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THE ROSSI α VALIDATION SUITE FOR MCNP

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ABSTRACT

A Rossi α validation suite has been created for the MCNP Monte Carlo code. The suite includes 13 benchmarks based on specifications given in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. The benchmarks are divided into four categories of fuel – ^{233}U, highly enriched uranium, intermediate enriched uranium, and plutonium. The benchmarks also cover fast, intermediate, and thermal spectra. Succinct descriptions are provided for each benchmark, along with computed values for Rossi α using ENDF/B-VI and ENDF/B-VII.0 nuclear data libraries.

Key Words: MCNP, validation, suite, Rossi α, benchmarks

1 INTRODUCTION

The MCNP code developers have assembled more than a dozen verification and validation suites for testing general classes of problems, including installation, radiation shielding, electrons, photons, variance reduction, and criticality. These suites provide a general indication of the overall performance of the code in conjunction with one or more specific nuclear data libraries. Furthermore, they can provide warnings of unexpected or unintended consequences that result from changes to nuclear data or to the code itself.

The MCNP5 Monte Carlo code [1] version 1.60, released from RSICC in November 2010, is capable of computing Rossi α in criticality calculations [2]. As part of the validation of that capability, a Rossi α validation suite has been developed to complement the existing validation suites for MCNP. As an indication of its usefulness, that suite currently is being used to test β versions of the ENDF/B-VII.1 nuclear data library to help assess the impact of proposed changes to nuclear data.

2 ROSSI α

Rossi α characterizes the exponential rate of change in the population of prompt neutrons that produce fissions in a system that is close to delayed critical:

$$n_{pf}(t) = n_{pf}(o)e^{\alpha_R t} \tag{1}$$

where α_R is Rossi α, n_{pf} is the population of prompt neutrons that produce fissions, and t is time. By definition, Rossi α is zero at prompt critical, negative below it, and positive above it. It is straightforward to show that

$$\alpha_R = \frac{k_p - 1}{\Lambda_{pf}} \cong -\frac{\beta_{eff}}{\Lambda_{pf}} \tag{2}$$

where k_p is the multiplication factor for prompt neutrons, Λ_{pf} is the generation time for prompt neutrons that produce fission, and β_{eff} is the effective delayed neutron fraction. MCNP5 1.60 calculates β_{eff} and Λ_{pf} and then determines Ross α as the negative ratio of those two parameters, as indicated in Eq. (2). A technique to measure Rossi α using correlated fission chains was developed by Bruno Rossi in the 1950s [3].

3 DESCRIPTION OF THE ROSSI α VALIDATION SUITE

The Rossi α validation suite includes ^{233}U, highly enriched uranium (HEU), intermediate enriched uranium (IEU), and plutonium benchmarks. Those benchmarks include systems with thermal, intermediate, and fast spectra. Some of the benchmarks are unreflected, while the others are reflected by normal uranium, depleted uranium, thorium, copper, or water. Succinct descriptions of the 13 benchmarks in the suite are given in Table I, and more detailed descriptions are provided below.

Specifications for each of the benchmarks are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [4], and the specific evaluations from which those specifications are taken are included in Table I. The measured values of Rossi α for eight of the benchmarks are taken from the CSEWG Benchmark Book [5]. The measured value for Zeus-1 is taken from the *Handbook*, the values for Zeus-5 and Zeus-6 are taken from the log books for those experiments, and the values for STACY-30 and STACY-46 are taken from a journal article [6].

3.1 ^{233}U Benchmarks

The Jezebel-233 benchmark is a bare, homogeneous sphere of ^{233}U with a radius of 5.9838 cm. The uranium is 98.13 at.% ^{233}U. It is based on the Jezebel-233 experiment that was performed in 1961 at Los Alamos Scientific Laboratory (LASL), now known as Los Alamos National Laboratory (LANL).

The Flattop-23 benchmark contains an inner sphere of ^{233}U enclosed in an annulus of normal uranium. The ^{233}U content of the inner sphere is 98.13 wt.%, and its radius is 4.2058 cm. The outer radius of the annulus of normal uranium is 19.9136 cm. This benchmark is based on the Flattop-23 experiment that was performed in 1964 at LASL.

