The Case for and Against a Gadolinium Bias in SCALE: Round 2**

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ABSTRACT

The "Opening Arguments" for and against a gadolinium bias in SCALE were presented at the American Nuclear Society Annual Meeting in Philadelphia, Pennsylvania, in June, 2018. Some critical experiments included in the Oak Ridge National Laboratory Verified, Archived Library of Inputs and Data (VALID) indicate a significant bias as a function of gadolinium concentration. Other experiments indicate that no significant bias exists. The work presented here develops a larger suite of gadolinium-bearing benchmark models to further examine code, data, and benchmark performance. The new benchmark models have been reviewed for accuracy, but documentation and review for addition to the VALID library have not been completed. The problematic benchmarks included in VALID are HEU-SOL-THERM-014 and -016. These are two evaluations from a series of experiments from the Institute for Physics and Power Engineering (IPPE), Russia, documented in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook. The entire set of evaluations also includes HEU-SOL-THERM-015, -017, -018, -019, and -025. Each evaluation contains a different uranium concentration, and different configurations within each evaluation include different gadolinium concentrations. These 7 evaluations contain a total of 52 configurations and form the largest subset of experiments considered, and they allow for a more complete assessment of the performance of these benchmarks than has historically been possible using just the HEU-SOL-THERM-014 and -016 results.

Additional solution experiments are considered, including MIX-SOL-THERM-006 and -007 and PU-SOL-THERM-034. MIX-SOL-THERM-007 is in the VALID library, whereas MIX-SOL-THERM-006 and PU-SOL-THERM-034 are not. The results for MIX-SOL-THERM-007 have not shown a gadolinium trend. These mixed- and plutonium-fueled solutions include 28 configurations. Some experiments including solid fuel and solid gadolinium are also included. These experiments include highly enriched uranium (HEU) foils moderated with polyethylene in HEU-MET-THERM-010, -016, and -034, and low-enriched uranium (LEU) pin arrays with gadolinia absorber rods in LEU-COMP-THERM-036 and -043. A total 32 cases with solid fuel are included. The IPPE solution benchmarks show a fairly high degree of variability, but no clear trend as a function of gadolinium concentration can be observed. The mixed- and plutonium-fueled solutions show less variability than the HEU solutions and also no trend relative to gadolinium concentration. The solid-fueled experiments also show no trend as a function of gadolinium content. The entire set of benchmarks shows no clear trend on gadolinium content or the energy of the average neutron lethargy causing fission.

KEYWORDS

Validation, gadolinium, SCALE, KENO

1. INTRODUCTION

Validation of the KENO codes within the SCALE code system [1] has been documented in many publications over the years [2]–[4]. These recent validation reports are based on models of critical experiments evaluated in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [5] that have been included in the Verified, Archived Library of Inputs and Data (VALID) [6] maintained in the Nuclear Energy and Fuel Cycle Division at Oak Ridge National Laboratory (ORNL). A limited number of evaluations included in each of these validation reports includes Gd. Some of the benchmarks indicate a significant potential bias in the Gd cross sections, whereas others do not, as summarized in an "Opening Arguments" paper from the summer of 2018 [7].

An effort to create additional benchmark models for Gd-bearing experiments was executed in the summer of 2022 at ORNL. Another source of additional validation cases was work reported in Shaw et al. [8] examining updated nuclear data evaluations in the ENDF/B-VIII.0 library [9]. These models have not yet been integrated into the VALID library, but reviews have been performed to confirm their accuracy. The models may be included in the VALID library pending further documentation. The model reviews are deemed sufficient to allow the use of these models alongside the VALID data in performing a more extensive assessment of the performance of Gd nuclear data in the SCALE code system.

This paper describes the new benchmark models that are available and the results of the calculations using them. These results support a tentative conclusion from the authors [7] that it is more likely that some of the ICSBEP evaluations are discrepant than that the nuclear data contain significant errors.

