Benchmark of WIMS-IST Against MCNP for CANDU Pressure Tube Fast Fluxes

R. E. Donders[*], S.R. Douglas[**]

[*]Reactor and Radiation Physics Branch
[**]Deformation Technology Branch
Atomic Energy of Canada Limited
Chalk River Laboratories
Chalk River, Ontario, Canada
KOJ 1J0
dondersr@aecl.ca

ABSTRACT

Pressure tube fast-flux data in CANDU are currently calculated using the multi-group neutron transport code WIMS-IST. In this study, the WIMS-IST fast flux calculations are benchmarked against MCNP calculations (a Monte Carlo particle transport code), over the range of fuel burnup and coolant density in CANDU. The comparison shows good agreement between WIMS and MCNP, with WIMS fast fluxes being 1.5% to 4% lower than the MCNP values. The difference is smallest for fresh fuel, and increases with burnup. The fast flux gradient across the pressure tube (factor of 1.23 from inner edge to outer edge) is accurately calculated by WIMS.

When reporting fast fluxes in pressure tubes, these are generally given as >1.000 MeV fluxes. For WIMS, this requires an extra conversion step, since the WIMS ENDF/B libraries do not have a group boundary at 1 MeV. The conversion step is based on a fictitious isotope ONEMEV in the WIMS nuclear data library. The conversion factor in WIMS was found to be about one percent too high. When providing >1 MeV fluxes from WIMS, this partially compensates for the slight under prediction of the fast flux. Pressure tube >1 MeV fluxes from WIMS are therefore 0.5% to 3% lower than MCNP values.

To obtain accurate fast flux data, neutron transport calculations must be performed on a critical cell. For this study, all calculations were performed with radial albedo boundary conditions giving a critical cell. This required the use of an albedo version of MCNP, developed at AECL.

1. Introduction

Fast neutrons affect the behavior of pressure tubes in CANDU reactors. Pressure tube fast fluxes have been previously calculated using the multi-group two-dimensional neutron-transport code WIMS-IST [1] (referred to as WIMS for the remainder of this document). As a benchmark of the WIMS calculations, fast fluxes calculated using MCNP were compared with WIMS values. All MCNP calculations were performed using version MCNP-4C [2]. The MCNP code was modified at AECL to allow for the application of albedo boundary conditions, allowing for critical cell calculations (needed to produce accurate fast to thermal flux ratios). The MCNP calculations use point-wise cross sections, which do not include the group structure approximations needed for the multi-group transport calculations.

2. Method for Calculating Pressure Tube Fast Fluxes

MCNP is a general purpose Monte Carlo radiation transport code, which can calculate neutron, photon, and beta particle transport in complex geometries. To provide an accurate and consistent comparison of fast flux data for a CANDU cell, the following methodologies were adopted:

1. The AECL multi-temperature ENDF/B-6 neutron library for MCNP was used for the MCNP calculations. The WIMS calculations were performed with the ENDF/B-6 based NDAS library Version 1A (the WIMS-IST library).
2. The MCNP and WIMS calculations were performed using an energy-independent radial albedo boundary condition that established a critical cell within 2 mk. No other leakage treatments were applied in the calculations. For each MCNP calculation, the number of particles (neutrons) was chosen to be about one million, giving an uncertainty of less than 0.5 mk in the k-effective value. In MCNP, the boundary was set as “specular reflective”, to best represent an infinite lattice cell. WIMS assumes “white” reflection over a circular boundary. The impact of the boundary condition is discussed in Section 4.
3. Fast flux data were normalized to a bundle linear power of one kilowatt per cm. The MCNP powers were calculated by multiplying MCNP isotopic fission rates with the corresponding isotope fission Q values from WIMS ENDF/B-6 library. This provides a consistent relationship between the fission rates and the bundle power for the two codes. (Note that fission energy Q values in WIMS include delayed-photon and beta-particle energy, and energy from parasitic neutron captures. MCNP fission energy Q values do <u>not</u> include delayed-photon or beta-particle energy, nor do they fully account for energy in parasitic neutron captures).
4. Consistent input geometries were established for the WIMS and MCNP models. The bundle geometry is that of a CANDU 6 37-element bundle. The fuel compositions at the different burnups were based on WIMS calculations of the fuel compositions. Some of the materials from the WIMS burnup calculations are not available in the MCNP libraries. To establish complete consistency between the WIMS and MCNP models, materials not available in the MCNP library were removed from the WIMS model (giving identical material compositions for both the WIMS and MCNP calculations). All material temperatures in the WIMS and MCNP models were set at the same values. These values were chosen to be consistent with the temperatures available in the MCNP library as follows: fuel and sheath 900K; coolant and pressure tube 500K; calandria and moderator 300K.
5. The WIMS calculations were performed in 89 groups (full library groups), with fine mesh coolant and moderator regions (coolant: 2 mm mesh spacing; moderator: 2 mm from pressure tube to 10 cm radius, 4 mm from 10 cm radius to cell boundary).

