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THE ORSPHERE BENCHMARK EVALUATION AND ITS POTENTIAL IMPACT ON NUCLEAR CRITICALITY SAFETY

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ABSTRACT

In the early 1970's, critical experiments using an unreflected metal sphere of highly enriched uranium (HEU) were performed with the focus to provide a "very accurate description…as an ideal benchmark for calculational methods and cross-section data files." Two near-critical configurations of the Oak Ridge Sphere (ORSphere) were evaluated as acceptable benchmark experiments for inclusion in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (ICSBEP Handbook). The results from those benchmark experiments were then compared with additional unmoderated and unreflected HEU metal benchmark experiment configurations currently found in the ICSBEP Handbook. For basic geometries (spheres, cylinders, and slabs) the eigenvalues calculated using MCNP5 and ENDF/B-VII.0 were within 3σ of their respective benchmark values. There appears to be generally good agreement between calculated and benchmark values for spherical and slab geometry systems. Cylindrical geometry configurations tend to calculate low, including more complex bare HEU metal systems containing cylinders. The ORSphere experiments do not calculate within their 1σ uncertainty and there is a possibility that the effect of the measured uncertainties for the GODIVA I benchmark may need reevaluation. There is significant scatter in the calculations for the highly-correlated ORCEF cylinder experiments, which are constructed from close-fitting HEU discs and annuli. Selection of a nuclear data library can have a larger impact on calculated eigenvalue results than the variation found within calculations of a given experimental series, such as the ORCEF cylinders, using a single nuclear data set.

Key Words: Benchmark, HEU, ICSBEP, ORSphere

1 INTRODUCTION

In the early 1970's, the Oak Ridge Sphere (ORSphere) experiments [1,2] were performed at the Oak Ridge Critical Experiments Facility (ORCEF) with highly enriched uranium (HEU) metal, also called Oak Ridge Alloy (ORALLOY) to recreate GODIVA I results with greater accuracy than the experiments performed at Los Alamos National Laboratory (LANL) in the 1950's [3]. The ORSphere experiments included two near-critical configurations, one slightly above delayed criticality and the other slightly below; this was done by machining the parts to reduce the radius slightly between experiments. Various reactivity effects and imperfections from spherical were also experimentally evaluated. The purpose of those two configurations was to provide quality experimental data to validate one-dimensional transport theory methods as well as verification of Monte Carlo methods using the as-assembled descriptions. Those assemblies provided better estimates of the unreflected and unmoderated pure HEU spherical critical mass since high precision was used to characterize the components utilized in the experiments. Benchmark evaluation of those two ORSphere configurations was recently performed for inclusion in the September 2013 edition of the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (ICSBEP Handbook) [4]. A third configuration, which employs the second sphere configuration with some additional HEU mass adjustment buttons, was later performed, representing a very near-critical configuration. This configuration has yet to be evaluated as a benchmark experiment.

A comparison study was prepared in which all unmoderated and unreflected HEU metal benchmark experiment configurations, without significant amounts of specialized alloy materials, that are currently available in the ICSBEP Handbook were evaluated. The variability and discrepancies in our computational analysis of the various bare HEU configurations has an impact on how we address the application of advanced modeling and simulation methods in nuclear criticality safety activities. A summary of the ORSphere benchmark evaluation and its comparison with other bare HEU benchmark experiment data is provided.

2 ANALYSIS AND RESULTS

2.1 Benchmark Evaluation of the ORSphere Configurations

The process of evaluating the nominal 3.4465-in.-radius sphere (Case 1) and the 3.4420-in.-radius sphere (Case 2) included the compilation of all available experiment information, the evaluation of the experimental uncertainty, and the development of detailed and simple benchmark models. Sample calculation results for the benchmark models were also generated using various codes and neutron cross section libraries. The detailed compilation of the benchmark analysis can be found in the 2013 edition of the ICSBEP Handbook with the identifier HEU-MET-FAST-100 [4]. The ORSphere was a five part sphere with two pairs of plates pinned together using HEU pins to create three sections that were then assembled on a vertical assembly machine. Configurations 1 and 2 had respective total masses of HEU (~93.2 wt.% ^{235}U) metal of approximately 53.476 and 52.351 kg. A photograph of an assembled sphere is shown in Fig. 1.

While performing the ORSphere experiments care was taken to accurately document component dimensions (±0.0001 in. for non-spherical parts), masses (±0.01 g), and material data. The experiment was also set up to minimize the amount of structural material in the sphere proximity. A comprehensive evaluation of the experimental uncertainty was performed, including the uncertainty in the reactivity measurement, dimensions, mass, and material data. The small, total uncertainty for both configurations is approximately 70 pcm. Most of the uncertainty in the various experimental parameters had a negligible impact on k_{eff}; the primary uncertainty is derived from the deviation in the curvature of the ellipsoidal parts and the modeling approximations necessary to accurately depict the total volumes of the spheres' components. A summary of the evaluated benchmark uncertainties of the ORSphere experiments is shown in Table I.

