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Title: Excluding Benchmark Statistical Outliers in Nuclear Criticality Safety Validation: A Comparison Study of Upper Subcritical Limits for Plutonium Systems using Whisper-1.1

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Excluding Benchmark Experiment Statistical Outliers in Nuclear Criticality Safety Validation: A Comparison Study of Upper Subcritical Limits for Plutonium Systems using Whisper-1.1

Introduction

Neutron transport methods used to establish subcriticality require validation by comparison to critical experiments considered to be benchmarks. Whisper is a sensitivity/uncertainty analysis tool developed to assist with the task of validation in nuclear criticality safety. Details on the Whisper methodology can be found in References 1-3 on the MCNP® reference collection website at https://mcnp.lanl.gov. During the process of validation there can be cases where a benchmark experiment may be found to be a statistical outlier, in which the calculated k-effective value and the experiment k-effective value differ by an amount atypical for similar experiments. A methodology optionally employed by Whisper is the exclusion of statistical outliers based upon the iterative diagonal chi-squared statistical rejection technique. Alternatively, there is an option to include all benchmarks in the Whisper library collection, even those benchmarks found to be statistical outliers, when computing the bias, bias uncertainty and margin of subcriticality (MOS) leading to establishment of the baseline upper subcritical limit (USL). A comparison study has been done to compute USLs with and without statistical outliers in the Whisper benchmark collection to determine what effect rejection of statistical outliers has on the recommended USL. The results show little overall difference in the recommended baseline USLs developed by Whisper when excluding statistical outliers. Additionally, there does not appear to be a clear trend in predicting whether the baseline USL will be higher or lower when rejecting statistical outliers from the benchmark critical experiment collection used for validation.

Whisper-1.0 was originally developed in 2014 and used for validation support at Los Alamos National Laboratory. Whisper was upgraded in 2016 to Whisper-1.1 and prepared for release with MCNP6.2 [References 3-5]. In December 2017 a revised ANSI/ANS-8.24-2017 *Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations* [Reference 6] was approved. It included a modification to the language in the standard on the topic of rejection of statistical outliers stating:

"*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.*"

Previous to ANSI/ANS-8.24-2017 the language in ANSI/ANS-8.24-2007 [Reference 7] was:

"Rejection of data outliers shall be based on the inconsistency of the data with known physical behavior or on established statistical rejection methods."

This paper examines the effect of exclusion of benchmarks which are found to be statistical outliers from the collection of benchmarks used by Whisper-1.1. The primary focus of this study is on nuclear criticality safety validation for ^{239}Pu. The baseline recommended USL, calculational margin and margin of subcriticality for nuclear data uncertainty is presented for many plutonium application cases ranging from fast metal systems to intermediate moist oxide systems to thermal solution systems. Results show there is little difference in baseline USL when using a reduced benchmark collection due to statistical rejection of outliers. Overall maximum difference in baseline USL between the two methods:

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = 0.00021$ for plutonium metal systems,

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00234$ for plutonium oxide systems, and

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00026$ for plutonium solution systems.

There is slight nonconservatism, i.e., the baseline USL is greater, when including all the benchmarks in the Whisper-1.1 collection and not using the available statistical rejection technique to exclude benchmark outliers for oxide and solution systems.

^{239}Pu Study

Application models used for this study are those from the validation report contained in Reference 2 for various plutonium systems, -metal, -solution, and -oxide. These models are described below, along with illustrations from MCNP6.2. Results were computed on the Los Alamos National Laboratory High Performance Computing (HPC) platform Snow. This platform is based on Linux OS with Intel Xeon Broadwell processors and 36 CPU nodes per core. The MCNP6.2 calculations were done using 18 Slurm tasks.

Pu Metal cases

The plutonium metal cases were conducted as a parameter study to cover a range of applicable process models. The process models consisted of three Pu-metal right circular cylinders on a stainless steel floor reflected radially by 1-inch thick water to represent personnel and incidental reflection. The three identical cylinders were placed touching in a triangular pattern with their bases sitting on the ½-inch thick stainless steel floor. The plutonium was modeled as 100% ^{239}Pu at a density of 19.85 g/cm^3. Various masses of plutonium in the cylinders and height-to-diameter (H/D) ratio of the cylinders were modeled. The plutonium mass modeled in each cylinder was 2300, 2500, 3300, 3000, 3500, 4000, and 4500 grams per cylinder. The H/D ratios varied from 1.0 to 2.2 in increments of 0.1. Parameterizing the mass per cylinder and H/D ratio as described resulted in 91 different cases. Internal to each individual case the cylinder mass and H/D were identical to one another; there was no variation amongst cylinders in an individual case and therefore the total mass in cases varied from 6,900 to 13,500 g Pu. The model geometry is shown below in Figure 1.

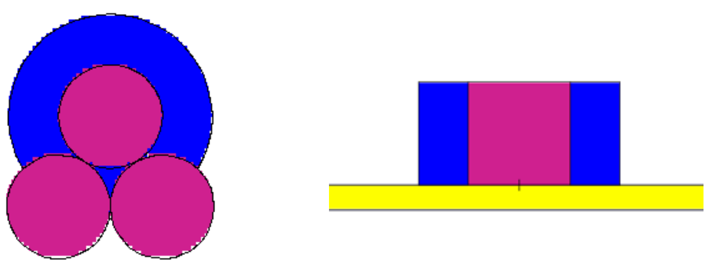

Figure 1. MCNP6.2 top and side view illustrations, respectively, of model geometry. Pu metal is shown in magenta; water in blue and steel in yellow.

MCNP6.2 was used to determine k-effective, the average energy of neutrons causing fission, the energy of the average lethargy of neutrons causing fission, and sensitivity profiles for each of the 91 process model cases. Whisper was used to find benchmarks neutronically similar to each process model case using sensitivity profiles, determine the calculational margin and portions of the margin of subcriticality leading to the baseline USL.

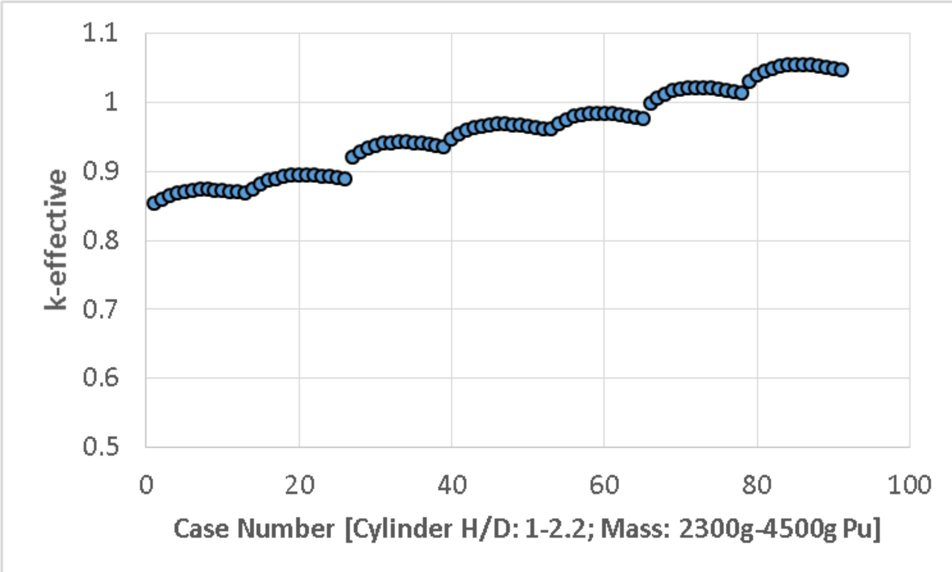

Figure 2. MCNP6.2 k-effective results for Pu metal cases

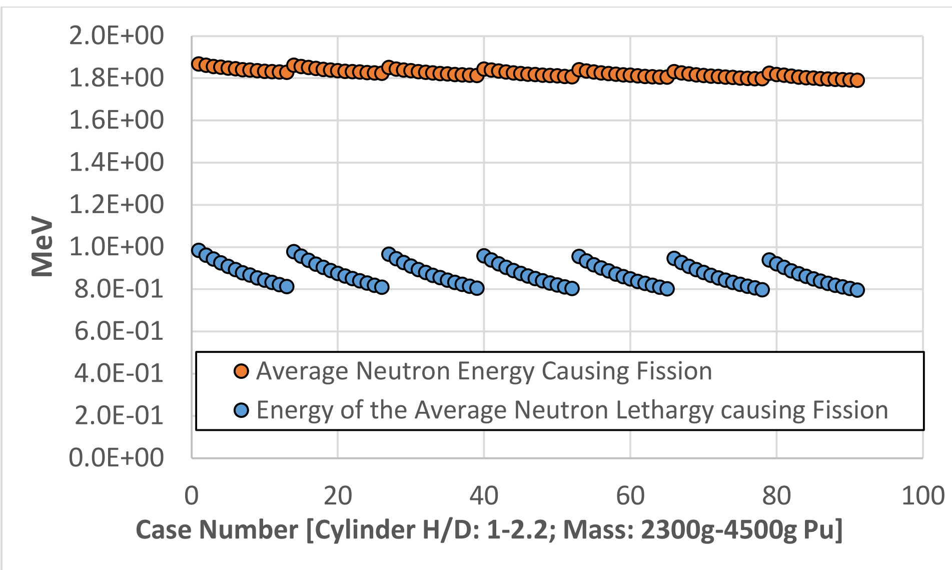

Figure 3. MCNP6.2 ANECF and EALF results for Pu metal cases

The results for the Whisper-1.1 baseline USL are reported below. A separate USL was computed for each process model case using a benchmark collection reduced due to exclusions based upon the iterative diagonal chi-squared rejection method. Then the USL was computed for each process model case using a benchmark collection consisting of all 1101 benchmark experiments contained in the Whisper-1.1 library.

The baseline USL is slightly higher when excluding benchmarks. The difference between the baseline USL when excluding benchmarks and the baseline USL when using all benchmarks in the library ranges from 0.00017 to 0.00021.

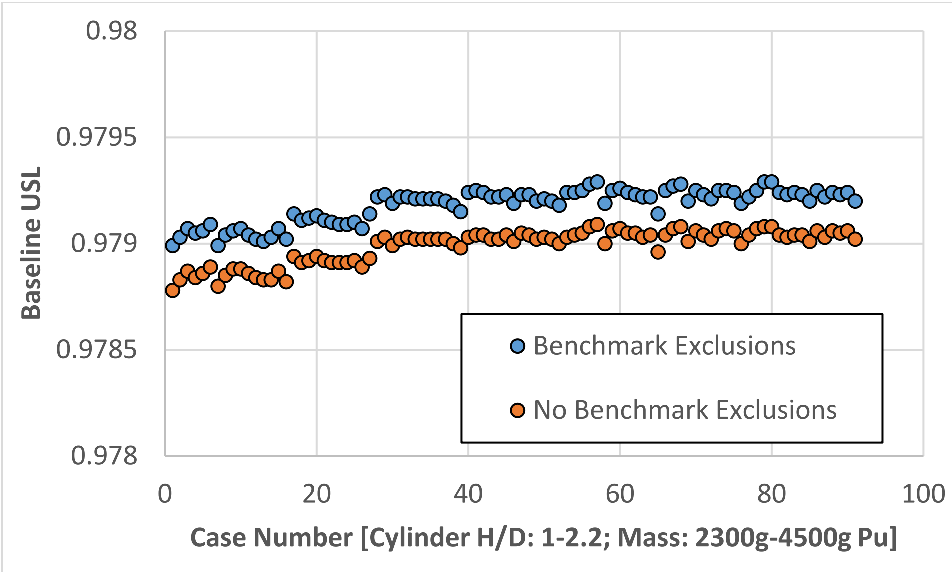

Figure 4. Whisper-1.1 baseline USL results for Pu metal cases when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The calculational margin calculated by Whisper is shown below. The calculational margin is slightly larger when there are no benchmark exclusions. The difference between the calculational margin when excluding benchmarks and the baseline USL when using all benchmarks in the library ranges from -0.00017 to -0.00021. The magnitude of the difference in the baseline USL computed by Whisper when using all benchmarks versus the baseline USL computed by Whisper when excluding outliers is due to the calculational margin (bias and bias uncertainty) and not due to the margin of subcriticality for to nuclear data.

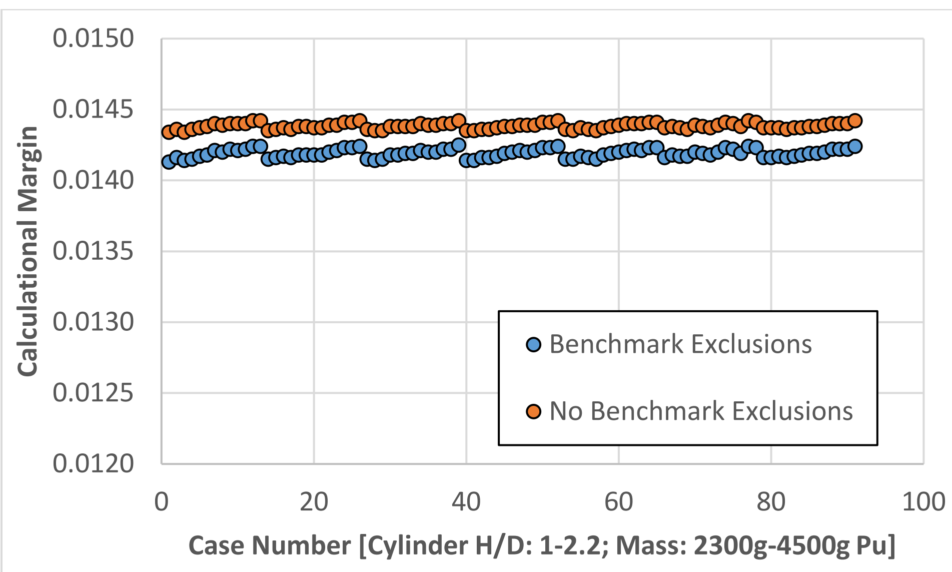

Figure 5. Whisper-1.1 calculational margin results for Pu metal cases when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The margin of subcriticality due to nuclear data uncertainty is shown below. The $MOS_{nuclear\ data}$ is calculated from the sensitivity profile created by MCNP6.2 and the nuclear data covariances. GLLS adjustment of nuclear data covariances may be influenced by the benchmark collection. Therefore, two studies of nuclear data covariance adjustment were done. The initial study was conducted using the reduced benchmark set that does not include rejected outliers. In the subsequent study, Whisper nuclear data covariance adjustment was also done using the entire benchmark suite, keeping the benchmarks that were found to be outliers in the set. It was found that there are insignificant differences in the $MOS_{nuclear\ data}$ computed by Whisper whether or not the benchmark collection excludes outliers. For this reason the $MOS_{nuclear\ data}$ is the same for the case in which all benchmarks in the library are used versus the case in which benchmarks may be excluded based upon statistical rejection. Differences in the Whisper USLs generated when using a benchmark suite that excludes outliers versus the Whisper USLs generated when using a benchmark suite containing the entire library of 1101 benchmarks is due to differences in the Whisper calculational margin and not the $MOS_{nuclear\ data}$.

