DETERMINISTIC AND MONTE CARLO CALCULATIONS FOR THE BUDAPEST RESEARCH REACTOR

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ABSTRACT

The upgraded VVR-SM type (Russian design) Budapest Research Reactor using 36% enriched uranium serves both research and practical applications. As a by-product of the experimental methods used in the field of the neutron activation analysis a unique opportunity arose for benchmarking the neutron physical algorithms against measurements. The two dimensional MULTICELL transport code was tested against foil activity measurements and Monte Carlo calculations. The comparison indicated the need of three-dimensional treatment even in case of calculating local spectrum characteristics. The application of the few-group spectrum calculated with the DIF3D diffusion code improved the accuracy of the calculated reaction rate ratios.

INTRODUCTION

The reconstructed and upgraded VVR-SM type research reactor in Budapest began its regular operation in November 1993. Besides improved reactor safety the power of the Budapest Research Reactor was increased to 10 MW. The maximum achievable thermal neutron flux is about $2.5\ 10^{14}$ cm^{-2}s^{-1}.

The reactor serves for basic and applied research (condensed matter, radiochemistry, biological irradiations, reactor technology), technological and commercial applications (production of radioisotopes, neutron radiography, activation analysis, pressure vessel surveillance) furthermore education and training: (undergraduates, PhD students, IAEA training courses, public information).

THE BUDAPEST RESEARCH REACTOR

The Budapest Research Reactor is a pool type reactor, moderated and cooled by light water. The fuel is composed of 36% enriched uranium and aluminium. The clad is made of aluminum.

The fuel elements contain two concentric cylindrical fuel plates and a surrounding hexagonal one (see Figure 1).

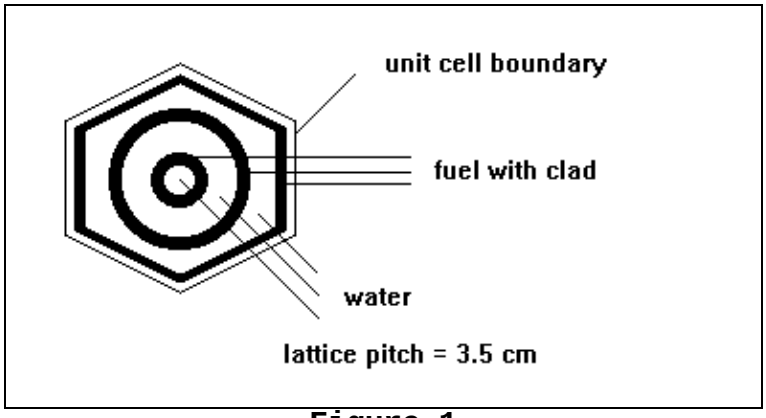

Figure 1
VVR-SM fuel geometry

The fuel elements, the control rods, the inner irradiation channels and beryllum displacers are arranged into a hexagonal lattice with 3.5 cm pitch. Irradiations may be carried out by inserting samples into more than 40 special vertical channels and six flux traps with various geometrical and spectral parameters. The reactor has 10 horizontal beam tubes (8 radial and 2 tangential ones). The core is enclosed with solid ^{9}Be reflector.

THE FOIL ACTIVITY MEASUREMENTS

A unique opportunity arose for benchmarking the neutron physical algorithms against measurements as a by-product of the experimental methods used in the field of neutron activation analysis.

Since its introduction in 1976 [1], the use of zirconium has received wide interest mainly in absolute neutron activation analysis. Some of the outstanding characteristics of zirconium:
- When measuring F_{th}/F_{epi} flux ratios the ^{94}Zr-^{96}Zr pair gives better precision than any other monitor combination due to the largest known difference in relevant I_0/S_0 ratios.
- Due to the low thermal and epithermal neutron absorption cross sections thin foils require no neutron self-shielding corrections thus considered to be infinitely dilute.