The detailed benchmark models include all details of the spheres as well as the brass bolt that held the bottom section of sphere to the lower support structure. Experimentally measured corrections were used to account for the surrounding support structure and a bias was calculated to account for the atmosphere and room return as well as the steel table of the vertical assembly machine. The simple benchmark models are simple, solid spheres of homogenized HEU with only Si, B, and C impurities. The enrichment and material density were averaged to maintain total mass and HEU metal volume. The bias of the simple model simplifications was calculated. Table II contains a summary of the benchmark experiment values and sample calculations using MCNP5-1.60 [5] and ENDF/B-VII.0 neutron cross section data [6]. See Fig. 2 for a depiction of the assembled benchmark model for Case 1, demonstrating the complexity of the sphere itself.

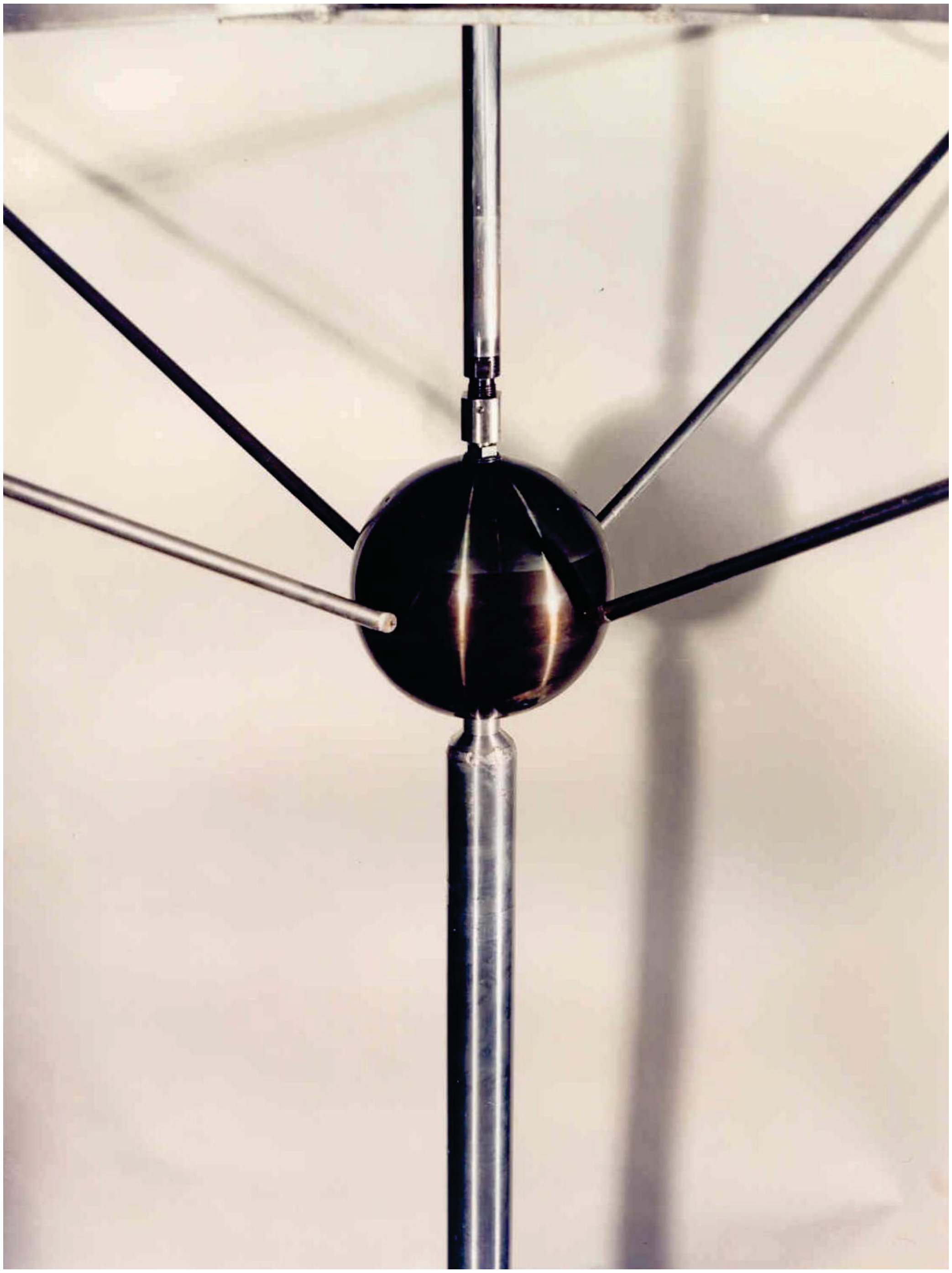

Figure 1. Photograph of the Assembled ORSphere.

Table I. Total Experimental Uncertainty in ORSphere Benchmark.

