KAPL-P-000089
(K98083)

CONF-981003--

MONTE CARLO TESTING OF UNRESOLVED RESONANCE TREATMENT FOR FAST AND INTERMEDIATE CRITICAL ASSEMBLIES

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October 1998

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INTRODUCTION

The purpose of this study is to investigate the eigenvalue sensitivity to changes in unresolved resonance treatment by comparing RACER[1] Monte Carlo calculations for several fast and intermediate spectrum critical experiments. Calculations performed using smooth, dilute-average, tabulated cross sections were compared with calculations using the probability table method to produce stochastically generated resonance cross sections in the unresolved resonance region. The use of the probability table method is superior to the dilute-average cross section method for representing the unresolved resonance region because the table method properly accounts for resonance self shielding; thereby, reducing the effectiveness of the cross sections in the region. The unresolved resonance region is typically found in the intermediate and fast energy range. Eleven benchmark critical assemblies[2,3,4] that span a range of ^{235}U enrichments (93.8 to 10.2%) and four highly enriched ^{239}Pu and ^{233}U assemblies[2] were analyzed. These benchmarks were chosen to accentuate the reactivity importance of the unresolved resonance range.

SUMMARY

Only small differences in eigenvalues were observed between calculations utilizing the two unresolved resonance treatments for the benchmarks with highly enriched ^{235}U, ^{233}U, or ^{239}Pu fuel systems. Eigenvalue differences between calculations were typically within the 95% confidence interval ($\pm$ 0.0005 Δk_{eff}). The largest eigenvalue differences were observed for low enriched uranium fuel systems. Eigenvalue differences as large as +0.0059 Δk_{eff} were calculated for enrichments lower than 15% with the probability table method producing the higher eigenvalue. The pseudo-resonances generated by the probability table method cause the ^{238}U capture cross sections to be self-shielded, reducing the capture reaction rate, which in turn causes an increase in the eigenvalue for the low enriched uranium systems. In all cases but one, the increase in eigenvalues for the low enriched critical assemblies resulted in an increase in the Monte Carlo-to-experiment reactivity bias.

Many of the benchmark assemblies utilized for this analysis, including the low enriched uranium assemblies, have an intermediate-hardness spectrum, which have calculated k_{eff} values that are high compared with 1.0. The higher k_{eff} values produced when the unresolved resonance treatment is applied to the low enriched uranium assemblies, are consistent with the higher calculated k_{eff} values observed in conjunction with the highly enriched uranium assemblies of intermediate-spectra such as UH3 and HISS-HUG[9,10] (See Table 2). These results indicate that there exists a reactivity bias with experiment for intermediate-spectra benchmark criticals that needs further investigation.

DESCRIPTION of RACER

RACER is a three-dimensional, continuous-energy, neutron Monte Carlo code originally based on the Oak Ridge National Laboratory (ORNL) O5R Monte Carlo code[5]. The neutron tracking and cross section processing routines[1] have been highly vectorized and utilize multiple levels of parallel processing. The ENDF/B-VI.4 cross sections are processed with the NJOY system[6], Doppler broadened to 293 K, and fitted onto 21,248 energy mesh points between 0.625 eV and 20 MeV. The thermal model utilized for this study is based on 32 multigroups with moderators represented by P0 and P1 scattering kernels, evaluated at 296 K.

