Evaluation of Supercell Methodologies Using ZED-2 Measurements

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ABSTRACT

As part of an effort to assess the supercell methods used to calculate the incremental cross sections representing reactivity devices, a benchmark study was performed by comparison with ZED-2 measurements. ZED-2 is a research reactor used to measure criticality, fine-flux and core-flux distributions for a given lattice arrangement. The measurements selected for the study included various absorbers similar to the light-water liquid-zone controllers and adjuster rods used in CANDU® reactors. Two types of supercell calculations were tested by comparison with measurements: the DRAGON code and the WIMS-AECL/SPH/Modified-MULTICELL suite of codes. The flux shape calculated with the supercell codes inside and outside the absorbers was compared with available copper-activation measurements. A full-core ZED-2 model was set up for Reactor Fuelling Simulation Program (RFSP) calculations. The calculated global flux distributions were compared with measurements. The error in modelling the reactivity effect was expressed in terms of the error in the prediction of the change in critical height.

1. Introduction

A decision has been made to use the multigroup transport code WIMS-AECL (Reference 1) for lattice-cell calculations in all future CANDU reactor-physics analyses. Within this framework, 2-group device incremental cross sections, compatible with WIMS-AECL lattice cross sections are required for core simulations. A full-2-energy-group option in the Reactor Fuelling Simulation Program (RFSP) (Reference 2), for static and dynamic core simulations has been developed, and functionally tested, and is currently being validated. Two supercell methods have emerged as candidates for generating 2-group incremental cross sections: the WIMS-AECL/SPH/Modified-MULTICELL suite of codes (Reference 3) and the DRAGON transport code (Reference 4).

An AECL R&D program was initiated to evaluate the supercell methodologies for calculating 2-group device incremental cross sections. In one component of this program, the supercell methods were tested using available ZED-2 measurements performed with various absorbers similar to the light-water liquid controllers and adjusters used in CANDU reactors.

2.0 Experimental Set-up in ZED-2

ZED-2 is an experimental reactor used to measure criticality, fine-flux and core-flux distributions for various lattice arrangements. It has an open aluminum vessel, surrounded by a graphite reflector. The circular side wall of the calandria vessel has an inside diameter of 336 cm, a thickness of 0.635 cm, and a height of 334 cm. The bottom plate of the calandria vessel is 2.97 cm thick. The graphite reflector surrounding the calandria has a mean thickness of 60 cm. There is a 2.86-cm gap between the calandria vessel and the radial graphite reflector. Below the calandria vessel, there is a bottom graphite reflector, 90 cm thick.

In many experiments, the fuel consisted of 28-element bundles. The fuel stacks were hung vertically down into the core from support rails positioned above the moderator. Each bundle stack was contained in an aluminum pressure tube containing heavy-water coolant, identical to moderator heavy water.

The moderator critical height was measured for the reference lattice without the reactivity device. The reactivity device was then introduced into the core, typically, interstitially at the core centre. If the device was a neutron absorber, it would require an increase in moderator height to maintain criticality. The change in critical height was a measure of the reactivity effect of the device.

3.0 Analysis Methodology

The validation of the supercell methodologies involves two levels of comparison of the flux distribution for each absorbing device. The first level is the comparison of the microscopic flux distribution calculated by the supercell codes with the measurement data. The second level is the comparison of the macroscopic flux distribution obtained by solving the diffusion equation in core simulations using RFSP. It also involves the comparison of the predicted reactivity effect of the device with measured values in terms of the change in critical moderator height.

3.1 Basic Lattice-Cell Properties

The ZED-2 reactor was modelled using the RFSP code. The lattice properties provided to the RFSP core model for the reference 28-element fuel lattice were generated using WIMS-AECL version 2-5a. The 89-energy-group ENDF/B-V library was used for this analysis.

3.2 Supercell Methods

Incremental cross sections were calculated for the absorbing devices using both the DRAGON code and the WIMS-AECL/SPH/Modified-MULTICELL suite. The calculations performed with each of these methods were completely independent, and are described in the following subsections.

