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# Qualification of MCNP Coolant Void Reactivity Calculations using ZED-2 Measurements

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Several sets of fuel-substitution and reference-lattice measurements performed in the ZED-2 zero-power reactor were simulated with MCNP to test its reliability for CANDU coolant-void-reactivity calculations when used with an AECL-generated, continuous-energy data library based on ENDF/B-VI release 5. The reactivity results were analyzed to estimate the bias in coolant-void-reactivity calculations for pure lattices of fresh-natural-uranium and MOX (simulated irradiated natural uranium) CANDU fuels using an approximate methodology derived from perturbation theory. It was found that MCNP overestimates the coolant void reactivity for pure lattices of 28-element and 37-element CANDU fuel at room temperature by 0.7 to 1.7 mk, amounts which are generally consistent with corresponding bias values established for WIMS-IST lattice-cell calculations.

***KEYWORDS: MCNP, CANDU, coolant void reactivity, ZED-2***

## 1. Introduction

MCNP (Monte Carlo N-Particle [1]) calculations are often used to benchmark the reactor physics results of the deterministic methods normally used for CANDU®* reactor design and safety assessment, such as WIMS-AECL/RFSP (Winfrith Improved Multigroup Scheme – Atomic Energy of Canada Limited [2]/ Reactor Fuelling Simulation Program [3]). Many of the benchmark comparisons have examined the coolant-void reactivity (CVR), which is positive for current CANDU reactors and is an important parameter in the assessment of large-break loss-of-coolant accidents. Comparisons of the CVR results from the two calculation methods show good agreement for current CANDU reactor designs, typically to within a few tenths of a mk [4] (1 mk = 0.1 % $\Delta$k = 100 pcm). However, a need existed to qualify the MCNP calculation methodology and its associated nuclear data against pertinent experimental data. This paper describes the simulation of experiments related to CANDU coolant voiding using MCNP and the analysis of the results to extract the MCNP CVR bias information for a uniform critical lattice of CANDU fuel.

The primary source of experimental data concerning CANDU coolant voiding is sets of measurements performed in the ZED-2 (Zero Energy Deuterium) zero-power reactor at AECL's Chalk River Laboratories (CRL). The ZED-2 facility consists of an open, cylindrical aluminium tank, filled with heavy-water ($D_2O$) neutron moderator and reflected by graphite. Vertical fuel assemblies are arranged on an adjustable regular lattice pitch within the tank. The reactor is brought to a low-power critical-core state by adjusting the moderator level.

* CANDU: CANada Deuterium Uranium; registered trademark of AECL

The ZED-2 CVR measurements are designed to determine the critical lattice bucklings of $D_2O$-cooled and air-cooled (i.e., voided) lattices of CANDU fuel. Two types of CVR measurements are performed:

- Flux-map measurements. If sufficient test fuel is available to form a large uniform lattice region, the radial and axial components of the critical buckling are determined directly by fitting Bessel and cosine functions to the measured radial and axial flux profiles without involving lattice-cell or reactor-core calculations.
- Fuel-substitution measurements. If only a limited quantity of test fuel is available (generally thirty-five 0.5-m-long CANDU fuel bundles arranged into seven assemblies of five bundles each), the critical bucklings are determined using a progressive series of fuel-substitution measurements, in which one, three, five and seven test-fuel assemblies are inserted into the central core region. The results are then extrapolated to a pure lattice of test fuel. The analysis procedure involves core simulations and the application of a calibration correction based on comparisons of the critical bucklings obtained using the flux-map and fuel-substitution methods for various combinations of test fuel and reference fuel.

When the measured critical buckling is used as input in a WIMS-AECL lattice-cell calculation for the test fuel, the difference of the calculated effective multiplication constant from unity (i.e., the $k_{eff}$ bias) provides an estimate of the systematic error in the calculation of the absolute reactivity. Similarly, the difference between the $k_{eff}$ bias values for the voided and cooled states gives an estimate of the bias in the calculated CVR.

