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ASSESSMENT OF CANDU REACTOR PHYSICS EFFECTS USING A SIMPLIFIED WHOLE-CORE MCNP MODEL

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ABSTRACT

A whole-core Monte Carlo n-particle (MCNP) model of a simplified CANDU® reactor was developed and used to study core configurations and reactor physics phenomena of interest in CANDU safety analysis. The resulting reactivity data were compared with values derived from corresponding WIMS-AECL/RFSP, two-neutron-energy-group diffusion theory core simulations, thereby extending the range of CANDU-related code-to-code benchmark comparisons to include whole-core representations. These comparisons show a systematic discrepancy of about 6 mk between the respective absolute $k_{effective}$ values, but very good agreement to within about -0.15 ± 0.06 mk for the reactivity perturbation induced by ¼-core checkerboard coolant voiding. These findings are generally consistent with the results of much simpler uniform-lattice comparisons involving only WIMS-AECL and MCNP. In addition, MCNP fission-energy tallies were used to evaluate other core-wide properties, such as fuel bundle and total-channel power distributions, as well as intra-bundle details, such as outer-fuel-ring relative power densities and outer-ring fuel element azimuthal power variations, which cannot be determined directly from WIMS-AECL/RFSP core calculations. The average MCNP values for the ratio of outer fuel element to average fuel element power density agreed well with corresponding values derived from WIMS-AECL lattice-cell cases, showing a small systematic discrepancy of about 0.5 %, independent of fuel burn-up. For fuel bundles containing the highest-power fuel elements, the maximum peak-to-average outer-element azimuthal power variation was about 2.5% for cases where a statistically significant trend was observed, while much larger peak-to-average outer-element azimuthal power variations of up to around 42% were observed in low-power fuel bundles at the core/radial-neutron-reflector interface.

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1. INTRODUCTION

In CANDU® reactor physics analysis, Monte Carlo n-particle (MCNP) [1] neutron transport calculations are often used as reference points for calculation methods that are used for core design, operation and safety assessment, especially when experimental validation data are lacking. Typically, this has involved infinite-lattice cell calculations [2], although comparisons have been made occasionally for finite lattices [3], including simplified core sub-region models [4] or symmetrical core segments [5]. The present work extends these MCNP benchmark applications to include a full three-dimensional representation of a CANDU 6 reactor core.

Although certain simplifications must still be made, a full-core MCNP CANDU model enables a realistic simulation of complex core configurations and states. For example, this model enables the determination of the static reactivity perturbation associated with coolant voiding of alternate fuel channels on one side of the reactor core, as would occur in the early stages of a hypothetical large-loss-of-coolant accident (LLOCA) in a CANDU 6 reactor. The same simulations can also be used to determine core power distributions, including some details, such as intra-bundle fuel element power distributions, that cannot be obtained directly using the diffusion-theory calculation methods normally used for whole-core analyses.

Some of these whole-core MCNP calculations pose significant numerical data processing challenges and require considerable running times to achieve adequate statistical precision in the CANDU case. Nevertheless, the benchmark data obtained provide useful reactor physics information for testing the simpler calculation methods used for routine reactor-core analysis, particularly for circumstances where it would not be practicable to obtain comparable information from real power reactors.

2. METHOD

The present whole-core MCNP model of a CANDU 6 reactor was developed specifically to perform code-to-code benchmark comparisons with corresponding two-neutron-energy-group diffusion theory results obtained using the WIMS-AECL/RFSP [6–8] (Winfrith Improved Multigroup Scheme–Atomic Energy of Canada Limited / Reactor Fuelling Simulation Program) code suite normally used in CANDU studies. The whole-core model approach was used so that complex core configurations of particular interest in CANDU safety analyses and involving non-uniform fuel burn-up distributions, local absorbers and asymmetric, non-uniform core perturbations could be simulated in a reasonably realistic manner.

