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Plutonium Critical Mass Curve Comparison to Mass at Upper Subcritical Limit (USL) Using Whisper

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Introduction

Whisper is computational software designed to assist the nuclear criticality safety analyst with validation studies with the MCNP® Monte Carlo radiation transport package. Standard approaches to validation rely on the selection of benchmarks based upon expert judgment. Whisper uses sensitivity/uncertainty (S/U) methods to select relevant benchmarks to a particular application or set of applications being analyzed. Using these benchmarks, Whisper computes a calculational margin. Whisper attempts to quantify the margin of subcriticality (MOS) from errors in software and uncertainties in nuclear data. The combination of the Whisper-derived calculational margin and MOS comprise the baseline upper subcritical limit (USL) to which an additional margin may be applied by the nuclear criticality safety analyst as appropriate to ensure subcriticality.

A series of critical mass curves for plutonium, similar to those found in Figure 31 of LA-10860-MS, have been generated using MCNP6.1.1 and the iterative parameter study software, WORM_Solver. The baseline USL for each of the data points of the curves was then computed using Whisper 1.1. The USL was then used to determine the equivalent mass for plutonium metal-water system. ANSI/ANS-8.1 states that it is acceptable to use handbook data, such as the data directly from the LA-10860-MS, as it is already considered validated (Section 4.3 $_{4)}$ *"Use of subcritical limit data provided in ANSI/ANS standards or accepted reference publications does not require further validation.").* This paper attempts to take a novel approach to visualize traditional critical mass curves and allows comparison with the amount of mass for which the k_{eff} is equal to the USL (calculational margin + margin of subcriticality). However, the intent is to plot the critical mass data along with USL, not to suggest that already accepted handbook data should have new and more rigorous requirements for validation.

Critical Mass Curve Study

Critical mass curves in LA-10860-MS are used extensively for an understanding of the critical mass of plutonium systems moderated with water, both bare and water reflected. The curves presented in LA-10860-MS allow the criticality safety analyst to visualize the changes to the system with changes in various parameters, such as moderation and reflection. By following the critical mass curve from pure plutonium metal to the limiting critical concentration one can begin to gain an understanding of the competing effects of changes in density, moderation, and absorption on the plutonium system.

Additional understanding of the system can be gained by comparing the actual critical mass (the mass at which k_{eff} = 1.0) with the mass at the USL (the mass at which k_{eff} = USL). The data for the curves were generated by modeling a plutonium sphere uniformly mixed with various amounts of water. Three different curves were computed using MCNP6.1.1; the bare plutonium-water sphere, the plutonium-water sphere reflected in all directions by 2 cm of water, and the plutonium-water sphere reflected in all directions by 30 cm of water. The data point corresponding to 19.84 g/cm^3 indicates a pure plutonium sphere, the points moving to the left at the x-axis indicate a plutonium-water mixture with increasing amounts of water, stated as concentration of Pu in the mixture, g Pu/cm^3. It is necessary to point out that a plutonium-water mixture does not exist as a practical reality, some amount of solvent is necessary to dissolve plutonium into solution. For the purposes of a critical mass curve, a fictitious plutonium-water mixture is useful and often conservative of plutonium solutions in a practical sense.

The generation of the critical mass curves using MCNP6.1.1 is an iterative process calculated using MCNP6.1.1, WORM, WORM_solver, and Microsoft Excel.

MCNP6.1.1 allows for the calculation of the system eigenvalue, k_{eff} of the system. A system is defined to be critical when k_{eff} value equals 1.0.

WORM is a perl script that generates a suite of MCNP6.1.1 input decks based on the user defined input parameter values.

WORM_solver is a wrapper script that that uses iterative method to "solve" to a particular k_{eff} value. If the user defines the value k_{eff} to be 1.0, WORM_solver will use a brute force iterative method to solve for a mass (also as defined by user) which is used to obtain a k_{eff} value closest to 1.0, within a convergence criteria.

WORM_solver only solves to a certain convergence criteria. Once the result, in this case mass, is within the convergence criteria, WORM_solver considers the problem finished. The concern may be that the result doesn't quiet produce a k_{eff} value of exactly 1.0, perhaps it is 1.00005 or 0.99997. In order to further obtain a value closest to k_{eff} of 1.0, Excel was used. The user takes the calculated k_{eff} and mass to plot the mass as a function of k_{eff}. A 3rd order polynomial curve fit was then performed on the given data. Using the equation obtained from the curve fit, the critical mass value result for a k_{eff} of 1.0 is obtained.

Once the critical mass values (k_{eff} = 1) for the each concentration is obtained from the process described above, these mass values were used as an input for MCNP6.1.1 followed by Whisper 1.1. In order to determine the mass at the USL, several steps are necessary. First, for every concentration, the critical mass calculated previously was used as an input and is submitted to Whisper 1.1 and the baseline USL recommended by Whisper is computed using sensitivity/uncertainty techniques, more information about Whisper can be found in References 1 through 8. Once the USL (a k_{eff} value) for each concentration is obtained, the mass corresponding to the Whisper-generated USL is then determined using an Excel polynomial curve fit using the same technique that was used to determine the mass corresponding to k_{eff} = 1.0.

Results

The critical mass and USL mass curves are presented in Figures 1 through 3 below. The baseline USL calculated by Whisper is also shown in the curves. It is necessary to point out that the baseline USL does not include margin for extending the area of applicability or application of other additional margin due to considerations judged by criticality safety analysts when applying this study to their application.

It is also useful to plot the curves with data such as the average neutron energy causing fission (ANECF) and the energy of the average lethargy of neutron causing fission (EALF) generated by MCNP6.1.1. This data is presented in Figures 6 through 8.