The magnitude of the bias in a WIMS-AECL CVR calculation will depend on the accuracy and detail of the input model, the code options selected and the nuclear data used. A specific set of CANDU physics calculation conditions, termed the 'Industry Standard Toolset' (IST), has been adopted and subjected to extensive validation [5]. The IST lattice-calculation configuration uses WIMS-IST (WIMS-AECL Release 2-5d, used with the 89-group ENDF/B-VI-based NDAS library Version 1a) and a set of standard lattice-cell model and transport-equation solution options that are used in typical calculations for CANDU power reactors.

The analysis of a substantial set of ZED-2 CVR measurements has established WIMS-IST CVR bias values for 37-element CANDU fuel (used in CANDU 6 power reactors and the CANDU reactors at the Bruce and Darlington Nuclear Generating Stations) and 28-element CANDU fuel (used at the Pickering Nuclear Generating Station) at room temperature. CVR bias values were determined for fresh-natural-uranium (FNU) fuel and, in the case of 37-element CANDU fuel, mixed-oxide (MOX) fuel representing simulated irradiated natural uranium. The latter fuel consists of a mixture of depleted uranium dioxide, plutonium dioxide and dysprosia ($Dy_2O_3$) that approximates the reactivity properties of irradiated CANDU fuel near mid-life burnup (about 3.8 GWd/Mg(U)). The WIMS-IST CVR bias values for these fuel types are listed in Table 1 along with the estimated uncertainties. A positive CVR bias value implies that WIMS-IST overestimates the CVR.

The remainder of this paper concerns the simulation of several sets of ZED-2 fuel-substitution and reference-lattice core configurations using MCNP and the analysis of the results to obtain MCNP CVR bias estimates for pure lattices of test fuel, that can be compared with the WIMS-IST CVR bias values presented in Table 1.

**Table 1** WIMS-IST CVR bias values for 28- and 37-element CANDU fuel [5]

| CANDU fuel type | | Estimated WIMS-IST CVR bias and uncertainty (mk) |
|---|---|---|
| 28 element | FNU | 0.8 ± 0.8 |
| 37 element | FNU | 1.9 ± 0.8 |
| 37 element | MOX | 1.5 ± 0.8 |

## 2. MCNP Simulation of ZED-2 Critical Lattices

MCNP was used to simulate five sets of ZED-2 room-temperature critical-core configurations involving the substitution of $D_2O$-cooled and air-cooled, FNU and MOX, 37-element CANDU test fuel into various reference lattices. Each set of measurements involved a different combination of test fuel, test-fuel channels and reference lattice (see Table 3). For four of the sets of measurements, the 37-element test fuel was inserted into 'CANDU channels', consisting of concentric zirconium-alloy tubes having dimensions and compositions similar to CANDU pressure tubes and calandria tubes. The remaining set of measurements involved 37-element MOX fuel inserted into 'ZED-2 hot channels', which are similar to the CANDU channels, but have aluminium thermal shields located in the gap between the pressure tube and the calandria tube.

Four distinct reference lattices were involved, consisting of fifty-five rods of $D_2O$-cooled or voided 28-element natural $UO_2$ CANDU fuel in aluminium channels, surrounded by an outer zone of thirty uranium-metal-based "booster" fuel rods (see Figure 1). Two types of booster fuel assemblies were used: either ZEEP (Zero Energy Experimental Pile) fuel rods, consisting of a single uranium-metal rod clad in aluminium, or $D_2O$-cooled 19-element uranium-metal fuel in aluminium channels. The unperturbed reference lattices were also simulated with MCNP and the results used to derive MCNP CVR bias estimates for 28-element $UO_2$ fuel.

The ZED-2 fuel assemblies were arranged on a 31-cm hexagonal lattice pitch. This arrangement provides a similar moderator-to-fuel ratio to that in CANDU power reactors, which have fuel channels arranged on a square lattice pitch of 28.575 cm. All fuel was FNU except for the 37-element MOX fuel.

The 'recommended critical heights' from the experimental data reports were used in the MCNP simulations for each configuration. These moderator heights include a small adjustment (<1.2 cm or <0.6% of the critical height for the range of cases studied) to bring a sequence of fuel-substitution measurements to a common set of conditions with respect to moderator and coolant temperature and purity.