The MCNP reactor core model includes all 380 fuel channels in the CANDU 6 core; the channels are arranged in a regular square lattice (pitch = 28.575 cm), with 22 horizontal rows (labelled A through W, excluding I) and 22 vertical columns (labelled 1 through 22). The specific representation used in MCNP consisted of a lattice of hexahedra with a pitch of 14.2875 cm, with the fuel channels being located at the centre of their respective lattice cells, as shown in Figure 1 (cross-sectional view near the reactor end face). At the coarse spatial resolution used in Figure 1, each calculation lattice cell containing a fuel channel appears essentially as a black square surrounded by eight interstitial white squares containing heavy-water moderator. An MCNP model with interstitial moderator lattice cells between fuel

channels was used to facilitate the simulation of reactivity devices, specifically vertical, cylindrical adjuster rods that are located at and near the core axial midplane (see Figure 2, which shows the adjuster rods as three horizontal sets of circles).

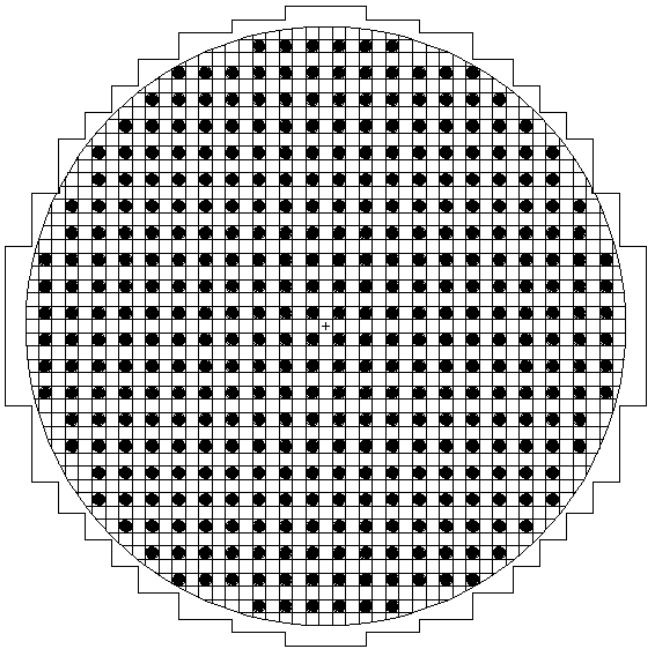

Figure 1. Cross-section of the CANDU 6 MCNP model (near the end face).

A jagged-edge radial boundary surface with vacuum flux boundary conditions (i.e., zero neutron importance outside) was used for this code-to-code benchmark problem, even though a circular radial boundary surface corresponding to the inside edge of the calandria vessel would have provided a more realistic representation of the CANDU radial reflector. The MCNP radial boundary surface replicates the jagged exterior of the standard RFSP CANDU 6 model (having 42, 34 and 22 active, rectangular mesh cells in the horizontal, vertical and axial directions, respectively). In turn, the RFSP calculations were performed with vacuum flux-extrapolation factors applied at each plane facet of the radial boundary surface.

Each fuel channel contains twelve 49.53-cm-long fuel bundles (total of 4560 bundles), as seen in the top view of the MCNP model near the vertical mid plane (see Figure 2). This figure also shows three banks of seven vertical, cylindrical, stainless-steel adjuster rods arranged at the core axial midplane and at a 80-cm axial distance from this midplane, on either side. Other devices that are normally inserted into the core, such as the liquid zone controllers, were excluded from the present model. Note the axial notches in the radial neutron reflector in Figure 2, such that the reflector is much thicker for axial bundle planes 3 through 10.

Vacuum boundary conditions are used at the axial plane surfaces. Note that, while both MCNP and RFSP used plane vacuum boundary conditions for this benchmark problem, in typical CANDU studies, RFSP is usually used with empirical, non-vacuum radial and axial flux-extrapolation factors (independent of neutron energy), with the radial flux extrapolating to zero on a hypothetical circular boundary surface.

