Expanded COG Criticality Validation Suite for Inter-Laboratory Benchmark Data Comparison

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The COG suite of criticality benchmarks has been formally expanded from 591 to 3,395 to cover the entire energy range from thermal to fast neutron spectra under a variety of reflector and moderator conditions and fissile materials. COG results have been compared with benchmark values from the International Criticality Safety Benchmark Evaluation Project Handbook for ENDF/B-VII.1, ENDF/B-VIII.0 and JEFF-3.3. COG results have been also compared with a MERCURY validation suite. Most of the results agreed with the benchmark values within ±3σ. Among the three cross section data, cases with ENDF/B-VIII.0 performed best with about 85% of the total cases within ±3σ range. A major inter-comparison project between COG, MCNP, MORET, and SCALE for ENDF/B-VIII.0 and JEFF-3.3 is in progress.

Introduction

COG is a general purpose, multi-particle, high-fidelity Monte Carlo code developed by LLNL. Since 2017, LLNL has focused on expanding COG benchmark cases as part of a collaborative effort of the benchmark inter-laboratory comparison study between the US Department of Energy (DOE) Nuclear Criticality Safety Program (NCSP) and the French Institut de Radioprotection et de Sûreté Nucléaire (IRSN). The benchmark cases fully cover the entire range from thermal to fast neutron spectra for a wide variety of fissionable material forms in a variety of reflector and moderator conditions described in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook.

The original number of LLNL 591 benchmark cases (143 PU, 358 ^{235}U, and 90 ^{233}U) was expanded to 3,395 PU, HEU (Highly Enriched Uranium), IEU (Intermediate Enriched Uranium), LEU (Low Enriched Uranium), ^{233}U, Mixed fuel, and SMF (Special Metal Fast) cases, providing valuable data for the inter-laboratory benchmark data comparison.

Category	Number of Cases
PU	766
HEU	1,056
IEU	207
LEU	807
^{233}U	193
Mixed	356
SMF	10
Total	3,395

Table 1. Number of Benchmark Cases.

Comparison with ICSBEP Benchmarks

SD	PU	HEU	IEU	LEU	^{233}U	Mixed	SMF
< 1σ	295	544	137	345	119	195	7
1σ - 2σ	174	165	28	171	39	61	1
2σ -3σ	147	116	11	114	16	40	2
> 3σ	150	231	31	177	19	60	0
Total	766	1,056	207	807	193	356	10

Table 2. COG Results Compared with Benchmark Values for ENDF/B-VII.1.

SD	Pu	HEU	IEU	LEU	^{233}U	Mixed	SMF
< 1σ	484	576	157	391	123	174	5
1σ - 2σ	137	181	38	183	37	85	3
2σ -3σ	53	100	3	117	18	36	2
> 3σ	92	199	9	116	15	61	0
Total	766	1,056	207	807	193	356	10

Table 3. COG Results Compared with Benchmark Values for ENDF/B-VIII.0.

SD	PU	HEU	IEU	LEU	^{233}U	Mixed	SMF
< 1σ	488	541	145	383	111	184	3
1σ - 2σ	139	180	28	165	46	83	2
2σ -3σ	47	108	12	89	16	47	3
> 3σ	92	227	22	170	20	42	2
Total	766	1,056	207	807	193	356	10

Table 4. COG Results Compared with Benchmark Values for JEFF-3.3.

- 668 cases with ENDF/B-VII.1, 492 cases with ENDF/B-VIII.0 data and 573 cases with JEFF-3.3 data exceed ± 3σ range.
- For PU, ENDF/B-VIII.0 and JEFF-3.3 performed better than ENDF/B-VII.1.
- For HEU, ENDF/B-VIII.0 performed better than ENDF/B-VII.1 and JEFF-3.3. COG results with ENDF/B-VIII.0 for LEU and IEU were better than those with JEFF-3.3 and ENDF/B-VII.1 data.
- For ^{233}U, ENDF/B-VIII.0 performed better than ENDF/B-VII.1 and JEFF-3.3.
- For Mixed cases, JEFF-3.3 performed better than ENDF/B-VII.1 and ENDF/B-VIII.0.