DESCRIPTION of UNRESOLVED RESONANCE TREATMENT

The unresolved resonance region (URR) is generally in the intermediate and fast energy range where the resonances are too numerous and too close in energy to experimentally resolve. The ^{235}U unresolved resonance region spans an energy of 2.25 keV to 25 keV. Whereas, the ^{238}U unresolved resonance region spans an energy of 10 keV to 300 keV. The table below lists, for the uranium and plutonium isotopes that are found in the benchmark critical assemblies, the energy ranges for the unresolved resonance region[7], the average capture width of the resonances (Γ_γ)[8], and the average level spacing of the s-wave resonances (D_o)[8]. This region is often represented by a set of smooth, dilute-average, tabulated cross section data which does not represent the resonances explicitly. In some cross section sets, average unresolved resonance parameters, which specify distribution functions for the resonance spacings and widths, are tabulated over an energy band covering the entire unresolved resonance range, or energy points within the unresolved resonance range. The number of energy bands or points can be as few as one band or as many as 70 points, as with the ^{240}Pu cross sections. The probability table method utilizes the average parameters to create sets of stochastically-generated resonances utilizing the single-level Breit-Wigner approximation. The generated resonances are Doppler broadened to 293 K. In the RACER Monte Carlo implementation, the resonance integral associated with the dilute-average cross section is conserved. This allows for an unbiased comparison between the two unresolved resonance treatments. RACER utilizes the probability tables to randomly sample a band within the unresolved resonance region to obtain total and partial cross sections at the neutron exit energy for each nuclide.

Element	Isotope	Start of URR keV	End of URR keV	Average Capture Width (Γ_γ) meV	s-wave Average Level Spacing (D_0) eV
Uranium	^{233}U	0.060	10.0	40.0	0.55
	^{234}U	1.5	100.0	26.0	10.6
	^{235}U	2.25	25.0	35.0	0.44
	^{236}U	1.5	100.0	23.0	14.7
	^{238}U	10.0	300.0	23.2	20.9
Plutonium	^{239}Pu	2.5	30.0	43.0	2.3
	^{240}Pu	5.7	40.0	31.0	13.6
	^{241}Pu	0.300	40.2	42.0	0.9

DESCRIPTION of EXPERIMENTS

Specifications of the ^{235}U / ^{238}U critical assemblies were taken from the Cross Section Evaluation Working Committee (CSEWG) benchmark compilation[2]. GODIVA is the only bare enriched uranium reactor evaluated here; the remaining are reflected with either depleted or natural uranium. GODIVA and FLAT-TOP are modeled with the correct spherical geometry and exact compositions, while the remaining ones are modeled using the benchmark specifications (equivalent cylinders and homogenized compositions). The specifications for these benchmark models have been adjusted to match the experimentally measured critical experiments[2]. GODIVA, FLAT-TOP-25, and VERA-1B contain highly enriched (~93%) ^{235}U fuel, whereas ZPR-III 6F has an enrichment of ~46%. The remaining cores, ZPR-III 12, ZEBRA-2, ZPR-III 11, and BIGTEN contain low enriched fuel with enrichments of 10% to 20%. ZPR-III 12, VERA-1B, and ZEBRA-2 are diluted with graphite in the fuel which softens the spectrum. The neutron leakage fraction varies considerably among the experiments tested. GODIVA, the smallest assembly, has the highest leakage (56%); FLAT-TOP-25 has 30% leakage; and the remaining large heterogeneous assemblies have leakages of less than 10%. The energy spectra of these critical assemblies are very hard, with essentially no neutron interactions in the thermal energy range.

The intermediate spectrum UH3-UR and UH3-NI critical assemblies[3] consist of a 93 weight percent ^{235}U-hydride powder and polyethylene mixture with an eight inch reflector shell of natural uranium or nickel, respectively. The HISS-HUG central region experiment[4] is modeled as an infinite homogeneous uranium-graphite-boron mixture. The UH3 and HISS-HUG assemblies have a softer spectrum than the fast critical assemblies, with fissions occurring throughout the energy range from 10 eV to the MeV.

Specifications of the ^{233}U and ^{239}Pu critical assemblies were also taken from the CSEWG benchmark compilation[2]. The JEZEBEL-23 and JEZEBEL- Pu critical assemblies are bare, metallic spheres, whereas the FLAT-TOP-23 and FLAT-TOP-Pu critical assemblies are metallic spheres reflected with natural uranium. The ^{233}U critical assemblies are 98% enriched and the ^{239}Pu critical assemblies are 95% enriched.

The three sets of experiments are useful for testing the unresolved resonance cross sections for the different fuel systems and spectra. Table 1 lists the geometry description and dimensions for the benchmark critical assemblies studied.