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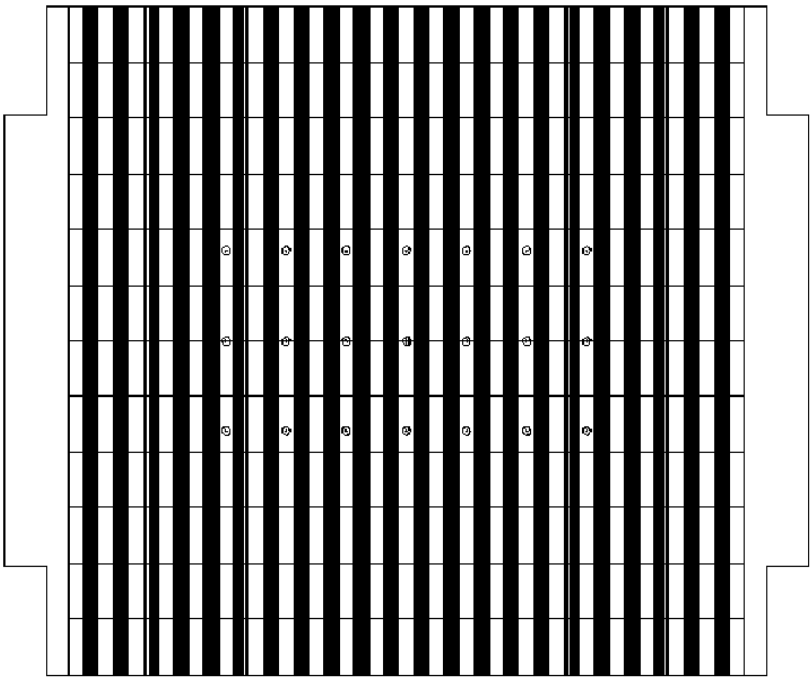

Figure 2. Top view of the CANDU 6 MCNP model (near the vertical midplane).

A typical equilibrium core, fuel bundle irradiation distribution was simulated based on a 'snapshot' of the Pt. Lepreau reactor state on 1984 December 31, as obtained from an earlier WIMS-AECL/RFSP core-follow study [9]. Both the MCNP and the present WIMS-AECL/RFSP calculations used a simplified burn-up distribution, with eleven representative fuel bundle burn-up values from 0.5 to 10.5 GW_td/tU in steps of 1.0 GW_td/tU. The approximate equilibrium-core burn-up distribution was obtained by rounding the detailed fuel burn-up values to the nearest representative value.

Each CANDU 6 fuel bundle contains 37 cylindrical fuel elements arranged in four annular fuel rings, as shown in Figure 3. All fuel bundles in the MCNP model had the same azimuthal orientation. Distinct fuel compositions were used in each of the four fuel rings, with 64 nuclides for each fuel material. The nuclide concentrations for each fuel ring and burn-up were derived from a separate WIMS-AECL fuel-depletion calculation.

Because not all of the nuclides used to describe the irradiated fuel composition in WIMS-AECL are available in the MCNP data library (e.g., pseudofission-product nuclides used to represent collective residual fission-product behaviour in WIMS-AECL), those that were not available in both codes were eliminated from both WIMS-AECL and MCNP calculations. This truncation increased the WIMS-AECL absolute k_{eff} values by about 1.2 mk (1 mk represents a change in $k_{effective}$ of 0.001); however, the effect on lattice-cell coolant void reactivity (CVR) was negligible.

