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MCNP CALCULATIONS FOR KRITZ 2 BENCHMARKS USING JEF-2.2 AND ENDF/B-VI.5

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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 MCNP-4B calculations for the KRITZ 2 experiments, using two different nuclear data libraries (JEF-2.2 and ENDF/B-VI.5). The calculated results are compared with experimental results for both K_{eff} and pin powers in different cores (UO_2 and MOX fuelled cores). The influence of the nuclear data libraries on calculated results are examined.

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 (Johansson 1990, Remec 2000a, Remec 2000b).

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 measured also. The KRITZ 2 experimental data can be used for the validation of both the nuclear data and calculation methods in different temperatures. Therefore, 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), within the framework of its Task Force on Reactor-Based Plutonium Disposition (TFRPD).

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 MCNP-4B calculations for the three KRITZ 2 cores using both JEF-2.2 and ENDF/B-VI.5 libraries. Section 2 briefly describes the KRITZ 2 experiments comprising the geometry, materials composition, etc. Section 3 presents the calculation modelling and assumptions made for MCNP calculations, and the nuclear data processing method used. The main results and discussions are summarized in Section 4, followed by the conclusions in Section 5.

2. KRITZ 2 DESCRIPTION

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 in 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 summarized in Table 1. More details can be found in references (Johansson 1990, Remec 2000a, Remec 200b).

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.

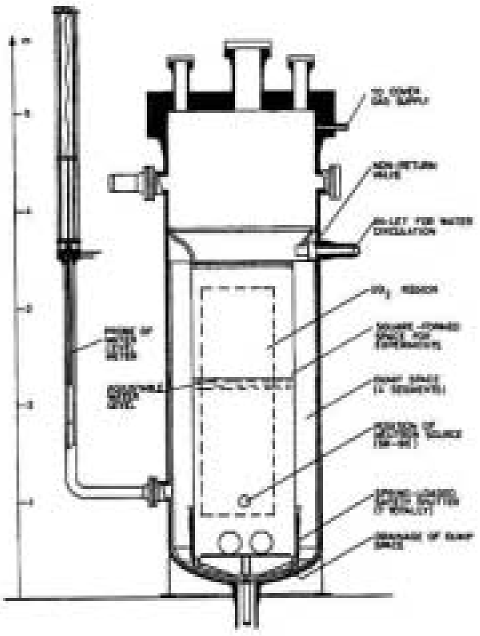

Fig. 1 Vertical cross-section of KRITZ core

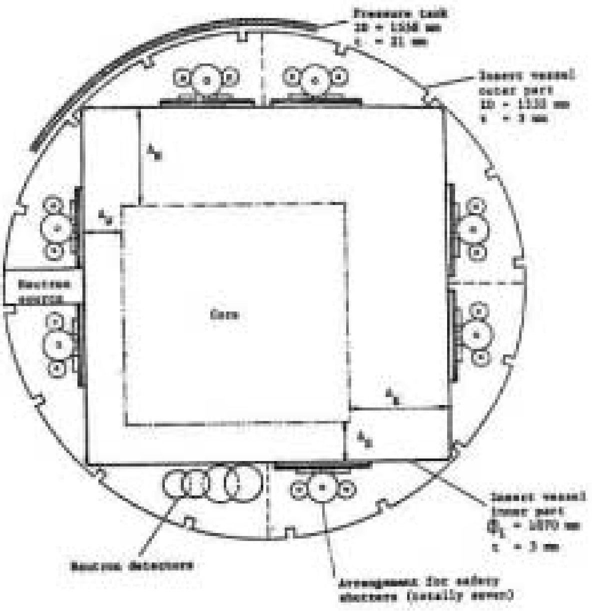

Fig. 2 Horizontal cross-section of KRITZ core

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_∞ 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

3.1 Nuclear data

For each temperature case, a set of cross-sections is generated by using the data processing system NJOY (version 97.114). The nuclear data used were based mainly on JEF-2.2 and ENDF/B-VI (release 5) evaluations for all isotopes except for Ni, Cr and Fe (from JENDL-3.2) and Sn (from BROND-2). The resonance reconstruction and linearization accuracy in generating the data was generally 0.1%. Concerning the neutron thermal scattering for H_2O, the data were prepared based on both ENDF/B-VI and JEF-2.2 for the eight temperature points. When specific temperature data were not available, interpolated values for cross-sections between the nearest temperatures were applied.

