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TESTING WIMS-D4M CROSS SECTIONS AND THE ANL ENDF/B-V 69-GROUP LIBRARY

Results from Global Diffusion and Monte Carlo Calculations Compared with Measurements in the Romanian 14-MW TRIGA Reactor*

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ABSTRACT

The WIMS-D4 code has been modified (WIMS-D4M) to produce microscopic isotopic cross sections in ISOTXS format for use in diffusion and transport calculations. Beginning with 69-group libraries based on ENDF/B-V data, numerous cell calculations have been made to prepare a set of broad group cross sections for use in diffusion calculations. Global calculations have been made for two control rod states of the Romanian steady state TRIGA reactor with 29 fresh HEU fuel clusters. Detailed Monte Carlo calculations also have been performed for the same reactor configurations using data based on ENDF/B-V. Results from these global calculations are compared with each other and with the measured excess reactivities. Although region-averaged macroscopic principal cross sections obtained from WIMS-D4M are in good agreement with the corresponding Monte Carlo values, problems exist with the high energy (E>10 keV) microscopic hydrogen transport cross sections.

INTRODUCTION

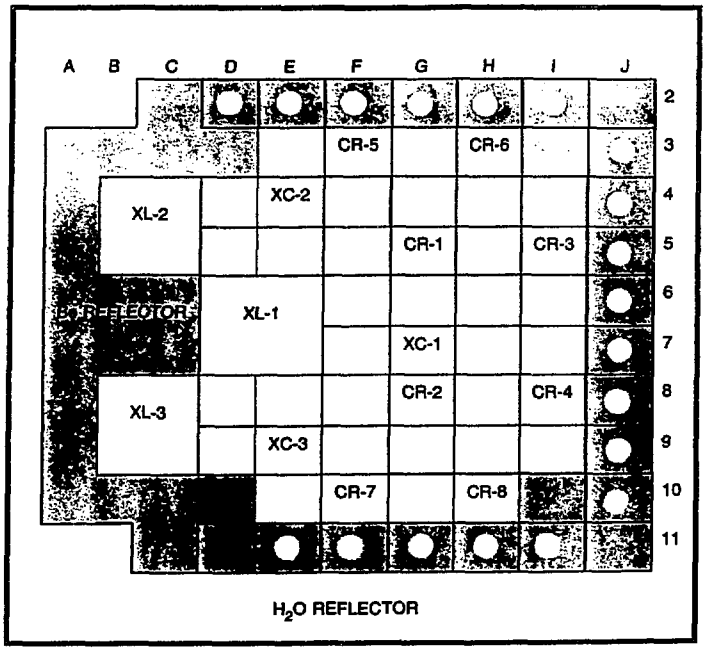
The WIMS-D4 code[1] has been modified[2] and improved to make it more useful to the research reactor community. Major modifications include the ability to produce broad group microscopic cross sections in ISOTXS format and to average them over any desired combination of material regions. A supercell option has been added to the code and is currently being tested. This option should allow the calculation of improved cross sections for thick experimental regions, reflectors, and strongly absorbing control rods. Based on ENDF/B-V data, a new 69-group 96-material library[3] has been prepared for use with WIMS. In a paper[4] presented at the last RERTR meeting principal microscopic cross sections generated by WIMS-D4M were found to compare very favorably with corresponding VIM[5]-Monte Carlo cell calculations.

To test the quality of the broad group cross sections produced by WIMS-D4M with the new ENDF/B-V-based library, diffusion calculations have been performed for well-defined initial startup configurations of the Romanian 14-MW TRIGA steady state reactor (SSR). Results from these global diffusion calculations are compared with parallel Monte Carlo calculations and with measured excess reactivities.

THE SSR REACTOR

The SSR reactor is located in Pitesti, Romania, and is operated by the Institute for Nuclear Research. Initially, the beryllium-reflected core contained 29 HEU fuel clusters each consisting of a square 5x5 array of Incoloy-clad uranium-zirconium hydride-erbium fuel pins enclosed within an aluminum shroud 8.753 cm on a side. Figure 1 shows the configuration of this initial core. With all