For monitoring the fast flux the (n,p) reaction of the ^{58}Ni isotope was selected. The neutron capture in ^{176}Lu and ^{197}Au was utilized at only few measuring positions.

The reaction rates of the following measured reactions were used in the comparison:
^{94}Zr(n,?)^{95}Zr, ^{96}Zr(n,?)^{97}Zr/^{97m}Nb, ^{58}Ni(n,p)^{58}Co, ^{176}Lu(n,?)^{177}Lu and ^{197}Au(n,?)^{198}Au.

The monitors in the form of foils and wires were placed into 23 inner irradiation channels at five axial positions and 2 irradiation channels were used in the beryllum reflector. After a 12 hour irradiation the selected gamma lines of the induced isotopes were measured with the help of Ge-Li gamma-ray spectrometers. On the basis of the measured peak areas, the detector efficiency and calculating the isotopic chains during irradiation, cooling and measurement, the reaction rates of the monitor isotopes can be evaluated. As the above reaction rates were measured at the same positions, the measured and calculated reaction rate ratios can be compared even on the level of the multigroup MULTICELL calculations. The absolute values of the reaction rates corresponding to the reactor power are comparable only by using detailed 3D calculations for the whole core.

THE KARATE MULTICELL CODE

The MULTICELL code which is integrated into the KARATE program system uses the multicell collision probability method [2] which has been applied for hexagonal lattices [3]. The multigroup calculations are performed in 35 epithermal and 35 thermal groups on the basis of a cross section library generated from the ENDF/B-IV file. For the calculation of the shielded cross sections of ^{235}U, ^{238}U and ^{239}Pu the equivalence theory is used [4] or an ultra fine energy group transport method is applied. In the thermal groups the Doppler broadening of ^{240}Pu is calculated, the shielding effects are taken into account explicitly. To get multicell CP's which pertain to the i'th region of the A'th cell type, the following assumptions are made: The distribution of the incoming neutrons on the boundary of the cells is isotropic and can be made smooth (i.e. the neutron exchange between the cells can be calculated from their contact ratios). For the calculation of the black collision probabilities of the individual cells the cylindrization can be used.The flux distribution is calculated using the CP equations of the MGCP program. The B-1 equations are solved optionally to take into account the leakage in asymptotic approximation. The code calculates the transmutation of fuel regions, too.

The MULTICELL code has been developed originally for calculating VVER fuel assemblies. It was tested against measurements performed on ZR-6 lattices [5]. As the VVR-SM fuel elements are radically different from the VVER cells, there is a need to assess the adequacy of the MULTICELL code for this new situation. The accuracy of the MULTICELL code for the research reactor has been tested by comparative Monte Carlo calculations.

MONTE CARLO CALCULATIONS

The Monte Carlo calculations were made by the MCNP4A code [6]. The power distributions and the reaction rates were taken from criticality calculations. To achieve the desired accuracy, in case of the power distribution about one million, in the case of the reaction rates about fourteen million neutron histories were used. The large number of neutron histories in the second case was necessary because of the sharp resonances in the (n,?) cross sections of ^{96}Zr and ^{94}Zr, and it took about one week on an IBM RISC 6000 machine. For the sake of the consistent comparison with the MULTICELL calculations, the cross sections for ^{94}Zr, ^{96}Zr, ^{58}Ni and ^{176}Lu were derived from ENDF/B-VI by the NJOY code and the cross sections for all the other materials were taken from ENDF/B-IV based MCNP4A libraries. For the same reason the outermost hexagonal shell of the fuel element was replaced by a cylindrical one.

Five different configurations were investigated by the MCNP4A to compare the results with MULTICELL calculations. In these configurations the fuel elements, absorber rods, water holes and the monitor were positioned into a hexagonal array and this array was bounded by a hexagon with horizontal planes on top and bottom. Reflective boundary conditions were prescribed on each boundary planes. K_{inf} and the power distributions were calculated for all the cases. The investigated configurations are as follows:

Case 1: An absorber rod in the centre surrounded by 18 fuel elements.

