KRITZ-2 BENCHMARK CALCULATIONS USING DIFFERENT NUCLEAR DATA LIBRARIES

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ABSTRACT

A set of KRITZ-2 experiments with light water moderated lattices with uranium rods and mixed-oxide rods, at room and elevated temperatures, were performed in the early 1970's. Using the results of these experiments, an international benchmark was developed and launched by the OECD/NEA in co-operation with ORNL. This paper presents the results obtained from two versions of MCNP calculations (4C and 4B) for the KRITZ-2 experiments, using three different nuclear data libraries (JEF-2.2, ENDF/B-VI.5 and JENDL-3.2). For the MCNP library generation, the nuclear data processing system NJOY (version 97.114) is used. For both sets of calculations, the three KRITZ-2 cores are explicitly modelled in 3-D geometry. The linear thermal expansion coefficients given in the specification are used to determine the dimensions of the core geometry, the material densities, and the atomic number densities of the materials at high temperatures. The calculated results are compared with experimental results for both k_{eff} and pin powers in different cores (two UO_2- and one MOX-fuelled cores). The influence of the nuclear data libraries on calculated results are examined. The calculated k_{eff} results show a strong dependence on the basic data libraries used. The calculated pin powers are in general in good agreement with the experimental values within ±2% of discrepancy for most of the fuel pin positions.

1. INTRODUCTION

The KRITZ reactor operated at Studsvik, Sweden, during the early 1970's. The KRITZ-2 experiments included a series of light water moderated lattices with uranium rods and mixed-oxide rods, at room temperature (19.7, 21.1 and 22.1°C) and elevated temperature (235.9, 243 and 248.5 °C). Criticality was attained by controlling the boron content in the water and by adjusting the water level [1, 2, 3].

The critical levels were measured at low power, often as low as 10W, to minimize the activation of the fuel, and relative powers for selected rods were also measured. The KRITZ-2 experimental data can be used for the validation of both the nuclear data and calculation methods at different temperatures. Therefore, within the framework of its Nuclear Science Committee (NSC), the OECD/NEA, in co-operation with ORNL, launched a benchmark based on the four following experiments: three with uranium rods (KRITZ-1, KRITZ-2:1 and KRITZ-2:13 cores) and one with mixed-oxide rods (KRITZ-2:19 core).

The benchmark requested the determination of the k_{eff} values for different critical configurations and the calculation of the pin power distribution of measured pin positions. This paper presents the results obtained from the MCNP-4C calculation with JEF-2.2 and from the MCNP-4B calculations using JEF-2.2, ENDF/B-VI.5 and JENDL-3.2 libraries for the three KRITZ-2 cores. Section 2 briefly describes the KRITZ-2 experiments comprising the geometry, materials composition, etc. Section 3 presents the nuclear data and processing method used and calculation modelling and assumptions made for the MCNP calculations. The main results and discussions are summarised in Section 4, followed by the conclusions in Section 5.

2. DESCRIPTION OF KRITZ-2 EXPERIMENTS

The vertical and horizontal cross-sections of the KRITZ reactor are shown in Figures 1 and 2. The KRITZ reactor consisted of a ~5m high cylindrical pressure tank with a 1.5 cm diameter. The fuel rods were placed inside the inner part of the insert vessel, which had a square cross-section with a side length of ~1m. The tank contained the insert vessel. The outer part of the insert vessel was cylindrical with only a slightly smaller diameter than the pressure tank. The square shaped part was filled with water up the level required to obtain criticality. The typical water level at criticality was below the top of the fuel, so the top portions of the fuel rods were extended into the steam region. The pressure tank and the insert vessel (the inner and the outer parts) are both made of Stainless Steel (SS-304). The thin annulus between them was filled with water up to the same level as the square-shaped part. The space between the outer and the inner part of the insert vessel (dump region) was filled by saturated steam during normal reactor operation.

The array of fuel rods was placed eccentrically in the square-shaped region as shown in Figure 2. The position of the core in the insert vessel differs depending on the pin pitch and the number of rods. The core of both KRITZ-2:1 and KRITZ-2:13 experiments was square whereas that of KRITZ-2:19 was rectangular; they all consisted of a regular lattice of fuel rods of the same type. The fuel rods were supported by cylindrical steel beam and kept in place by spacer grids which were made of stainless steel. The core characteristics of each of the experiments is summarised in Table 1. More details can be found in references [1, 2, 3].

For the KRITZ-2 experiments, besides the critical height of the fuel under water (H_w), the axial buckling B_z^2 and the boron content, the rod-to-rod distribution were also measured with gamma scanning.