2. EXPERIMENT DESCRIPTIONS

As mentioned above, there are three sources of the critical benchmark models used in this work: the VALID library maintained at ORNL, the work documented in Shaw et al. [8], and an effort at ORNL in 2022 focused on a training rotation for two students from the United States Naval Academy. A synopsis of each of the benchmark experiments included in this study is presented in the remainder of this section.

2.1. VALID Models

Three evaluations from the ICSBEP Handbook including soluble gadolinium in solution experiments are included in VALID. These evaluations are HEU-SOL-THERM-014 (HST-014), HST-016, and MIX-SOL-THERM-007 (MST-007).

The HST-014 and HST-016 evaluations are part of a series of six evaluations of experiments performed at the Institute of Physics and Power Engineering (IPPE) in Russia. All the experiments involve solutions of highly enriched uranium (HEU), and many of the experiments also include Gd dissolved into the solution. Each evaluation contains experiments with a specific uranium concentration, and that uranium concentration varies between experiments from 70 g U/l in HST-014 to 400 g U/l in HST-019. HST-016 has a uranium concentration of 150 g U/l. Each evaluation includes several experiments with different concentrations of soluble Gd. The three experiments in HST-014 include 0, 0.1, and 0.193 g/l of Gd. The three HST-016 experiments include Gd concentrations of 0, 0.3, and 0.525 g/l.

The MST-007 evaluation documents a series of 10 experiments including a mixture of Pu and U nitrates, all with approximately 76 g/l of Pu and 175 g/l of U. Three cases are judged to be unacceptable as benchmarks because of large uncertainties in the dissolved Gd concentration. The primary variables among the 7 remaining cases are the Gd concentration, ranging from 0.042 to 1.01 g/l, and the solution height, which ranges from 19 to 62 cm. All cases include a water reflector with a thickness of 20 cm below the solution tank and about 19 cm around the tank.

2.2. Shaw et. al [8] Models

Several evaluations were modeled in the work described in Shaw et al. [8], as its primary purpose was to evaluate data changes in ENDF/B-VIII.0 [9]. Some of those models included Gd, so the inclusion of those benchmarks here was a logical decision. The relevant models for this work are HST-015, HST-017, HST-018, HST-019, and PST-034.

The HST benchmarks complete the initial set of IPPE Gd benchmarks. HST-015 has a uranium concentration of 100 g/l, and the other three HSTs have concentrations of 200, 300, and 400 g U/l. The HST-015 evaluation contains 5 cases, HST-017 has 8 cases, HST-018 has 12 cases, and HST-019 has 3. These evaluations contain 28 critical configurations, of which 19 contain soluble Gd. The Gd concentrations range up to almost 2 g/l.

The other models from Shaw et al. [8] included in this work come from the PST-034 evaluation. This evaluation contains 15 cases, with Pu concentrations of 116 or 363 g Pu/l. The Gd concentrations vary up to 20.25 g/l; case 1 includes no Gd. The solution height is increased as the Gd concentration increases to maintain criticality. The experiments were performed in the same tank used in the MST-007 evaluation discussed above and were reflected with light water in the same reflector tank used in the MST-007 experiments.

2.3. New Models

A number of new models were generated by two students from the United States Naval Academy on a training rotation at ORNL in the summer of 2022. Experiments containing Gd were identified in the ICSBEP Handbook to expand the coverage for this effort while also simple enough to be generated by novice code users. The evaluations selected were HST-025, MST-006, HEU-MET-THERM-010 (HMT-010), HMT-016, HMT-034, LEU-COMP-THERM-036 (LCT-036), and LCT-043.

The HST-025 evaluation completes the HEU solution experiments containing Gd performed at IPPE, along with the experiments documented in HST-014 through HST-019. In the HST-025 experiments, the uranium concentration varied from 51 to 395 g/l, and Gd concentrations range from 0 to 10.37 g/l. In some cases, the experiment contains a middle tank with either 50 or 77 g U/l. In most cases, there is a bottom and radial water reflector in a third tank. This series of experiments contains a wider range of both uranium and Gd concentrations than the rest of the HST series from IPPE.