Case 2: An absorber rod in the centre surrounded by 36 fuel elements.

Case 3: An absorber rod in the centre surrounded by 30 fuel elements and by 6 water holes

placed with 30^0 symmetry among the fuel elements.

Case 4: A monitor cell in the centre surrounded by 30 fuel elements and by 6 water holes placed with 30^0 symmetry among the fuel elements. The reaction rates in the monitor wire were also calculated in case 4 and 5.

Case 5: Similar to configuration No. 4, but surrounded by a layer of cells filled with ^{9}Be.

The 30^o sector of these configurations with the MCNP4A power distributions and the MULTICELL relative deviations[%] can be seen in Figures 2-6. The applied notations:

FU : Fuel cells
MO : Monitor cell
WA : Cell containing water and absorber rod guide tube
AB : Cell with inserted absorber rod
BE : Cell containing beryllium

The leftmost cell is the centre of the considered configuration. The bottom and the right side symmetry lines halve the cells.

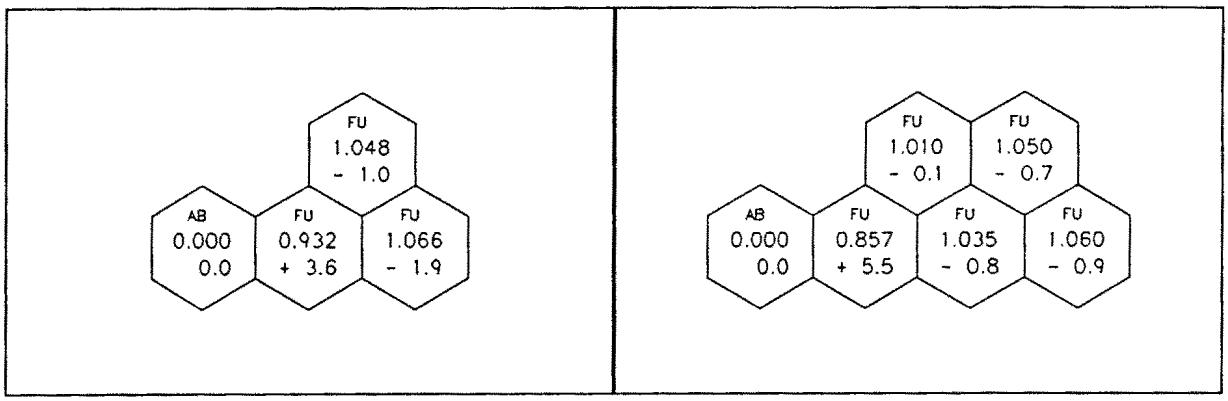

Figure 2
Relative power , case 1

Figure 3
Relative power , case 2

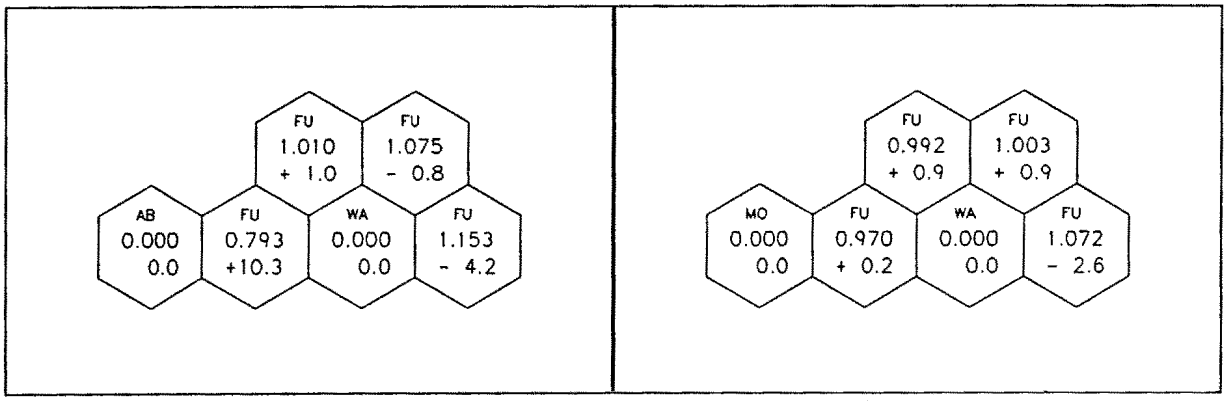

Figure 4
Relative power , case 3

Figure 5
Relative power , case 4

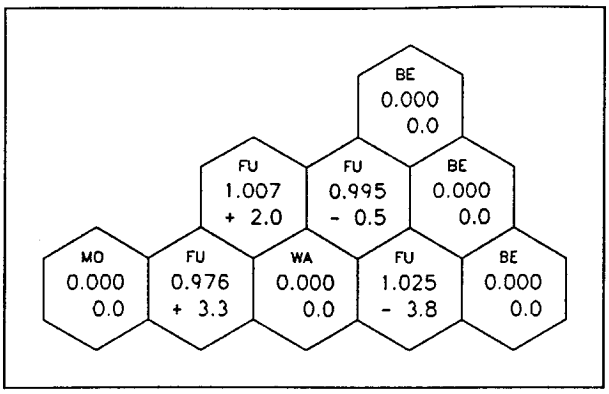

Figure 6 Relative power, case 5

The typical relative error of the power density from MCNP4A in the 1st case is 0.005, in the 2nd case is 0.01 and it is 0.001 for the last 3 cases. The maximum deviation from the reference MCNP4A relative power is observed in case 3, near the strongly absorbing B_4C rod with 2.5 cm diameter. The reason of the difference is probably the application of the flat flux approximation along the periphery of the cylindrized cells for this wide lattice pitch.