Parameter	**Perturbation ±1σ**	**Case 1 $\pm\Delta k_{eff}$ (1σ)**	**Case 2 $\pm\Delta k_{eff}$ (1σ)**
Reactivity Measurement[(a)]	2.0 ¢	0.00013	0.00013
Radius	2.54×10^{-4} cm	0.00005	0.00005
Curve of Ellipsoidal Parts	0.12 % (volume)	0.00066	0.00066
Lower Polar Cap/Lower Plate Gap	2.54×10^{-4} cm	0.00004	0.00004
Lower Plate/Center Plate Gap	2.54×10^{-4} cm	0.00007	0.00011
Center Plate/Upper Plate Gap	2.54×10^{-4} cm	0.00009	0.00008
Upper Plate/Upper Plate Cap Gap	2.54×10^{-4} cm	0.00006	0.00005
Tilt Angle	Effect of No Gap ÷ 2√3	-0.00011	NA
Diametral Hole Diameter	2.54×10^{-4} cm	<0.00001	<0.00001
Diametral Rod Diameter	2.54×10^{-4} cm	<0.00001	<0.00001
Diametral Rod Length	2.54×10^{-4} cm	<0.00001	<0.00001
Brass Bolt Diameter	0.033274 ÷ 2√3 cm	<0.00001	<0.00001
Brass Bolt Height	2.54×10^{-4} cm	0.00001	0.00001
Bottom Section Mass	1 g (Case 1) 0.01 g (Case 2)	0.00006	<0.00001
Center Section Mass	0.01 g	<0.00001	<0.00001
Top Section Mass	0.01 g	<0.00001	<0.00001
Diametral Filler Rod Mass	0.014 g	<0.00001	<0.00001
Parts and Voids within Sphere	2.54×10^{-4} cm	<0.00001	<0.00001
Uranium Fraction	0.0005 gU/g Total	0.00003	0.00003
Silicon	20% ÷ √3	0.00001	0.00001
Boron	70% ÷ √3	0.00002	0.00002
Carbon	20% ÷ √3	-0.00003	-0.00003
Other Impurities	70% ÷ (√11 × √3)	-0.00004	-0.00004
^{234}U Content	1%	-0.00004	-0.00004
^{235}U Content	0.0177 wt.%	-0.00009	-0.00009
^{236}U Content	0.0130 wt.%	0.00002	0.00002
Brass Density	0.2 g/cm^3	0.00006	0.00006
Brass Composition	Red vs. Yellow Brass	0.00001	0.00001
Temperature	2 ºC	0.00004	0.00004
Total Experimental Uncertainty		**0.00071**	**0.00070**

(a) Reactivity uncertainty includes reproducibility, reactor period measurement, and delayed neutron parameter uncertainties.

Table II. ORSphere Benchmark Values and Sample Calculations.

Case	Model	Benchmark Experiment			Calculated[(a)]			$\frac{C-E}{E}$ %
		k_{eff}	±	σ	k_{eff}	±	σ	
1	Detailed	1.0026	±	0.0007	1.00385	±	0.00002	0.13
	Simple	1.0031	±	0.0007	1.00441	±	0.00002	0.18
2	Detailed	0.9966	±	0.0007	0.99821	±	0.00002	0.17
	Simple	0.9966	±	0.0007	0.99826	±	0.00002	0.17

(a) Results obtained using 500,000 histories for 2650 cycles, skipping the first 150 cycles using MCNP5-1.60 [5] and ENDF/B-VII.0 neutron cross section libraries [6].