The MST-006 evaluation contains a series of six experiments performed at the critical experiment facility in Valduc, France. All six cases contain a similar solution with approximately 91 g Pu/l and 213 g U/l. The Gd concentration varies from 0.03 to 0.7 g/l, and the solution tank is water-reflected.

The HMT-010, HMT-016, and HMT-034 evaluations contain similar experiments containing HEU foils moderated and reflected with polyethylene. HMT-010 contains two cases, with Gd foils of 7.5 mil and 15 mil (0.1905 and 0.381 mm) thicknesses. The HMT-016 and HMT-034 evaluations each contain one case. Each of these experiments contains an alloy of Gd with Ni, Cr, and Mo.

The LCT-036 evaluation documents experiments performed in Hungary as part of the VVER critical experiment series. The evaluation contains 69 critical configurations; 19 were selected and modeled. The selected models are cases 27–45, and cases 27, 31, 32, and 33 contain no gadolinium. The remaining 15 cases contain Gd absorber rods of different concentration located at different locations within the array lattice.

The LCT-043 evaluation contains 9 experiments performed at the IPEN/MB-01 reactor in São Paulo, Brazil. Each configuration contains either 4 or 6 gadolinia rods; the number and location of the absorber rods vary among the cases. The gadolinia rods are identical in dimensions and loading, so the only variation in Gd present among the cases is based on the number of rods. The worth of the rods varies based on their location within the core.

3. CODES AND DATA

All results presented in this paper used the KENO V.a or KENO-VI 3D Monte Carlo transport codes within the SCALE 6.3.0 code system [1]. The results are presented together regardless of transport code used because it has been shown that the two transport solvers generate equivalent biases given the same set of benchmark experiments [3]. The stochastic uncertainty was less than 0.00020 Δk in all cases, and in most cases it was approximately 0.00010 Δk. Several different combinations of calculation parameters were used, but indications of source convergence were confirmed in all calculations. At least 10,000 particles were used in each generation for each calculation. All calculations were performed in continuous energy (CE) and used nuclear data based on ENDF/B-VIII.0 [9].

4. RESULTS

The results presented here are organized into four subsets: the IPPE experiments, all solution benchmarks, the HEU and polyethylene cases, and the LCT arrays. Results are also presented for the complete set of models. The results presented here are ratios of the calculated k_{eff} value to the expected benchmark k_{eff} from the evaluation. These ratios are referred to as C/E ratios. The difference of these C/E ratios from unity represents the misprediction of the benchmark by the code and data. An examination of multiple benchmarks is needed to make a reliable assessment of code and data performance. It is often informative to generate trends of the C/E values with respect to each of a number of different parameters to investigate the behavior of the mispredictions with respect to that parameter. In this work, the C/E values are examined with respect to the energy of the average lethargy causing fission (EALF) and the Gd concentration. These parameters are the most likely parameters to indicate the presence of a bias in the Gd nuclear data, and the energy range in which such a bias occurs.

4.1. Subset 1: IPPE HEU Solution Experiments

The IPPE HEU solution experiments are evaluated in HST-014 through HST-019 and HST-025. This subset consists of 52 experiments with varying uranium and Gd concentrations among the models. The results show significant variation; in many cases, the variation is greater than the evaluated uncertainty in the experiments. The results are presented graphically in Fig. 1 and Fig. 2 as a function of Gd concentration and the EALF, respectively.

There is no clear trend in the results presented as a function of Gd concentration in Fig. 1. Each evaluation is shown with a separate line to help distinguish the different uranium concentrations. The Gd concentration increases with case number, so the lines are monotonically increasing with Gd concentration. The calculated-to-evaluation (C/E) ratios do not always increase with increasing Gd concentration. In the majority of evaluations, the last C/E value is less positive than the previous case. It appears that the primary indication of a Gd bias resulting from the HST-014 and HST-016 results was not justified and is not generally supported by the more complete data set from the IPPE experiments.

