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Monte Carlo Cross Section Testing for Thermal and Intermediate $^{235}U/^{238}U$ Critical Assemblies, ENDF/B-V vs ENDF/B-VI

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MONTE CARLO CROSS SECTION TESTING FOR THERMAL and INTERMEDIATE ^{235}U / ^{238}U CRITICAL ASSEMBLIES, ENDF/B-V vs ENDF/B-VI

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INTRODUCTION

The purpose of this study is to investigate the eigenvalue sensitivity to changes in ENDF/B-V and ENDF/B-VI cross section data sets by comparing RACER[1] vectorized Monte Carlo calculations for several thermal and intermediate spectrum critical experiments. Nineteen Oak Ridge and Rocky Flats thermal solution benchmark critical assemblies[2,3,4] that span a range of hydrogen-to-^{235}U (H/U) concentrations (2052 to 27.1) and above-thermal neutron leakage fractions (0.555 to 0.011) were analyzed. In addition, three intermediate spectrum critical assemblies (UH3-UR, UH3-NI, and HISS-HUG)[5,6] were studied.

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[7]. The neutron tracking and cross section processing routines[1] have been highly vectorized and utilize multiple levels of parallel processing. The epithermal neutron physics treatment consists of the following features. The ENDF cross sections are processed with the NJOY system[8], Doppler broadened to 73F, and fitted onto 21,248 energy mesh points between 0.625 eV and 20 MeV. The unresolved resonance region utilizes pointwise dilute average cross sections. Elastic scattering angular distributions are represented anisotropically, using up to 20 angular (P_n) moments in the center-of-mass system. The angular distributions are fitted by up to 31 equally probable step functions per energy interval. Inelastic scattering is represented above 5530 eV as isotropic in the laboratory system with a 25 multigroup transfer matrix . Bound-hydrogen scattering above 0.625 eV is represented by a modified free gas model with upscattering replaced by scattering with no energy change. The thermal model utilized for this study is based on 32 multigroups and P_1 scattering data with moderators represented by a scattering kernel, evaluated at 73F, and consisting of group-to-group energy and angular transfer probabilities. The recommended ENDF/B-V or ENDF/B-VI ^{235}U fission spectra were utilized in conjunction with the corresponding cross section set.

DESCRIPTION of EXPERIMENTS

Specifications of the thermal critical assemblies were taken from References 2 through 4. The analyzed critical assemblies consist of: six large Oak Ridge National Laboratory (ORNL) spheres and cylinders containing uranyl nitrate solutions with high hydrogen-to-^{235}U ratios (H/U), six small ORNL spheres and cylinders containing uranyl fluoride solutions with low H/U ratios, and seven small Rocky Flats cylinders containing uranyl nitrate solutions with low H/U ratios. All the solution tank critical assemblies utilize a uranium enrichment of 93 weight percent ^{235}U. The neutron leakage fraction varies considerably among the analyzed experiments. The large cylindrical ORNL 23 critical assembly has an above-thermal leakage fraction of 0.011 whereas the small reflected sphere ORNL L7 has a 0.555 leakage fraction. The six large ORNL critical assemblies have over 98% of fissions occurring in the thermal energy range (<0.625 eV), whereas most of the ORNL L-series and Rocky Flats critical assemblies are less thermal with as few as 55% of the fissions occurring in the thermal range.

The intermediate spectrum UH3-UR and UH3-NI critical assemblies are modeled as equivalent spheres, with 3.067 and 3.07 inch radii, respectively. The assemblies 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 UH3 critical assemblies have a harder spectrum than the solution critical assemblies, with fissions occurring at fairly uniformly distributed energies from 10 eV to the MeV range. The above-thermal leakage fractions are 0.198 and 0.325 for UH3-UR and UH3-NI, respectively. The HISS-HUG central experiment is modeled as an infinite homogeneous uranium-graphite-boron mixture. The HISS-HUG experiment has a softer spectrum, with most of the fissions occurring at incident energies from 10 eV to 10 keV. The three experiments are useful for testing the resolved and unresolved ^{235}U resonance cross sections.