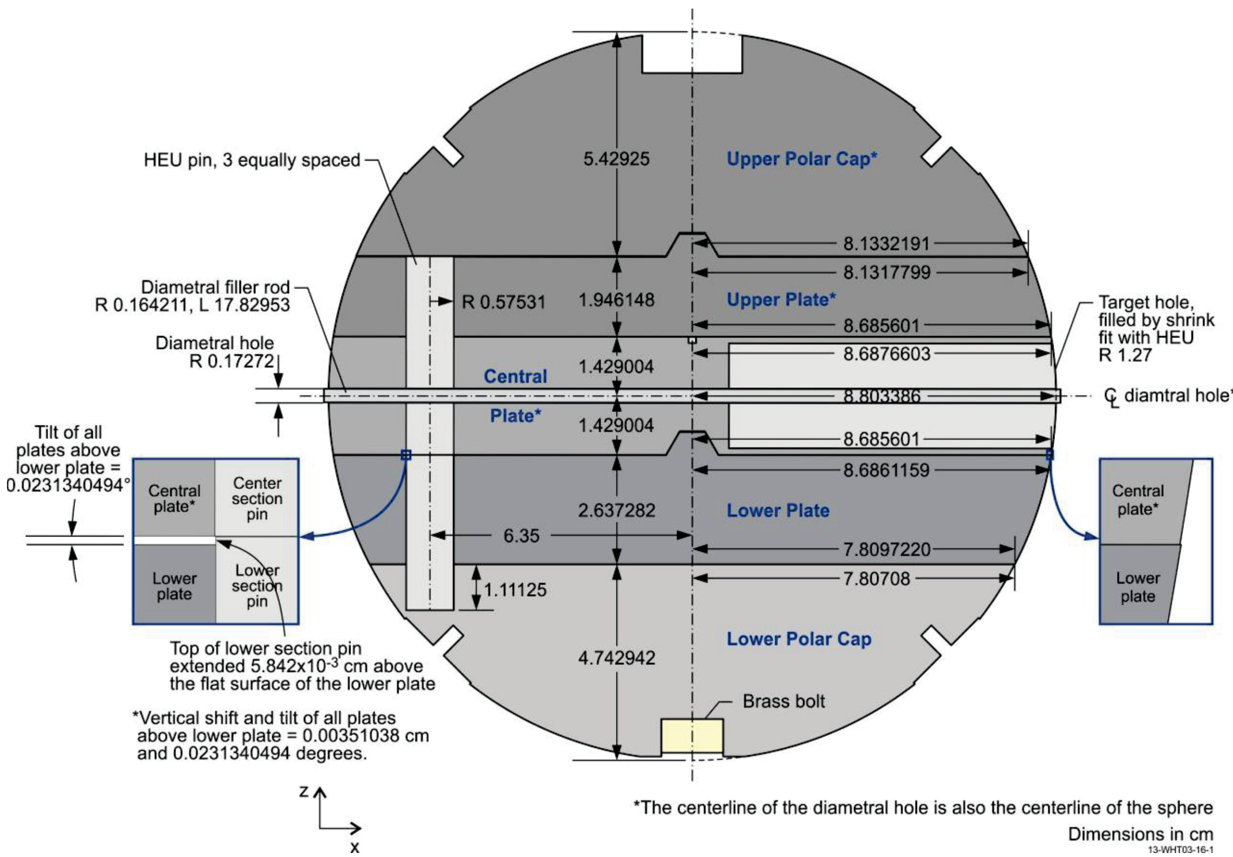

Figure 2. Depiction of Benchmark Model for Fully Assembled ORSphere, Case 1.

2.2 Comparison of Bare HEU Metal Benchmark Experiment Data

A total of 46 unreflected and unmoderated HEU metal experiments (enriched between 90 and 96 wt.% ^{235}U) were included in a comparison study. These experiments include the GODIVA I ("Lady Godiva"), COMET, and GODIVA IV (5 configurations) from Los Alamos National Laboratory (LANL); a sphere and two cylinders from the Russian Federal Nuclear Center – Institute of Technical Physics (RFNC-VNIITF); a sphere from the Russian Federal Nuclear Center – Institute of Experimental Physics (RFNC-VNIIEF); as well as TINKERTOY

(12 configurations), two slabs, 18 cylinders, GROTESQUE, and ORSphere (2 configurations) from ORCEF. Descriptions and benchmark specifications can be found in the ICSBEP Handbook [4].

Eigenvalues were calculated with MCNP5 and ENDF/B-VII.0 using benchmark model specifications provided in respective benchmark reports. The differences between the calculated and benchmark experiment eigenvalues, (C-E)/E %, are shown in Fig. 3; shaded error bars represent 1σ and 3σ uncertainties. Many of the calculated eigenvalues fall below their respective benchmark values with the largest negative difference of -1.18 % for the fifth GODIVA IV configuration. The second ORSphere configuration calculates with a positive difference of 0.18 %. On average (variance weighted mean) the difference between calculated and experimental eigenvalues is -0.22 %, which is dominated by the computational discrepancy with low benchmark uncertainties for the ORCEF cylinder experiments.