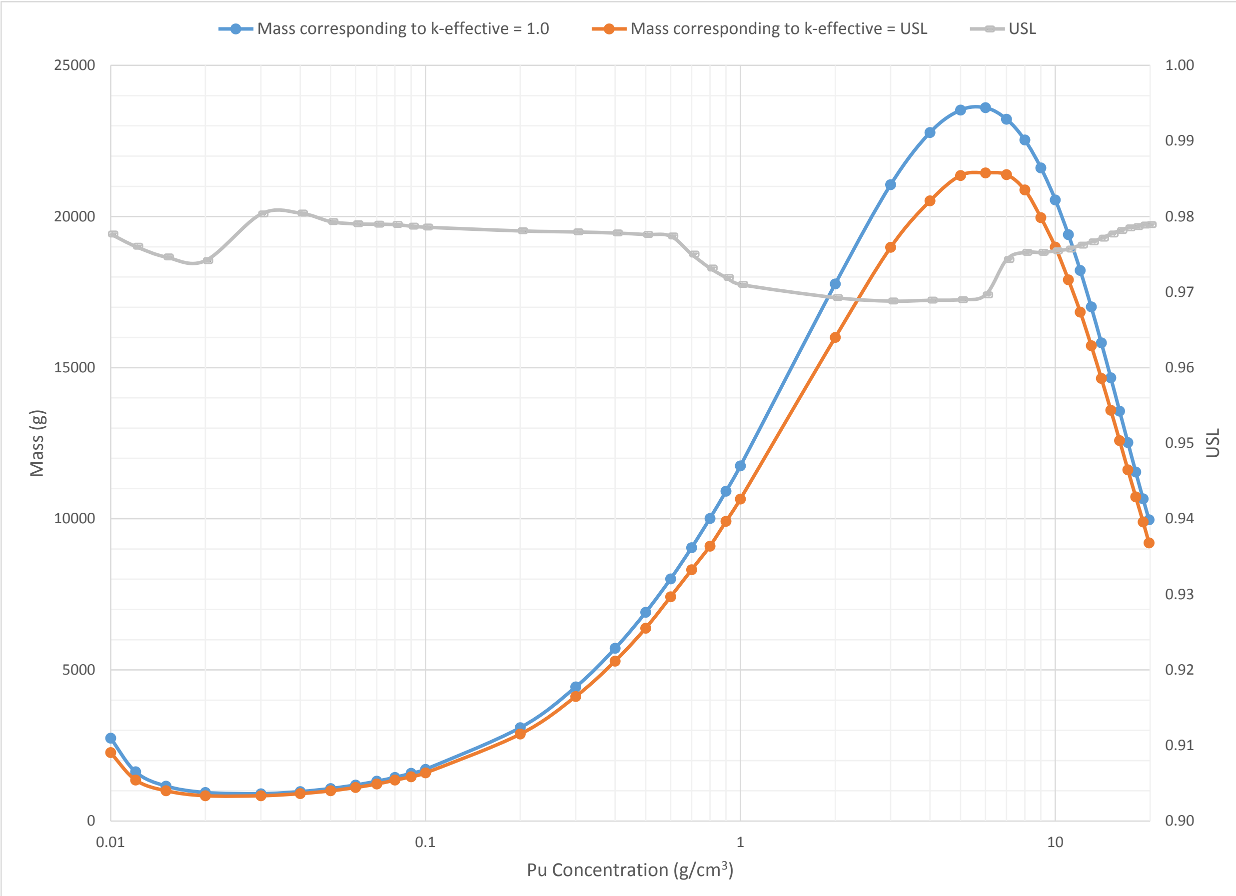

Figure 1. Pu critical mass and USL-mass for water-moderated plutonium bare spheres

