## ENERGY AND SPATIAL DEPENDENCE OF MCNP SIMULATIONS FOR ZED-2 CRITICAL EXPERIMENTS

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# ABSTRACT

MCNP simulations of ZED-2 critical experiments provide a good test of the reliability of the nuclear data involved in the simulation of reactor physics phenomena of importance to CANDU reactors, particularly the coolant void reactivity. Recent work has therefore focused on the impact of the new ENDF/B-VII.0 nuclear data library. One feature of this library is the provision of thermal scattering law data for UO<sub>2</sub>. Initial MCNP results using preliminary ACE-format data files for UO<sub>2</sub> thermal scattering suggested that a consistent reduction was obtained in the coolant void reactivity simulation bias, especially for ZED-2 critical experiments involving slightly enriched uranium (0.95 wt%<sup>235</sup>U) and H<sub>2</sub>O/air coolant. However, subsequent work using UO<sub>2</sub> thermal scattering data files that correctly include the coherent elastic scattering component indicated that the net reactivity impact is quite small. The present work extends this investigation to examine in detail the energy dependence of the impact of the  $UO_2$  thermal scattering data and, more generally, the energy and spatial dependence of the coolant void reactivity simulation bias for some of these experiments. In addition, results are presented using MCNPX with an improved treatment for thermal scattering. It is found that the net reactivity impact results from the cancellation of larger positive and negative effects at different energies and in different fuel regions, and which generally highlight the reactor physics changes that occur when the coolant is removed.

# I. INTRODUCTION

The ZED-2<sup>[1]</sup> (Zero Energy Deuterium) facility at Atomic Energy of Canada Limited's (AECL) Chalk River Laboratory (CRL) is used primarily for critical experiments supporting the validation of reactor physics codes used in the design and safety analysis of CANDU<sup>®1</sup> and ACR<sup>TM2</sup> power reactors, for which the coolant void reactivity (CVR) is an important parameter. The simulation of ZED-2 critical experiments with a stochastic code, such as MCNP<sup>[2]</sup> (Monte Carlo N-Particle), that uses continuous-energy cross sections and a detailed geometric representation, can be made sufficiently precise, that residual differences mainly reflect the experimental measurement uncertainties as well as errors arising from uncertainties in the nuclear data. In ZED-2 CVR experiments involving pairs of critical moderator height measurements for lattice configurations that differ only in the type of coolant in the fuel channels (i.e., heavy water (D<sub>2</sub>O), light water (H<sub>2</sub>O) or air), the estimated experimental uncertainty is quite small (about ±0.3 mk) owing to the cancellation of systematic error components.

<sup>&</sup>lt;sup>1</sup> CANDU<sup>®</sup> (CANada Deuterium Uranium) is a registered trademark of AECL.

<sup>&</sup>lt;sup>2</sup> ACR<sup>TM</sup> (Advanced CANDU Reactor<sup>TM</sup>) is a trademark of AECL.

Thus, the ZED-2 CVR measurements provide a sensitive integral test of the reliability of the underlying nuclear data.

The nuclear data libraries used for various applications at AECL are based primarily on the ENDF (Evaluated Nuclear Data File) system, for which a major revision, ENDF/B-VII.0<sup>[3]</sup>, was released in 2006 December. Recent work at AECL has therefore focused on evaluating the impact of the new ENDF/B-VII.0 nuclear data library for ZED-2 CVR simulations<sup>[4]</sup>. The official release of ENDF/B-VII.0 was accompanied by a preliminary set of ACE (A Compact ENDF) format files, which are needed to perform MCNP calculations. These files were distributed on a limited basis by RSICC (Radiation Safety Information Computational Center) for initial testing and evaluation.