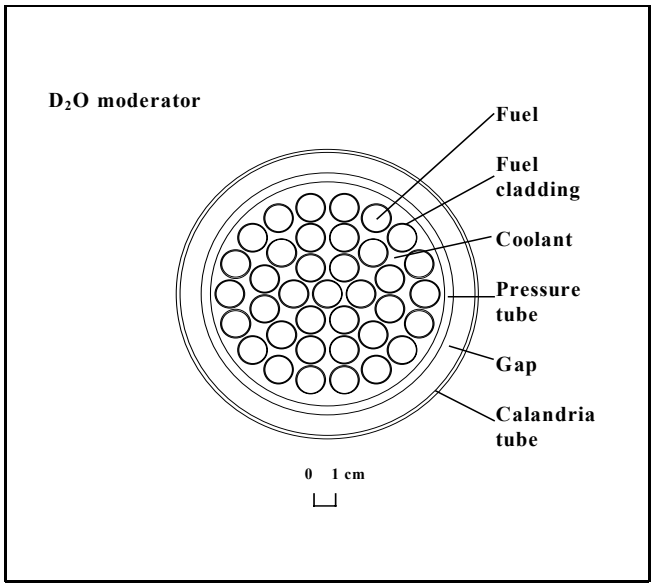

Figure 3. Cross-Section of a 37-Element CANDU Fuel Bundle

MCNP version 4B [1] was used with nuclear cross-section data obtained from the ENDF/B-VI (Evaluated Nuclear Data File Version B-VI, up to Release 5) library, using files prepared at AECL. These data include most of the nuclides needed to simulate structural and irradiated fuel material compositions at temperatures that are representative of the hot operating reactor condition.

Nominal fixed temperature values of 300, 600 and 900 K were used for the moderator, coolant and fuel, respectively. However, moderator and coolant nuclide number densities correspond to the values at 341.16 and 563.96 K, respectively, obtained from the reference WIMS-AECL case.

The WIMS-AECL comparison calculations used nuclear data that were based on ENDF/B-VI, Release 4 for ^{235}U and Release 2 for other nuclides. It is important to note that the WIMS-AECL lattice-cell calculations were performed using data, methods and approximations (e.g., 33 neutron energy groups for the main transport solution) that are normally used in typical CANDU studies (selected as a compromise between accuracy and speed) and that do not reflect the most accurate capabilities of the code. The sensitivity of the WIMS-AECL results to some of these approximations was studied in Reference [3].

The incremental cross-sections that were used to represent the adjuster rods in RFSP are typical CANDU values that were prepared using the DRAGON [10] code, but were not generated specifically to match the precise conditions used in the MCNP simulations.

Some of the simplifications and approximations of potential significance that remain in the whole-core MCNP model include the following:

- Other reactivity devices, such as the local zone controllers, which contain significant amounts of light water (H_2O), are not modelled.
- Neutron reflection associated with the stainless-steel calandria vessel and other ex-core materials is not simulated.
- The material temperature distribution within a fuel channel is assumed to be the same everywhere in the core, independent of local fuel bundle power.
- The same nominal fuel temperature (900 K) is used uniformly within a fuel element for all fuel rings in a bundle, irrespective of element power.
- Both the WIMS-AECL and MCNP calculations assume a uniform distribution of the fuel constituents, such as ^{235}U, ^{239}Pu and fission products, within each fuel element, even though the flux is depressed in the element interior. Similarly, the fuel composition is kept fixed around each fuel ring, even though azimuthal variations exist due to the radial location within the core and due to the presence of local neutron absorbers. In addition, the axial fuel composition is assumed to be uniform within a bundle.
- The coolant density and temperature are assumed to be constant along a fuel channel and the same for all fuel channels in the core.
- The concentrations of saturating fission products in both the MCNP and WIMS-AECL/RFSP calculations are based on a nominal power rating and do not reflect local power variations throughout the core.
- No fuel bundle end regions are modelled in MCNP (or in WIMS-AECL).

The whole-core CANDU MCNP model was used to simulate four core configurations, representing the fully cooled and ¼-core checkerboard coolant-voiding core states (i.e., voiding alternate channels on the right hand side of Figure 1), with the adjuster rods inserted (ARI) and withdrawn (ARW). The ¼-core checkerboard coolant-voiding pattern is relevant to the early stages of a hypothetical LLOCA, as a result of the configuration used for the primary heat transport system in a CANDU 6 reactor.

A converged MCNP starting neutron source distribution was built up for each core configuration in a series of steps, starting with a case having a single source neutron at the centre of each of the 4560 fuel bundles. The final MCNP k_{eff} values for each configuration were determined from a weighted average of the results from 22 to 34 separate MCNP cases involving 182 to 346 million total neutron histories (Mh) per data point. Each successive MCNP case used the most recent starting neutron source distribution, together with a new value for the starting pseudorandom number. Many of these MCNP cases used 250 active cycles of 60 000 neutron source particles each, while the subset used to calculate power distributions used 30 to100 active cycles of 150 000 neutron source particles each, which was the largest neutron source that could be used with the core models and computer platforms involved.

