COMPARISON OF BARE-LATTICE CALCULATIONS USING MCNP AGAINST MEASUREMENTS WITH CANFLEX®*-LEU IN ZED-2

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Abstract

This paper summarizes bare-lattice calculations performed using MCNP5 and compared against full-core measurements performed in the ZED-2 Critical Facility at Atomic Energy of Canada Limited's Chalk River Laboratories. The results demonstrate that the total buckling calculated from a bare-lattice model in MCNP5 with the axial and radial dimensions adjusted to match the k-effective offset of a full-core post-test simulation matches the total buckling value measured in ZED-2 within the uncertainties of the calculation and measurement. The study shows that the calculated k-effective offset of a post-test simulation of a ZED-2 lattice modeled using MCNP5 is solely a property of the lattice and is not related to the large radial and axial leakage in ZED-2 and the surrounding D_2O and graphite reflector.

1. Introduction

This paper describes the analysis of substitution experiments performed in the ZED-2 reactor at Chalk River Laboratories [1] to provide data for checking the accuracy of reactor physics codes and associated nuclear data libraries that are used in the design and safety analysis of the Advanced CANDU Reactor™ (ACR™)•[2].

A substitution experiment is a mixed lattice of test fuel, which has unknown lattice physics properties, and reference fuel, which has known properties. In a substitution experiment, the size of the mixed lattice is adjusted (usually by adjusting the moderator height) such that the reactor becomes just critical (k_{eff} =1.000). The critical size of the mixed lattice is determined by the characteristic lattice physics properties (e.g., material buckling) of both the test fuel and the reference fuel. The objective is to isolate and determine the characteristic lattice physics properties of the test fuel alone through the analysis of the substitution experiments. The approach used and described in this paper for analysing substitution experiments makes use of MCNP [3], instead of older deterministic methods [4], and builds on previous development work [5].

Substitution analysis makes it possible to isolate the offset in the calculation of k_{eff} by MCNP for a lattice of pure test fuel from the offset in k_{eff} determined from the simulation of a mixed lattice (test fuel and reference fuel) in a substitution experiment. After determination of the offset in k_{eff} for the test fuel by analysis, an MCNP simulation for a bare lattice of pure test fuel sized to give the same offset in k_{eff} can be used to determine the material buckling (B^2) of the test fuel by fitting cosine and Bessel functions to the calculated neutron flux

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• ACR™ (Advanced CANDU Reactor™) is a trademark of AECL.

distributions. Subsequently, the buckling can be used in a deterministic lattice physics code such as WIMS-AECL [6] to calculate k_{eff} and its offset. Thus, by performing a substitution analysis, it is possible to determine the offsets in k_{eff} for both MCNP5 [3] (the probabilistic code) and for WIMS-AECL (the deterministic code), for a small amount of test fuel in a given lattice.

2. General description of the ZED-2 reactor

Figure 1 shows a side view of the ZED-2 reactor. ZED-2 is a tank-type critical facility used to study the physics of heavy-water moderated lattices. The cylindrical calandria is constructed out of aluminium and has a diameter of approximately 3.36 m and is 3.34 m deep. Fuel assemblies are suspended in the calandria from movable steel beams that are positioned across the top of the reactor. The reactor is made critical by pumping heavy water into the calandria, and is controlled by adjusting the heavy-water level.

3. Substitution experiments

The substitution experiments analysed were progressive substitutions of test fuel channels into a reference lattice to obtain critical height data for multiple substitution arrangements. For the duration of the progressive substitution experiments, ZED-2 was operated continuously to minimize changes in moderator purity and temperature. Data from two substitution measurements are presented. The first was H_2O-cooled CANFLEX-LEU fuel substituted into an air-cooled CANFLEX-LEU fuel reference lattice. The air-cooled reference lattice (Figure 2) was progressively flooded from the centre with a sequence of 4, 12, 16, 32, and finally 52 flooded fuel channels as shown in Figure 3 through Figure 6. The CANFLEX-LEU fuel is a 43-element bundle with 0.95 wt% ^{235}U/U enriched uranium dioxide. The lattice pitch was 24-cm square.

The second substitution experiment involved air-cooled CANFLEX-LEU fuel substituted into an H_2O-cooled CANFLEX-LEU fuel reference lattice. This was performed by progressively flooding the air-cooled reference lattice from the outside towards the centre of the core with a sequence of 20, 36, 40, 48 and finally 52-flooded fuel channels. This sequence is equivalent to starting with an H_2O-cooled reference lattice, and then progressively voiding channels from the centre to the outside in the sequence of 4, 12, 16, 32, and then 52.

