COMPARISON OF MCNP CALCULATIONS AGAINST MEASUREMENTS IN MODERATOR TEMPERATURE EXPERIMENTS WITH CANFLEX-LEU IN ZED-2

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Abstract

This paper summarizes sample calculations of MCNP5 compared against measurements of moderator temperature coefficient experiments in the ZED-2 critical facility with CANFLEX®-LEU fuel. MCNP5 is tested for key parameters associated with various reactor physics phenomena of interest for CANDU®/ ACR-1000® reactors, including reactivity changes with coolant density, moderator density, and moderator temperature, and also normalized flux distributions. The experimental data for these comparisons were obtained from critical experiments in AECL's ZED-2 critical facility using CANFLEX-LEU fuel in a 24-cm square lattice pitch. These comparisons establish biases/uncertainties in the calculation of k-eff, coolant void reactivity, and moderator temperature coefficient of reactivity. Results show very little bias in the moderator temperature coefficient of reactivity, and very good agreement in the calculation of normalized flux distributions.

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1. Introduction

Experiments were performed in AECL's ZED-2 critical facility [1] (see Figure 1) to provide experimental data for validation of reactor physics codes being used in the design and safety analysis of the Advanced CANDU Reactor 1000 (ACR-1000) [2]. Critical moderator heights and foil activation rate distributions were measured in 52-channel, 24.00 cm square lattice pitch experiments with both air and light water (H_2O) coolants.

The main test fuel was the 43-element CANFLEX-LEU fuel bundle (see Figure 2), made with slightly enriched uranium oxide (approximately 0.95 wt% ^{235}U/U). 4 outer channels contained 43-element CANFLEX-RU, which is made from recovered Light-Water Reactor (LWR) fuel, and is very similar to CANFLEX-LEU in terms of enrichment (approximately 0.96 wt% ^{235}U/U).

The heavy water (D_2O) moderator temperature was varied during the experiments, and the effects on the critical moderator height and normalized flux distributions (as inferred by the normalized activation foil distributions) were measured. These measurements were then used to check the reactivity (k_{eff}) calculations and flux distributions computed by MCNP [3], and how they changed with coolant density (air or H_2O) and moderator temperature.

The MCNP code used was MCNP5 v.1.30 [3] and was run in a parallel mode on various upgraded computer clusters at AECL. The nuclear data library used with MCNP was based on ENDF/B-VI, Release 8 [4].

2. Experiments

Figure 1 shows the 52-channel, 24.00 cm square lattice arrangement for the ZED-2 critical experiments, including the 48 central channels (housing stacks of 5 CANFLEX-LEU fuel bundles) and the 4 corner channels (housing stacks of 5 CANFLEX-RU fuel bundles). The CANFLEX-LEU/RU fuel bundle and accompanying Al CANDU-type channel (pressure tube and calandria tube) are shown in Figure 2. As noted, the CANFLEX-LEU was made from fresh 0.95wt% ^{235}U/U, while the CANFLEX-RU was made from recovered LWR uranium, with a comparable enrichment of ^{235}U (0.96wt% ^{235}U/U), with slightly higher concentrations of ^{234}U and some ^{236}U. A total of 6 foil (tallied) experiments and 8 non-foil (untallied) experiments were performed with the conditions of the experiment (moderator purity/temperature, coolant temperature, critical moderator height) being recorded. The moderator purity ranged from approximately 99.06 wt%D_2O to 99.03 wt%D_2O, while the moderator temperature was adjusted from approximately 20°C to 50°C. The coolant temperature lagged behind the moderator temperature, varying from approximately 25°C to 35°C.

These experiments were modeled in MCNP, using up to 30 million neutron histories for the non-foil (untallied) experiments and 300 million neutron histories for the foil (tallied) experiments. (Extra histories were required for modeling the foil experiments in order to obtain low statistical uncertainties in the simulated foil activation rates.)

2.1 (Tallied) Experiments with Activation Foils

For the foil (tallied) experiments, stringers with Cu foils were positioned in the test lattice at specified locations to measure the neutron flux via neutron activation of the foils. The foils were positioned at 10-cm intervals along the lengths of the stringers. The experiments used a mix of "long" and "short" stringers in order to map out both the axial and radial neutron fluxes, respectively.

