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Excluding Benchmark Statistical Outliers in Nuclear Criticality Safety Validation

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INTRODUCTION

Neutron transport methods used to establish subcriticality require validation by comparison to benchmark critical experiments. A collection of benchmark experiments may include statistical outliers where the calculated k-effective and the experiment k-effective differ by an amount atypical for similar experiments. Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations, ANSI/ANS-8.24-2017[1] states:

> *"Identification of data outliers may be based on established statistical rejection methods; rejection of outliers shall be based on the inconsistency of the data with known physical behavior in the experimental data."*

Whisper is a sensitivity/uncertainty analysis tool developed to assist with the task of validation in nuclear criticality safety [2-4]. Details on the Whisper methodology can be found on the MCNP® reference collection website at https://mcnp.lanl.gov. Whisper-1.1, released with MCNP6.2 in the spring of 2018, contains a library with more than 1100 benchmark critical experiments. A methodology optionally employed by Whisper is the exclusion of benchmark statistical outliers based upon the iterative diagonal chi-squared statistical rejection technique.

This paper discusses studies done to determine the impact of excluding benchmark outliers on validation for nuclear criticality safety. The studies include ^{239}Pu and highly enriched uranium (HEU) systems. The systems range in energy from fast to thermal and include metal, oxide with varying moisture levels, and solution. They were chosen to be representative of applications relevant to criticality safety analysis.

The studies show that there is little change to the baseline upper subcritical limit (USL), calculational margin (CM), and margin of subcriticality (MOS) for nuclear data when excluding benchmark statistical outliers. Furthermore, inclusion of all benchmarks from the library does not appear to be conservative; the baseline USL may be higher when including all benchmarks than when rejecting benchmark outliers.

METHODOLOGY AND BACKGROUND

Application Cases

Parameterized models, built for use with MCNP6.2, are described in the sub-paragraphs below. The models were run as kcode calculations and k-effective results were collected, along with the average energy of neutrons causing fission (ANECF), energy of the average neutron lethargy causing fission (EALF), and k-effective sensitivity profiles. Results were utilized by Whisper-1.1 to select neutronically similar benchmarks and calculate a baseline USL from the CM plus MOS for nuclear data plus MOS for code errors. The final USL used for an application is determined by the criticality safety analyst using judgment for additional MOS considering area of applicability and other issues.

^{239}Pu Metal Cases

The plutonium metal cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of three right circular cylinders of plutonium metal placed touching in a triangular pattern with their bases resting on a ½-inch thick stainless steel floor. Radial reflection was modeled as a 1-inch thick layer of water around one cylinder. The plutonium was modeled as 100% ^{239}Pu at a density of 19.85 g/cm^3. The mass of plutonium in each cylinder was varied from 2300 grams to 4500 grams and the height-to-diameter ratio of each cylinder was varied from 1.0 to 2.2. Parameterizing the mass and height-to-diameter resulted in 91 cases.

^{239}Pu Oxide Cases

The plutonium metal cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of three right circular cylinders of plutonium oxide-water mixture placed touching in a triangular pattern with their bases resting on a ½-inch thick stainless steel floor. Radial reflection was modeled as a 1-inch thick layer of water around one cylinder. The plutonium was modeled as 100% ^{239}Pu. The mass of each cylinder was 3500 grams and the water atom fraction varied from 1e-6 (effectively zero for a dry powder) to 0.999 (which resembles a solution). The height-to-diameter ratio of each cylinder was 1.6. Parameterizing the atom fraction of water resulted in 106 cases.

^{239}Pu Solution Cases

The plutonium solution cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of two right circular cylinders of plutonium metal-water mixture placed touching with their bases resting on a ½-inch thick stainless steel floor. The plutonium was modeled as 100% ^{239}Pu at a density of 19.85

g/cm^3 mechanically mixed with water at a density of 1.0 g/cm^3. Radial reflection was modeled as ½-inch thick offset cylinder of water. The concentration of plutonium in each cylinder ranged from 5 to 300 g/L. The height-to-diameter ratio of each cylinder was varied from 0.5 to 2.0. Parameterizing the concentration and height-to-diameter resulted in 518 cases.