3.2.1 The DRAGON Code

The DRAGON code was developed by École Polytechnique of Montréal and allows 2-dimensional (2D) and 3-dimensional (3D) lattice-cell and supercell calculations (References 5 and 6). The code solves the transport equation (References 7 and 8). The main characteristics of the code are

- access to multi-energy-group libraries (the 2D and 3D transport calculation can be performed with the same number of energy groups),
- self-shielding calculation capability,
- neutron flux calculation in multi-energy groups from the fundamental mode (using the Bn equation),
- calculation and editing of nuclear properties,
- burnup calculation capability, and
- collision-probability solution.

The DRAGON supercell model allows a 3D, mixed cylindrical and Cartesian representation: cylindrical geometry for the absorber and for the fuel channel and Cartesian geometry for the moderator. The latest version used in this study, DRAGON971124.zed2 (References 9 and 10), also allows the rectangular meshes to intersect with the cylindrical mesh. The 89-energy-group ENDF/B-V library was used for all the calculations.

Using a DRAGON supercell model with a fine-mesh structure (especially where a 3D representation is necessary) and a full 89-energy-group calculation is very demanding on computation-hardware resources and computation time. This demand is primarily due to the large size of the collision-probability matrices (region-to-region and region-to-surface) and the large number of energy groups. A standard procedure for the device-incremental-cross-section calculations has therefore been developed and tested. The procedure is sufficiently general to be suitable for all reactivity devices in most configurations. The 3-step process is described as follows:

1) A 2D basic lattice cell with cluster geometry is treated, and the maximum number of energy groups from the microscopic library is used to calculate the fine-flux distribution. The cross sections are condensed to the number of energy groups specified by the user (typically 33) to be used in Step 3, and are also homogenized over 3 regions: the moderator, the pressure-tube-and-calandria-tube annulus region, and the fuel-coolant-cladding region.
2) With a coarse-mesh supercell model, a full 89-energy-group flux solution is sought. The flux distribution is used to condense the absorber properties to the number of energy groups specified by the user (typically 33 groups). The 89-energy-group properties used in the coarse-mesh supercell model for the fuel, annulus, and moderator regions are obtained from the 2D cluster calculation of Step 1. The 33-group macroscopic cross sections calculated for the absorber device are used in Step 3.
3) A calculation is then performed with a fine-mesh model using the few-energy-group structure (typically 33 groups) to generate the detailed spatial flux distribution and the incremental cross sections homogenized in 2 energy groups.

3.2.2 WIMS-AECL/SPH/Modified-MULTICELL

In this method, the calculation of the supercell properties is based on the solution of the diffusion equation throughout the supercell, but with the absorber material properties formed in such a manner that the reaction rates calculated in the supercell are matched to those predicted by using a simplified WIMS-AECL model through SuPer Homogenization (SPH) techniques (Reference 11).

In the first step, a WIMS-AECL 1-dimensional (1D) model is set up with the absorber surrounded by a fuel annulus at an appropriate distance, typically representing the average distance of the neighbouring fuel channels. With this 1D model, the reaction rates in the absorber are calculated by a detailed transport calculation, using typically 33 energy groups. In the second step, an equivalent model with the same geometry is treated in a diffusion calculation in 2 energy groups to determine the SPH factors to be applied to the absorber cross sections so that the various reaction rates in the absorber match those calculated in the transport-based WIMS-AECL calculations.

A 3D supercell model is then set up for flux calculation in 2 energy groups using the modified MULTICELL. The cylindrical absorber and fuel channels are rectangularized since only Cartesian geometry is allowed. A full 2-group flux solution is sought for all regions delineated by the meshes including the absorber and the fuel channels.

The basic premise of this method is that the correct reaction rates in the absorber are being reproduced in the supercell calculation and that the reactivity rates determined from the 1D WIMS-AECL model are correct.

3.3 RFSP ZED-2 Core Model

A full-core ZED-2 model was set up for 2-group RFSP calculations. The radial and bottom graphite reflectors, the aluminum tank, the D_2O reflector, and the lattice properties were all included in the calculation model. The top of the core was cut off at the moderator free surface, and an appropriate extrapolation distance imposed. The air gap separating the graphite and the tank was smeared with the aluminum tank wall in the model. The axial extrapolation distance was specified to cater to the moderator surface, but was also applied at the bottom end of the ZED-2 model, because RFSP does not distinguish between top and bottom extrapolation distances. This did not introduce any error, since, in any case, the flux drops quickly at the boundary between the core and the 90-cm-thick reflector. The extrapolation distance at the top of each core configuration was established by a cosine fit to the measured axial flux shape.