The optimum neutron source size presents somewhat of a numerical dilemma. On the one hand, MCNP k_{eff} values have a small negative bias that is inversely proportional to the number of source particles per generation [1], and even a neutron source of 150 000 neutrons represents less than one starting neutron on average for each of the 168 720 fuel elements in a CANDU 6 core. On the other hand, Reference [1] recommends that a minimum of 30 cycles, and more typically, 200 to 400 cycles be used for a single MCNP case to limit the potential for a negative bias in the estimated standard deviation of the MCNP k_{eff} values for systems with dominance ratios (second largest to largest eigenvalue) close to unity.

For certain cases, fission-energy tallies were accumulated for each of the 4560 fuel bundles, 18 240 fuel rings and 82 080 outer-ring fuel elements. The final power-distribution results were based on combining the results from 21 to 23 separate MCNP cases totalling 167 to 197 Mh per core configuration. Typical uncertainty values of about ±0.7% for the bundle powers and about ±2.0% for the outer-element powers were obtained.

Channel powers were calculated from the sum of the MCNP bundle powers in a fuel channel. The typical uncertainty in the channel power was estimated to be about ±1.6%, assuming that the axial bundle powers are statistically independent.

CANDU MCNP calculations are time consuming, in part because each source neutron typically undergoes around 180 collisions (primarily as thermal neutrons in the D_2O moderator) before termination. In addition, the MCNP cases with fission-energy tallies had execution times about four times longer than the same cases without these tallies. Moreover, the 'outp' MCNP output files for the cases with fission-energy tallies were too large to be imported into a spreadsheet (such as Microsoft® Excel) as a single file for subsequent data processing. However, the 'mctal' tally output file is formatted with more data entries per line (35 944 total lines for the cases studied) and can be successfully imported into Excel without exceeding the limit on the maximum number of lines. Once these files were imported into Excel, customized Visual Basic® macro routines were used to combine the tally data from multiple cases and to calculate derived quantities.

3. RESULTS

The MCNP CVR results are shown in Table 1 and are compared with corresponding values from WIMS-AECL/RFSP for both the ARW and ARI core configurations. Both sets of comparisons show similar results, namely a systematic discrepancy of 5.8 to 6.4 mk between the absolute k_{eff} values, but very good agreement to within about -0.15 ± 0.06 mk for the reactivity perturbation induced by ¼-core checkerboard coolant voiding.

Notably, this level of agreement is consistent with that obtained between the MCNP and WIMS-AECL reactivity results for much simpler infinite and axially finite uniform-lattice cases [3] that do not involve a two-group RFSP model. Thus, the complexities introduced by the whole-core simulation do not appear to alter the degree of agreement appreciably. In particular, the presence of the adjuster rods influences the level of agreement between the absolute k_{eff} values somewhat (by about 0.5 mk), but does not affect the agreement for the CVR values significantly.

The primary reason for the relatively large discrepancies between the absolute k_{eff} values is believed to be inconsistencies in the nuclear data used by WIMS-AECL and MCNP. For example, the current WIMS-AECL ENDF/B-VI data library uses an earlier vintage of ENDF/B-VI (Release 4 for ^{235}U and Release 2 for ^{238}U and the Pu nuclides), customized cross-sections for Zr that take into account self-shielding, and a data file for ^{238}U that was processed in a manner to be consistent with earlier files prepared from ENDF/B-V.

Table 1. Comparison of WIMS-AECL/RFSP and MCNP Reactivity Results

	WIMS-AECL/RFSP	**MCNP**	**Difference (mk)**
k_{eff}: ARW, ¼-core checkerboard coolant voiding	1.028398	1.022620 ± 0.000040	5.778 ± 0.040
k_{eff}: ARW, fully cooled	1.023813	1.017929 ± 0.000048	5.884 ± 0.048
CVR*: ARW, ρ (mk)	4.355	4.506 ± 0.060	-0.151 ± 0.060
k_{eff}: ARI, ¼-core checkerboard coolant voiding	1.013154	1.006820 ± 0.000043	6.334 ± 0.043
k_{eff}: ARI, fully cooled	1.008264	1.001842 ± 0.000036	6.422 ± 0.036
CVR*: ARI, ρ (mk)	4.787	4.935 ± 0.055	-0.148 ± 0.055