MCNP version 4C was used with an AECL-generated, continuous-energy nuclear data library (designated ENDF65MT-AECL) that is consistent with ENDF/B-VI release 5. Cross-section data corresponding to 300 K were used with the entries on the MCNP TMP0 card adjusted to correspond to the ambient temperature for a specific set the measurements.

The probability-table treatment of unresolved resonances that is available with MCNP4C was not used in this work, primarily for consistency with earlier work involving comparisons of CANDU-related calculations using MCNP versions 4B and 4C and WIMS-AECL/RFSP. However, a sensitivity study was performed for the ZED-2 reference-lattice core configurations involving $D_2O$-cooled and voided 28-element $UO_2$ fuel with ZEEP booster fuel. It was found that the probability-table treatment reduced the MCNP4C core $k_{eff}$ bias values (i.e., increased the calculated core $k_{eff}$ values) systematically by about 1.6 mk but reduced the MCNP4C core CVR bias by only a small amount (0.10 ± 0.11 mk (1σ)).

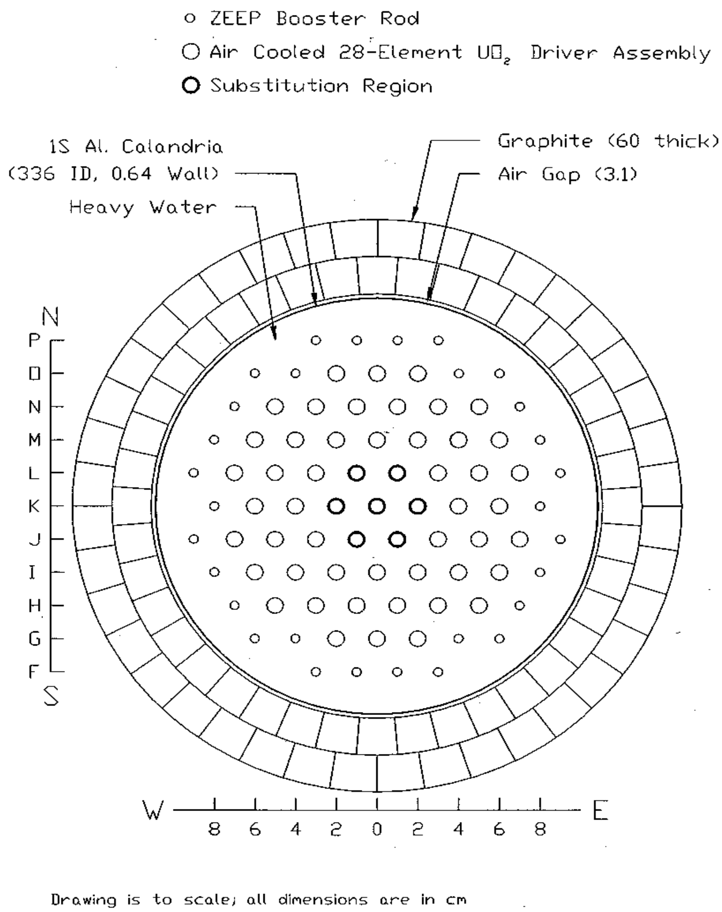


**Fig.1** Plan view of ZED-2 experimental lattice

The initial neutron source distribution was established for the case of a $D_2O$-cooled 28-element $UO_2$ reference lattice with ZEEP booster rods starting with one fission neutron near the centre of each 28-element $UO_2$ fuel bundle or ZEEP fuel rod. The neutron source size was then evolved in progressive steps up to a case involving 50 cycles of 60 000 source neutrons.

The neutron source distribution thus established was used as the starting point for each core configuration studied. The first MCNP case for each core configuration allowed 50 inactive cycles of 60 000 neutrons each for the neutron source to adapt to the new configuration, followed by a further 250 active cycles. Subsequent cases for the same configuration used no inactive cycles and 250 active cycles of 60 000 neutrons. These latter cases used the latest available neutron source file with a different starting random number for each case.