The 2-group cross sections for 28-element-fuel, the D_2O reflector, the aluminum tank (bottom), the homogenized air gap and aluminum tank wall, and the graphite reflector were calculated using the WIMS-AECL code. The RFSP code version 2-15HP was used throughout this study.

3.4 Benchmarking of the Supercell Methods

The accuracy of the supercell method can be gauged from the fine-flux-shape and global-flux-shape comparisons with measurements and from the comparison of the reactivity effect in terms of change in critical height in the measurements. These criteria are described below.

a) Fine-Flux-Shape Comparisons

The thermal fluxes calculated with the supercell model inside the absorber, along the absorber tube or around its circumference, and in the neighbouring moderator can be compared to available copper-wire-activation measurements. These comparisons validate the local flux perturbation that is due to neutron absorption and scattering by the absorber materials, and the escape of neutrons from inside the absorber back to the moderator region. The measurements of flux shape were in terms of ^{64}Cu activity. Thus a proper comparison is with the total absorption rate in ^{63}Cu, computed by the supercell code.

For comparison purposes, the calculated ^{63}Cu absorption rates and measured ^{64}Cu activity were normalized to the same value at the surface of the absorber. With DRAGON, in addition to fluxes for each mesh region in the supercell model, a computation of reaction rates can be performed. Thus the ^{63}Cu neutron-absorption rates were computed and compared directly with measured data. With WIMS-AECL/SPH/Modified-MULTICELL, the comparisons were more involved. Inside the absorber, ^{63}Cu absorption rates obtained from the WIMS-AECL 1D model were compared with the measured ^{64}Cu activity. Outside the absorber, the calculated flux shape obtained from the Modified-MULTICELL supercell code was used in the comparisons. The two sets of reaction rates were normalized to the same value (measurement value) at the surface of the absorber.

b) Reactivity-Effect Comparisons

The reactivity effect of the absorber was measured in terms of change in critical height in the experiment. The error in modelling of the reactivity effect, expressed in terms of error in prediction of critical-height change, was inferred in the following manner. The reference core (without the absorber) was simulated using an RFSP model with an axial core height that corresponded to the measured critical height, and an upper extrapolation distance deduced from global flux-shape measurements. The perturbed core with the absorber inserted was also simulated with an axial core length that corresponded to the measured critical height, and an upper extrapolation distance deduced from global flux-shape measurements. The difference between the two calculated k_{eff} values indicated the error in modelling the reactivity effect of the absorber. It was, however, necessary to translate this k_{eff} error into an error in critical-height change. A moderator-level reactivity coefficient was determined using the perturbed-core configuration but with an arbitrary (1 cm) change in moderator level. Using this coefficient, the error in k_{eff} was converted to an error in critical-height change, which was then expressed as a percent error in the total measured critical-height change.

c) Global Flux-Shape Perturbation

Insertion of an absorber into the core causes a change in the global flux shape. In the experiments, the global flux perturbations were measured with copper wires placed at strategic interstitial locations, both for the reference core and for the perturbed core. These measurements allowed comparisons to the RFSP-computed flux shape, indicating whether

- the core model was properly set up to account for symmetry, and whether the relative neutron production and absorption in the fuel region, the heavy-water reflector and the graphite regions were reasonably predicted, hence adequately reproducing the flux shapes.
- the perturbation caused by the absorber was adequately captured via the set of incremental cross sections.

4.0 Results

This section compares results obtained with a set of light-water-absorber and stainless-steel adjuster measurements.