One feature of the ENDF/B-VII.0 library is the provision of thermal scattering law (TSL; i.e.,  $S(\alpha,\beta)$ ) data for additional materials, such as for oxygen and uranium bound in UO<sub>2</sub>. Initial test results using ENDF/B-VII.0 with the preliminary UO<sub>2</sub> TSL ACE data files showed a significant reduction in the MCNP ZED-2 CVR simulation bias, especially when the coolant combination was H<sub>2</sub>O/air. However, it was subsequently learned that the preliminary UO<sub>2</sub> TSL ACE files did not include the elastic scattering component. Correcting this oversight for the UO<sub>2</sub> TSL data (as well as for Al and Fe) gives results that, in marked contrast, show relatively little sensitivity to the UO<sub>2</sub> TSL data.

Although the net reactivity impact of the UO<sub>2</sub> TSL data on the MCNP ZED-2 CVR simulation bias is indeed small (<0.1 mk), detailed examination of its energy dependence shows that it results from the cancellation of larger positive and negative components associated with the shift in the critical neutron flux spectrum at thermal neutron energies that accompanies coolant voiding. Examination of the energy and spatial dependence of these reactivity changes is the main subject of this work. In addition, the ZED-2 calculations were repeated using MCNPX (version 2-6a) together with ENDF-B/VII.0 TSL ACE files downloaded from the LANL (Los Alamos National Laboratory) T2 thermal data web page<sup>[5]</sup>. MCNPX incorporates an improved S( $\alpha$ , $\beta$ ) treatment based on an algorithm provided by Little and Pitcher of LANL<sup>[6]</sup>, which removes the non-physical discontinuous 'spikes' that are sometimes observed at thermal energies and which is not currently available for use with MCNP5.

#### **II. ZED-2 CVR EXPERIMENTS**

The ZED-2 facility consists of a large cylindrical aluminum tank containing  $D_2O$  moderator and surrounded in the radial and lower axial directions by a graphite reflector. Lattice arrays are formed by suspending vertical fuel assemblies within the tank on a regular lattice pitch. Criticality is achieved by raising the  $D_2O$  moderator level.

Two groups of ZED-2 critical experiments were simulated with MCNP for this study:

- H<sub>2</sub>O/air-cooled configurations with 48 five-bundle assemblies of 43-element CANFLEX<sup>®3</sup> SEU (slightly enriched uranium; 0.95 weight % <sup>235</sup>U) UO<sub>2</sub> fuel and four similar corner assemblies containing RU (recovered uranium; 0.96 weight % <sup>235</sup>U) UO<sub>2</sub> fuel on square lattice pitches of 20.0 and 24.0 cm.
- D<sub>2</sub>O/air-cooled configurations with 55 five-bundle assemblies of 28-element natural uranium (NU) UO<sub>2</sub> fuel on a hexagonal lattice pitch of 31.0 cm and

<sup>&</sup>lt;sup>3</sup> CANFLEX<sup>®</sup> (CANDU Flexible Fuelling) is a registered trademark of AECL and the Korea Atomic Energy Research Institute.

surrounded by 30 NU U-metal 'booster' fuel assemblies consisting of either single-element ZEEP (Zero Energy Experimental Pile) rods or 19-element single-bundle assemblies.

## **III. MCNP SIMULATIONS**

Most of the ZED-2 simulations were initially performed using MCNP5 version 1.40 with 2,100 cycles of 60,000 source neutrons per cycle and skipping the first 100 cycles (i.e., 120 million active neutron histories); however, some earlier results using the ENDF/B-VI.8 library for the NU experiments, which involved only 60 million active neutron histories, are included for comparison. Since these ZED-2 measurements were performed at room temperature (22.24 to 25.95°C), the 'reference standard' ENDF/B-VII.0 ACE files<sup>[7]</sup>, prepared at the U.S. National Nuclear Data Center (NNDC) at 300 K (26.85°C) and distributed by RSICC, were used directly. Corresponding results based on ENDF/B-VI.8 were obtained using the ACE files distributed with MCNP5.

