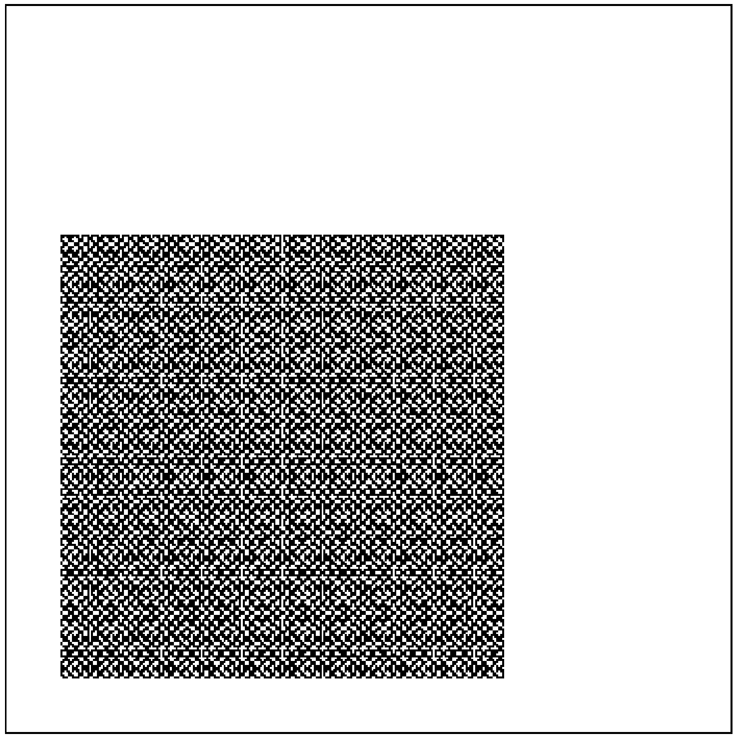

Fig. 2.1. Core 2:1 geometry model.

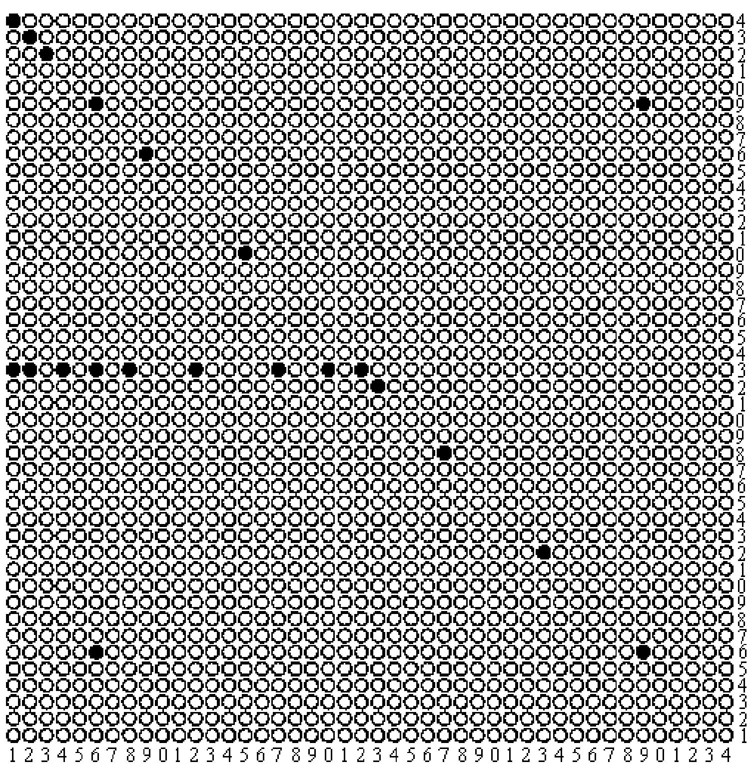

Fig. 2.2. Core 2:1 measured pin locations.
(Left bottom pin position is X = 1, Y = 1 according to Ref. 1)

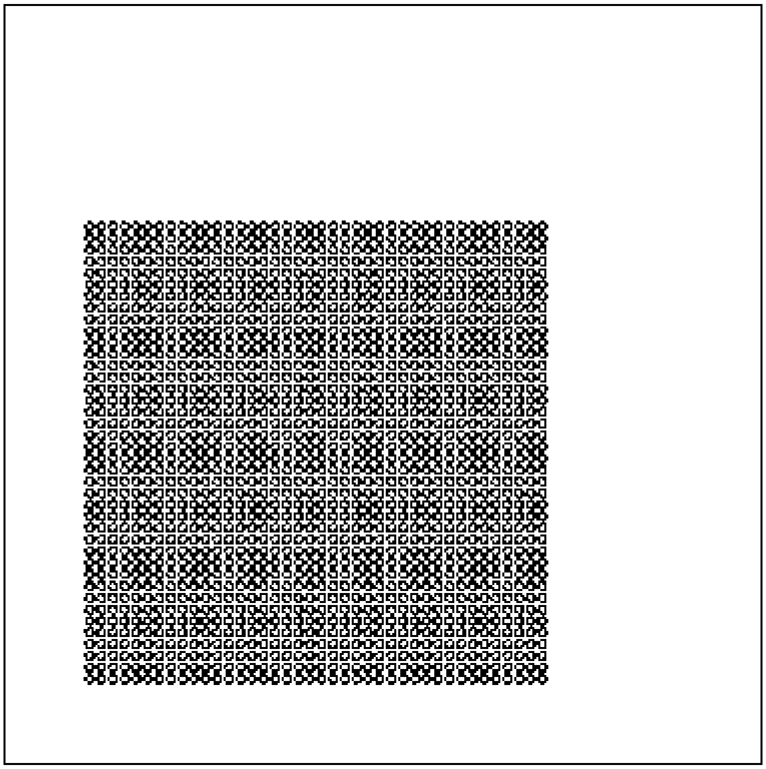

Fig. 2.3. Core 2:13 geometry model.

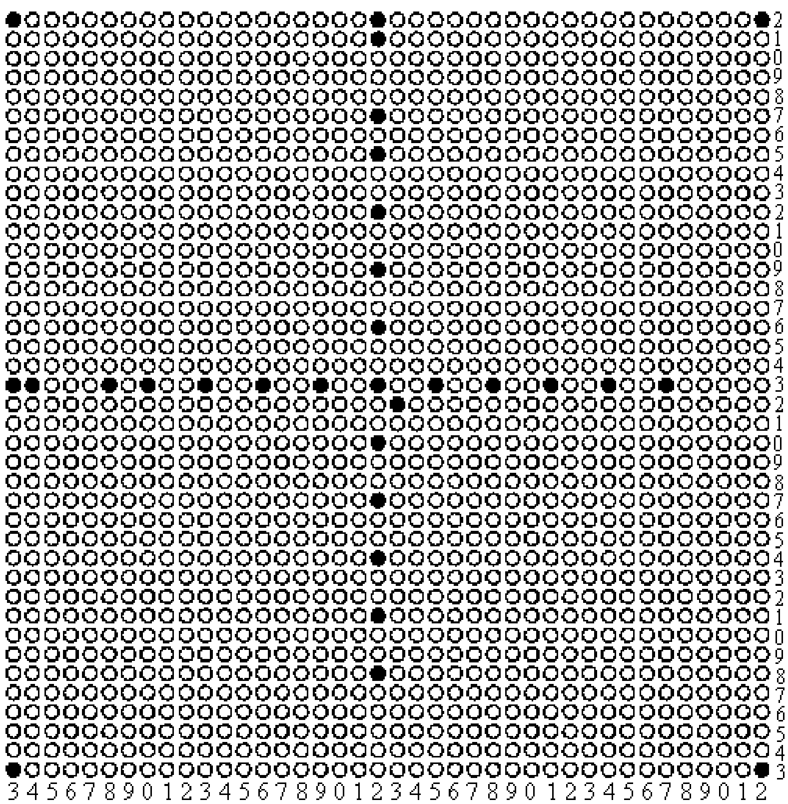

Fig. 2.4. Core 2:13 measured pins locations.
(Left bottom pin position is X = 3, Y = 3 according to [1])