Similarly, there is no clear trend for the C/E values as a function of EALF, as shown in Fig. 2. Each evaluation is shown with a unique set of markers, though in this case data markers are used instead of lines because the EALF values are not monotonically increasing with case number.

The average C/E for these 52 experiments is 1.00272 ± 0.00075. This can be compared with the average C/E value of the 52 HST cases included in VALID for CE ENDF/B-VIII.0 calculations of 0.99824 ± 0.00074, taken from Greene and Marshall [10]. The 6 configurations included in HST-014 and HST-016 are included in both sets, but the remaining 48 cases are unique. The difference of the two averages is statistically significant at 0.00448 ± 0.00106. Although no bias in the Gd nuclear data is apparent from the trend shown in Fig. 1, it is still possible that one exists. A sensitivity analysis such as that performed in Rearden and Marshall [11] would likely indicate that the difference between these two sets cannot be related to the Gd absorption cross section without manifesting a trend as a function of concentration.

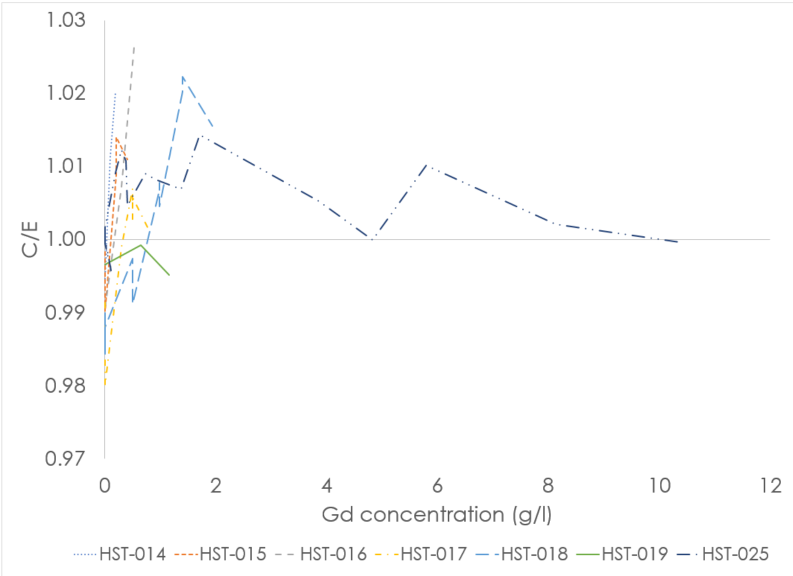

Figure 1. C/E versus Gd concentration for the IPPE HST experiments

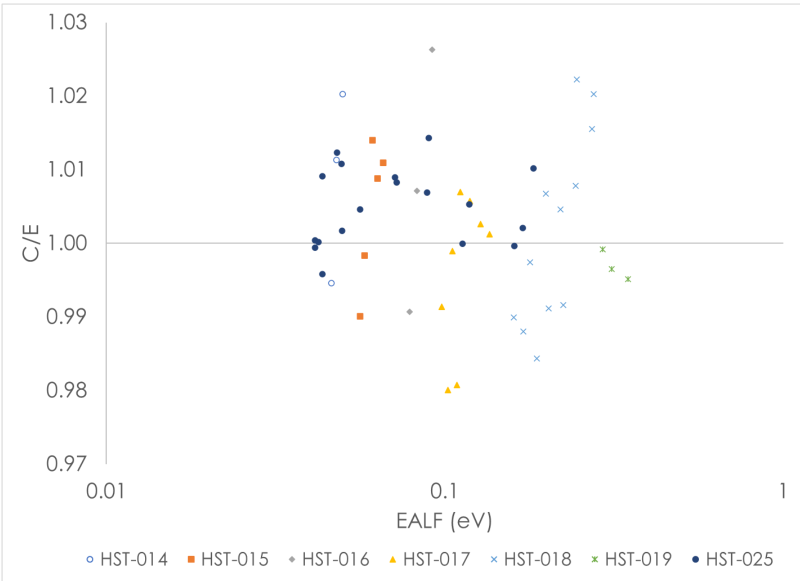

Figure 2. C/E versus EALF for the IPPE HST experiments

4.2. All Solution Benchmarks

The results for the MST-006, MST-007, and PST-034 evaluations are added to the IPPE HST results to assess the performance of the Gd-bearing solution experiments. As with the results presented above, the results are considered both as a function of Gd concentration and EALF, in Figs. 3 and 4, respectively.

A Gd bias should show itself most clearly in a trend as a function of Gd concentration, but none is evident in Fig. 3. The wide range of concentrations used in PST-034 may obscure some of the results at low Gd concentrations, but it should also provide a strong indication of a bias if one were present. The significant variability in the IPPE results is apparent in Fig. 3 just as it was in Fig. 1. Neither the MST nor the PST results provide any indication of a Gd bias.

The results for all solutions as a function of EALF also show no trend. The different Pu concentrations in PST-034 are evident with the higher concentration also having a harder neutron energy spectrum. The lower concentration experiments overlap well with the HST and MST results.

The average C/E for all solution benchmarks used here is 1.00021 ± 0.00057, compared to 0.99759 ± 0.00042 from Greene and Marshall [10]. As with the HST solutions presented above, this is a statistically significant difference of 0.00262 ± 0.00071. This is not a surprising result given that 52 of the 80 solution benchmarks are the IPPE HST cases. As mentioned above, a sensitivity analysis would provide insight into whether or not the Gd data could be the culprit without introducing a trend in the C/E results.