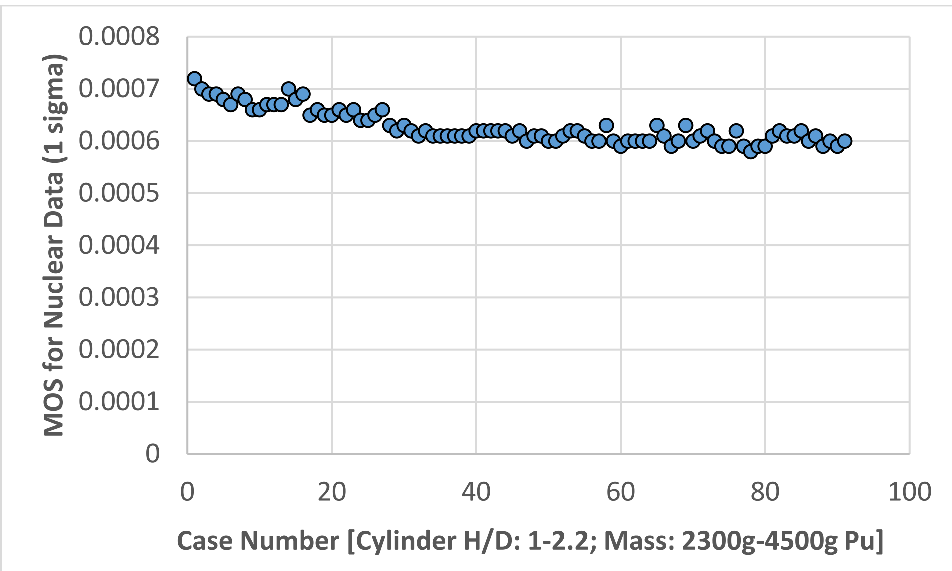

Figure 6. Whisper-1.1 margin of subcriticality due to nuclear data uncertainty for Pu metal cases

The preceding results are for MCNP6.2 calculations with 100,000 neutrons per cycle. For comparison the results shown in the figure below were done with 10,000 neutrons per cycle. While the magnitude of the difference in USL when excluding benchmarks vs. including all benchmarks is the same, 0.00022, the variation in the baseline USL for cases is greater. When calculating the baseline USL and excluding benchmarks based upon statistical rejection the lowest baseline USL = 0.97814 and the highest 0.97929. When including all benchmarks the lowest baseline USL = 0.97796 and the highest = 0.9791.

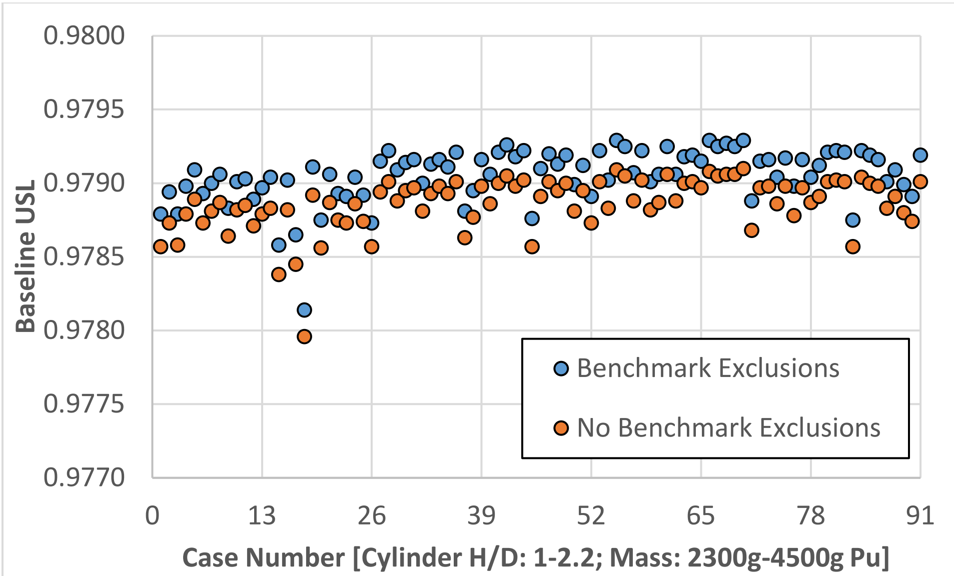

Figure 7. Whisper-1.1 baseline USL results for Pu metal cases (using MCNP6.2 calculations with 10,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

It is important to note that only a subset of the benchmarks in the collection, enough found to be neutronically similar for valid statistical analysis in each case, are used to compute the baseline USL. For the plutonium metal cases the series of relevant benchmark experiments are those from PU-MET-FAST and MIX-MET-FAST. From those sets of experiments there are four benchmark experiments which were found to be statistical outliers: PU-MET-FAST-016-001, PU-MET-FAST-039-001, PU-MET-FAST-041-001, and MIX-MET-FAST-007-002. When using Whisper to determine experiments similar to the application and including all 1101 benchmark experiments in the collection (not rejecting outliers) the only benchmark, which would have been rejected if allowed, found to be neutronically similar to the plutonium metal application cases was PU-MET-FAST-039-001. This benchmark was chosen for each of the 91 process model cases with the highest $c_k = 0.9956$. A $c_k = 1$ implies perfect correlation, therefore PU-MET-FAST-039-001 was found to be highly correlated, or to have high neutronic similarity, to the plutonium metal application cases.

The difference in baseline USL for a benchmark collection with exclusions versus a benchmark collection without exclusions was from 0.00017 to 0.00021. The maximum $USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = 0.00021$ occurred in 9 cases, including case 1 which represents the lowest USL at $USL_{\text{No Benchmark Exclusions}} = 0.97878$. The highest $USL_{\text{No Benchmark Exclusions}} = 0.97909$ for case 57. A comparison table for Case 1 is shown below in Table 1, with the benchmark which would have been excluded based upon the statistical rejection method, PU-MET-FAST-039-001, shown in bold text.

Table 1. Comparison of Whisper output for Case 1 with and without exclusions based upon statistical rejection of the benchmark collection. Benchmark which is excluded using the rejection technique shown in bold text.

Benchmark Exclusions	No Benchmark Exclusions
Baseline USL = 0.97899	Baseline USL = 0.97878
Bias = 0.00697	Bias = 0.00859
Bias Uncertainty = 0.00716	Bias Uncertainty = 0.00575
Nuclear Data Uncertainty = 0.00072	Nuclear Data Uncertainty = 0.00072

Benchmark	C_k	Weight	Benchmark	C_k	Weight
pu-met-fast-022-001.i	0.9961	1.0000	pu-met-fast-022-001.i	0.9961	1.0000
pu-met-fast-001-001.i	0.9957	0.9860	pu-met-fast-001-001.i	0.9957	0.9854
mix-met-fast-009-001.i	0.9955	0.9799	mix-met-fast-009-001.i	0.9955	0.9790
pu-met-fast-023-001.i	0.9949	0.9630	pu-met-fast-023-001.i	0.9949	0.9613
pu-met-fast-025-001.i	0.9948	0.9612	pu-met-fast-025-001.i	0.9948	0.9595
			pu-met-fast-039-001.i	**0.9937**	**0.9236**
pu-met-fast-035-001.i	0.9937	0.9253	pu-met-fast-035-001.i	0.9937	0.9220
pu-met-fast-036-001.i	0.9923	0.8837	pu-met-fast-036-001.i	0.9923	0.8784
pu-met-fast-024-001.i	0.9908	0.8387	pu-met-fast-024-001.i	0.9908	0.8315
pu-met-fast-009-001.i	0.9901	0.8175	pu-met-fast-009-001.i	0.9901	0.8093
pu-met-fast-029-001.i	0.9897	0.8062	pu-met-fast-029-001.i	0.9897	0.7975
pu-met-fast-044-002.i	0.9886	0.7735	pu-met-fast-044-002.i	0.9886	0.7634
pu-met-fast-030-001.i	0.9882	0.7595	pu-met-fast-030-001.i	0.9882	0.7487
pu-met-fast-044-005.i	0.9865	0.7096	pu-met-fast-044-005.i	0.9865	0.6966
pu-met-fast-044-003.i	0.9849	0.6624	pu-met-fast-044-003.i	0.9849	0.6472
pu-met-fast-021-002.i	0.9849	0.6605	pu-met-fast-021-002.i	0.9849	0.6453
pu-met-fast-003-103.i	0.9836	0.6234	pu-met-fast-003-103.i	0.9836	0.6065
pu-met-fast-021-001.i	0.9830	0.6036	pu-met-fast-021-001.i	0.9830	0.5858
pu-met-fast-044-004.i	0.9827	0.5951	pu-met-fast-044-004.i	0.9827	0.5769
pu-met-fast-042-012.i	0.9819	0.5697	pu-met-fast-042-012.i	0.9819	0.5504
pu-met-fast-042-009.i	0.9817	0.5648	pu-met-fast-042-009.i	0.9817	0.5453
pu-met-fast-042-015.i	0.9816	0.5612	pu-met-fast-042-015.i	0.9816	0.5415
pu-met-fast-042-013.i	0.9813	0.5531	pu-met-fast-042-013.i	0.9813	0.5330
pu-met-fast-042-007.i	0.9813	0.5529	pu-met-fast-042-007.i	0.9813	0.5329
pu-met-fast-042-011.i	0.9813	0.5515	pu-met-fast-042-011.i	0.9813	0.5314
pu-met-fast-042-010.i	0.9812	0.5503	pu-met-fast-042-010.i	0.9812	0.5302
pu-met-fast-042-006.i	0.9811	0.5477	pu-met-fast-042-006.i	0.9811	0.5274
pu-met-fast-042-014.i	0.9811	0.5466	pu-met-fast-042-014.i	0.9811	0.5262
pu-met-fast-042-008.i	0.9809	0.5407	pu-met-fast-042-008.i	0.9809	0.5201
pu-met-fast-042-005.i	0.9799	0.5100	pu-met-fast-042-005.i	0.9799	0.4880
pu-met-fast-042-004.i	0.9790	0.4841	pu-met-fast-042-004.i	0.9790	0.4610
pu-met-fast-031-001.i	0.9788	0.4778	pu-met-fast-031-001.i	0.9788	0.4543
pu-met-fast-042-003.i	0.9776	0.4408	pu-met-fast-042-003.i	0.9776	0.4157
mix-met-fast-007-022.i	0.9757	0.3844	mix-met-fast-007-022.i	0.9757	0.3567
mix-met-fast-007-023.i	0.9751	0.3670	mix-met-fast-007-023.i	0.9751	0.3386
pu-met-fast-011-001.i	0.9748	0.3558	pu-met-fast-011-001.i	0.9748	0.3269
pu-met-fast-032-001.i	0.9747	0.3541	pu-met-fast-032-001.i	0.9747	0.3251
pu-met-fast-042-002.i	0.9743	0.3406	pu-met-fast-042-002.i	0.9743	0.3110
mix-met-fast-001-001.i	0.9742	0.3376	mix-met-fast-001-001.i	0.9742	0.3079
pu-met-fast-018-001.i	0.9728	0.2966	pu-met-fast-018-001.i	0.9728	0.2651
pu-met-fast-044-001.i	0.9708	0.2347	pu-met-fast-044-001.i	0.9708	0.2004
pu-met-fast-026-001.i	0.9700	0.2114	pu-met-fast-026-001.i	0.9700	0.1761
pu-met-fast-045-005.i	0.9670	0.1230	pu-met-fast-045-005.i	0.9670	0.0837
pu-met-fast-027-001.i	0.9670	0.1204	pu-met-fast-027-001.i	0.9670	0.0809
pu-met-fast-042-001.i	0.9662	0.0981	pu-met-fast-042-001.i	0.9662	0.0576

mix-met-fast-005-001.i	0.9659	0.0878	mix-met-fast-005-001.i	0.9659	0.0469
pu-met-fast-008-001.i	0.9655	0.0776	pu-met-fast-008-001.i	0.9655	0.0362

Pu Solution Cases

The plutonium solution cases consist of two right circular cylinders of plutonium metal-water mixture that are touching and resting atop a ½-inch thick stainless steel floor. The plutonium in each of the cylinders is 520 grams of 100% ^{239}Pu. Radial reflection is modeled as ½-inch thick offset annulus of full-density (1.0 g/cm^3) water. The H/D of the cylinders is varied from 0.5 to 2.0 in increments of 0.25. For each H/D the plutonium concentration is varied from 5 to 300 g/L (the density of the metal-water mix is a linear combination of Pu metal at 19.84 g/cm^3 and water at 1.0 g/cm^3). Parameterizing the plutonium concentration in the cylinder and H/D ratio as described resulted in 518 different cases. Internal to each individual case the cylinder concentration and H/D were identical to one another; there was no variation amongst cylinders in an individual case. The model geometry is shown below in Figure 8.

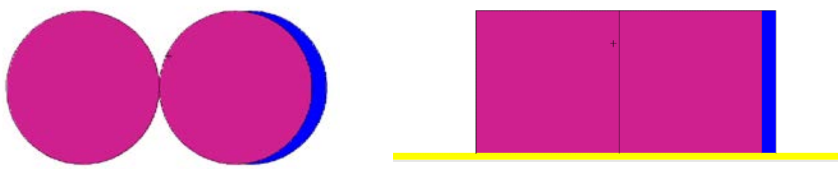

Figure 8. MCNP6.2 top and side view illustrations, respectively, of model geometry. Pu metal-water mixture is shown in magenta; water in blue and steel in yellow.

MCNP6.2 was used to determine k-effective, the average energy of neutrons causing fission, the energy of the average lethargy of neutrons causing fission, and sensitivity profiles for each of the 518 process model cases. The results are shown below in Figures 9 and 10. Whisper-1.1 was used to find benchmarks neutronically similar to each process model case using sensitivity profiles, determine the calculational margin and portions of the margin of subcriticality leading to the baseline USL.

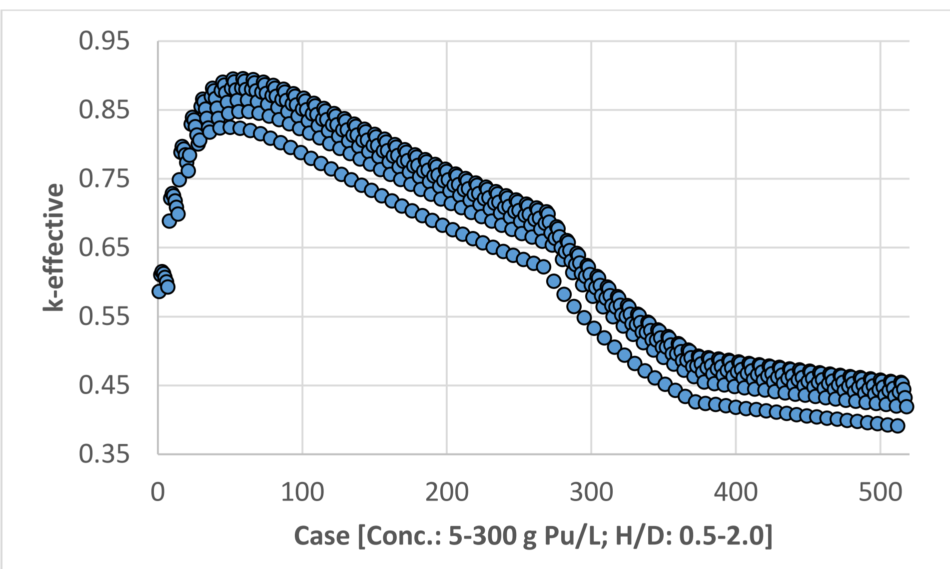

Figure 9. MCNP6.2 k-effective results for Pu metal-water mixture "solution" cases

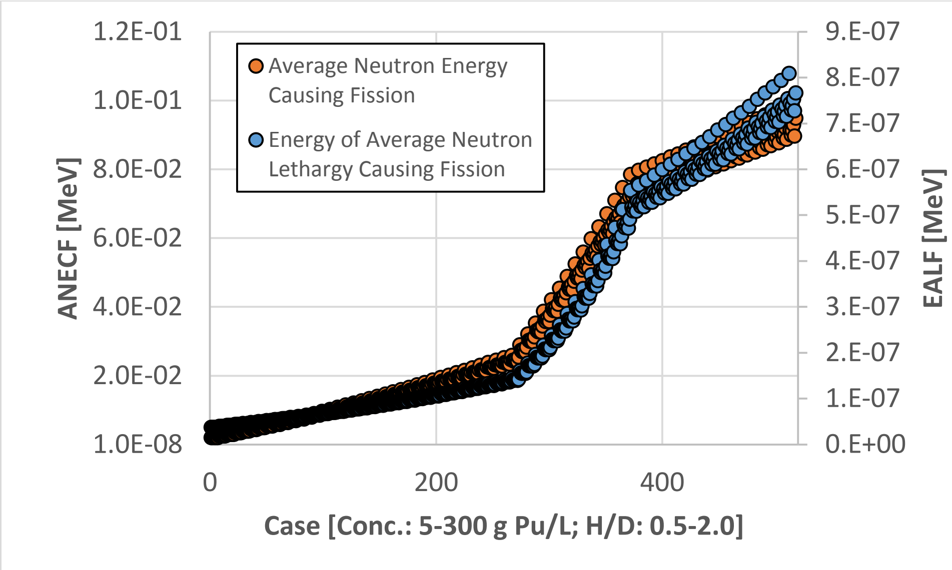

Figure 10. MCNP6.2 ANECF and EALF results for Pu metal-water mixture "solution" cases

The results for the Whisper-1.1 baseline USL are reported below in Figure 11. A separate USL was computed for each process model case using a benchmark collection with exclusions based upon the iterative diagonal chi-squared rejection method. Then the baseline USL was computed for each process model case using a benchmark collection consisting of all 1101 benchmark experiments contained in the Whisper-1.1 library.