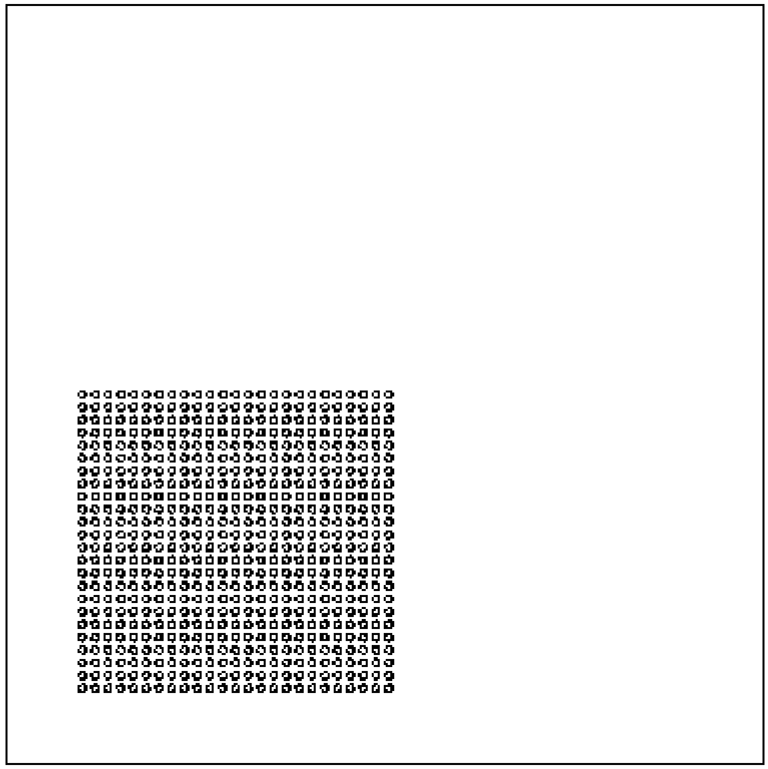

Fig. 2.5. Core 2:19 geometry model.

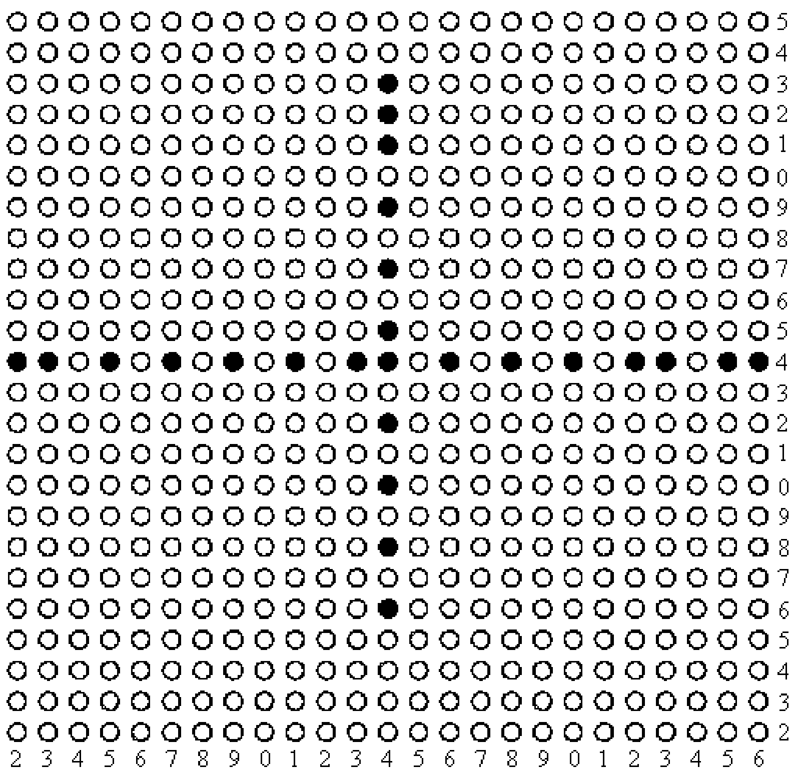

Fig. 2.6. Core 2:19 measured pin locations.
(Left bottom pin position is X = 2, Y = 2 according to [1])

3. CALCULATED RESULTS AND COMPARISON

For each variant 12 million histories were used in the calculation resulting in a statistical error for k_{eff} calculations of less than 0.0003, which is much less than the experimental error in k_{eff} of 0.0008 (Ref. 1). There was no detailed study of the experimental error (according to Ref. 1)) and the error was taken from the “earlier reports.” The statistical error of fission rate distribution calculations was less than 1% (1σ). Experimental error of radial fission rate distribution determination is 1% (1σ).

3.1 MULTIPLICATION FACTOR AND TOTAL TEMPERATURE EFFECT RESULTS

Results of k_{eff} calculations obtained by means of the MCU-REA code are presented in Tables 3.1–3.3 Results calculated by means of other codes (obtained from Ref. 5) are given in the same table. Maximal deviation from the experimental data for k_{eff} is 0.0067 (absolute value) for Core 2:1 245°C. The deviation does not exceed 0.0037 for the other five cores.

Table 3.2 presents total temperature effect values calculated by MCU-REA for three cores of KRITZ-2. The hot variant in this table is the cold variant heated isothermally up to 245°C with changed water density, but with the boron concentration from the cold variant, which is not the critical condition.

Table 3.3 presents the difference between k_{eff} values of the cold and hot KRITZ-2 cores. This value may serve as the characteristic of the precision of difference effect calculation (in this case—total temperature effect at isothermal heating). Resuls from MCU-REA and other codes[5] are given in the table. It is seen from this table that maximal uncertainty of MCU calculated value for total temperature effect is 100*(0.3/2.9) = 10%, which is quite satisfactory.

3.2 FISSION RATE DISTRIBUTION

Results of fission rate distribution calculations and the comparison with experimental data are given in Tables 3.4–3.9. Deviations of the calculational results from experimental data and graphical presentation of the fission rate in rods’ rows are given in Figs. 3.1–3.15.

Calculated values of fission rates are normalized in such a way that the sum of the calculated values equals the sum of the experimental values. The deviation reaches 8% for three rods (marked by bold font in Tables 3.4–3.8). However, these rods are marked in Ref. 1 as rods with measured fission rate “clearly outside the 1σ uncertainty ±1%.” Table 3.9 presents root mean square deviations (RMS) δ calculated by the formula:

$$\delta = 100\% * \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(\frac{MCU}{EXP} - 1\right)^2} \quad ,$$

Where N is the number of experimental points. The maximal root mean square deviation from the experiment for Core 2:1 245C is 3.6%. If the above-mention out-lying pins are excluded the RMS deviation is 3.2%. The value for the other five cores does not exceed 2.4%, which is comparable with statistical error of the calculations.

Table 3.1. Calculational results for KRITZ-2 cores from MCU-REA and other codes
(results for other codes from Ref. 5)

Zone	MCU-REA	CASMO	APOLLO Bz	WIMS6/JEF2 172	WIMS6/JEF2 69	APOLLO Br
2:1 20C	0.9963	1.0005	0.9993	0.9997	1.0003	0.9984
2:1 245C	0.9933	0.9983	0.9989	0.9986	0.9995	0.9980
2:13 20C	0.9972	1.0007	1.0013	1.0002	0.9995	1.0024
2:13 245C	0.9968	1.0015	1.0014	0.9988	0.9996	1.0001
2:19 20C	0.9975			1.0005	1.0014	
2:19 245C	0.9975			0.9979	0.9981	

Table 3.2. Total temperature effect obtained from MCU-REA calculations

Core	k_{eff} (Hot state)	k_{eff} (Cold state)	100*(hot-cold)
2:1	0.96734	0.9963	-2.90
2:13	0.96943	0.9972	-2.78
2:19	0.99847	0.9975	0.10

Table 3.3. Comparison of KRITZ-2 calculation results of hot-cold reactivity difference
(results for other codes from Ref. 5).