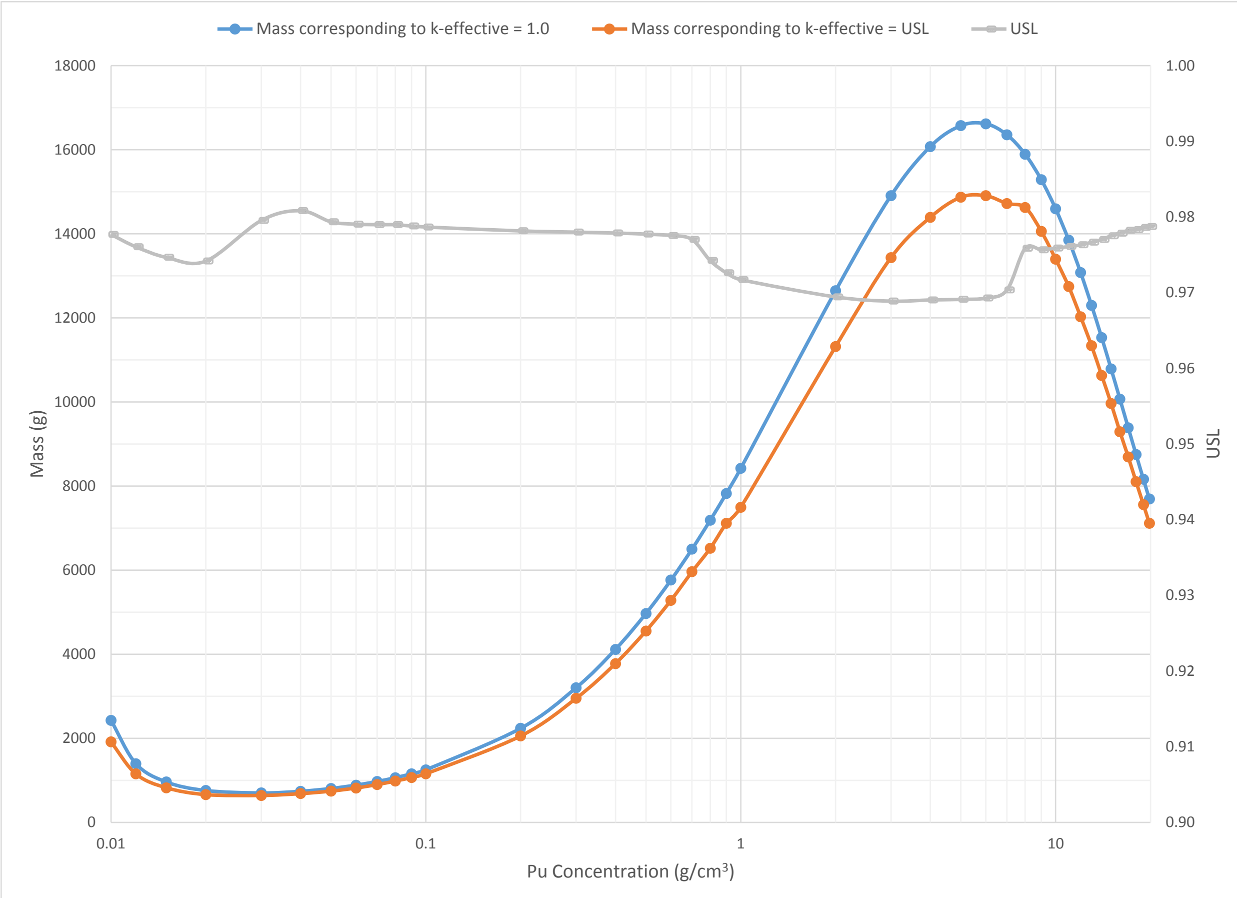

Figure 2. Pu critical mass and USL-mass for water-moderated plutonium spheres reflected with 2 cm water on all sides

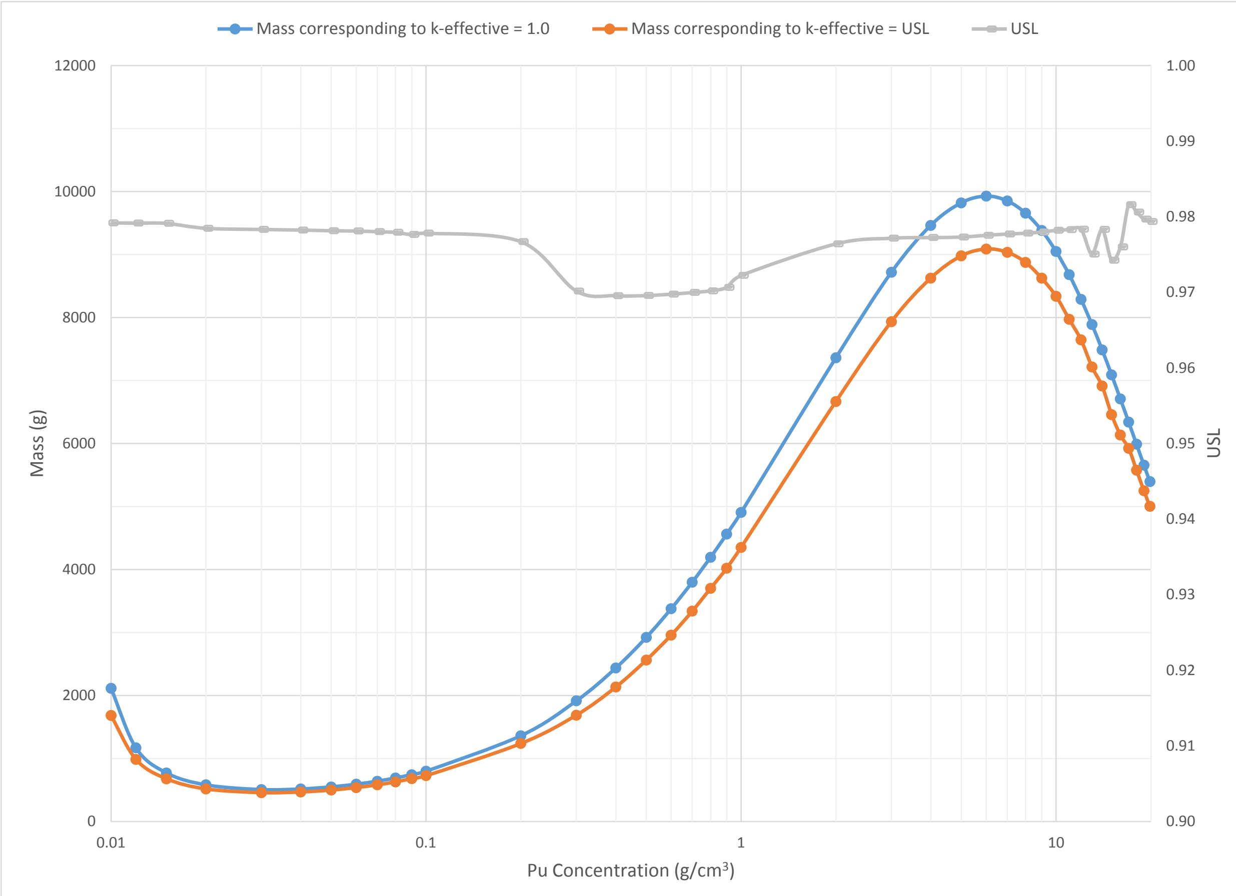

Figure 3 . Pu critical mass and USL-mass for water-moderated plutonium spheres reflected with 30 cm water on all sides

The data presented above was alternatively plotted on log-log scale in order to be most similar to the original LA-10860-MS Figure 31 curves, shown in Figure 4. The curves from Figure 31 of LA-10860-MS are also superimposed on the bare and 30-cm reflected cases for comparison. As can be seen in Figure 4, the water-reflected curve does not completely overlap the curve obtained from LA-10860-MS. This is due to the fact that some of the LA-10860-MS experimental data was done for PuO_2 and polystyrene systems rather that the plutonium metal-water systems represented in the water-reflected calculated critical mass curve. This accounts for the lack of a complete fit from the intermediate to fast energy part of the curve in Figure 4.