The baseline USL is slightly higher when there were no benchmark exclusions. When calculating the baseline USL with a reduced set of benchmarks in the Whisper collection due to statistical rejection the lowest baseline USL = 0.97317 and the highest 0.98079. When including all benchmarks in the Whisper collection the lowest baseline USL = 0.97317 and the highest = 0.98089.The largest difference in the baseline USL when comparing using all benchmarks with the Whisper results when using a reduced set of benchmarks due to statistical rejection, $USL_{Benchmark\ Exclusions} - USL_{No\ Benchmark\ Exclusions}$ = -0.00027 for Case 67 with a plutonium concentration of 27.5 g/L and H/D of 1.25. It should be noted that in this case, and many other cases, it is slightly non-conservative to include all benchmarks because the baseline USL is actually higher when including all benchmarks. For Case 67 the recommended baseline USL is 0.97925 when rejecting benchmark outliers and 0.97952 when including all benchmarks. A comparison of similar benchmarks for this case is studied to attempt to determine the specific benchmarks leading to the baseline USL differences and is shown in Table 2.

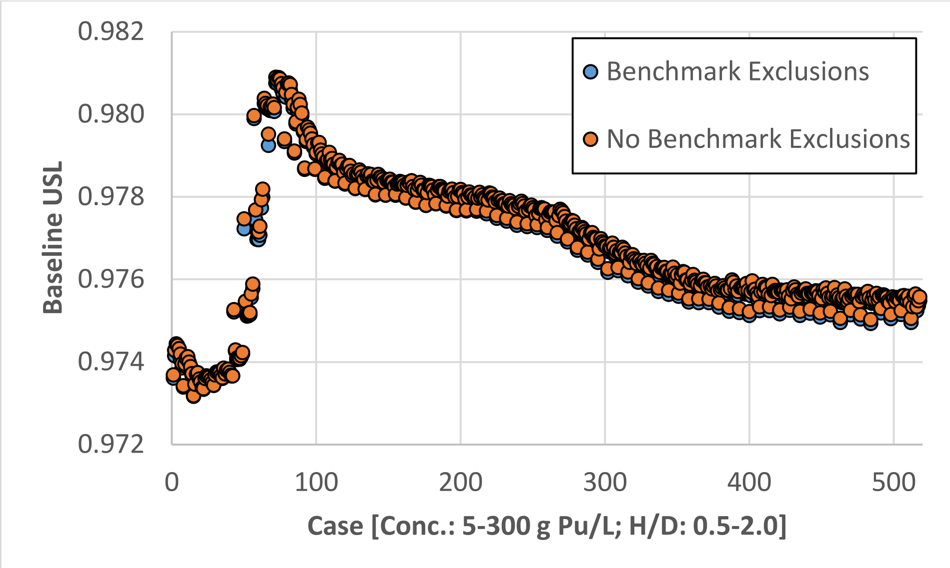

Figure 11. Whisper-1.1 baseline USL results for Pu metal-water mixture "solution" cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

In order to examine the differences in the USL more closely, the $USL_{\text{No Benchmark Exclusions}}$-$USL_{\text{Benchmark Exclusions}}$ is shown in Figure 12 below. As discussed in the preceding paragraph**,** it is non-conservative in the solution cases modeled to include all benchmarks because the baseline USL is slightly higher when including all benchmarks.

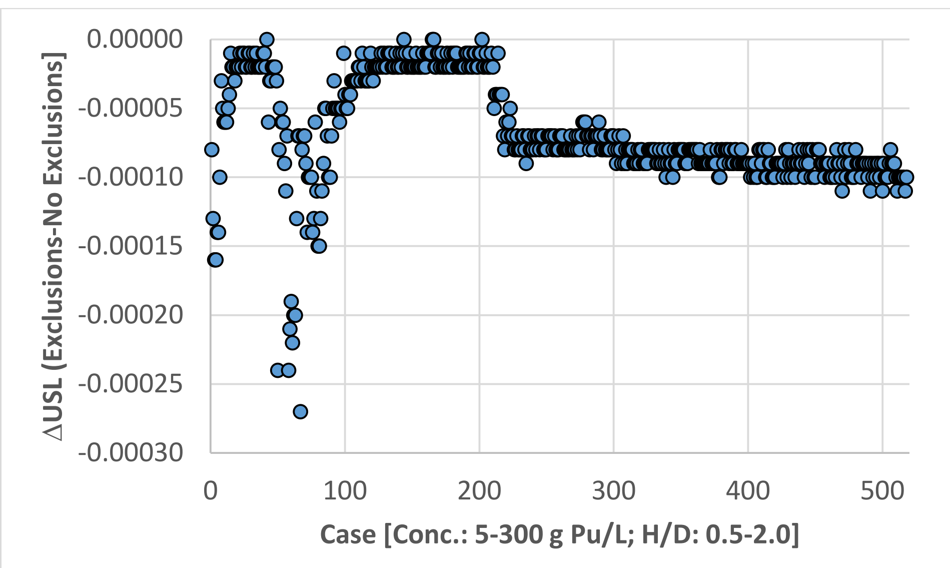

Figure 12. Whisper-1.1 baseline USL result differences for Pu metal-water mixture "solution" cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The calculational margin calculated by Whisper is shown below in Figure 13. The calculational margin is slightly larger when using a reduced benchmark collection due to statistical rejection leading to benchmark exclusions. The calculational margin ranges from 0.01236-0.01954. The difference between the calculational margin when excluding benchmarks vs. using all benchmarks in the library ranges from 0 to 0.00026. The magnitude of the difference in the baseline USL computed by Whisper when using all benchmarks versus the baseline USL computed by Whisper when excluding outliers is due to the calculational margin (bias and bias uncertainty) and not due to the margin of subcriticality for nuclear data.

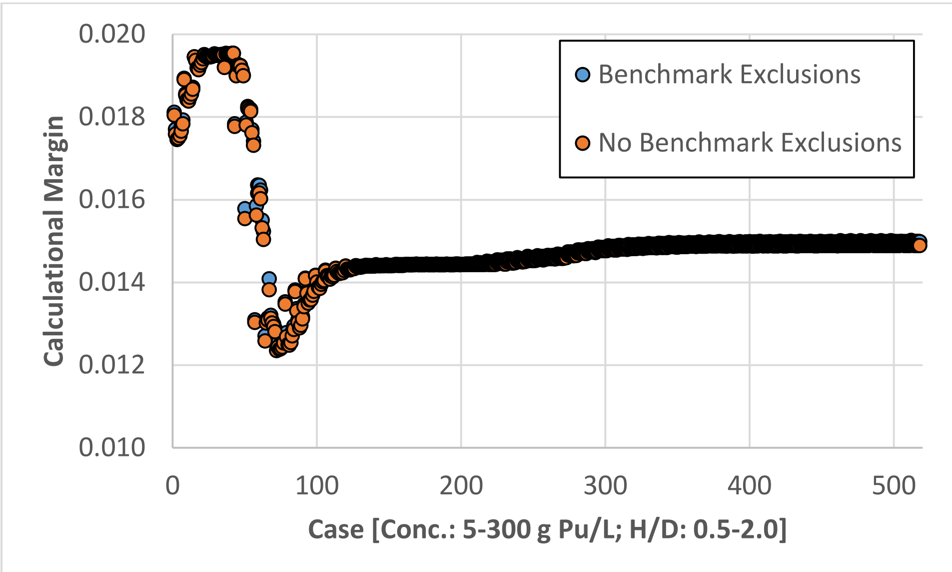

Figure 13. Whisper-1.1 calculational margin results for Pu metal-water mixture "solution" cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The margin of subcriticality due to nuclear data uncertainty is shown below in Figure 14. The $MOS_{nuclear\ data}$ is calculated from the sensitivity profile created by MCNP6.2 and the nuclear data covariances. GLLS adjustment of nuclear data covariances may be influenced by the benchmark collection. Therefore, two studies of nuclear data covariance adjustment were done. The initial study was conducted using the reduced benchmark set that does not include rejected outliers. In the subsequent study, Whisper nuclear data covariance adjustment was also done using the entire benchmark suite, keeping the benchmarks that were found to be outliers in the set. It was found that there are insignificant differences in the $MOS_{nuclear\ data}$ computed by Whisper whether or not the benchmark collection excludes outliers. For this reason the $MOS_{nuclear\ data}$ is the same for the case in which all benchmarks in the library are used versus the case in which benchmarks may be excluded based upon statistical rejection. Differences in the Whisper USLs generated when using a benchmark suite that excludes outliers versus the Whisper USLs generated when using a benchmark suite containing the entire library of 1101 benchmarks is due to differences in the Whisper calculational margin and not the $MOS_{nuclear\ data}$.

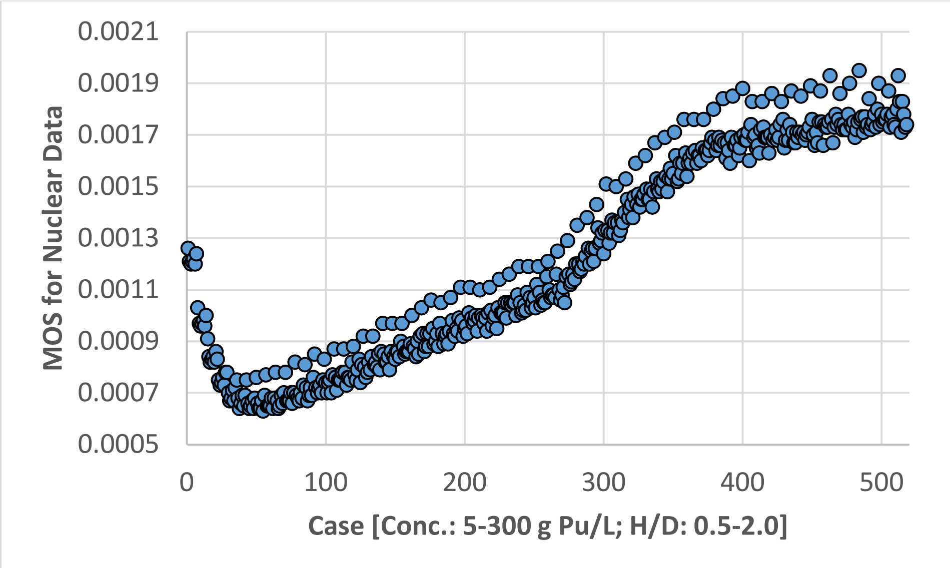

Figure 14. Whisper-1.1 margin of subcriticality for nuclear data results for Pu metal-water mixture "solution" cases (using MCNP6.2 calculations with 100,000 neutrons per cycle)

The preceding results are for MCNP6.2 calculations with 100,000 neutrons per cycle. For comparison the results shown in Figure 15 below were done with 10,000 neutrons per cycle. While the magnitude of the difference in USL when excluding benchmarks vs. including all benchmarks is about the same, 0.00026 for 100,000 neutrons per cycle vs. 0.00025 for 10,000 neutrons per cycle, the variation in the baseline USL for cases is greater. When calculating the baseline USL and excluding benchmarks based upon statistical rejection the lowest baseline USL = 0.97318 and the highest 0.98085. When including all benchmarks the lowest baseline USL = 0.97319 and the highest = 0.98096.

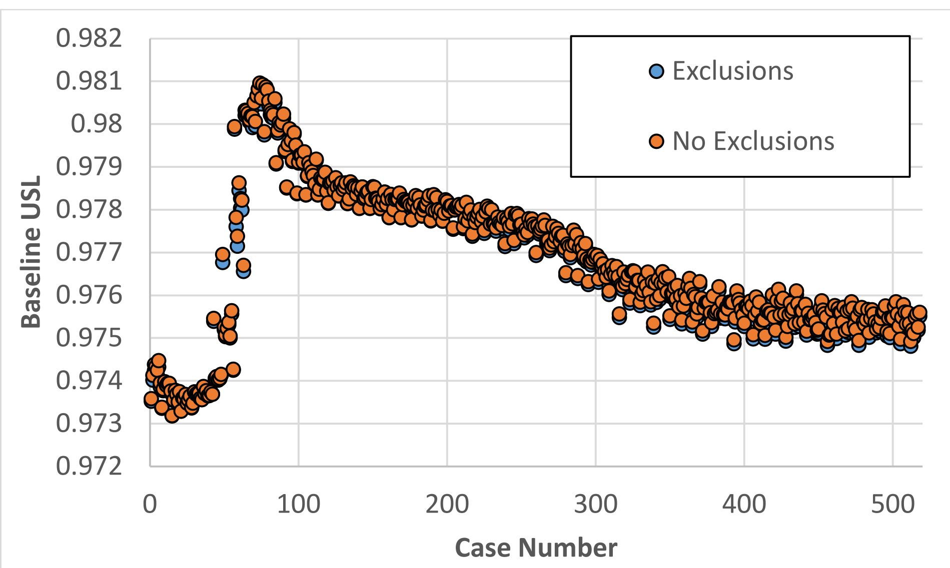

Figure 15. Whisper-1.1 baseline USL results for Pu metal-water mixture "solution" cases (using MCNP6.2 calculations with 10,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

It is important to note that only a subset of the benchmarks in the collection, enough found to be neutronically similar for valid statistical analysis in each case, are used to compute the baseline USL. For the plutonium metal-water mixture “solution” cases the series of relevant benchmark experiments are those from PU-SOL-THERM and MIX-SOL-THERM. From those sets of experiments there are twenty-four benchmark experiments which were found to be statistical outliers and they are shown in Table 3, with the number of times chosen as neutronically similar to an application and the highest correlation coefficient. A $c_k = 1$ implies perfect correlation and many of the benchmarks in Table 3 are found to be highly correlated, or to have high neutronic similarity, to the plutonium metal-water mixture application cases.

The maximum magnitude $USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00026$ occurred in Case 66, for a plutonium concentration of 27.5 g/L and H/D=1.25. A comparison table for Case 66 is shown below in Table 2, with benchmarks which would have been excluded based upon the statistical rejection method shown in bold text.

Table 2. Comparison of Whisper output for Case 66 with and without exclusions based upon statistical rejection of the benchmark collection. Excluded benchmarks using statistical rejection technique shown in bold text.