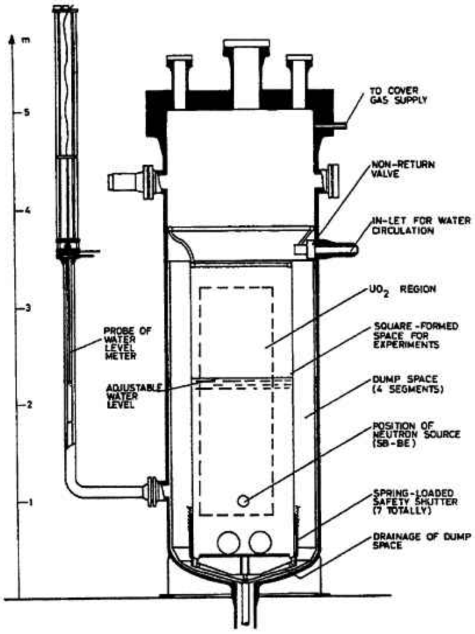

Figure 1. Vertical cross-section of KRITZ core

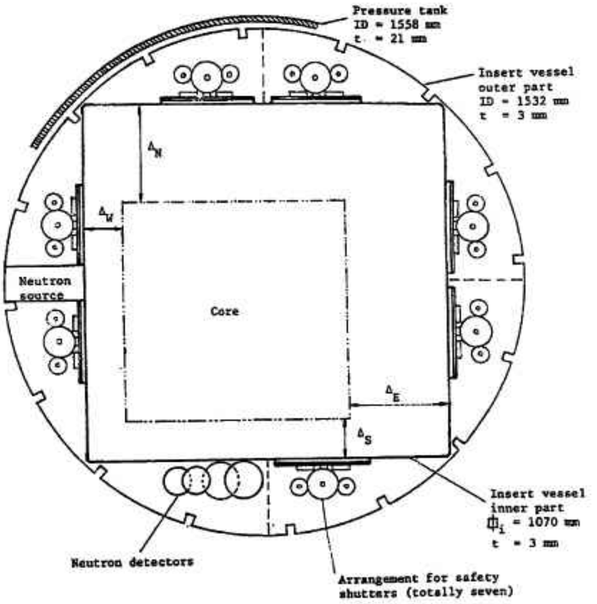

Figure 2. Horizontal cross-section of KRITZ core

Table 1. Main characteristics of the KRITZ-2 cores

Core	KRITZ-2:1	KRITZ-2:13	KRITZ-2:19
Fuel material	UO_2	UO_2	UO_2-PuO_2
Fuel density (g/cm^3)	10.145	10.145	9.58
^{235}U (wt. %)	1.86	1.86	0.16
PuO_2 (wt. %)	-	-	1.50
Canning material	Zircaloy-2	Zircaloy-2	Zircaloy-2
Rod pitch (mm)	18.0	14.85	16.35
No. of rods	44×44	40×40	25×24
Temperature (°C)	19.7 248.5	22.1 243.0	21.1 235.9
Boron concentration (ppm)	217.9 26.2	451.9 280.1	4.8 5.2
H_w* (mm)	652.8 1055.2	961.7 1109.6	665.6 1000.1

* height of active fuel under water

The following results were requested for the benchmark exercise: from cell calculations, k_{inf} and absorption/fission reaction rates per isotope in one group were to be reported at room temperature (20°C) and elevated temperature (245°C) for each of the fuel cells (MOX and UO_2). From core calculations, k_{eff} and pin-by-pin group integrated power for some specific rods (for which the measured values are available) were requested. The powers of 21 pins were measured in KRITZ-2:1, those of 30 pins in KRITZ-2:13 and those of 25 pins in KRITZ-2:19.

3. NUCLEAR DATA AND CALCULATION MODELLING

Two different sets of Monte Calo calculations are carried out using the two versions (4C and 4B) of the MCNP code [4, 5]. For the MCNP library generation, the nuclear data processing system NJOY (version 97.114) is used. The resonance reconstruction and linearization accuracy in generating the data is generally 0.1%.