Core	% hot-cold					
	MCU-REA	CASMO	APOLLO Bz	WIMS6/JEF2 172	WIMS6/JEF2 69	APOLLO Br
2:1	-0.30	-0.22	-0.04	-0.11	-0.08	-0.04
2:13	-0.04	0.08	0.02	-0.14	0.01	-0.23
2:19	0.00	-	-	-0.26	-0.33	

3.3 FUEL HETEROGENEITY CALCULATIONS

Core 2:19 contains rods with vibro-compacted PuO_2UO_2 fuel. Such fuel consists of two materials: UO_2 matrix, which contains spherical grains of PuO_2 with 25 μm size. The total volume of the grains is 1.5% from the overall volume of the fuel with the grains are randomly positioned in the matrix. The replacement of the grain structure by homogeneous matter may lead to noticeable errors. The MCU-REA code allows the direct modeling of the neutron transport in the matter with double heterogeneity[6]. An infinite lattice of the cells of the Core 2:19 20°C was calculated by means of MCU-REA. Two variants of such lattice were calculated: homogeneous fuel and heterogeneous fuel, which is UO_2 matrix containing PuO_2 grains. The difference between k_{eff} values of these two variants characterizes the double heterogeneity effect. The results are given in Table 3.10. The value of the effect is 0.0067 in k_{eff} for such system. The double heterogeneity effect need be studied in more detail using full-scale models of KRITZ cores with PuO_2UO_2 fuel.

Table 3.4. MCU-REA calculational results of fission rate distribution for Core 2:1 at 245°C

N	Pin X	Pin Y	Fission rate (EXP)	Fission rate (MCU)	Deviation (MCU/EXP-1)
1	1	23	0.7133	0.7050	-0.0116
2	1	44	0.4309	0.4184	-0.0290
3	2	23	0.5899	0.5703	-0.0332
4	2	43	0.3431	0.3293	-0.0403
5	3	42	0.3140	0.3022	-0.0375
6	4	23	0.5689	0.5449	-0.0422
7	6	6	0.3763	0.3522	-0.0641
8	6	23	0.6231	0.6165	-0.0106
9	6	39	0.3954	0.3789	-0.0418
10	8	23	0.7074	0.6928	-0.0207
11	9	36	0.5653	0.5374	-0.0494
12	12	23	0.8602	0.8441	-0.0188
13	**15**	**30**	**0.7902**	**0.8588**	**0.0868**
14	17	23	0.9670	0.9837	0.0173
15	20	23	0.9868	1.0120	0.0255
16	22	23	1.0000	1.0336	0.0336
17	23	22	0.9965	1.0220	0.0256
18	27	18	0.9679	0.9797	0.0121
19	33	12	0.7071	0.7198	0.0179
20	39	6	0.3832	0.3757	-0.0195
21	39	39	0.4025	0.4118	0.0232

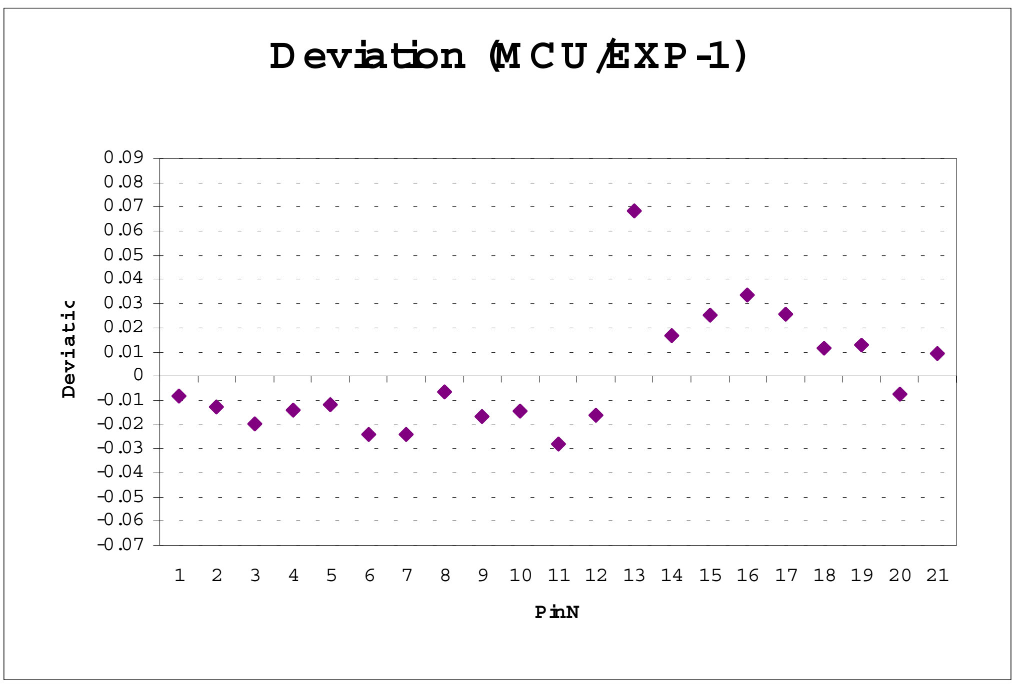

Fig. 3.1. Deviation of calculation from experiment for Core 2:1 at 245°C.

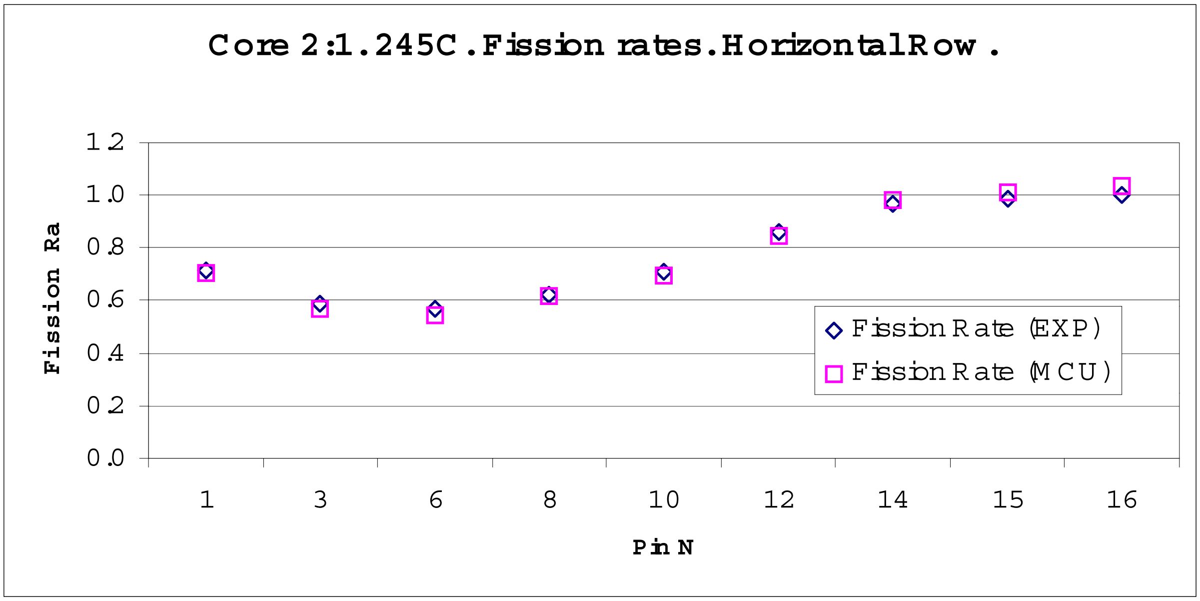

Fig. 3.2. Comparison of relative fission rates in horizontal row for Core 2:1. 245°C.