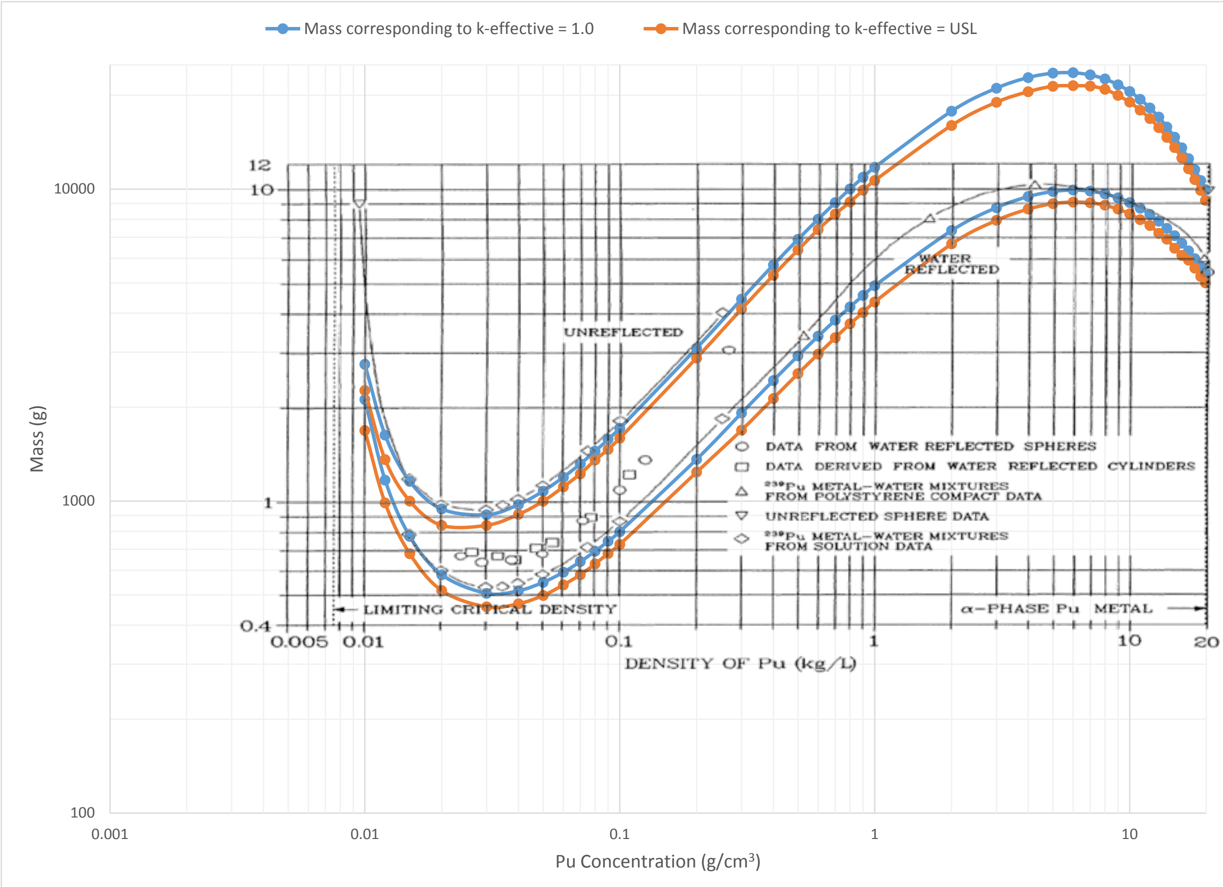

Figure 4. Pu critical mass and USL-mass for water-moderated bare spheres and water-moderated 30 cm water reflected spheres, the curve from Figure 31 of LA-10860-MS is superimposed in the figure

The critical volume curves from Figure 32 of LA-10860-MS have been superimposed on the bare and 30-cm reflected cases in Figure 5 below. These curves use the same critical mass, USL-mass and concentration data as that presented in Figure 4, manipulated to show volume instead of mass.