INITIAL SSR CORE CONFIGURATION
WITH 29 FRESH HEU TRIGA (5X5) FUEL CLUSTERS



ALL EXPERIMENT LOCATIONS (XL-1, 2, 3; XC-1, 2, 3;
AND THE HOLES IN THE BERYLLIUM REFLECTOR) ARE FILLED WITH WATER

Figure 1

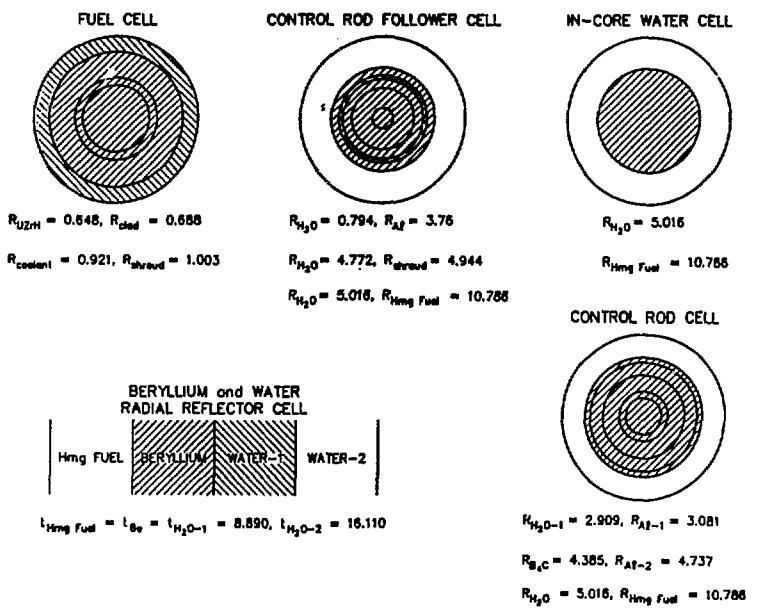


Figure 2. Single Cells for SSR Cross Section Generation
(Dimensions in cm. Shaded areas correspond to combined material edit regions.)

experiment positions filled with water and with fresh fuel in the xenon-free core, careful measurements were made at low power to determine the excess reactivity and the elevation of the control rod bank when the reactor was observed to be just critical. This experimental information was provided by the SSR staff[6]. Detailed SSR geometric information is provided in reference (7) while the method used to determine the fuel pin atom densities is discussed elsewhere[8]. The standard 29-cluster SSR core configuration was chosen for this benchmark test of WIMS-D4M cross sections generated from the new 69-group library because it is a clean core with a well-defined geometry and for which fundamental experimental data are available.

MULTIGROUP CROSS SECTIONS

Broad group cross sections were generated for the various SSR regions shown in Figure 1. An 8-group structure simulating that used for the SSR SAR[7] was used for these studies. Figure 2 shows the single cell models used to generate WIMS-D4M and VIM cross sections. The outer region of the the fuel cell is a thin homogenized Al-H_2O mixture used to approximate the effect of the alumunium shroud surrounding the 25 pin square array. However, this outer region was not included in the calculation of the DANCOFF factor. Cross sections were homogenized over the fuel, clad and coolant regions of the fuel cell and in a second calculation over the shroud/water ring. An homogenized fuel ring served as a driver for the other cells but was excluded from the cross section material edit regions. Improved cross sections for these auxillary cells are expected from the use of the supercell option in WIMS-D4M when it becomes fully operational. This option should be especially useful for the control rod cell where fluxes and spectra change rapidly from the outer to the inner surface of the thick natural boron carbide absorber. VIM/Monte Carlo cross sections were obtained from both cell calculations and from a very detailed 3D global calculation of the entire SSR reactor shown in Figure 1. For this global calculation, a retally of the neutron history data was performed in order to combine similar edit regions of identical composition and thus obtain region-averaged cross sections that can be directly compared with the cell calculations.

Tables 1-4 compare SSR region-dependent macroscopic cross sections obtained from the WIMS-D4M microscopic data and from both VIM/Monte Carlo cell and global computations. The first table shows good agreement between WIMS and VIM cell calculation for the production and absorption cross sections for the homogenized fuel. Generally speaking, the Monte Carlo cell and global cross sections are very similar with the largest differences (5%) appearing in group 8. Infinite multiplication factors obtained from the WIMS and VIM cell calculations are 1.3222 and 1.3203 ± 0.0010, respectively. Table 2 shows a similar comparison of macroscopic absorption cross sections for the thin shroud regions surrounding the 25 pin fuel clusters. Macroscopic absorption cross section comparisons for the in-core water regions, the aluminum control rod followers, and the beryllium and water reflectors are given in Tables 3 and 4. With few exceptions the WIMS-VIM comparisons are very satisfactory. Taken together, the results in Tables 1-4 show that WIMS-D4M with the new 69-group library produces reliable reaction rate cross sections, even when simple single cell geometries are used. However, cross sections averaged over the strongly absorbing boron carbide control rod cell are not well calculated by WIMS with the single cell model shown in Figure 2. Table 5 shows a WIMS-VIM comparison of the hydrogen elastic scattering matrix for the XC-H_2O positions. Although most of the elements are in good agreement, VIM shows more up-scatter than WIMS. However, the group-dependent total cross sections are in good agreement.