4. ZED-2 MCNP model

The MCNP model consisted of a detailed three-dimensional representation of the ZED-2 reactor. The aluminium calandria, air gap, graphite reflector, dump lines, and borated polyethylene neutron shields were all included in the MCNP model of ZED-2. The 52 fuel channels were included in the model with 5 fuel bundles in each channel. The bottom of the fuel was located at 15 cm from the top of the calandria floor. For the post-simulations of the measurements that were done with flooded channels, the light water was modeled up to the top of the fifth bundle. The heavy water was modeled up to the measured critical height and the mixture of air and heavy-water vapour above the critical height was modeled as air. The model did not include the stainless steel support beams from which the fuel channels are suspended.

5. Neutron production correction factors

In MCNP, the calculated effective multiplication factor (k_{eff}) values for critical experiments performed in ZED-2 are not equal to unity (i.e., there is a non-zero bias in the calculated k_{eff} values). A neutron production correction factor (NPCF) is a scaling factor that may be used to adjust the calculated k_{eff} to 1.000. MCNP was modified such that the weight of the fission neutrons born in the fuel are multiplied by the NPCF, and the value of the NPCF is adjusted until the value of k_{eff} calculated by MCNP is equal to unity within the combined uncertainties of the calculations, which are statistical, and the uncertainties in k_{eff} due to the uncertainties in the key measured parameters in the experiment (e.g., moderator purity, critical height). The method used to determine the NPCF values for the different fuel types at different coolant conditions consists of running full-core MCNP simulations of critical experiments performed in ZED-2 using the measured operational conditions (e.g., moderator purity and temperature) and critical moderator height. The NPCF value of a reference fuel type at a given coolant condition is equal to $1/k_{eff}$. NPCFs were determined for the following reference lattices:

- air-cooled CANFLEX-LEU at 24-cm square lattice pitch
- H_2O-cooled CANFLEX-LEU at 24-cm square lattice pitch

Normally, in the analysis of a substitution experiment, the NPCF for a full-core of reference fuel is determined (which makes k_{eff} =1.000 for the reference lattice). After the NPCF that was derived from the full-core experiment is applied to the reference fuel an NPCF for the test region is derived which results in k_{eff} for the entire lattice to equal 1.000. The buckling for the test region is then determined by creating a full-core of test fuel, with the NPCF for that fuel, and adjusting the size of the core until k_{eff}=1.000. The buckling is then determined from the axial and radial flux distributions.

The current study allowed the NPCF values of the test fuel and the reference fuel to be determined from simulations of full-core lattice measurements in ZED-2. Hence, the NPCF values for the test fuel and reference fuel were determined with the highest accuracy possible from ZED-2 measurements. By applying the NPCF for the test fuel that was determined from the analysis of a full-core of test fuel to various sizes of substitution cores, the sensitivity of the NPCF to the size of the substitution region can be determined. Ideally, k_{eff} would equal 1.000 for all substitution cores.

The NPCF values determined for the H_2O-cooled and air-cooled CANFLEX-LEU lattices at 24-cm pitch from the simulations of the full-core experiments were subsequently used in the simulations of the progressive substitution experiments since the method allows for different fuel types to be given different NPCF values. Table 1 and Table 2 give the results of the substitution analyses in terms of the k_{eff} values with their associated uncertainties. The values of k_{eff} calculated for the MCNP simulations of the substitution experiments using the NPCFs derived from the analysis of the full-core experiments were found to range from 0.99983 to 1.00023. The remaining offsets in k_{eff} (-0.17 mk to + 0.23 mk) are generally within the uncertainty of the analysis (within two standard deviations), where the combined one-sigma uncertainties ranged from ±0.10 mk to ±0.12 mk. The NPCF value for test fuel in a substitution experiment is insensitive to the size of the test region to within the uncertainty of the analysis as shown in Table 1 and Table 2.

The older deterministic methods [4] relied on extrapolation of the results from progressive substitution experiments. The new method using MCNP requires only a single substitution core.

5.1 Theory behind the use of the NPCF

MCNP can predict the neutron flux distributions in ZED-2 within the combined uncertainties of the calculations and the measurements (usually less than ±1%) as illustrated in Figure 7 and Figure 8. Hence the radial and axial leakages of the lattice are properly modeled in the full-core MCNP model of the ZED-2 reactor. In principle, the calculated values of k_{eff} in the MCNP simulations should be exactly equal to unity to balance the neutron productions to the sum of the neutrons being absorbed and leaking out of the system. According to the fundamental modified one-group diffusion theory, as shown in Equation 1, k_{eff} is proportional to the infinite multiplication factor (k_∞) and inversely proportional to geometric buckling (B^2). For a critical reactor, the material buckling and geometric buckling are equivalent.

$$k_{eff} = \frac{k_\infty}{1 + M^2 B^2} \quad (1)$$

Where

k_{eff} is the neutron multiplication factor of a system that has leakage

k_∞ is the neutron multiplication factor in an infinite medium

M is the neutron migration length (cm)

B^2 is the geometrical buckling (cm^{-2})