For the first set of MCNP-4C calculations, the nuclear data used are mainly based on the JEF-2.2 library for all isotopes except for Ni, Cr and Fe from JENDL-3.2, and Sn from BROND-2. Libraries are generated for each high temperature. However, for low temperatures, only one library generated at 20 °C are used for 19.7 °C, 21.1 °C and 20 °C cases. Self-shielding effects in the unresolved resonance range are taken into account by a probability table treatment for some isotopes. The thermal scattering data at 20.45 °C (293.6 K) and at 250.45 °C (523.6 K) from JEF-2.2 are used for the thermal scattering cross-section generation at low and high temperatures, respectively. The pin-cell was modelled in two-dimensional geometry with square sides using the reflective boundary condition. The fuel gap was modelled explicitly in the UO_2 fuel cells (no gap in the MOX fuel cell). For the high temperature cases of UO_2 fuel lattices (2:1, 2:13), the thermal expansion was considered both in radial and axial directions. For the MOX case (i.e., vibrocompacted fuel), the thermal expansion of the fuel was considered in radial direction only following the radial expansion of the cladding and the material density was reduced accordingly. The MCNP-4C calculations for all pin-cell lattices were undertaken with 5000 particles per cycle and 1000 active cycles after 100 inactive cycles, i.e., the total number of histories used for cell calculations is 5 millions. For core calculations, 12.5 10^6 histories (50000 histories per cycle with 300 cycles including 50 inactive cycles) are used.

For the second set of MCNP-4B calculations, three different cross-section libraries based on ENDF-B/VI Release 5 (^{14}N, $^{120, 122, 124}$Sn from JENDL-3.2), JEF-2.2 (^{112}Sn from ENDF/B-VI Release 5), and JENDL-3.2 (C_{nat} from ENDF/B-VI Release 5) are generated for all temperatures. The thermal scattering data are taken from ENDF/B-VI Release 5 and the LEAPR module of NJOY is used for generating thermal scattering law data at specific temperature points. The same number of cell calculation histories is used as in the MCNP-4C calculations. However, for core calculations, the number of histories is increased to 25 10^6 (50000 histories per cycle with 500 cycles after 100 inactive cycles).

For both sets of calculations, the three KRITZ-2 cores are explicitly modelled in 3-D geometry up to the pressure tank. Nevertheless, some simplifications in the geometry are made as follows:

- The structure above the top of the fuel was modelled. It was assumed that the reflection from the vapor area above the top of the fuel rods as well as the structure in this region could be neglected.
- The spacer grids (SS316), supporting the fuel rods, were modelled.
- The bottom reflector extended to 50 cm below the bottom of the fuel.

The linear thermal expansion coefficients given in the specification are used to determine the dimensions of the core geometry, the material densities, and the atomic number densities of the materials at high temperatures.

4. RESULTS AND DISCUSSIONS

4.1. CELL CALCULATIONS

A comparison of calculated k_{inf} values with different libraries is summarised in Table 2. The comparison is made in taking the MCNP-4B (JEF) calculations as the reference. Two JEF-based results show a good agreement (within 30 pcm of differences for all the three cores) at room temperature. However, the differences between them become larger (up to about 150 pcm for the UO_2 cores and about 50 pcm for the MOX core) at higher temperature. Use of probability tables in the MCNP-4C calculations does not seem to affect the results very much. In the MCNP-4B calculations, ENDF-based results for the two UO_2 cores give much smaller k_{inf} values compared to those based on JEF. For the MOX core, the agreement between ENDF- and JEF-based results is better. The JENDL-based results produce more than 500 pcm higher k_{inf} values than those based on JEF for the MOX core. The differences between ENDF- and JENDL-based results are always more than 350 pcm for all the cores.

Table 2. Comparison of the calculated k_{inf} values (pcm)

Temperature	Core	(MCNP-4C JEF) - (MCNP-4B JEF)	MCNP-4B (ENDF) - (JEF)	MCNP-4B (JENDL) - (JEF)
20 °C	KRITZ-2:1	-30	-442	-67
	KRITZ-2:13	25	-247	109
	KRITZ-2:19	25	120	547
245 °C	KRITZ-2:1	-146	-620	-153
	KRITZ-2:13	-139	-455	45
	KRITZ-2:19	47	10	510

NOTE: In all the calculations, statistical errors are between ±0.00020 and ±0.00024.

Concerning the reaction rates, in the UO_2 cores, some differences are observed for ^{234}U absorption and fission rates between the JEF-based MCNP-4C and MCNP-4B calculations. However, the absolute contributions of ^{234}U to the total neutronic balance are small. ENDF gives larger absorption rates of ^{235}U and JENDL produces larger fission rates of ^{235}U compared to the other libraries in the UO_2 cores. The two JEF calculations give consistent absorption and fission rates of ^{235}U. The absorption reaction rates of ^{238}U are consistent in all libraries, even though ENDF gives slightly larger fission rates of ^{238}U than other libraries and JENDL gives smaller values. ^{238}U fission rates produced by the two JEF calculations are consistent.