Although the above results are very encouraging, the hyrogen microscopic transport cross sections in the high energy range (E > 10 keV) calculated by WIMS-D4M with the 69-group library prepared from ENDF/B-V appear to be very low. Table 6 illustrates this problem. The first two columns in this table compare the hydrogen (as bound in water) transport cross sections calculated by WIMS-D4M using the Winfrith[1] 69-group library with those obtained from the new library[3] based on ENDF/B-V data. The Winfrith library produces substantially larger transport cross sections in groups 1 and 2 whose energy boundaries (in eV) are 10.0+6, 5.0+5, and 9.118+3. Figure 3 compares the high energy H(in H_2O) transport cross sections in the two 69-group libraries. Why this large difference exists is still under study. Transport cross sections calculated from the broad group values of the total cross section and the P_1

Table 1.
Macroscopic Cross Sections for SSR Homogenized HEU Fuel Region

Group*	NU Fission			Absorption		
	WIMS (Cell)	VIM (Cell)	VIM (Global)	WIMS (Cell)	VIM (Cell)	VIM (Global)
1	2.4613-3	2.4463-3	2.4906-3	1.4694-3	1.4626-3	1.4767-3
2	2.9062-3	2.8910-3	2.8961-3	2.0736-3	2.0510-3	2.0515-3
3	3.5024-2	3.5432-2	3.5159-2	3.5279-2	3.5507-2	3.5209-2
4	4.0431-2	3.9668-2	3.9631-2	3.2029-2	3.1578-2	3.1553-2
5	1.1426-1	1.1517-1	1.1481-1	2.2177-1	2.2565-1	2.2383-1
6	2.8295-1	2.8515-1	2.8273-1	2.1979-1	2.1941-1	2.1619-1
7	4.3131-1	4.2986-1	4.2108-1	2.6124-1	2.6055-1	2.5557-1
8	6.7152-1	6.8624-1	6.5297-1	3.9788-1	4.0539-1	3.8726-1
	1 σ range (%):	0.06-0.21	0.03-0.23		0.07-0.17	0.05-0.21
K-INF:	1.3222	1.3203 ±0.0010				

*Group Boundaries (eV): 10.0+6, 5.0+5, 9.118+3, 2.100, 1.150, 0.400, 0.140, 0.058, 1.0-5

Table 2.
Macroscopic Absorption Cross Sections
Fuel Cluster Shroud/Water Region

Group	WIMS (Cell)	VIM (Cell)	VIM (Global)
1	2.9479-4	2.8793-4	2.7786-4
2	7.2649-5	7.0867-5	6.9502-5
3	4.9755-4	4.8751-4	4.8883-4
4	2.3912-3	2.3824-3	2.3890-3
5	3.5939-3	3.5938-3	3.6082-3
6	6.2703-3	6.2594-3	6.3682-3
7	1.0083-2	9.9799-3	1.0123-2
8	1.8990-2	1.8968-2	1.9256-2
	1 σ range (%):	0.03-0.73	0.15-1.3

Table 3.
Macroscopic Absorption Cross Sections
In-Core Water and Control Rod Follower Regions

	In-Core Water		Control Rod Followers	
Group	WIMS (Cell)	VIM (Global)	WIMS (Cell)	VIM (Global)
1	3.2200-4	2.9970-4	2.7388-4	2.5369-4
2	1.0128-5	1.0183-5	1.0100-4	8.1909-5
3	5.7152-4	5.6856-4	4.9662-4	4.7505-4
4	2.8572-3	2.8380-3	2.2231-3	2.2206-3
5	4.3514-3	4.3573-3	3.3667-3	3.3653-3
6	7.8557-3	7.8891-3	5.9005-3	6.0067-3
7	1.2325-2	1.2238-2	9.4467-3	9.4769-3
8	2.3245-2	2.3195-2	1.7749-2	1.7936-2
	1 σ range (%):	0.02 - 1.9		0.12 - 1.4