CALCULATIONS

All calculations were performed on the CRAY-C90 computer. The RACER Monte Carlo calculations were run in the fission iterated mode, with the first 2.5 million histories 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. The 95% (~2σ) confidence intervals were between ±.0002 and ±.0010. RACER calculated about 15 million histories per hour for the leakier, harder spectrum critical assemblies such as ORNL L5. The larger, softer spectrum critical assemblies such as ORNL 23, RACER calculated about 2 million histories per hour.

DISCUSSION of RESULTS

Table I shows a comparison of k_{eff} values computed using ENDF/B-V and ENDF/B-VI (for both releases 1 and 3) cross sections for the nineteen solution critical assemblies versus above-thermal leakage fraction (ATL). The solution tank critical assemblies are useful for determining reactivity sensitivity to changes in hydrogen, oxygen, and ^{235}U cross sections versus spectrum indicators such as ATL.

The following observations are made concerning changes to the three cross section libraries. The 2200 m/s hydrogen capture cross section increased from 332.0 mb in ENDF/B-V to 332.6 mb in ENDF/B-VI; this caused a decrease of as much as 0.0008 Δk for the very thermal critical assemblies such as ORNL 23. Below 2.35 MeV, the P_1 scattering moment in ENDF/B-VI oxygen is considerably more positive than in ENDF/B-V; this increased both the forward scattering and fast leakage for the harder spectrum critical assemblies such as ORNL L5. As a result, the k_{eff} value for ORNL L5 decreased by 0.0040 Δk. The ^{235}U above-thermal α (capture/fission) decreased from 0.4940 in ENDF/B-V to 0.4782 in ENDF/B-VI (release 1), this caused an increase of as much as 0.0107 Δk for the harder spectrum ORNL L5 critical assembly. Lastly, the ^{235}U 2200 m/s eta (ν fission/absorption) decreased from 2.085 in ENDF/B-V to 2.080 in ENDF/B-VI (release 1); this caused a decrease of 0.0012 Δk for the softer spectrum ORNL 1 critical assembly. A least-squares fit of the k_{eff} values versus ATL for the nineteen critical assemblies showed a net increase in the slope with ENDF/B-VI cross sections. Also, a decrease of about 0.0025 Δk was observed for the more thermal critical assemblies with ENDF/B-VI which resulted in k_{eff} values below critical by about the same amount.

The ENDF/B-VI release 3 ^{235}U library by Lubitz[9] succeeds in correcting the observed trends in k_{eff}. This is accomplished by adjusting the ^{235}U capture, fission, and nubar cross section parameters up to 900 eV. The adjusted values are within the experimental uncertainty of the fitted data and match experimentally measured integral data over broad energy bins. The resulting cross section library has an above-thermal α of 0.5167 and a thermal η of 2.083. The new ^{235}U library significantly reduced the least-squares k_{eff} trend with ATL, and resulted in an average k_{eff} for the ensemble of critical assemblies closest to unity.

Table 2 shows a comparison of k_{eff} values computed using ENDF/B-V and ENDF/B-VI (for both releases 1 and 3) cross sections for three intermediate spectrum critical assemblies versus above-thermal leakage fraction. The intermediate spectrum critical assemblies are useful for determining the reactivity sensitivity to changes in above-thermal ^{235}U cross sections parameters. The ENDF/B-VI release 3 cross sections produce the most consistent k_{eff} values with an average closest to unity (1.0116 ±0.0018). ENDF/B-V k_{eff} values are more variable (1.0141 ±0.0188) and ENDF/B-VI release 1 k_{eff} values are considerably higher (1.0261±0.0058).

In conclusion, the ENDF/B-VI cross sections, in conjunction with the Lubitz ENDF/B-VI release 3 ^{235}U library, produce k_{eff} values which are closer to unity and reduce the trend with above-thermal leakage for both the thermal and intermediate spectrum critical assemblies when compared with the other libraries. In addition, it is observed that returning to the ENDF/B-V hydrogen 2200 m/s capture cross section (332.0 mb) would help to reduce any residual bias for the very thermal ORNL solution critical assemblies.