HEU Metal Cases

The HEU metal cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of three right circular cylinders of plutonium metal placed touching in a triangular pattern with their bases resting on a ½-inch thick stainless steel floor. . Radial reflection was modeled as a 1-inch thick layer of water around one cylinder. The HEU was modeled as 93% ^{235}U and 7% ^{238}U at a density of 18.75 g/cm^3. The mass of plutonium in each cylinder was varied from 10000 grams to 20000 grams and the height-to-diameter ratio of each cylinder was varied from 0.5 to 2.5. Parameterizing the mass and height-to-diameter resulted in 25 cases.

HEU Oxide Cases

The HEU oxide cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of three right circular cylinders of HEU oxide-water mixture placed touching in a triangular pattern with their bases resting on a ½-inch thick stainless steel floor. Radial reflection was modeled as a 1-inch thick layer of water around one cylinder. The HEU was modeled as 93% ^{235}U and 7% ^{238}U at a density of 18.75 g/cm^3. The HEU oxide mass of each cylinder was 10000 grams and the water atom fraction varied from 1e-6 (effectively zero for a dry powder) to 0.999 (which resembles a solution). The height-to-diameter ratio of each cylinder was 1.6. Parameterizing the atom fraction of water resulted in 106 cases.

HEU Solution Cases

The HEU solution cases were conducted as a parameter study to cover a range of applicable process models. The models consisted of two right circular cylinders of HEU metal-water mixture placed touching with their bases resting on a ½-inch thick stainless steel floor. The HEU was modeled at a density of 18.755 g/cm^3 mechanically mixed with water at a density of 1.0 g/cm^3. Radial reflection was modeled as ½-inch thick offset cylinder of water. The concentration of HEU in each cylinder ranged from 5 to 1000 g/L. The height-to-diameter ratio of each cylinder was 1.6. Parameterizing the concentration and height-to-diameter resulted in 29 cases.

RESULTS

The baseline USLs computed by Whisper are shown below in Fig. 1 for plutonium and HEU systems over a range of EALF.

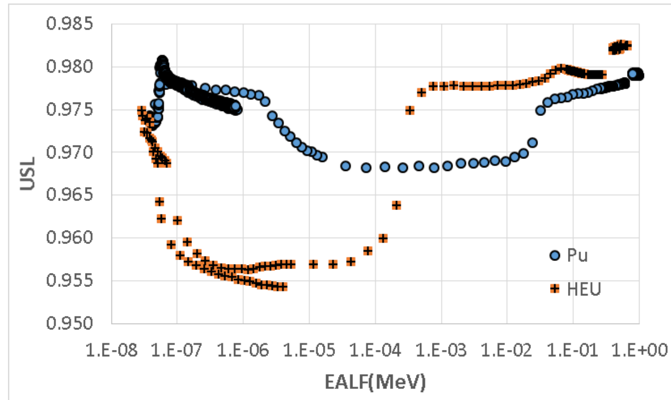

Fig. 1. Baseline USLs for Pu and HEU systems.

^{239}Pu Metal Cases

The baseline USL for the plutonium metal cases ranges from 0.97999 to 0.97929 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly lower, 0.97878 to 0.97909, when including all benchmarks in the validation collection. The difference in baseline USL ranges from 0.00017 to 0.00021. Only a subset of the entire benchmark collection is neutronically similar to the plutonium metal cases and of that subset one benchmark outlier, PMF-039-001, was found to be neutronically similar in all cases with a maximum correlation coefficient of 0.9956.

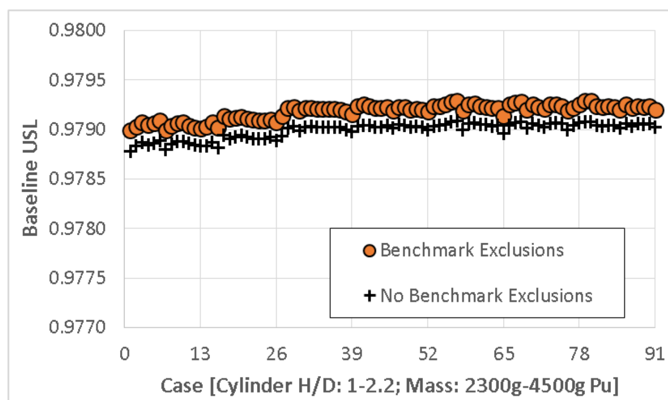

Fig. 2. Baseline USL for Pu metal cases.

