Benchmark Model Temperatures Incorporated into DICE

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INTRODUCTION

SCALE 6.2 introduced a new Doppler broadening treatment in continuous-energy (CE) KENO [1,2]. The validation of this capability has been attempted to a small degree, but it is hampered by the limited availability of critical benchmark experiments performed at nonambient temperatures [1]. One known set of experiments from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [3], which was previously used for validation [4], has been shown to have deficiencies in the evaluation that make their use problematic. The identification of other potential benchmarks has been hampered because the benchmark models have not been available in the Database of the ICSBEP (DICE). This paper documents work performed to extract the benchmark model temperatures from all ICSBEP evaluations and incorporate them into DICE. A summary of available data is also presented, along with results of two experiments which could be useful in temperature-dependent validation. Currently, the benchmark model temperature can be used as a search criterion in the web-based DICE interface [5] and it is also included on the 2017 DVD release.

BENCHMARK MODEL TEMPERATURES

The benchmark model temperatures have been collected for each case in the ICSBEP Handbook [3]. The temperatures were taken from Section 3.4 in the handbook and are included in DICE. Many evaluations do not provide an unambiguous temperature, and others use cross sections that have not been processed to the temperature at which the experiment was conducted. In the first case, the description provided in Section 3.4 of the handbook is typically a statement that the experiments were conducted at room temperature, without any specification as to what that temperature is. “Room temperature” is assumed to be 293K for this release. In other cases, the temperature at which the cross sections were processed, typically 300K, is specified instead of the temperature of the experiment. The cross section temperature is provided for these cases.

Temperature is now an available search parameter in the “Themes” tree of the “Critical/Subcritical” tab within DICE. Model temperatures are tabulated in Kelvin, and users can search for a specific temperature with a specified tolerance, or users can search for cases above or below a desired temperature. This capability greatly facilitates the identification of potentially applicable benchmark experiments at specific temperatures. The number of cases not at ambient temperature is discussed in the next paragraph. Temperature data can also be displayed in the subcase panel of the search results. Some evaluations provide unique temperatures for each experiment, so inclusion with the specific case details is appropriate.

A total of 143 cases in 21 evaluations contain benchmark temperatures greater than or above 301K. These evaluations and the number of cases in each evaluation are provided in Table I. Only 43 cases in 11 evaluations have benchmark model temperatures of 310K or higher. These cases are also included in Table I. Many of these cases come from the LEU-COMP-THERM-046 evaluations, which is known to have errors in the temperature-dependent thermal expansion factors. These evaluation errors should be fixed so that analysts can use the benchmark as provided in the ICSBEP Handbook without further analysis or justification. Some evaluations contain multiple cases at elevated but effectively identical temperatures. The limited number of available benchmarks, the variability of system characteristics, and the small temperature range covered all indicate that temperature-dependent validation of computational methods for criticality safety will continue to be problematic in the near future.

PU-SOL-THERM-038 AND -039

The PU-SOL-THERM-038 (PST-038) and -039 (PST-039) experiments were performed at the Institut de Radioprotection et de Sûreté Nucléaire (IRSN) critical experiment facility at Valduc on the Apparatus B machine [3]. The PST-038 evaluations pertain to experiments performed with plutonium solutions at room temperature, and the PST-039 evaluation contains similar experiments at elevated temperatures. The experiments were identified through a review of available cases at elevated temperature, and they provide an opportunity to detect a temperature-dependent bias in a computational method. The benchmark models for PST-038 are at 295K, and for PST-039, they range between 301 and 313K. Five of the eight cases in PST-039 are at 313K, so these experiments provide a very limited range of temperatures

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for evaluation. Both the 252-group (multigroup [MG]) and CE libraries based on ENDF/B-VII.1 cross sections will be tested with these experiments. The Doppler broadening methods used for the CE data are described in detail in [1]; the MG data is interpolated in $\sqrt{T}$.

The calculated/experimental (C/E) values for all five cases of PST-038 are above 1 with both the MG and CE libraries. The CE results show slightly more variation, with C/E values ranging from 1.00088 to 1.00301. The MG results vary from 1.00143 to 1.00250. The Monte Carlo uncertainty in all cases is approximately 0.01% Δk, and the uncertainty in the evaluation k_{eff} is approximately 0.15% Δk. Therefore, the results can all be considered statistically indistinguishable from each other at the 1-σ level for both libraries. The C/E values are shown with blue markers in Figure 1. The closed diamond markers are the CE results, and the open circles are the MG C/E values. Cases 1 and 2 both yield a C/E of 1.00250 for the MG library, so only 4 open circle markers are evident in Figure 1. The average C/E value is 1.00192 for the CE library and 1.00205 for the MG library, demonstrating excellent agreement between the two libraries for these cases.