For each core configuration and coolant state, multiple MCNP cases were executed and the results combined in a weighted average. At least five separate MCNP cases were executed. The core $k_{eff}$ value for each MCNP case was the recommended combined-average value of the collision, absorption and track-length estimates. The largest statistical uncertainty in the weighted-average core $k_{eff}$ value for each core configuration and coolant state was ±0.064 mk.

**3. Results and Analysis**

The $k_{eff}$ results from the MCNP simulations generally underestimated criticality by about 5 mk, with the core $k_{eff}$ bias varying in a near linear manner as test fuel was added. Sample $k_{eff}$ bias results for the sequence involving $D_2O$-cooled and voided 37-element MOX fuel in CANDU channels substituted into a $D_2O$-cooled 28-element $UO_2$ reference lattice with ZEEP booster fuel are shown in Figure 2. Corresponding MCNP core CVR bias values determined from the difference between the voided and cooled $k_{eff}$ bias values are shown in Figure 3.

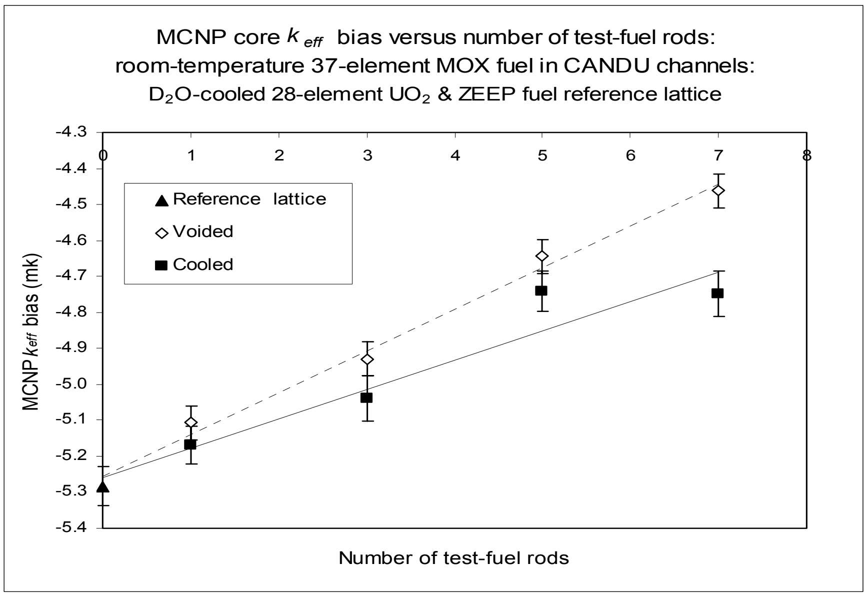


**Fig. 2** MCNP core $k_{eff}$ bias versus number of test-fuel rods

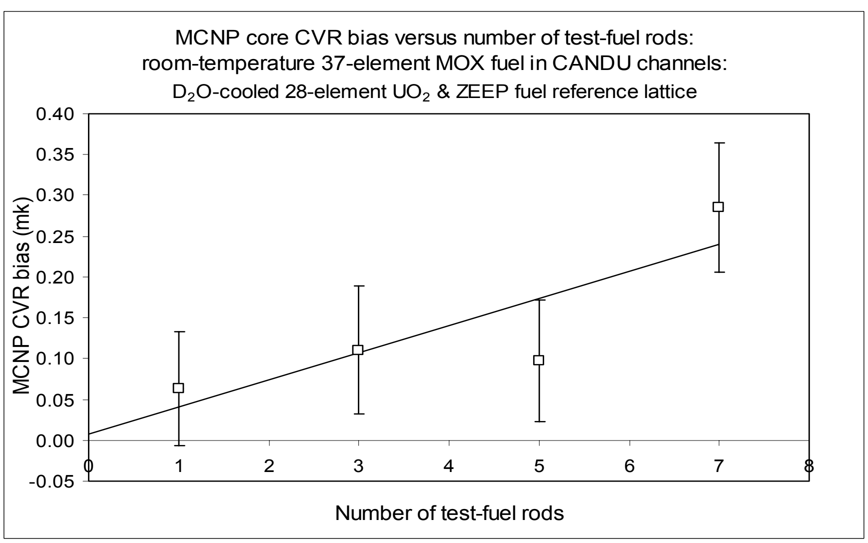


**Fig. 3** MCNP core CVR bias versus number of test-fuel rods

From first-order perturbation theory [6], the perturbed $k_{eff}$ value, $k_n$, for a ZED-2 core configuration involving the substitution of $n$ test-fuel rods into a reference lattice containing a total of $N$ lattice sites of equal volume and having an unperturbed $k_{eff}$ value, $k_r$, is given by