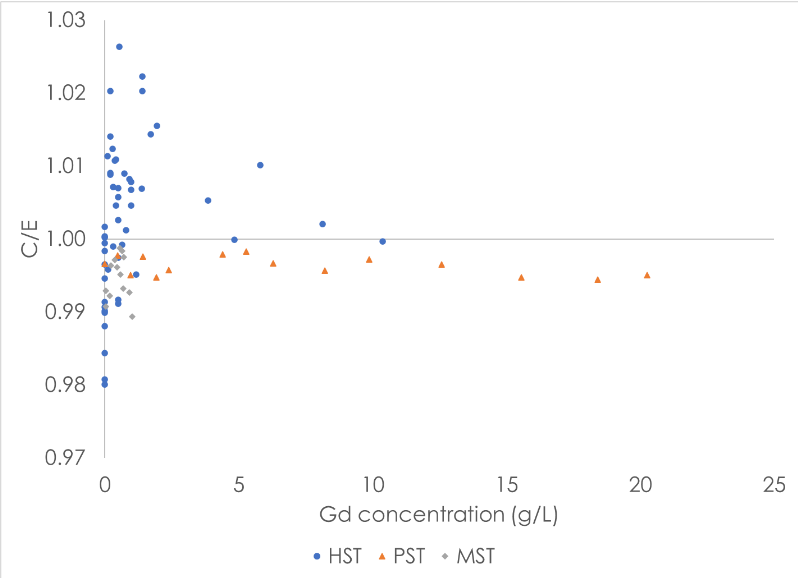

Figure 3. C/E versus Gd concentration for all solution experiments

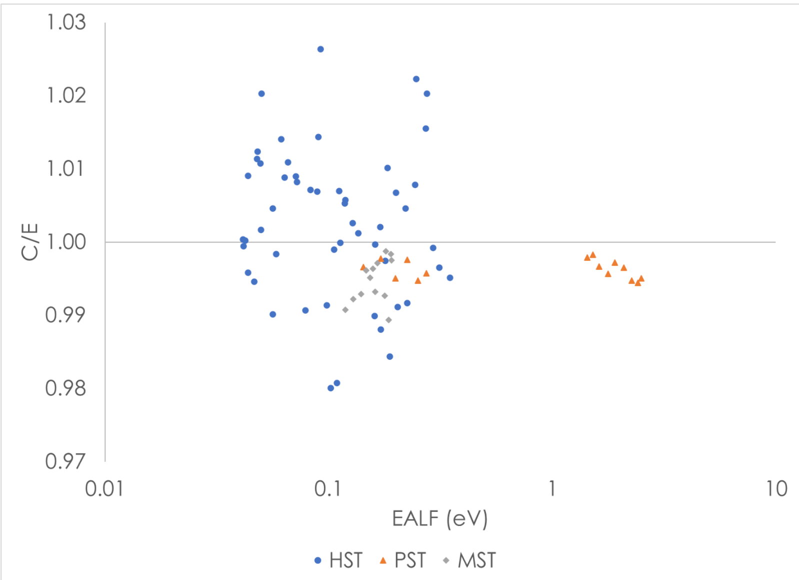

Figure 4. C/E versus EALF for all solution experiments

4.3. HEU and polyethylene experiments

The HEU and polyethylene experiments included in HMT-010, HMT-016, and HMT-034 include only 4 experiments. HMT-010 has two cases, the first with 14 foils that are each 15 mils (0.381 mm) thick. The second case has 13 foils that are 7.5 mils (0.1905 mm) thick. The HMT-016 and HMT-034 evaluations use plates made of a Ni-Cr-Mo-Gd alloy along with HEU foils, moderated and reflected with polyethylene. The C/E results for these systems are shown in Table I and as a function of EALF in Fig. 5. No analogue of concentration is derived for the solid systems, though surface area might be appropriate for these black absorbers.

The results presented in Table I and Fig. 5 show no clear trends as a function of EALF. The variability of the experiments' EALF values is quite small, which limits the usefulness of this trend. No other trending parameters are clearly applicable, and many potential interpretations could be made among only 4 points. The HMT-016 and HMT-034 results are clearly overpredicted, but this is consistent with other polyethylene-moderated systems in the ICSBEP Handbook.

No HEU systems with polyethylene moderation are currently in VALID, so no comparison of these results with other similar benchmarks in VALID is possible.

Table I. HEU foil and polyethylene results

Case	C/E	C/E Unc.	EALF (eV)
HMT-010-001	1.00515	0.00722	0.077
HMT-010-002	1.00146	0.00717	0.078
HMT-016-001	1.01183	0.00162	0.067
HMT-034-001	1.01352	0.00057	0.069