3.2 HEU Benchmarks

The Godiva benchmark is a bare, homogeneous sphere of HEU with a radius of 8.7407 cm and an enrichment of 93.71 wt.%. It is based on the Godiva experiment that was operated during the 1950s at LASL.

The FLATTOP-25 benchmark contains a solid, homogeneous sphere of HEU reflected by an annulus of normal uranium. The enrichment of the sphere is 93.24 wt.%. The radius of the sphere is 6.1156 cm, and the thickness of the annulus is 18.0086 cm. This benchmark is based on the Flattop-25 experiment that was operated at LASL in the mid 1960s.

The Zeus benchmarks are based on some of the Zeus experiments that were conducted at LANL from 1999 through 2003. In the Zeus-1 and Zeus-6 cores, cylindrical HEU platters are separated by graphite or iron platters, respectively. In the Zeus-5 core, the HEU platters are stacked directly on top of each other. In all three cases, the core is enclosed in a copper reflector.

Table I. Benchmarks in the Rossi α Benchmark Suite

Fuel	Name	Spectrum	*Handbook* Identifier	Description
^{233}U	Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
	Flattop-23	Fast	U233-MET-FAST-006	^{233}U sphere reflected by normal U
HEU	Godiva	Fast	HEU-MET-FAST-001	Bare sphere of HEU
	Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
	Zeus-1	Intermediate	HEU-MET-INTER-006	Stacked HEU and graphite platters reflected by copper
	Zeus-5	Fast	HEU-MET-FAST-073	HEU platters reflected by copper
	Zeus-6	Fast	HEU-MET-FAST-072	Stacked HEU and steel platters reflected by copper
IEU	BIG TEN	Fast	IEU-MET-FAST-007	Stacked cylinders of IEU reflected by depleted U
	STACY-30	Thermal	LEU-SOL-THERM-007	Unreflected cylinder of IEU solution
	STACY-46	Thermal	LEU-SOL-THERM-004	Cylinder of IEU solution reflected by water
Pu	Jezebel	Fast	PU-MET-FAST-001	Bare sphere of Pu
	Flattop-Pu	Fast	PU-MET-FAST-006	Pu sphere reflected by normal U
	THOR	Fast	PU-MET-FAST-008	Pu sphere reflected by thorium

The HEU, graphite, and steel platters all have outer radii of 26.67 cm. Each HEU platter is slightly less than 0.3 cm thick. In Zeus-1 there is slightly more than 8.0 cm of graphite between neighboring HEU platters, and in Zeus-6 there is slightly less than 2.4 cm of steel between neighboring HEU platters. The average thickness of the copper is slightly less than 14.5 cm. A vertical slice through the center of the Zeus-1 benchmark is shown in Figure 1.

3.3 IEU Benchmarks

The BIG TEN benchmark is based on the BIG TEN experiment that was operated at LASL in the 1970s. Four IEU cylinders are stacked on top of each other and surrounded by annuli of normal uranium or a homogeneous mixture of HEU and normal uranium. A depleted-uranium reflector encloses those regions. Dimensions and enrichments for the various regions are given in Table II, and a slice through the center of the benchmark configuration is shown in Figure 2.