4.1 Comparison with Light-Water Absorber Measurements

A set of light-water-absorber measurements in ZED-2 is described in References 12 and 13. The absorbers used in these experiments were aluminum tubes containing pure or borated light water, inserted vertically at the centre of the core. Measurements were made with two different square lattice arrangements, with lattice pitches of 22.86 cm and 27.94 cm. Three sizes of liquid-absorber tubes were used, the largest being of outer diameter 6.35 cm, and wall thickness 0.147 cm. Measurements with this tube size were selected for this study because it is the most similar to the dimensions of the liquid-zone controllers in CANDU reactors. The light water in the absorber had 3 different boron concentrations:

1. B0 - Pure H_2O
2. B1 - H_2O + boron (2.5 mg/mL)
3. B2 - H_2O + boron (8.0 mg/mL)

The fine-flux distributions obtained from the supercell simulations were compared with measurements in the radial direction, from the centre of the absorber toward the centre of a fuel channel. The global flux distributions calculated with RFSP were compared against the measurements in the axial direction, on a line intersecting the centre of the absorber and the mid-point between two fuel channels.

4.1.1 DRAGON Results

The supercell model was 2D, and consisted of four channels with or without the absorber at the centre. The ^{63}Cu absorption rate inside the absorber and in the moderator region was calculated and compared with measured ^{64}Cu activity. Table 1 gives the comparison of the calculated fine-flux distributions with the measurements.

Comparisons of the fine-flux distribution can be considered separately for the region inside the absorber and for the neighbouring moderator region. Inside the absorber, with pure light water, the scattering process competes with absorption. The flux peaking or depression inside the absorber is sensitive to the relative reaction rates, and it is a fairly stringent test of the code to accurately represent the two competing reactions and reproduce the flux shape. On the other hand, when the light water is borated, the absorption reaction becomes dominant.

In the moderator region, the trend of the flux shapes is generally well reproduced by the calculations. The agreement for the B0 absorber case is within 1.76%. With the B1 absorber, the agreement deteriorates but is still within a reasonable range of 5.13%. With the strong B2 absorber, the predicted flux shape in the moderator generally agrees with the measured data, but the absolute magnitude differs substantially.

Table 2 shows, however, that the reactivity effect is very well reproduced for the B2 absorber, to within 1%, which is comparable to measurement uncertainty. For the B1 absorber, the agreement is within 2%. For the B0 absorber, the percent error in critical-height change prediction is equal to +6.8%. A positive sign for the calculation error means the reactivity effect is underestimated.

The measured global flux shape for the reference core in the axial direction at a location near the core radial centre at an elevation near the axial-flux peak is compared with the thermal flux shape computed by RFSP in Table 3. The results show that the calculation scheme over estimates the absorption rate with increasing boron concentration.

4.1.2 WIMS-AECL/SPH/Modified-MULTICELL Results

The fine-flux distributions calculated by the WIMS-AECL/SPH/Modified-MULTICELL method are compared with measurements in Table 1. The flux shape inside the absorber is from the WIMS-AECL model, whereas the flux shape outside the absorber in the moderator region is from the Modified-MULTICELL model. The flux shape inside the B0 unborated light-water absorber is most difficult to predict. WIMS-AECL overestimates the flux increase substantially. This discrepancy is not too surprising, given that the balance between scattering and absorption is sensitive to the spectrum, which in turn is dependent on neutron sources. These are modelled rather crudely in the 1D WIMS-AECL calculation.

Table 2 shows that the reactivity effect is predicted quite well for the B0 absorber. However, the agreement deteriorates as the absorption strength increases, and the reactivity effect of the B2 absorber is overestimated by 17.5%

The calculated global flux shape with the absorber inserted is compared with the measurements in Table 3. The results show that the calculation scheme over estimates the absorption rate with increasing boron concentration.

4.2 Comparison with Stainless-Steel Adjuster Measurements

The adjuster rods in CANDU reactors consist of stainless-steel tubes, either with or without a concentric stainless-steel shim rod. In Reference 14, ZED-2 experiments with stainless-steel adjusters of similar design to those of power reactors are described. Measurements of the reactivity effect and flux perturbations were performed with a variety of tube thicknesses and shim-rod sizes, with the adjusters placed vertically (parallel to the fuel) at the core centre.