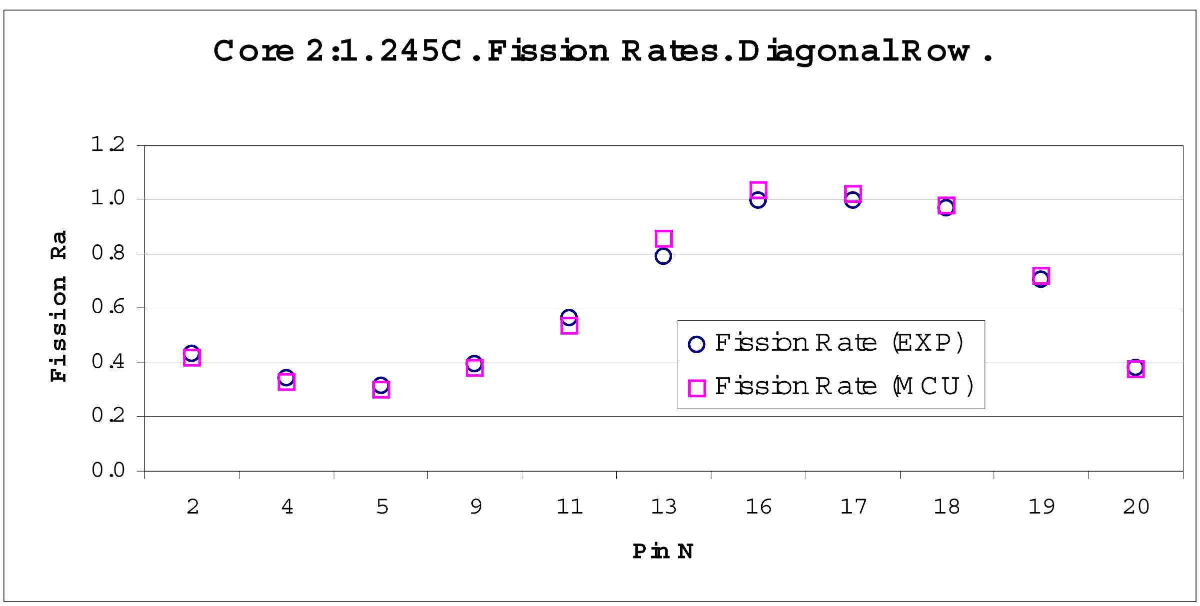

Fig. 3.3. Comparison of relative fission rates in diagonal row for Core 2:1. 245°C.

Table 3.5. MCU-REA calculational results of fission rate distribution for Core 2:13 at 20°C

N	Pin X	Pin Y	Fission rate (EXP)	Fission rate (MCU)	Deviation (MCU/EXP-1)
1	3	3	0.1570	0.1599	0.0184
2	3	23	0.4167	0.4132	-0.0084
3	3	42	0.1554	0.1572	0.0118
4	4	23	0.3846	0.3782	-0.0166
5	8	23	0.5573	0.5669	0.0172
6	10	23	0.6646	0.6615	-0.0046
7	13	23	0.8021	0.7953	-0.0085
8	16	23	0.9228	0.8981	-0.0268
9	19	23	0.9608	0.9668	0.0062
10	22	8	0.5653	0.5680	0.0047
11	22	11	0.7174	0.7156	-0.0025
12	22	14	0.8347	0.8230	-0.0141
13	22	17	0.9192	0.9142	-0.0055
14	22	20	0.9859	0.9618	-0.0244
15	22	23	0.9656	0.9644	-0.0012
16	22	26	0.9522	0.9612	0.0095
17	22	29	0.8907	0.9022	0.0129
18	22	32	0.8129	0.8069	-0.0074
19	22	35	0.6667	0.6727	0.0090
20	22	37	0.5647	0.5650	0.0005
21	22	41	0.3802	0.3945	0.0377
22	22	42	0.4032	0.4138	0.0264
23	23	22	1.0000	0.9891	-0.0109
24	25	23	0.9640	0.9814	0.0180
25	28	23	0.9256	0.9185	-0.0077
26	31	23	0.8196	0.8457	0.0319
27	34	23	0.7140	0.7141	0.0002
28	37	23	0.5711	0.5654	-0.0100
29	42	3	0.1536	0.1532	-0.0025
30	42	42	0.1547	0.1548	0.0005

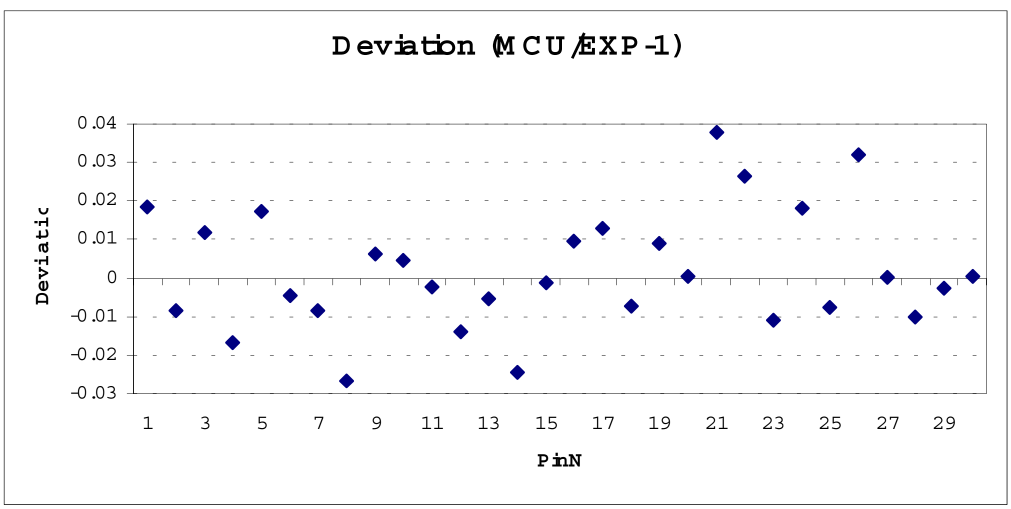

Fig. 3.4. Deviation of calculation from experiment for Core 2:13 at 20°C.

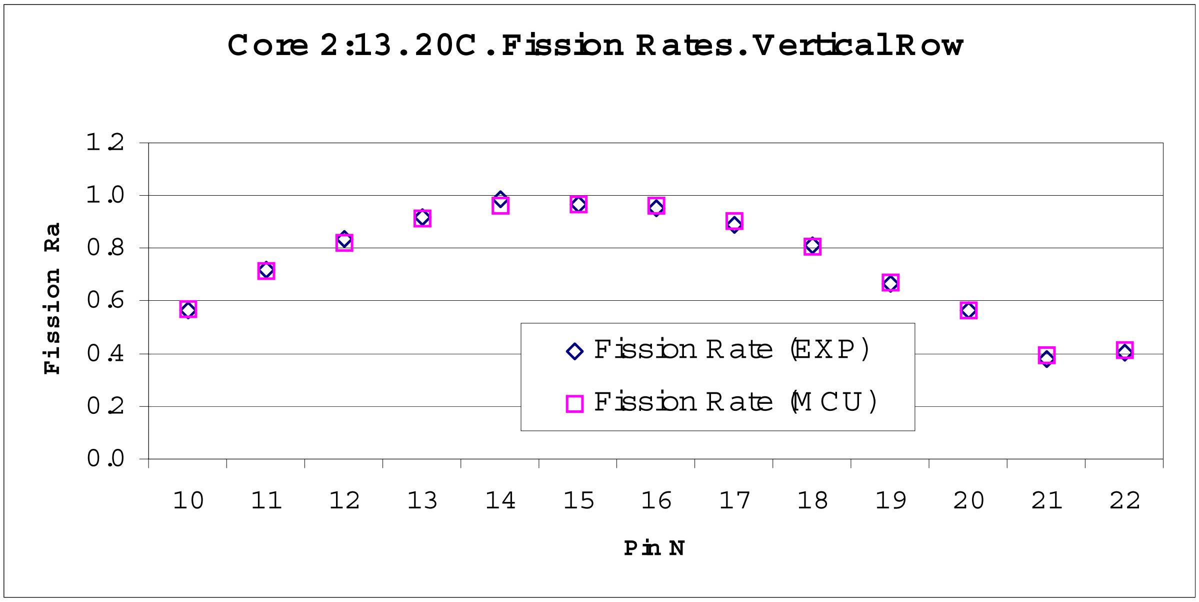

Fig. 3.5. Comparison of relative fission rates in vertical row for Core 2:13. 20°C.