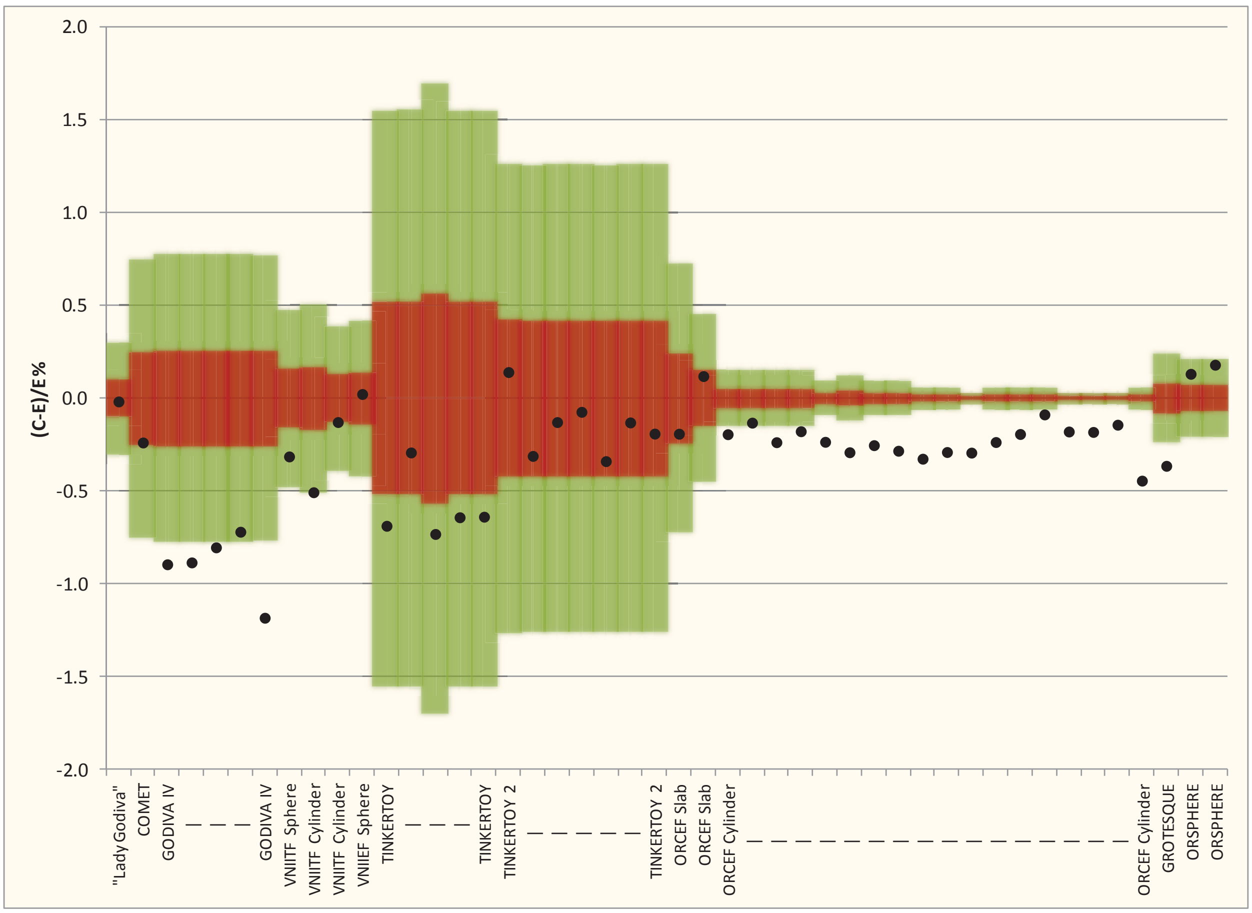

Figure 3. Comparison of the Difference between Calculated and Benchmark Experiment Eigenvalues for Bare HEU Configurations [4]. Calculations were performed with MCNP5 [5] and ENDF/B-VII.0 [6]. Shaded error bars represent 1σ and 3σ.

The dominant sources of experimental uncertainty for the benchmarks with larger uncertainties are generally due to fuel mass, fuel dimensions, or the measured distances between assembly components. Many of the ORCEF experiments were reported with a high degree of precision in their measured masses, dimensions, impurity content, and isotopics [7]. When those sources of uncertainty are significantly reduced in a benchmark experiment, the remaining uncertainty is due to experimental method or measurements (which are typically eclipsed by fuel mass and dimension uncertainties in non-ORCEF experiments), and the physical placement of experiment components that was not as precisely measured as the properties of the components themselves.

Further inspection of the results requires a consolidation of pertinent data. The GODIVA IV benchmark models include significant quantities of structural support materials (steels and aluminum) and the HEU is comprised of an alloy with ~1.5 wt.% molybdenum and can therefore be removed from the comparison. The purpose of the TINKERTOY measurements was to evaluate the impact of spacing within arrays of HEU cylinders and was not intended for use to optimize integral nuclear data. The GROTESQUE experiment was developed to test complex modeling capabilities and also not intended for integral data adjustment. The remaining spheres, cylinders, and slabs can be further consolidated into their respective experimental series due to correlation effects among the individual experiments when multiple experiments were performed. Computing a variance-weighted mean value for the (C-E)/E value of a given set of experiments provides an unreasonably low uncertainty for the ORCEF cylinder experiments, especially when significant variability exists between the experiments within the series. The standard deviation of the average (non-weighted) (C-E)/E value is summed in quadrature with the variance-weighted uncertainty; the standard deviation is used to capture the variability in modeling highly-correlated experiments. The revised comparison chart is shown in Fig. 4.

Inspection of the consolidated comparison of simple bare HEU configurations (Fig. 4) indicates that all calculated results fall within a 3σ band from the benchmark values if the variability in correlated experiments is accounted for in the combined uncertainty. The ENDF/B-VII.0 integral nuclear data is calibrated to provide a (C-E)/E value of ~0.0 % for the Lady Godiva experiment using MCNP5. Not all benchmark experiments should also produce this same result (i.e. (C-E)/E ~0.0 %) as a distribution around some mean value should exist. It is not currently clear why the ORSphere configurations, which were performed to a higher degree of precision, do not calculate within their 1σ uncertainty. Furthermore, the reported mass correction uncertainty for the ORSphere is 60 % smaller than the reported uncertainty for the GODIVA I benchmark [1]; comparison of the ~70 pcm uncertainty in the ORSphere configurations to the ~100 pcm (technically ~90 pcm when recalculated using MCNP5 and ENDF/B-VII.0) indicates that a reevaluation of the effect of the uncertainty in the Lady Godiva benchmark might be necessary.