The reference core contained 52 fuel rods arranged in a square lattice of 28.575-cm pitch. The fuel rods consisted of 28-element natural-uranium fuel. Three adjuster types, with different tube-and-rod combinations, were analyzed. All three types have a stainless-steel tube of outside diameter 7.62 cm and a wall thickness of 1.713 mm, which are representative of the dimensions of adjusters in the power reactors:

1. Vertical Adjuster Type V1: No Shim Rod
2. Vertical Adjuster Type V2: Shim Rod O.D. 19.08 mm

3. Vertical Adjuster Type V3: Shim Rod O.D. 12.73 mm

The fine-flux distributions obtained from the supercell simulations were compared with the measurements in the radial direction, from the centre of the absorber toward the centre of a fuel channel. The global flux distribution calculated with RFSP was compared with measurements in the axial direction, on a line intersecting the centre of the absorber and the mid-point between two fuel channels.

4.2.1 DRAGON Results

Table 4 shows the comparison of the fine-flux distribution calculation with measurements. The results of the calculation were normalized to be the same as the measurements at the surface of the adjuster tubes. In the cases of the V2 and V3 adjusters, which have a central shim rod, the fine-flux distribution inside the adjuster was also compared and showed very reasonable agreement. The flux shapes in the nearby moderator region are also in general good agreement, with a maximum difference of about 5%.

The RFSP simulation results for all cases are summarized in Table 5. The agreement between the measured and calculated reactivity effect is very close in all cases, with or without the shim rod, and for different sizes of the shim rod.

The comparison of the RFSP-calculated global-flux-shape distribution with the measurements is given in Table 6. In general, the agreement is very satisfactory with a maximum error of -4.33%.

4.2.2 WIMS-AECL/SPH/Modified-MULTICELL

The fine flux-shape comparisons are presented in Table 4. The results of the calculations were normalized to the measurement values at the surface of the adjuster tube. The flux shape in the nearby moderator region is in good agreement, with a maximum difference of 4.4%.

The reactivity effect comparison is given in Table 5. The agreement with the measured reactivity effect is very good, the worst case being the 6.3% overestimate for the V1 (tube-only) adjuster. The degree of agreement is quite comparable to that obtained using DRAGON increments.

Comparisons of the global flux-shape distribution are presented in Table 6. The same degree of agreement with measurement data as obtained using DRAGON incremental cross sections is observed.

5.0 Conclusion

Based on the results presented in the tables, DRAGON supercell calculations gave very good overall agreement in the case of liquid absorbers with a range of absorption strengths and in the case of various adjuster rod-and-tube designs. Good agreement is shown in fine- and global-flux-shape comparisons, as well as in reactivity-effect comparisons. The WIMS-AECL/SPH/Modified-MULTICELL calculations gave good overall agreement in the case of the unborated liquid absorber and in the case of various rod-and-tube adjuster designs. However, with borated light-water absorbers, the reactivity-effect comparison shows a maximum calculation error of about 20%.

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Table 1: Comparison of the Fine-flux Distributions with the Measurements for the Liquid Absorbers (Surface of the Absorber at 0.0 cm).

	(Measured-Simulated) / Measured (%)					
	DRAGON			WIMS-AECL/SPH/Modified-MULTICELL		
Distance (cm)	B0	B1	B2	B0	B1	B2
-2.575	+2.78	+0.00	-9.09	-4.03	+1.92	-4.54
-1.908	+2.07	-3.64	-12.00	-4.77	-1.82	-4.00
-0.956	+0.82	-7.24	-11.63	-5.82	-4.35	-2.32
0.163	+1.76	-1.90	-1.94	+0.00	+2.83	+9.71
1.565	+0.85	-1.72	-6.45	-1.98	+1.72	+8.06
1.985	+0.57	-1.69	-6.25	-2.46	+1.69	+7.81
3.695	-0.09	-2.48	-10.45	-3.89	-1.65	+1.49
5.035	-0.10	-4.17	-11.76	-4.80	-4.17	-1.47
6.225	-0.63	-5.13	-13.33	-6.56	-6.84	-4.44

