## S/U Comparison Study with a Focus on USLs

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### INTRODUCTION

Under a DOE Nuclear Criticality Safety Program (NCSP) task involving Analytical Methods, three Laboratories collaborated in a comparison of results obtained from Sensitivity/Uncertainty (S/U) packages relevant to validation of transport codes. The task involves Institut de Radioprotection et de Sûreté Nucléaire (IRSN), Los Alamos National Laboratory (LANL), and Oak Ridge National Laboratory (ORNL) comparing results of MORET 5/MACSENS V3.0, MCNP6.2/Whisper-1.1, and SCALE 6.2.3/TSUNAMI/USLSTATS respectively. All Monte Carlo transport code results utilize ENDF/B-VII.1.

Four cases from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP Handbook) [1] were selected as application models: HEU-MET-FAST-013-001, HEU-SOL-THERM-001-008, PU-MET-FAST-022-001, and PU-SOL-THERM-001-001. Ultimately, comparison is made between Upper Subcritical Limits (USLs) obtained using each code package for each application case. Since differences exist in whether packages take into account margin of subcriticality (MOS), the USL may be computed using bias and bias uncertainty, also known as the calculational margin (CM) in ANSI/ANS-8.24 [2]. Application of portions of MOS to the USL for nuclear data uncertainty of and potential code margin is referred to as USL* herein. In either case, additional MOS is considered for actual application cases.

$$USL = 1.0 + bias - bias\ uncertainty \quad (1)$$

$$USL^* = 1.0 + bias - bias\ uncertainty - MOS_{ND} - MOS_{code} \quad (2)$$

### Case Descriptions and k-effective Results

The set of benchmark problems (applications) were selected by comparing the libraries of existing benchmark models each laboratory uses for validation of their own radiation transport codes and nuclear data and selecting benchmarks in common. Four cases were selected to include highly enriched uranium (HEU) and plutonium systems, each with a fast and a thermal system. Selecting benchmarks to use as cases allows for the additional comparison of the actual benchmark bias and bias uncertainty with the results obtained using each code package. Application case descriptions and results follow.

*HEU-MET-FAST-013-001*

HMF-013-001 is a critical assembly that consists of a sphere of HEU metal reflected by steel.

| | |
|---|---|
| Experimental k-effective: | 0.9990 ± 0.0015 |
| MORET k-effective: | 0.99655 ± 0.00010 |
| MCNP6.2 k-effective: | 0.99752 ± 0.00009 |
| SCALE 6.2.3 k-effective: | 0.99730 ± 0.00010 |

*HEU-SOL-THERM-001-008*

HST-001-008 is a critical assembly that consists of a minimally reflected cylinder of HEU solution of uranyl nitrate with a concentration of 145.68 g U/liter and acid molarity of 0.294 moles/liter.

| | |
|---|---|
| Experimental k-effective: | 0.9998 ± 0.0038 |
| MORET k-effective: | 0.99779 ± 0.00010 |
| MCNP6.2 k-effective: | 0.99823 ± 0.00015 |
| SCALE 6.2.3 k-effective: | 0.99590 ± 0.00010 |

*PU-MET-FAST-022-001*

PMF-022-002 is a critical assembly that consists of a bare plutonium metal sphere with a small central cavity.

| | |
|---|---|
| Experimental k-effective: | 1.0000 ± 0.0023 |
| MORET k-effective: | 0.99794 ± 0.00010 |
| MCNP6.2 k-effective: | 0.99830 ± 0.00008 |
| SCALE 6.2.3 k-effective: | 0.99860 ± 0.00010 |

*PU-SOL-THERM-001-001*

PST-001-001 is a critical assembly that consists of a spherical tank of plutonium nitrate solution with a concentration of 73 g Pu/liter and acid molarity of 0.2 N nitrate reflected by water.

| | |
|---|---|
| Experimental k-effective: | 1.0000 ± 0.0050 |
| MORET k-effective: | 1.00492 ± 0.00010 |
| MCNP6.2 k-effective: | 1.00578 ± 0.00013 |
| SCALE 6.2.3 k-effective: | 1.00390 ± 0.00010 |

### S/U METHODS

Various methods employed for this study are described below. Not all methods calculate portions of the margin of subcriticality (MOS); therefore, MOS is excluded in some USL comparisons in this study. The bias and bias uncertainty are presented at the 95% confidence level. The similarity coefficient, $c_k$, quantifies how neutronically similar an application is compared with each benchmark.