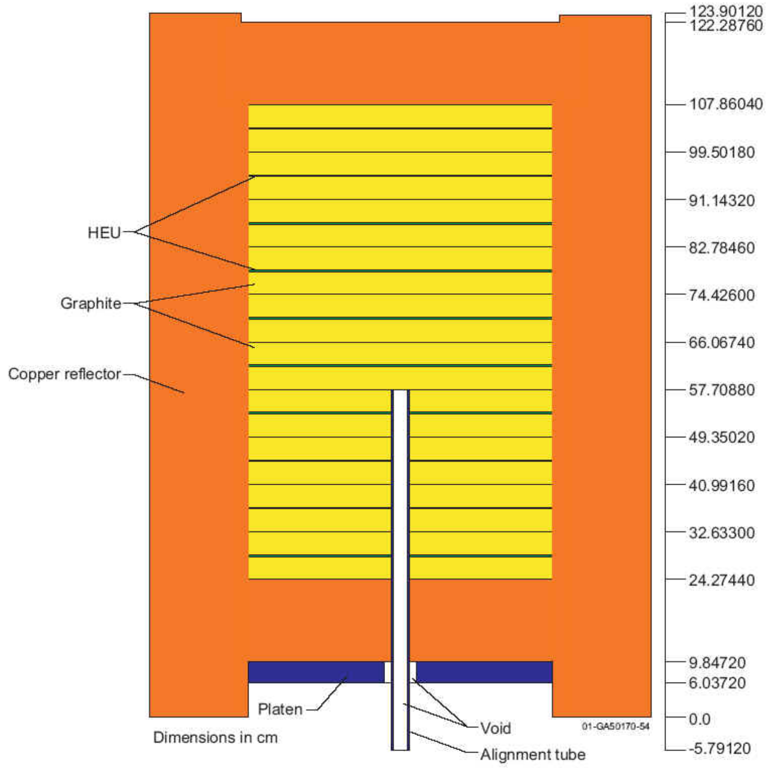

Figure 1. Vertical slice through the center of Zeus-1.

Table II. Enrichments and dimensions for the BIG TEN benchmark

Region	^{235}U (wt.%)	Outer Radius (cm)	Height (cm)
Central IEU	10.06	2.25014	15.24
		3.10996	19.46148
		7.62	26.74112
		12.54604	19.34351
Normal Uranium	0.711	26.67	3.48717
Homogenized HEU and Normal Uranium	10.23	26.67	55.41309
Normal Uranium	0.711	26.67	6.64585
Depleted Uranium	0.21	26.67	15.24
		41.91	96.52
		26.67	15.73389

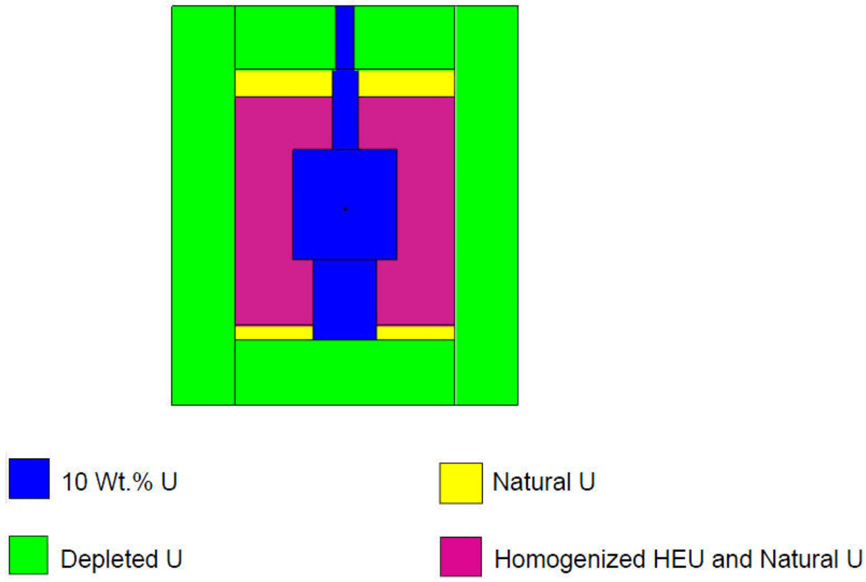

Figure 2. Slice through the center of the BIG TEN benchmark

The STACY-30 and STACY-46 benchmarks are included here as IEU benchmarks because they have an enrichment of 9.97 wt.%, and 5 wt.% is the current limit for fuel used in commercial reactors in the United States. They are based on the STACY-30 and STACY-46 experiments that were performed at the Japan Atomic Energy Research Institute in 1995. The benchmarks contain a uranium nitrate solution inside a cylindrical tank made of stainless steel 304. The inner radius of the tank is 29.5 cm, and it is 0.3 cm thick. STACY-30 is unreflected, but STACY-46 has a water reflector outside the stainless steel tank that is 30 cm thick. The critical heights, solution densities, and uranium concentrations for the two benchmarks are given in Table III.

Table III. Characteristics of the STACY benchmarks

Benchmark	Critical Height (cm)	Uranium Content (g/l)	Solution Density (g/cm^3)
STACY-30	54.20	290.7	1.4571
STACY-46	78.56	241.9	1.3936

3.4 Plutonium Benchmarks

The Jezebel benchmark contains a bare, homogeneous sphere of plutonium with a radius of 6.3849 cm and a ^{240}Pu content of 4.5 at.%. It is based on the Jezebel experiment that was operated at LASL during the 1950s.