The axial flux measurements used 'long' stringers with 12 or 17 foils (12 for air-cooled tallies, 17 for H_2O-cooled), covering ranges of 20 cm to 130 cm (for the air-cooled tallies) or 20 cm to 180 cm (for the H_2O-cooled tallies) above the reactor bottom, and were located at positions[†] K2W and K2E as well as K12W and K12E (see Figure 1). The radial flux measurements used 'short' stringers with 3 sets of Cu foils, covering ranges of 50 cm to 70 cm (for the air-cooled tallies) and 80 cm to 100 cm (for the H_2O-cooled tallies) above the reactor bottom. These radial flux measurements were made using short stringers located at radial positions K10W to K10E in the West-East direction, and also at positions O/N0 to H/G0 in the North-South direction.

Measurements were made of the foil activations, and both axial and radial components of buckling were found by fitting the normalized activation data to a joint zero-order Bessel function/cosine curve in the asymptotic region of the core where the neutron energy spectrum remains constant. Axial data were taken from the long stringers (leaving out the top 2 and bottom 2 foil measurements), while radial data were taken from the short stringers inside the core (from K6W to K6E and O/N0 to H/G0).

2.2 Measurement Uncertainties and k_{eff} Sensitivities

The D_2O moderator purity was known to within ±0.005wt%. Thermometers used in the experiment were digital, with an uncertainty of ±0.2°C, while the instruments used to measure moderator height were analogue, with an uncertainty of ±0.2 cm. The stringer positions were measured with a ruler, with uncertainties of ±0.1 cm.

The uncertainties of these parameters propagate into the uncertainty of k_{eff} calculated by MCNP. The sensitivity of k_{eff} to D_2O moderator purity for these particular models was found to be approximately 25 mk/wt%D_2O, and was relatively independent of coolant type. This results in an uncertainty in k_{eff} of ±0.13 mk due to the ±0.005wt% uncertainty in moderator purity. The sensitivity of k_{eff} to D_2O moderator height was found to be approximately 1.6 mk/cm for the air-cooled cases, and 0.54 mk/cm for the H_2O-cooled cases. Since the uncertainty in the D_2O moderator height is ±0.20 cm, these yield uncertainties in k_{eff} of ±0.33 mk and ±0.11 mk for the air- and H_2O-cooled cases, respectively. Finally, the statistical MCNP uncertainties in k_{eff} ranged from approximately ±0.03 mk to ±0.04 mk (for 300 million history tallied runs) to approximately ±0.09 mk to ±0.11 mk (for 30 million history untallied runs). Thus, the overall uncertainties in k_{eff} ranged from about ±0.2 mk for the H_2O-cooled runs to about ±0.4 mk for air-cooled runs (combining MCNP statistical uncertainties in quadrature with the D_2O-induced uncertainties).

[†] See Figure 1 for layout of ZED-2's *alpha-numeric* locations.

3. MCNP Models

The MCNP models used were a precise approximation of the actual experimental set-up. A detailed model of the 43-element fuel bundle with cylindrical fuel elements was created for both the CANFLEX-LEU and CANFLEX-RU fuel types. The Al-backed Cu-foil and Zr-wire stringers were also modeled for these experiments, using rectangular prisms for the Al backers and circular cells for the Cu foils. Since their orientations could vary from location to location (and from time to time), the orientation of the Al backers alternated orientations from N-S to W-E in the MCNP model.

As noted, in this experiment, the core (moderator) temperature varied from approximately 20°C to 50°C. There were 4 sets of temperatures for the non-foil (untallied) air- and H_2O-cooled cases: 20°C, 35°C, 40°C, and 50°C, and there were 3 sets of temperatures for the foil (tallied) air- and H_2O-cooled cases: 20°C, 40°C, and 50°C.

Much detail was put into the material cards in the MCNP modeling, to ensure both the correct compositions of the materials and to ensure that the material temperatures matched those of the experiment. Since the MCNP libraries are generated at fixed temperatures that may differ from those of the experiment, material cards were created using mixes of isotope files at two different fixed temperatures (represented by different isotopic cross-section library extensions) in linear proportion to the actual temperature between the fixed nuclear data library temperatures.