While the sphere and slab calculations appear, on average, to calculate within reasonable agreement distributed about the benchmark values, the cylinder configurations noticeably calculate low. It is unclear if this occurrence is an anomaly or if there is a fundamental difference in how current modeling capabilities apply towards HEU metal systems of different basic geometries. Even the GODIVA IV, TINKERTOY, and GROTESQUE experiments (Fig. 3) are cylindrical systems that similarly calculate lower than the benchmark experiment eigenvalues. The scatter in the calculation of the eigenvalues for the 18 ORCEF cylinder configurations may also indicate that further investigation be warranted to assess what is driving said effect in these highly correlated experiments. These cylinders are constructed from various discs and annuli components (see Fig. 5 for an example of the smallest (7 in.) and largest (15 in.) diameter cylinders, experiments 14 and 18, respectively); many of the ORALLOY metal parts were utilized in more than one assembled configuration.

Another comparative study was performed repeating the MCNP5 eigenvalue calculations using various contemporary nuclear data libraries (Fig. 6). There is significant differences between the results obtained using the different libraries. Even within results from a given library there is still some variation when comparing trends between libraries. The variation in calculated results using the various nuclear data libraries is greater than the variation in calculations for the ORCEF cylinders within a given nuclear data set. The library that calculates most in alignment with the benchmark values is CENDL-3.1, followed by JENDL-3.3 and ENDF/B-VII.0. Therefore even when using the same available integral nuclear data, the selection of the nuclear data library can have quite an impact on calculated eigenvalues for given critical configurations.

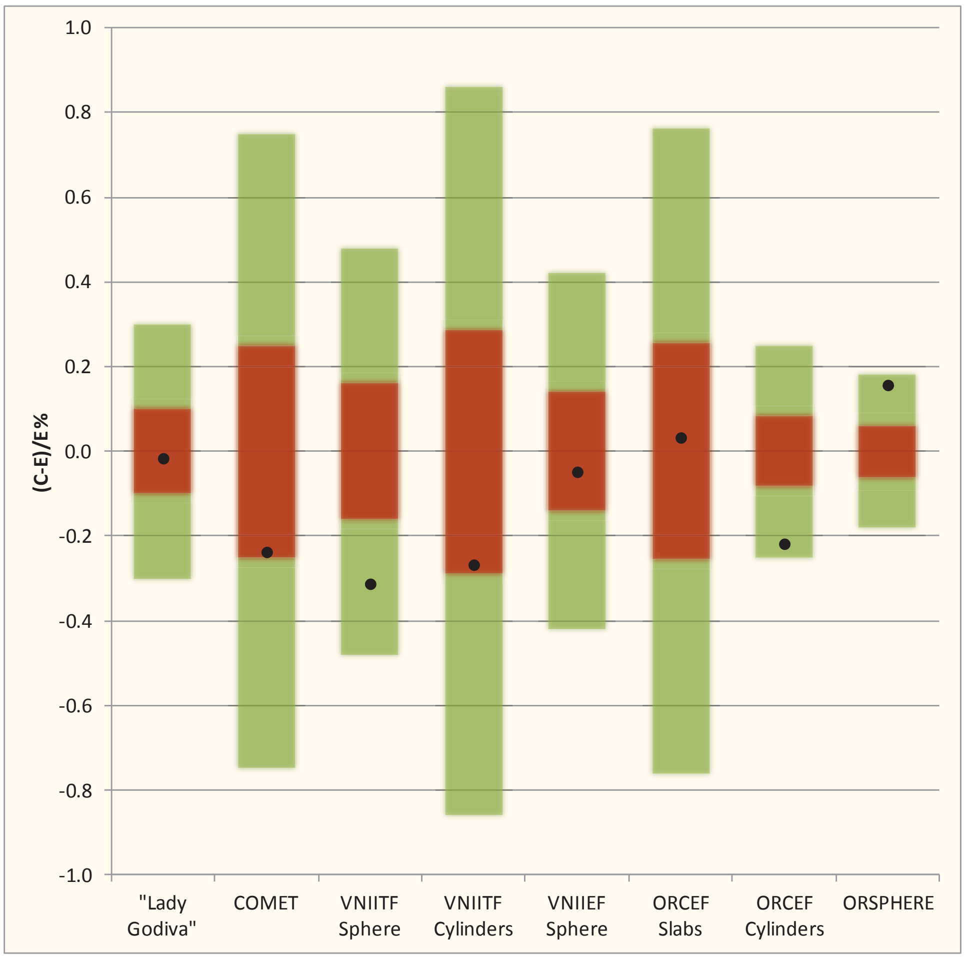

Figure 4. Consolidated Comparison of the Difference between Calculated and Benchmark Experiment Eigenvalues for Select Bare HEU Experimental Series. Calculations were performed with MCNP5 [5] and ENDF/B-VII.0 [6]. Shaded error bars represent 1σ and 3σ.