CALCULATIONS

All calculations were performed on a CRAY-J90 computer. The RACER Monte Carlo calculations were run in the fission iterated mode. The first 2.5 million histories were discarded to obtain a converged source distribution. Subsequently, 25 million histories were analyzed in 500 batches of 50,000 neutrons per batch, which led to very small statistical uncertainties on the eigenvalue. All calculations were run with ENDF/B-VI release 4 cross sections.

DISCUSSION of RESULTS

Table 2 shows a comparison of k_{eff} values computed using both smooth, dilute-average, cross sections and the probability table method in the unresolved resonance region versus atom percent enrichment of ^{235}U, ^{233}U, or ^{239}Pu for the fifteen critical assemblies analyzed. The largest eigenvalue differences were observed for low enriched uranium fuel systems. Eigenvalue differences as large as +0.0059 Δk_{eff} (ZEBRA-2 critical benchmark assembly) were calculated for enrichments lower than 15%, with the probability table method producing the higher eigenvalue. Differences less than ±0.0005 Δk_{eff} were observed between calculations with highly enriched ^{235}U, ^{233}U, or ^{239}Pu fuel systems. In all cases but one (ZEBRA-2), the increase in eigenvalues for the low enriched critical assemblies resulted in an increase in the Monte Carlo-to-experiment reactivity bias.

Table 3 shows a detailed comparison of total ν-fission reaction rates and ^{238}U absorption reaction rates versus energy for the ZEBRA-2 critical assembly. The ^{238}U unresolved resonance region spans an energy of 10 keV to 300 keV. The data in Table 3 show that the ^{238}U absorption reaction rate was reduced by over 4% in the 10-50 keV energy range when the probability table method was utilized. Because of the very narrow width, widely spaced resonances in ^{238}U capture cross section (see table on second page) in the unresolved resonance region, the use of the probability table method results in greater shielding of the ^{238}U capture cross sections thus creating a reduced effective cross section and an increase in the resonance escape probability. As a result of the reduced neutron capture in the ^{238}U (at this energy, all the absorptions in ^{238}U lead to capture), more neutrons are available for ^{235}U fission within the same energy range.

The reduction in ^{238}U capture results in an increase of the slowing down of neutrons to the next energy range due to increased resonance escape probability. The data presented in Table 3 show an increase in both total ν fission and ^{238}U capture in the 1-10 keV energy range as a result of the increase in available neutrons. The net result was an increase in the calculated eigenvalue of +0.0059 Δk_{eff} for the ZEBRA-2 critical assembly when utilizing the probability table method for the unresolved resonance region.

In contrast, Table 4 shows the effect of the probability table method for GODIVA, the highly enriched ^{235}U bare critical benchmark assembly. Shown is a detailed comparison of total ν-fission and ^{235}U capture reaction rates versus energy for the GODIVA critical assembly. The ^{235}U unresolved resonance region spans an energy of 2.25 keV to 25 keV. Table 4 shows no effect from the self shielding of the ^{235}U cross sections due to the probability table method treatment of the unresolved resonances. The effect of resonance self shielding is small in ^{235}U capture and fission cross sections because of the wider resonance widths and closer spacing of the resonances that are found in ^{235}U compared with the ^{238}U capture resonances.

The last example, shown in Table 5, demonstrates the effect of the probability table method for VERA-1B, the highly enriched ^{235}U critical benchmark assembly with a natural uranium reflector. The data in Table 5 show that the ^{238}U absorption reaction rate in the natural uranium reflector region was reduced by nearly 4% in the 10-50 keV energy range when the probability table method was utilized. As a result of the reduced neutron capture in the ^{238}U, more neutrons are reflected back into the highly enriched core region (the net leakage from the core region was reduced by -.0017) where increased ^{235}U fission is observed within the same energy range. Also, neutron leakage from the outer boundary of the critical assembly increases by +.0049. The reactivity effect is smaller for the VERA-1B benchmark (+0.0016 Δk_{eff}) than for the low enriched assemblies.

CONCLUSIONS

The reactivity effect of stochastically representing the resonances in the unresolved resonance region by utilizing the probability table method is significant for low enriched ^{235}U intermediate and fast critical benchmark assemblies. The use of the probability table method is important because it correctly represents the resonance self shielding of the ^{238}U capture cross sections in the unresolved resonance region which causes the observed reactivity differences.