In the MOX core, the reaction rates of ^{235}U are very consistent for both absorption and fission. For the absorption rates of ^{238}U, all four calculations give consistent values, but for the fission rates of ^{238}U, ENDF and JENDL give larger values than those from the two JEF-based calculations. For ^{239}Pu, two JEF results produce slightly higher values of absorption and fission rates than ENDF and JENDL; however the differences between them are very small. For ^{240}Pu absorption rates, MCNP-4C (JEF) and MCNP-4B (ENDF) give similar values, and MCNP-4B (JEF) and MCNP-4B (JENDL) produce slightly smaller values than the former. For the ^{240}Pu fission rates, JENDL give smaller values than the other libraries. For ^{241}Pu, the two JEF results are very similar, and ENDF and JENDL give the similar results, but they are smaller than the two JEF results. For ^{242}Pu, ENDF gives larger absorption rates while JENDL produces smaller fission rates than the other libraries. For ^{241}Am, larger differences of both reaction rates are observed among the three libraries. However, the two JEF results are consistent in both absorption and fission rates. Compared to other isotopes, the absolute contributions of ^{241}Pu, ^{242}Pu, and ^{241}Am are very small to the total neutronic balance; hence the relatively large deviations observed for these isotopes would not play an important role.

4.2. CORE CALCULATIONS

Multiplication factor, k_{eff}

As shown in Table 3, the two JEF-based calculations give similar k_{eff} results. However, for the KRITZ-2:1 cores, the JEF library produces about 500 pcm smaller k_{eff} values compared to 1 (experimental value) at low temperature and the differences become larger up to 600 pcm at high temperature. For the KRITZ-2:13 cores, the agreements are better than for the KRITZ-

2:1 cores. However, there are still about up to 300 pcm of difference between the experimental and calculated k_{eff} values. The ENDF-based results show the largest discrepancies for all the cores, especially about 1200 pcm smaller k_{eff} value for the KRITZ-2:1 core at high temperature. Interestingly, the results for the KRITZ-2:19 MOX cores are always better than those for the two UO_2 cores in all cases. The JENDL-based results are slightly better than those based on JEF for most of the cores. Regarding the two JEF-based calculations, they give very similar k_{eff} values, even though the MCNP-4C calculations used twice the less number of cycles than the MCNP-4B calculations: 250 cycles (50000 histories per cycle) in the MCNP-4C calculations and 500 cycles (50000 histories/cycle) in the MCNP-4B calculations.

Table 3. Calculated k_{eff} values compared to the experimental value (k_{eff} - 1) (pcm)

Core	T (°C)	MCNP-4C	MCNP-4B		
		JEF	ENDF	JEF	JENDL
KRITZ-2:1	19.7	-490	-916	-474	-394
	248.5	-613	-1168	-540	-505
KRITZ-2:13	22.1	-271	-536	-212	-79
	243.0	-296	-813	-284	-155
KRITZ-2:19	21.1	17	-291	-24	141
	235.9	-61	-469	-170	11

NOTE: Statistical errors are between ±0.00017 and ±0.00019 in the MCNP-4C calculations and between ±0.00013 and ±0.00014 in the MCNP-4B calculations.

Table 4 summarises the temperature coefficients derived from the calculated k_{eff} values. The temperature coefficient is defined as $[(k_{eff}\,(hot)-k_{eff}\,(cold))/(T_{hot} - T_{cold})]$. Since the measured k_{eff} values are 1 for both cores, the smaller the temperature coefficient values are, the better they are. MCNP-4C (JEF), MCNP-4B (JEF) and MCNP-4B (JENDL) calculations give relatively good results, but the MCNP-4B (ENDF) calculations produce higher values than other calculations

Table 4. Temperature coefficients (pcm/°C)

Core	MCNP-4C	MCNP-4B		
	JEF	ENDF	JEF	JENDL
KRITZ-2:1	-0.538	-1.101	-0.288	-0.485
KRITZ-2:13	-0.113	-1.254	-0.326	-0.344
KRITZ-2:19	-0.363	-0.829	-0.680	-0.605

Pin power distributions

For the KRITZ-2:1 core (44×44 UO_2 rods with pitch of 14.85 mm), the experiments were carried out at 19.7°C and 248.5°C, but relative powers only at 248.5°C for 21 rods are available. For the KRITZ-2:13 core (40×40 UO_2 rods with pitch of 16.35 mm), relative powers were measured at 22.1°C and 243.0°C for 30 rods. For the KRITZ-2:19 core (25×24 MOX rods with pitch of 18.0 mm), relative powers were measured at 21.1°C and 235.9°C for 25 rods.