For each material, the two library temperatures closest to the 'actual' temperature (core or channel) were identified, specifically, the temperature immediately below (T_{lo}) and immediately above (T_{hi}) the actual temperature (T). These were then used to create 'fractional multipliers' according to

$$f_{lo} = [T_{hi} - T]/[T_{hi} - T_{lo}]$$

$$f_{hi} = [T - T_{lo}]/[T_{hi} - T_{lo}]$$

where f_{lo} represents the 'lo' fractional multiplier, and f_{hi} the 'hi' fractional multiplier. For each isotope, two cross-section library extensions were chosen, corresponding to T_{lo} and T_{hi}. The isotopic compositions for T_{lo} and T_{hi} were then adjusted according to f_{lo} and f_{hi}, respectively. The result is an isotopic composition precisely at temperature T.

For example, the composition for material #43 ('pure aluminum') at 40°C is given as

```
C     pure Al   2.702g/cc [T=40C]

m43    13027.21c -0.415

       13027.22c -0.585
```

The .21c library (corresponding to 310 K) here represents 41.5% of m43, while the .22c library (corresponding to 320 K) here represents 58.5% of m43. The result is pure Al-27 (13027) at a temperature of 315.85 K = 42.7°C (the moderator temperature of the *(nominal)* 40°C H_2O-cooled tallied case).

4. Results

In total, 8 non-foil (untallied) and 6 foil (tallied) MCNP simulations were completed, corresponding to the ZED-2 critical experiments. In each MCNP run, the first 100 cycles were dropped for tally convergence, and the subsequent 3000 cycles were used for tally (and k_{eff}) convergence. In the tallied cases, 10^5 histories per cycle were used, while, in the untallied cases, 10^4 histories per cycle were used, giving totals of 30×10^6 histories and 300×10^6 histories per untallied and tallied runs, respectively.

The tallies used were cellular flux tallies, and, to further ensure low statistical uncertainty, they were tallied on both the thin circular foil-cells, and also on the cylindrical D_2O-filled cells surrounding the Al backers. These D_2O cells were given the same neutron-reaction rate as the foils as a method of reducing statistical uncertainties.

Two sets of measurements were made: k_{eff} for all runs, and neutron flux counts for the tallied runs. The latter were used to determine bucklings for the tallied runs.

4.1 k_{eff} Results

The k_{eff}'s were found to be about 7.5 to 11 mk below criticality for all runs, about 7.5 mk below criticality for the air-cooled runs and about 11 mk below criticality for the H_2O-cooled runs. (The H_2O-cooled cases having a larger offset from unity.) The calculated values of k_{eff} for all cases and their associated uncertainties are shown in Table 1 and plotted in Figure 3.

For the air-cooled runs, the average k_{eff} bias was found to be approximately[•] -7.46 ± 0.37 mk for the untallied cases, and -7.51 ± 0.35 mk for the tallied cases. For the H_2O-cooled cases, the average k_{eff} bias was found to be approximately -11.11 ± 0.19 mk for the untallied cases, and -10.91 ± 0.17 mk for the tallied cases.

The air-cooled k_{eff}'s (both tallied and untallied) show a very small change with moderator temperature. Based on a least-squares linear fit, the slopes of these plots (the biases in moderator temperature coefficients; MTCs) were found to be $+0.023\pm0.017$ mk/^{o}C for the untallied cases and $+0.013\pm0.018$ mk/^{o}C for the tallied cases. Both are consistent with each other, and (nearly) consistent with zero.

The H_2O-cooled k_{eff}'s also show a very small change with moderator temperature. The least-squares linear fit for the H_2O-cooled slopes (biases in MTCs) were found to yield $+0.009\pm0.009$ mk/^{o}C for the untallied cases and $+0.022\pm0.008$ mk/^{o}C for the tallied cases, which were both consistent with each other and close to zero. Clearly, the biases in moderator temperature coefficients are close to zero, independent of coolant.

The coolant-void reactivity bias was found to range from approximately +2.8 mk to +4.3 mk, with an average uncertainty of approximately ±0.4 mk. (Based on subsequent error analyses, these biases are thought to be due to errors in the ENDF/B-VI Release 8 nuclear data library used in MCNP.) However, the slope of the coolant-void reactivity bias with moderator temperature was smaller than its uncertainty ($+0.014\pm0.020$ mk/^{o}C). Thus, within statistical

[•] The uncertainties here only include the MCNP and D_2O-induced uncertainties in k_{eff} combined in quadrature. They do *not* also include the standard deviational spread in k_{eff}'s (see Conclusion for *full* k_{eff} uncertainties).

uncertainties, the coolant-void reactivity bias remained essentially constant against changing moderator temperature.