*Coolant void reactivity (CVR) = $1000*(1/k_{cooled} - 1/k_{voided})$

The static, whole-core, MCNP total channel fission energy distributions (proportional to the power distributions) for the ARI core configurations are shown in Figure 4, normalized to a total core power of 2061.4 MW_t. The fully cooled, nominal-reference-core values in the left foreground of Figure 4 exhibit the pronounced radial flattening at the core centre that occurs for the ARI core configurations. The results to the right and slightly behind show a side-to-side tilt in the static core power profile, which is caused by simulating ¼-core checkerboard coolant voiding (on the right hand side of Figure 1).

The MCNP values for the outer-fuel-ring relative power density (RPD, i.e., the ratio of the average power density in the outer ring fuel elements to the average power density in the bundle) are shown in Figure 5 as a function of fuel burn-up for the ¼-core checkerboard coolant-voiding ARI configuration. This figure shows two distinct bands of data: a dense upper band corresponding to the 75% of the fuel bundles that remain fully cooled and a diffuse lower band corresponding to the 25% that are voided. Coolant voiding decreases the outer-ring RPD as a result of the hardening of the neutron spectrum and the redistribution of the radial flux (and hence power) that occurs within the fuel channel.

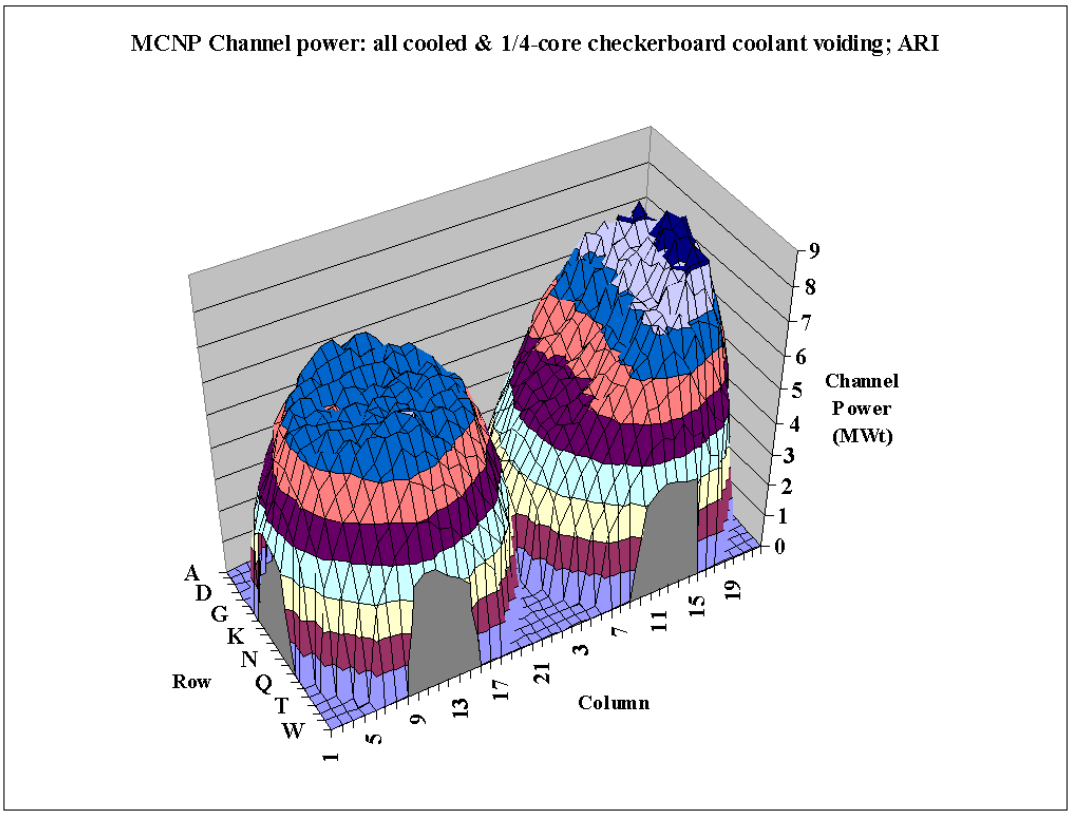

Figure 4. MCNP ARI Channel Power Distributions

Figure 5 shows that the average outer-ring MCNP RPD values agree well with corresponding values derived from WIMS-AECL lattice-cell cases, showing a small systematic discrepancy of about 0.5%, independent of fuel burn-up.