Table 1- k_{eff}[1] - ^{235}U / ^{238}U THERMAL BENCHMARKS ENDF/B-V, ENDF/B-VI(Rel. 1), and ENDF/B-VI(Rel. 3)

Benchmark	ENDF/B-V	ENDF/B-VI Release 1	ENDF/B-VI Release 3	ABOVE THERMAL LEAKAGE
ORNL 23	1.0008(2)	0.9983(2)	0.9995(2)	.011
ORNL 22	0.9984(2)	0.9960(2)	0.9970(2)	.021
ORNL 16	0.9993(2)	0.9967(2)	0.9973(2)	.025
ORNL 10	0.9995(2)	0.9968(3)	0.9975(3)	.054
ORNL 12	1.0013(3)	0.9986(3)	0.9995(3)	.096
ORNL 1	1.0003(3)	0.9966(3)	0.9971(6)	.143
Average	0.9999(11)	0.9972(11)	0.9980(12)	
ORNL L9	1.0031(3)	1.0000(3)	1.0007(3)	.141
ORNL L8	1.0085(3)	1.0049(4)	1.0057(3)	.196
ORNL L11	1.0024(3)	0.9987(3)	0.9996(3)	.207
ORNL L5	1.0069(6)	1.0129(5)	1.0032(4)	.436
ORNL L6	1.0069(5)	1.0098(10)	1.0030(4)	.443
ORNL L7	1.0056(5)	1.0030(4)	0.9999(4)	.555
Average	1.0056(25)	1.0049(58)	1.0020(25)	
RF 5	1.0048(7)	0.9995(4)	0.9999(7)	.334
RF 6	1.0083(4)	1.0032(4)	1.0031(7)	.342
RF 7	1.0049(5)	1.0005(7)	0.9997(5)	.411
RF 3	1.0082(7)	1.0043(8)	1.0034(5)	.413
RF 8	1.0052(4)	1.0014(5)	0.9996(5)	.415
RF 4	1.0051(4)	1.0044(5)	0.9997(5)	.437
RF 9	1.0009(5)	1.0008(5)	0.9961(5)	.438
Average	1.0053(23)	1.0020(18)	1.0002(23)	
Total Av	1.0037(16)	1.0014(22)	1.0001(12)	

1. 95% (~2σ) confidence interval x10^{-4} in parenthesis

Table 2 - k_{eff} - ^{235}U / ^{238}U INTERMEDIATE BENCHMARKS ENDF/B-V, ENDF/B-VI(Rel. 1), and ENDF/B-VI(Rel. 3)

critical assembly	ENDF/B-V	ENDF/B-VI Release 1	ENDF/B-VI Release 3	ABOVE THERMAL LEAKAGE
HISS-HUG	1.0228(1)	1.0266(1)	1.0122(1)	0.0
UH3-UR	1.0106(3)	1.0236(3)	1.0108(6)	.198
UH3-NI	1.0090(3)	1.0282(4)	1.0118(4)	.325
Average	1.0141(188)	1.0261(58)	1.0116(18)	

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REFERENCES:

1. F.B. Brown, "Vectorization of 3-D General-Geometry Monte Carlo," *Trans. Am. Nucl. Soc.*, **53**, 283 (1986).

2. R. Gwin and D.W. Magnuson, "The Measurement of Eta and Other Nuclear Properties of U^{233} and U^{235} Critical Aqueous Solutions," *Nuc. Sci. Eng.*, **12**, 364 (1962).

3. J.K. Fox, L.W. Gilley, and D. Callihan, "Critical Mass Studies, Paret IX, Aqueous U235 Solutions," ORNL-2367, 22 (1958).

4. R.E. Rothe and Inki Oh, "Benchmark Critical Experiments on High Enriched Uranyl Nitrate Solution Systems," *Nucl. Tech.*, **41**, 207 (1978).

5. G.A. Linenberger et al., "Enriched-Uranium Hydride Critical Assemblies," *Nuc. Sci. Eng.*, **7**, 44-57 (1960).

6. 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).

7. D.C. Irving et al., "O5R. A General-Purpose Monte Carlo Neutron Transport Code, ORNL-3622," Oak Ridge National Laboratory (1965).

8. R.E. MacFarlane et al., "The NJOY Nuclear Data Processing System," LA-9303-M (ENDF-324), Los Alamos National Laboratory (1982).

9. C.R. Lubitz, "A Modification to ENDF6 U235 To Increase Epithermal Alpha and K1," *Proc. Int. Conf. Nucl. Data for Sci. and Tech.*, Gatlinburg, Tennessee (1994).