APPLICATIONS AND RESULTS FOR THE SUPERCELL OPTION OF THE WIMS-D4M CODE*

W. L. Woodruff

Argonne National Laboratory
Argonne, Illinois 60439-4841 USA

and

C. I. Costescu

University of Illinois
Urbana-Champaign, Illinois 61801-2984 USA

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W. L. Woodruff
Argonne National Laboratory
Argonne, Illinois 60439-4841, USA
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C. I. Costescu
University of Illinois
Urbana-Champaign, Illinois 61801-2984, USA

ABSTRACT

The Supercell option of the WIMS-D4M code is used with a model for the Advanced Neutron Source design to illustrate the capability, and the results are compared with Monte Carlo. The capability is also used to successfully model Russian designed fuel assemblies with concentric tubes. The capability to model homogenized and resonance corrected fuel and to properly treat secondary regions containing resonance materials is particularly useful. The Supercell option is well suited to modeling non-lattice regions, such as, reflector, control and/or experimental regions of research reactors.

Introduction

While the WIMS-D4[1] code is well suited to the treatment of regular lattices, the conventional WIMS method does not deal well with non-lattice regions, such as, reflector, control or experimental regions. The Supercell option in the WIMS-D4M code[2] provides a capability for treating non-lattice geometry by providing properly homogenized and resonance corrected fuel regions, improved spectra for non-fueled regions and proper treatment for regions containing experimental fuel or other resonance material. This new option is applied to several diverse geometries and compared with VIM[3] Monte Carlo data.

Supercell Method

The Supercell option uses a variation of the multicell structure in a manner that allows the user to construct a detailed model of the desired geometry in a single cell and define a set of supporting auxiliary cells that provide improved spectra for selected regions of the supercell geometry. Auxiliary cells can be used to provide 1) homogenized and properly resonance shielded fuel data for use in the supercell fuel region(s) and/or as a driver source in other auxiliary cells, 2) a proper spectrum and resonance treatment for fuel or other resonance absorber in an experimental region or a resonance material in a control region, and 3) an improved spectrum and data for the reflector region or other regions of interest.

The supercell geometry may be either slab or annular, and the auxiliary cells may be any mix of geometries. The Supercell option is not a single fixed prescription that can be applied to all problems, but rather a collection of tools that allow the user to break down a complex supercell geometry into simpler auxiliary cells that provide improved spectra, resonance corrections and homogenization for the supercell regions. The possibilities for auxiliary cells are seemingly without limit, however, many of the choices may have little or no impact or give essentially the same spectrum as other choices. Only a few auxiliary cells are usually needed to describe the important regions of the supercell.

The fuel auxiliary cell for the initial spectrum and resonance treatment may be a simple unit cell or a more complex geometry. With the unit cell the conventional SPECTROX method may still be used, but for more complex geometries a new generalized S_n solution may be selected with a detailed mesh. This generalized solution removes the SPECTROX limitation which forces all materials into either fuel, clad, coolant and optionally moderator regions. The conventional WIMS solution if applied to the supercell geometry is also subject to this limitation. The conventional WIMS solution would also lump all of the resonance materials in the problem into the fuel region rather than applying a proper treatment for each separate region containing resonance material(s).

A model of the Oak Ridge National Laboratory's Advanced Neutron Source (ANS) design can serve to illustrate the use of the Supercell option. Figure 1 shows a section of the radial model of the ANS core, where the Hf control rods have been rendered as equivalent cylinders, and the fuel for the lower fuel assembly is homogenized. The shared side plates for the upper and middle fuel assemblies are shown on either side of the fuel together with the flow channels and companion side plates. Various other vessel walls are shown in the model. The actual Supercell model does not include all of the outer D_2O reflector and vessel but truncates the full model at the dashed line. Four auxiliary cells have been selected for this example.

The first auxiliary cell is a unit cell reflecting the dimensions of the fuel plates and channels together with a moderator region of D_2O representing the additional moderator surrounding the fuel assembly. This cell provides not only properly homogenized and resonance corrected data for the supercell fuel region but a source for the other auxiliary cells, as well.