$$k_n \approx k_r + k_r^2 \cdot \frac{<\phi^*(\Delta P/k_r - \Delta L)\phi>}{<\phi^* P_r \phi>} \tag{1}$$

where:

| | | |
|---|---|---|
| $P$ | = | neutron production cross section, |
| $L$ | = | neutron loss cross section, |
| $\phi, \phi^*$ | = | unperturbed regular and adjoint neutron flux, respectively. |

With the additional approximations that: (1) a one-neutron-energy-group treatment is adequate, (2) the unperturbed axial flux profile has the same shape in all lattice positions (i.e., cosine function determined by the $D_2O$ moderator level), and (3) the adjoint flux has the same radial profile as the regular flux, and defining

$k_t$ = $P_t/L_t$ = derived $k_{eff}$ value for a pure lattice of test fuel,

$$W_n = \frac{\sum_{i=1}^{n} \phi_i^2(r)}{\sum_{i=1}^{N} \phi_i^2(r)}$$ = flux-squared weighting factor for $n$ test-fuel rods,

Equation 1 may then be rewritten as

$$k_n \approx k_r + W_n \cdot (1 + \Delta L / L_r) \cdot (k_t - k_r) \tag{2}$$

Dropping the higher-order term, $\Delta L/L_r$, and rearranging the remaining terms to obtain an estimate of the $k_{eff}$ bias for a pure test-fuel lattice, $k_{t\text{-}bias}$, gives

$$k_{t-bias} = k_t - 1 \approx W_n^{-1} \cdot k_{n-bias} + (1 - W_n^{-1}) \cdot k_{r-bias} \tag{3}$$

The $\Delta k$-on-coolant-voiding, or CVR, bias is then given by

$$\Delta k_{t-bias} = k_{t-bias-voided} - k_{t-bias-cooled} \approx W_n^{-1} \cdot (k_{n-bias-voided} - k_{n-bias-cooled}) \tag{4}$$

The weighting factors, $W_n$, were determined from flux values calculated at the centres of the fuel channels using a $J_o$ Bessel function and the measured radial bucklings for the unperturbed reference lattices from the experimental data reports. The measured radial bucklings are determined by fitting a $J_o$ Bessel function to the measured thermal flux at locations in the moderator between the fuel channels and have experimental uncertainties of less than 0.04 $m^{-2}$ (less than 3 %).

Equations 3 and 4 were used to estimate the test-fuel MCNP $k_{eff}$ and CVR bias values for each fuel-substitution configuration. Sample results are listed in Table 2 for the same set of results shown in Figures 2 and 3. The final value of the MCNP CVR bias estimate for each data set was determined using a weighted average of the individual CVR bias values obtained for the four substitution measurements (e.g., see the last line of Table 2).

Applying this methodology to the five sets of fuel-substitution data involving 37-element CANDU fuel produced the MCNP CVR bias estimates shown in Table 3. The MCNP test-fuel CVR bias estimates range from 0.74 ± 0.27 mk to 1.70 ± 0.43 mk. The three values for MOX fuel show good agreement to within one standard deviation. The two values for FNU fuel differ by slightly less than two standard deviations of their combined uncertainties and their mean compares well with the values obtained for MOX fuel.

MCNP CVR bias estimates for 28-element CANDU test-fuel were similarly derived from the $k_{eff}$ bias values for the reference lattices. Values of 1.18 ± 0.10 mk and 1.41 ± 0.11 mk were obtained as shown in Table 3.