As part of a related study<sup>[4]</sup>, the ENDF/B-VII.0-based ZED-2 simulations were repeated using new ACE files prepared at 300 K using a slightly modified version of NJOY-99.161<sup>[8]</sup>. MCNP5  $k_{eff}$  results using this dataset agreed with those calculated using the RSICC ENDF-B/VII.0 ACE files to within about 0.063 mk. These calculations were also repeated using new TSL ACE files for O-in-UO<sub>2</sub>, U-in-UO<sub>2</sub>, Al and Fe that include the coherent elastic neutron scattering component. As shown in Figure 1 for the case of O-in-UO<sub>2</sub> at 296 K, the elastic scattering component of the TSL file has a noticeable impact on the total cross section in the neutron energy range from about  $2x10^{-9}$  to  $10^{-6}$  MeV. Similar calculations were also performed without using the UO<sub>2</sub> TSL data.



Figure 1: O-in-UO<sub>2</sub> TSL cross-section data components.

As a final test, the ZED-2 calculations were repeated using MCNPX (version 2-6a) with ENDF-B/VII.0 TSL ACE files from the LANL T2 thermal data web page<sup>[5]</sup>. In the case of the SEU/RU experiments, the MCNPX calculations were performed with and without the UO<sub>2</sub> TSL data.

Fission-yield tallies (using the same 89-group structure as in WIMS-AECL) were performed for all ENDF/B-VII.0-based MCNP simulations of the NU experiments, as well as for the MCNPX simulations of the SEU/RU experiments.

## **IV. MCNP SIMULATION RESULTS**

### IV.A MCNP keff and CVR Simulation Bias

The MCNP  $k_{eff}$  simulation bias is the difference between the calculated  $k_{eff}$  for a given ZED-2 critical core configuration and the known value of 1.0. In this paper, the CVR simulation bias is defined as the  $\Delta k_{eff}$  difference between the  $k_{eff}$  calculated for core configurations in which the fuel channels are cooled by air and that for corresponding configurations with the coolant being H<sub>2</sub>O or D<sub>2</sub>O. The  $k_{eff}$  and CVR simulation biases for the SEU/RU and NU UO<sub>2</sub> measurements are shown in Tables 1 and 2, respectively, based on the combined-average (collision/absorption/track-length)  $k_{eff}$  values and corresponding uncertainties (1 sigma).

		Lattice	$S(\alpha,\beta)$ for $O$ in UO <sub>2</sub>	Elastic UO <sub>2</sub>			
Nuclear data		nitch	& Uin	component	$k_{eff}$ bias	CVR bias	
library and code	Coolant				(mk)	(mk)	
-		(cm)	$UO_2$	included	. ,	. ,	
ENDF/B-VI.8;	Air		No	No	$-6.466 \pm 0.052$	$2670 \pm 0.070$	
MCNP5	$H_2O$		INU	NO	$-9.136 \pm 0.047$	2.070 ± 0.070	
	Air		No	No	$-1.007 \pm 0.053$	$1.851 \pm 0.071$	
	H <sub>2</sub> O	20.0	INO	INO	$-2.858 \pm 0.047$	$1.031 \pm 0.0/1$	
ENDF/B-VII.0;	Air		Yes	No	$0.235 \pm 0.055$	$1.196 \pm 0.073$	
MCNP5	H <sub>2</sub> O				$-0.961 \pm 0.048$		
	Air		Yes	Yes	$-1.142 \pm 0.055$	$1.901 \pm 0.072$	
	H <sub>2</sub> O				$-3.043 \pm 0.047$		
ENDF/B-VII.0; MCNPX	Air		No	No	$-1.484 \pm 0.053$	$1.798 \pm 0.071$	
	H <sub>2</sub> O				$-3.282 \pm 0.047$		
	Air		Yes	Yes	$-1.154 \pm 0.054$	$1.870 \pm 0.073$	
	H <sub>2</sub> O				$-3.024 \pm 0.048$		
ENDF/B-VI.8;	Air		No	No	$-4.934 \pm 0.055$	$5.067 \pm 0.072$	
MCNP5	H <sub>2</sub> O		INU	NO	$-10.001 \pm 0.047$	5.007 ± 0.072	
ENDF/B-VII.0; MCNP5	Air	24.0	No	No	$0.213 \pm 0.055$	$3.988 \pm 0.073$	
	H <sub>2</sub> O				$-3.775 \pm 0.047$		
	Air		Yes	No	$0.716 \pm 0.054$	$1.445 \pm 0.071$	
	H <sub>2</sub> O				$-0.729 \pm 0.047$	$1.445 \pm 0.071$	
	Air		Yes	Yes	$-0.002 \pm 0.057$	$3.980 \pm 0.073$	
	H <sub>2</sub> O				$-3.982 \pm 0.046$		
ENDF/B-VII.0; MCNPX	Air		No	No	$-0.176 \pm 0.054$	$3.964 \pm 0.070$	
	H <sub>2</sub> O				$-4.140 \pm 0.045$		
	Air		Yes	Yes	$-0.137 \pm 0.054$	$4.011 \pm 0.072$	
	H <sub>2</sub> O				$-4.148 \pm 0.047$		