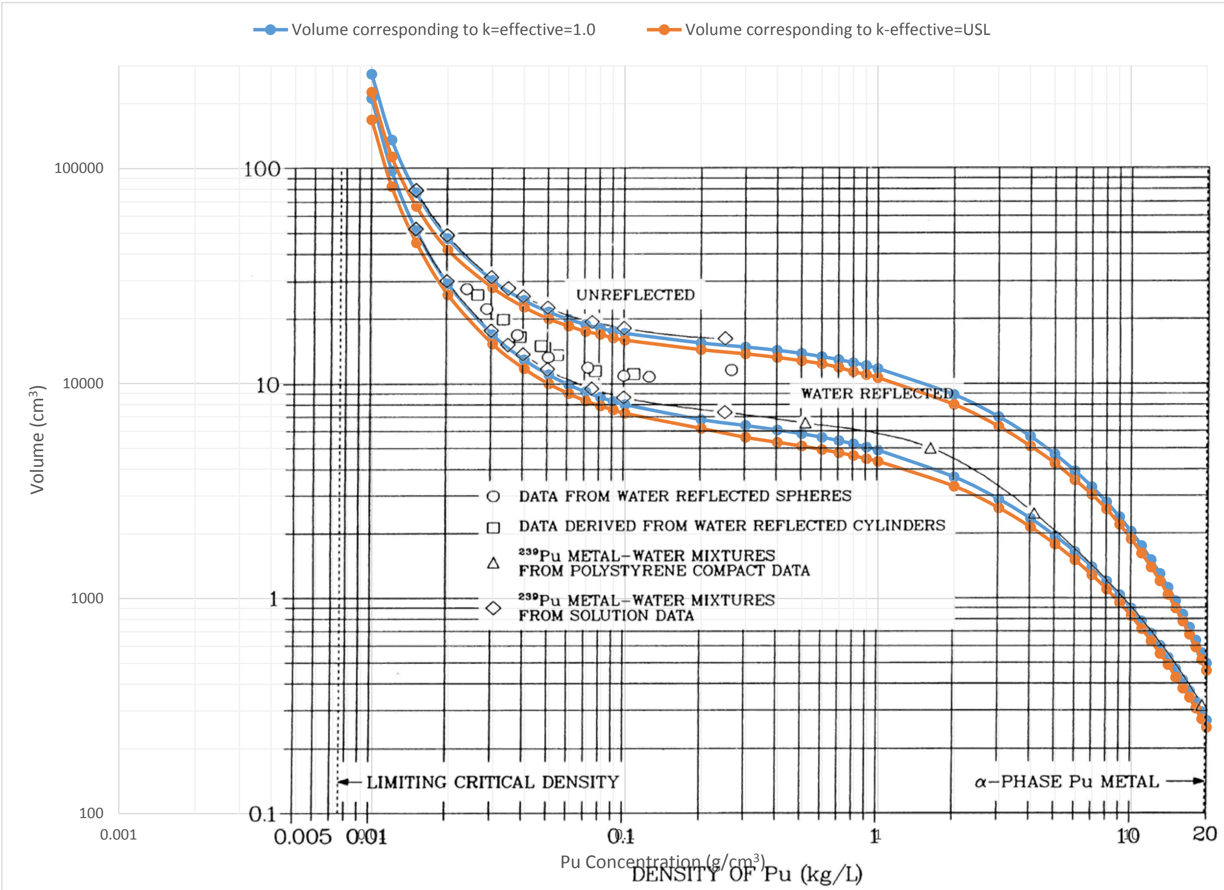

Figure 5. Pu critical volume and USL-volume for water-moderated bare spheres and water-moderated 30 cm water reflected spheres, the curve from Figure 32 of LA-10860-MS is superimposed in the figure

In addition to the data presented above, the curves are presented below along with the USL, the average energy of neutron causing fission and the energy of the average neutron lethargy causing fission.

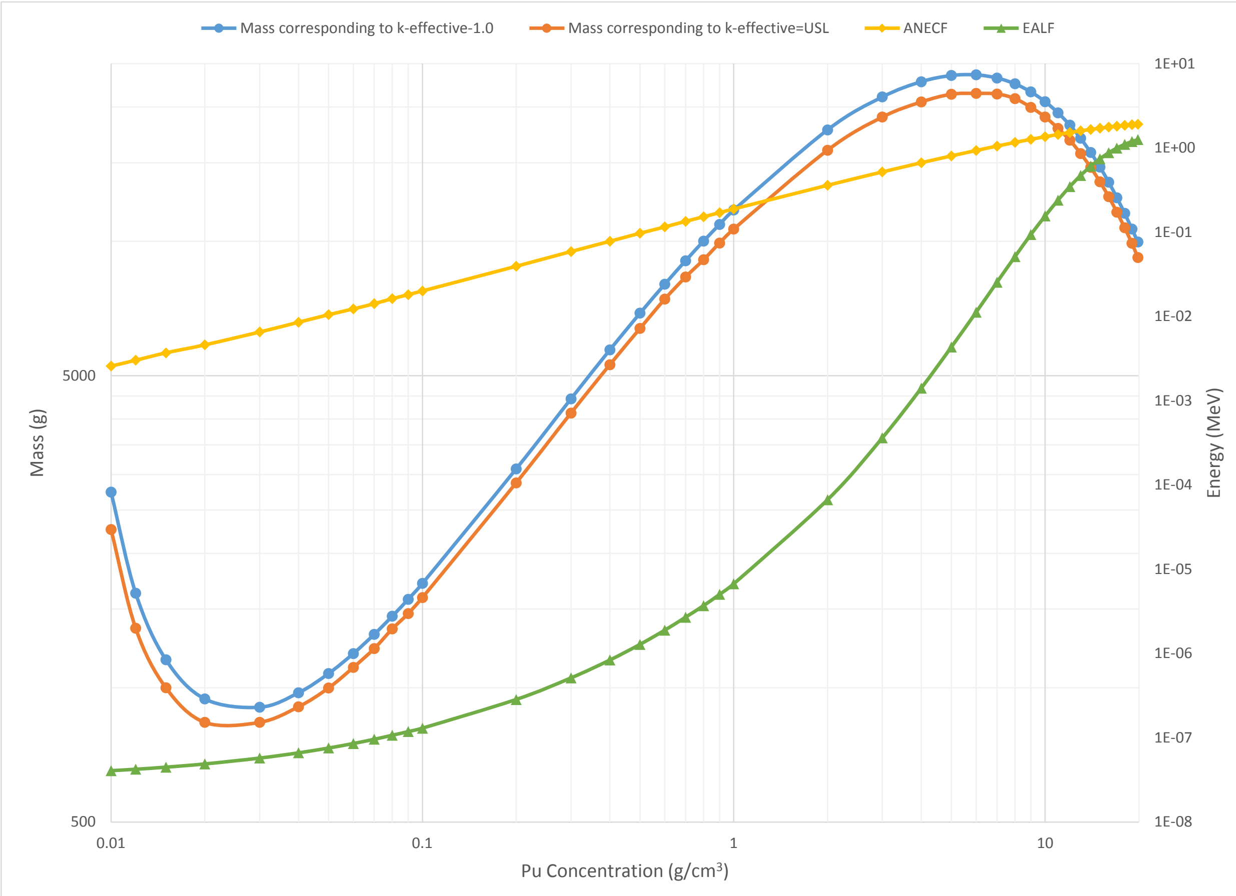

Figure 6. Critical mass and USL mass curves for bare Pu-water mixture shown in comparison to average neutron energy causing fission (ANECF) and energy corresponding to the average neutron lethargy causing fission (EALF)