3. Calculated Pressure Tube Fast Fluxes

Fast fluxes in the pressure tube were calculated for the CANDU 6 fuel channels. To investigate the effect of fuel burnup and coolant density, three bundle burnups (0, 100, 300 MWh/kgIHE) and two coolant densities (0.862, 0.761 g/cm^3) were considered. The coolant densities represent the range of coolant densities typically found in CANDU 6 reactors (there is zero steam quality throughout the channel, and the densities correspond to coolant temperatures of 539K and 583K, respectively). The bundle burnups also represent the range typically found in CANDU, with 300 MWh/kgIHE being somewhat higher than the typical exit burnup value.

Material compositions as a function of burnup were calculated by WIMS using an average coolant temperature of 562K. During the burnup, the radial albedo was adjusted to maintain the cell within 2 mk of critical. Calculated fluxes are listed in Table 1. Albedos and corresponding k-effectives for the calculations are presented in Table 2.

Table 1. Neutron fluxes, averaged over the pressure tube volume, for a CANDU 6 channel. Statistical uncertainties in the MCNP fluxes are all less than 0.2%.

Coolant Density (g/cm^3)	**Bundle Burnup (MWh/kgIHE)**	**Neutron Fluxes (1E+16 n·m^{-2}·s^{-1}) for a Bundle Fission Power of 1 kW/cm**								
		>1.0540 MeV Flux			**<0.625 eV Flux**			**Total Flux**		
		WIMS	**MCNP**	**W/M Ratio***	**WIMS**	**MCNP**	**W/M Ratio***	**WIMS**	**MCNP**	**W/M Ratio***
0.862 (inlet)	0	1.990	2.023	98.4%	14.50	14.65	99.0%	26.64	26.93	98.9%
	100	2.117	2.186	96.9%	14.33	14.52	98.7%	27.24	27.55	98.9%
	300	2.205	2.289	96.3%	16.43	16.67	98.6%	29.91	30.32	98.7%
0.761 (outlet)	0	2.033	2.067	98.4%	14.35	14.52	98.9%	26.57	26.88	98.9%
	100	2.161	2.235	96.7%	14.19	14.34	98.9%	27.18	27.48	98.9%
	300	2.251	2.335	96.4%	16.27	16.56	98.3%	29.84	30.26	98.6%

* Ratio of the WIMS to MCNP value.

Table 2. Albedos for the WIMS and MCNP calculations. The MCNP boundary is square with specular reflection. The WIMS code assumes a circular boundary with "white" reflection.

Coolant Density (g/cm^3)	**Bundle Burnup (MWH/kgIHE)**	**WIMS**		**MCNP**	
		Albedo	**k-effective**	**Albedo**	**k-effective**
0.862	0	0.98970	0.99999	0.99133	0.99985 ± 0.00017
"	100	0.99576	0.99995	0.99665	1.00003 ± 0.00044
"	300	1.00740	0.99997	1.00685	0.99990 ± 0.00022
0.761	0	0.98946	1.00003	0.99125	1.00079 ± 0.00039
"	100	0.99556	1.00001	0.99641	0.99855 ± 0.00042
"	300	1.00725	1.00000	1.00680	1.00192 ± 0.00048

There is a considerable fast flux gradient across the pressure tube in CANDU reactors. WIMS and MCNP fast fluxes at the inner and outer edges of the pressure tube are presented in Table 3. The fast flux ratio across the pressure tube is about a factor of 1.23.

Table 3. Fast fluxes at the inner and outer edges of the pressure tube in CANDU 6 fuel channels. Statistical uncertainties in the MCNP fluxes are all less than 0.2%.