Azimuthal variations in the outer-element relative power densities (OERPDs) were observed; these variations depend on the location of the fuel bundle in the core. For fuel bundles containing the highest-power fuel elements, the maximum peak-to-average OERPD azimuthal variation observed was about 2.5% (for cases where a statistically significant trend was observed), as shown in Figure 6 for channel Q17, axial plane 6 for the ¼-core checkerboard coolant-voiding ARI configuration.

The fitted sine curve in Figure 6 (95% confidence limits are shown as dashed lines) assumes that the azimuthal variation is governed by a single flux gradient across the bundle, which, in this instance, is aligned from the top to the bottom of the core (i.e., approximately along a line from channel P17 to channel R17). As expected, this observed direction for the OERPD gradient in the fuel bundle in channel Q17, plane 6 is reasonably consistent with local variations in total bundle power in plane 6, which shows a bundle-power decrease of 1.3% from channels P17 to Q17, and a further decline of 7.8% from channels Q17 to R17.

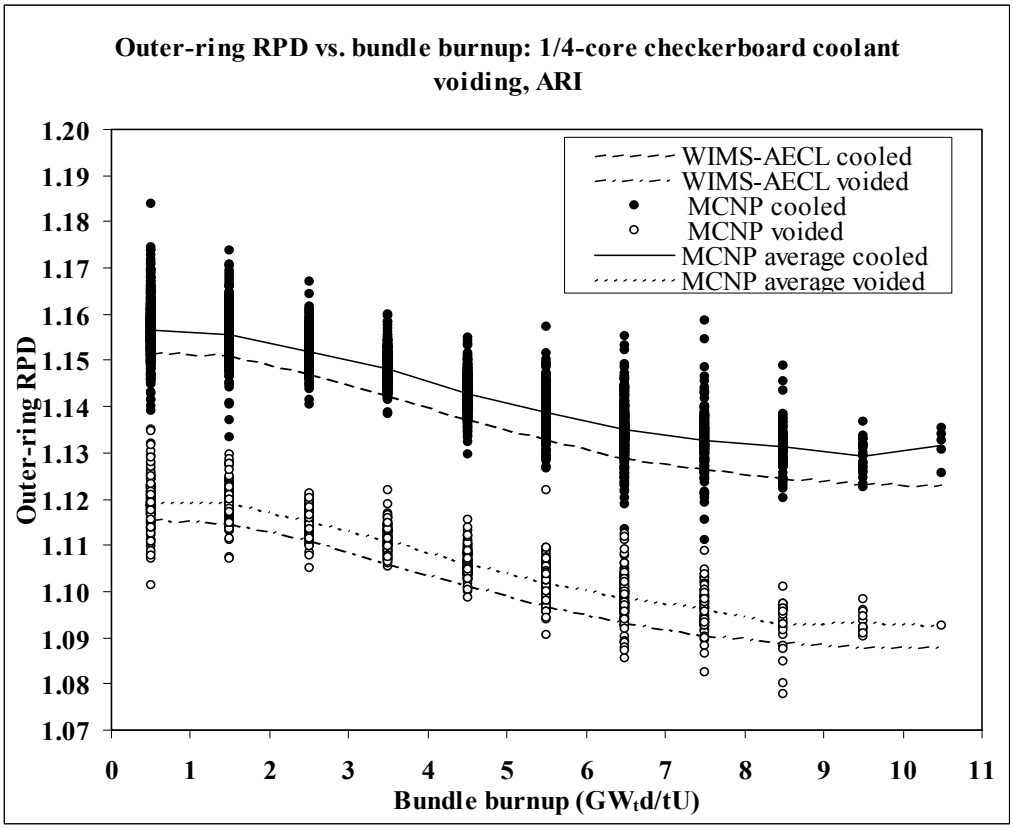

Figure 5. Outer-ring RPD as a function of bundle burn-up, ¼-core checkerboard coolant voiding, ARI.