Table 1
Fast and Intermediate Critical Benchmarks
Model Description

CRITICAL BENCHMARK	TYPE	CORE RADIUS cm.	CORE HEIGHT cm.	REFL.	REFL. RADIUS cm.	REFL. HEIGHT cm.
GODIVA	SPHERE	8.741	---	NONE	---	---
FLATTOP-25	SPHERE	6.116	---	NAT. U	24.130	---
BIGTEN	CYL	26.67	55.88	DEPL. U	41.91	96.52
ZPR-III 6F	CYL	20.293	40.884	DEPL. U	51.983	101.984
ZPR-III 11	CYL	29.640	51.000	DEPL. U	64.200	112.000
VERA-1B[a]	CYL	19.107	13.573	NAT. U	60.907	101.350
ZPR-III 12[a]	CYL	26.960	45.920	DEPL. U	57.460	106.920
ZEBRA-2[a]	CYL	40.270	83.440	NAT. U	73.530	144.400
HISS-HUG[b]	INFINITE MEDIUM	---	---	---	---	---
UH3-UR[c]	SPHERE	7.7902	---	NAT. U	28.1102	---
UH3-NI[c]	SPHERE	7.7978	---	NICKEL	28.1178	---
JEZEBEL-PU	SPHERE	6.3849	---	NONE	---	---
FLATTOP-PU	SPHERE	4.533	---	NAT. U	24.130	---
JEZEBEL-23	SPHERE	5.9838	---	NONE	---	---
FLATTOP-23	SPHERE	4.2058	---	NAT. U	24.1194	---

a. Graphite moderated
b. Graphite moderated with homogenous boron
c. Uranium-hydride with Polyethylene moderator

Table 2
RACER Monte Carlo Reactivity Worth of Unresolved Resonance Treatment (URT) for Fast and Intermediate Critical Benchmarks

Critical Benchmark	Atom Percent Enrichment	Keff with Smooth Unresolved Cross Sections	Keff with Unresolved Resonance Treatment	$\Delta K/\overline{K}$* (URT - Smooth)
Fast ^{235}U Critical Benchmarks				
GODIVA	93.8	0.9981(3)	0.9978(2)	-0.0003(4)
FLAT-TOP-25	93.3	1.0059(3)	1.0054(3)	-0.0005(4)
BIGTEN	10.2	1.0011(2)	1.0065(2)	+0.0054(3)
ZPR-III 6F	46.8	1.0020(3)	1.0049(2)	+0.0029(4)
ZPR-III 11	11.7	1.0050(2)	1.0100(2)	+0.0050(3)
Fast ^{235}U Critical Benchmarks with Graphite Moderator				
VERA-1B	92.9	1.0022(3)	1.0038(3)	+0.0016(4)
ZPR-III 12	20.1	1.0022(3)	1.0058(2)	+0.0036(4)
ZEBRA-2	13.9	0.9935(3)	0.9994(2)	+0.0059(4)
Intermediate ^{235}U Critical Benchmarks				
HISS-HUG[a]	93.4	1.0135(1)	1.0134(1)	-0.0001(1)
UH3-UR[b]	93.2	1.0110(3)	1.0107(6)	-0.0003(7)
UH3-NI[b]	93.2	1.0120(3)	1.0118(3)	-0.0002(4)
Fast ^{239}Pu and ^{233}U Critical Benchmarks				
JEZEBEL-PU	94.9	0.9910(2)	0.9909(2)	-0.0001(3)
FLAT-TOP-PU	95.2	1.0025(5)	1.0023(3)	-0.0002(6)
JEZEBEL-23	98.1	0.9917(2)	0.9919(2)	+0.0002(3)
FLAT-TOP-23	98.1	1.0038(3)	1.0042(4)	+0.0004(5)

* 95% (~2σ) confidence interval $\times 10^{-4}$ in parenthesis

a. Graphite moderated with homogenous boron
b. Uranium-hydride with Polyethylene moderator