Coolant Density (g/cm^3)	Bundle Burnup (MWh/kgIHE)	>1.0540 MeV Neutron Fluxes (1E+16 n·m^{-2}·s^{-1}) for a Bundle Fission Power of 1 kW/cm								
		Inner Edge of PT			Outer Edge of PT			Inner/Outer Ratio		
		WIMS*	MCNP	W/M Ratio	WIMS*	MCNP	W/M Ratio	WIMS**	MCNP	W/M Ratio
0.862 (inlet)	0	2.200	2.240	98.2%	1.785	1.821	98.0%	1.235	1.230	100.4%
	100	2.340	2.420	96.7%	1.899	1.968	96.4%	1.235	1.230	100.4%
	300	2.436	2.530	96.3%	1.978	2.060	96.0%	1.234	1.228	100.5%
0.761 (outlet)	0	2.247	2.291	98.1%	1.822	1.856	98.2%	1.236	1.234	100.2%
	100	2.389	2.475	96.5%	1.938	2.012	96.3%	1.236	1.230	100.4%
	300	2.488	2.586	96.2%	2.019	2.101	96.1%	1.235	1.231	100.3%

* For WIMS, these are actually the fluxes in the inner and outer 0.05 mm thick regions of the pressure tube.

** The WIMS ratios have been adjusted for the 0.05 mm thickness of the inner and outer regions, assuming a linear relationship between the fast flux and radial position. In a CANDU pressure tube, the relationship between fast flux and radial position is essentially linear, as has been shown previously.

When reporting fast fluxes, >1 MeV fluxes are often presented. Since the WIMS library structure does not have an energy boundary at 1 MeV, the ratio of >1 MeV flux to >1.054 MeV flux is usually provided from the WIMS edit routine, which includes a "ONEMEV" reaction rate to provide an estimate of the >1 MeV flux. As a check of this ratio, MCNP tallies of the >1.054 and >1.0 MeV fluxes were performed for fuel with 0 and 300 MWh/kgIHE burnup. Results are summarized in Table 4.

Table 4. Comparison of the >1 MeV to >1.054 MeV ratio, as calculated using WIMS and MCNP. Data are for a coolant density of 0.862 g/cm^3.

Bundle Burnup (MWh/kgIHE)	Ratio of >1 MeV to >1.054 MeV flux								
	Inner Edge of PT			Average in PT			Outer Edge of PT		
	WIMS	MCNP	W/M Ratio	WIMS	MCNP	W/M Ratio	WIMS	MCNP	W/M Ratio
0	1.039	1.028 ± 0.001	101.0%	1.039	1.029 ± 0.001	101.0%	1.039	1.029 ± 0.001	101.0%
300	1.039	1.027 ± 0.001	101.1%	1.039	1.028 ± 0.000	101.1%	1.039	1.028 ± 0.001	101.1%

4. Discussion of Results

The pressure tube fast fluxes calculated by WIMS are 1.5% to 4% lower than the MCNP values. The discrepancy is smallest at zero burnup, and increases with increasing burnup. WIMS and

MCNP calculate the same impact of coolant density change (~2%) and flux gradient across the pressure tube (inner- to outer-edge factor of 1.23).

When converting the WIMS >1.054 MeV group flux to a >1 MeV group flux, the WIMS reaction rate edit overestimates the conversion factor by one percent. When providing >1 MeV fluxes from WIMS, this partially compensates for the slight under prediction of the >1.054 MeV flux.

The boundary conditions applied within the WIMS code are different from those used in the MCNP calculation (which were selected to most closely represent the cells within a CANDU lattice). The albedo boundary condition for WIMS calculations is white reflection (i.e., reflected with a cosine distribution relative to the surface normal). The calculations were performed with a Pij boundary at about 3.5 cm outside the calandria tube. Although a square cell geometry is input into WIMS, the calculation is actually performed with a circular boundary (with the cell volume conserved).

The impact of the boundary conditions was studied by applying different boundary conditions to the MCNP code, as presented in Table 5. Albedos and corresponding k-effectives for the different boundary conditions are presented in Table 6.

Table 5. WIMS and MCNP pressure tube fluxes for a CANDU 6 channel, calculated with different boundary conditions. All calculations are for unirradiated fuel with a coolant density of 0.862 g/cm^3. Statistical uncertainties in the MCNP fluxes are all less than 0.2%.

Code	Boundary Condition	Neutron Fluxes (1E+16 $n \cdot m^{-2} \cdot s^{-1}$) for a Bundle Fission Power of 1 kW/cm					
		>1.0540 MeV Flux		<0.625 eV Flux		Total Flux	
			W/M Ratio		W/M Ratio		W/M Ratio
WIMS	circular/white	1.990		14.50		26.64	
MCNP	square/specular	2.023	98.4%	14.65	99.0%	26.93	98.9%
MCNP	square/white	2.017	98.7%	14.67	98.8%	26.99	98.7%
MCNP	circular/ specular	2.012	98.9%	14.63	99.1%	26.92	99.0%
MCNP	circular/white	2.008	99.1%	14.66	98.9%	26.80	99.4%

Table 6. Albedos and k-effectives for the MCNP boundary conditions study. All calculations are for unirradiated fuel with a coolant density of 0.862 g/cm^3.