^{239}Pu Oxide Cases

The baseline USL for the plutonium oxide cases ranges from 0.96799 to 0.97817 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly lower, 0.96821 to 0.97819, when including all benchmarks in the validation collection. The difference in baseline USL ranges from 0.001 to 0.00234. Only a subset of the entire benchmark collection is neutronically similar to the plutonium oxide cases and of that subset 37 benchmark outliers were found to be neutronically similar a total of 817 for all 106 application cases with a maximum correlation coefficient of 0.9870.

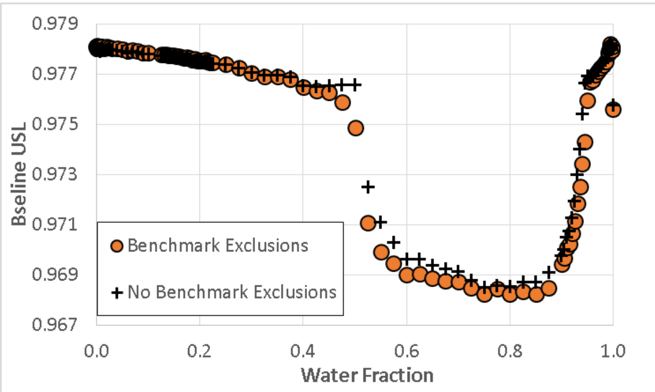

Fig. 3. Baseline USL for Pu oxide cases.

^{239}Pu Solution Cases

The baseline USL for the plutonium solution cases ranges from 0.97317 to 0.98079 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly higher, 0.97317 to 0.98089, when including all benchmarks in the validation collection. The difference in baseline USL ranges from 0 to 0.00027. Only a subset of the entire benchmark collection is neutronically similar to the plutonium solution cases and of that subset 12 benchmark outliers were found to be neutronically similar a total of 2146 times for all 518 application cases with a maximum correlation coefficient of 0.9974.

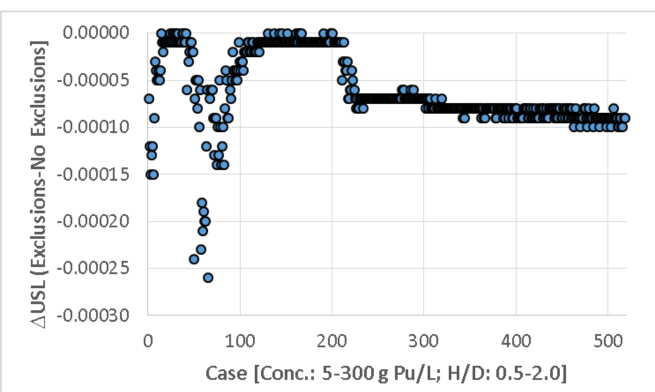

Fig. 4. Difference in baseline USL for Pu solution cases when including or excluding benchmark outliers.

HEU Metal Cases

The baseline USL for the HEU metal cases ranges from 0.98194 to 0.98264 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly higher, 0.98196 to 0.98315, when including all benchmarks in the validation collection. The difference in baseline USL ranges from 0.00002 to 0.00058. Only a subset of the entire benchmark collection is neutronically similar to the HEU metal cases and of that subset 10 benchmark outliers were found to be neutronically similar a total of 188 times for all 25 application cases with a maximum correlation coefficient of 0.9864.

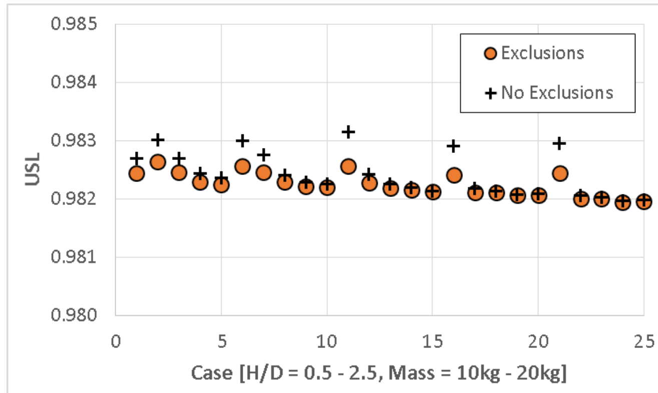

Fig. 5. Baseline USL for HEU metal cases.