Root Mean Squared Errors (RMSE) and chi-squared values were used to compare the performance and the degree of differences where,

$$\mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{N}(K_{c,i}-K_{b,i})^2}{N}}, \qquad \chi^2 = \frac{1}{\nu}\sum_{i=1}^{N}\frac{(K_{c,i}-K_{b,i})^2}{\sigma_i^2}$$

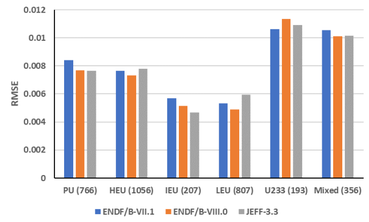

Figure 1. RMSE for ENDF/B-VII.1, ENDF/B-VIII.0, and JEFF-3.3.

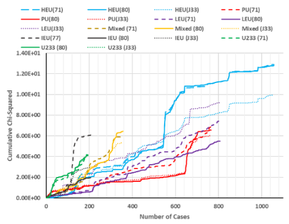

Figure 2. Cumulative Chi-Squared Values for Six Different Categories.

Comparison with MERCURY Validation Suites

To validate the newly expanded benchmark data set, COG input decks are translated into the MERCURY input decks. From this effort, errors from the benchmark models, if any, cannot be identified. However, results from different (MERCURY) cross section data processing can be compared. The selected 3,350 COG benchmark cases are compared.

Category	Number of Cases
PU	753
HEU	1,034
IEU	207
LEU	797
^{233}U	193
Mixed	356
SMF	10
Total	3,350

Table 5. Number of Benchmark Cases.

SD	Code	Pu	HEU	IEU	LEU	^{233}U	Mixed	SMF
< 1σ	COG	475	570	157	390	123	174	5
	MERCURY	391	560	140	425	120	190	4
1σ - 2σ	COG	134	180	38	178	37	85	3
	MERCURY	184	177	40	148	40	87	4
2σ -3σ	COG	52	98	3	113	18	36	2
	MERCURY	68	107	5	107	13	31	2
> 3σ	COG	92	186	9	116	15	61	0
	MERCURY	110	190	22	117	20	48	0
Total	COG	753	1,034	207	797	193	356	10
	MERCURY	753	1,034	207	797	193	356	10

Table 6. COG Results Compared with Benchmark Values for ENDF/B-VIII.0.

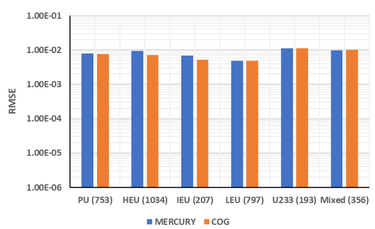

Figure 3. RMSE for ENDF/B-VIII.0.

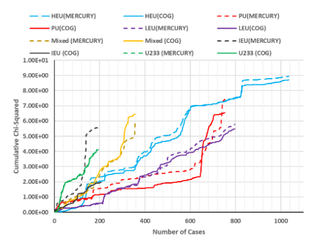

Figure 4. Cumulative Chi-Squared Values for Six Different Categories.

Conclusions

COG11.3 comparison with benchmark values from the ICSBEP Handbook and MERCURY results showed quite good agreement with each other. Sources of discrepant results may come from 1) errors in the cross section data, 2) possible errors from the modeling of the benchmark experiments, or 3) errors in the benchmark measurement data itself or its evaluated biases and uncertainties.

An inter-laboratory comparison project with different Monte Carlo codes such as MCNP, MORET, and SCALE for ENDF/B-VIII.0 and JEFF-3.3 is in progress. LLNL participation in this project will result in development of significantly more COG benchmark cases as our goal is to overlap the VALID, WHISPER, and IRSN compendia of criticality benchmarks to the extent possible, which will be beneficial to international code user communities.

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