4.2 Neutron Flux Distributions

Results of the Cu foil tallies from the tallied MCNP runs were compared with the experimental Cu foil activation data and are shown in a sample case (T_{mod} = 40°C, air- and H_2O-cooled) in Figure 4 (showing axial distributions) and in Figure 5 (showing radial distributions). In both sets (experimental and computer-generated), the neutron counts from each tally were normalized to the average of all counts within a given tally except for counts outside the central core region (*i.e.*, outside K6W or K6E) and near the top or bottom (*i.e.*, the top 2 and bottom 2 tallies) as these tallies were thought to be too close to the edges to be considered reliable.

In examining these plots, the first notable thing one sees are the small 'upticks' that occur near the bottom of the channels in the axial plots for the K2 Cu data. These 'upticks' appear higher for air-cooled than H_2O-cooled. Since Cu is activated by thermal neutrons, it's reasonable to assume that neutrons that are being reflected back from the water at the end of the channel are being thermalized as a result of their scattering. The Cu foils would then be activated by such neutrons, yielding these bottom-axial 'upticks'. That these 'upticks' are higher for the *air*-cooled rather than the H_2O-cooled indicates that this thermalized-scattering is most likely being done by the *heavy* water just outside the end of the channel, and *not* by any *light* water inside it.

From the radial neutron-flux plots, one can further see that the Cu distributions are, indeed, those of a thermal distribution (*i.e.*, triple-humped), which is consistent with neutron back-scatter from the moderator.

Finally, the root-mean-square (RMS) errors in the normalized Cu activation rate distributions (between the experimental and MCNP tallies) were determined to be approximately 1%, with the errors being slightly higher for the air-cooled cases than the H_2O-cooled cases. Thus, the agreement between MCNP and the experiment for the normalized flux distributions was found to be very good.

4.3 Buckling Comparisons

The normalized flux distributions for both the foil experiments and the corresponding tallied MCNP simulations were then fit by least squares to combined Bessel/cosine functions [$\phi\{r,z\} = A_0 J_0\{\lambda r\} \cos\{\alpha(z-z_{max})\}$] in the asymptotic region of the ZED-2 core to obtain the axial (α^2) and radial (λ^2) components of buckling, and hence the total buckling ($B^2 = \alpha^2+\lambda^2$). The asymptotic region is defined where the neutron energy spectrum remains unchanging, and was found to be inside the core region leaving out the top 2 and bottom 2 axial foils (tallies), and also by excluding the radial foils (tallies) outside K6W/K6E. The uncertainties in the fitting parameters A_0, z_{max}, α and λ were found using a chi-squared variance.

Results for the total buckling determined from the foil experiments and from the corresponding MCNP simulations are shown in Table 2. The uncertainties for the axial and radial bucklings were then taken as $\pm\delta\alpha^2=\pm2\alpha\delta\alpha$ and $\pm\delta\lambda^2=\pm2\lambda\delta\lambda$. The uncertainty for the total buckling was that of the components combined in quadrature, $\delta B^2=[(\delta\alpha^2)^2+(\delta\lambda^2)^2]^{½}$.

The total buckling for the air-cooled cases ranged from approximately 7.0 m^{-2} to 6.8 m^{-2}, decreasing with moderator temperature, while the H_2O-cooled cases ranged from approximately 5.5 m^{-2} to 5.4 m^{-2}, also decreasing with increasing moderator temperature.

When plotted against moderator temperature, the variation of MCNP (experimental†) buckling with T_{mod} was found to be –0.004±0.007 $m^{-2}/^{o}C$ (–0.008±0.006 $m^{-2}/^{o}C$) for the air-cooled, and –0.008±0.005 $m^{-2}/^{o}C$ (–0.002±0.004 $m^{-2}/^{o}C$) for the H_2O-cooled. Not only are the MCNP and experimental values consistent with each other, they are also (mostly) consistent with zero. Thus, there appears to be little/no variation of buckling with moderator temperature (at least, at these temperatures).

The differences between MCNP and experiment for the total buckling were usually less than 0.1 m^{-2}, or usually less than 1% (with a tendency for the MCNP buckling to be less than the experimental buckling). If the quadrature-combined uncertainties in the experimental and MCNP bucklings are taken into account, the buckling differences between MCNP and experiment was usually less than two standard deviations.