HEU Oxide Cases

The baseline USL for the HEU oxide cases ranges from 0.95633 to 0.97940 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly higher, 0.95633 to 0.97970, when including all benchmarks in the validation collection. The magnitude of the difference in baseline USL, rejecting outliers versus including outliers, ranges from 0 to 0.00208. Only a subset of the entire benchmark collection is neutronically similar to the HEU metal cases and of that subset 17 benchmark outliers were found to be neutronically similar a total of 611 times for all 106 application cases with a maximum correlation coefficient of 0.9997.

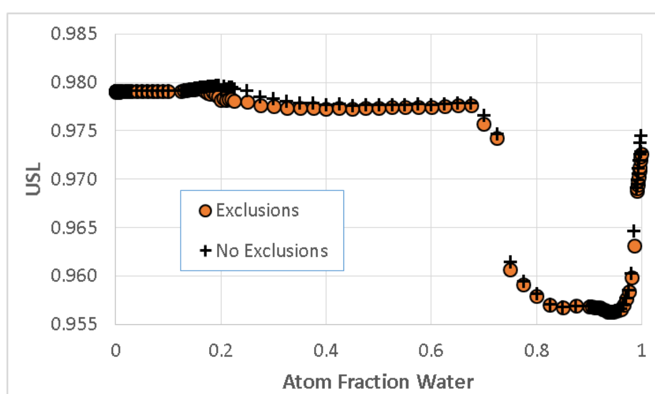

Fig. 6. Baseline USL for HEU oxide cases.

HEU Solution Cases

The baseline USL for the HEU solution cases ranges from 0.95427 to 0.97494 when benchmark outliers are excluded from the validation collection. The baseline USL is slightly higher, 0.95427 to 0.97538, when including all benchmarks in the validation collection. The magnitude of the difference in baseline USL, rejecting outliers versus including outliers, ranges from 0 to 0.00307. Only a subset of the entire benchmark collection is neutronically similar to the HEU solution cases and of that subset 8 benchmark outliers were found to be neutronically similar a total of 104 times for all 29 application cases with a maximum correlation coefficient of 0.9995.

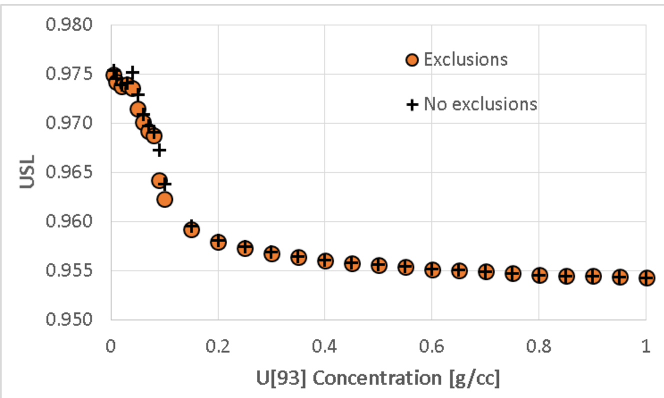

Fig. 7. Baseline USL for HEU solution cases.

RESULTS

A comparison study has been done to compute baseline USLs with and without benchmark outliers in the validation collection using Whisper-1.1 to determine what effect rejection of outliers has on nuclear criticality safety validation. The effect of excluding benchmark outliers is small. There does not appear to be a clear trend in predicting the most conservative method; sometimes the baseline USL is higher when including all benchmarks and sometimes it is lower. The overall magnitude of the difference in the baseline USL, rejecting outliers versus including outliers, in this study was found to be:

- Pu metal systems = 0.00021,
- Pu oxide systems = 0.00234,
- Pu solution systems = 0.00026,
- HEU metal systems = 0.0005,
- HEU oxide systems = 0.00208, and
- HEU solution systems = 0.00307.

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