Benchmark Exclusions			No Benchmark Exclusions		
Baseline USL = 0.97925			Baseline USL = 0.97951		
Bias = 0.00599			Bias = 0.00586		
Bias Uncertainty = 0.0081			Bias Uncertainty = 0.00797		
Nuclear Data Uncertainty = 0.00064			Nuclear Data Uncertainty = 0.00064		
Benchmark	**C_k**	**Weight**	**Benchmark**	**C_k**	**Weight**
pu-sol-therm-011-161.i	0.9986	1.0000	pu-sol-therm-011-161.i	0.9986	1.0000
pu-sol-therm-011-162.i	0.9985	0.9830	pu-sol-therm-011-162.i	0.9985	0.9827
pu-sol-therm-003-008.i	0.9982	0.9117	pu-sol-therm-003-008.i	0.9982	0.9101
pu-sol-therm-011-164.i	0.9981	0.8971	pu-sol-therm-011-164.i	0.9981	0.8952
pu-sol-therm-011-163.i	0.9981	0.8908	pu-sol-therm-011-163.i	0.9981	0.8888
pu-sol-therm-003-007.i	0.9980	0.8740	pu-sol-therm-003-007.i	0.998	0.8717
pu-sol-therm-003-002.i	0.9975	0.7695	pu-sol-therm-003-002.i	0.9975	0.7653
pu-sol-therm-003-001.i	0.9975	0.7625	pu-sol-therm-003-001.i	0.9975	0.7581
pu-sol-therm-003-003.i	0.9973	0.7147	pu-sol-therm-003-003.i	0.9973	0.7095
pu-sol-therm-003-004.i	0.9973	0.7037	pu-sol-therm-003-004.i	0.9973	0.6983
pu-sol-therm-002-001.i	0.9972	0.7017	pu-sol-therm-002-001.i	0.9972	0.6963
pu-sol-therm-010-012.i	0.9971	0.6633	pu-sol-therm-010-012.i	0.9971	0.6572
pu-sol-therm-010-006.i	0.9970	0.6533	pu-sol-therm-010-006.i	0.997	0.6470
pu-sol-therm-003-005.i	0.9970	0.6495	pu-sol-therm-003-005.i	0.997	0.6431
pu-sol-therm-002-002.i	0.9970	0.6430	pu-sol-therm-002-002.i	0.997	0.6365
pu-sol-therm-011-165.i	0.9969	0.6332	pu-sol-therm-011-165.i	0.9969	0.6265
pu-sol-therm-010-011.i	0.9969	0.6132	pu-sol-therm-010-011.i	0.9969	0.6062
pu-sol-therm-010-010.i	0.9969	0.6127	pu-sol-therm-010-010.i	0.9969	0.6056
pu-sol-therm-003-006.i	0.9966	0.5627	pu-sol-therm-003-006.i	0.9966	0.5547
			pu-sol-therm-010-013.i	**0.9966**	**0.5481**
pu-sol-therm-010-007.i	0.9966	0.5454	pu-sol-therm-010-007.i	0.9966	0.5371
pu-sol-therm-002-003.i	0.9963	0.4993	pu-sol-therm-002-003.i	0.9963	0.4902
pu-sol-therm-010-003.i	0.9963	0.4796	pu-sol-therm-010-003.i	0.9963	0.4701

pu-sol-therm-010-005.i	0.9962	0.4742	pu-sol-therm-010-005.i	0.9962	0.4646
pu-sol-therm-004-002.i	0.9958	0.3822	pu-sol-therm-004-002.i	0.9958	0.3709
pu-sol-therm-005-003.i	0.9958	0.3791	pu-sol-therm-005-003.i	0.9958	0.3678
pu-sol-therm-004-012.i	0.9958	0.3682	pu-sol-therm-004-012.i	0.9958	0.3567
pu-sol-therm-004-003.i	0.9958	0.3680	pu-sol-therm-004-003.i	0.9958	0.3564
pu-sol-therm-004-004.i	0.9958	0.3673	pu-sol-therm-004-004.i	0.9958	0.3558
pu-sol-therm-004-008.i	0.9957	0.3609	pu-sol-therm-004-008.i	0.9957	0.3492
pu-sol-therm-010-004.i	0.9957	0.3590	pu-sol-therm-010-004.i	0.9957	0.3472
pu-sol-therm-002-004.i	0.9957	0.3536	pu-sol-therm-002-004.i	0.9957	0.3418
pu-sol-therm-005-004.i	0.9957	0.3433	pu-sol-therm-005-004.i	0.9957	0.3313
pu-sol-therm-005-001.i	0.9956	0.3406	pu-sol-therm-005-001.i	0.9956	0.3286
pu-sol-therm-004-009.i	0.9956	0.3399	pu-sol-therm-004-009.i	0.9956	0.3279
pu-sol-therm-004-007.i	0.9956	0.3386	pu-sol-therm-004-007.i	0.9956	0.3265
pu-sol-therm-005-009.i	0.9956	0.3306	pu-sol-therm-005-009.i	0.9956	0.3184
pu-sol-therm-005-002.i	0.9956	0.3290	pu-sol-therm-005-002.i	0.9956	0.3167
pu-sol-therm-010-009.i	0.9956	0.3270	pu-sol-therm-010-009.i	0.9956	0.3147
pu-sol-therm-004-013.i	0.9956	0.3221	pu-sol-therm-004-013.i	0.9956	0.3097
pu-sol-therm-004-001.i	0.9955	0.3142	pu-sol-therm-004-001.i	0.9955	0.3017
pu-sol-therm-004-005.i	0.9955	0.3017	pu-sol-therm-004-005.i	0.9955	0.2890
pu-sol-therm-005-008.i	0.9954	0.2953	pu-sol-therm-005-008.i	0.9954	0.2825
pu-sol-therm-004-006.i	0.9954	0.2917	pu-sol-therm-004-006.i	0.9954	0.2788
pu-sol-therm-005-005.i	0.9954	0.2759	pu-sol-therm-005-005.i	0.9954	0.2627
pu-sol-therm-004-010.i	0.9953	0.2663	pu-sol-therm-004-010.i	0.9953	0.2529
pu-sol-therm-005-006.i	0.9953	0.2576	pu-sol-therm-005-006.i	0.9953	0.2441
pu-sol-therm-002-005.i	0.9951	0.2238	pu-sol-therm-002-005.i	0.9951	0.2096
pu-sol-therm-010-014.i	0.9951	0.2158	pu-sol-therm-010-014.i	0.9951	0.2014
pu-sol-therm-004-011.i	0.995	0.2009	pu-sol-therm-004-011.i	0.9950	0.1863
pu-sol-therm-001-001.i	0.9949	0.1856	pu-sol-therm-001-001.i	0.9949	0.1707
pu-sol-therm-010-008.i	0.9948	0.1558	pu-sol-therm-010-008.i	0.9948	0.1404
pu-sol-therm-005-007.i	0.9948	0.1457	pu-sol-therm-005-007.i	0.9948	0.1301
pu-sol-therm-011-184.i	0.9944	0.0549	pu-sol-therm-011-184.i	0.9944	0.0377
pu-sol-therm-011-186.i	0.9944	0.0530	pu-sol-therm-011-186.i	0.9944	0.0357
pu-sol-therm-011-187.i	0.9943	0.0506	pu-sol-therm-011-187.i	0.9943	0.0333
pu-sol-therm-010-002.i	0.9943	0.0462	pu-sol-therm-010-002.i	0.9943	0.0287

Table 3. Critical Benchmark Experiment outliers chosen as neutronically similar to plutonium-metal water mixture "solution" application cases when included in the Whisper benchmark collection

Benchmark Outlier	Times Benchmark is Neutronically Similar to Application	Maximum c_k
pu-sol-therm-009-003.i	7	0.9727
pu-sol-therm-010-001.i	445	0.9945
pu-sol-therm-010-013.i	297	0.9974
pu-sol-therm-012-006.i	0	n/a
pu-sol-therm-012-007.i	0	n/a
pu-sol-therm-018-002.i	0	n/a

pu-sol-therm-028-001.i	218	0.9445
pu-sol-therm-028-002.i	178	0.932
pu-sol-therm-028-003.i	0	n/a
pu-sol-therm-028-004.i	0	n/a
pu-sol-therm-028-005.i	0	n/a
pu-sol-therm-028-006.i	19	0.9828
pu-sol-therm-028-007.i	0	n/a
pu-sol-therm-028-008.i	0	n/a
pu-sol-therm-028-009.i	0	n/a
mix-sol-therm-001-003.i	0	n/a
mix-sol-therm-001-004.i	0	n/a
mix-sol-therm-001-011.i	0	n/a
mix-sol-therm-003-001.i	243	0.9605
mix-sol-therm-003-002.i	272	0.9664
mix-sol-therm-003-003.i	255	0.9517
mix-sol-therm-003-004.i	145	0.9253
mix-sol-therm-003-006.i	34	0.994
mix-sol-therm-003-007.i	33	0.9929
	Total Times Similar = 2146	**Overall Max. C_k = 0.9974**

Pu Oxide Cases

The plutonium oxide cases were conducted as a parameter study to cover a range of applicable process models. The process models consisted of three right circular cylinders of plutonium oxide-water mixture on a stainless steel floor reflected radially by 1-inch thick water to represent personnel and incidental reflection. The three identical cylinders were placed touching in a triangular pattern with their bases sitting on the ½-inch thick stainless steel floor. The plutonium was modeled as 100% ^{239}Pu. The mass of the Pu oxide-water mix is fixed at 3500 g. The oxide-water mix has a varied water atomic fraction from 1e-6 (effectively zero for a dry powder) to 0.999 (which looks like a solution). This corresponds to varying the concentration of the plutonium from 1014.2 to 1.32 g/L. The density of the oxide-water mix is a linear combination of theoretical density oxide at 11.5 g/cm^3 and water at 1.0 g/cm^3. The H/D ratio of the cylinders was kept constant at 1.6. Parameterizing the oxide-water mix concentration per cylinder as described resulted in 106 different cases.

MCNP6.2 was used to determine k-effective, the average energy of neutrons causing fission, the energy of the average lethargy of neutrons causing fission, and sensitivity profiles for each of the 106 process model cases. The results are shown below in Figures 16 and 17. Whisper-1.1 was used to find benchmarks neutronically similar to each process model case using sensitivity profiles, determine the calculational margin and portions of the margin of subcriticality leading to the baseline USL.

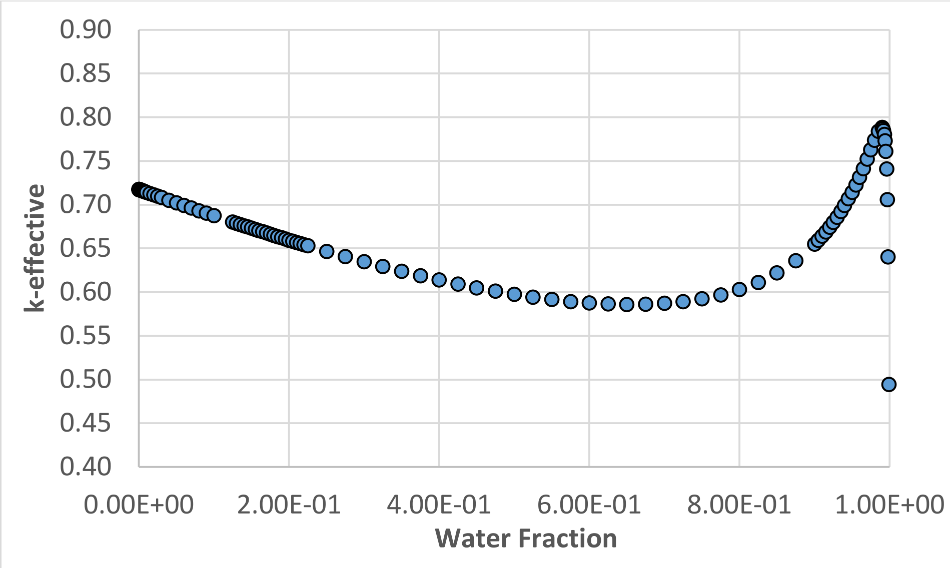

Figure 16. MCNP6.2 k-effective results for Pu oxide-water mixture cases

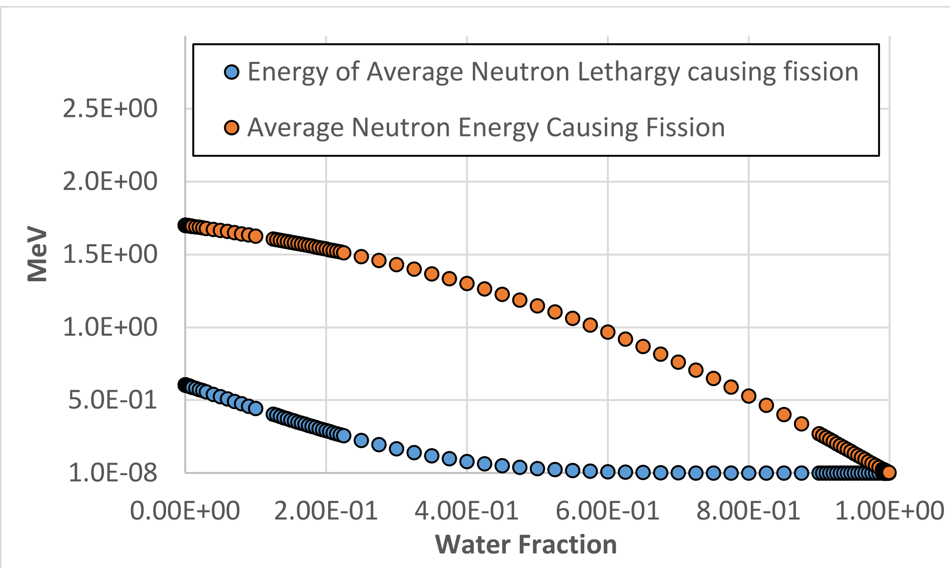

Figure 17. MCNP6.2 ANECF and EALF results for Pu oxide-water mixture cases

The results for the Whisper-1.1 baseline USL are reported below. A separate USL was computed for each process model case using a benchmark collection with exclusions based upon the iterative diagonal chi-squared rejection method. Then the baseline USL was computed for each process model case using a benchmark collection consisting of all 1101 benchmark experiments contained in the Whisper-1.1 library. The results are shown below in Figures 18-21. The largest difference in the baseline USL when comparing results with a full set of all benchmarks in the Whisper collection versus results when using a reduced set of benchmarks due to statistical rejection, $USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}}$ = -0.00234 for the case with water fraction 0.945. It should be noted that in this case, and all oxide-water mix cases where the water fraction is ≥ 0.3, it is non-conservative to include all benchmarks because the baseline USL is actually higher when including all benchmarks. For the case with water fraction = 0.945

the recommended baseline USL is 0.97429 when rejecting benchmark outliers and 0.97663 when including all benchmarks. A comparison of similar benchmarks for this case is studied to attempt to determine the specific benchmarks leading to the baseline USL differences, the results of which are shown in Table 4.