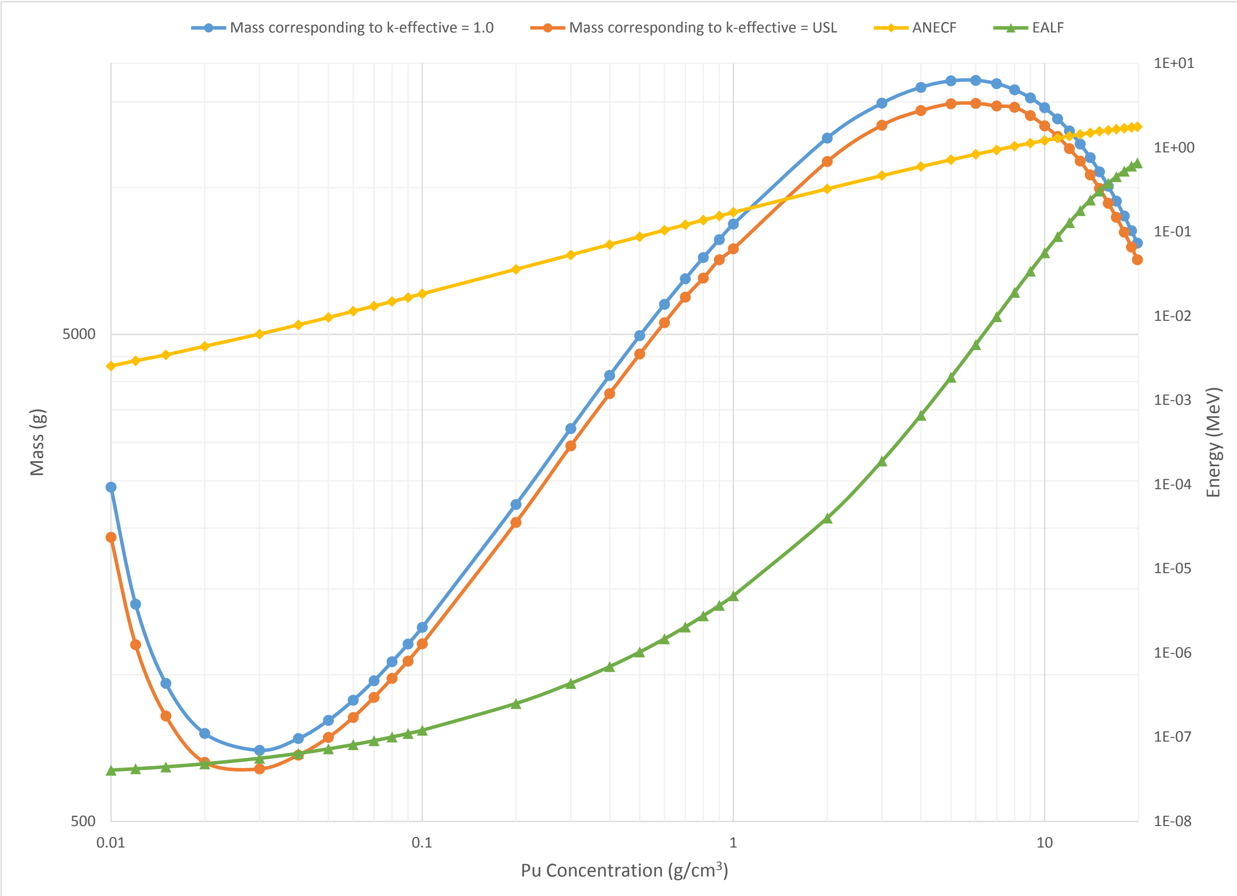

Figure 7. Critical mass and USL mass curves for 2 cm water-reflected Pu-water mixture shown in comparison to average neutron energy causing fission (ANECF) and energy corresponding to the average neutron lethargy causing fission (EALF)