5. Conclusions

MCNP-generated computer runs were performed to simulate the air- and H_2O-cooled moderator-temperature experiments performed in ZED-2. The resulting k_{eff}'s were found for all runs, while neutron flux tallies, to simulate Cu activation data, were also found for the foil (tallied) runs.

The overall average* air-cooled k_{eff} bias was found to be• –7.51±0.39 mk, while the overall average H_2O-cooled k_{eff} bias was found to be –10.95±0.61 mk. (The reproducibility uncertainty for k_{eff} is typically ~0.2 to 0.3 mk for repeat measurements on *nominally* the same lattice.) The bias in the coolant-void reactivity was found to range from approximately +2.8 mk to +4.3 mk, with an uncertainty of approximately ±0.4 mk.

The coolant-void reactivity bias was also found to be essentially constant when plotted against changing moderator temperature (+0.014±0.020 $mk/^{o}C$). The dependencies of k_{eff}'s on moderator temperature (biases in MTCs) were found to be close to zero for all cases. For the tallied (untallied‡) cases, the biases in air-cooled MTCs were found to be +0.013±0.018 $mk/^{o}C$ (+0.023±0.017 $mk/^{o}C$), while the biases in H_2O-cooled MTCs were found to be +0.022±0.008 $mk/^{o}C$ (+0.009±0.009 $mk/^{o}C$).

Plots of normalized copper activation distributions demonstrate that MCNP accurately predicts the thermal neutron flux distribution (since copper activation is dominated by thermal neutron absorption). In addition, comparison of buckling calculations shows close agreement between MCNP and the experiment, within combined uncertainties.

† The experimental values being shown in (*brackets*).

* The 'overall averages' here combine tallied and untallied k_{eff}'s, (in a weighted fashion).

• The uncertainties of k_{eff} here include the standard deviational spread in k_{eff}'s with the MCNP and D_2O-induced uncertainties in k_{eff}, all combined in quadrature.

‡ The untallied values being shown in (*brackets*).

6. References

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[4] Lane,V. and Members of the Cross Section Evaluation Working Group; "ENDF-201 ENDF/B-VI Summary Documentation Supplement I (4th Ed.)", App.A; National Nuclear Data Center, Brookhaven National Laboratory, Upton, New York, USA, 11973-5000; BNL-NCS-17541; 2001, Nov. 2.

Table 1: MCNP Calculations of k_{eff} for Moderator Temperature Experiments

Nominal T_{mod} [°C]	Foils?	H_2O			Air		
		T_{mod} [°C]	k_{eff}	$\pm\delta k_{eff}$	T_{mod} [°C]	k_{eff}	$\pm\delta k_{eff}$
20	No	20.06	0.98848	0.00019	20.93	0.99226	0.00037
20	Yes	20.22	0.98856	0.00017	21.50	0.99230	0.00035
35	No	34.68	0.98921	0.00019	34.26	0.99225	0.00037
40	No	40.55	0.98925	0.00019	41.22	0.99282	0.00037
40	Yes	42.70	0.98978	0.00017	40.09	0.99250	0.00035
50	No	49.62	0.98862	0.00019	49.80	0.99282	0.00037
50	Yes	49.98	0.98893	0.00017	49.32	0.99266	0.00035

Table 2: Comparison of Experimental and MCNP Bucklings

T_{mod} [°C]	Coolant	Exp't $B^2 \pm d(B^2)$	MCNP $B^2 \pm d(B^2)$	% Diff.	$\|\Delta(B^2)/\delta(B^2)\|$
21.50	Air	7.035 ± 0.047	7.000 ± 0.039	–0.51	0.58
40.09	Air	6.844 ± 0.043	6.853 ± 0.037	0.13	0.16
49.32	Air	6.793 ± 0.044	6.874 ± 0.055	1.20	1.15
20.22	H_2O	5.552 ± 0.024	5.511 ± 0.028	–0.74	1.12
42.70	H_2O	5.515 ± 0.026	5.499 ± 0.029	–0.30	0.43
49.98	H_2O	5.490 ± 0.026	5.373 ± 0.030	–2.10	2.93