The second auxiliary cell models the inner Hf control ring surrounded by an annulus of homogenized fuel from the first auxiliary cell. The geometry replicates that of the supercell geometry, but users will find that the results are rather insensitive to the exact geometry (a reasonable spectrum is still obtained). The Hf control material represents a second resonance material in addition to the fuel. A properly shielded set of cross sections for Hf is generated independent of the fuel resonance treatment.

The third auxiliary cell represents the outer Hf ring together with the surrounding Al vessel and D_2O. Again a surrounding annulus of homogenized fuel from the first auxiliary cell is used, and the inner ring of Hf is replaced with pure D_2O. Note: It would probably be sufficient to use the same data from the second auxiliary cell for this region of the Supercell model.

The last auxiliary cell represents the outer vessels and D_2O reflector. Here a slab of homogenized fuel from the first auxiliary cell is used together with an Al vessel and inner and outer regions of D_2O. The inner D_2O and Al vessel data are used in the supercell materials for the side plates and adjacent coolant, and the outer D_2O is used for the reflector region.

The actual input for this example is provided in the WIMS-D4M User Manual[4] as one of the sample problems, and some of the results from this case are provided in the following section. This example illustrates much of the capability available with the Supercell option.

Results

Some of the results for the Supercell analysis of the ANS reactor model (described in the previous section) are provided in Table I. Table I shows a comparison of the capture cross section and spectrum with VIM for the inner ring of Hf and shows a similar comparisons for the outer ring of Hf. Also shown is a comparison of the values of k-infinity between the Supercell and VIM. The Supercell is overestimating the eigenvalue by more than 1%. In the 15 group structure used in this study, groups 4-9 cover the resonance range treated by WIMS-D4M. The cross sections and spectrum for groups 1-8 are in reasonably good agreement with VIM, but some of the lower energy resonances in Hf have no resonance correction applied in WIMS-D4M and the agreement is not as good. The spectrum, however, shows that these groups have a very small population of neutrons. The conventional WIMS method would not be able to deal with the separate resonance regions for Hf and fuel in any reasonable way. The next two cases better illustrate the shortcomings of the conventional methods.

The Supercell option has been found to be particularly useful in treating some of the Russian designed fuel assemblies. Two are considered in this paper the VVR-M2 and the IRT-2M fuel assemblies. The VVR-M2[5] design consists of two concentric cylinders surrounded by an outer hexagonal tube, and the IRT-2M[6] design consists of four concentric boxes of fuel with a central circular tube without fuel (See Figure 2). In each case the fuel tubes are converted to equivalent cylinders preserving volumes in the supercell geometry. The fuel and clad thickness is the same for each tube in the fuel assembly in each case, so that a single fuel auxiliary cell can be used. This is the only auxiliary cell used in the VVR-M2 model. The fuel auxiliary cell consists of a simple slab unit cell with representative dimensions. The IRT-2M Supercell model uses a second auxiliary cell to get an improved spectrum for the central tube. These two cases have also been included as sample problems in the WIMS-D4M User Manual.

The first concern is the impact of changing the geometry to all cylindrical geometry. Table II shows a comparison of two VIM cases for the VVR-M2 assembly, one with as built geometry and the other with all cylindrical geometry. The results are identical within the statistical limits. This is a good approximation for the Supercell model. The Supercell comparisons with VIM are all done with a consistent cylindrical geometry.

The results for the VVR-M2 assembly in Table III show a comparison of the conventional WIMS methods with a simple unit cell and with the full supercell geometry, the Supercell model and VIM for ^{235}U fission, ^{238}U capture and spectra, respectively. The results with a simple unit cell give reasonably good agreement with VIM. The results when conventional methods are used for the full assembly show some of the limitations that the Supercell option overcomes. The poor resonance treatment with the conventional SPECTROX method has a small effect on the fission data and a larger effect on the capture data and eigenvalue results. Lumping the fuel, clad and coolant from all of the annuli in the assembly to form a unit cell is not a good approximation for the resonance treatment. The spectra are in good agreement for all of the methods. The Supercell option gives the best overall agreement with the VIM data.