3.2 Calculation modelling

Both cell and core calculations were performed by using the Monte Carlo code MCNP-4B (Briesmeister, 1997).

Fuel cells were modeled in 2-D explicit square lattice geometry (including the gap for UO_2 cell) using reflective boundary conditions. At elevated temperatures, the calculation needed to take into account the thermal expansion, so dimensions of geometry and material densities at higher temperatures were determined by following the thermal expansion coefficients given in the specification. The thermal expansion coefficients used were 7.0 (10^{-6}/K) for zircaloy-2 and 18.0 (10^{-6}/K) for stainless steel. For the UO_2 fuel, the thermal expansion coefficient reported was 11.0 (10^{-6}/K) whereas it was not available for the vibrocompacted MOX fuel. In consequence, in the modellings of the KRITZ 2:1 and KRITZ 2:13 cores (with oxide uranium fuel) both radial and axial thermal expansion of the cores were considered. However, for the KRITZ 2:19 core (with mixed oxide fuel), it was assumed that the vibrocompacted MOX fuel expanded in radial direction only, following the radial thermal expansion of the clad.

In the MCNP core calculations, the core was explicitly represented in 3-D geometry up to the pressure tank. Nevertheless, some simplifications in the geometry were made as follows:

- The structure above the top of the fuel was modeled. 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 modeled.
- The bottom reflector extended to 50 cm below the bottom of the fuel.

In core calculations, more than 12 million neutron histories were considered, i. e., 50000 neutrons per cycle and 350 cycles were used, including 50 inactive cycles.

4. RESULTS AND DISCUSSIONS

4.1. Effective multiplication factor

Tables 2 and 3 summarize the calculated values of K_{eff} and corresponding statistical errors. The JEF-2.2 and the ENDF/B-VI.5 based results fit both well the experimental critical value (K_{eff}=1). The uncertainty (1σ) of the experimental value of K_{eff} is about 80 pcm for all three KRITZ 2 cores.

The calculated results are within less than 0.4% of the experimental value for both evaluations. The maximum discrepancy observed with the JEF-2.2 set is about +171 pcm for the KRITZ 2:1 UO_2 core, and +370 pcm for the KRITZ 2:19 MOX core. The ENDF/B-VI.5 data give lower values of K_{eff} except for the MOX core; this trend was also observed in a different study (Joneba, 2001). Indeed, the cell calculations show that the JEF-2.2 evaluation predicts higher K_∞ values than the END/B-VI.5 data independently of the temperature for UO_2 cores. This result is in agreement with the study done by (Bernnat, 2000).

The JEF-2.2 library overpredicts the UO_2 core reactivity with standard deviations (1σ) less than 23 pcm for most cases.

With the ENDF/B-VI.5 evaluation, K_{eff} value of the MOX core at elevated temperature shows a discrepancy of about +406 pcm compared with the experimental value but this value is higher than that obtained with the JEF-2.2 evaluation. The cell calculation shows the same tendency. This could be explained by the difference (3%) observed in the resonance integral for the fission to capture ratio of ^{239}Pu between JEF-2.2 and ENDF/B-VI data as is shown in reference (JEF Report 14, 1994). ^{239}Pu capture and fission cross-sections have a large resonance (at 0.29 eV) just above the thermal Maxwellian peak of the flux spectrum in thermal reactor. A recent study (Campbell, 2000) observes the same trend and indicates that the uncertainty in the cross-sections of this isotope is large enough to be of concern in terms of reactivity effects.