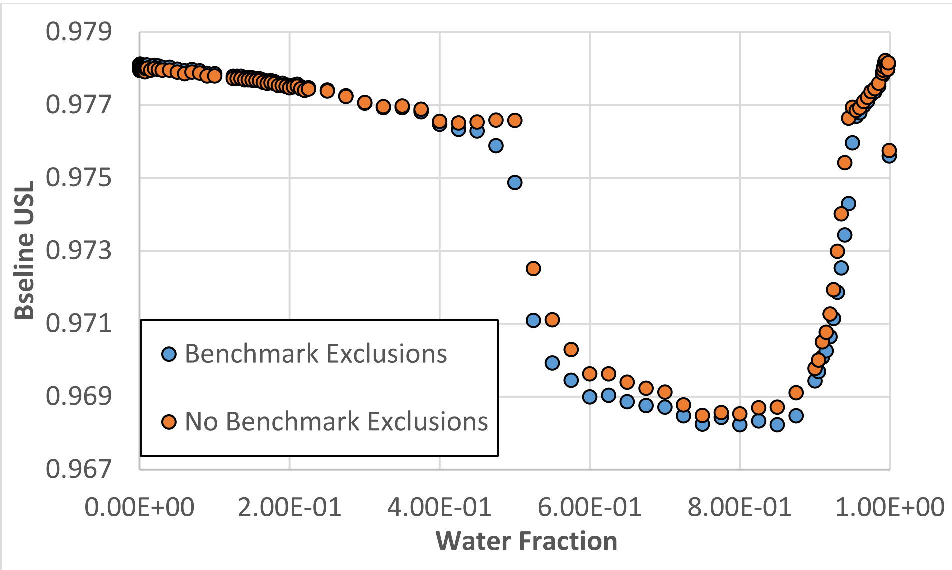

Figure 18. Whisper-1.1 baseline USL results for Pu metal-oxide mixture cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The calculational margin (bias and bias uncertainty) calculated by Whisper is shown below in Figure 19. The calculational margin is slightly smaller when there are no benchmark exclusions for water fraction ≥0.3. The difference between the calculational margin when excluding benchmarks and the baseline USL when using all benchmarks in the library ranges from -0.0001 to 0.00234. The magnitude of the difference in the baseline USL computed by Whisper when using all benchmarks versus the baseline USL computed by Whisper when excluding outliers is due to the calculational margin (bias and bias uncertainty) and not due to the margin of subcriticality for to nuclear data.

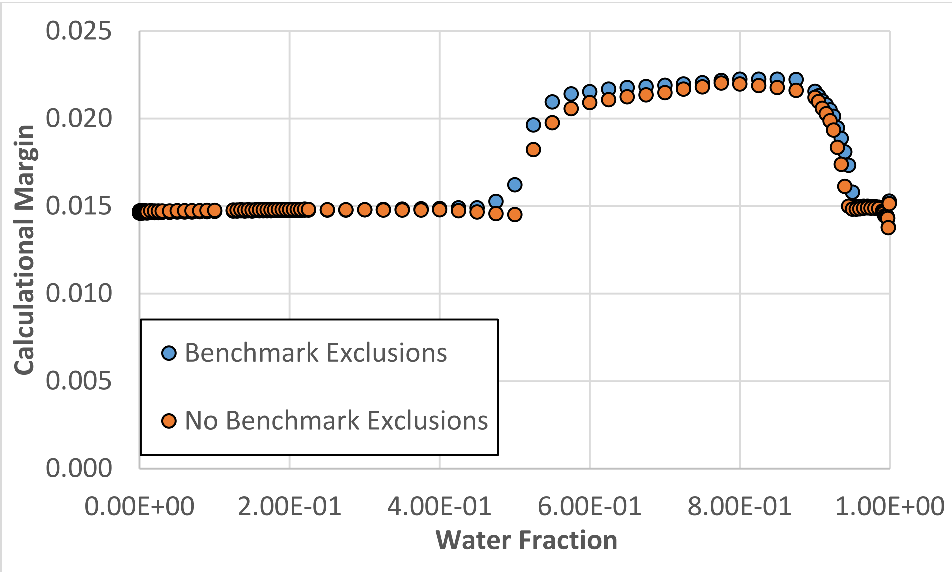

Figure 19. Whisper-1.1 calculational margin results for Pu metal-oxide mixture cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The margin of subcriticality due to nuclear data uncertainty is shown below in Figure 20. The $MOS_{nuclear\ data}$ is calculated from the sensitivity profile created by MCNP6.2 and the nuclear data covariances. GLLS adjustment of nuclear data covariances may be influenced by the benchmark collection. Therefore, two studies of nuclear data covariance adjustment were done. The initial study was conducted using the reduced benchmark set that does not include rejected outliers. In the subsequent study, Whisper nuclear data covariance adjustment was also done using the entire benchmark suite, keeping the benchmarks that were found to be outliers in the set. It was found that there are insignificant differences in the $MOS_{nuclear\ data}$ computed by Whisper whether or not the benchmark collection excludes outliers. For this reason the $MOS_{nuclear\ data}$ is the same for the case in which all benchmarks in the library are used versus the case in which benchmarks may be excluded based upon statistical rejection. Differences in the Whisper USLs generated when using a benchmark suite that excludes outliers versus the Whisper USLs generated when using a benchmark suite containing the entire library of 1101 benchmarks is due to differences in the Whisper calculational margin and not the $MOS_{nuclear\ data}$.

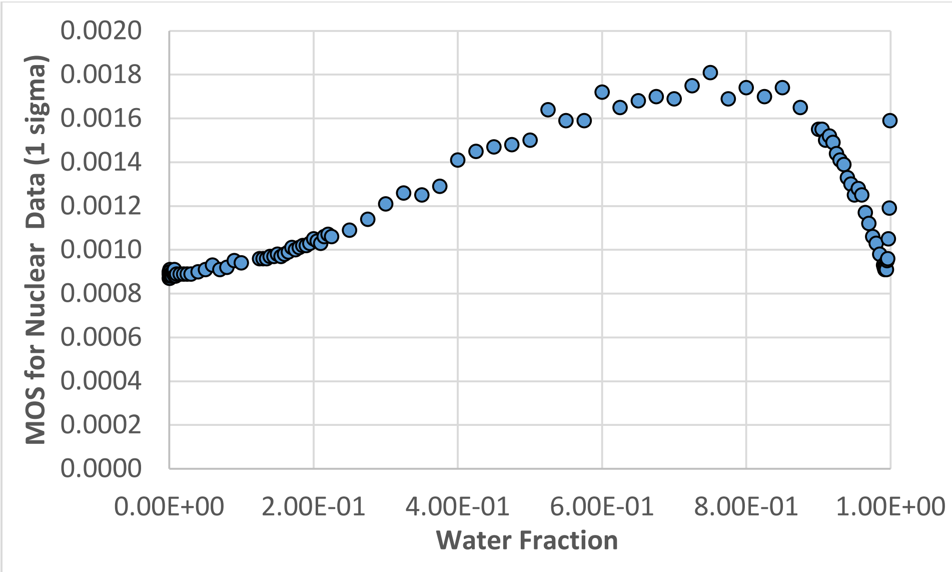

Figure 20. Whisper-1.1 margin of subcriticality for nuclear data uncertainty results for Pu metal-oxide mixture cases (using MCNP6.2 calculations with 100,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

The preceding results are for MCNP6.2 calculations with 100,000 neutrons per cycle. For comparison the results shown in Figure 21 below were done with 10,000 neutrons per cycle. While the magnitude of the difference in USL when excluding benchmarks vs. including all benchmarks is the about same, $USL_{Benchmark\ Exclusions} - USL_{No\ Benchmark\ Exclusions}$ = -0.00157, the variation in the baseline USL between individual cases is greater. When calculating the baseline USL and excluding benchmarks based upon statistical rejection the lowest baseline USL = 0.96799 and the highest 0.97817. When including all benchmarks the lowest baseline USL = 0.96821 and the highest = 0.97819.

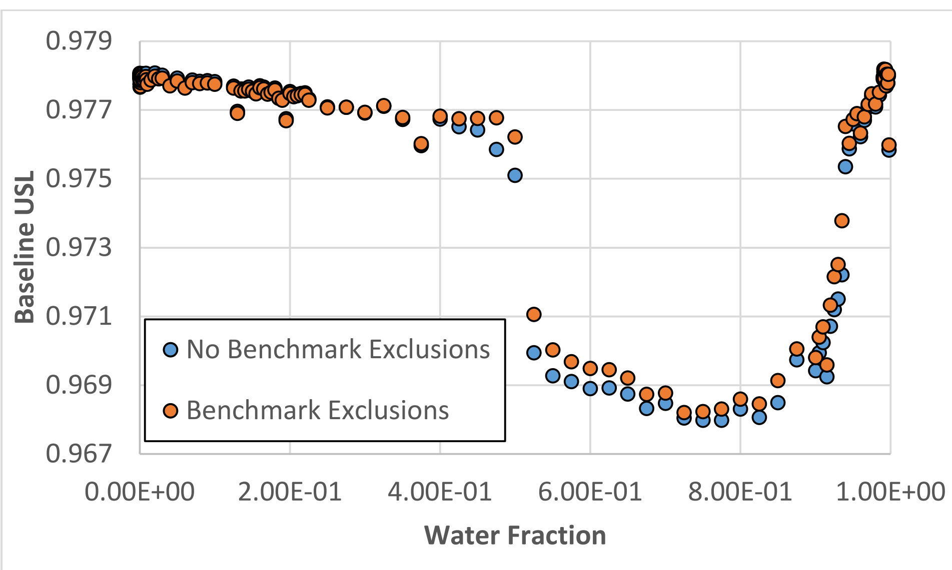

Figure 21. Whisper-1.1 calculational margin results for Pu metal-oxide mixture cases (using MCNP6.2 calculations with 10,000 neutrons per cycle) when using all benchmarks in the collection versus excluding benchmark outliers based upon statistical rejection.

It is important to note that only a subset of the benchmarks in the collection, enough found to be neutronically similar for valid statistical analysis in each case, are used to compute the baseline USL. For the plutonium oxide-water mixture cases the energy spectrum ranges from fast to intermediate and thermal depending on the amount of water in the mixture, and the series of relevant benchmark experiments are those from PU-COMP-MIXED, PU-MET-FAST, MIX-MET-FAST, PU-SOL-THERM, and MIX-SOL-THERM. From those sets of experiments there are forty-four benchmark experiments which were found to be statistical outliers and they are shown in Table 4, with the number of times chosen as neutronically similar to an application and the highest correlation coefficient. A $c_k = 1$ implies perfect correlation and many of the benchmarks in Table 4 are found to be highly correlated, or to have high neutronic similarity, to the plutonium-oxide water mixture application cases.

The maximum magnitude $USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00234$ occurred in Case 88. A comparison table for Case 88 is shown below in Table 1, with benchmarks which would have been excluded based upon the statistical rejection method shown in bold text.

Table 4. Critical Benchmark Experiment outliers chosen as neutronically similar to plutonium-oxide water mixture application cases when included in the Whisper benchmark collection

Benchmark Outlier	Times Benchmark is Neutronically Similar to Application	Maximum c_k
mix-met-fast-007-002.i	0	n/a
mix-sol-therm-001-003.i	9	0.8376
mix-sol-therm-001-004.i	5	0.7581
mix-sol-therm-001-011.i	0	n/a
mix-sol-therm-003-001.i	32	0.9715
mix-sol-therm-003-002.i	33	0.9728
mix-sol-therm-003-003.i	30	0.962
mix-sol-therm-003-004.i	28	0.9561
mix-sol-therm-003-006.i	3	0.721
mix-sol-therm-003-007.i	0	n/a
pu-comp-mixed-001-001.i	60	0.9549
pu-comp-mixed-001-002.i	17	0.9469
pu-comp-mixed-001-003.i	27	0.9549
pu-comp-mixed-002-001.i	25	0.9414
pu-comp-mixed-002-002.i	21	0.9382
pu-comp-mixed-002-003.i	19	0.9318
pu-comp-mixed-002-004.i	18	0.9273
pu-comp-mixed-002-005.i	18	0.9162
pu-comp-mixed-002-006.i	17	0.9335
pu-comp-mixed-002-010.i	25	0.9342
pu-comp-mixed-002-011.i	26	0.9402
pu-comp-mixed-002-012.i	29	0.9454
pu-comp-mixed-002-013.i	29	0.9494
pu-comp-mixed-002-014.i	29	0.9495
pu-comp-mixed-002-015.i	29	0.9501
pu-comp-mixed-002-016.i	29	0.9456
pu-met-fast-016-001.i	35	0.9355

pu-met-fast-039-001.i	66	0.9648
pu-met-fast-041-001.i	0	n/a
pu-sol-therm-009-003.i	0	n/a
pu-sol-therm-010-001.i	39	0.987
pu-sol-therm-010-013.i	23	0.9787
pu-sol-therm-012-006.i	7	0.7863
pu-sol-therm-012-007.i	5	0.7627
pu-sol-therm-018-002.i	0	n/a
pu-sol-therm-028-001.i	30	0.9598
pu-sol-therm-028-002.i	24	0.9563
pu-sol-therm-028-003.i	10	0.8416
pu-sol-therm-028-004.i	5	0.7623
pu-sol-therm-028-005.i	3	0.7237
pu-sol-therm-028-006.i	0	n/a
pu-sol-therm-028-007.i	6	0.7888
pu-sol-therm-028-008.i	5	0.7603
pu-sol-therm-028-009.i	1	0.6741
	Total Times Similar = 817	**Overall Max. c_k = 0.987**

Table 5. Comparison of Whisper output for plutonium-oxide water mixture case with the greatest difference in baseline USL, Case 88 [corresponding to 0.945 atom fraction water], with and without exclusions based upon statistical rejection of the benchmark collection. Excluded benchmarks using statistical rejection technique shown in bold text.

Benchmark Exclusions			**No Benchmark Exclusions**		
Baseline USL = 0.97429			Baseline USL = 0.97663		
Bias = 0.00692			Bias = 0.00612		
Bias Uncertainty = 0.01042			Bias Uncertainty = 0.00888		
Nuclear Data Uncertainty = 0.0013			Nuclear Data Uncertainty = 0.0013		
Benchmark	**C_k**	**Weight**	**Benchmark**	**C_k**	**Weight**
pu-sol-therm-007-003.i	0.9697	1.0000	pu-sol-therm-007-003.i	0.9697	1.0000
pu-sol-therm-001-006.i	0.9685	0.9759	pu-sol-therm-001-006.i	0.9685	0.9724
pu-sol-therm-007-002.i	0.9683	0.9708	pu-sol-therm-007-002.i	0.9683	0.9666
pu-sol-therm-001-005.i	0.9641	0.8866	pu-sol-therm-001-005.i	0.9641	0.8703
pu-sol-therm-001-004.i	0.9635	0.8742	pu-sol-therm-001-004.i	0.9635	0.8560
pu-sol-therm-001-003.i	0.9620	0.8425	pu-sol-therm-001-003.i	0.9620	0.8198
pu-sol-therm-007-008.i	0.9612	0.8269	pu-sol-therm-007-008.i	0.9612	0.8020
pu-sol-therm-007-009.i	0.9612	0.8264	pu-sol-therm-007-009.i	0.9612	0.8014
pu-sol-therm-007-007.i	0.9608	0.8180	pu-sol-therm-007-007.i	0.9608	0.7917
pu-sol-therm-007-006.i	0.9608	0.8176	pu-sol-therm-007-006.i	0.9608	0.7913
pu-sol-therm-007-010.i	0.9601	0.8042	pu-sol-therm-007-010.i	0.9601	0.7760
pu-sol-therm-007-005.i	0.9599	0.7993	pu-sol-therm-007-005.i	0.9599	0.7704
pu-sol-therm-001-002.i	0.9596	0.7930	pu-sol-therm-001-002.i	0.9596	0.7631
			pu-sol-therm-010-001.i	**0.9587**	**0.7435**
pu-sol-therm-002-007.i	0.9564	0.7289	pu-sol-therm-002-007.i	0.9564	0.6898
pu-sol-therm-002-006.i	0.9553	0.7066	pu-sol-therm-002-006.i	0.9553	0.6643
pu-sol-therm-001-001.i	0.9545	0.6890	pu-sol-therm-001-001.i	0.9545	0.6441