**IRSN**

The Monte Carlo MORET 5.D.1 [10] radiation transport code was used with the ENDF-B/VII.1 continuous energy library for calculation of k-effective and collection of sensitivity profiles [11] in the SCALE 44-group energy structure. The MACSENS V3.0 tool, based on the General Linear Least Square Method (GLLSM), was used for calculation of the bias and its associated uncertainty using MORET 5 sensitivity profiles and the SCALE 6.2 44-group covariance data based largely on ENDF/B-VII.0. The IRSN calculation models are from the MORET 5 validation database [13], which contains 1566 ICSBEP benchmarks. Selection of similar benchmarks is based on expert judgement for the results in this study, considering mainly the different nuclides involved and the energy spectrum of the studied cases. MACSENS gives the bias and the associated uncertainties due to nuclear data. No additional margins of safety are included.

**LANL**

MCNP6.2 Monte Carlo code [3] was used for calculation of k-effective and collection of sensitivity profiles in 44 energy groups for use with the BLO 44-group covariance library, based largely on the Low-fidelity Covariance Project [4]. Whisper-1.1 contains a benchmark library with over 1100 benchmarks. Benchmarks in the Whisper library that are found to be most neutronically similar for each application case, using correlation coefficients, are used for calculation of the bias and bias uncertainty [5]. Whisper has a built-in user option that allows the user to specify whether to reject statistical benchmark outliers from the library using GLLS. Rejection of outliers is not employed for the results presented in this paper. Whisper uses extreme value theory (EVT) to calculate combined bias and bias uncertainty, CM, at a specified confidence level. As mentioned above, a 95% confidence level is chosen for consistency in comparing results in this study, in which case Whisper calculation encompasses the worst-case bias and bias uncertainty at a 95% confidence level. Whisper also uses GLLS to estimate MOS for nuclear data uncertainty. Further results of USLs for the cases studied can be found in [6].

**ORNL**

Comprehensive case results of USLs studied for this work are presented in [7]. The Tools for Sensitivity Uncertainty Analysis Methodology Implementation (TSUNAMI) from the SCALE 6.2.3 code suite [8] were utilized for the ORNL portion of this task. The calculational models are from the ORNL Verified, Archived Library of Inputs and Data (VALID) [9]. The VALID library includes sensitivity data files (sdfs) generated using the TSUNAMI-3D sequence. For each application, TSUNAMI-IP was used to compare the sdfs between applications and available benchmark experiments and calculate the correlation coefficient, $c_k$, which indicates the degree of similarity between the systems. TSUNAMI-IP was also used to generate inputs for the Upper Subcritical Limit Statistical Software (USLSTATS) trending analysis in which the $c_k$ values are used as a trending parameter to determine the bias and bias uncertainty, which are then used to determine the USL. No additional margins of safety are included. Typically, $c_k$ values greater than 0.9 are accepted as indicative of similar systems. For the work presented here, $c_k$ thresholds of 0.8, 0.9, and 0.95 are used. The SCALE 252-group covariance library, based largely on ENDF/B-VII.1, was used for covariance data.

**S/U METHOD RESULTS**

Results are presented below for the four application cases. An advantage of using benchmark experiments as application cases is the ability to calculate the bias in the case using the benchmark k-effective result and the calculated k-effective result, referred to herein as $B_{bmk}$. The bias and bias uncertainty calculated using a set of benchmarks which are neutronically similar to each application case are referred to as the statistical bias ($B_{statistical}$) and statistical uncertainty ($\sigma_{statistical}$), respectively.

$$B_{bmk} = \text{calculated } k_{eff} - \text{benchmark } k_{eff} \quad (3)$$

Results for HMF-013-001 are shown in Table I. The most conservative statistical bias is found with the ORNL method. The IRSN and ORNL USLs are nearly identical at 0.9835 and 0.9828, respectively. MOS has not yet been applied but would be considered for actual application cases. The LANL USL takes into account an additional 0.00100 MOS for nuclear data and 0.00500 MOS for code resulting in a USL of 0.9858, higher than IRSN and ORNL due to the lower bias uncertainty using the LANL method. Without any MOS, the LANL USL would be 0.9917.

The ORNL results shown in Table I are for minimum $c_k$ value of 0.9 without the dcov option and 40 benchmarks were chosen. The LANL results presented include 75 benchmarks selected with $c_k$ ranging from 0.999 to 0.972. There were 12 benchmarks selected in common between with LANL and ORNL. It is interesting that an additional 14 of the 40 benchmarks selected by ORNL exist in the LANL collection, but were not selected by LANL. The IRSN method chose 303 benchmarks, 9 in common with LANL and 3 in common with ORNL. The calculation bias estimated by the IRSN MACSENS tool (-0.00358) is consistent with the actual bias (-0.00245) regarding the benchmark uncertainty (0.00150).