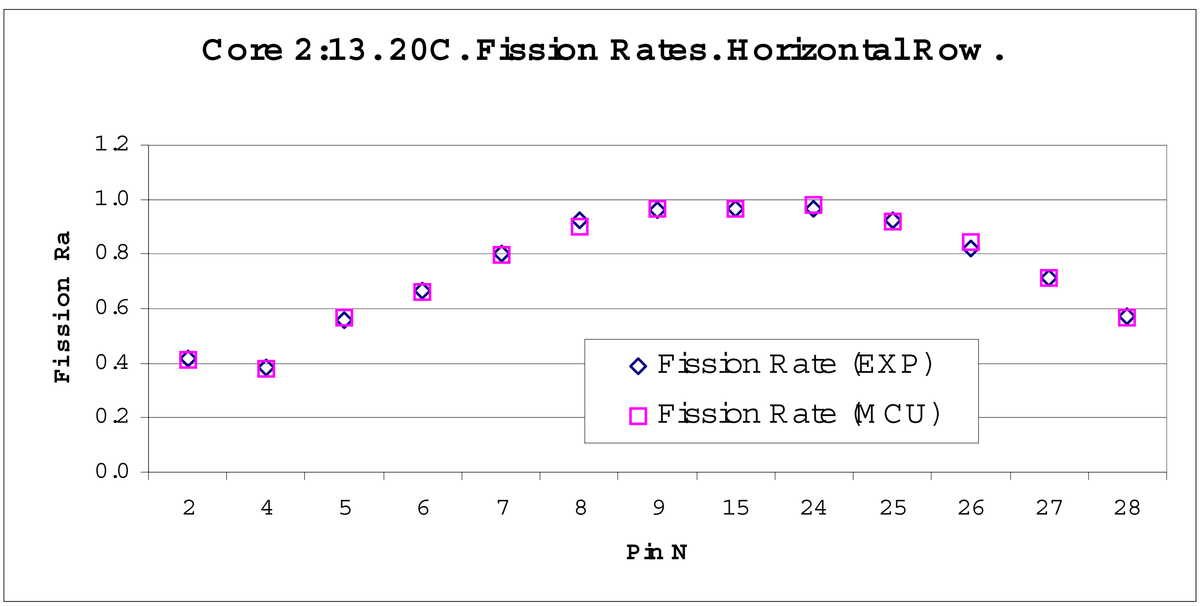

Fig. 3.6. Comparison of relative fission rates in horizontal row for Core 2:13. 20°C.

Table 3.6. MCU-REA calculational results of fission rate distribution for Core 2:13 at 245°C

N	Pin X	Pin Y	Fission rate (EXP)	Fission rate (MCU)	Deviation (MCU/EXP-1)
1	3	3	0.2601	0.2392	-0.0804
2	3	23	0.5427	0.5369	-0.0107
3	3	42	0.2563	0.2676	0.0443
4	4	23	0.4858	0.4763	-0.0196
5	8	23	0.5929	0.6006	0.0129
6	10	23	0.6903	0.6989	0.0125
7	13	23	0.8214	0.8090	-0.0151
8	16	23	0.8951	0.8887	-0.0071
9	19	23	0.9519	0.9482	-0.0039
10	22	8	0.6048	0.6017	-0.0051
11	22	11	0.7332	0.7439	0.0147
12	22	14	0.8563	0.8493	-0.0081
13	22	17	0.9145	0.9370	0.0246
14	22	20	0.9640	0.9512	-0.0133
15	22	23	0.9784	0.9771	-0.0013
16	22	26	0.9375	0.9596	0.0236
17	22	29	0.9085	0.9202	0.0129
18	22	32	0.8405	0.7929	-0.0566
19	22	35	0.6960	0.6922	-0.0055
20	22	37	0.5983	0.6120	0.0229
21	22	41	0.4763	0.4810	0.0098
22	22	42	0.5406	0.5518	0.0208
23	23	22	1.0000	0.9813	-0.0187
24	25	23	0.9628	0.9731	0.0107
25	28	23	0.9177	0.9235	0.0063
26	31	23	0.8218	0.8442	0.0272
27	34	23	0.7469	0.7314	-0.0208
28	37	23	0.5985	0.6076	0.0151
29	42	3	0.2555	0.2541	-0.0054
30	42	42	0.2609	0.2590	-0.0072

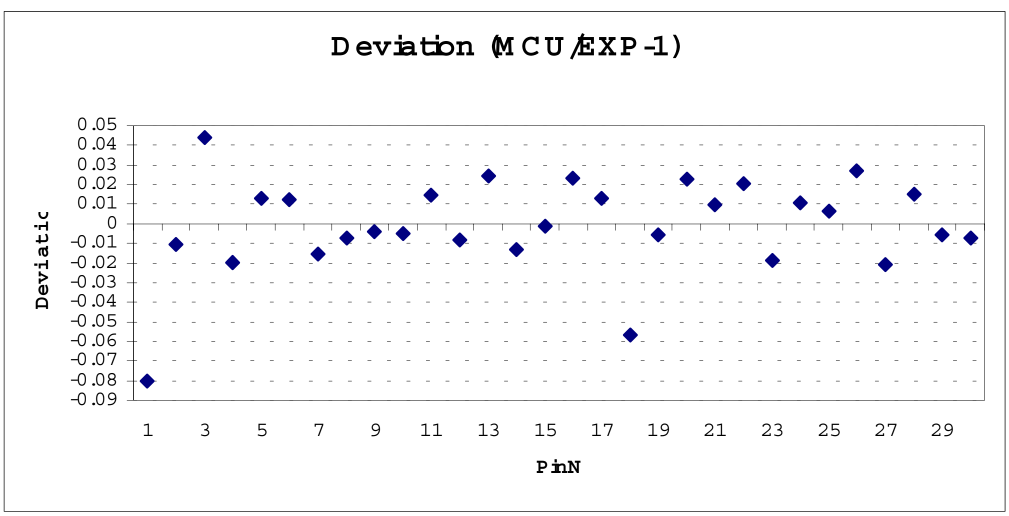

Fig. 3.7. Deviation of calculation from experiment for Core 2:13 at 245°C.

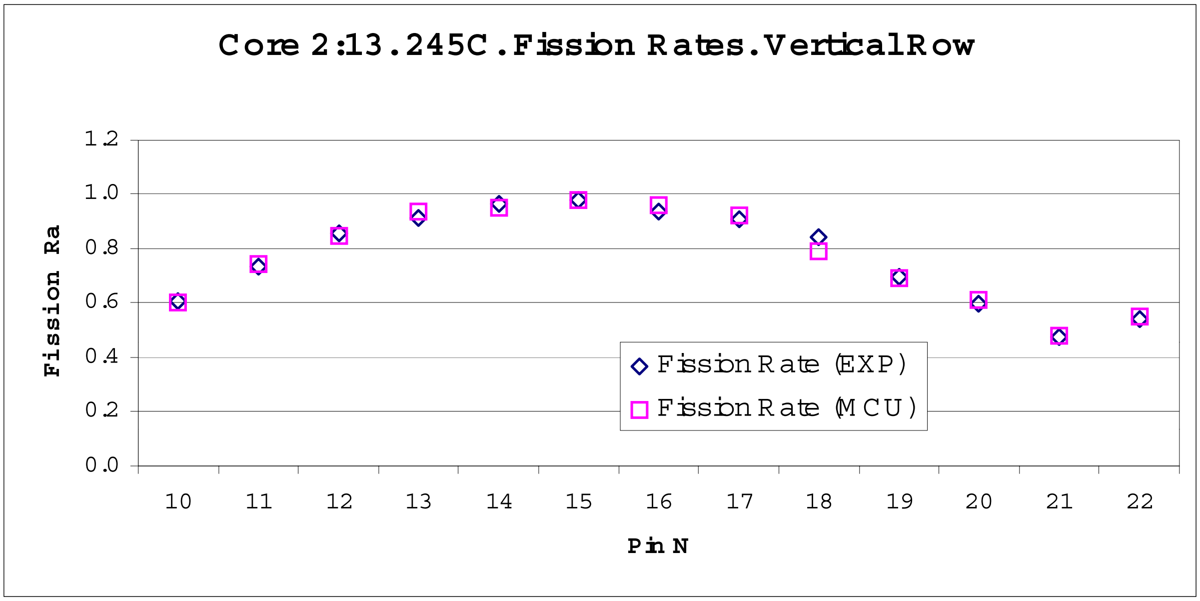

Fig. 3.8. Comparison of fission rates in vertical row for Core 2:13. 245°C.

