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Criticality Benchmark Calculations using PARTISN: Comparisons using MENDF5 and MENDF6 Nuclear Data Libraries

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INTRODUCTION

A project was undertaken to assess the MENDF5 and MENDF6 [1] nuclear data libraries through the analysis of 86 critical assembly benchmarks using the LANL discrete ordinates transport code PARTISN [2]. As an initial analysis of the effects of some limitations in the MENDF libraries, this current work assesses differences in k_{eff} calculations between the PARTISN cases (with MENDF5 and MENDF6 nuclear data libraries) and MCNP [3] cases, and compares these results to the experimental data.

COMPUTATIONAL MODEL

The suite [4-6] of 86 criticality benchmarks was developed at LANL to be suitable for the validation of nuclear data. As mentioned above, in addition to the PARTISN calculations, the suite of critical assembly benchmarks [4] was analyzed using MCNP with ENDF/B-V and ENDF60 (ENDF/B-VI Release 2) [7] nuclear data libraries.

The suite of criticality benchmark cases [4] comprises one-, two-, and three-dimensional models of U.S. and Russian criticality experiments. For consistency and completeness, the ICSBEP (International Criticality Safety Benchmark Evaluation Project) [8] criticality benchmark experimental data compendium was used. CSEWG (Cross Section Evaluation Working Group) data were not explicitly used. The benchmarks represent a wide range of neutron energy spectra, and can be categorized as fast, intermediate, and thermal systems. The benchmarks involved several types of fissile material, and a variety of reflector materials including Be, BeO, C, Al, Fe, Ni, W, Th, ^{233}U, natural uranium, as well as bare and solution cases. The critical benchmarks are sorted into five general groupings of cases: ^{233}U [Jezebel, Flattop, ORNL], intermediate enrichment ^{235}U (IEU) [Jemima], high enrichment ^{235}U (HEU) [Godiva, Bigten, Flattop, ORNL], ^{239}Pu [Jezebel, Flattop, Thor, PNL], and mixed metal fueled cores [Zebra]. The materials used in the benchmark case input files are specified by isotopic atom densities. Consistency in geometry and materials and the region masses between the PARTISN and MCNP case models was verified.

The MCNP4C [3] Monte-Carlo transport code was used to analyze the criticality benchmark cases with ENDF/B-V and ENDF60 nuclear data libraries. The suite of 86 criticality benchmark cases was initially prepared as a means of validating nuclear data using MCNP. The 86 cases are actually represented by 91 input files, as several benchmarks are modeled in two different ways.

PARTISN is a discrete ordinates radiation transport simulation code developed from the DANTSYS [9] code system. The benchmark cases were run with PARTISN beta release 1.38 using both MENDF5 and MENDF6 nuclear data libraries. The PARTISN code provides neutron transport solutions on orthogonal meshes with adaptive mesh refinement (AMR) in one, two, and three dimensions. A multigroup energy treatment is used in conjunction with the S_N angular approximation. DANTSYS (the predecessor of PARTISN) has been widely distributed by RSICC (Radiation Safety Information Computation Center) at ORNL.

CROSS SECTION LIBRARIES

The MENDF5 and MENDF6 nuclear data libraries were prepared as binary files primarily from ENDF/B-V (up to the final release update in 1987) and ENDF/B-VI (up to release 3 in 1995) nuclear evaluation data, respectively, as multigroup, isotopic nuclear data libraries. The nuclear data in MENDF5 and MENDF6 is also augmented by LANL T-2 and LLNL evaluation data. MENDF5 has data for 99 nuclides and MENDF6 has data for 167 nuclides. The MENDF5 and MENDF6 libraries were produced using the code NJOY [10] and applying the LANL TD-Division Weighting Function (in module GROUPR) to collapse the cross sections to 30 neutron energy groups.

The MENDF5 and MENDF6 libraries include prompt data only which, depending on the case, would usually lead to a lower k_{eff} calculation than ENDF60 results. For fast spectrum cases, the MENDF criticality calculations should be good when consideration is given to the total vs prompt $\overline{\nu}$; however, the MENDF nuclear data libraries will not perform well for intermediate and especially thermal spectrum systems. The MENDF libraries include only limited detail in the thermal neutron energy range. There are no upscatter data included. No self-shielding effects were incorporated into the MENDF nuclear data libraries so all nuclides are treated as being at infinite dilution; this leads to an abnormally high neutron capture rate for some materials, in the resonance region.

In TABLE 1, the results from PARTISN (with MENDF5 and MENDF6 data) and MCNP4C (with ENDF/B-V and ENDF60 data) for some representative criticality benchmark cases are shown and compared with the experimental k_{eff} data.

TABLE 1: Comparisons of k_{eff} from Representative Criticality Benchmark Cases

Fissile Fuel	Benchmark Case Identifier	Case Description	Code and Nuclear Data Library				Experimental Benchmark
			PARTISN (MENDF5)	PARTISN (MENDF6)	MCNP (ENDF/B-V)	MCNP (ENDF60)	
^{233}U	U233-MET-FAST-001	Jezebel-23 ^{233}U sphere	0.98619	0.98498	0.99366±0.00051	0.99356±0.00044	1.000±0.001
^{233}U	233U-SOL-THERM-001 Case 2	ORNL-6 unrefl. sphere U nitrate sol w/boron	0.96091	0.96073	1.00044±0.00040	0.99767±0.00038	1.0005±0.0033
^{235}U	IEU-MET-FAST-005	Steel-reflected IEU sphere VNIEF	1.052016	1.041871	1.00982±0.00059	1.00070±0.00063	1.0000±0.0021
HE ^{235}U	HEU-MET-FAST-001	Godiva unrefl. sphere HEU	0.99274	0.99098	0.99856±0.00057	0.99615±0.00057	1.000±0.001
HE ^{235}U	HEU-SOL-THERM-032	ORNL-10 refl. sphere Uranyl Nitrate w/Boron	0.98419	0.98017	0.99960±0.00026	0.99664±0.00024	1.0015±0.0026
^{239}Pu	PU-MET-FAST-011	water-refl. alpha-phase Pu sphere	1.01176	1.00969	1.00136±0.00074	0.99747±0.00066	1.0000±0.001
^{239}Pu	PU-SOL-THERM-011 Case 18-1	PNL-3 18" Cd. Cov Bare sphere 2 wt% Pu240	0.95833	0.95076	1.00202±0.00052	0.99365±0.00052	1.0000±0.0052
Mixed-metal	MIX-MET-FAST-001	HEU reflected Pu sphere	0.99434	0.99415	0.99754±0.00058	0.99667±0.00057	1.0000±0.0016

CONCLUSIONS

The trend seems to be that k_{eff} is lower in the PARTISN calculations using MENDF6 nuclear data than with MENDF5; however, case IEU-MET-FAST-005 shows a large opposite effect. For most of the cases, the MCNP k_{eff} results are considerably larger than the PARTISN results; PU-MET-FAST-011 has the PARTISN results larger than the MCNP k_{eff} values. From Table 1, the benchmarks of critical solution reactors show low values for k_{eff} for the PARTISN calculations compared to the experimental data, with the results for MENDF6 lower than for MENDF5. A full summary will be presented of the k_{eff} results for the criticality benchmark cases between the discrete ordinates code PARTISN (using MENDF5 and MENDF6 nuclear data libraries), the Monte-Carlo code MCNP4C (using ENDF/B-V and ENDF60 nuclear data libraries) and the experimental benchmark critical data.

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