The reported uncertainty of the measured pin power values is less than 1% for the three cores. However, the uncertainty of some rods could be much larger than 1% due to bent rods and inhomogeneities in the material, which are particularly large for the MOX rods. For relative comparison of calculated pin power results, calculated/measured (C/M) values of pin powers are plotted in Figure 3 for KRITZ-2:1 (hot core), in Figures 4 and 5 for KRITZ-2:13 (cold and hot cores), and in Figures 6 and 7 for KRITZ-2:19 (cold and hot cores). In the KRITZ experiments, the measured fuel pin positions were defined as (x,y), where x is the column number and y is the row number of the fuel rod. For the KRITZ-2:13 core (regular lattice of 40×40 fuel rods) and the KRITZ-2:19 core (regular lattice of 25×24 fuel rods), the first rod positions were defined as (3, 3) and (2, 2), respectively. For the KRITZ-2:1 core (regular lattice of 44×44 fuel rods), this position was defined as (1, 1).

In the MCNP-4C pin power calculations, the average of the relative error (1σ) is less than 1% for the two UO_2 cores and about 0.6% for the MOX core. In the MCNP-4B pin power calculations, it becomes less due to an increased number of histories (about 0.6% for the UO_2 cores and 0.4% for the MOX core).

For the KRITZ-2:1 core, the measurement values of 21 pin powers only at high temperature are available. For most of the pin positions, the agreement between calculated and measured values is less than ±2%. The two JEF-based results are slightly better than the others, and followed by JENDL- and then by ENDF-based results. The number of pins that have C/M values less than ±2% are 15, 13, 18, 15 from MCNP-4C (JEF), MCNP-4B (ENDF), MCNP-4B (JEF) and MCNP-4B (JENDL) calculations, respectively (in other word, 71%, 62%, 86% and 71% of total number of pins). With the MCNP-4B (ENDF) calculations, 6 calculated pin powers show ±3% of discrepancy compared to the measured values. For the pin at position (15,30), all the calculations show systematically high discrepancies (up to 8%). This may be explained by possible error in the measurement.

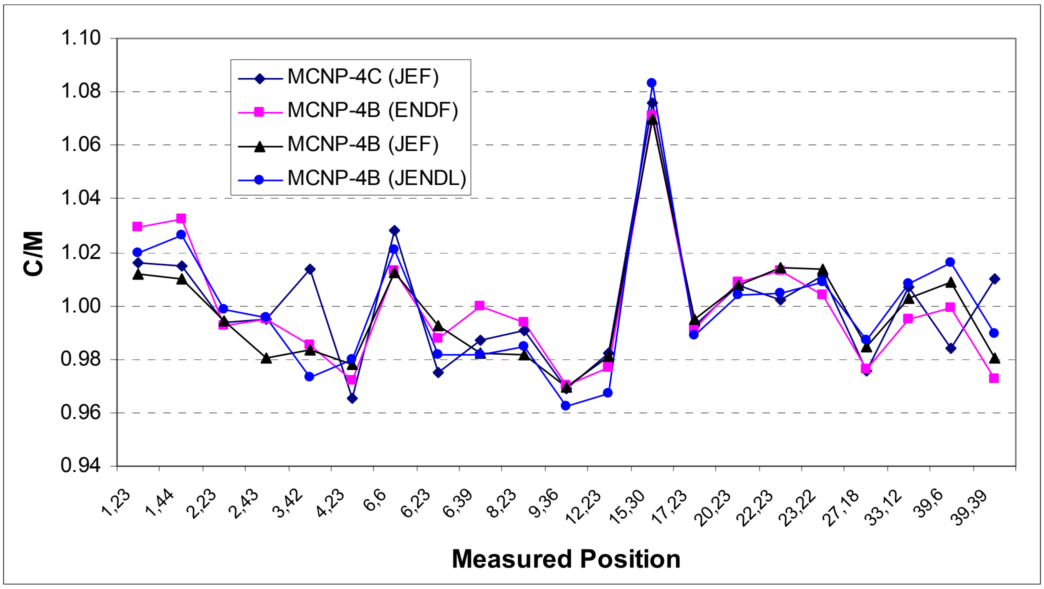

Figure 3. Pin Power Distribution in KRITZ-2:1 (Hot Core)