Table 2 Effective multiplication factor K_{eff}

Core type	**T (°C)**	**K_{eff} (JEF-2.2)**
KRITZ 2:1 (UO_2)	19.7	1.00171±0.00022
	248.5	0.99954±0.00019
KRITZ 2:13 (UO_2)	22.1	1.00014±0.00019
	243.0	1.00149±0.00019
KRITZ 2:19 (MOX)	21.1	1.00174±0.00019
	235.9	1.00370±0.00020

Table 3 Comparison of K_{eff} with JEF-2.2 and ENDF/B-VI.5

Core type	**T (°C)**	**K_{eff} (ENDF/B-VI.5)**	**ΔK_{eff} (pcm)** **K_{eff} (JEF-2.2) - K_{eff} (ENDF/B-VI)**
KRITZ 2:1 (UO_2)	248.5	0.99585±0.00019	+369
KRITZ 2:13 (UO_2)	22.1	0.99925±0.00019	+89
	243.0	0.99871±0.00019	+278
KRITZ 2:19 (MOX)	21.1	1.00285±0.00019	-111
	235.9	1.00406±0.00020	-36

4.2. Pin power results

The pin powers of the measured fuel pin positions were calculated and compared with the measured values as C/E. In the KRITZ 2 experiments, the measured fuel pin positions were defined as (X, Y), where X refers to the column number and Y to 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, this position was defined as (1, 1).

For KRITZ 2:1, the measured pin powers are available in the hot core (248.5°C) only whereas for KRITZ 2:13 and KRITZ 2:19, those of the hot and cold cores are available. The uncertainty (1σ) of the experimental pin powers is below 1% for the three cores, but the uncertainty of some rod powers could be much large than 1% due to bent rods and inhomogeneities in the material (e. g. rod 15, 30 in KRITZ 2:1, and rod 14, 6 and 14, 14 in KRITZ 2:19).

The C/E values of pin powers for each KRITZ core and comparative results between JEF-2.2 and ENDF/B-VI.5 evaluations are shown in Figures 3 to 9.

For KRITZ 2:1 and KRITZ 2:13 loaded with UO_2 fuel, the calculated pin power based on JEF-2.2 cross-sections fit the experimental values sufficiently well at room temperature and elevated temperature (See Figures 3 and 4). Indeed, most of the calculated results show discrepancies within ±2%. For KRITZ 2:13, only a few fuel pins show about 4% of discrepancy in both cold and hot cores.

The calculated results based on ENDF/B-VI.5 evaluations are also in good agreement with the experimental values for both KRITZ 2:1 and KRITZ 2:13. As shown in Figure 4, the two evaluations give almost the same results for most pin positions in KRITZ 2:1 core. But for KRITZ 2:13, the result based on ENDF/B-VI data are slightly higher than those for JEF-2.2 data except for a few fuel pin positions (See Figures 5 and 6).

For the KRITZ 2:19 MOX fuel core, as shown in Figure 7, the JEF-2.2 based results fit very well with the experimental values for both temperatures (21.1°C and 235.9°C). At room temperature, most of the results show discrepancies of less than ±2%.

In Figures 8 and 9, the ENDF/B-VI.5 based results for KRITZ 2:19 at room temperature and elevated temperature are compared with those from JEF-2.2. In fact, for most of the pin power positions, the C/E ratio is closed to the unity. The results from the JEF-2.2 evaluation are slightly better than those from ENDF/B-VI.5 for the hot core. For the cold core, the discrepancies observed from the two libraries are almost the same.

The relative errors (1σ) concerning MCNP calculation results are small for most of the calculated pins. For the UO_2 cores (KRITZ 2:1 and KRITZ 2:13), the average of the relative error is less than 1% whereas for the MOX core (KRITZ 2:19), this value is about 0.6%.