The Flattop-Pu benchmark contains a sphere of plutonium reflected by an annulus of normal uranium. The sphere has a radius of 4.5332 cm and contains 4.83 at.% ^{240}Pu. The annulus of normal uranium is 19.6088 cm thick. This benchmark is based on the Flattop-Pu experiment that was operated at LASL during the mid 1960s.

The Thor benchmark contains a sphere of plutonium enclosed in the center of a right circular cylinder of thorium. The sphere has a radius of 5.31 cm, while the cylinder has a radius of 26.67 cm and is 53.34 cm high. The plutonium contains 5.13 at.% ^{240}Pu. This benchmark is based on the Thor experiment that was operated at LASL in 1961 and 1962.

4 ENDF/B-VII and ENDF/B-VII RESULTS

Rossi α is obtained as part of a criticality (kcode) calculation in MCNP5 1.60. Calculated values for k_{eff} for the benchmarks in the Rossi α validation suite are compared with their benchmark values in Table IV. The ENDF/B-VII.0 data are taken from the ENDF70 nuclear data library [7] distributed with MCNP5 1.51 and later. The ENDF/B-VI data are taken from the ACTI [8] and ENDF66 [9] nuclear data libraries included in the same distribution. In combination, those two libraries correspond to the final release of ENDF/B-VI for the cases in the suite. Overall, ENDF/B-VII.0 clearly produces better agreement with the benchmark values for k_{eff} than ENDF/B-VI does.

Table IV. Comparison of Measured and Calculated Values for Rossi α

Benchmark Name	Benchmark k_{eff}	Calculated k_{eff} from MCNP5 1.60	
		ENDF/B-VI	ENDF/B-VII.0
Jezebel-233	1.0000 ± 0.0010	0.9928 ± 0.0001	0.9996 ± 0.0001
Flattop-23	1.0000 ± 0.0014	1.0004 ± 0.0001	0.9994 ± 0.0001
Godiva	1.0000 ± 0.0010	0.9965 ± 0.0001	0.9999 ± 0.0001
Flattop-25	1.0000 ± 0.0030	1.0017 ± 0.0001	1.0029 ± 0.0001
Zeus-1	0.9977 ± 0.0008	0.9919 ± 0.0001	0.9936 ± 0.0001
Zeus-5	1.0004 ± 0.0016	1.0080 ± 0.0001	1.0115 ± 0.0001
Zeus-6	0.9991 ± 0.0024	1.0065 ± 0.0001	1.0088 ± 0.0001
BIG TEN	1.0049 ± 0.0008	1.0167 ± 0.0001	1.0048 ± 0.0001
STACY-30	0.9973 ± 0.0009	0.9976 ± 0.0001	0.9973 ± 0.0001
STACY-46	0.9999 ± 0.0010	1.0015 ± 0.0001	1.0019 ± 0.0001
Jezebel	1.0000 ± 0.0020	0.9974 ± 0.0001	0.9999 ± 0.0001
Flattop-Pu	1.0000 ± 0.0030	1.0018 ± 0.0001	1.0001 ± 0.0001
THOR	1.0000 ± 0.0006	1.0058 ± 0.0001	0.9981 ± 0.0001

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

The Zeus benchmarks continue to produce poor agreement with the benchmark values for k_{eff} [10]. Zeus-1 has an intermediate spectrum, and the principal reason for its poor agreement is believed to be the nuclear data for ^{235}U in the unresolved resonance range (2.25 to 25 keV). Zeus-5 and Zeus-6 both have fast spectra, and the principal reason for their poor agreement is believed to be the nuclear data for copper in the fast range (above 100 keV).

Calculated values for Rossi α from the benchmarks in the suite were obtained with MCNP5 and its ENDF/B-VI and ENDF/B-VII.0 nuclear data libraries. Those values are presented in Table V. The Zeus cases are the most problematic for Rossi α as well. Overall, ENDF/B-VII.0 produces marginally better results than ENDF/B-VI.