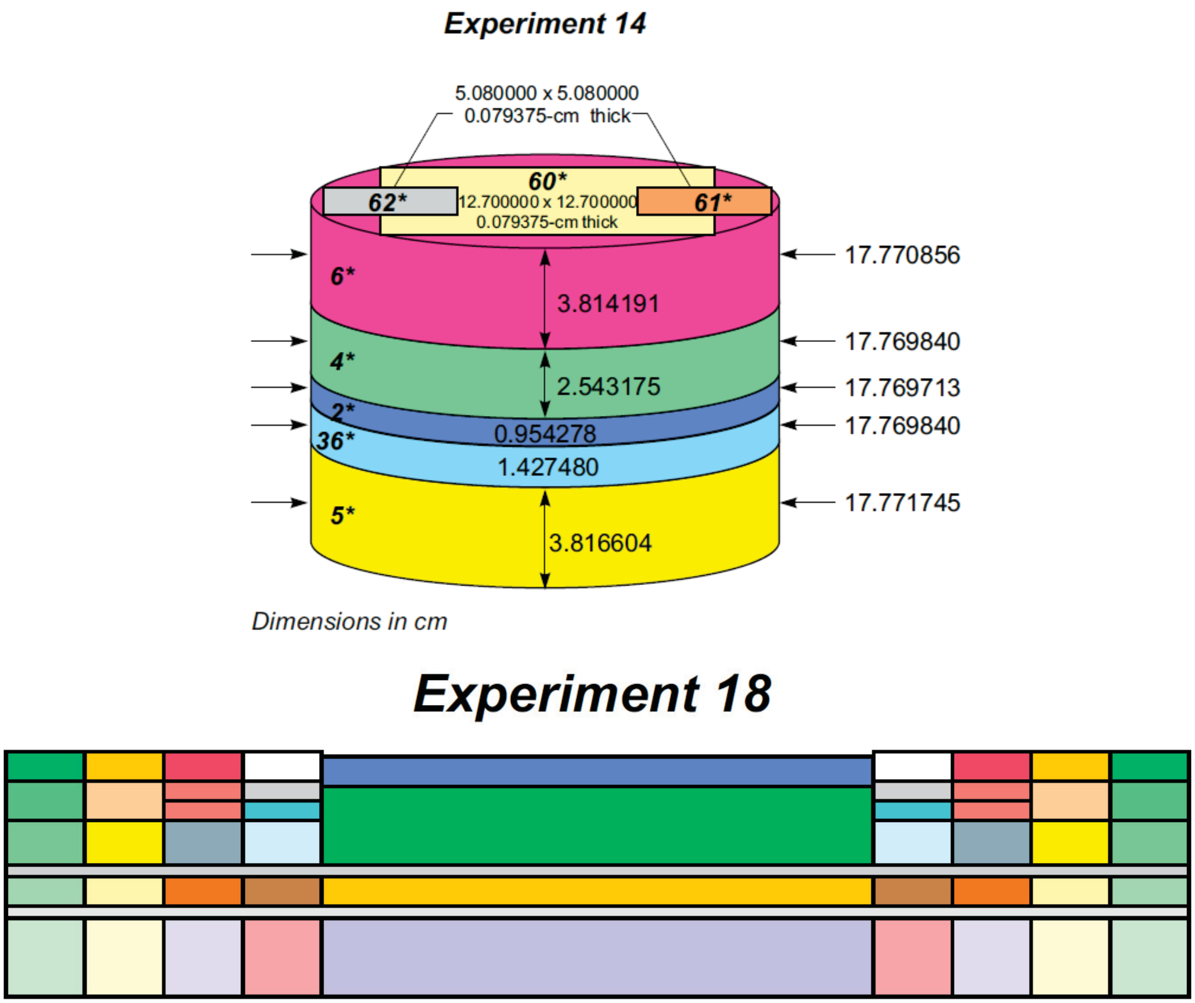

Figure 5. Example Benchmark Configurations for ORCEF Cylinder Experiments.