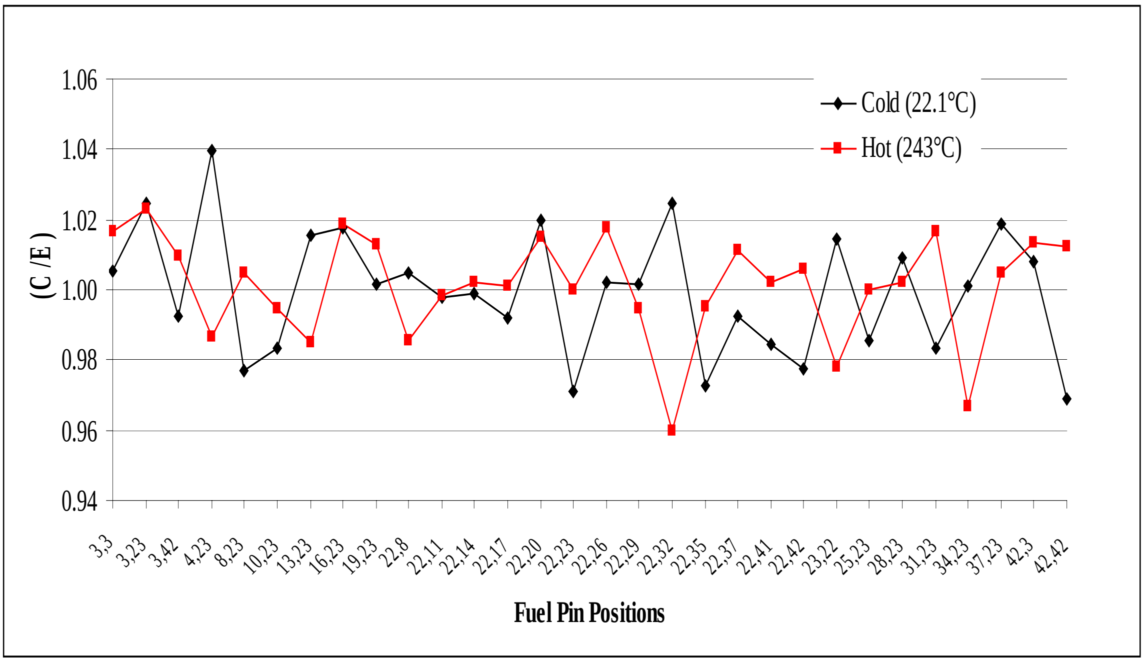

Fig. 3 KRITZ 2:13 core pin power comparison (JEF-2.2)