The results of the k_{inf} calculations are summarized and compared with MULTICELL in Table 1. The relative errors (one standard deviation divided by the mean) of the MCNP4A results are shown parallel with the calculated values of the multiplication factor.

configuration	k MCNP4A		k MULTICELL	$\Delta k/k$ %
1	1.2330	0.0009	1.2128	-1.7
2	1.4577	0.0008	1.4450	-0.9
3	1.3783	0.0006	1.3659	-0.9
4	1.5389	0.0001	1.5527	+ 0.9
5	1.5987	0.0001	1.6048	+ 0.4

Table 1
Comparison of k_{inf} values

The MULTICELL k_{inf} values except the 1st extremely rodded case seem to be satisfactory.

The reaction rates are normalized by the $^{58}Ni(n,p)$ reaction, which has the lowest relative error. The reaction rate ratios for configuration 4 are given in Table 2.

Reaction	MCNP4A		MULTICELL	?r/r %
^{94}Zr(n,?)	0.878	0.01	0.732	-17
^{96}Zr(n,?)	5.93	0.05	5.183	-13
^{176}Lu(n,?)	40401.	0.005	33956.	-16

Table 2
Reaction rate ratios, case 4

The same data for configuration 5 can be found in Table 3.

Reaction	MCNP4A		MULTICELL	?r/r %
^{94}Zr(n,?)	1.001	0.01	0.780	-22
^{96}Zr(n,?)	6.525	0.05	5.415	-17
^{176}Lu(n,?)	47723.	0.005	37647.	-21

Table 3
Reaction rate ratios, case 5

The MULTICELL reaction rates normalized by the ^{58}Ni(n,p) reaction show systematic underprediction compared to the MCNP4A results. The cause of the difference is not obvious. According to the expectations, normalzing by any of the isotopes indicated in the tables, the highest deviations do not exceed 6% for allbut the ^{58}Ni isotope, where the overprediction is about 20%. From now on we normalze with the ^{94}Zr(n,?) reaction rate which is available at all the measured positions.