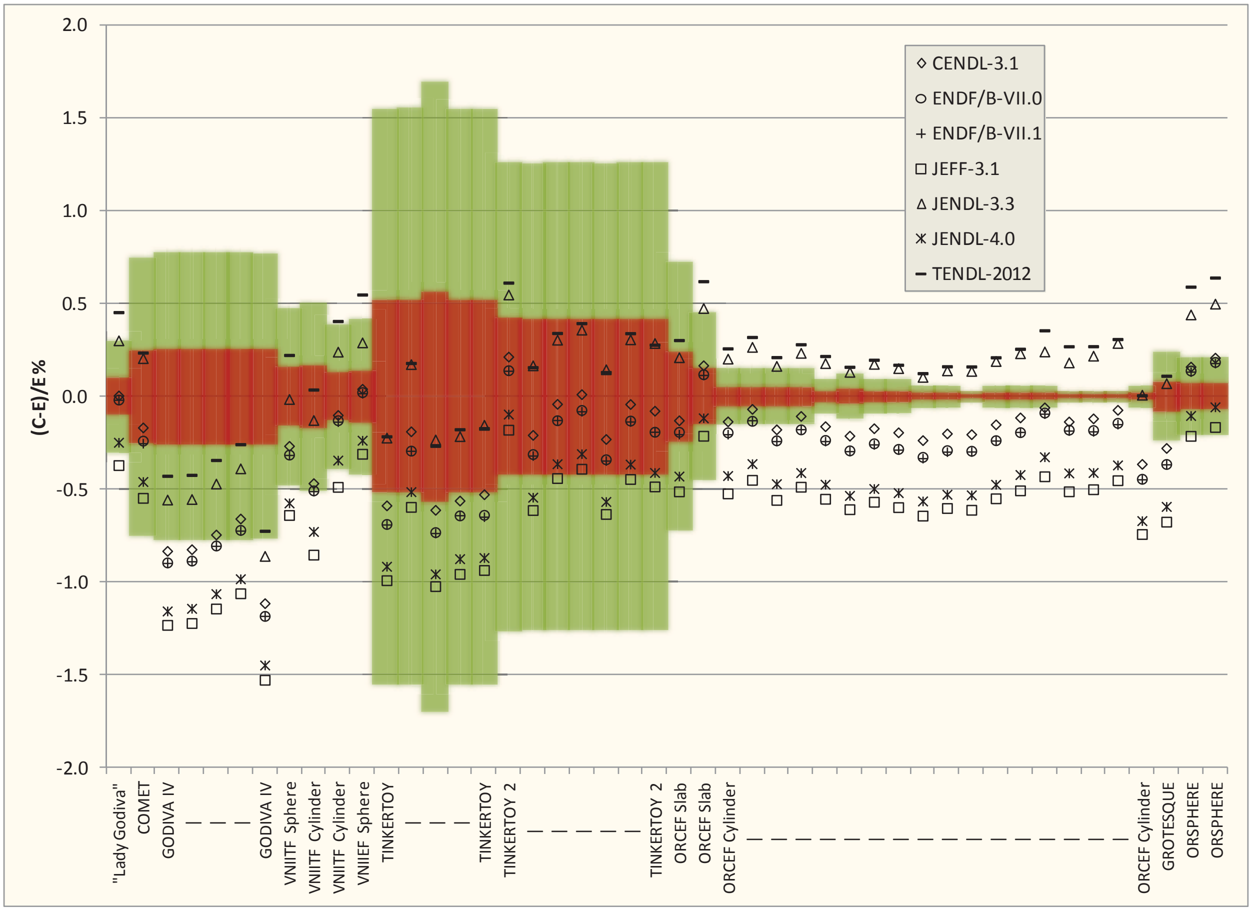

Figure 6. Comparison of the Difference between Calculated and Benchmark Experiment Eigenvalues for Bare HEU Configurations [4]. Calculations were performed with MCNP5 [5] and various nuclear data libraries. Shaded error bars represent 1σ and 3σ.

3 CONCLUSIONS

Two high-quality ORSphere near-critical configurations have been evaluated as acceptable benchmark experiments and made available in the ICSBEP Handbook. The uncertainty in these highly-correlated experiments is ~70 pcm and calculations with MCNP5 and ENDF/B-VII.0 are within 0.2% (3σ) of the benchmark eigenvalues. Even though the ORSphere configurations were performed to a higher degree of precision, they do not calculate within their 1σ uncertainty.

A comparison of the percent difference between computed and benchmark eigenvalues was performed for 46 unreflected and unmoderated HEU metal configurations. Calculated eigenvalues for basic spherical, slab, or cylindrical geometries are within 3σ of the benchmark values, when the uncertainties are increased to account for the variation in modeling highly-correlated experiments within a series.

While spherical and slab configurations appear to calculate, on average, within reasonable agreement of the benchmark values, there is a noticeable bias in the cylindrical configurations in that calculations are slightly low. Even the more complex bare HEU systems that include cylindrical geometries calculate below their expected benchmark eigenvalues.

There is significant scatter in the calculations for the highly-correlated ORCEF cylinder experiments, which are constructed from close-fitting HEU discs and annuli; further investigation may be necessary to address this issue.

There is a possibility that the GODIVA I benchmark, upon which modern ENDF/B-VII HEU data is tailored to fit, may need to be revised to properly address the impact of the measured uncertainties on the benchmark eigenvalue.

Selection of a nuclear data library can have a larger impact on calculated eigenvalue results than the variation found within calculations of a given experimental series, such as the ORCEF cylinders, using a single nuclear data set.

The variability and discrepancies in our computational analysis of the various bare HEU configurations has an impact on how we address the application of advanced modeling and simulation methods in nuclear criticality safety activities.

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