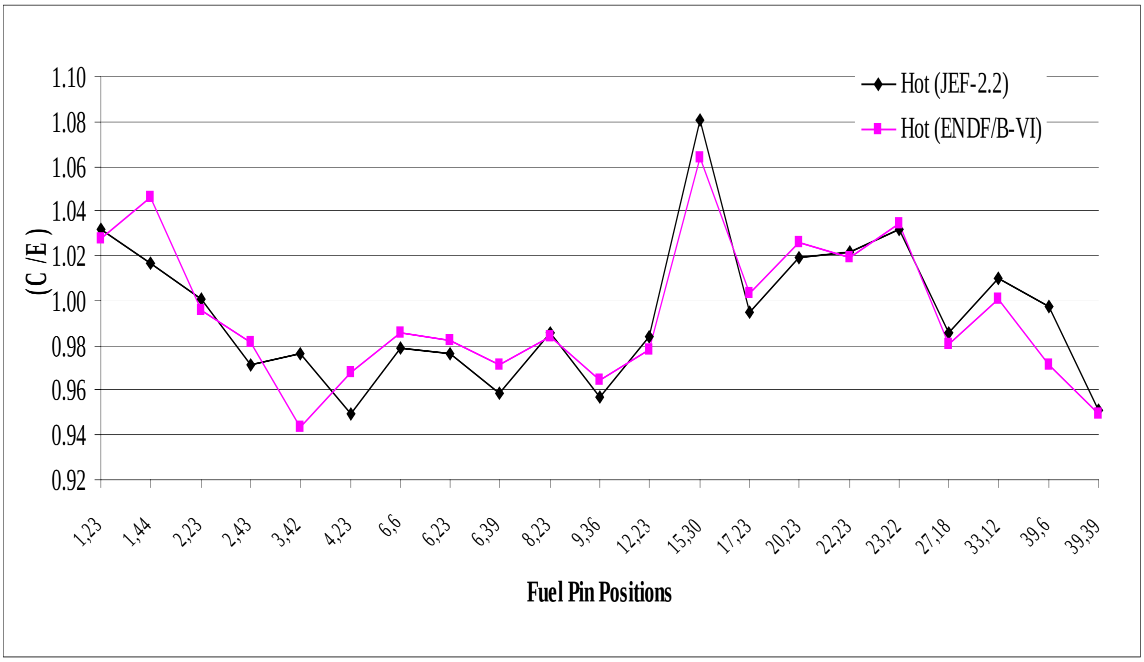

Fig. 4 KRITZ 2:1 (hot core) pin power comparison with both libraries

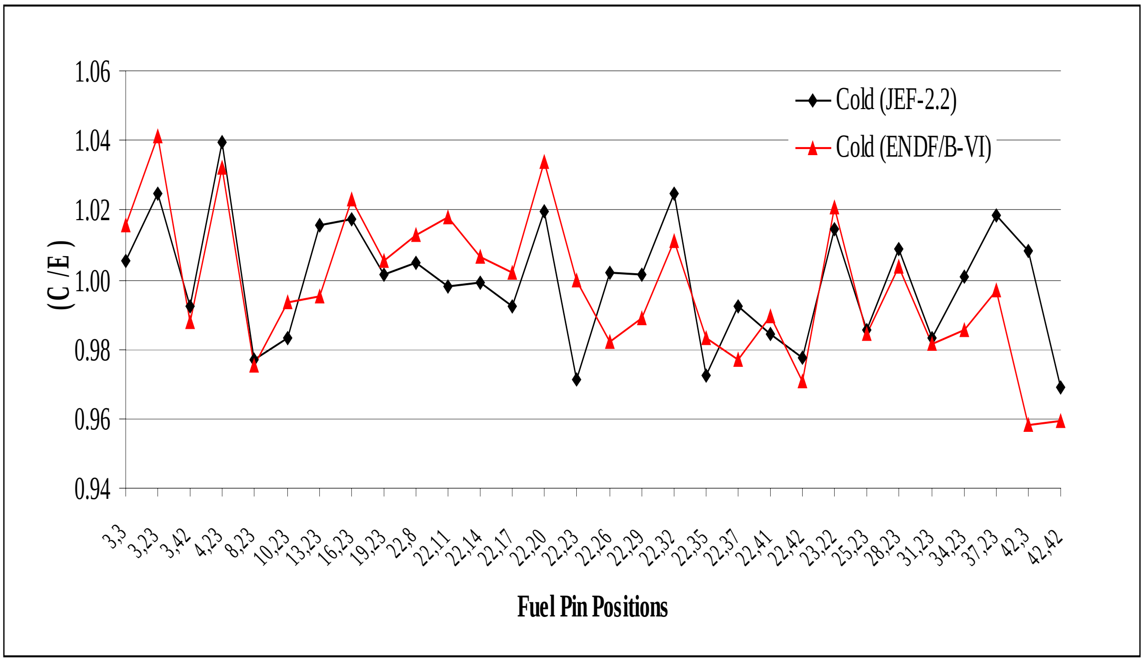

Fig. 5 KRITZ 2:13 (cold core) pin power comparison with both libraries