For the KRITZ-2:13 cores, 30 measured pin powers are compared to the calculated values and all the calculated results are slightly better than those for the KRITZ-2:1 hot core. For the both cores at room and high temperatures, C/M values are less than ±2% for most of the pins. For the core at room temperature, the three MCNP-4B calculations give 87% (i.e., 26 pins) of calculated pin powers less than ±2% of discrepancy when compared to measured results and 80% of calculated pin powers are less than ±2% of discrepancy from the MCNP-4C calculation. The better pin power distribution results from the MCNP-4B calculations than those from the MCNP-4C results may be explained by the number of cycles used twice the in the former (500 cycles and 50000 histories/cycle) than in the latter (250 cycles and 50000 histories/cycle). If the number of cycles were to be increased in the MCNP-4C calculations, the calculations would give similar results of the pin power distribution as the other calculations. For the pin position (16,23), all four calculations give more than ±3% of discrepancy. The maximum discrepancy of about 4% is shown for one pin position from all four calculations, but the position of that pin is different in all four calculations: (3,42) from MCNP-4C (JEF), (42,3) from MCNP-4B (ENDF), (16,23) from MCNP-4B (JEF) and (22,42) from MCNP-4B (JENDL).

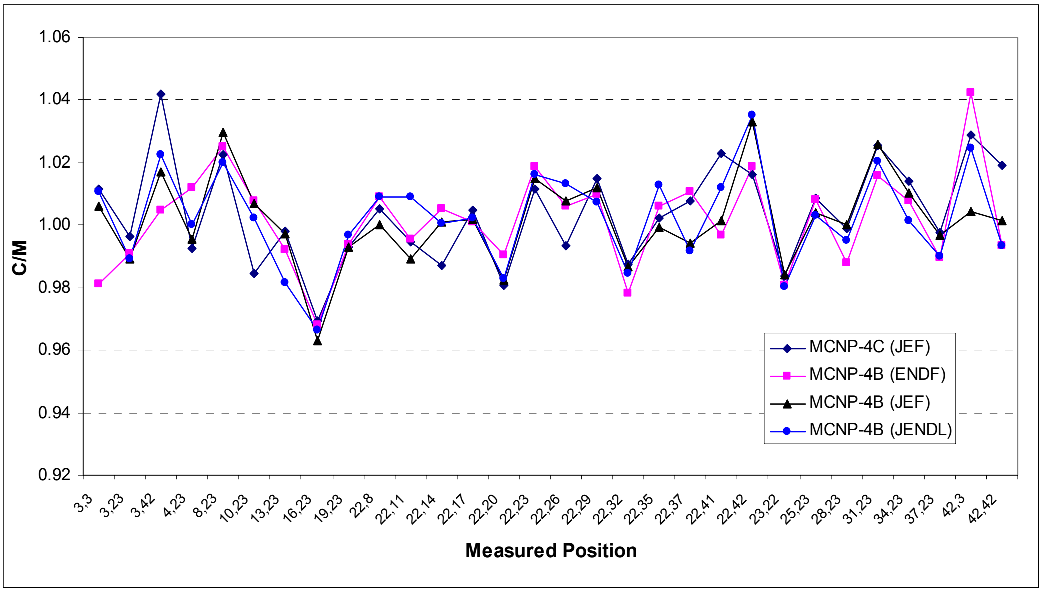

Figure 4. Pin Power Distribution in KRITZ-2:13 (Cold Core)

For the KRITZ-2:13 hot core, the trend of calculated results is slightly worse than for the cold core. The best solution is obtained from the MCNP-4B (JEF) calculation from which 83 % (25 pins) of calculated pin powers are within ±2% of discrepancy, followed by MCNP-4B (JENDL). The latter gives 80% of calculated pin powers within ±2% of discrepancy. Both MCNP-4B (ENDF) and MCNP-4C (JEF) produce very similar results giving 73 % of pin powers within ±2% of discrepancy and the maximum discrepancy of ±5% is shown for the pin at position (3,42). All four calculations give about ±4% of discrepancy for the pin at position (22,32).