Table 2: B0, B1 and B2 Absorbers / RFSP Simulation Results

	Measured Critical Height H_c (cm)	Measured Critical Height Change ΔH_c (cm)	RFSP Computed K_{eff}	Reactivity Error - $\Delta\rho$ (mk)	Moderator Level Coef. (mk/cm)	Calculation Error in ΔH_c (cm)	Calculation Error in ΔH_c (%)
	Incremental Cross Sections from DRAGON						
Reference Core	309.264	–	1.00252	--	–	–	–
With B0	321.232	11.968	1.00285	+0.338	0.416	+0.813	+6.8
With B1	340.584	31.320	1.00270	+0.189	0.348	+0.540	+1.7
With B2	351.049	41.785	1.00244	-0.080	0.309	-0.258	-0.6
	Incremental Cross Sections From WIMS-AECL/SPH/Modified-MULTICELL						
Reference Core	309.264	–	1.00252	--	–	–	–
With B0	321.232	11.968	1.00263	+0.109	0.416	+0.263	+2.2
With B1	340.584	31.320	1.00124	-1.275	0.348	-3.664	-11.7
With B2	351.049	41.785	1.00025	-2.264	0.309	-7.326	-17.5

Table 3: Comparison of the Global Flux Distributions with the Measurements for the Liquid Absorbers. (Measured-Simulated) / Measured (%)

	DRAGON			WIMS-AECL/SPH/Modified-MULTICELL		
Distance from Core Centre (cm)	B0	B1	B2	B0	B1	B2
13.97	-1.77	-7.69	-10.18	-2.18	-6.24	-6.51
41.91	+1.39	-0.34	+1.42	+1.45	+0.21	+3.20
69.85	+1.61	+2.04	+2.87	+1.70	+1.89	+3.54
97.79	+0.74	-0.69	+0.66	+0.74	-1.19	+0.76

Table 4: Comparison of the Fine-flux Distributions with the Measurements for the Vertical Adjusters (Surface of the Adjuster at 0.0 cm).

	(Measured-Simulated) / Measured (%)					
	DRAGON			WIMS-AECL/SPH/Modified-MULTICELL		
Distance (cm)	V1	V2	V3	V1	V2	V3
-2.583	–	-2.91	-0.87	–	-0.61	-2.83
-1.970	–	-1.02	+0.42	–	+1.87	-0.68
-0.786	–	-1.32	+0.57	–	+1.27	-0.78
0.440	-0.10	-3.09	+3.08	+0.10	+0.00	+1.48
1.700	+1.70	+1.93	+2.77	+2.59	+4.44	+3.76
2.410	+1.96	+2.37	+3.20	+2.61	+4.12	+3.71
3.830	+2.20	+2.58	+3.57	+1.68	+4.31	+3.03
5.350	+1.73	+2.32	+4.04	-2.10	+3.59	+1.95
6.510	+1.53	+2.29	+4.79	-1.54	+2.83	+1.47

Table 5: V1, V2 and V3 Adjusters / RFSP Simulation Results

	Measured Critical Height H_c (cm)	Measured Critical Height Change ΔH_c (cm)	RFSP Computed K_{eff}	Reactivity Error - $\Delta\rho$ (mk)	Moderator Level Coef. (mk/cm)	Calculation Error in ΔH_c (cm)	Calculation Error in ΔH_c (%)
	Incremental Cross Sections from DRAGON						
Reference Core	308.611	–	1.00462	--	–	–	–
With V1	323.665	15.054	1.00491	+0.287	0.366	+0.784	+5.2
With V2	329.181	20.570	1.00458	-0.040	0.357	-0.111	-0.5
With V3	326.581	17.970	1.00441	-0.208	0.386	-0.539	-3.0
	Incremental Cross Sections From WIMS-AECL/SPH/Modified-MULTICELL						
Reference Core	308.611	–	1.00462	--	–	–	–
With V1	323.665	15.054	1.00497	+0.347	0.366	+0.947	+6.3
With V2	329.181	20.570	1.00447	-0.149	0.357	-0.417	-2.0
With V3	326.581	17.970	1.00463	+0.010	0.386	+0.026	+0.1

Table 6: Comparison of the Global Flux Distributions with the Measurements for the Vertical Adjusters. (Measured - Simulated) / Measured (%)

	DRAGON			WIMS-AECL/SPH/Modified-MULTICELL		
Distance from Core Centre (cm)	V1	V2	V3	V1	V2	V3
14.29	-0.18	-2.34	-4.33	-2.22	-2.51	-4.50
42.86	+1.73	+2.55	+0.56	+1.69	+2.55	+0.56
71.44	+1.91	+2.42	+0.42	+1.91	+2.38	+0.46
100.01	-0.78	-0.59	-1.96	-0.78	-0.30	-1.90