The range of C/E values for the 8 cases in PST-039 is similar for both libraries. The range for the CE library is from 0.99754 to 1.00429, and for the MG library the range is from 0.99772 to 1.00397. The Monte Carlo and experimental uncertainties are nearly identical between the PST-038 and -039. Both libraries indicate that Case 8 is an outlier, with results approximately 0.33% Δk lower than the next lowest C/E value. Case 8 is also the only C/E value less than unity in either evaluation. The C/E values for PST-039 are shown with red markers in Figure 1. As with the PST-038 results, the closed diamond markers are the CE results, and the open circles are the MG results. The average of the C/E values for the CE library is 1.00187, and for the MG library, the average is 1.00196. Again, the two libraries demonstrate excellent agreement for the average C/E value.

Figure 1 shows the results of PST-038 and -039 as a function of temperature to provide potential indications of a temperature-dependent bias in the results. There is no clear bias in the result, though as mentioned earlier, there is a very small range of temperatures examined with these experiments. Both MG and CE results are similar at all temperatures and for all cases, including the outlier case PST-039-008. The exclusion of the outlier does not indicate a trend. The only conclusion that can be readily drawn from these results is that more study is needed; proving a negative, in this case that there is not a temperature-dependent bias, is always difficult. A number of other plutonium solution experiments are available above 300K, but only PST-039 contains cases above 310K. It is doubtful, therefore, that the additional cases available in the ICSBEP Handbook will provide any indications of a temperature-dependent bias. The range of available temperatures is also not wide enough to provide clear evidence that there is no such bias present within the MG or CE libraries with SCALE 6.2.

CONCLUSIONS

The primary purpose of this paper is to make the criticality safety community aware that benchmark model temperature data are now available in DICE. The benchmark model temperature can be displayed with other search results, or it can be used as a search criterion. A limited number of experiments are available in the ICSBEP Handbook at non-room temperature. As demonstrated through the use of the PST-038 and -039 evaluations, it is unlikely that definitive conclusions can be reached regarding temperature-dependent biases from the available data in the handbook. The benchmarks currently available in the ICSBEP Handbook should be expanded to cover a wider range of temperatures, especially for LEU fuel rod array systems.

ACKNOWLEDGMENT

The preparation and presentation of this paper was supported by the US Department of Energy Nuclear Criticality Safety Program (NCSP). The NCSP also funded Ms. Clifton's summer appointment at ORNL through the HERE Program, which was administered by Oak Ridge Associated Universities.

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TABLE I. Experiments in the ICSBEP Handbook with a Benchmark Model Temperature of 301K or Greater