pu-sol-therm-010-002.i	0.9526	0.6510	pu-sol-therm-010-002.i	0.9526	0.6007
pu-sol-therm-002-005.i	0.9514	0.6268	pu-sol-therm-002-005.i	0.9514	0.573
pu-sol-therm-002-004.i	0.9501	0.5989	pu-sol-therm-002-004.i	0.9501	0.5411
pu-sol-therm-010-009.i	0.9500	0.5982	pu-sol-therm-010-009.i	0.95	0.5403
pu-sol-therm-002-003.i	0.9492	0.5811	pu-sol-therm-002-003.i	0.9492	0.5207
			pu-comp-mixed-002-015.i	**0.9476**	**0.4828**
			pu-comp-mixed-002-014.i	**0.9473**	**0.4753**
			pu-comp-mixed-002-013.i	**0.9472**	**0.4733**
pu-sol-therm-002-002.i	0.9457	0.5094	pu-sol-therm-002-002.i	0.9457	0.4387
pu-sol-therm-011-165.i	0.9456	0.5075	pu-sol-therm-011-165.i	0.9456	0.4366
pu-sol-therm-010-004.i	0.9447	0.4897	pu-sol-therm-010-004.i	0.9447	0.4162
pu-sol-therm-034-001.i	0.9443	0.4809	pu-sol-therm-034-001.i	0.9443	0.4060
pu-sol-therm-002-001.i	0.9442	0.4788	pu-sol-therm-002-001.i	0.9442	0.4037
pu-sol-therm-010-003.i	0.9436	0.4659	pu-sol-therm-010-003.i	0.9436	0.3889
			pu-comp-mixed-002-016.i	**0.9435**	**0.3873**
			pu-comp-mixed-001-003.i	**0.9433**	**0.3831**
			pu-comp-mixed-002-012.i	**0.9432**	**0.3800**
			mix-sol-therm-003-002.i	**0.9426**	**0.3657**
pu-sol-therm-010-010.i	0.9424	0.4413	pu-sol-therm-010-010.i	0.9424	0.3608
pu-sol-therm-010-011.i	0.9413	0.4185	pu-sol-therm-010-011.i	0.9413	0.3346
			mix-sol-therm-003-001.i	**0.9404**	**0.3140**
pu-sol-therm-010-006.i	0.9403	0.3998	pu-sol-therm-010-006.i	0.9403	0.3133
pu-sol-therm-011-164.i	0.9398	0.3883	pu-sol-therm-011-164.i	0.9398	0.3001
pu-sol-therm-010-005.i	0.9397	0.3874	pu-sol-therm-010-005.i	0.9397	0.2991
pu-sol-therm-003-006.i	0.9389	0.3697	pu-sol-therm-003-006.i	0.9389	0.2789
			pu-comp-mixed-002-011.i	**0.9387**	**0.2756**
pu-sol-therm-011-163.i	0.9387	0.3666	pu-sol-therm-011-163.i	0.9387	0.2753
			mix-sol-therm-003-003.i	**0.9385**	**0.2710**
pu-sol-therm-011-162.i	0.9375	0.3419	pu-sol-therm-011-162.i	0.9375	0.2471
pu-sol-therm-011-161.i	0.9366	0.3229	pu-sol-therm-011-161.i	0.9366	0.2253
pu-sol-therm-010-012.i	0.9362	0.3143	pu-sol-therm-010-012.i	0.9362	0.2155
mix-sol-therm-001-007.i	0.9357	0.3046	mix-sol-therm-001-007.i	0.9357	0.2044
pu-sol-therm-010-007.i	0.9354	0.2978	pu-sol-therm-010-007.i	0.9354	0.1966
pu-sol-therm-003-005.i	0.9352	0.2935	pu-sol-therm-003-005.i	0.9352	0.1917
			pu-sol-therm-028-001.i	**0.9347**	**0.1814**
pu-sol-therm-003-008.i	0.9333	0.2553	pu-sol-therm-003-008.i	0.9333	0.1479
			pu-comp-mixed-002-010.i	**0.9330**	**0.1410**
pu-sol-therm-004-011.i	0.9328	0.2463	pu-sol-therm-004-011.i	0.9328	0.1377
pu-sol-therm-003-004.i	0.9328	0.2451	pu-sol-therm-003-004.i	0.9328	0.1363
mix-sol-therm-001-008.i	0.9321	0.2308	mix-sol-therm-001-008.i	0.9321	0.1200
pu-sol-therm-005-007.i	0.9319	0.2272	pu-sol-therm-005-007.i	0.9319	0.1158
			mix-sol-therm-003-004.i	**0.9317**	**0.1113**
pu-sol-therm-003-003.i	0.9316	0.2219	pu-sol-therm-003-003.i	0.9316	0.1097
pu-sol-therm-003-007.i	0.9309	0.2062	pu-sol-therm-003-007.i	0.9309	0.0918
pu-comp-mixed-002-020.i	0.9301	0.1912	pu-comp-mixed-002-020.i	0.9301	0.0747
pu-sol-therm-003-002.i	0.9300	0.1892	pu-sol-therm-003-002.i	0.9300	0.0723

			pu-sol-therm-028-002.i	**0.9300**	**0.0721**
pu-sol-therm-005-006.i	0.9296	0.1806	pu-sol-therm-005-006.i	0.9296	0.0625
pu-comp-mixed-002-021.i	0.9292	0.1714	pu-comp-mixed-002-021.i	0.9292	0.0519
pu-sol-therm-032-001.i	0.9288	0.1637	pu-sol-therm-032-001.i	0.9288	0.0432
pu-comp-mixed-002-019.i	0.9287	0.1609	pu-comp-mixed-002-019.i	0.9287	0.0400
pu-sol-therm-003-001.i	0.9285	0.1581	pu-sol-therm-003-001.i	0.9285	0.0368
pu-sol-therm-034-002.i	0.9281	0.1499	pu-sol-therm-034-002.i	0.9281	0.0274
			pu-sol-therm-010-013.i	**0.9277**	**0.0168**
pu-comp-mixed-001-004.i	0.9274	0.1353	pu-comp-mixed-001-004.i	0.9274	0.0107
pu-sol-therm-004-010.i	0.9269	0.1238			
pu-sol-therm-010-008.i	0.9265	0.1159			
pu-comp-mixed-002-018.i	0.9264	0.1146			
pu-sol-therm-005-005.i	0.9259	0.1038			
pu-comp-mixed-002-022.i	0.9257	0.1010			
pu-sol-therm-022-001.i	0.9256	0.0974			
pu-sol-therm-032-002.i	0.9253	0.0930			
pu-sol-therm-005-004.i	0.9233	0.0521			
mix-sol-therm-001-006.i	0.9231	0.0461			
pu-sol-therm-022-002.i	0.9224	0.0332			
pu-sol-therm-004-009.i	0.9216	0.0172			
pu-sol-therm-034-007.i	0.9213	0.0110			

Summary

A comparison study has been done to compute USLs with and without statistical outliers in the Whisper-1.1 benchmark collection to determine what effect rejection of statistical outliers has on the recommended USL. The effect of exclusion of benchmarks which are found to be statistical outliers from the collection of benchmarks used by Whisper-1.1 on nuclear criticality safety validation for ^{239}Pu is found to be small. The results show little overall difference in the recommended baseline USLs developed by Whisper when excluding statistical outliers. Additionally, there does not appear to be a clear trend in predicting whether the baseline USL will be higher or lower when rejecting statistical outliers from the benchmark critical experiment collection used for validation.

The baseline recommended USL, calculational margin and margin of subcriticality for nuclear data uncertainty was presented for many plutonium application cases ranging from fast metal systems to intermediate moist oxide systems to thermal solution systems. Results show there is little difference in baseline USL when using a reduced benchmark collection due to statistical rejection of outliers. Overall maximum difference in baseline USL between the two methods:

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = 0.00021$ for plutonium metal systems,

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00234$ for plutonium oxide systems, and

$USL_{\text{Benchmark Exclusions}} - USL_{\text{No Benchmark Exclusions}} = -0.00026$ for plutonium solution systems.

There is slight nonconservatism, i.e., the baseline USL is greater, when including all the benchmarks in the Whisper-1.1 collection and not using the available statistical rejection technique to exclude benchmark outliers. The magnitude of the difference in the baseline USL computed by Whisper when using all benchmarks versus the baseline USL computed by Whisper when excluding outliers is due to the calculational margin (bias and bias uncertainty) and not due to the margin of subcriticality for to nuclear data.

References

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Appendix- Whisper-1.1 Benchmark Collection Relevant to Plutonium Systems

Table 6. Plutonium system benchmark experiments, bold text indicates benchmarks found to be statistical outliers.

Benchmark	k_{exp}	σ_{exp}	k_{calc}	σ_{calc}	Bias	Bias uncert.
mix-comp-fast-001-001.i	0.9866	0.0023	0.98716	0.00007	-0.00056	0.0023
mix-comp-fast-002-001.i	0.9874	0.0022	0.98544	0.00007	0.00196	0.0022
mix-comp-inter-005-001.i	1.1602	0.0055	1.16715	0.00009	-0.00695	0.0055
mix-comp-therm-001-001.i	1.0000	0.0025	1.00086	0.00012	-0.00086	0.0025
mix-comp-therm-001-002.i	1.0000	0.0026	0.99988	0.00011	0.00012	0.0026
mix-comp-therm-001-003.i	1.0000	0.0032	0.99968	0.00012	0.00032	0.0032
mix-comp-therm-001-004.i	1.0000	0.0039	1.00138	0.00011	-0.00138	0.0039
mix-comp-therm-002-001.i	1.0010	0.0059	1.00099	0.00011	0.00001	0.0059
mix-comp-therm-002-002.i	1.0009	0.0045	1.00155	0.00011	-0.00065	0.0045
mix-comp-therm-002-003.i	1.0024	0.0029	1.00242	0.00011	-0.00002	0.0029
mix-comp-therm-002-004.i	1.0024	0.0021	1.00594	0.00011	-0.00354	0.0021
mix-comp-therm-002-005.i	1.0038	0.0022	1.00348	0.0001	0.00032	0.0022
mix-comp-therm-003-001.i	1.0000	0.0071	1.0001	0.00011	-0.0001	0.0071
mix-comp-therm-003-002.i	1.0000	0.0057	1.00067	0.00012	-0.00067	0.0057
mix-comp-therm-003-003.i	1.0000	0.0052	1.00346	0.00013	-0.00346	0.0052
mix-comp-therm-003-004.i	1.0000	0.0024	1.00003	0.00012	-0.00003	0.0024
mix-comp-therm-003-005.i	1.0000	0.0028	1.0003	0.00011	-0.0003	0.0028
mix-comp-therm-003-006.i	1.0000	0.002	1.00096	0.00011	-0.00096	0.002
mix-met-fast-001-001.i	1.0000	0.0016	0.99951	0.00008	0.00049	0.0016
mix-met-fast-002-001.i	1.0000	0.0042	1.00529	0.0001	-0.00529	0.0042
mix-met-fast-002-002.i	1.0000	0.0044	1.0052	0.0001	-0.0052	0.0044
mix-met-fast-002-003.i	1.0000	0.0048	1.00549	0.0001	-0.00549	0.0048
mix-met-fast-003-001.i	0.9993	0.0017	1.0008	0.00009	-0.0015	0.0017
mix-met-fast-004-001.i	0.9993	0.0013	1.0005	0.00009	-0.0012	0.0013
mix-met-fast-004-002.i	0.9993	0.0013	0.99939	0.00009	-0.00009	0.0013
mix-met-fast-005-001.i	0.9990	0.0017	1.00393	0.00009	-0.00493	0.0017
mix-met-fast-007-001.i	1.0000	0.0045	1.00313	0.00011	-0.00313	0.0045
mix-met-fast-007-002.i	**1.0000**	**0.0023**	**1.00794**	**0.00011**	**-0.00794**	**0.0023**
mix-met-fast-007-003.i	1.0000	0.0028	1.00645	0.0001	-0.00645	0.0028
mix-met-fast-007-004.i	1.0000	0.0028	1.00536	0.0001	-0.00536	0.0028
mix-met-fast-007-005.i	1.0000	0.0032	1.00246	0.00009	-0.00246	0.0032
mix-met-fast-007-006.i	1.0000	0.0035	1.00101	0.00009	-0.00101	0.0035
mix-met-fast-007-007.i	1.0000	0.0032	1.00611	0.00011	-0.00611	0.0032
mix-met-fast-007-008.i	1.0000	0.003	1.00507	0.00011	-0.00507	0.003
mix-met-fast-007-009.i	1.0000	0.0028	1.0051	0.0001	-0.0051	0.0028
mix-met-fast-007-010.i	1.0000	0.0027	1.00506	0.0001	-0.00506	0.0027
mix-met-fast-007-011.i	1.0000	0.0026	1.00373	0.0001	-0.00373	0.0026
mix-met-fast-007-012.i	1.0000	0.003	1.00261	0.00009	-0.00261	0.003
mix-met-fast-007-013.i	1.0000	0.0033	1.00073	0.00009	-0.00073	0.0033
mix-met-fast-007-014.i	1.0000	0.0032	1.00804	0.0001	-0.00804	0.0032
mix-met-fast-007-015.i	1.0000	0.0032	1.00757	0.0001	-0.00757	0.0032