Table 1: MCNP results for ZED-2 SEU/RU UO2 measurements

Most of the MCNP5  $k_{eff}$  simulation bias results from Tables 1 and 2 are shown as a function of MCNP5 calculated neutron leakage (particle weight loss to escape) in Figure 2. In this figure, cooled and voided pairs of measurements are joined by straight

lines with square and triangular data points representing SEU/RU and NU simulation results, respectively. The SEU/RU and NU  $k_{eff}$  simulation bias results tend to be correlated, suggesting that they may be related to a common phenomenon or nuclear data issue. Thus, the SEU/RU experiments appear to involve larger CVR bias values than the NU cases primarily because they involve larger perturbations of the neutron leakage.

Nuclear data library and code	Coolant	Booster fuel	$S(\alpha,\beta)$ for O in UO <sub>2</sub> & U in UO <sub>2</sub>	Elastic UO <sub>2</sub> TSL component included	k <sub>eff</sub> bias (mk)	CVR bias (mk)
ENDF/B-VI.8; MCNP5	Air D <sub>2</sub> O		No	No	$-3.815 \pm 0.066 \\ -4.596 \pm 0.060$	$0.781 \pm 0.089$
	Air D <sub>2</sub> O		No	No	$\frac{1.703 \pm 0.047}{0.749 \pm 0.047}$	$0.954 \pm 0.067$
ENDF/B-VII.0; MCNP5	Air D <sub>2</sub> O		Yes	No	$\begin{array}{c} 3.194 \pm 0.049 \\ 2.797 \pm 0.049 \end{array}$	$0.397 \pm 0.069$
	Air D <sub>2</sub> O	ZEEP	Yes	Yes	$\frac{1.434 \pm 0.047}{0.797 \pm 0.046}$	$0.637 \pm 0.066$
ENDF/B-VII.0; MCNPX	Air D <sub>2</sub> O		Yes	Yes	$\frac{1.329 \pm 0.048}{0.608 \pm 0.048}$	$0.721 \pm 0.067$
ENDF/B-VI.8; MCNP5	Air D <sub>2</sub> O		No	No	$-4.048 \pm 0.070 \\ -5.240 \pm 0.065$	$1.192 \pm 0.095$
	Air D <sub>2</sub> O		No	No	$\frac{1.260 \pm 0.046}{0.039 \pm 0.044}$	$1.221 \pm 0.064$
ENDF/B-VII.0; MCNP5	Air D <sub>2</sub> O		Yes	No	$\begin{array}{c} 2.956 \pm 0.047 \\ 2.202 \pm 0.049 \end{array}$	$0.754 \pm 0.068$
	Air D <sub>2</sub> O	U19	Yes	Yes	$\frac{1.031 \pm 0.047}{-0.142 \pm 0.046}$	$1.173 \pm 0.066$
ENDF/B-VII.0; MCNPX	Air D <sub>2</sub> O		Yes	Yes	$\begin{array}{c} 0.949 \pm 0.047 \\ \text{-}0.181 \pm 0.044 \end{array}$	$1.130 \pm 0.065$

Table 2: MCNP results for ZED-2 NU measurements.