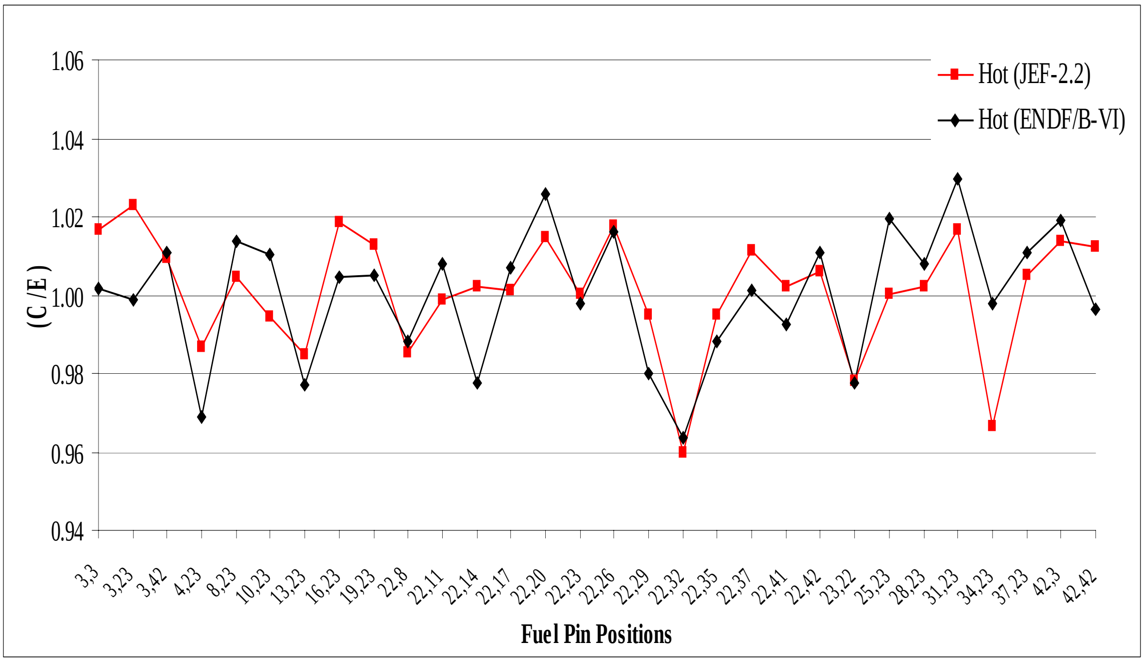

Fig. 6 KRITZ 2:13 (hot core) pin power comparison with both libraries

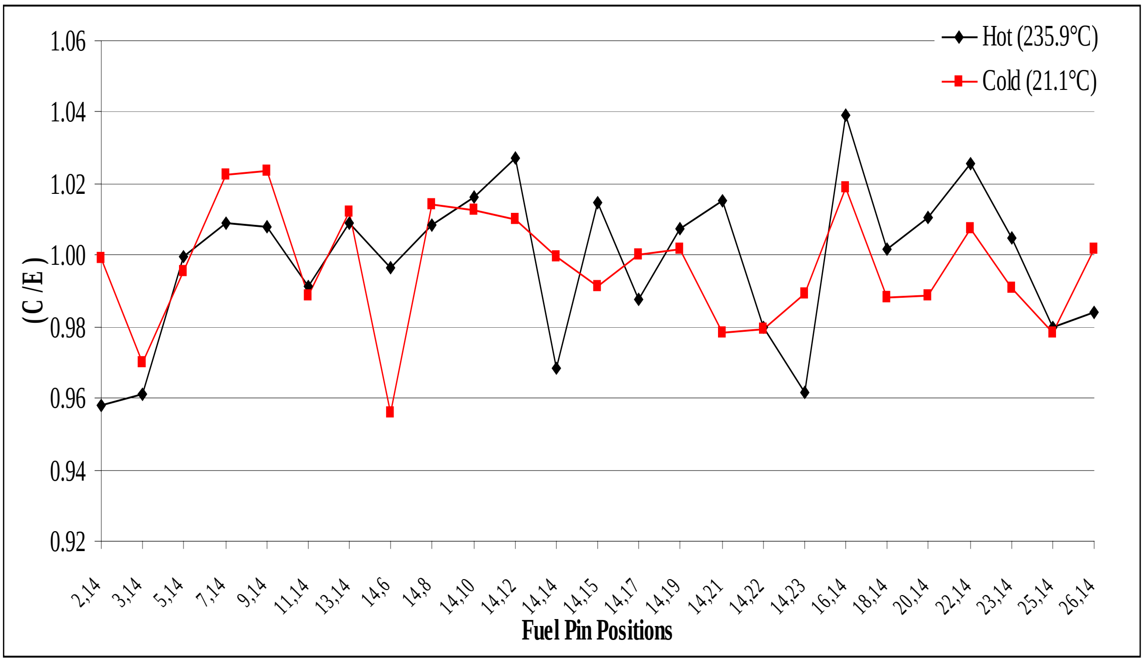

Fig. 7 KRITZ 2:19 pin power comparison (JEF-2.2)