Table 3
ZEBRA-2 CRITICAL BENCHMARK ASSEMBLY
EFFECT of UNRESOLVED RESONANCE TREATMENT (URT)
FRACTION of TOTAL ν FISSIONS and ^{238}U ABSORPTIONS
by ENERGY RANGE

	Total ν Fissions[a]			^{238}U Absorptions		
ENERGY RANGE	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ν Fission (URT - Smooth)	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ^{238}U Absorptions (URT - Smooth)
20 MeV - 10 MeV	0.0013	0.0013	--	0.0003	0.0003	--
10 MeV - 1 MeV	0.3084	0.3084	--	0.0946	0.0946	--
1 MeV - 150 keV	0.2075	0.2073	-0.0002	0.1098	0.1100	+0.0002
150 keV - 100 keV	0.0494	0.0496	+0.0002	0.0329	0.0329	--
100 keV - 50 keV	0.0814	0.0819	+0.0005	0.0700	0.0692	-0.0008
50 keV - 10 keV	0.1610	0.1635	+0.0025	0.1810	0.1735	-0.0075
10 keV - 1 keV	0.1398	0.1420	+0.0022	0.0774	0.0796	+0.0022
1 keV - 110 eV	0.0404	0.0411	+0.0006	0.0107	0.0109	+0.0002
110 eV - 10 eV	0.0037	0.0038	+0.0001	0.0010	0.0010	--
10 eV - 0.625 eV	0.0003	0.0003	--	0.0001	0.0001	--
0.625 eV - 10^{-5} eV	0.0	0.0	--	0.0	0.0	--
TOTAL	0.9935(3)	0.9994(2)	+0.0059(4)	0.5778(1)	0.5720(1)	-0.0058(2)

a. 95% (~2σ) confidence interval x10^{-4} in parenthesis, 95% C.I. < 10^{-4} not shown

Table 4
GODIVA CRITICAL BENCHMARK ASSEMBLY
EFFECT of UNRESOLVED RESONANCE TREATMENT (URT)
FRACTION of TOTAL ν FISSIONS and ^{235}U CAPTURE
by ENERGY RANGE

	Total ν Fissions[a]			^{235}U Captures		
ENERGY RANGE	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ν Fission (URT - Smooth)	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ^{235}U Capture (URT - Smooth)
20 MeV - 10 MeV	0.0019	0.0019	--	0.0	0.0	--
10 - 6.0653 MeV	0.0251	0.0251	--	0.0	0.0	--
6.0653 - 2.865 MeV	0.1361	0.1361	--	0.0006	0.0006	--
2.865 - 1.0 MeV	0.3413	0.3411	-0.0002	0.0075	0.0075	--
1.0 - 0.58 MeV	0.1539	0.1539	--	0.0067	0.0067	--
580 keV - 320 keV	0.1400	0.1399	-0.0001	0.0086	0.0086	--
320 keV - 150 keV	0.1144	0.1145	+0.0001	0.0096	0.0096	--
150 keV - 100 keV	0.0351	0.0351	--	0.0037	0.0036	-0.0001
100 keV - 50 keV	0.0312	0.0311	-0.0001	0.0037	0.00037	--
50 keV - 10 keV	0.0179	0.0179	--	0.0024	0.0024	--
10 keV - 1.0 keV	0.0013	0.0013	--	0.0002	0.0002	--
1.0 keV - 10^{-5} eV	--	--		--	--	
TOTAL	0.9981(3)	0.9978(2)	-0.0003(3)	0.0893(1)	0.0893(1)	--

a. 95% (~2σ) confidence interval x10^{-4} in parenthesis, 95% C.I. < 10^{-4} not shown

Table 5
VERA-1B CRITICAL BENCHMARK ASSEMBLY
EFFECT of UNRESOLVED RESONANCE TREATMENT (URT)
FRACTION of TOTAL ν FISSIONS and ^{238}U ABSORPTIONS
by ENERGY RANGE