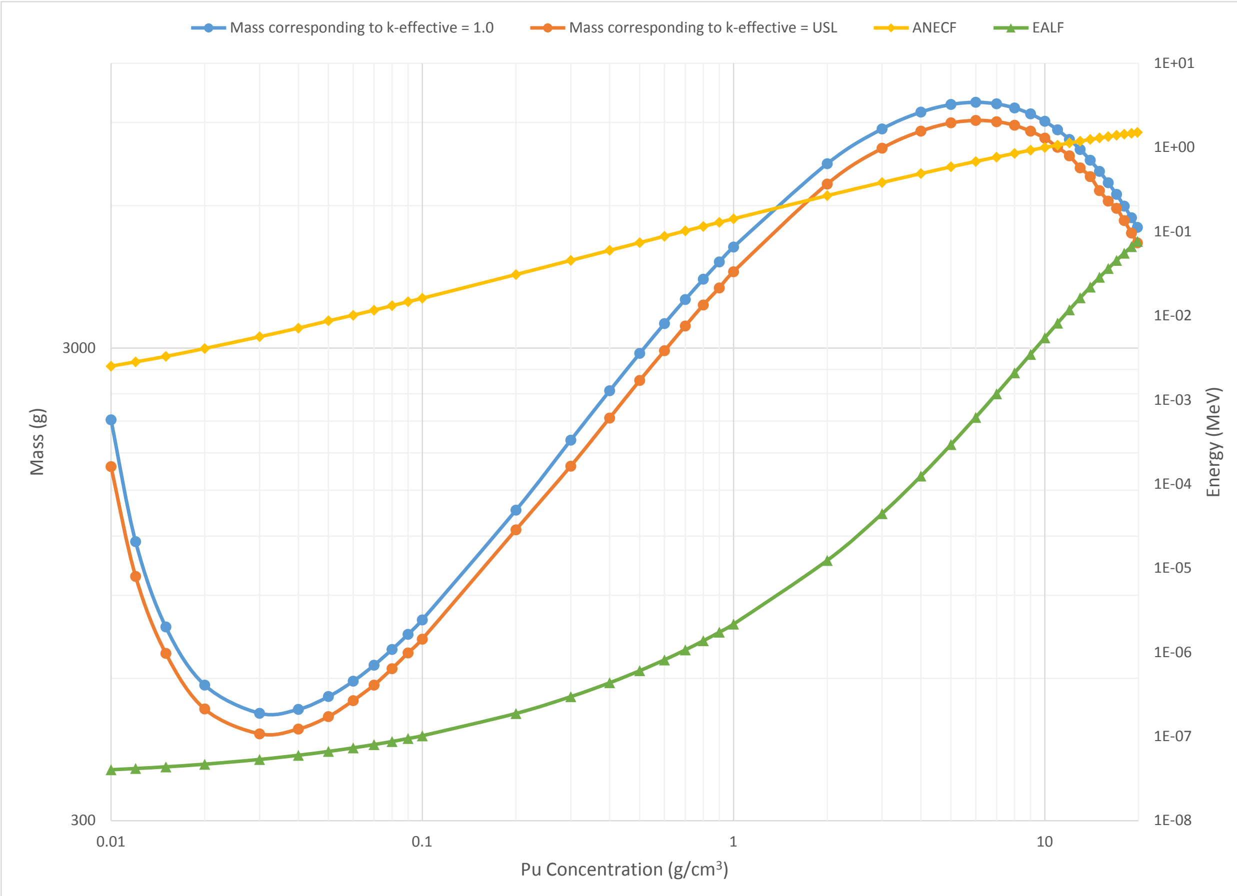

Figure 8. Critical mass and USL mass curves for 30 cm water-reflected Pu-water mixture shown in comparison to average neutron energy causing fission (ANECF) and energy corresponding to the average neutron lethargy causing fission (EALF)

Whisper uses correlation coefficients to identify the benchmarks experiments that most closely match the system. Tables 1-3 below present the chosen benchmarks along with correlation coefficients and weight for the bare Pu-water curves at 0.030 g/cm^3; 1.00 g/cm^3, and 19.84 g/cm^3, respectively.

For the bare curve these data show the various benchmarks selected as similar to pure plutonium sphere with no water (fast system), plutonium-water mixture with 1.00 g Pu/cm^3 (intermediate energy system), and the optimally moderated 0.030 g Pu/cm^3 (thermal system). As expected Whisper has identified PU-MET-FAST benchmarks as similar to the pure plutonium sphere, and PU-SOL-THERM benchmarks as similar to the moderated system, and a combination of PU-COMP and PU-SOL benchmarks as similar to the intermediate energy. There are fewer benchmarks that closely match the intermediate energy spectrum well than there were for the fast and moderated systems.

Table 1. Data from Whisper for bare 0.030 g/cm^3 Pu water mixture		
Baseline USL=0.98032	Benchmark population=53	Population weight=25.11247

benchmark	ck	weight
pu-sol-therm-011-161.i	0.9994	1.0000
pu-sol-therm-011-162.i	0.9993	0.9888
pu-sol-therm-003-008.i	0.9992	0.9526
pu-sol-therm-003-007.i	0.9991	0.9346
pu-sol-therm-011-163.i	0.9990	0.8964
pu-sol-therm-011-164.i	0.9990	0.8893
pu-sol-therm-003-002.i	0.9986	0.7935
pu-sol-therm-003-001.i	0.9986	0.7855
pu-sol-therm-003-003.i	0.9985	0.7544
pu-sol-therm-003-004.i	0.9984	0.7286
pu-sol-therm-002-001.i	0.9982	0.6915
pu-sol-therm-003-005.i	0.9982	0.6772
pu-sol-therm-010-012.i	0.9982	0.6720
pu-sol-therm-010-006.i	0.9981	0.6463
pu-sol-therm-002-002.i	0.9980	0.6187
pu-sol-therm-010-011.i	0.9979	0.6047
pu-sol-therm-010-010.i	0.9979	0.5960
pu-sol-therm-010-013.i	0.9979	0.5862
pu-sol-therm-011-165.i	0.9978	0.5806
pu-sol-therm-003-006.i	0.9978	0.5595
pu-sol-therm-010-007.i	0.9977	0.5503
pu-sol-therm-010-003.i	0.9974	0.4637
pu-sol-therm-010-005.i	0.9973	0.4376
pu-sol-therm-002-003.i	0.9973	0.4328
pu-sol-therm-005-003.i	0.9971	0.3858
pu-sol-therm-004-012.i	0.9971	0.3672
pu-sol-therm-004-008.i	0.9971	0.3657
pu-sol-therm-005-004.i	0.9971	0.3618
pu-sol-therm-004-007.i	0.9970	0.3524
pu-sol-therm-005-009.i	0.9970	0.3463
pu-sol-therm-004-002.i	0.9970	0.3462
pu-sol-therm-005-001.i	0.9970	0.3448
pu-sol-therm-004-003.i	0.9970	0.3401
pu-sol-therm-005-002.i	0.9970	0.3389
pu-sol-therm-004-009.i	0.9970	0.3384
pu-sol-therm-004-004.i	0.9969	0.3312
pu-sol-therm-004-013.i	0.9969	0.3242
pu-sol-therm-005-008.i	0.9969	0.3105
pu-sol-therm-010-004.i	0.9968	0.3016
pu-sol-therm-004-005.i	0.9968	0.2937
pu-sol-therm-005-005.i	0.9968	0.2936
pu-sol-therm-004-006.i	0.9968	0.2920
pu-sol-therm-002-004.i	0.9968	0.2910
pu-sol-therm-004-001.i	0.9968	0.2878
pu-sol-therm-004-010.i	0.9967	0.2608
pu-sol-therm-005-006.i	0.9967	0.2555
pu-sol-therm-010-009.i	0.9966	0.2460
pu-sol-therm-010-014.i	0.9966	0.2357
pu-sol-therm-004-011.i	0.9963	0.1561
pu-sol-therm-010-008.i	0.9963	0.1536
pu-sol-therm-005-007.i	0.9963	0.1412
pu-sol-therm-002-005.i	0.9963	0.1407
pu-sol-therm-001-001.i	0.9960	0.0689