TABLE I. Experimental and statistical bias and bias uncertainty for HMF-013-001

| | $B_{bmk}$ | $B_{statistical}$ | $\sigma_{bmk}$ | $\sigma_{statistical}$ | USL |
|---|---|---|---|---|---|
| IRSN | -0.00245 | -0.00358 | 0.00150 | 0.01294 | 0.9835[1] |
| LANL | -0.00148 | -0.00571 | 0.00150 | 0.00253 | 0.9858[2] |
| ORNL | -0.00170 | -0.00780 | 0.00150 | 0.00940 | 0.9828[1] |

[1]$USL=1+B_{statistical}-\sigma_{statistical}$

[2]$USL^{*}=1+B_{statistical}-\sigma_{statistical}-MOS_{ND}-MOS_{code}$

Results for HST-001-008 are shown in Table II. In all cases, the statistical bias and bias uncertainty used for validation conservatively encompass the actual bias and bias uncertainty. The most conservative statistical bias is found with the LANL EVT method. The IRSN and ORNL USLs are quite similar at 0.9866 and 0.9846, respectively; MOS has not yet been applied but would be considered for actual application cases. The LANL USL takes into account an additional 0.00112 MOS for nuclear data and 0.00500 MOS for code resulting in a USL of 0.9688. Without application of MOS the LANL USL would be 0.9749, lower than IRSN and ORNL due to the statistical bias calculated using the EVT method.

The ORNL results shown in Table II are for a minimum $c_k$ value of 0.9 without the dcov option and 46 benchmarks were chosen from the benchmark library. The LANL results presented include 51 benchmarks selected with $c_k$ ranging from 1.0 to 0.972. Of the 46 benchmarks selected by ORNL 8 were also chosen by LANL. The IRSN method chose 100 benchmarks, 9 of which were chosen by all, and 8 additional chosen by LANL.

TABLE II. Experimental and statistical bias and bias uncertainty for HST-001-008

| | $B_{bmk}$ | $B_{statistical}$ | $\sigma_{bmk}$ | $\sigma_{statistical}$ | USL |
|---|---|---|---|---|---|
| IRSN | -0.00201 | -0.00631 | 0.00380 | 0.00708 | 0.9866[1] |
| LANL | -0.00157 | -0.01462 | 0.00380 | 0.01048 | 0.9688[2] |
| ORNL | -0.00390 | -0.00500 | 0.00380 | 0.01040 | 0.9846[1] |

[1]$USL=1+B_{statistical}-\sigma_{statistical}$

[2]$USL^{*}=1+B_{statistical}-\sigma_{statistical}-MOS_{ND}-MOS_{code}$

Results for PMF-022-001 are shown in Table III. In all cases, the statistical uncertainty used for validation conservatively encompasses the actual bias uncertainty. The most conservative statistical bias is found with the LANL EVT method. The ORNL method results in a slightly positive bias, which is set to zero for the calculation of the USL. IRSN and ORNL USLs are quite similar at 0.9925 and 0.9916, respectively, and MOS has not yet been applied to the resultant USL but would be considered for actual application cases. The LANL USL takes into account portions of additional MOS, 0.00116 for nuclear data and 0.00500 for code resulting in a USL of 0.9816. Without application of MOS, the LANL USL would be 0.9878, lower than IRSN and ORNL due to the statistical bias value calculated using the EVT method.

The ORNL results shown in Table III are for a minimum $c_k$ value of 0.9 without the dcov option and 4 benchmarks were chosen from the benchmark library. When those same benchmarks are used from the Whisper library to calculate the bias and bias uncertainty with Whisper, identical results are obtained. This demonstrates the effect of using the same benchmarks with different methods for this PMF case. The LANL results presented include 51 benchmarks selected with $c_k$ ranging from 0.999 to 0.956. Of the 4 benchmarks chosen by ORNL, there were 3 in common with LANL of which 2 were also selected by IRSN. The IRSN method chose 7 benchmarks; all were in common with the LANL selection and 2 with the ORNL selection.