mix-met-fast-007-016.i	1.0000	0.0028	1.00588	0.00009	-0.00588	0.0028
mix-met-fast-007-017.i	1.0000	0.0028	1.00594	0.00009	-0.00594	0.0028
mix-met-fast-007-018.i	1.0000	0.003	1.00798	0.00009	-0.00798	0.003
mix-met-fast-007-019.i	1.0000	0.0034	1.00696	0.00009	-0.00696	0.0034
mix-met-fast-007-020.i	1.0000	0.003	1.00473	0.00009	-0.00473	0.003
mix-met-fast-007-021.i	1.0000	0.0031	1.00504	0.00009	-0.00504	0.0031
mix-met-fast-007-022.i	1.0000	0.003	1.00403	0.00009	-0.00403	0.003
mix-met-fast-007-023.i	1.0000	0.0028	1.00336	0.00009	-0.00336	0.0028
mix-met-fast-009-001.i	1.0000	0.001	1.00006	0.00008	-0.00006	0.001
mix-met-fast-010-001.i	1.0000	0.0009	0.9998	0.00009	0.0002	0.0009
mix-met-mixed-001-001.i	0.9991	0.0013	0.99973	0.00012	-0.00063	0.00131
mix-sol-therm-001-001.i	1.0000	0.0016	0.99514	0.00013	0.00486	0.00161
mix-sol-therm-001-002.i	1.0000	0.0016	0.99507	0.00012	0.00493	0.0016
mix-sol-therm-001-003.i	**1.0000**	**0.0016**	**0.98879**	**0.00013**	**0.01121**	**0.00161**
mix-sol-therm-001-004.i	**1.0000**	**0.0016**	**0.99435**	**0.00012**	**0.00565**	**0.0016**
mix-sol-therm-001-005.i	1.0000	0.0016	0.99793	0.00012	0.00207	0.0016
mix-sol-therm-001-006.i	1.0000	0.0016	0.99557	0.00012	0.00443	0.0016
mix-sol-therm-001-007.i	1.0000	0.0016	1.00026	0.00013	-0.00026	0.00161
mix-sol-therm-001-008.i	1.0000	0.0016	0.99963	0.00013	0.00037	0.00161
mix-sol-therm-001-009.i	1.0000	0.0016	0.99913	0.00012	0.00087	0.0016
mix-sol-therm-001-010.i	1.0000	0.0016	0.99971	0.00012	0.00029	0.0016
mix-sol-therm-001-011.i	**1.0000**	**0.0052**	**1.03581**	**0.00012**	**-0.03581**	**0.0052**
mix-sol-therm-003-001.i	**0.9985**	**0.002**	**1.0125**	**0.00013**	**-0.014**	**0.002**
mix-sol-therm-003-002.i	**0.9960**	**0.002**	**1.01012**	**0.00013**	**-0.01412**	**0.002**
mix-sol-therm-003-003.i	**0.9935**	**0.002**	**1.00927**	**0.00013**	**-0.01577**	**0.002**
mix-sol-therm-003-004.i	**0.9909**	**0.002**	**1.00201**	**0.00013**	**-0.01111**	**0.002**
mix-sol-therm-003-005.i	0.9981	0.0022	1.00386	0.00011	-0.00576	0.0022
mix-sol-therm-003-006.i	**0.9959**	**0.0022**	**1.00708**	**0.00012**	**-0.01118**	**0.0022**
mix-sol-therm-003-007.i	**0.9935**	**0.002**	**1.00231**	**0.00012**	**-0.00881**	**0.002**
mix-sol-therm-003-008.i	0.9988	0.0025	1.00655	0.00009	-0.00775	0.0025
mix-sol-therm-003-009.i	0.9958	0.0025	1.00328	0.0001	-0.00748	0.0025
mix-sol-therm-003-010.i	0.9964	0.0025	1.00337	0.00009	-0.00697	0.0025
pu-comp-fast-004-001.i	1.0004	0.0044	0.99324	0.00009	0.00716	0.0044
pu-comp-inter-001-001.i	1.0000	0.011	1.01174	0.00007	-0.01174	0.011
pu-comp-mixed-001-001.i	**0.9986**	**0.0041**	**1.02461**	**0.00009**	**-0.02601**	**0.0041**
pu-comp-mixed-001-002.i	**1.0000**	**0.0068**	**1.02764**	**0.00013**	**-0.02764**	**0.0068**
pu-comp-mixed-001-003.i	**0.9990**	**0.0067**	**1.02383**	**0.00015**	**-0.02483**	**0.0067**
pu-comp-mixed-001-004.i	1.0000	0.0066	0.99315	0.00014	0.00685	0.0066
pu-comp-mixed-001-005.i	0.9989	0.0072	1.00865	0.00014	-0.00975	0.0072
pu-comp-mixed-002-001.i	**0.9990**	**0.0046**	**1.0311**	**0.00012**	**-0.0321**	**0.0046**
pu-comp-mixed-002-002.i	**0.9990**	**0.0046**	**1.0294**	**0.00012**	**-0.0304**	**0.0046**
pu-comp-mixed-002-003.i	**0.9990**	**0.0046**	**1.02466**	**0.00011**	**-0.02566**	**0.0046**
pu-comp-mixed-002-004.i	**0.9990**	**0.0046**	**1.01474**	**0.00012**	**-0.01574**	**0.0046**
pu-comp-mixed-002-005.i	**0.9990**	**0.0046**	**1.01479**	**0.00012**	**-0.01579**	**0.0046**
pu-comp-mixed-002-006.i	**1.0000**	**0.0075**	**1.02531**	**0.00012**	**-0.02531**	**0.0075**
pu-comp-mixed-002-007.i	1.0000	0.0075	1.02368	0.00012	-0.02368	0.0075

pu-comp-mixed-002-008.i	1.0000	0.0075	1.02227	0.00013	-0.02227	0.0075
pu-comp-mixed-002-009.i	1.0000	0.0075	1.02258	0.00013	-0.02258	0.0075
pu-comp-mixed-002-010.i	**1.0000**	**0.0073**	**1.03211**	**0.00013**	**-0.03211**	**0.0073**
pu-comp-mixed-002-011.i	**1.0000**	**0.0073**	**1.02949**	**0.00013**	**-0.02949**	**0.0073**
pu-comp-mixed-002-012.i	**1.0000**	**0.0073**	**1.02973**	**0.00012**	**-0.02973**	**0.0073**
pu-comp-mixed-002-013.i	**1.0000**	**0.0073**	**1.02782**	**0.00014**	**-0.02782**	**0.0073**
pu-comp-mixed-002-014.i	**1.0000**	**0.0073**	**1.03191**	**0.00013**	**-0.03191**	**0.0073**
pu-comp-mixed-002-015.i	**1.0000**	**0.0073**	**1.02977**	**0.00013**	**-0.02977**	**0.0073**
pu-comp-mixed-002-016.i	**1.0000**	**0.0073**	**1.02553**	**0.00013**	**-0.02553**	**0.0073**
pu-comp-mixed-002-017.i	0.9988	0.0055	1.00738	0.00013	-0.00858	0.0055
pu-comp-mixed-002-018.i	0.9988	0.0055	1.01126	0.00012	-0.01246	0.0055
pu-comp-mixed-002-019.i	0.9988	0.0055	1.01046	0.00013	-0.01166	0.0055
pu-comp-mixed-002-020.i	0.9988	0.0055	1.0105	0.00013	-0.0117	0.0055
pu-comp-mixed-002-021.i	0.9988	0.0055	1.01119	0.00012	-0.01239	0.0055
pu-comp-mixed-002-022.i	0.9988	0.0055	1.01511	0.00013	-0.01631	0.0055
pu-comp-mixed-002-023.i	1.0000	0.0068	1.0069	0.00012	-0.0069	0.0068
pu-comp-mixed-002-024.i	1.0000	0.0068	1.00761	0.00013	-0.00761	0.0068
pu-comp-mixed-002-025.i	1.0000	0.0068	1.00764	0.00014	-0.00764	0.0068
pu-comp-mixed-002-026.i	1.0000	0.0068	1.00871	0.00014	-0.00871	0.0068
pu-comp-mixed-002-027.i	1.0000	0.0068	1.00917	0.00013	-0.00917	0.0068
pu-comp-mixed-002-028.i	1.0000	0.0068	1.00916	0.00013	-0.00916	0.0068
pu-comp-mixed-002-029.i	1.0000	0.0068	1.01014	0.00013	-0.01014	0.0068
pu-met-fast-001-001.i	1.0000	0.002	1.00001	0.00008	-0.00001	0.002
pu-met-fast-002-001.i	1.0000	0.002	1	0.00008	0	0.002
pu-met-fast-003-103.i	1.0000	0.003	0.99873	0.00009	0.00127	0.003
pu-met-fast-005-001.i	1.0000	0.0013	1.00125	0.00009	-0.00125	0.0013
pu-met-fast-006-001.i	1.0000	0.003	1.00107	0.0001	-0.00107	0.003
pu-met-fast-008-001.i	1.0000	0.0006	0.99814	0.00008	0.00186	0.00061
pu-met-fast-009-001.i	1.0000	0.0027	1.00573	0.00009	-0.00573	0.0027
pu-met-fast-010-001.i	1.0000	0.0018	0.99968	0.00009	0.00032	0.0018
pu-met-fast-011-001.i	1.0000	0.001	1.00014	0.00011	-0.00014	0.00101
pu-met-fast-012-001.i	1.0009	0.0021	1.003	0.0001	-0.0021	0.0021
pu-met-fast-013-001.i	1.0034	0.0023	1.0082	0.00009	-0.0048	0.0023
pu-met-fast-014-001.i	1.0037	0.0031	1.00646	0.0001	-0.00276	0.0031
pu-met-fast-015-001.i	1.0041	0.0026	0.99995	0.00009	0.00415	0.0026
pu-met-fast-016-001.i	**0.9976**	**0.0042**	**1.01764**	**0.00012**	**-0.02004**	**0.0042**
pu-met-fast-016-002.i	1.0000	0.0038	1.00711	0.00011	-0.00711	0.0038
pu-met-fast-016-003.i	1.0000	0.0033	1.00513	0.00011	-0.00513	0.0033
pu-met-fast-016-004.i	1.0000	0.003	1.00478	0.00011	-0.00478	0.003
pu-met-fast-016-005.i	1.0000	0.0034	1.00455	0.00011	-0.00455	0.0034
pu-met-fast-016-006.i	1.0000	0.0032	1.00681	0.0001	-0.00681	0.0032
pu-met-fast-018-001.i	1.0000	0.003	0.99942	0.0001	0.00058	0.003
pu-met-fast-019-001.i	0.9992	0.0015	1.00098	0.0001	-0.00178	0.0015
pu-met-fast-020-001.i	0.9993	0.0017	0.99789	0.00009	0.00141	0.0017
pu-met-fast-021-001.i	1.0000	0.0026	1.00458	0.00009	-0.00458	0.0026
pu-met-fast-021-002.i	1.0000	0.0026	0.99341	0.0001	0.00659	0.0026

pu-met-fast-022-001.i	1.0000	0.0021	0.9983	0.00008	0.0017	0.0021
pu-met-fast-023-001.i	1.0000	0.0022	0.99998	0.00009	0.00002	0.0022
pu-met-fast-024-001.i	1.0000	0.0022	1.00176	0.00009	-0.00176	0.0022
pu-met-fast-025-001.i	1.0000	0.0022	0.99886	0.00009	0.00114	0.0022
pu-met-fast-026-001.i	1.0000	0.0022	0.99867	0.00009	0.00133	0.0022
pu-met-fast-027-001.i	1.0000	0.0024	1.00321	0.0001	-0.00321	0.0024
pu-met-fast-028-001.i	1.0000	0.0024	0.99911	0.00009	0.00089	0.0024
pu-met-fast-029-001.i	1.0000	0.0024	0.9958	0.00008	0.0042	0.0024
pu-met-fast-030-001.i	1.0000	0.0023	1.00325	0.00009	-0.00325	0.0023
pu-met-fast-031-001.i	1.0000	0.0023	1.00441	0.0001	-0.00441	0.0023
pu-met-fast-032-001.i	1.0000	0.0022	0.99855	0.00009	0.00145	0.0022
pu-met-fast-035-001.i	1.0000	0.0016	0.9977	0.00008	0.0023	0.0016
pu-met-fast-036-001.i	1.0000	0.0031	1.00639	0.00009	-0.00639	0.0031
pu-met-fast-038-001.i	1.0007	0.0019	1.00253	0.0001	-0.00183	0.0019
pu-met-fast-039-001.i	**1.0000**	**0.0022**	**0.9922**	**0.00009**	**0.0078**	**0.0022**
pu-met-fast-040-001.i	1.0000	0.0038	0.99667	0.00009	0.00333	0.0038
pu-met-fast-041-001.i	**1.0000**	**0.0016**	**1.00574**	**0.0001**	**-0.00574**	**0.0016**
pu-met-fast-042-001.i	1.0004	0.0077	1.01849	0.00012	-0.01809	0.0077
pu-met-fast-042-002.i	1.0007	0.0074	1.01271	0.00011	-0.01201	0.0074
pu-met-fast-042-003.i	1.0013	0.008	1.01214	0.00011	-0.01084	0.008
pu-met-fast-042-004.i	1.0026	0.008	1.01021	0.0001	-0.00761	0.008
pu-met-fast-042-005.i	1.0013	0.008	1.01021	0.0001	-0.00891	0.008
pu-met-fast-042-006.i	1.0015	0.0079	1.00915	0.0001	-0.00765	0.0079
pu-met-fast-042-007.i	1.0006	0.0075	1.0085	0.0001	-0.0079	0.0075
pu-met-fast-042-008.i	1.0019	0.008	1.0114	0.00011	-0.0095	0.008
pu-met-fast-042-009.i	1.0019	0.0073	1.01067	0.0001	-0.00877	0.0073
pu-met-fast-042-010.i	1.0015	0.0079	1.01295	0.00011	-0.01145	0.0079
pu-met-fast-042-011.i	1.0010	0.0078	1.01214	0.0001	-0.01114	0.0078
pu-met-fast-042-012.i	1.0016	0.0076	1.01212	0.0001	-0.01052	0.0076
pu-met-fast-042-013.i	1.0016	0.0074	1.01203	0.00011	-0.01043	0.0074
pu-met-fast-042-014.i	1.0016	0.0078	1.01273	0.0001	-0.01113	0.0078
pu-met-fast-042-015.i	1.0014	0.0076	1.01243	0.0001	-0.01103	0.0076
pu-met-fast-044-001.i	0.9977	0.0021	1.00054	0.00009	-0.00284	0.0021
pu-met-fast-044-002.i	0.9980	0.0022	0.99997	0.0001	-0.00197	0.0022
pu-met-fast-044-003.i	0.9927	0.0021	0.99938	0.0001	-0.00668	0.0021
pu-met-fast-044-004.i	0.9978	0.0026	1.00002	0.0001	-0.00222	0.0026
pu-met-fast-044-005.i	0.9977	0.0024	0.99927	0.00011	-0.00157	0.0024
pu-met-fast-045-001.i	1.0000	0.0047	1.00164	0.00009	-0.00164	0.0047
pu-met-fast-045-002.i	1.0000	0.0046	1.00785	0.0001	-0.00785	0.0046
pu-met-fast-045-003.i	1.0000	0.0044	1.00536	0.00009	-0.00536	0.0044
pu-met-fast-045-004.i	1.0000	0.0046	1.00462	0.00009	-0.00462	0.0046
pu-met-fast-045-005.i	1.0000	0.0045	1.00858	0.00009	-0.00858	0.0045
pu-met-fast-045-006.i	1.0000	0.0049	1.00483	0.00009	-0.00483	0.0049
pu-met-fast-045-007.i	1.0000	0.005	1.00541	0.00009	-0.00541	0.005
pu-sol-therm-001-001.i	1.0000	0.005	1.00578	0.00013	-0.00578	0.005
pu-sol-therm-001-002.i	1.0000	0.005	1.0073	0.00012	-0.0073	0.005