The results in Table IV for the IRT-2M fuel assembly show even more dramatic differences. Here the simple unit cell model is not such a good choice for the full fuel assembly but serves well as an auxiliary cell in the Supercell model. A second auxiliary cell is provided for the central tube and water hole with homogenized fuel from the first auxiliary cell used as a source. The Supercell option again gives the best agreement with VIM for the full fuel assembly. The spectrum and the hydrogen capture in the central water hole is compared in Table V, and the agreement with the VIM data is excellent. Only the lowest energy groups for hydrogen capture are signiicant and shown in the table.

Conclusions

The Supercell option of the WIMS-D4M code has been shown to be a very useful tool in modeling complex geometries and non-lattice regions. The ANS reactor design serves as a good platform for illustrating some of the capabilities for producing homogenized and resonance-corrected fuel data, treating separate regions containing resonance material and providing good spectra for control, reflector and experimental regions. The Supercell option proves to be an essential tool for modeling the complex geometry of the VVR-M2 and IRT-2M Russian designed fuel assemblies. The eigenvalues for these assemblies are in remarkably good agreement, but this is partially due to compensating differences in the ^{235}U fission data and the ^{238}U capture data. The differences observed are not due to limitations in the Supercell option but rather to other inherent limitations in the WIMS code itself. These results were generated prior to any fine tuning of the cross section library.

Figure 1. Supercell Model for Advanced Neutron Source Design

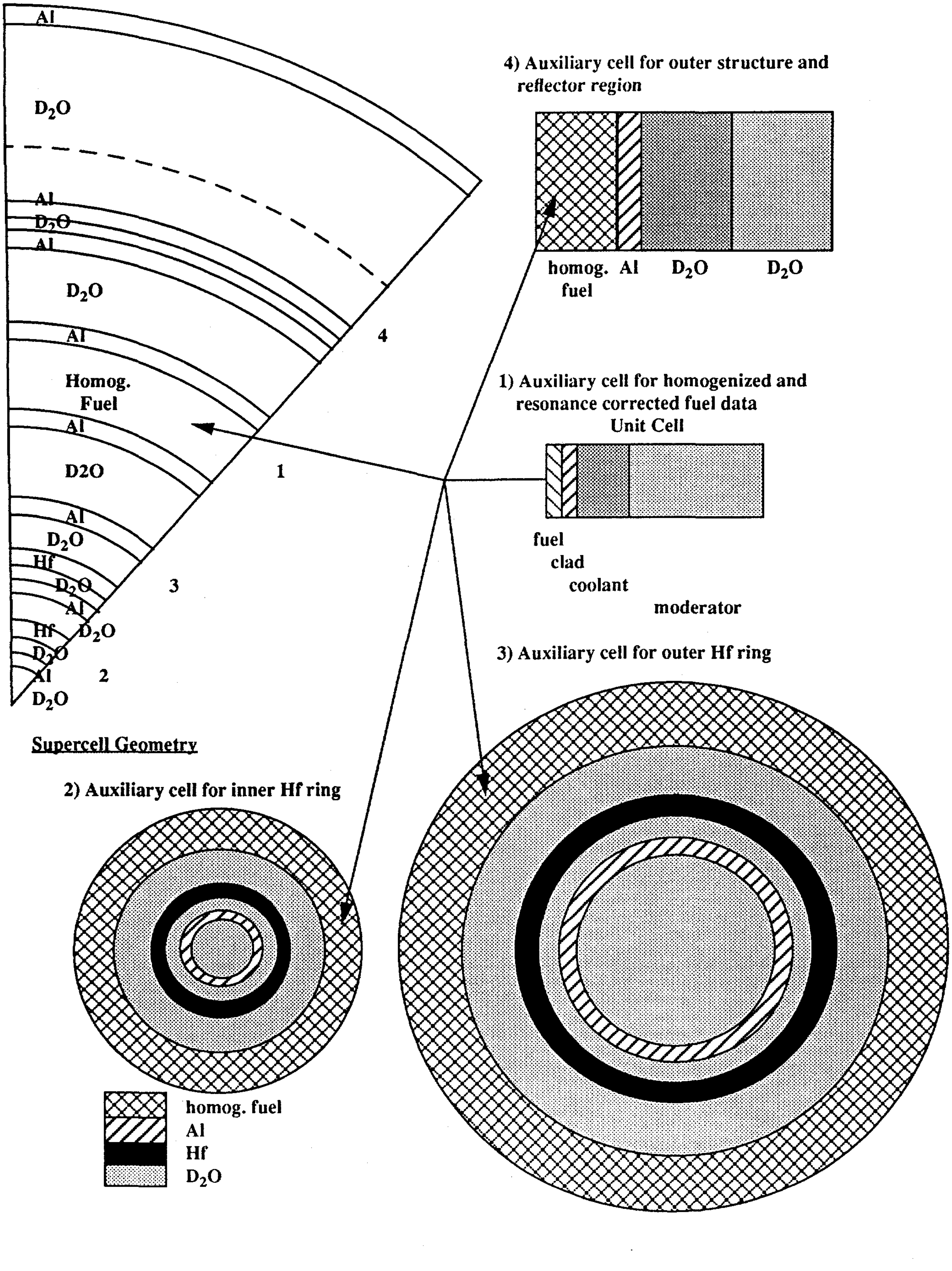
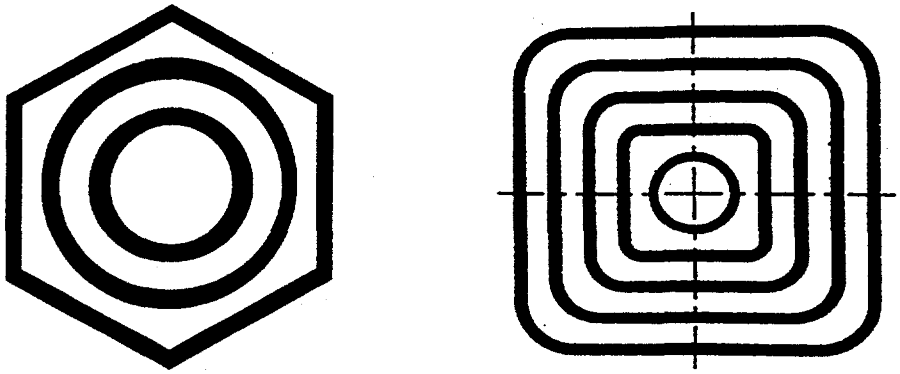