MCNP Boundary Condition*	Albedo	k-effective		
square/specular	0.99133	0.99985	±	0.00017
square/white	0.99133	0.99875	±	0.00038
circular/specular	0.99014	1.00133	±	0.00036
circular/white	0.99010	1.00040	±	0.00026

* Boundary shape / type of reflection coefficient.

The data in Table 5 show that the boundary conditions affect the fast fluxes by up to two percent. The MCNP calculations with the same boundary conditions as WIMS (circular/white) give the best agreement with WIMS. The critical-cell albedo for the MCNP circular/white boundary condition is also in closest agreement with the WIMS albedo. Based on this boundary condition study, it appears that the application of a circular boundary with white reflection underestimates the pressure tube fast flux by about one percent. For the fresh fuel case this accounts for most of the discrepancy between WIMS and MCNP.

Fast fluxes in the pressure tube depend on several parameters, including: a) the power distribution within the bundle, especially the power of the outer elements, b) the fission neutron spectra for the important fissionable isotopes, and c) neutron scattering cross sections. Comparisons of the fission rates (U-235 and Pu-239) in CANDU 37-element bundles, as calculated with WIMS and MCNP, have been performed previously. The study showed that the WIMS and MCNP codes calculate relative pin powers within one percent, and outer element powers within 0.5%.

5. Summary and Conclusions

Cases with coolant densities and fuel compositions spanning the full range of CANDU conditions were constructed, and the fast neutron fluxes generated by the critical albedo versions of WIMS and MCNP were compared. The calculated fast neutron fluxes in the pressure tube agreed very well using these two codes, with the MCNP predictions about 1.5% higher at low burnup and about 3.5% higher at high burnup. A significant tilt of 23% in fast neutron flux across the thickness of a pressure tube was calculated by both codes. The above conclusions were insensitive to the change in coolant density from inlet to outlet conditions.

Boundary conditions in the WIMS and MCNP models differ slightly, which results in slight differences in the critical albedo. WIMS uses a circular boundary with "white" reflection, whereas the MCNP model used a square boundary with specular reflection. The MCNP boundary condition is closer to a real lattice cell situation. The effect of the boundary condition choice was investigated by running MCNP with a circular “white” boundary for unirradiated fuel. The white boundary condition reduces the pressure tube fast flux by about one percent, improving the agreement between WIMS and MCNP calculations. Note that the use of an energy-independent albedo is not necessarily appropriate for reactor calculations, although for CANDU cells, which are very similar, they represent a reasonable approximation.

A final small difference in fast flux was tracked to the conversion from the WIMS energy boundary of 1.054 MeV to the 1.000 MeV boundary prescribed by the fictitious isotope ONEMEV in the WIMS nuclear data library. The >1 MeV flux is often used by material scientists to describe the fast neutron flux. The WIMS >1.054 to >1.000 fast flux conversion is about one percent higher than that calculated by MCNP. This bias partially compensates for the underestimate in the WIMS fast flux discussed above. Pressure tube >1 MeV fluxes from WIMS are therefore 0.5% to 3% lower than MCNP values.

With the use of the albedo option in both MCNP and WIMS calculations, the agreement in fast neutron flux in the pressure tube is excellent between the two codes.

It is worth noting two important factors that must be considered when calculating and benchmarking neutron fluxes from neutron transport codes:

1. When calculating neutron fluxes in reactors, care must be taken to ensure that the cell is a critical lattice cell. In this study, criticality was established using energy independent radial albedos.
2. When comparing MCNP and WIMS fluxes, a consistent normalization method must be chosen for use in both codes. For this study, the WIMS "energy per fission" Q values (applied to each fissionable isotope) were used in both codes.

MCNP input files, WIMS input files, and the spreadsheet for the flux calculations have been archived under FFC-03310-253-002.

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NOMENCLATURE

MWh/kgIHE – MegaWatt hours per kilogram initial heavy element. In the 37-element CANDU 6 bundles, the initial heavy element mass is the initial uranium mass.
W/M Ratio – Ratio of WIMS value to corresponding MCNP value.

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