Figure 2: MCNP5  $k_{eff}$  simulation bias for ZED-2 critical experiments.

The results in Figure 2 show three distinct groups, the lowest set corresponding to the earlier ENDF/B-VI.8 data library, for which larger negative  $k_{eff}$  biases of up to -10 mk are observed. For the SEU/RU simulations, this group also shows the largest CVR simulation bias of +5.1 mk for the 24-cm pitch case.

The middle group of data in Figure 2 corresponds to the ENDF/B-VII.0 data, but without using the TSL data for UO<sub>2</sub>. The  $k_{eff}$  biases are reduced substantially in every case and the CVR biases for the SEU/RU experiments are reduced modestly by about 0.9 mk. Since the calculated leakage values do not change substantially with the different nuclear data sets, a lower CVR bias corresponds to a reduced slope for the lines joining the pairs of data points.

Finally, the top data group shows the results obtained when the preliminary UO<sub>2</sub> TSL ACE files are used. Although the correlation between the SEU/RU and NU results is much reduced, the  $k_{eff}$  and CVR biases are reduced for the SEU/RU simulations, as is the CVR bias for the NU simulations.

Examining the MCNPX  $k_{eff}$  bias results in Table 1 with and without the UO<sub>2</sub> TSL data shows that the reactivity impact is small, up to about +0.33 ± 0.08 mk for the aircooled 20-cm SEU/RU case. However, the impact on the CVR simulation bias is less than about 0.08 mk and, hence, is statistically insignificant.

#### IV.B Energy Dependence

The effective neutron multiplication constant,  $k_{eff}$ , can be defined as the ratio of total fission neutron yields (i.e.,  $v\Sigma_f \phi$  integrated over all energies and volumes containing fissionable materials) to total neutron losses (i.e., fissions plus captures minus (n,xn) reactions integrated over all energies and volumes, plus leakage). Since total neutron losses are effectively normalized to unity in MCNP (see p. 2-168 of Reference 2),  $k_{eff}$  is numerically equivalent to the total neutron yields. However, while  $k_{eff}$  is a single, spatially independent, integral value, fission yields vary considerably with neutron energy and position. Thus, MCNP fission-yield tallies grouped into appropriate neutron-energy bins and summed over the fuel regions of interest can be used to explore the energy and spatial dependence of these individual contributions to  $k_{eff}$ .

There are two provisos

- The fission-yield tallies must involve sufficient events in each neutron-energy group and sub-region of interest such that the associated statistical uncertainties are sufficiently small to minimize insignificant/spurious results.
- Since the fission-yield tallies are derived from flux values, the  $k_{eff}$  obtained corresponds numerically only to the MCNP 'track-length'  $k_{eff}$  estimator (see Note 6 on p. 5-103 of Reference 2). This is not a major concern provided that the associated uncertainty is sufficiently small for the application.

On this basis, the energy dependencies of the various contributions to  $k_{eff}$  are shown in Figure 3 for sample cooled and voided cases involving the NU UO<sub>2</sub>/ZEEP and SEU/RU 24-cm-pitch simulations. One caveat is that the contributions to  $k_{eff}$  are based on the numerical sum of the fission-yield tallies and not the fission-yield per unit lethargy values depicted. Although the shape of figures based on the former are rather similar, the results obtained depend on the choice of energy-group boundaries, such that results based on the latter values (i.e., per unit lethargy) are generally smoother.



Figure 3: Energy dependence of MCNP track-length  $k_{eff}$  based on fission-yield tallies for air/D<sub>2</sub>O-cooled NU UO<sub>2</sub>/ZEEP and air/H<sub>2</sub>O-cooled SEU/RU 24-cm-pitch simulations.

The left side of Figure 3 shows that the perturbation in the energy distribution of the fission yields associated with  $D_2O$  coolant voiding is barely discernable. The right side of Figure 3 shows that the basic spectrum of fission yields for the SEU/RU cases is essentially the same as for the NU cases with a very slightly reduced thermal peak, while the perturbation associated with H<sub>2</sub>O coolant voiding is more readily apparent.