COMPARING THE MULTICELL CALCULATIONS WITH THE MEASUREMENTS

Several 2D calculations have been made with the MULTICELL code to simulate the measured reaction rate ratios. The geometry of calculating the reaction rates for the monitor at the VVR-SM position No. 408 can be seen in Figure 7. The new notations:

FT : Flux trap (three adjoining water cells)

BD : Beryllium displacer (cellcontaining beryllum and water)

As the MULTICELL code uses periodic boundary condition at symmetry lines which halve the peripheralcells, the cells at the opposite sides of the outermost string are identical.

The measured and calculated reaction rates normalized with the ^{94}Zr(n,?) reaction can be found in tables 4-6 for positions 312, 408 and 342. The dry irradiation channelat position 312 has a hard spectrum while in positions 342 and 408 which are at the edge and at the corner of the core the spectrum is much softer.

Reaction	Measurement		MULTICELL/M-DIF3D	?r/r [%]
^{58}Ni(n,p)	1.392	0.010	1.424 1.280	+ 2.3 -8.0
^{96}Zr(n,?)	6.548	0.019	8.044 6.584	+ 22.8 + 0.5

Table 4
Reaction rate ratios, position 312

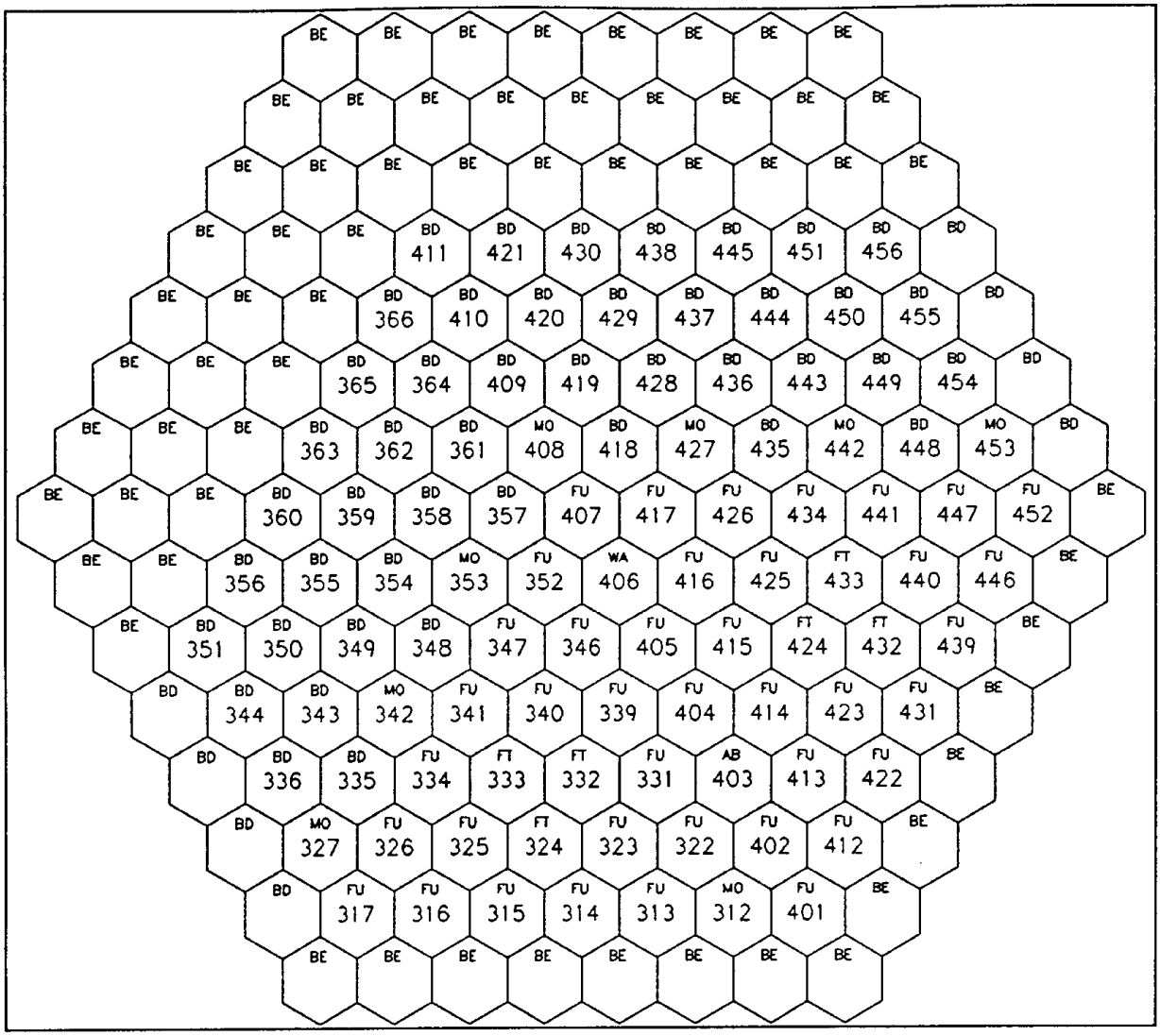

Figure 7 Map for the reaction rate calculations at position No. 408

Reaction	Measurement		MULTICELL,M-DIF3D	?r/r [%]
^{58}Ni(n,p)	0.3995	0.011	0.3511 0.415	-12.1 + 3.9
^{96}Zr(n,?)	3.471	0.019	4.193 3.577	+ 20.8 + 3.0

Table 5. Reaction rate ratios, position 408

Reaction	Measurement		MULTICELL,M-DIF3D	?r/r [%]
^{58}Ni(n,p)	0.6188	0.006	0.5213 0.5967	-15.7 -3.6
^{96}Zr(n,?)	4.387	0.008	4.502 4.181	+ 2.6 -4.7
^{176}Lu(n,?)	56819.	0.006	64307. 64282.	+ 13.2 + 13.1
^{197}Au(n,?)	2537.	0.005	2611. 2519.	+ 2.9 -0.7

Table 6. Reaction rate ratios, position 342

Studying Tables 4-6, one can not observe the same tendency seen at the comparative Monte Carlo calculations. Some methodic calculations were also carried out to clarify the drawbacks to the current procedure.