Since MCNP can predict the flux distribution (and hence B^2) quite accurately, it may be assumed that the non-leakage probability term, $1/\left(1 + M^2 B^2\right)$, is also predicted accurately. Hence it can be presumed that most of the discrepancy in the calculation of k_{eff} is attributable to an under-estimate (or over-estimate) of the value of k_∞. The value of k_∞ is calculated with Equation 2.

$$k_\infty = \frac{\nu \Sigma_f}{\Sigma_a} \quad (2)$$

Where

ν is the fission-neutron yield

Σ_f is the fission cross section (1/cm)

Σ_a is the absorption cross section (1/cm)

The weight of the neutrons born in the fuel is scaled up (or down) by an NPCF value, which has the equivalent effect of changing ν and therefore changes the value of k_∞ calculated by MCNP. The physical effect of the implementation of the NPCF in the MCNP simulation is to artificially increase (or decrease) the value of k_∞, such that k_{eff} will become unity. The NPCF helps correct for any errors that might exist in the nuclear cross-section data that cause discrepancies in the calculation of k_{eff}.

The NPCF values for the two lattice types were determined from MCNP simulations of full-core experiments using 50,000 neutron histories per cycle, 200 inactive cycles and 400 active cycles.

6. Bare lattice calculations

Once the NPCF is obtained for the test fuel a bare lattice of the fuel is modeled in MCNP as shown in Figure 9 and the NPCF is applied to the test fuel. The axial and radial dimensions

are adjusted until the calculated k_{eff} value is unity. In this analysis, NPCF values derived from a full-core of test fuel were used.

Virtual surfaces were set up in various equi-distant positions in the MCNP model of ZED-2 in the axial and radial directions to tally the neutron flux distributions. The neutron fluxes were tallied at those positions and then multiplied by the copper-capture cross section. This technique corresponds to using the infinite dilution model where foils are not explicitly modeled to avoid perturbing the global neutron flux distribution. Each MCNP run typically consisted of up to 60,000 neutron histories per cycle, 200 inactive cycles, and 5,800 active cycles, for a total of 6,000 cycles.

The copper-capture tallies were fitted to a cosine function axially, and a Bessel function radially. The radial buckling was determined by fitting the radial distributions of copper activation rates to a Bessel function. The fitted curve was used to extrapolate to the point of zero flux. This defines the extrapolated radius R_{ex}. The axial buckling was determined by fitting the axial distributions of copper activation rates to a cosine function. The fitted curve was used to extrapolate to the point of zero flux above and below the lattice. The distance separating these points defines the extrapolated height H_{ex}. The buckling was then determined using the following expression:

$$B^2 = (2.405/R_{ex})^2 + (\pi/H_{ex})^2$$

The results of the bare-lattice calculations shown in Table 3 demonstrate that the material buckling derived from a bare-lattice model in MCNP is in good agreement (within 1%) with the total buckling value measured in ZED-2 determined using the traditional flux-map method (The uncertainty in the substitution derived buckling in Table 3 is based only on the fit to the expression above). A flow chart of the MCNP-based substitution analysis method is shown in Figure 10.

8. Conclusion

This paper describes the analysis of substitution experiments performed in the ZED-2 reactor at Chalk River Laboratories using a modified version of MCNP5. The results demonstrate that applying an NPCF value derived from a full-core of test fuel to substitution lattices, the resulting k_{eff} is insensitive to the size of the test region. Therefore, implying that the NPCF is insensitive to the size of the test region. Material bucklings obtained using the substitution method for the cores analysed are within 1% of the values derived from full-core flux maps in ZED-2.

9. References

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9. Acknowledgements

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Table 1
k_{eff} values for the 24-cm H_2O-cooled LEU fuel substituted into voided LEU core

Lattice	Reference Fuel Coolant	Test Fuel Coolant	k-effective	±δk-effective			
				Effect of the Uncertainty in NPCF Values	Uncertainty in MCNP	Experimental Uncertainty	Total Uncertainty
Reference	Air	-	1.00000	NA	0.00006	0.00003	0.00007
4-rod sub	Air	H_2O	1.00022	0.00010	0.00006	0.00003	0.00012
12-rod sub	Air	H_2O	1.00023	0.00009	0.00006	0.00002	0.00011
16-rod sub	Air	H_2O	1.00020	0.00008	0.00006	0.00002	0.00010
32-rod sub	Air	H_2O	1.00020	0.00008	0.00006	0.00001	0.00010
Reference	H_2O	-	1.00000	NA	0.00006	0.00001	0.00006

Table 2
k_{eff} values for the 24-cm voided LEU fuel substituted into H_2O LEU core