TABLE III. Experimental and statistical bias and bias uncertainty for PMF-022-001

| | $B_{bmk}$ | $B_{statistical}$ | $\sigma_{bmk}$ | $\sigma_{statistical}$ | USL |
|---|---|---|---|---|---|
| IRSN | -0.00206 | -0.00013 | 0.00210 | 0.00740 | 0.9925[1] |
| LANL | -0.00170 | -0.00857 | 0.00210 | 0.00253 | 0.9816[2] |
| ORNL | -0.00140 | +0.00070[3] | 0.00210 | 0.00840 | 0.9916[3] |

[1]$USL=1+B_{statistical}-\sigma_{statistical}$

[2]$USL^{*}=1+B_{statistical}-\sigma_{statistical}-MOS_{ND}-MOS_{code}$

[3]$B_{statistical} > 1 \rightarrow 0$, $USL=1-\sigma_{statistical}$

Results for PST-001-001 are shown in Table IV. In all cases, the bias is positive with MORET5.D.1, MCNP6.2, and SCALE6.2.3 calculating k-effective results higher than the experimental k-effective of 1.0000 using ENDF/B-VII.1. The positive statistical bias calculated by the IRSN and ORNL methods is not used for calculation of the USL. In all cases, the statistical uncertainty used for validation conservatively encompasses the actual bias uncertainty. The most conservative statistical bias is found with the LANL EVT method. IRSN and ORNL USLs are 0.9913 and 0.9892, respectively, and MOS has not yet been applied to the resultant USL but would be considered for actual application cases. The LANL USL takes into account portions of additional MOS, 0.00078 for nuclear data and 0.00500 for code, resulting in a USL of 0.9800. Without application of MOS the LANL USL would be 0.9857, lower than IRSN and ORNL due to the statistical bias value calculated using the EVT method.

The ORNL results shown in Table IV are for a minimum $c_k$ value of 0.9 without the dcov option and 85 benchmarks were chosen from the benchmark library. The LANL results shown in Table IV have $c_k$ ranging from 0.999 to 0.996 and 38 benchmarks were chosen. Of the 85 benchmarks chosen by ORNL, 20 were also chosen by LANL method, although 10 of them exist in the Whisper library and were not chosen by the Whisper method. The IRSN results shown in Table IV are using 100 benchmarks, 4 of which were also chosen by LANL, and 6 chosen in common with ORNL. It is mainly due to the benchmarks available in the validation databases of the different codes and not to the selection process. Indeed, very few PST benchmarks are common to IRSN, ORNL and LANL validation databases [11].

TABLE IV. Experimental and statistical bias and bias uncertainty for PST-001-001

| | $B_{bmk}$ | $B_{statistical}$ | $\sigma_{bmk}$ | $\sigma_{statistical}$ | USL |
|---|---|---|---|---|---|
| IRSN | 0.00492 | +0.00878 | 0.00500 | 0.00868 | 0.9913[1] |
| LANL | 0.00578 | -0.00597 | 0.00500 | 0.00829 | 0.9800[2] |
| ORNL | 0.00390 | +0.00430 | 0.00500 | 0.01080 | 0.9892[1] |

[1]$B_{statistical} > 1 \rightarrow 0$, USL=1- $\sigma_{statistical}$

[2]$USL^* = 1 + B_{statistical} - \sigma_{statistical} - MOS_{ND} - MOS_{code}$

## CONCLUSIONS

A comparison study of four cases of HEU and Pu with fast and thermal energy spectrum using S/U methods for resultant USL reveals similar values for what may be considered subcritical. Overall USL* differences for the HMF case shows 0.9% difference when comparing the results obtained by LANL and ORNL, 0.1% difference between ORNL and IRSN, and 1% difference between LANL and IRSN. Overall USL* differences for the HST case show 1% difference between LANL and ORNL, 0.2% difference between ORNL and IRSN, and 1.2% difference between LANL and IRSN. Overall USL* differences for the PMF case show 0.4% difference between LANL and ORNL, 0.1% difference between ORNL and IRSN, and 0.5% difference between LANL and IRSN. Overall USL* differences for the PST case show 0.4% difference between LANL and ORNL, 0.21% difference between ORNL and IRSN, and 0.57% difference between LANL and IRSN. The biggest difference was 1.2% for the HST case, which is likely due to differences in benchmarks held in common between libraries.

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## NOMENCLATURE

$B_{bmk}$=bias of the benchmark according to Eq. 3
$B_{statistical}$=bias computed using a set of similar benchmarks
$\sigma_{bmk}$=benchmark uncertainty
$\sigma_{statistical}$= bias uncertainty computed using a set of similar benchmarks
$C_k$=correlation coefficient or similarity coefficient
CM=Calculational Margin
GLLSM=Generalized Linear Least Squares Method
MOS=margin of subcriticality
$MOS_{code}$=MOS considered for unknown code errors
$MOS_{ND}$=MOS considered for nuclear data uncertainty
NCSP=Nuclear Criticality Safety Program
S/U=Sensitivity/Uncertainty
USL=Upper Subcritical Limit, taking into account bias and bias uncertainty
USL*=USL taking into account bias, bias uncertainty, MOS for nuclear data and MOS for unknown code errors

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