Table I. Data for Inner and Outer Rings of Hf

Inner Ring:	Capture		Spectra	
Group	Supercell	VIM	Supercell	VIM
1	0.070	0.071	0.0661	0.0711
2	0.324	0.330	0.1263	0.1311
3	0.837	0.878	0.1297	0.1324
4	1.179	1.425	0.0989	0.1034
5	1.805	2.886	0.1446	0.1429
6	3.135	5.908	0.1444	0.1261
7	9.326	8.842	0.1951	0.1856
8	10.02	9.433	0.0584	0.0597
9	83.44	36.88	0.0102	0.0131
10	92.36	59.95	0.0079	0.0141
11	142.6	130.6	0.0012	0.0015
12	46.18	46.29	0.0045	0.0051
13	43.85	43.92	0.0035	0.0040
14	58.68	58.42	0.0079	0.0083
15	106.3	104.4	0.0014	0.0015

Outer Ring:	Capture		Spectra	
Group	Supercell	VIM	Supercell	VIM
1	0.071	0.071	0.0695	0.0709
2	0.323	0.330	0.1326	0.1333
3	0.836	0.879	0.1261	0.1271
4	1.179	1.423	0.0924	0.0962
5	1.803	2.926	0.1319	0.1317
6	3.133	6.163	0.1285	0.1178
7	9.420	9.609	0.1807	0.1758
8	10.01	10.17	0.0570	0.0580
9	83.44	41.23	0.0141	0.0154
10	116.0	73.46	0.0120	0.0187
11	142.2	126.3	0.0034	0.0039
12	46.25	46.34	0.0111	0.0114
13	43.86	43.99	0.0084	0.0088
14	59.95	60.11	0.0253	0.0244
15	108.8	108.6	0.0072	0.0065
K-infinity	1.3199	1.3006 ± 0.0007		