$\Delta(B^2) \equiv$ *buckling differences* $\equiv B^2_{MCNP} - B^2_{Expt}$

$\delta(B^2) \equiv$ *quadrature-combined buckling uncertainties* $\equiv [d(B^2_{MCNP})^2 + d(B^2_{Expt})^2]^{1/2}$

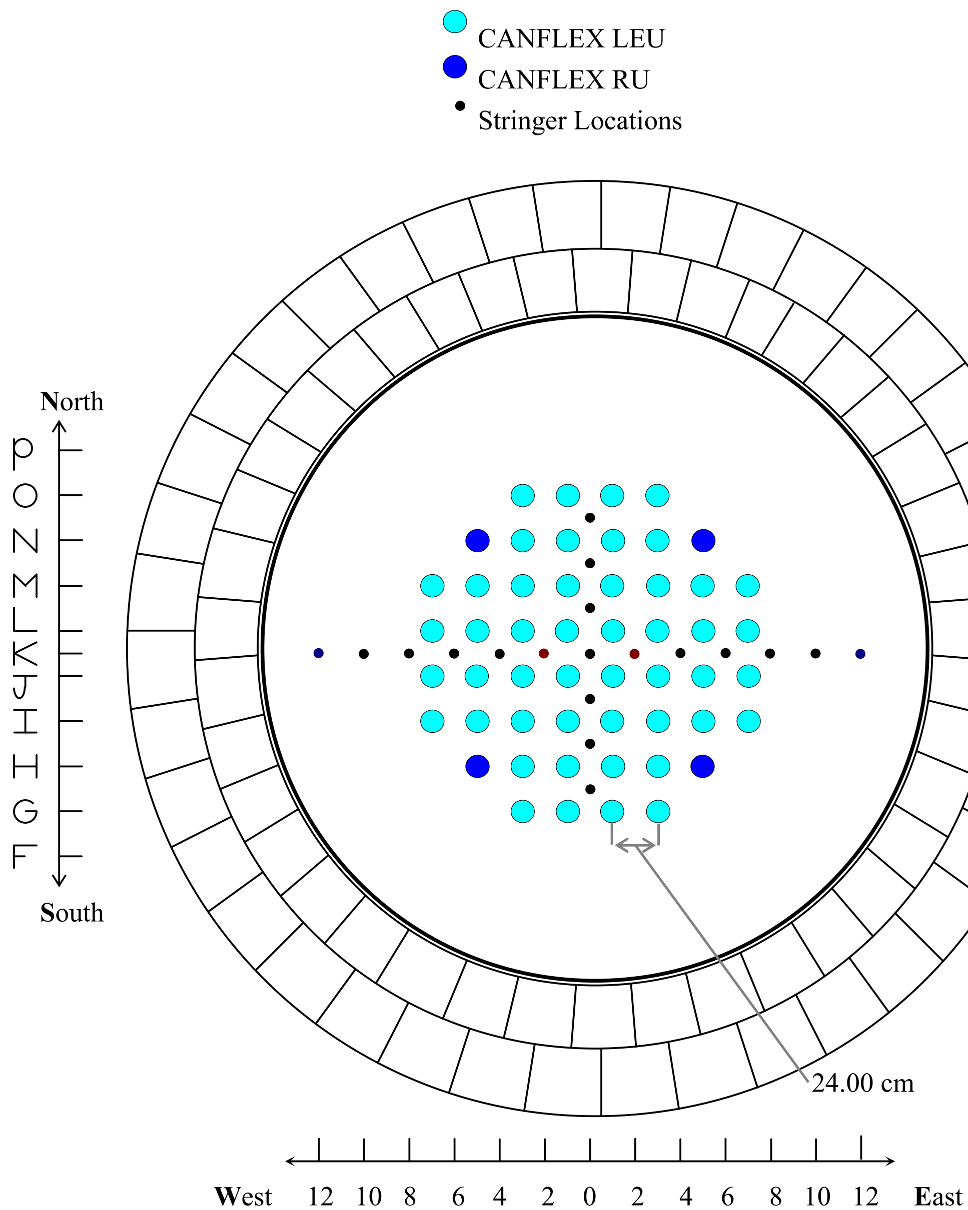