Larger (and statistically more significant) peak-to-average outer-element azimuthal power gradients of up to 42% (for channel B06, plane 1, 1/4-core checkerboard coolant voiding, ARI configuration) were observed in low-power channels at the core/reflector interface, where flux and power gradients are substantial (see Figure 4).

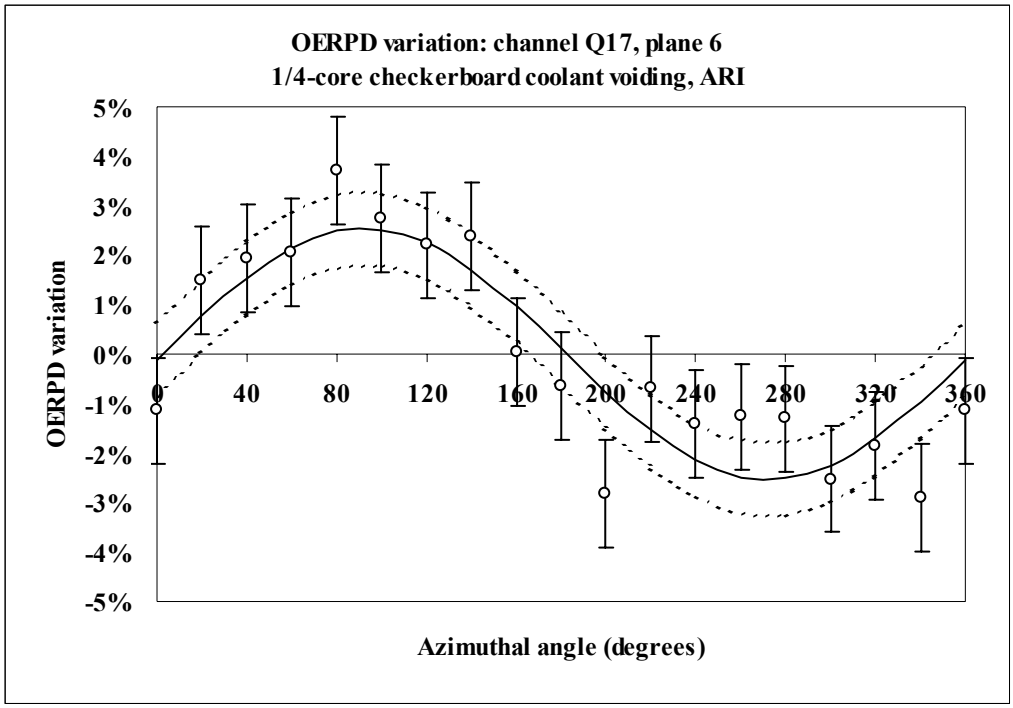

Figure 6. Azimuthal variations in OERPD, channel Q17, plane 6, ¼-core checkerboard coolant voiding, ARI.

4. CONCLUSIONS

A whole-core MCNP model of a simplified CANDU core was developed and used to study core configurations of interest in safety analysis, particularly the hypothetical case of ¼-core checkerboard coolant voiding. The MCNP results were compared with those from corresponding WIMS-AECL/RFSP simulations. The key findings are that

- the WIMS-AECL/RFSP and MCNP results show a systematic discrepancy of 5.8 to 6.4 mk between the absolute k_{eff} values, but very good agreement to within about -0.15 ± 0.06 mk for the reactivity perturbation induced by ¼-core checkerboard coolant voiding.
- the MCNP outer-ring RPD values agree well with corresponding WIMS-AECL lattice-cell values, showing a small (about 0.5%) systematic discrepancy that is independent of fuel burn-up.
- the largest peak-to-average OERPD azimuthal variation observed in high-power fuel bundles was about 2.5%, but larger variations of up to around 42% occurred in low-power bundles at the core/reflector interface.

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