Table 4.
Macroscopic Absorption and N,2N Cross Sections
Beryllium and Water Radial Reflector Regions

	Beryllium		Water	
Group	WIMS (Cell)	VIM (Global)	WIMS (Cell)	VIM (Global)
1	3.7297-3	3.6882-3	3.6838-4	3.6043-4
2	1.2349-5	1.2322-5	1.0876-5	1.0550-5
3	3.2173-5	3.2524-5	6.1601-4	6.1663-4
4	1.5147-4	1.5025-4	2.8578-3	2.8395-3
5	2.2978-4	2.3111-4	4.3658-3	4.3705-3
6	4.1218-4	4.1857-4	8.0309-3	8.1966-3
7	6.4638-4	6.4940-4	1.2352-2	1.2282-2
8	1.2071-3	1.2248-3	2.3248-2	2.3192-2
	1 σ range (%):	0.03 - 0.41		0.02 - 2.6
N, 2N Cross Section				
1	9.8051-3	9.8753-3		
	1 σ (%):	0.86		

Table 5.
Hydrogen Elastic Scattering Matrix
SSR XC-H_20 Positions

Code	Group (E_n-ev)	From Group								σ_{tot}
		1	2	3	4	5	6	7	8	
WIMS:	1	1.8360								3.3746
VIM:	(1.0+7)	1.8453								3.4221
%:		1.12								0.18
WIMS:	2	1.5104	9.3367							12.4600
VIM:	(5.0+5)	1.5507	9.3508							12.503
%:		1.20	0.90							0.11
WIMS:	3	2.8113-2	3.1324	17.943	8.5019-3					20.3294
VIM:	(9.118+3)	2.7763-2	3.1530	17.896						20.333
%:		4.43	0.93	0.85						0.002
WIMS:	4	2.9406-6	3.2732-4	1.0863	6.3897	1.5075-2				20.8634
VIM:	(2.10)		3.4955-4	1.1108	6.5013	4.8611-2				20.978
%:			48.8	1.08	1.46	9.01				0.005
WIMS:	5		2.6181-4	8.6241-1	9.9242	11.1449	8.4268-2	4.0444-5	8.3692-6	22.2300
VIM:	(1.150)		3.4955-4	8.6824-1	9.8654	11.158	1.1862-1			22.352
%:			48.8	1.08	1.47	1.35	4.51			0.020
WIMS:	6		9.05288-5	2.9390-1	3.2840	8.1681	15.6358	1.1304	1.7580-1	28.2485
VIM:	(0.400)		1.7478-4	3.0222-1	3.3690	8.174	15.474	1.3315	1.8463-1	28.452
%:			70.2	1.53	1.95	1.24	1.00	1.21	1.80	0.029
WIMS:	7		2.8338-5	8.4706-2	8.4887-1	2.0133	9.1974	24.2409	5.2324	36.0731
VIM:	(0.140)			9.4763-2	8.8667-1	2.0013	9.5562	23.879	5.6020	36.041
%:				2.60	2.88	1.65	1.11	1.03	1.11	0.012
WIMS:	8		1.1455-5	5.0363-2	3.6536-1	8.2350-1	3.2132	10.5171	47.5216	53.2781
VIM:	(0.058)			5.5538-2	3.7311-1	8.5909-1	3.1878	10.544	47.237	53.375
%				3.66	5.43	2.35	1.34	1.03	1.08	0.030

Table 6.
$H(H_2O)$ Microscopic Transport Cross Sections
Homogenized Fuel Region

Group	WIMS			VIM	
	Winfrith Lib	ANL-V5 Lib	ANL-V5*	Cell*	Global*
1	1.6799	0.9795	1.1020	1.1125	1.0890
2	5.0734	3.6658	4.0540	4.0553	4.0089
3	6.9338	6.9088	6.9014	6.9364	6.8899
4	9.0234	8.7382	8.7516	8.8313	8.6928
5	11.722	11.345	11.443	11.610	11.669
6	17.874	17.295	17.644	18.294	18.622
7	26.006	26.933	27.246	28.295	29.069
8	49.244	53.414	59.974	57.990	60.076

*$\sigma_{tr,g} = \sigma_{tot,g} - \Sigma_{g'} [\sigma_{s1\text{-}el}(g \rightarrow g') + \sigma_{s1\text{-}inel}(g \rightarrow g')]$