Figure 2. VVR-M2 and IRT-2M Russian Fuel Assemblies



VVR-M2 IRT-2M

Table II. VIM Reaction Rates for VVR-M2 Fuel Assembly

Group	Fission		Capture	
	As Built	Cylindrical	As Built	Cylindrical
1	3.4522E-3	3.4636E-3	3.9056E-3	3.9302E-3
2	1.7222E-3	1.7207E-3	8.7006E-4	8.6917E-4
3	7.5237E-4	7.5325E-4	8.2087E-4	8.2190E-4
4	6.4269E-4	6.4105E-4	8.5264E-4	8.4931E-4
5	1.4713E-3	1.4695E-3	1.4166E-3	1.4112E-3
6	2.9029E-3	2.9101E-3	2.7406E-3	2.7410E-3
7	1.4409E-2	1.4408E-2	1.9352E-2	1.9347E-2
8	8.5516E-3	8.5280E-3	1.5139E-2	1.4910E-2
9	6.2686E-3	6.2386E-3	2.1779E-2	2.1551E-2
10	7.0634E-3	7.0761E-3	6.1721E-3	6.1734E-3
11	6.3156E-3	6.3261E-3	2.9931E-3	2.9982E-3
12	1.7878E-2	1.7896E-2	7.7297E-3	7.7350E-3
13	2.3797E-2	2.3775E-2	1.0700E-2	1.0691E-2
14	2.5719E-1	2.5744E-1	1.0410E-1	1.0427E-1
15	3.2286E-1	3.2228E-1	1.2527E-1	1.2531E-1
Total	6.7527E-1	6.7492E-1	3.2384E-1	3.2361E-1
K-infinity	1.6465 $\pm$0.0006	1.6467 $\pm$0.0005		

Table III. Full Fuel Assembly Data for VVR-M2

Group	U-235 Fission (Table III - Part 1)			
	Unit Cell	Full Cell	Supercell	VIM
1	1.2857	1.2585	1.2587	1.2834
2	1.3279	1.3147	1.3156	1.3253
3	2.0104	2.0073	2.0084	2.0135
4	2.9829	2.9856	2.9848	2.9756
5	5.2265	5.2311	5.2280	5.2227
6	10.566	10.539	10.578	10.559
7	28.112	26.808	28.238	28.308
8	44.091	39.451	44.443	44.187
9	36.911	31.266	37.294	38.410
10	27.763	27.621	27.837	27.531
11	59.522	59.686	59.692	59.404
12	111.39	111.68	111.91	111.16
13	179.72	180.77	180.78	178.67
14	292.65	296.62	295.43	288.32
15	624.72	622.70	629.77	613.91
K-infinity	1.6550	1.6838	1.6522	1.6467

Group	U-238 Capture (Table III - Part 2)			
	Unit Cell	Full Cell	Supercell	VIM
1	0.0555	0.0542	0.0542	0.0564
2	0.1380	0.1366	0.1368	0.1378
3	0.4363	0.4354	0.4358	0.4341
4	0.7295	0.7215	0.7302	0.7248
5	1.2948	1.1904	1.2991	1.2927
6	2.6903	2.2216	2.7125	2.7075
7	11.715	6.3565	12.122	12.160
8	21.899	10.214	22.832	22.280
9	52.250	24.164	54.526	54.652
10	0.5046	0.5054	0.5056	0.5054
11	0.5475	0.5490	0.5491	0.5470
12	0.6974	0.7000	0.7004	0.6953
13	0.9174	0.9233	0.9230	0.9104
14	1.5240	1.5387	1.5379	1.5027
15	2.8633	2.8565	2.8865	2.8135

Group	Spectra (Table III - Part 3)			
	Unit Cell	Full Cell	Supercell	VIM
1	0.2512	0.2475	0.2501	0.2452
2	0.1813	0.1784	0.1800	0.1818
3	0.0528	0.0522	0.0526	0.0524
4	0.0303	0.0300	0.0303	0.0302
5	0.0398	0.0393	0.0397	0.0394
6	0.0388	0.0384	0.0388	0.0386
7	0.0718	0.0714	0.0717	0.0714
8	0.0272	0.0275	0.0272	0.0271
9	0.0230	0.0236	0.0230	0.0228
10	0.0365	0.0370	0.0364	0.0360
11	0.0150	0.0152	0.0150	0.0149
12	0.0225	0.0229	0.0225	0.0226
13	0.0178	0.0181	0.0179	0.0187
14	0.1198	0.1230	0.1212	0.1252
15	0.0721	0.0755	0.0736	0.0736