Figure 1: Top View of Lattice in ZED-2 with Locations of Foil Stringers

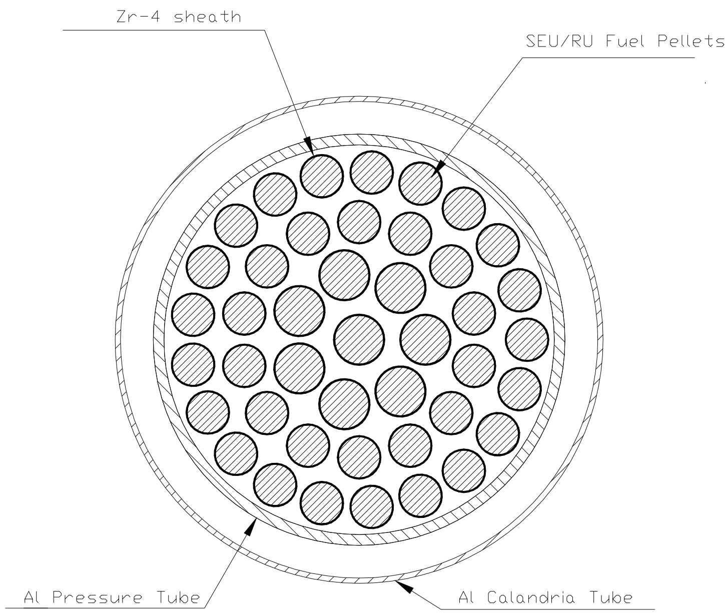

Figure 2: CANFLEX Fuel Bundle

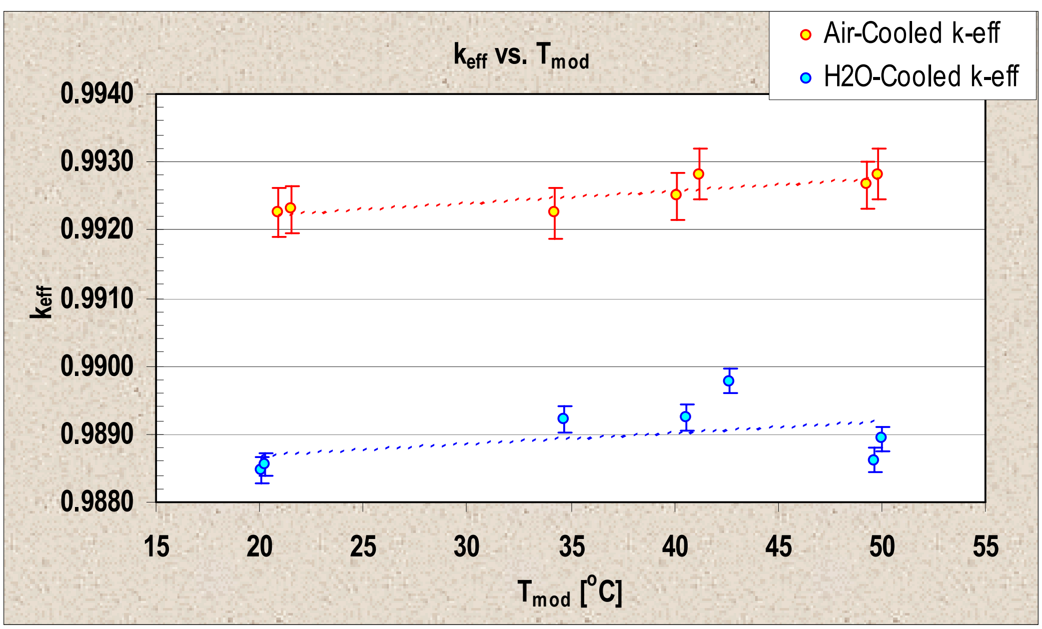

Figure 3: k_{eff} vs. Moderator Temperature