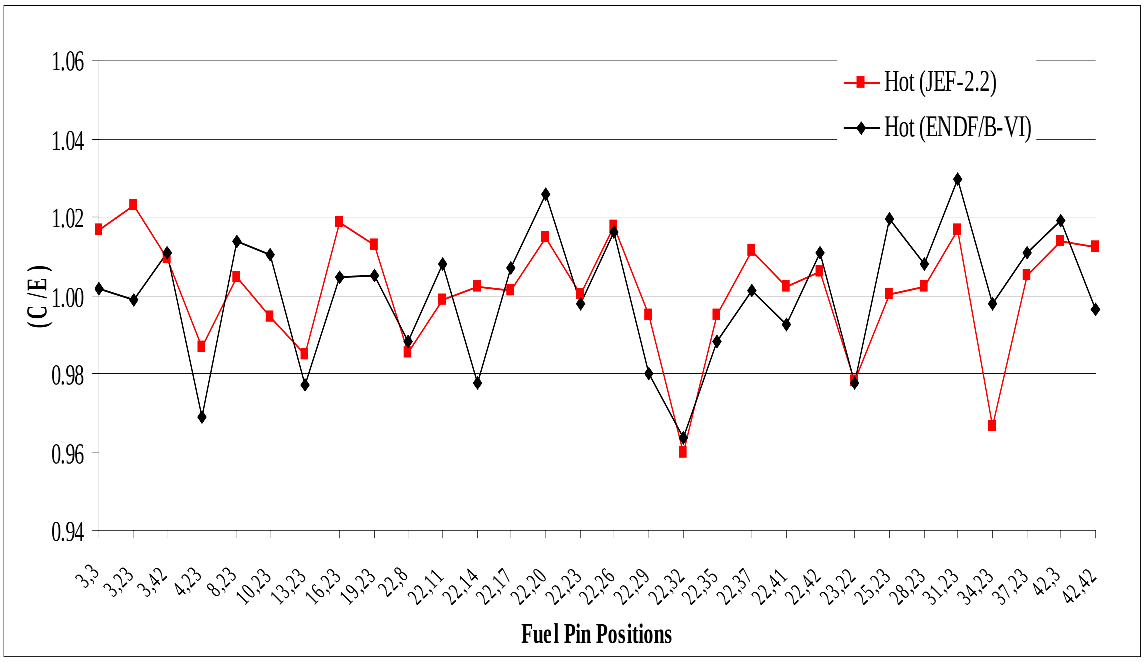

Fig. 8 KRITZ 2:19 (hot core) pin power comparison with both libraries

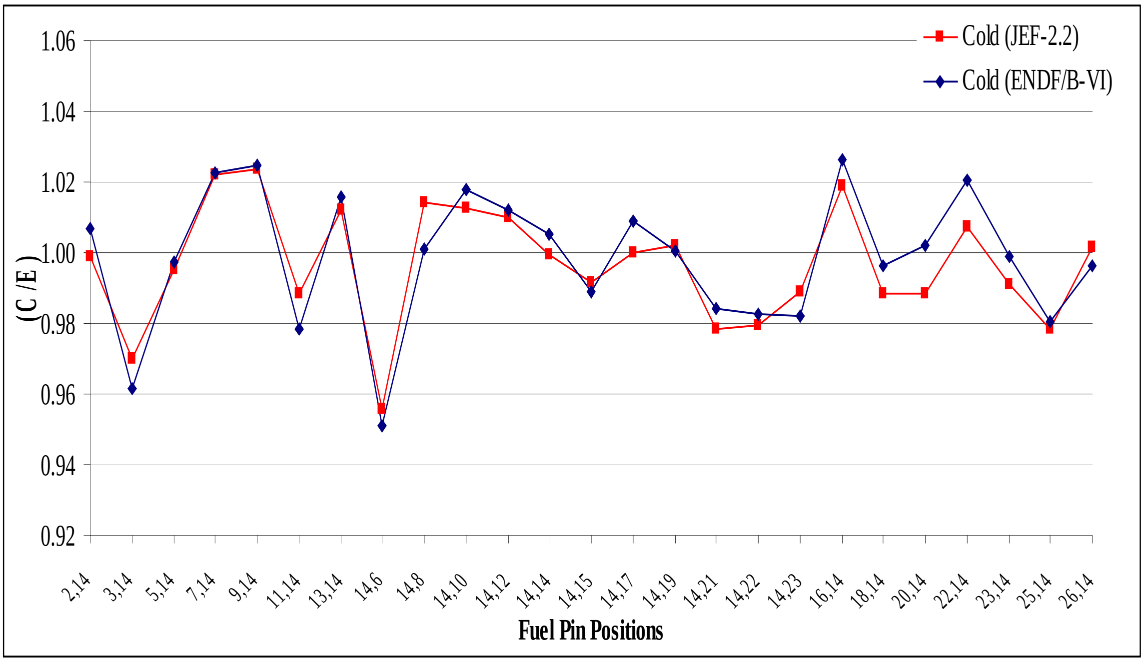

Fig. 9 KRITZ 2:19 (cold core) pin power comparison with both libraries

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).

This paper presents the results of MCNP-4B calculations for the three KRITZ 2 cores. K_{eff} values and the pin power distributions are investigated by using two different nuclear data based on JEF-2.2 and ENDF/B-VI.5.

The calculated K_{eff} values with both evaluations (JEF-2.2 and ENDF/B-VI.5) show a good agreement with the experimental values. However, the JEF-2.2 based K_{eff} values are higher than those with ENDF/B-VI.5, except for the MOX fuelled core. The same trend is observed for K_{∞} calculated from the cell calculations. The highest discrepancies of K_{eff} compared with the experimental value are +406 pcm for the KRITZ 2:19 core at elevated temperature and -415 pcm for KRITZ 2:1 at high temperature both with the ENDF/B-VI.5 data.

For pin power calculations, the JEF-2.2 based results fit the experimental values sufficiently well for KRITZ 2:1 and KRITZ 2:13 with UO_2 fuel. Most results show discrepancies within ±2% for KRITZ 2:1 and for KRITZ 2:13. For a few pins, the maximum discrepancy of about 4% is observed in both cold and hot core KRITZ 2:13.

The same trend is observed for the MOX fuel core KRITZ 2:19; most of the results show discrepancies less than ±2%.

The calculated results based on the ENDF/B-VI.5 evaluations are also in good agreement with the experimental values but they are slightly higher than those with JEF-2.2 data except for a few fuel pin positions.