Table IV. Full Fuel Assembly Data for IRT-2M

Group	U-235 Fission (Table IV - Part 1)			
	Unit Cell	Full Cell	Supercell	VIM
1	1.4042	1.2686	1.2690	1.3844
2	1.3908	1.3216	1.3230	1.3535
3	2.0224	2.0089	2.0127	2.0204
4	2.9852	2.9926	2.9903	2.9830
5	5.2239	5.2371	5.2320	5.2247
6	10.542	10.455	10.579	10.454
7	27.950	24.999	28.146	27.961
8	43.524	35.363	44.073	42.904
9	36.319	26.353	36.876	37.077
10	27.628	27.266	27.772	27.366
11	58.979	59.501	59.493	58.585
12	109.73	110,65	111.20	109.17
13	174.67	178.41	178.38	174.41
14	283.68	285.10	285.58	274.33
15	562.40	563.24	570.63	549.02
K-infinity	1.5920	1.7250	1.6858	1.6796

Group	U-238 Capture (Table IV - Part 2)			
	Unit Cell	Full Cell	Supercell	VIM
1	0.0584	0.0532	0.0531	0.0579
2	0.1443	0.1371	0.1376	0.1406
3	0.4387	0.4349	0.4366	0.4363
4	0.7301	0.7106	0.7318	0.7246
5	1.2945	1.0813	1.3044	1.2852
6	2.6851	1.8201	2.7336	2.6602
7	11.676	4.4586	12.497	11.491
8	21.609	6.7719	23.587	18.852
9	51.496	15.776	56.248	47.160
10	0.5016	0.5042	0.5043	0.5025
11	0.5426	0.5474	0.5472	0.5398
12	0.6863	0.6954	0.6961	0.6840
13	0.8949	0.9126	0.9118	0.8898
14	1.4712	1.4830	1.4847	1.4289
15	2.5777	2.5859	2.6169	2.5178

Group	Spectra (Table IV - Part 3)			
	Unit Cell	Full Cell	Supercell	VIM
1	0.2326	0.2537	0.2582	0.2540
2	0.1508	0.1698	0.1722	0.1738
3	0.0437	0.0495	0.0502	0.0495
4	0.0253	0.0286	0.0290	0.0286
5	0.0329	0.0373	0.0379	0.0373
6	0.0323	0.0366	0.0370	0.0365
7	0.0603	0.0681	0.0685	0.0673
8	0.0234	0.0264	0.0260	0.0257
9	0.0200	0.0228	0.0220	0.0219
10	0.0318	0.0357	0.0350	0.0346
11	0.0132	0.0147	0.0144	0.0143
12	0.0201	0.0222	0.0217	0.0217
13	0.0173	0.0176	0.0174	0.0183
14	0.1728	0.1316	0.1283	0.1340
15	0.1236	0.0853	0.0821	0.0826

Table V. Central Water Hole in IRT-2M Assembly

Group	Spectra		Hydrogen Capture	
	Supercell	VIM	Supercell	VIM
1	0.2179	0.2059	--	--
2	0.1504	0.1534	--	--
3	0.0460	0.0464	--	--
4	0.0269	0.0274	--	--
5	0.0354	0.0355	--	--
6	0.0349	0.0348	--	--
7	0.0656	0.0659	--	--
8	0.0255	0.0258	--	--
9	0.0218	0.0222	--	--
10	0.0341	0.0340	--	--
11	0.0141	0.0140	--	--
12	0.0216	0.0218	--	--
13	0.0181	0.0194	0.11141	0.11103 $\pm$0.00007
14	0.1637	0.1708	0.19541	0.19326 $\pm$0.00011
15	0.1240	0.1239	0.38861	0.38891 $\pm$0.00056

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