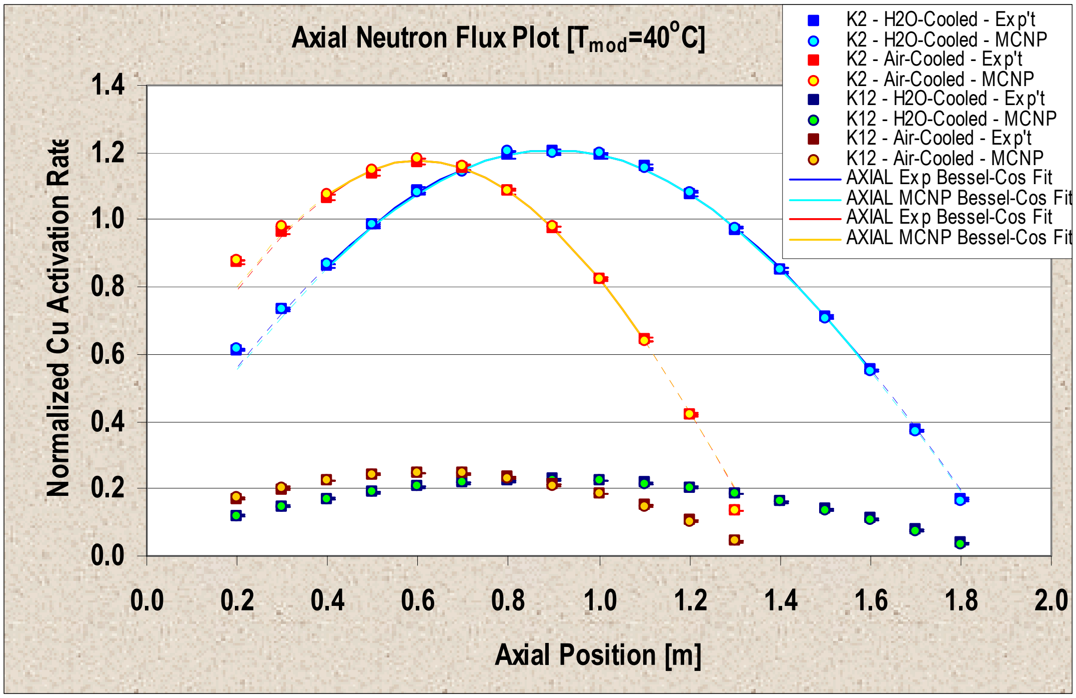

Figure 4: Normalized Cu Axial Flux Distributions at $T_{mod} = 40^{o}C$

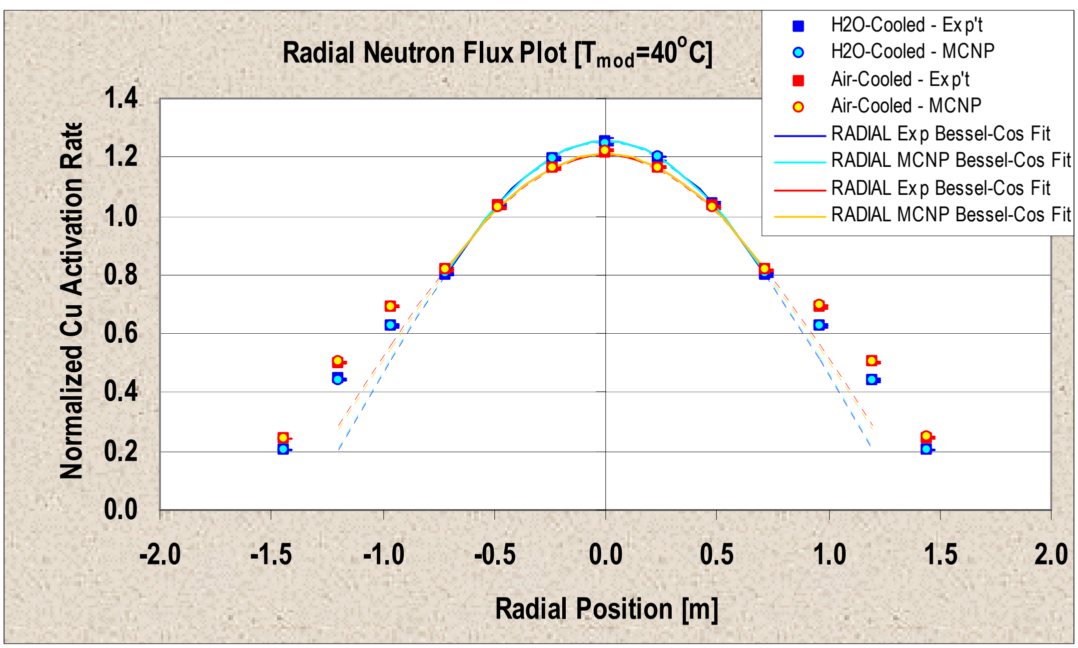

Figure 5: Normalized Cu radial Flux Distributions at $T_{mod} = 40^{o}C$