Lattice	Reference Fuel Coolant	Test Fuel Coolant	k-effective	±δk-effective			
				Effect of the Uncertainty in NPCF Values	Uncertainty in MCNP	Experimental Uncertainty	Total Uncertainty
Reference	H_2O	-	1.00000	NA	0.00006	0.00001	0.00006
4-rod sub	H_2O	Air	1.00018	0.00010	0.00006	0.00001	0.00011
12-rod sub	H_2O	Air	1.00014	0.00009	0.00006	0.00002	0.00011
16-rod sub	H_2O	Air	1.00014	0.00009	0.00006	0.00002	0.00011
32-rod sub	H_2O	Air	0.99983	0.00010	0.00006	0.00003	0.00012
Reference	Air	-	1.00000	NA	0.00006	0.00003	0.00007

Table 3
Bare-lattice calculated buckling compared against measured buckling

Lattice Pitch	Coolant	Substitution Derived Buckling (m^{-2})	Measured Buckling (m^{-2})	Difference (Calc.-Meas.)*100%/ Measured
24.0	Air	6.971 ± 0.030	6.962 ± 0.061	0.13
24.0	H_2O	5.241 ± 0.012	5.210 ± 0.016	0.60

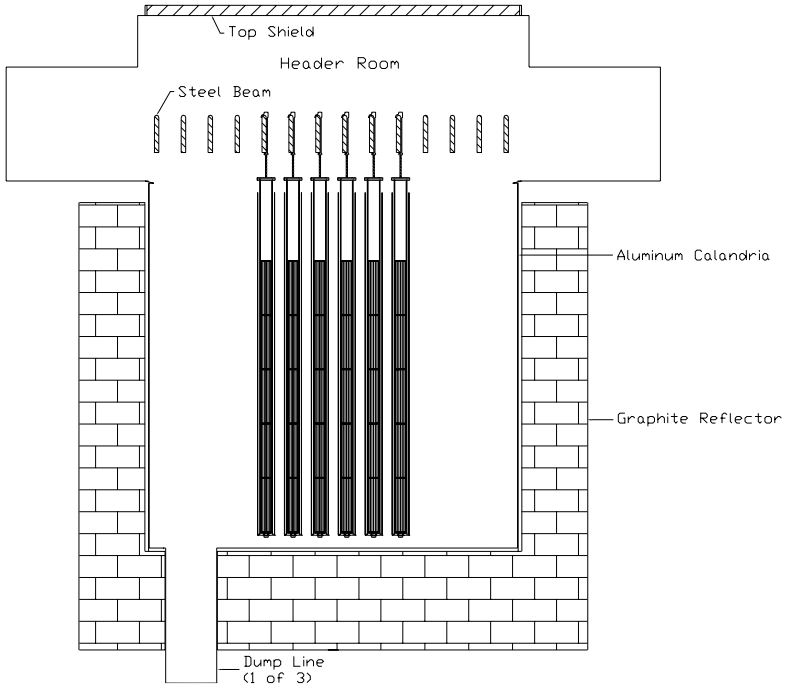


Figure 1 Side view of ZED-2