Table V. Comparison of Measured and Calculated Values for Rossi α

Benchmark Name	Rossi α (10^4 generations/second) at Delayed Critical		
		Calculated with MCNP5 1.60	
	Measured	ENDF/B-VI	ENDF/B-VII.0
Jezebel-233	-100 ± 1	-109 ± 1	-108 ± 1
Flattop-23	-26.7 ± 0.5	-30.9 ± 0.4	-30.2 ± 0.4
Godiva	-111 ± 2	-114 ± 1	-113 ± 1
Flattop-25	-38.2 ± 0.2	-40.9 ± 0.2	-39.7 ± 0.2
Zeus-1	-0.338 ± 0.008	-0.373 ± 0.002	-0.363 ± 0.002
Zeus-5	-7.96 ± 0.08	-10.94 ± 0.07	-10.76 ± 0.07
Zeus-6	-3.73 ± 0.05	-4.12 ± 0.03	-4.14 ± 0.03
BIG TEN	-11.7 ± 0.1	-12.6 ± 0.1	-11.8 ± 0.1
STACY-30	-0.0127 ± 0.0003	-0.0133 ± 0.0003	-0.0133 ± 0.0003
STACY-46	-0.0106 ± 0.0004	-0.0110 ± 0.0002	-0.0104 ± 0.0002
Jezebel	-64 ± 1	-64 ± 1	-65 ± 1
Flattop-Pu	-21.4 ± 0.5	-21.6 ± 0.3	-21.0 ± 0.3
THOR	-19 ± 1	-20 ± 1	-20 ± 1

The measured values for Rossi α cannot be considered as true benchmark values, because they do not contain allowances for physical uncertainties (in, e.g., dimensions and densities) or for the biases and uncertainties that accrue during the incorporation of simplifications into the benchmark models. Consequently, acceptable agreement must be judged subjectively rather than on a true quantitative basis.

Unfortunately, the sensitivity studies that would be required to determine the uncertainties for Rossi α that are associated with physical uncertainties would require resources that are beyond the scope of this study. However, the *Handbook* contains both detailed and benchmark models for some of the cases in the suite. Consequently, the biases and uncertainties associated with the simplifications incorporated into the benchmark models for those cases can be determined by comparing the results from the detailed and benchmark models. Those comparisons, based on ENDF/B-VII.0 nuclear data, are presented in Table VI.

Table VI. Comparison of Rossi α from benchmark and detailed models.

Benchmark Name	Rossi α (10^4 generations/second) at Delayed Critical		
	Calculated with MCNP5 1.60		
	Benchmark	Detailed	Bias
Godiva	-113 ± 1	-115 ± 1	2 ± 1
Zeus-1	-0.363 ± 0.002	-0.379 ± 0.002	0.016 ± 0.003
Zeus-5	-10.76 ± 0.07	-10.75 ± 0.07	-0.01 ± 0.10
BIG TEN	-11.8 ± 0.1	-11.9 ± 0.1	0.1 ± 0.1

The biases for two of the four cases are within a single standard deviation and therefore can be considered negligible. The bias for Godiva is statistically significant, however, and the bias for Zeus-1 is proportionally much larger. The simplifications incorporated into the benchmark model for Zeus-1 are more substantial than those for the other three cases (its bias in k_{eff} is -0.0020 Δk, for example, whereas the magnitude of the bias for the other three cases is no larger than 0.0004 Δk). Consequently, these results suggest that the mean of the benchmark value for Rossi α for these cases would be the same as the mean of the measured value for Zeus-5 and BIG TEN. However, the mean of the benchmark value for Godiva would be -109 x 10^4 per second rather than -111 x 10^4, and the mean for Zeus-1 would be -0.322 x 10^4 per second instead of -0.338 x10^4.

5 SUMMARY AND CONCLUSIONS

The Rossi α validation suite contains 13 benchmarks whose calculated values can be compared against measured values. The specifications for the benchmark models are taken from the *International Handbook of Evaluated Criticality Safety Experiments*, and the measured values are taken from the CSEWG benchmark book, the *Handbook*, journal articles, or the log books for the experiments on which the benchmarks are based. The usefulness of the suite is illustrated by the fact that it currently is being used to test β versions of ENDF/B-VII.1 in order to assess the impact of proposed changes to nuclear data.

Results have been obtained for each of the cases in the suite using the MCNP5 Monte Carlo code and nuclear data libraries based on ENDF/B-VI and ENDF/B-VII.0. Overall, ENDF/B-VII.0 produces marginally better agreement with the measured values for Rossi α than ENDF/B-VI does.

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