Figure 4 shows the corresponding energy dependencies of the CVR simulation biases obtained from differences between the fission-yield tallies for the air- and D<sub>2</sub>O- or H<sub>2</sub>O- cooled cases in Figure 3, as well as some related comparisons. This figure highlights the basic reactor physics of coolant voiding, which primarily involves a slight hardening of the <sup>235</sup>U-related fission-yield spectrum at thermal energies (e.g., the energy corresponding to the average lethargy of neutrons causing fission increases by 13% from 1.0641x10<sup>-7</sup> to 1.2032x10<sup>-7</sup> MeV for the change from D<sub>2</sub>O to air coolant depicted on the left side of Figure 3) giving rise to negative and positive reactivity contributions below and above about  $4x10^{-8}$  MeV, respectively, and a small increase in fast fission yields from <sup>238</sup>U at high energies. Note that, whereas the vertical scales on the left and right sides of Figure 3 are identical, the vertical scale on the right side of Figure 4 for the air/H<sub>2</sub>O cases is about an order of magnitude larger than that on the left for the air/D<sub>2</sub>O cases. Also, note for the air/H<sub>2</sub>O cases that the positive peak just above  $4x10^{-8}$  MeV dominates the fast-fission peak, whereas they are of comparable magnitude for the air/D<sub>2</sub>O cases.

Three air/D<sub>2</sub>O cases are compared on the left side of Figure 4 corresponding to MCNP5 ENDF/B-VII.0 results using no UO<sub>2</sub> TSL data (dashed line; yellow triangles), UO<sub>2</sub> TSL data with elastic scattering (blue squares) and the preliminary UO<sub>2</sub> TSL ACE files (red diamonds) without elastic scattering. As expected, the UO<sub>2</sub> TSL data only has a noticeable impact at thermal energies. For the case of no UO<sub>2</sub> TSL data, the negative and positive peaks at low energies are roughly equal in magnitude. A very slight reduction in the CVR bias results for the case of the UO<sub>2</sub> TSL data with elastic scattering because the negative peak increases by more than the positive peak does. For the case of the preliminary UO<sub>2</sub> TSL ACE files, both the negative and positive peaks are noticeably

reduced and a somewhat larger reduction of the CVR bias occurs as a result of the greater disparity between the magnitude of the negative and positive thermal peaks.



Figure 4: Energy dependence of MCNP CVR simulation bias based on differences in fission-yield tallies for air/D<sub>2</sub>O-cooled NU UO<sub>2</sub>/ZEEP and air/H<sub>2</sub>O-cooled SEU/RU 24-cm-pitch simulations.

The right side of Figure 4 compares the energy dependence of the CVR bias for MCNPX simulations of the 24-cm SEU/RU cases with and without the UO<sub>2</sub> TSL data. Although the CVR biases for these two datasets are the same to within 0.05 mk (see Table 1), there are small systematic differences at low neutron energies as shown in Figure 5, which shows the difference between the CVR bias results from the right side of Figure 4 as a function of energy together with  $\pm 1$  sigma statistical uncertainty bands.



Figure 5: Energy dependence of the difference between MCNPX CVR biases for 24-cmpitch SEU/RU simulations with and without UO<sub>2</sub> TSL data.

As with the CVR biases, the net impact of the  $UO_2$  TSL data results from the cancellation of larger negative (about 2.8 mk mainly at energies  $<3x10^{-8}$  MeV, based on

summing the negative differences between the  $\Delta$ fission-yield values) and positive (also about 2.8 mk, but at energies >3x10<sup>-8</sup> MeV) contributions. While the irregularity observed near 1.5x10<sup>-8</sup> MeV in Figure 5 appears to be statistically significant, the fluctuations between about 3x10<sup>-8</sup> and 7x10<sup>-8</sup> MeV are likely due to the statistical uncertainties associated with these differences of  $\Delta$ fission-yield tallies.