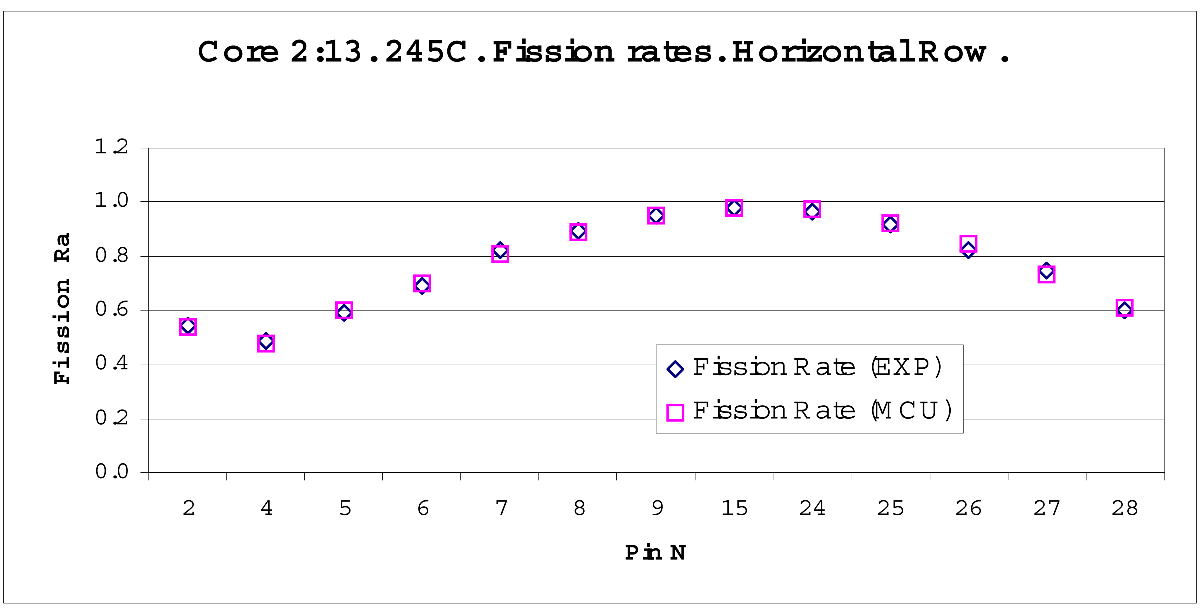

Fig. 3.9. Comparison of relative fission rates in horizontal row for Core 2:13. 245°C.

Table 3.7. MCU-REA calculated results of fission rate distribution for Core 2:19 at 20°C

N	Pin X	Pin Y	Fission rate (EXP)	Fission rate (MCU)	Deviation (MCU/EXP-1)
1	2	14	0.5571	0.5517	-0.0096
2	3	14	0.5360	0.5274	-0.0160
3	5	14	0.6412	0.6360	-0.0081
4	7	14	0.7648	0.7823	0.0229
5	9	14	0.8688	0.8731	0.0050
6	11	14	0.9731	0.9616	-0.0119
7	13	14	0.9774	0.9949	0.0179
8	**14**	**6**	**0.7679**	**0.7309**	**-0.0482**
9	14	8	0.8493	0.8539	0.0054
10	14	10	0.9275	0.9354	0.0085
11	14	12	0.9772	0.9726	-0.0047
12	14	14	1.0000	0.9964	-0.0036
13	14	15	0.9970	0.9994	0.0024
14	14	17	0.9367	0.9348	-0.0021
15	14	19	0.8522	0.8467	-0.0064
16	14	21	0.7369	0.7375	0.0008
17	14	22	0.6641	0.6652	0.0016
18	14	23	0.5941	0.5948	0.0012
19	16	14	0.9591	0.9695	0.0108
20	18	14	0.9344	0.9285	-0.0063
21	20	14	0.8359	0.8464	0.0126
22	22	14	0.7063	0.7043	-0.0029
23	23	14	0.6406	0.6431	0.0039
24	25	14	0.5265	0.5253	-0.0024
25	26	14	0.5580	0.5705	0.0224

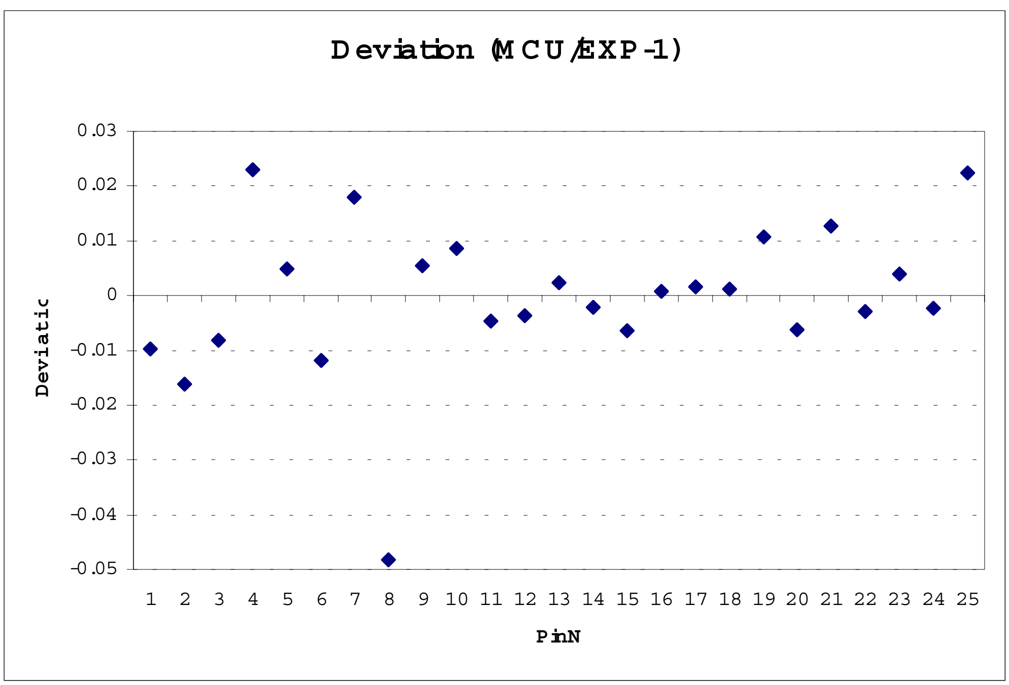

Fig. 3.10. Deviation of calculation from experiment for Core 2:19 at 20°C.

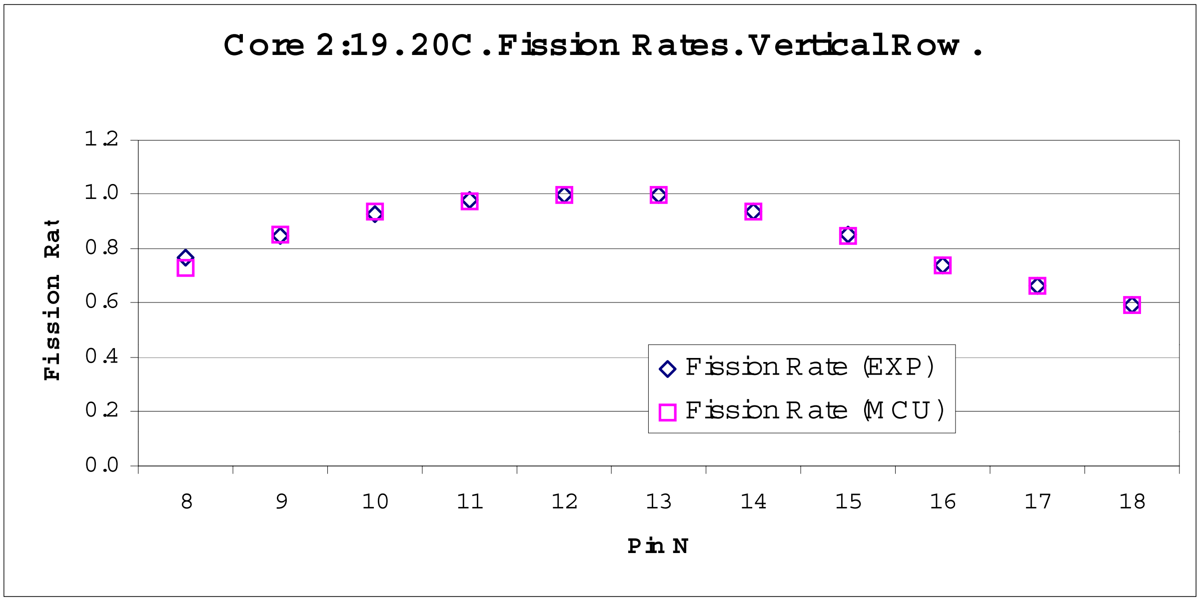

Fig. 3.11. Comparison of relative fission rates in vertical row Core 2:19. 20°C.