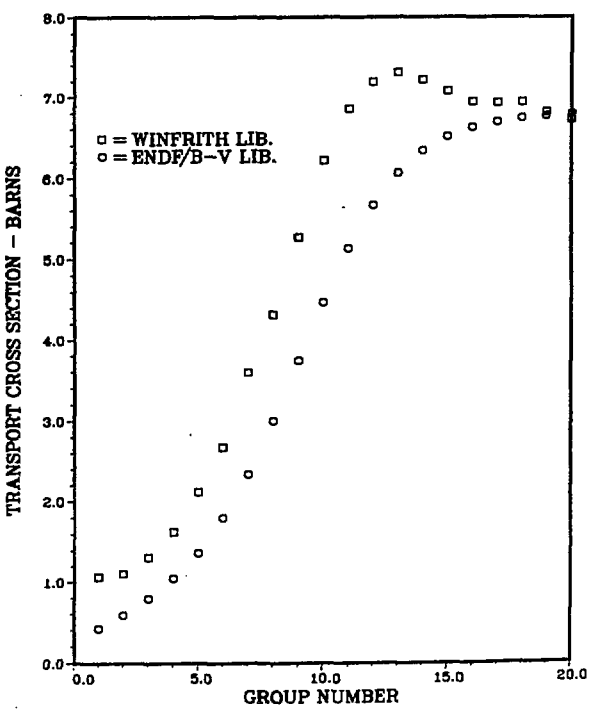


Figure 3.

scattering matrices are given in the last 3 columns of Table 6. This method allows a direct comparison of microscopic transport cross sections calculated from WIMS data and from VIM data and was the method used for most of the diffusion calculations to follow. Table 6 shows that on this basis the two codes give consistent results.

GLOBAL DIFFUSION AND MONTE CARLO RESULTS FOR THE SSR

Diffusion and Monte Carlo calculations have been performed for the SSR standard 29-element core configuration shown in Figure 1 with the control fully withdrawn and with the rods banked at the height where the reactor was critical. The diffusion calculations used the 8-group cross sections created by WIMS-4DM with the ENDF/B-V based library with the modified transport cross sections discussed in the previous section. The detailed Monte Carlo calculations modeled the fuel, clad, and coolant regions for each fuel pin and individually represented every fuel cluster, shroud, and beryllium reflector element. These calculations used the continuous energy code VIM and are also based on ENDF/B-V data.

Table 7 shows that the Monte Carlo results agree well with the experiment observations for both control rod elevation conditions. However, the DIF3D[9] results, which use the WIMS-D4M cross sections, significantly underpredict the eigenvalues. For these calculations the poison section of each control rod was treated by a set of internal boundary conditions (current-flux-ratios). The TWODANT code[10], with position-dependent boron carbide cross sections obtained from a set of WIMS-D4M calculations, was used to determine these boundary conditions. As was mentioned earlier, these cross sections are too small relative to VIM and underpredict the absorption in the B_4C material.

Because of the uncertainty in the high energy hydrogen transport cross sections (Table 6), a second set of diffusion calculations was performed. Here the hydrogen transport cross sections in the first two groups were replaced with WIMS-D4M-calculated values using the 69-group Winfrith library[1]. Table 6 shows that the eigenvalues obtained with this modified cross section set agree quite well with the Monte Carlo calculations and with the experimental observations. The somewhat large eigenvalue calculated for the critical state of the SSR is not surprising in view of the inadequate boron carbide cross sections discussed earlier.

Figure 4 shows the distribution of DIF3D/VIM reaction rate ratios for fission in the fuel clusters and for absorption in the water holes and the control rod followers. For this case, the control rods are withdrawn. The statistical errors (1 σ) in the Monte Carlo calculations are in the 1-2 % range. Somewhat improved distributions are obtained if the Winfrith-modified hydrogen transport cross sections are used.

CONCLUSIONS

Relative to cell and global VIM-Monte Carlo calculations, the region-averaged principal cross sections (i.e. production, fission, absorption, and total) obtained from the WIMS-D4M code with the new 69-group library based on ENDF/B-V appear to be of good quality. Once operational, the supercell option[2] holds the promise of giving improved cross sections in thick non-fuel regions, especially for the boron carbide control rods. The global Monte Carlo calculations for the standard 29-cluster SSR core configuration give eigenvalues for two different control rod states that are very consistent with the experimentally measured excess reactivities. However, the corresponding global diffusion calculations based on WIMS-D4M-ENDF/B V cross sections give eigenvalues that are too low by as much as 3%. About half of this discrepancy is removed if the transport cross sections are calculated from the broad group values for the total cross sections and the P_1 scattering matrices. The remaining discrepancy disappears if the high energy hydrogen (for H in H_2O and for H in ZrH) transport cross sections in broad groups 1 and 2 are replaced with those calculated by WIMS-D4M using the Winfrith 69-group library. For reasons that are still being studied, the Winfrith library of hydrogen transport cross sections in the fast