REFERENCES

Bernnat, W. *et al.*, 2000. Analysis of LWR Benchmarks Based on Different Methods and Nuclear Data Evaluations, Proc. of the 200 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium (PHYSOR 2000), Pittsburgh, Pennsylvania, USA, 7-11 May.

Briesmeister, J. F., editror, 1997. MCNP A General Monte Carlo Code N-Particle Transport Code, Los Alamos National Laboratory report, LA-12625-M, March 1997.

Campbell, J. *et al.*, 2000. Evaluation of Water-Moderated Lattices of UO_2-2.0 wt. % PuO_2 Rods, Proc. of the 200 ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium (PHYSOR 2000), Pittsburgh, Pennsylvania, USA, 7-11 May.

Johansson, E., 1990. Data and Results from KRITZ Experiments on Regular H2O/Fuel Pin Lattices at temperatures up to 245°C, STUDSVIK/NS-90/133, ISBN 91-7010-143-4, Studsvik AB, Sweden, 1990.

Joneba, O. P. *et al*., 2001. Validation of an MCNP4B whole-reactor Model for LWR-PROTEUS using ENDF/B-V, ENDF/B-VI and JEF-2.2 cross-section libraries. *Annals of Nuclear Energy*. **28**, 701-713.

Remec, I., Gehin, J. C. and Ellis, R. J., 2000a. KRITZ-2 and KRITZ-1 Experiments on Regular H2O/Fuel Pin Lattices with Low Enriched Uranium Fuel at Temperatures up to 245°C, Oak Ridge National Laboratory Report, September 2000.

Remec, I., Gehin, J. C. and Ellis, R. J., 2000b. KRITZ 2:19 Experiments on Regular H2O/Fuel Pin Lattices with Low Mixed Oxide Fuel at Temperatures up to 245°C, Oak Ridge National Laboratory Report, November 2000.

Table of Simple Integral Neutron Cross Section Data from JEF-2.2, ENDF/B-VI, JENDL-3.2, BROND-2 and CENDL-2, OECD/NEA report, JEF Report 14, 1994.