	Total ν Fission[a]			^{238}U Absorptions		
ENERGY RANGE	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ν Fission (URT - Smooth)	Run with Smooth Unresolved Cross Sections	Run with Unresolved Resonance Treatment	Delta ^{238}U Absorptions (URT - Smooth)
20 MeV - 10 MeV	0.0013	0.0013	--	0.0002	0.0002	--
10 MeV - 1 MeV	0.3517	0.3517	--	0.0725	0.0727	+0.0002
1 MeV - 150 keV	0.2759	0.2753	-0.0006	0.1354	0.1356	+0.0002
150 keV - 100 keV	0.0561	0.0563	+0.0002	0.0417	0.0418	+0.0001
100 keV - 50 keV	0.0868	0.0873	+0.0005	0.0843	0.0832	-0.0011
50 keV - 10 keV	0.1448	0.1462	+0.0014	0.1714	0.1650	-0.0064
10 keV - 1 keV	0.0786	0.0789	+0.0003	0.0255	0.0267	+0.0012
1 keV - 110 eV	0.0067	0.0068	+0.0001	0.0007	0.0007	--
110 eV - 10 eV	0.0001	0.0001	--	0.0	0.0	--
10 eV - 0.625 eV	0.0	0.0	--	0.0	0.0	--
0.625 eV - 10^{-5} eV	0.0	0.0	--	0.0	0.0	--
TOTAL	1.0022(3)	1.0038(3)	+0.0016(4)	0.5317(2)	0.5259(2)	-0.0058(3)

a. 95% (~2σ) confidence interval x10^{-4} in parenthesis, 95% C.I. < 10^{-4} not shown

REFERENCES:

1. F.B. Brown and T.M. Sutton, "Monte Carlo Fundamentals," Department of Energy - Office of Scientific Information, KAPL-4823 (1996).
2. National Neutron Cross Section Center, (1974), ENDF-202, "Cross Section Evaluation Working Group, Benchmark Specifications," Brookhaven National Laboratory.
3. G.A. Linenberger et al., "Enriched-Uranium Hydride Critical Assemblies," *Nuc. Sci. Eng.*, **7**, 44-57 (1960).
4. W.N. Fox et al., "Reactor Physics Measurements on ^{235}U and ^{239}Pu Fuels in an Intermediate Spectrum Assembly," *J. Brit. Nucl. Ener. Soc.*, **9** (1970).
5. D.C. Irving et al., "O5R. A General-Purpose Monte Carlo Neutron Transport Code, ORNL-3622," Oak Ridge National Laboratory (1965).
6. R.E. MacFarlane et al., "The NJOY Nuclear Data Processing System," LA-9303-M (ENDF-324), Los Alamos National Laboratory (1982).
7. P.F. Rose and C.L.Dunford, Eds., *ENDF-102: Data formats and procedures for the Evaluated Nuclear Data File ENDF-6*, BNL-NCS-44945, July 1990.
8. S.F. Mughabghab, "Neutron Cross Sections, " Volume 1, *Neutron Resonance Parameters and Thermal Cross Sections, Part B, Z = 61-100*, Academic Press, (1984).
9. R.Q. Wright and L.C. Leal, Benchmark Testing and Status of ENDF/B-VI Release-3 Evaluations," *Trans. Am. Nucl. Soc.*, **77**, 232 (1997).
10. J.P. Weinman, "Monte Carlo Cross Section Testing for Thermal and Intermediate $^{235}U/^{238}U$ Critical Assemblies - ENDF/B-V Versus ENDF/B-VI," *Trans. Am. Nucl. Soc.*, **76**, 325 (1997).

INTRODUCTION

PURPOSE

- Investigate reactivity sensitivity to unresolved resonance treatment
    - Smooth, dilute-average cross sections versus
    - Probability table method

METHOD

- Compare RACER Monte Carlo k_{eff} values
    - ^{235}U, ^{233}U, and ^{239}Pu fast and intermediate critical benchmark assemblies
    - Investigate causes of observed differences

BACKGROUND

- The probability table method is a superior method for representing unresolved resonance region because:
    - It stochastically represents the resonances
    - It accounts for the resonance self shielding of the cross sections
- Unresolved resonance region generally in keV range
    - ^{238}U - 10 keV to 300 keV
    - ^{235}U - 2.25 eV to 25 keV