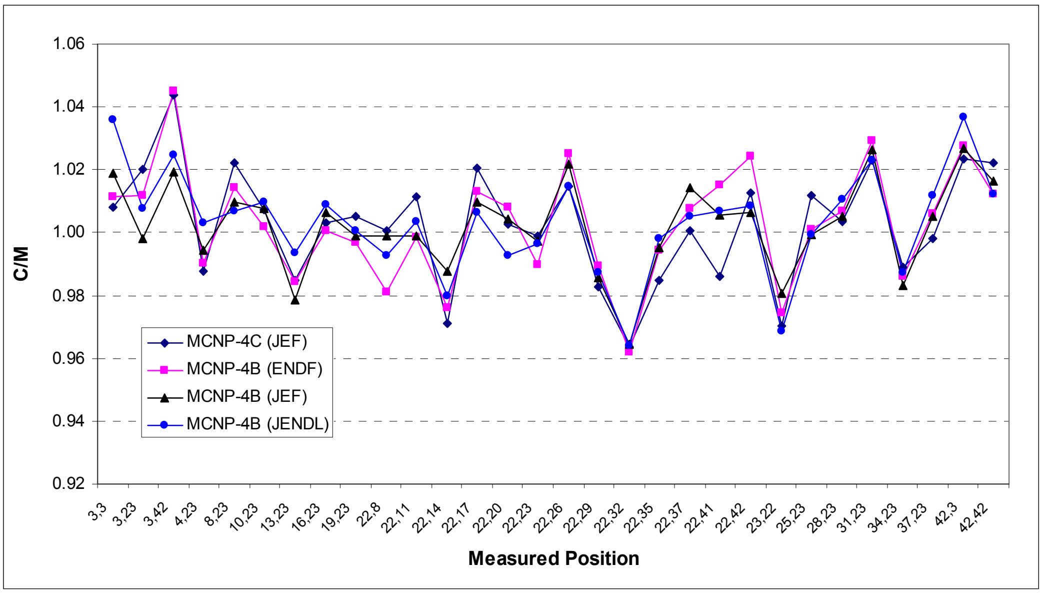

Figure 5. Pin Power Distribution in KRITZ-2:13 (Hot Core)

For the KRITZ-2:19 cold core, the results of all four calculations show an excellent agreement with the experimental results. Out of 25 measured pins, the calculated pin powers of more than 23 (92%) pins show less than ±2% of discrepancy compared to the measured values. For the pin at position (14,6) in this core, MCNP-4C (JEF), MCNP-4B (ENDF) and MCNP-4B (JENDL) give a discrepancy of about ±5% and MCNP-4B (JEF) shows a discrepancy of ±6%. For this pin position, a possible error in the measurement could be imagined.

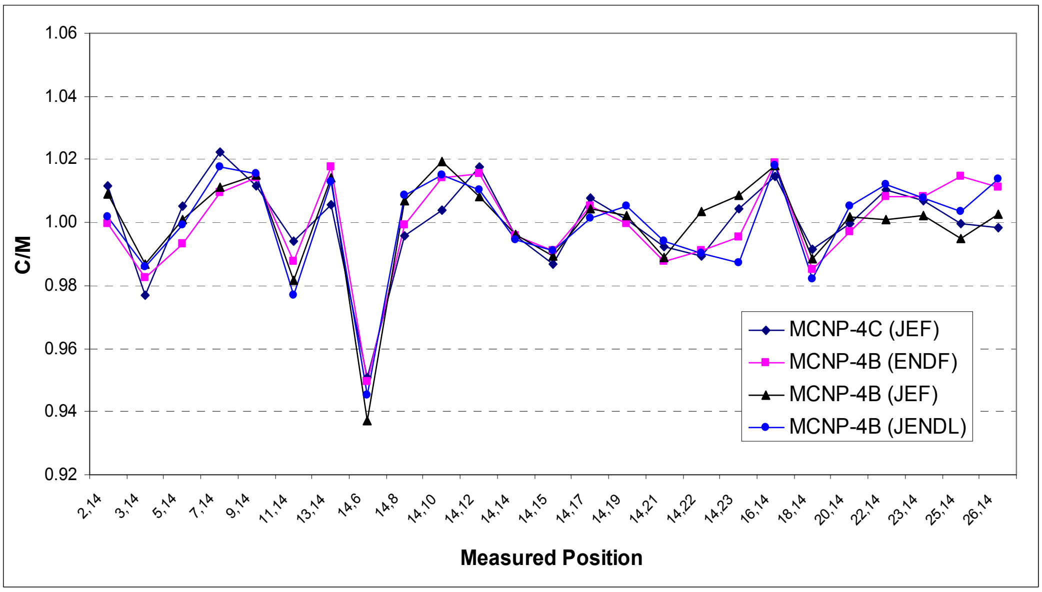

Figure 6. Pin Power Distribution in KRITZ-2:19 (Cold Core)

For the KRITZ-2:19 hot core, even though the calculated pin powers are in good agreement with the experimental values, they are slightly degraded compared to those for the cold core. Three MCNP-4B calculations give a discrepancy of about ±3% for the pin position (2,14). For the pin position (14,14), all four calculations show a discrepancy of about ±4% which could give a doubt on the accuracy of the measurement.