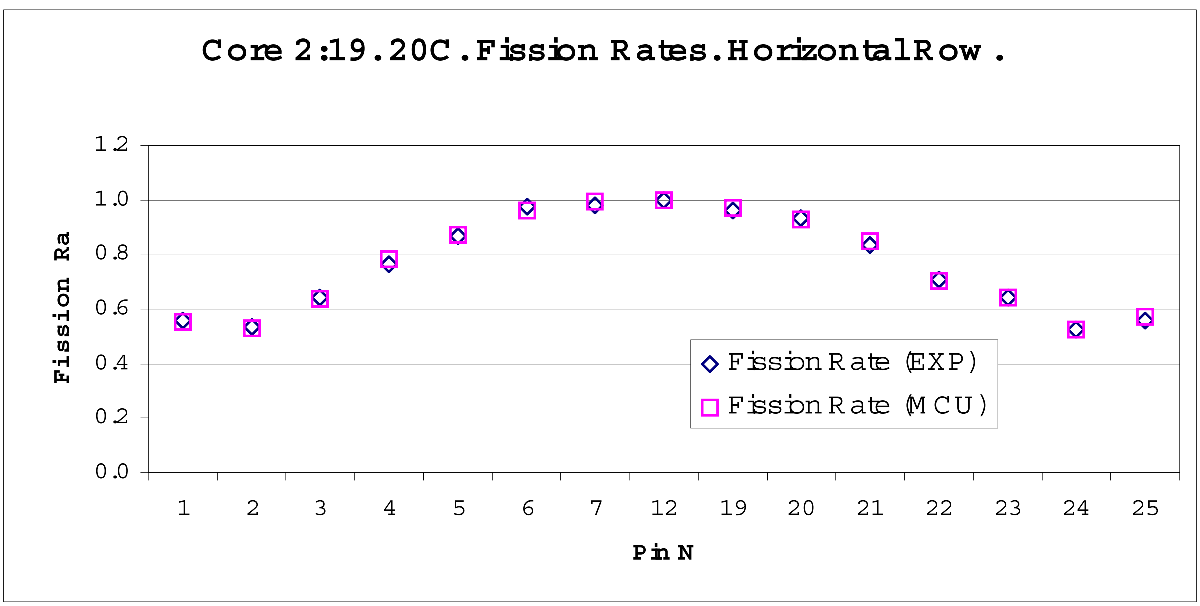

Fig. 3.12. Comparison of relative fission rates in horizontal row for Core 2:19 at 20°C.

Table 3.8. MCU-REA calculational results of fission rate distribution for Core 2:19 at 245°C

N	Pin X	Pin Y	Fission rate (EXP)	Fission rate (MCU)	Deviation (MCU/EXP-1)
1	2	14	0.6953	0.6655	-0.0429
2	3	14	0.5985	0.5936	-0.0081
3	5	14	0.6535	0.6600	0.0100
4	7	14	0.7644	0.7716	0.0094
5	9	14	0.8583	0.8584	0.0002
6	11	14	0.9297	0.9295	-0.0002
7	13	14	0.9486	0.9536	0.0052
8	14	6	0.7354	0.7306	-0.0065
9	14	8	0.8216	0.8215	-0.0002
10	14	10	0.8917	0.8975	0.0065
11	14	12	0.9384	0.9470	0.0092
12	**14**	**14**	**1.0000**	**0.9512**	**-0.0488**
13	14	15	0.9459	0.9472	0.0014
14	14	17	0.9230	0.9092	-0.0149
15	14	19	0.8329	0.8388	0.0070
16	14	21	0.7277	0.7354	0.0105
17	14	22	0.6856	0.6839	-0.0025
18	14	23	0.6435	0.6307	-0.0198
19	16	14	0.9217	0.9488	0.0294
20	18	14	0.9015	0.8910	-0.0116
21	20	14	0.8170	0.8202	0.0039
22	22	14	0.7045	0.7244	0.0283
23	23	14	0.6511	0.6570	0.0090
24	25	14	0.6054	0.6139	0.0140
25	26	14	0.6898	0.7044	0.0211

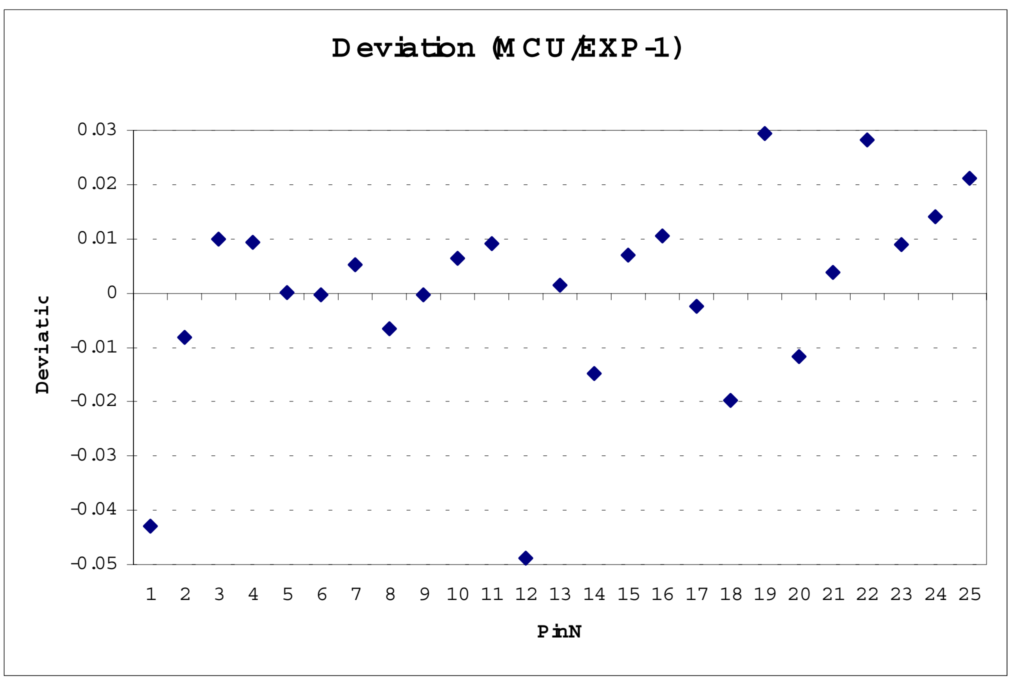

Fig. 3.13. Deviation of calculation from experiment for Core 2:19 at 245°C.

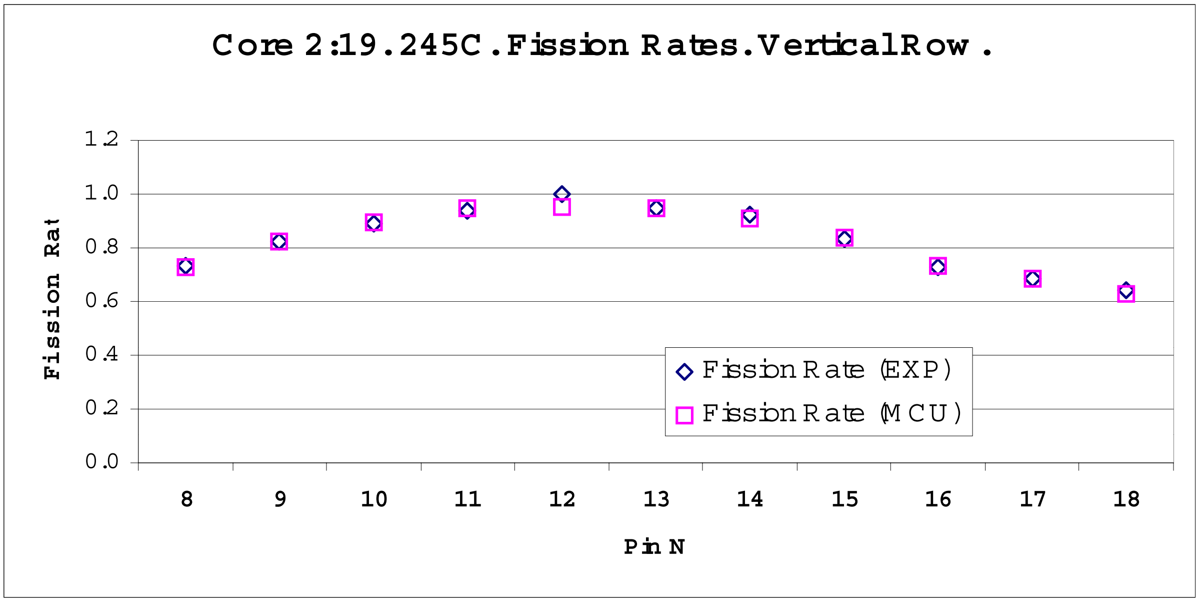

Fig. 3.14. Comparison of relative fission rates in vertical row for Core 2:19. 245°C.