## IV.C Spatial Dependence

The MCNP CVR simulation bias can also be examined on the basis of the differences in fission yields that occur in different fuelled regions of the critical lattices. Some examples are provided for the MCNPX simulations of the 24-cm SEU/RU measurements. Although space does not permit showing the detailed energy dependence of these differences, they are roughly similar to the differences shown in Figure 4, since this figure represents the cumulative effect. Nevertheless, the energy dependence is sufficiently different in different regions that quite different local net effects result as indicated in Table 3.

The first line of Table 3 shows the result of grouping all the positive changes in the fission yields (mainly above about  $4 \times 10^{-8}$  MeV, see Figure 4) and all negative changes (mainly below about  $4 \times 10^{-8}$  MeV) separately. The net CVR simulation bias of 4.00 mk results from the cancellation of much larger positive and negative reactivity effects. The next two rows in Table 3 sum the positive and negative reactivity changes separately according to fuel pin type. A large positive local net contribution is obtained for the large inner fuel elements, due to the relatively small decrease in fission yields in these fuel elements at low energies, whereas a large negative local net contribution occurs in the small outer elements due to a large decline in the yields at low energies. Finally, the last two rows in Table 3 sum the contributions according to fuel composition. A surprising result is obtained in that the local net contribution of the SEU fuel is negative and that for the lattice as a whole only becomes positive when the larger positive local net contribution for the four RU fuel channels is included. It is suspected that this difference between the SEU and RU results is due to the different neutron spectrum at the corners of the lattice (rather than arising from small differences in the SEU and RU fuel composition), but additional investigation would be needed to confirm this.

Region	Total positive contributions (mk)	Total negative contributions (mk)	Net contribution (mk)
Total for all fuel	65.48	-61.48	4.00
Large inner CANFLEX fuel elements	38.95	-5.05	33.90
Small outer CANFLEX fuel elements	36.63	-66.53	-29.90
All SEU fuel	59.11	60.36	-1.25
All RU fuel	7.21	-1.96	5.25

Table 3: Spatial dependence of MCNPX H<sub>2</sub>O CVR simulation bias for SEU/RU ZED-2 measurements at 24-cm lattice pitch.

# **V. CONCLUSION**

While adopting the ENDF/B-VII.0 nuclear data library reduces the MCNP  $k_{eff}$ simulation bias substantially for all the ZED-2 experiments studied, the improvement for the CVR bias is more modest (about 0.9 mk for the SEU/RU H<sub>2</sub>O CVR experiments and <0.1 mk for the NU UO<sub>2</sub> D<sub>2</sub>O CVR experiments). Although initial calculations using preliminary TSL ACE files for UO<sub>2</sub> suggested promising reductions of the CVR biases, correcting the data files to include the coherent elastic scattering component largely eliminated any net benefit. This finding was confirmed using MCNPX simulations with an improved thermal scattering treatment and TSL ACE files from LANL. Despite significant physical disparities among the experiments simulated (enrichment, bundle geometry, coolant, lattice type and pitch, etc.) the  $k_{eff}$  biases show a rising trend with calculated leakage, suggesting that the bias results from some common experimental factor or nuclear data issue. Additional insight is obtained by examining the detailed changes that occur between the calculated energy and spatial distributions of fissionneutron yields for the voided and cooled critical lattice configurations. Such investigation reveals that the CVR bias is associated with a hardening of the neutron spectrum in the fuel, causing a decrease in  $^{235}$ U fission yields below about  $4x10^{-8}$  MeV, a corresponding increase at thermal energies above this and an increase at energies >1 MeV arising from increased fast fissions in <sup>238</sup>U. Thus, the net CVR simulation bias arises from the cancellation of larger positive and negative changes in fission yields that occur at different energies and in different fuelled regions of the core. The net reactivity impact of the UO<sub>2</sub> TSL data, while negligible, involves a similar cancellation of larger negative and positive contributions at thermal energies.

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