a, MULTICELL is a 2D code, so can not represent axial phenomena, e.g. partially inserted control rods. The effect of rod insertion in the second neighbourhood of the monitor results in 4% difference in the reaction rate ratio of ^{96}Zr/^{94}Zr.

b, Because of the limited number of cells, the calculated domain is smaller than the whole core. The above reaction rate ratio is sensitive to the changes in the content of the outermost ring in the MULTICELL geometry. The deviation is about 4-7%.

The effect of the above two symptoms is comparable to the observed differences. Fortunately the monitor cell averaged few-group constants of foils remain nearly untouched, so a 3D diffusion calculation of the whole reactor was promising. The calculation was carried out using the well known DIF3D code [7] in 7 energy groups. The reaction rate ratios were evaluated with the spectrum of DIF3D at the positions of measurements. The results can be seen in Tables 4-6. With this method drawbacks a, and b, were removed, the calculated reaction rate ratios are in better agreement with the measurements.

SUMMARY AND CONCLUSIONS

The accuracy of the KARATE MULTICELL code for the VVR-SM type research reactor was tested by comparative Monte Carlo calculations. Some discrepancies were observed in the calculated reaction rate ratios of monitor foils. Comparing MULTICELL results to measurements does not show the same tendency, but deviations occur in roughly the same range. Some methodic drawbacks of the applied procedure have been enlightened. 3D diffusion method was applied even for the calculation of the reaction rate ratios. This procedure gives better agreement with the measurements.

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