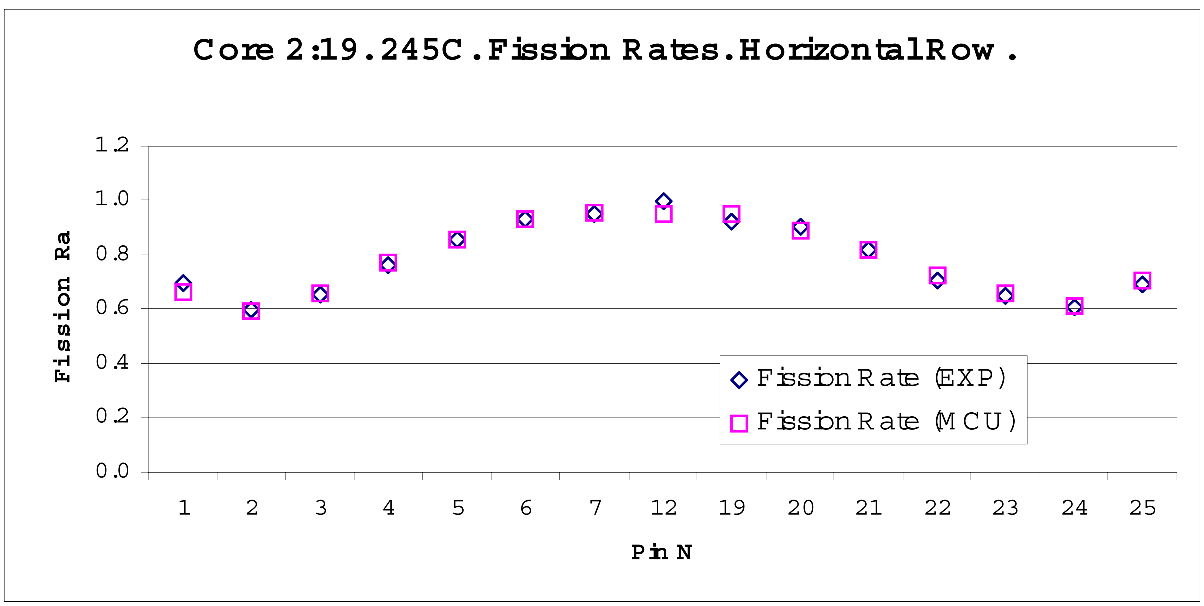

Fig. 3.15. comparison of relative fission rates in horizontal row for Core 2:19. 245°C.

Table 3.9. Root Mean Square deviation of calculated relative fission rates from experimental values

	Core/Temperature				
	2:1, 245°C	2:13, 20°C	2:13, 245°C	2:19, 20°C	2:19, 245°C
RMS Dev.	0.0363 (0.0318)[a]	0.0182	0.0242	0.0138 (0.0101)[a]	0.0179 (0.0153)[a]

[a]Rods with measured values labeled as "clearly outside 1σ" in Ref. 1 excluded.

Table 3.10. Heterogeneity effect calculated with MCU-REA as k_{eff} for a cell of the 2:19, 20°C core

Case	k_{eff}
Homogenous mixture	1.2025
Heterogeneous—25 μm grains	1.1958

4. CONCLUSIONS

This report presents results of KRITZ-2 experiments calculations performed using Russian MCU-REA code. The calculations were performed using 2D model with given experimental axial buckling.

Six experiments (Cores 2:1, 2:13, 2:19 at temperatures 20 and 245°C) have been calculated. Maximal deviation from the experiment for k_{eff} is 0.0067.

Maximal for 6 cores root mean square deviation of calculated fission rates from the experimental ones is 0.0363. It is 0.0318, if the rods with measured values "clearly outside the 1σ uncertainty ±1%" [1] are not taken into account.

The results of calculations are in good agreement with the experimental data.

The double heterogeneity effect has been evaluated for infinite lattice of cells of Core 2:19 20°C. The value of the effect is 0.0067 in k_{eff} for such a system.

The following work seems to be necessary:

1. Creation of 3D models for each of six configurations of the core. Calculations of the models by means of MCU. Determination of the calculational value of the critical buckling B_z.
2. Comparative analysis of the 2D and 3D calculations.
3. Study of MOX fuel double heterogeneity influence on k_{eff}.
4. Specification of experimental error considering technological uncertainty in fuel enrichment, dimensions, etc., and not only in the water level.
5. Specification of the cladding thickness for MOX rods.
6. Specification of isotopic composition of the cladding.

REFERENCES

1. Erik Johansson, *Data and Results for KRITZ Experiments on Regular H_2O Fuel Pin Lattices at Temperatures up to 245°C*, Studsvik Report, Studsvik AB, Sweden (1990).
2. M. A. Kalugin, L. V. Maiorov "ALIGR Technique for Reactor Fuel Burn-Up Calculations Using Monte-Carlo Method," *Trans. Am. Nuc. Soc.*, **79**, pp. 312–313 (1998).
3. E. A. Gomin, L. V. Maiorov, "The MCU Monte-Carlo Code for 3-D Depletion Calculation," *Proc. of the International Conference on Mathematics and Computation, Reactor Physics and Environmental Analysis in Nuclear Applications,* M&C'99-Madrid, Madrid, Spain, 1999, 16.2-12.
4. NIST WebBook, *Thermophysical Properties of Fluid Systems*, http://webbook.nist.gov/chemistry/fluid
5. *The JEF 2.2 Nuclear Data Library*, JEFF Report 17, OECD Nuclear Energy Agency (April 2000).
6. M. Gurevich, V. Brizgalov "The neutron flux density calculation by Monte-Carlo code for the double heterogeneity fuel," *Proc. of the Int-l Conf. on Reactor Phys. and Reactor Comp.*, Tel-Aviv, Jan. 23–26, 1994, p. 190–196.

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;
- $S(\alpha,\beta)$ 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.

Comments on *KRITZ-2 Experimental Benchmark Analysis With MCU-REA* by J. Gehin, Oak Ridge National Laboratory

ORNL Review Comments

1. These calculations are based on the experiment specifications given in Ref. 1 of the report. During the course of this work with the OECD/NEA TFRPD, a new set of specifications was developed by ORNL and used as the basis for the TFRPD KRITZ-2 benchmark. These specifications included a few details that were not specified in Ref. 1. The calculational model discussed in this report differs slightly from TFRPD specifications. These deviations from the specifications are minor and do not significantly affect the results. These additional details include such things as ^{241}Am that results from decay of ^{241}Pu, precise specifications of the temperatures rather than using the results adjusted to 20°C and 245°C, and the MOX pin clad thickness discussed in item 3 below.

2. The TFRPD benchmark includes variants for cell calculations for each type of rod that can be used in the benchmarking procedure to isolate difference between codes and libraries. These cell calculations have not been performed with MCU-REA.

3. The value for the canning thickness in Table 2.1 is indicated a "?" or unknown. Actually the fuels for the MOX rods were produced by vibrocompaction that resulted in no gap. As a result, the canning thickness is simply the difference of the canning outside radius and the pellet radius, which is 0.67 mm. This value is insignificantly different than the value of 0.65 used in these calculations as indicated on page 4.

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