pu-sol-therm-001-003.i	1.0000	0.005	1.01135	0.00013	-0.01135	0.005
pu-sol-therm-001-004.i	1.0000	0.005	1.00441	0.00013	-0.00441	0.005
pu-sol-therm-001-005.i	1.0000	0.005	1.0087	0.00013	-0.0087	0.005
pu-sol-therm-001-006.i	1.0000	0.005	1.00955	0.00014	-0.00955	0.005
pu-sol-therm-002-001.i	1.0000	0.0047	1.00384	0.00012	-0.00384	0.0047
pu-sol-therm-002-002.i	1.0000	0.0047	1.00475	0.00013	-0.00475	0.0047
pu-sol-therm-002-003.i	1.0000	0.0047	1.00385	0.00013	-0.00385	0.0047
pu-sol-therm-002-004.i	1.0000	0.0047	1.00667	0.00012	-0.00667	0.0047
pu-sol-therm-002-005.i	1.0000	0.0047	1.00941	0.00012	-0.00941	0.0047
pu-sol-therm-002-006.i	1.0000	0.0047	1.00518	0.00012	-0.00518	0.0047
pu-sol-therm-002-007.i	1.0000	0.0047	1.00772	0.00012	-0.00772	0.0047
pu-sol-therm-003-001.i	1.0000	0.0047	1.00268	0.00012	-0.00268	0.0047
pu-sol-therm-003-002.i	1.0000	0.0047	1.00238	0.00012	-0.00238	0.0047
pu-sol-therm-003-003.i	1.0000	0.0047	1.00513	0.00012	-0.00513	0.0047
pu-sol-therm-003-004.i	1.0000	0.0047	1.00433	0.00012	-0.00433	0.0047
pu-sol-therm-003-005.i	1.0000	0.0047	1.00568	0.00012	-0.00568	0.0047
pu-sol-therm-003-006.i	1.0000	0.0047	1.00605	0.00012	-0.00605	0.0047
pu-sol-therm-003-007.i	1.0000	0.0047	1.00668	0.00012	-0.00668	0.0047
pu-sol-therm-003-008.i	1.0000	0.0047	1.00536	0.00011	-0.00536	0.0047
pu-sol-therm-004-001.i	1.0000	0.0047	1.00399	0.00011	-0.00399	0.0047
pu-sol-therm-004-002.i	1.0000	0.0047	0.9987	0.00011	0.0013	0.0047
pu-sol-therm-004-003.i	1.0000	0.0047	1.0009	0.00011	-0.0009	0.0047
pu-sol-therm-004-004.i	1.0000	0.0047	0.99898	0.00011	0.00102	0.0047
pu-sol-therm-004-005.i	1.0000	0.0047	0.99983	0.00011	0.00017	0.0047
pu-sol-therm-004-006.i	1.0000	0.0047	1.00186	0.00011	-0.00186	0.0047
pu-sol-therm-004-007.i	1.0000	0.0047	1.00564	0.00011	-0.00564	0.0047
pu-sol-therm-004-008.i	1.0000	0.0047	1.00117	0.0001	-0.00117	0.0047
pu-sol-therm-004-009.i	1.0000	0.0047	1.00069	0.00011	-0.00069	0.0047
pu-sol-therm-004-010.i	1.0000	0.0047	1.00234	0.00011	-0.00234	0.0047
pu-sol-therm-004-011.i	1.0000	0.0047	1.00086	0.00012	-0.00086	0.0047
pu-sol-therm-004-012.i	1.0000	0.0047	1.00309	0.00012	-0.00309	0.0047
pu-sol-therm-004-013.i	1.0000	0.0047	1.00035	0.00011	-0.00035	0.0047
pu-sol-therm-005-001.i	1.0000	0.0047	1.00233	0.00012	-0.00233	0.0047
pu-sol-therm-005-002.i	1.0000	0.0047	1.00299	0.00012	-0.00299	0.0047
pu-sol-therm-005-003.i	1.0000	0.0047	1.00354	0.00011	-0.00354	0.0047
pu-sol-therm-005-004.i	1.0000	0.0047	1.00504	0.00011	-0.00504	0.0047
pu-sol-therm-005-005.i	1.0000	0.0047	1.00615	0.00011	-0.00615	0.0047
pu-sol-therm-005-006.i	1.0000	0.0047	1.00584	0.00012	-0.00584	0.0047
pu-sol-therm-005-007.i	1.0000	0.0047	1.0042	0.00012	-0.0042	0.0047
pu-sol-therm-005-008.i	1.0000	0.0047	0.99941	0.00011	0.00059	0.0047
pu-sol-therm-005-009.i	1.0000	0.0047	1.00215	0.00011	-0.00215	0.0047
pu-sol-therm-006-001.i	1.0000	0.0035	1.00073	0.00011	-0.00073	0.0035
pu-sol-therm-006-002.i	1.0000	0.0035	1.00202	0.00011	-0.00202	0.0035
pu-sol-therm-006-003.i	1.0000	0.0035	1.00158	0.00011	-0.00158	0.0035
pu-sol-therm-007-002.i	1.0000	0.0047	1.00956	0.00012	-0.00956	0.0047
pu-sol-therm-007-003.i	1.0000	0.0047	1.00361	0.00013	-0.00361	0.0047

pu-sol-therm-007-005.i	1.0000	0.0047	1.00928	0.00013	-0.00928	0.0047
pu-sol-therm-007-006.i	1.0000	0.0047	1.00313	0.00013	-0.00313	0.0047
pu-sol-therm-007-007.i	1.0000	0.0047	1.00524	0.00013	-0.00524	0.0047
pu-sol-therm-007-008.i	1.0000	0.0047	0.99868	0.00013	0.00132	0.0047
pu-sol-therm-007-009.i	1.0000	0.0047	0.9973	0.00013	0.0027	0.0047
pu-sol-therm-007-010.i	1.0000	0.0047	1.00092	0.00012	-0.00092	0.0047
pu-sol-therm-009-003.i	**1.0000**	**0.0033**	**1.01926**	**0.00006**	**-0.01926**	**0.0033**
pu-sol-therm-010-001.i	**1.0000**	**0.0048**	**1.01812**	**0.00013**	**-0.01812**	**0.0048**
pu-sol-therm-010-002.i	1.0000	0.0048	1.01428	0.00013	-0.01428	0.0048
pu-sol-therm-010-003.i	1.0000	0.0048	1.00818	0.00013	-0.00818	0.0048
pu-sol-therm-010-004.i	1.0000	0.0048	1.01261	0.00013	-0.01261	0.0048
pu-sol-therm-010-005.i	1.0000	0.0048	1.01057	0.00012	-0.01057	0.0048
pu-sol-therm-010-006.i	1.0000	0.0048	1.00954	0.00012	-0.00954	0.0048
pu-sol-therm-010-007.i	1.0000	0.0048	1.00241	0.00012	-0.00241	0.0048
pu-sol-therm-010-008.i	1.0000	0.0048	1.00377	0.00011	-0.00377	0.0048
pu-sol-therm-010-009.i	1.0000	0.0048	1.01445	0.00012	-0.01445	0.0048
pu-sol-therm-010-010.i	1.0000	0.0048	1.00259	0.00012	-0.00259	0.0048
pu-sol-therm-010-011.i	1.0000	0.0048	1.00985	0.00012	-0.00985	0.0048
pu-sol-therm-010-012.i	1.0000	0.0048	1.00953	0.00012	-0.00953	0.0048
pu-sol-therm-010-013.i	**1.0000**	**0.0048**	**1.01576**	**0.00011**	**-0.01576**	**0.0048**
pu-sol-therm-010-014.i	1.0000	0.0048	1.00967	0.00011	-0.00967	0.0048
pu-sol-therm-011-161.i	1.0000	0.0052	1.00962	0.00012	-0.00962	0.0052
pu-sol-therm-011-162.i	1.0000	0.0052	1.01483	0.00013	-0.01483	0.0052
pu-sol-therm-011-163.i	1.0000	0.0052	1.01657	0.00013	-0.01657	0.0052
pu-sol-therm-011-164.i	1.0000	0.0052	1.00927	0.00012	-0.00927	0.0052
pu-sol-therm-011-165.i	1.0000	0.0052	1.00642	0.00013	-0.00642	0.0052
pu-sol-therm-011-181.i	1.0000	0.0052	0.99435	0.00012	0.00565	0.0052
pu-sol-therm-011-182.i	1.0000	0.0052	1.00045	0.00012	-0.00045	0.0052
pu-sol-therm-011-183.i	1.0000	0.0052	0.99679	0.00011	0.00321	0.0052
pu-sol-therm-011-184.i	1.0000	0.0052	0.99366	0.00011	0.00634	0.0052
pu-sol-therm-011-185.i	1.0000	0.0052	1.00372	0.00012	-0.00372	0.0052
pu-sol-therm-011-186.i	1.0000	0.0052	1.00025	0.00012	-0.00025	0.0052
pu-sol-therm-011-187.i	1.0000	0.0052	0.9997	0.00011	0.0003	0.0052
pu-sol-therm-012-001.i	1.0000	0.0043	1.00536	0.00009	-0.00536	0.0043
pu-sol-therm-012-002.i	1.0000	0.0043	1.00615	0.00008	-0.00615	0.0043
pu-sol-therm-012-003.i	1.0000	0.0058	1.00736	0.00008	-0.00736	0.0058
pu-sol-therm-012-004.i	1.0000	0.0058	1.00746	0.00007	-0.00746	0.0058
pu-sol-therm-012-005.i	1.0000	0.0058	1.00981	0.00006	-0.00981	0.0058
pu-sol-therm-012-006.i	**1.0000**	**0.0007**	**1.00659**	**0.00013**	**-0.00659**	**0.00071**
pu-sol-therm-012-007.i	**1.0000**	**0.0013**	**1.00537**	**0.00013**	**-0.00537**	**0.00131**
pu-sol-therm-012-008.i	1.0000	0.0013	1.00417	0.00012	-0.00417	0.00131
pu-sol-therm-012-009.i	1.0000	0.0043	1.00966	0.00011	-0.00966	0.0043
pu-sol-therm-012-010.i	1.0000	0.0043	1.00409	0.0001	-0.00409	0.0043
pu-sol-therm-012-011.i	1.0000	0.0043	1.0067	0.0001	-0.0067	0.0043
pu-sol-therm-012-012.i	1.0000	0.0043	1.00721	0.00009	-0.00721	0.0043
pu-sol-therm-012-013.i	1.0000	0.0058	1.00964	0.00007	-0.00964	0.0058

pu-sol-therm-018-001.i	1.0000	0.0034	1.00849	0.00013	-0.00849	0.0034
pu-sol-therm-018-002.i	**1.0000**	**0.0034**	**1.01189**	**0.00012**	**-0.01189**	**0.0034**
pu-sol-therm-018-003.i	1.0000	0.0032	1.00938	0.00012	-0.00938	0.0032
pu-sol-therm-018-004.i	1.0000	0.003	1.00765	0.00012	-0.00765	0.003
pu-sol-therm-018-005.i	1.0000	0.003	1.00654	0.00011	-0.00654	0.003
pu-sol-therm-018-006.i	1.0000	0.0031	1.00462	0.00012	-0.00462	0.0031
pu-sol-therm-018-007.i	1.0000	0.0032	1.00399	0.0001	-0.00399	0.0032
pu-sol-therm-018-008.i	1.0000	0.0033	1.00356	0.00011	-0.00356	0.0033
pu-sol-therm-018-009.i	1.0000	0.0034	1.00176	0.0001	-0.00176	0.0034
pu-sol-therm-022-001.i	1.0000	0.002	0.99953	0.00013	0.00047	0.002
pu-sol-therm-022-002.i	1.0000	0.0016	1.00205	0.00013	-0.00205	0.00161
pu-sol-therm-022-003.i	1.0000	0.0015	1.00071	0.00012	-0.00071	0.0015
pu-sol-therm-022-004.i	1.0000	0.0017	1.00135	0.00012	-0.00135	0.0017
pu-sol-therm-022-005.i	1.0000	0.0019	1.00225	0.00011	-0.00225	0.0019
pu-sol-therm-022-006.i	1.0000	0.0021	1.00269	0.00011	-0.00269	0.0021
pu-sol-therm-022-007.i	1.0000	0.0021	1.00423	0.00011	-0.00423	0.0021
pu-sol-therm-022-008.i	1.0000	0.0023	1.00505	0.0001	-0.00505	0.0023
pu-sol-therm-022-009.i	1.0000	0.0024	1.00368	0.0001	-0.00368	0.0024
pu-sol-therm-028-001.i	**1.0000**	**0.0012**	**1.00788**	**0.00012**	**-0.00788**	**0.00121**
pu-sol-therm-028-002.i	**1.0000**	**0.0012**	**1.00708**	**0.00012**	**-0.00708**	**0.00121**
pu-sol-therm-028-003.i	**1.0000**	**0.0012**	**1.0089**	**0.00012**	**-0.0089**	**0.00121**
pu-sol-therm-028-004.i	**1.0000**	**0.0012**	**1.00871**	**0.00012**	**-0.00871**	**0.00121**
pu-sol-therm-028-005.i	**1.0000**	**0.0012**	**1.00991**	**0.00012**	**-0.00991**	**0.00121**
pu-sol-therm-028-006.i	**1.0000**	**0.0012**	**1.0107**	**0.00011**	**-0.0107**	**0.00121**
pu-sol-therm-028-007.i	**1.0000**	**0.0012**	**1.00815**	**0.00012**	**-0.00815**	**0.00121**
pu-sol-therm-028-008.i	**1.0000**	**0.0012**	**1.00826**	**0.00012**	**-0.00826**	**0.00121**
pu-sol-therm-028-009.i	**1.0000**	**0.0012**	**1.00989**	**0.00012**	**-0.00989**	**0.00121**
pu-sol-therm-032-001.i	1.0000	0.0019	0.99617	0.00013	0.00383	0.0019
pu-sol-therm-032-002.i	1.0000	0.0019	1.00142	0.00012	-0.00142	0.0019
pu-sol-therm-032-003.i	1.0000	0.0019	1.00264	0.00012	-0.00264	0.0019
pu-sol-therm-032-004.i	1.0000	0.0019	1.00255	0.00012	-0.00255	0.0019
pu-sol-therm-032-005.i	1.0000	0.0019	1.00439	0.00012	-0.00439	0.0019
pu-sol-therm-032-006.i	1.0000	0.0019	1.00477	0.00011	-0.00477	0.0019
pu-sol-therm-032-007.i	1.0000	0.0019	1.00496	0.00011	-0.00496	0.0019
pu-sol-therm-032-008.i	1.0000	0.0019	1.0044	0.00011	-0.0044	0.0019
pu-sol-therm-032-009.i	1.0000	0.0019	1.00326	0.00011	-0.00326	0.0019
pu-sol-therm-032-010.i	1.0000	0.0019	1.00514	0.00011	-0.00514	0.0019
pu-sol-therm-032-011.i	1.0000	0.0019	1.00448	0.0001	-0.00448	0.0019
pu-sol-therm-032-012.i	1.0000	0.0019	1.00347	0.0001	-0.00347	0.0019
pu-sol-therm-032-013.i	1.0000	0.0019	1.0023	0.00012	-0.0023	0.0019
pu-sol-therm-032-014.i	1.0000	0.0019	1.00212	0.00012	-0.00212	0.0019
pu-sol-therm-032-015.i	1.0000	0.0019	1.00402	0.00011	-0.00402	0.0019
pu-sol-therm-032-016.i	1.0000	0.0019	1.00382	0.00011	-0.00382	0.0019
pu-sol-therm-032-017.i	1.0000	0.0019	1.00389	0.00011	-0.00389	0.0019
pu-sol-therm-034-001.i	1.0000	0.0062	0.99995	0.00013	0.00005	0.0062
pu-sol-therm-034-002.i	1.0000	0.0044	1.00148	0.00012	-0.00148	0.0044

pu-sol-therm-034-003.i	1.0000	0.004	0.9995	0.00012	0.0005	0.004
pu-sol-therm-034-004.i	1.0000	0.0039	1.00248	0.00012	-0.00248	0.0039
pu-sol-therm-034-005.i	1.0000	0.004	0.99991	0.0001	0.00009	0.004
pu-sol-therm-034-006.i	1.0000	0.0042	1.00114	0.0001	-0.00114	0.0042
pu-sol-therm-034-007.i	1.0000	0.0057	0.9987	0.00012	0.0013	0.0057
pu-sol-therm-034-008.i	1.0000	0.0055	0.99889	0.00012	0.00111	0.0055
pu-sol-therm-034-009.i	1.0000	0.0052	0.99776	0.00011	0.00224	0.0052
pu-sol-therm-034-010.i	1.0000	0.0052	0.99732	0.00012	0.00268	0.0052
pu-sol-therm-034-011.i	1.0000	0.0048	0.99902	0.00011	0.00098	0.0048
pu-sol-therm-034-012.i	1.0000	0.0042	0.99847	0.00011	0.00153	0.0042
pu-sol-therm-034-013.i	1.0000	0.0043	0.99696	0.0001	0.00304	0.0043
pu-sol-therm-034-014.i	1.0000	0.0044	0.99681	0.00011	0.00319	0.0044
pu-sol-therm-034-015.i	1.0000	0.0042	0.99717	0.00011	0.00283	0.0042
pu-sol-therm-038-001.i	1.0005	0.0015	1.00318	0.00009	-0.00268	0.0015
pu-sol-therm-038-002.i	1.0005	0.0015	1.00365	0.00009	-0.00315	0.0015
pu-sol-therm-038-003.i	1.0005	0.0018	1.00359	0.00007	-0.00309	0.0018
pu-sol-therm-038-004.i	1.0005	0.0013	1.00173	0.00007	-0.00123	0.0013
pu-sol-therm-038-005.i	1.0005	0.0013	1.00192	0.00007	-0.00142	0.0013