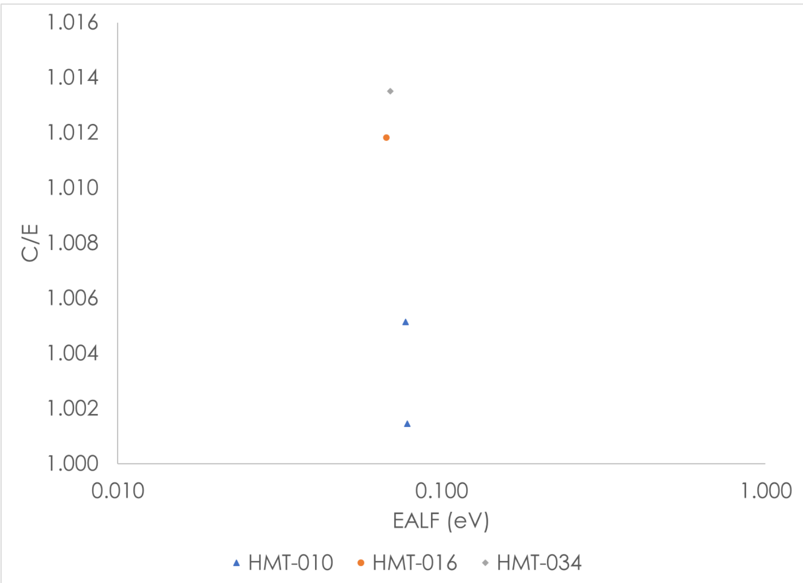

Figure 5. C/E versus EALF for HEU and polyethylene experiments

4.4. LEU Pin Array Systems

The last subset of results is the LEU pin array systems from LCT-036 and LCT-043. The results are presented as a function of EALF in Fig. 6, even though there is little variability in the EALF values in the experiments. The LCT-036 EALF values are all approximately 0.29 eV, and the LCT-043 are all around 0.16 eV. The results are also shown as a function of the number of absorber rods in Fig. 7.

There is no clear trend for either the LCT-036 or LCT-044 results as a function of EALF or the number of gadolinia rods present, as shown in Fig. 6 and Fig. 7, respectively. Both data sets are included in Fig. 7 as a matter of convenience, but the sets should be considered separately; the number of absorber rods is not a consistent basis for comparisons across the two different experimental configurations. Within each evaluation, the number of rods varies and provides an indication of the bias as a function of Gd loading. The loading per rod also varies in LCT-036; however, this trending parameter should be meaningful within an evaluation because the surface area scales with the number of rods.

The average C/E value for these 28 cases is 1.00097 ± 0.00019 compared to the average for the 140 LCT systems in VALID of 0.99921 ± 0.00018 [10]. This difference of 0.00176 ± 0.00026 is statistically significant, as were previous comparisons. The magnitude of the difference from the systems included in VALID is smaller for the LCT experiments than for the solution experiments, though in both cases the Gd-bearing experiments have a higher average C/E value. A sensitivity study would provide further indication of the potential for Gd to be the cause of this bias.