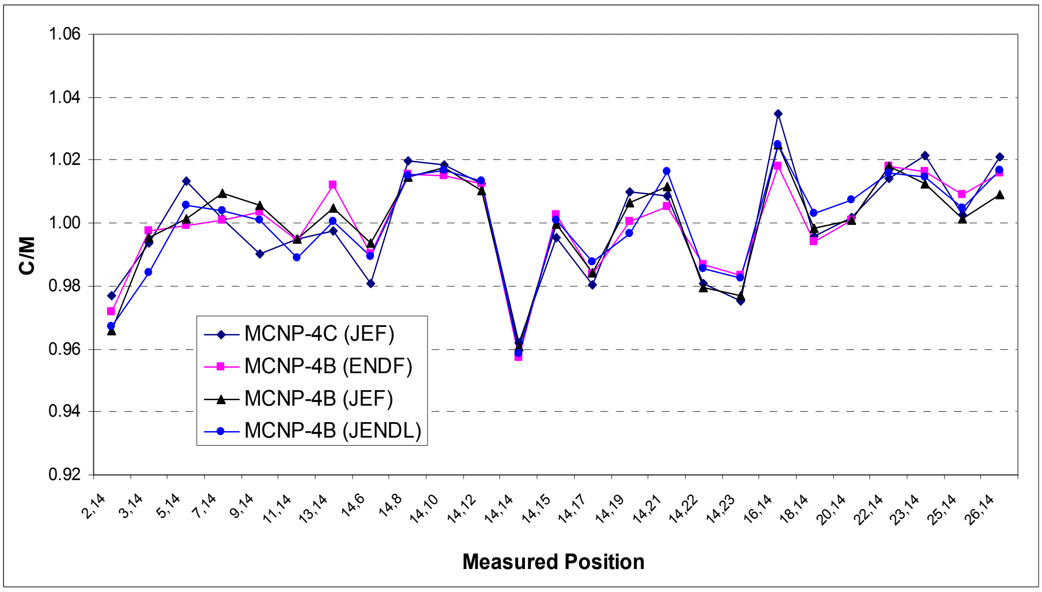

Figure 7. Pin Power Distribution in KRITZ-2:19 (Hot Core)

5. CONCLUSIONS

In the early 1970's, a set of KRITZ-2 experiments with light water moderated lattices with uranium rods and mixed-oxide rods, at room and elevated temperatures, were performed. Critical levels and relative powers for selected rods were measured. Using the experimental data released, a benchmark was developed based on the four following experiments: three with uranium rods (KRTIZ-1, KRITZ-2:1 and KRTIZ-2:13) and one with mixed-oxide rods (KRITZ-2:19).

Two sets of Monte Carlo calculations for the three KRITZ-2 cores are carried out using the two versions (4C and 4B) of the MCNP code. The basic nuclear data libraries used are mainly ENDF/B-VI, JEF-2.2 and JENDL-3.2. For the core calculations, the KRITZ-2 cores are explicitly modelled in 3-D geometry. The calculated k_{eff} values and the pin power distributions are compared with experimental data.

The calculated k_{eff} results show a strong dependence on the basic data libraries used. The JENDL-based results are slightly better than those based on JEF for most of the cores. The ENDF-based results strongly underestimate the k_{eff} for all the cores (up to –1200 pcm for the KRITZ-2:1 hot core). The results for the KRITZ-2:19 MOX cores are always better than those for the two UO_2 cores in all cases. The discrepancy in the hot core results are always higher than that in the cold cores, except for the JENDL-based results for KRITZ-2:19. Regarding the temperature coefficients, the ENDF-based results give the highest values, especially for the UO_2 cores.

In the MCNP-4C pin power calculations, the average of the relative error (1σ) is less than 1% for the two UO_2 cores and about 0.6% for the MOX core. In the MCNP-4B pin power calculations, it becomes less due to an increased number of histories (about 0.6% for the UO_2 cores and 0.4% for the MOX core).

All the calculations with the three different libraries show discrepancies within ±2% for most of the measured pin positions. For the KRITZ-2:1 (hot) core, the JEF (MCNP-4B) and JENDL-based results are slightly better than the others, followed by JEF (MCNP-4C) and ENDF-based results. For the KRITZ-2:13 cores, 30 measured pin powers are compared to the calculated values and all the calculated results are slightly better than those for the KRITZ-2:1 hot core. For both cores at room and high temperatures, C/M values are less than ±2% for most of the pins (for about 90% of pins). The agreements between calculated and measured pin powers are better for the KRITZ-2:19 MOX core than for the UO_2 cores. Out of 25 measured pins, the calculated pin powers of more than 23 (92%) pins show less than ±2% of discrepancy compared to the measured values. For both KRITZ-2:13 (UO_2) and KRITZ-2:19 (MOX), the results for the hot cores are always slightly degraded than for the cold cores. For a few pin positions, all the calculations show systematically high discrepancies (more than 4%). This could be explained by possible error in the measurement.

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