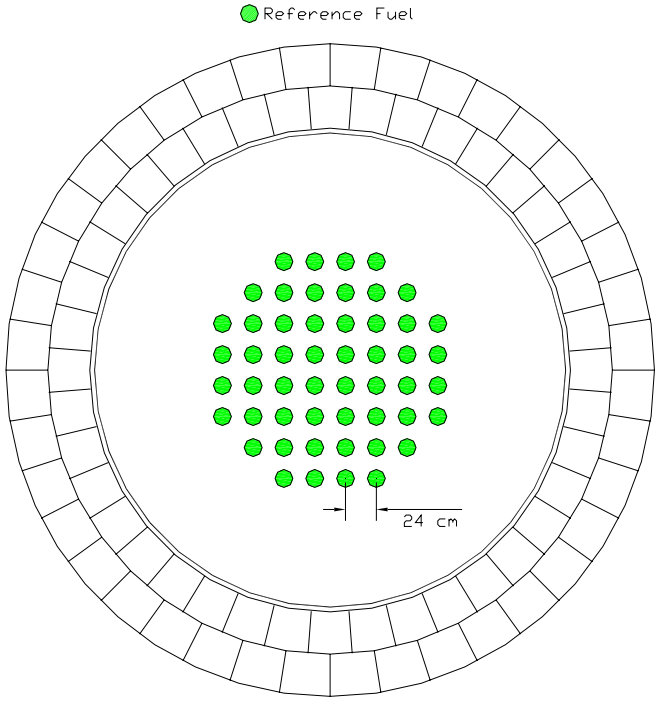


Figure 2 ZED-2 reference lattice

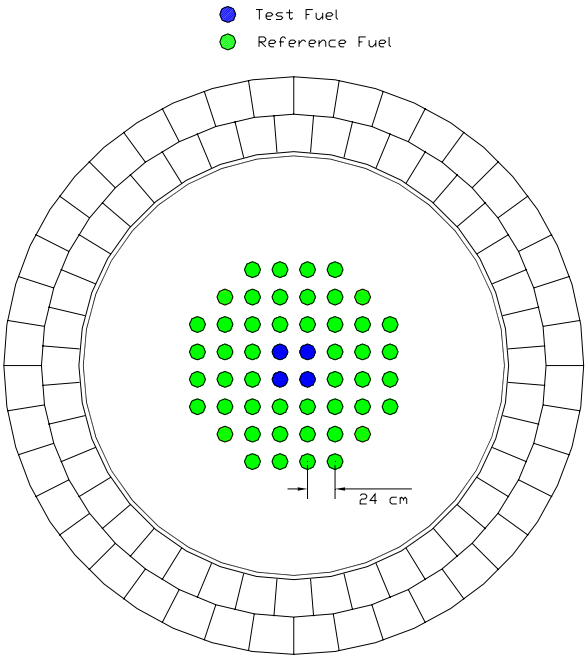


Figure 3 Four-channel substitution lattice

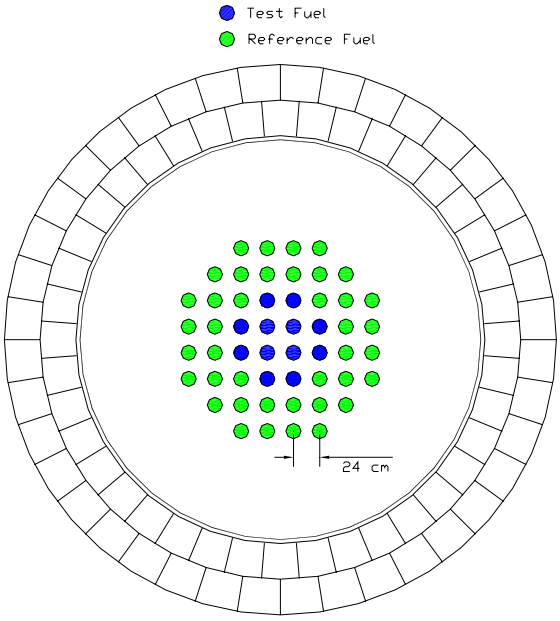


Figure 4 Twelve-channel substitution lattice

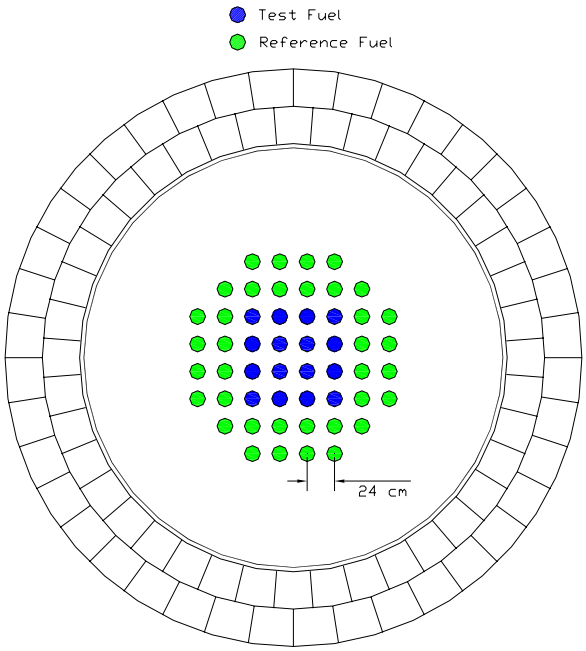


Figure 5 Sixteen-channel substitution lattice

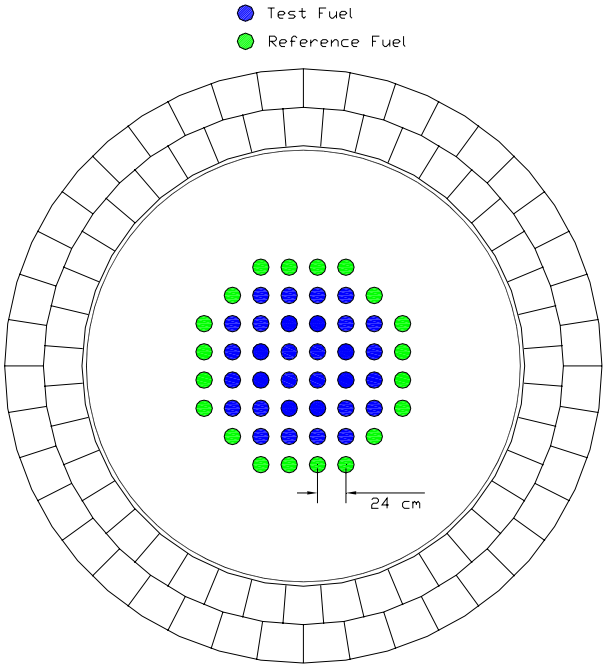
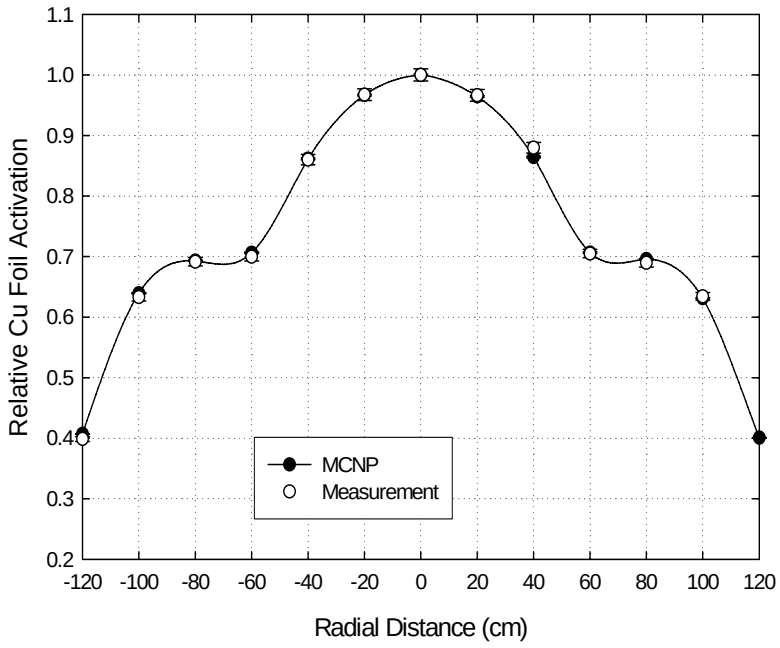
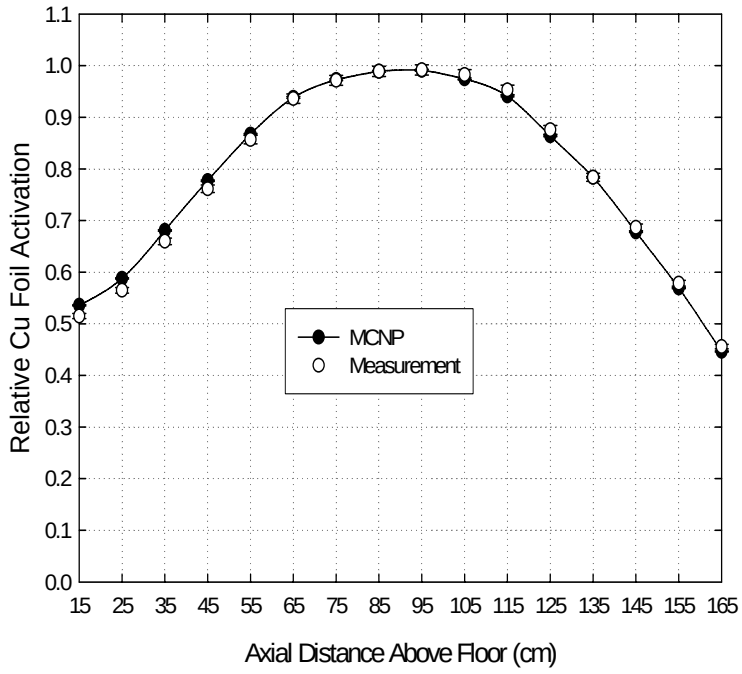