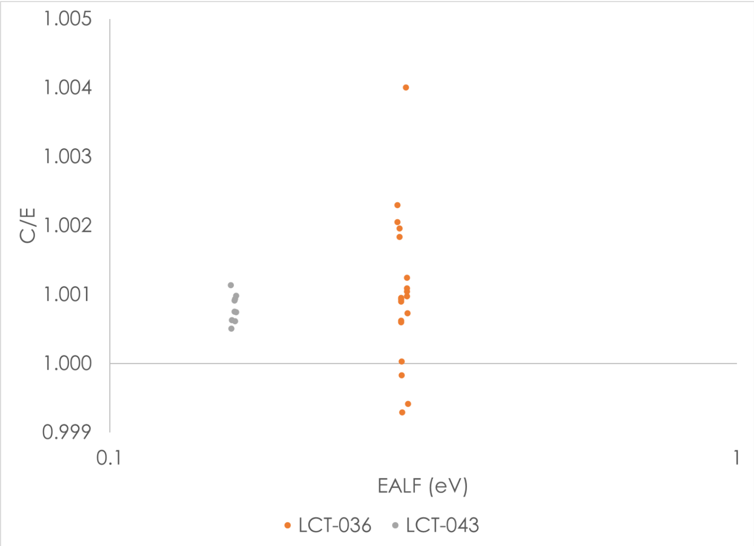

Figure 6. C/E versus EALF for the LCT experiments

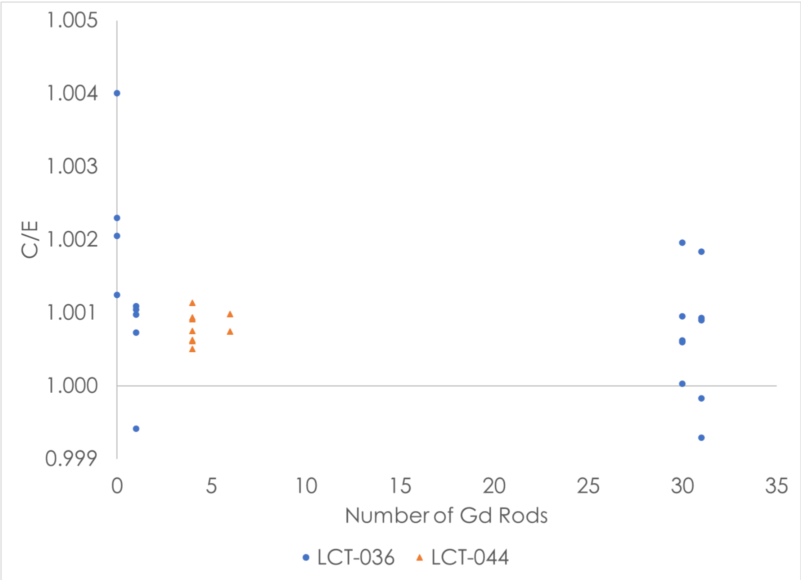

Figure 7. C/E versus number of Gd rods for LCT experiments

4.5. All Experiments

The results for all the Gd-bearing benchmarks considered in this work are shown as a function of EALF in Fig. 8. As with each of the subsets presented above, there is no clear indication of a trend in the C/E results as a function of EALF. There is no method for combining all the results in a trend as a function of Gd loading, mass, or concentration. A meaningful trend as a function of Gd sensitivity could be generated if sensitivity data are generated from the models in the future.

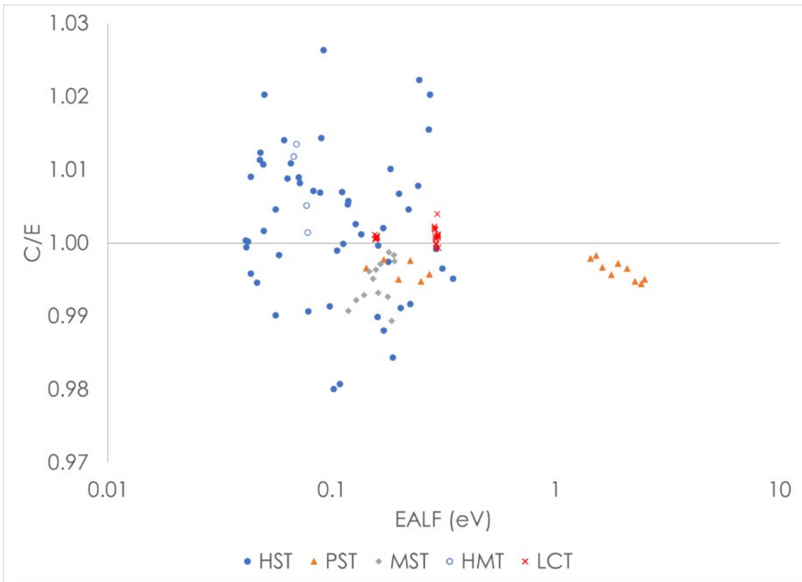

Figure 8. C/E versus EALF for all experiments

5. CONCLUSIONS AND FUTURE WORK

This work assembles a set of 112 critical experiments containing natural Gd as a neutron absorber to test the performance of the Gd nuclear data in ENDF/B-VIII.0 in the KENO Monte Carlo transport codes in SCALE 6.3.0. These experiments are solutions of HEU; Pu or a mixture of uranium and Pu; HEU foils moderated and reflected with polyethylene; or LEU fuel rod arrays moderated with light water. Section 4 presents the results for all of the experiments as well as the results for several subsets to examine similar results more closely. Neither the complete set of results nor any of the subsets provides any clear indications of a bias by trending the C/E values as a function of Gd content or neutron energy spectrum. The average C/E values for these experiments seem to be higher than the average values for similar experiments in the VALID library that do not include Gd.

A sensitivity analysis should be performed in the future to ensure that Gd is not the cause of this difference. It should also be noted that these experiments all contain natural Gd, so ^{157}Gd is the primary isotope being tested. Other experiments or measurements will be necessary to investigate the performance of nuclear data for other Gd isotopes.

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