Evaluation ID	Title	Total Cases	Cases ≥ 301K	Cases ≥ 310K
PU-MET-FAST-044	Plutonium (5.1 wt.% ^{240}Pu) Metal Sphere with Be, Graphite, Al, Fe, and Mo Tampers and Polyethylene Reflectors	5	5	0
PU-SOL-THERM-010	Water-Reflected 9-, 10-, 11-, and 12-Inch Diameter Cylinders of Plutonium Nitrate Solutions	35	3	0
PU-SOL-THERM-019	Plutonium Sulfate Solutions Reflected by Beryllium Oxide and Graphite: Prosperine Reactor – Saclay	11	11	0
PU-SOL-THERM-023	Plutonium (33.89% and 4.23% ^{240}Pu) Nitrate Solutions in Two Water-Reflected Cylindric Concentric Tanks	34	34	0
PU-SOL-THERM-039	Plutonium Temperature Effect Program – Low Concentration (20, 15 or 14.3 g/L) Plutonium Nitrate Solutions at Temperatures Varying from 28°C to 40°C	8	7	5
HEU-SOL-INTER-002*	Mixture of Uranium (93%) Hexafluoride and Hydrofluoric Acid (Low H/U Ratio) in a Hot-Water-Reflected Spherical Tank	1	1	1
HEU-SOL-THERM-034	Water-Moderated and -Reflected Slabs of Uranium Oxyfluoride	5	5	0
HEU-SOL-THERM-039	Mixture of Uranium (93%) Hexafluoride and Hydrofluoric Acid (Low H/U Ratio) in a Hot-Water-Reflected Spherical Tank	5	5	5
HEU-SOL-THERM-046	Highly Enriched Uranium (89.84% ^{235}U) Sulfate Solutions Reflected by Beryllium Oxide and Graphite: Prosperine Reactor – Saclay	13	13	0
HEU-COMP-THERM-016	IGR Reactor – Uranium-Graphite Blocks Reflected by Graphite	6	3	3
IEU-MET-FAST-014	ZPR-9 Assemblies 2 and 3: Cylindrical Assemblies of U Metal and Tungsten with Aluminum Reflectors	2	1	1
IEU-COMP-THERM-002	Water-Moderated U(17)O$_2$ Annular Fuel Rods Without Absorber and With Gadolinium or Cadmium Absorbers in 6.8 cm Pitch Hexagonal Lattices at Different Temperatures	6	3	3
IEU-COMP-THERM-009	Power Burst Facility: U(18)O$_2$-CaO-ZrO$_2$ Fuel Rods in Water	2	2	0
LEU-COMP-THERM-015	The VVER Experiments: Regular and Perturbed Hexagonal Lattices of Low-Enriched UO$_2$ Fuel Rods in Light Water	165	2	2
LEU-COMP-THERM-026	Water-Moderated U(4.92)O$_2$ Fuel Rods in 1.29, 1.09, and 1.01 cm Pitch Hexagonal Lattices at Different Temperatures	6	3	3
LEU-COMP-THERM-046	Critical Loading Configurations of the IPEN/MB-01 Reactor Considering Temperature Variation from 14°C to 85°C	22	19	17
U233-SOL-THERM-012	Water-Reflected Spherical Vessels Partially Filled or Filled with ^{233}UO$_2$(NO$_3$)$_2$ Solution	8	1	0
U233-SOL-THERM-013	Unreflected Spherical Vessels Partially Filled or Filled with ^{233}UO$_2$(NO$_3$)$_2$ Solution	21	6	0
U233-SOL-THERM-014	Lucite-Moderated and Unmoderated, Reflected and Non-reflected Arrays of Bottles Containing Uranyl Nitrate (98.2 wt. % ^{233}U) Solution	18	16	0
MIX-COMP-INTER-005	Undermoderated MOX (11 wt% PuO$_2$) Lattice in the EOLE Reactor	1	1	1
MIX-MISC-FAST-002	BFS-49 Assemblies: Critical Experiments with Heterogeneous Compositions of Plutonium, Depleted-Uranium Dioxide, and Polyethylene	2	2	2

*HSI-002 is a cross reference. The full experiment description is included in HST-039.

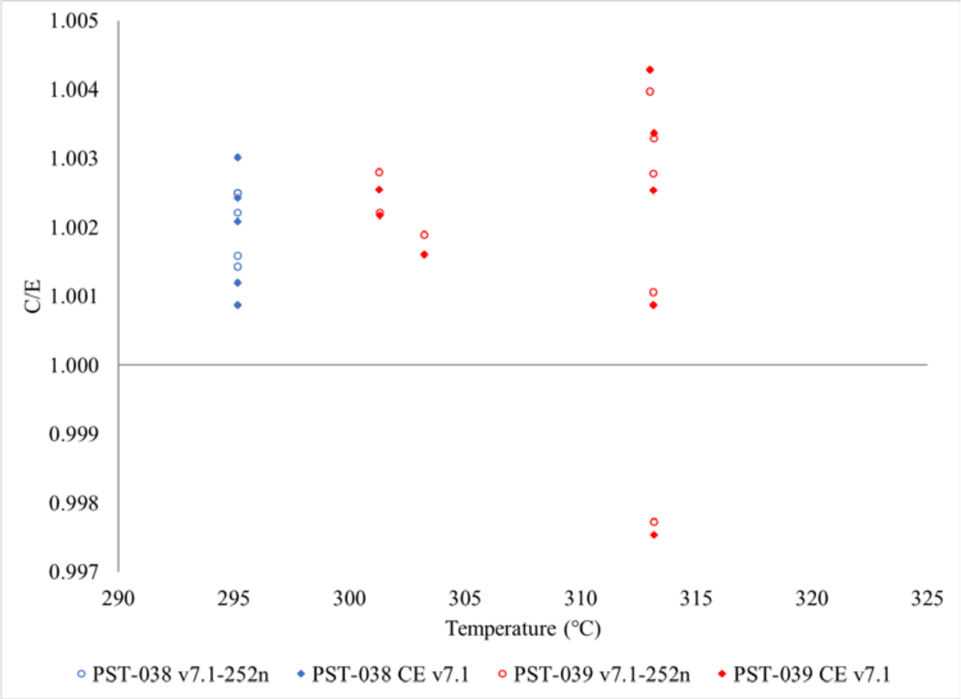

Fig. 1. Results for PST-038 and -039 evaluations.