Figure 6 Thirty-two-channel substitution lattice

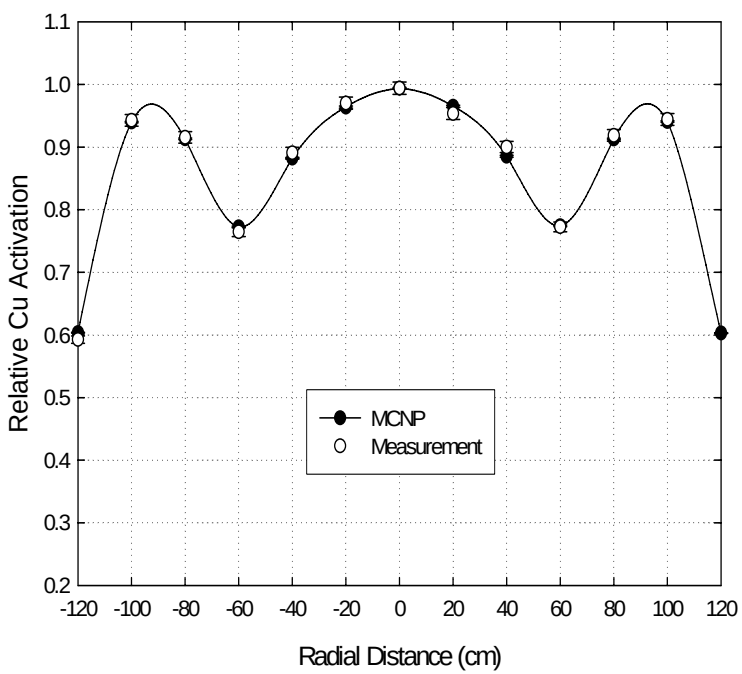


Radial Flux Distribution

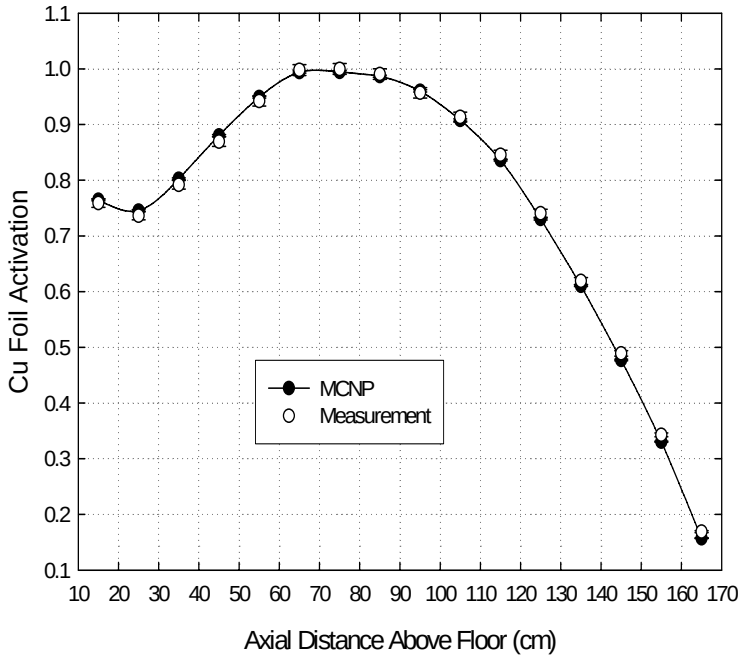


Axial Flux Distribution

Figure 7 Flux distributions in ZED-2 for reference lattice of H_2O-cooled CANFLEX-LEU



Radial Flux Distribution



Axial Flux Distribution

Figure 8 Flux distributions in ZED-2 for reference lattice of Air-cooled CANFLEX-LEU