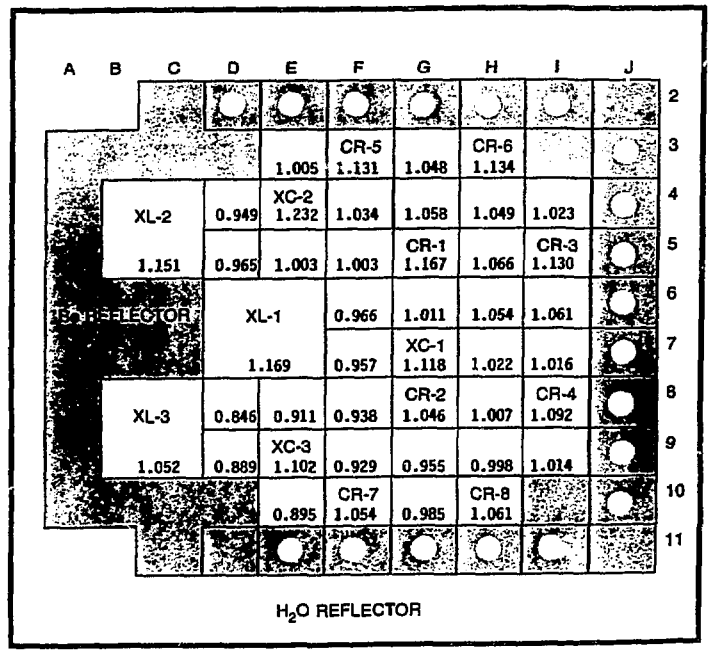
Table 7.
Neutron Balance Summary for Global SSR Calculations
(Normalization: Fission Rate = 1.0)

Control Rod Evaluations	Code	Fission Source	N2N Source	Absorption	Leakage	K-Eff (calc)	K-Eff (Exp)
Withdrawn	VIM	2.4398	0.0248	2.3280	0.0047	1.0565	1.0576
	1 σ:	±.0035	±.0002	±.0022	±.0022	±.0015	
	WIMS/ DIF3D	2.4396	0.0292	2.3623	0.0024	1.0440	
	**WIMS/ DIF3D	2.4396	0.0280	2.3299	0.0017	1.0583	
At critical	VIM	2.4399	0.0233	2.4539	0.0090	1.0001	1.0000
	1 σ:	±.0038	±.0002	±.0025	±.0025	±.0016	
	WIMS/ DIF3D	2.4397	0.0258	2.3409*	0.1479*	0.9907	
	**WIMS/ DIF3D	2.4398	0.0246	2.3098*	0.1391*	1.0063	

*The poison section (B_4C) of each control rod is treated by a set of group-dependent internal boundary conditions. Since these regions are non-diffusing regions, the total reactor absorption is too low, and the total leakage is too high. However, the sum of the two is correct.

**Uses H($H_2$0) and H(ZrH) transport cross sections in groups 1 and 2 calculated from the Winfrith library.

INITIAL SSR CORE CONFIGURATION
WITH 29 FRESH HEU TRIGA (5X5) FUEL CLUSTERS



ALL EXPERIMENT LOCATIONS (XL-1, 2, 3; XC-1, 2, 3;
AND THE HOLES IN THE BERYLLIUM REFLECTOR) ARE FILLED WITH WATER

Figure 4. WIMS-DIF3D/VIM Fission and Capture Rate Ratios

energy range has values that are appreciably larger (see Figure 3) than those in the new ENDF/B-V based library. Using standard WIMS-D4M methods for calculating broad group transport cross sections, this library difference for hydrogen (H in H_2O and H in ZrH) nearly accounts for the entire eigenvalue discrepancy. Trkov[11] emphasizes the importance of using Askew's[12] weighted column sum fonn of the P_1 scattering term in the transport cross section for very light materials. Kemshell[13] studied the sensitivity of the hydrogen transport cross sections to the choice of the weighting spectrum. We may need to apply some of these techniques to our current library. Meanwhile, the results presented in this paper must be regarded as preliminary.

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