**Table 2** MCNP $k_{eff}$ and CVR bias values for 37-element MOX fuel in CANDU channels

| MCNP $k_{eff}$ and CVR bias values: room-temperature 37-element MOX fuel in CANDU channels: $D_2O$-cooled 28-element $UO_2$ & ZEEP fuel reference lattice | | | | | |
|---|---|---|---|---|---|
| Number of test-fuel rods (n) | $1/W_n$ | $k_{n\text{-}bias}$ (mk) | uncertainty (mk) | $k_{t\text{-}bias}$ (mk) | uncertainty (mk) |
| 0 | 1 | -5.283 | 0.053 | n/a | n/a |
| 7 | 5.2986 | -4.462 | 0.047 | -0.935 | 0.338 |
| 5 | 7.3833 | -4.645 | 0.048 | -0.574 | 0.494 |
| 3 | 12.1720 | -4.929 | 0.046 | -0.977 | 0.815 |
| 1 | 34.6381 | -5.106 | 0.047 | 0.839 | 2.422 |
| Weighted average $k_{t\text{-}bias}$ voided (mk) | | | | -0.816 | 0.263 |
| 7 | 5.2986 | -4.748 | 0.064 | -2.447 | 0.408 |
| 5 | 7.3833 | -4.743 | 0.056 | -1.294 | 0.534 |
| 3 | 12.1720 | -5.040 | 0.063 | -2.323 | 0.969 |
| 1 | 34.6381 | -5.170 | 0.052 | -1.366 | 2.551 |
| Weighted average $k_{t\text{-}bias}$ cooled (mk) | | | | -2.043 | 0.310 |
| | | Number of substituted rods (n) | $1/W_n$ | $\Delta k_{t\text{-}bias}$ (mk) | uncertainty (mk) |
| | | 7 | 5.2986 | 1.513 | 0.419 |
| | | 5 | 7.3833 | 0.721 | 0.545 |
| | | 3 | 12.1720 | 1.346 | 0.945 |
| | | 1 | 34.6381 | 2.205 | 2.437 |
| Weighted average test-fuel CVR bias (mk) | | | | 1.248 | 0.311 |

**Table 3** MCNP CVR bias estimates for 28-element and 37-element CANDU fuel

| Experiment type | Test fuel | Reference fuel | Estimated MCNP CVR bias for test fuel (mk) |
|---|---|---|---|
| Substitution | 37-el. MOX in CANDU channels | $D_2O$-cooled 28-element $UO_2$ reference & ZEEP boosters | 1.25 ± 0.31 |
| Substitution | 37-el. MOX in CANDU channels | air-cooled 28-element $UO_2$ & ZEEP boosters | 1.04 ± 0.38 |
| Substitution | 37-el. MOX in ZED-2 hot channels | $D_2O$-cooled 28-element $UO_2$ & $D_2O$-cooled 19-element U-metal boosters | 0.89 ± 0.30 |
| Substitution | 37-el. FNU in CANDU channels | $D_2O$-cooled 28-element $UO_2$ & ZEEP boosters | 1.70 ± 0.43 |
| Substitution | 37-el. FNU in CANDU channels | air-cooled 28-element $UO_2$ & $D_2O$-cooled 19-element U-metal boosters | 0.74 ± 0.27 |
| Reference lattice | 28-el. UO2 in Al channels | 55 channels & ZEEP boosters | 1.18 ± 0.10 |
| Reference lattice | 28-el. UO2 in Al channels | 55 channels & $D_2O$-cooled 19-element U-metal boosters | 1.41 ± 0.11 |

Comparing the MCNP CVR bias results from Table 3 with those for WIMS-IST in Table 1 indicates good agreement to within one standard deviation of the uncertainties. This raises the possibility that the systematic overestimate of the CVR using the two distinct calculation systems originates in some common feature, perhaps a deficiency in the underlying ENDF/B-VI-based nuclear data.

## 4. Conclusion

MCNP, when used with an AECL-generated nuclear data library based on ENDF/B-VI release 5, was found to overestimate the CVR for pure lattices of 28-element and 37-element CANDU fuel by 0.7 to 1.7 mk, based on the simulation and analysis of ZED-2 CVR measurements. This result is broadly consistent with similar CVR overestimates that are obtained when the measured critical bucklings from these and other experiments are used with the deterministic lattice-cell code WIMS-IST.

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