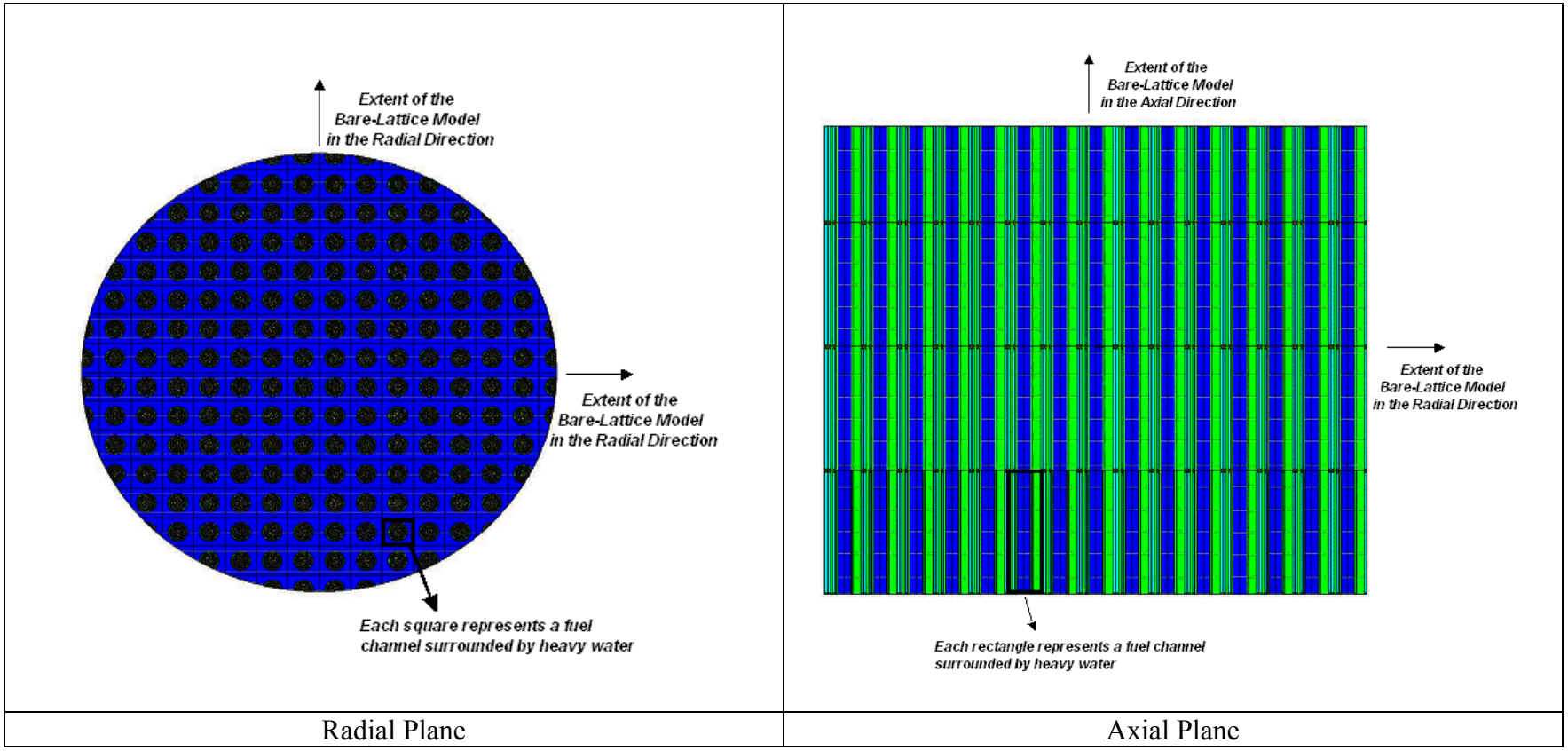


Figure 9 Bare-lattice Model in MCNP

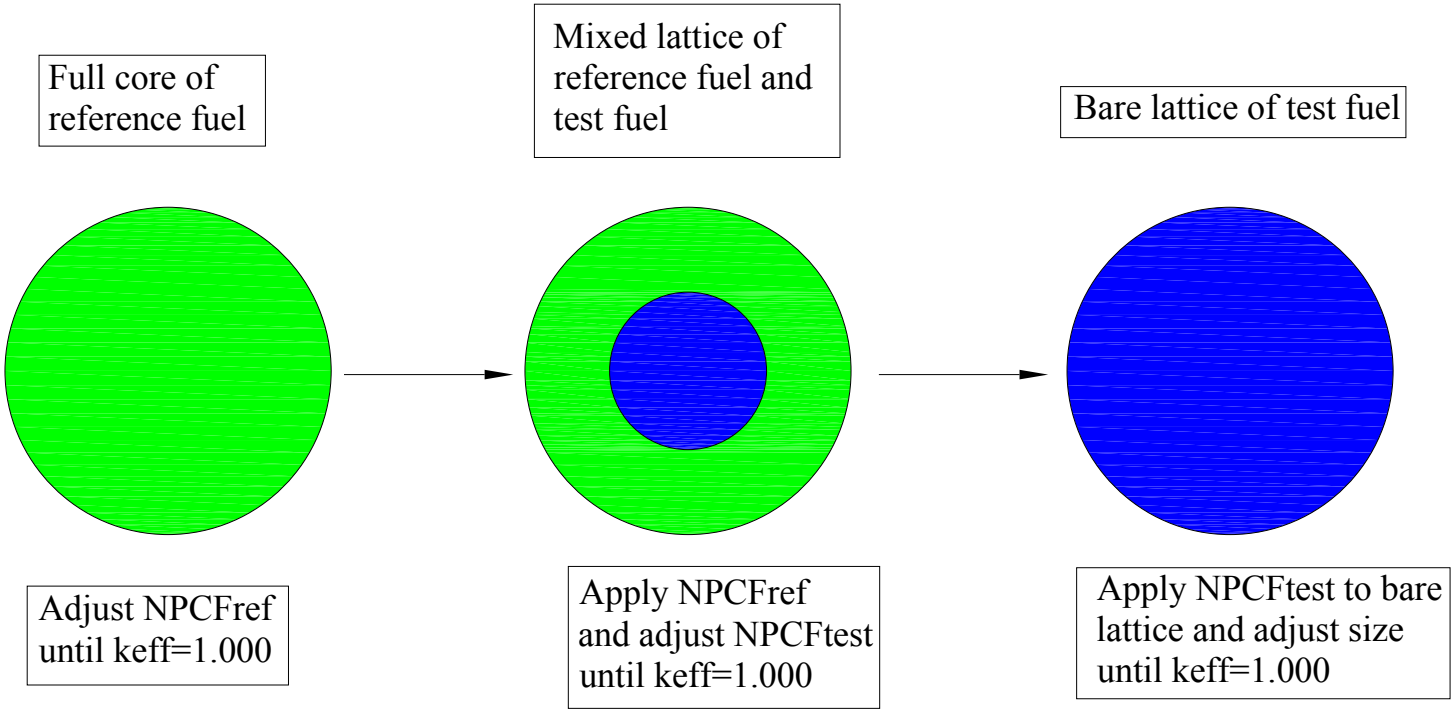


Figure 10 Simplified schematic description of MCNP-based substitution analysis method [5]