Table 2. Data from Whisper for bare 1 g/cm^3 Pu water mixture		
Baseline USL=0.97101	Benchmark population=60	Population weight=27.26843
benchmark	**ck**	**weight**
pu-comp-mixed-002-015.i	0.9774	1.0000
pu-sol-therm-001-006.i	0.9772	0.9949
pu-comp-mixed-002-013.i	0.9771	0.9907
pu-comp-mixed-002-014.i	0.9770	0.9891
pu-sol-therm-007-003.i	0.9758	0.9530
pu-sol-therm-007-002.i	0.9757	0.9514
pu-comp-mixed-001-003.i	0.9753	0.9391
pu-comp-mixed-002-012.i	0.9747	0.9198
pu-comp-mixed-002-016.i	0.9746	0.9168
pu-comp-mixed-002-011.i	0.9712	0.8195
pu-sol-therm-001-005.i	0.9686	0.7439
pu-sol-therm-001-004.i	0.9679	0.7210
pu-comp-mixed-002-010.i	0.9668	0.6913
pu-sol-therm-001-003.i	0.9660	0.6669
pu-comp-mixed-002-020.i	0.9658	0.6602
pu-comp-mixed-002-021.i	0.9652	0.6435
pu-comp-mixed-002-019.i	0.9648	0.6303
pu-comp-mixed-001-004.i	0.9645	0.6227
pu-sol-therm-007-008.i	0.9639	0.6040
pu-sol-therm-007-009.i	0.9637	0.5994
pu-sol-therm-007-006.i	0.9636	0.5960
pu-sol-therm-007-007.i	0.9634	0.5917
pu-comp-mixed-002-018.i	0.9632	0.5845
pu-sol-therm-007-005.i	0.9630	0.5781
pu-comp-mixed-002-022.i	0.9627	0.5707
pu-sol-therm-001-002.i	0.9625	0.5657
pu-sol-therm-007-010.i	0.9625	0.5637
pu-sol-therm-010-001.i	0.9619	0.5475
pu-sol-therm-002-007.i	0.9593	0.4711
pu-sol-therm-002-006.i	0.9578	0.4272
pu-sol-therm-001-001.i	0.9569	0.4008
pu-sol-therm-010-002.i	0.9560	0.3755
pu-sol-therm-034-001.i	0.9556	0.3621
mix-sol-therm-001-007.i	0.9556	0.3620
pu-comp-mixed-002-017.i	0.9550	0.3467
pu-sol-therm-002-005.i	0.9543	0.3259
mix-sol-therm-003-002.i	0.9536	0.3050
pu-sol-therm-010-009.i	0.9531	0.2885
pu-sol-therm-002-004.i	0.9530	0.2873
pu-sol-therm-034-007.i	0.9527	0.2792
mix-sol-therm-003-001.i	0.9523	0.2668
pu-sol-therm-002-003.i	0.9517	0.2487
mix-sol-therm-003-003.i	0.9509	0.2268
pu-sol-therm-034-008.i	0.9506	0.2157
pu-sol-therm-002-002.i	0.9488	0.1633
pu-sol-therm-011-165.i	0.9486	0.1581
pu-sol-therm-010-004.i	0.9484	0.1526
mix-sol-therm-001-008.i	0.9481	0.1452
pu-sol-therm-010-003.i	0.9477	0.1321
pu-sol-therm-002-001.i	0.9475	0.1277
pu-sol-therm-034-009.i	0.9467	0.1017
pu-sol-therm-010-010.i	0.9461	0.0840
mix-sol-therm-003-004.i	0.9459	0.0796
pu-sol-therm-034-002.i	0.9458	0.0753
pu-sol-therm-028-001.i	0.9456	0.0702
pu-sol-therm-010-011.i	0.9451	0.0573
pu-sol-therm-010-006.i	0.9444	0.0364
pu-sol-therm-010-005.i	0.9441	0.0258
pu-sol-therm-011-164.i	0.9435	0.0089
pu-sol-therm-003-006.i	0.9434	0.0055

Table 3. Data from Whisper for bare 19.84 g/cm^3 Pu water mixture		
Baseline USL=0.97891	Benchmark population=51	Population weight=25.06064
benchmark	**ck**	**weight**
pu-met-fast-022-001.i	0.9994	1.0000
pu-met-fast-001-001.i	0.9978	0.9678
pu-met-fast-024-001.i	0.9951	0.9111
pu-met-fast-036-001.i	0.9937	0.8839
mix-met-fast-009-001.i	0.9932	0.8741
pu-met-fast-023-001.i	0.9929	0.8671
pu-met-fast-039-001.i	0.9926	0.8607
pu-met-fast-035-001.i	0.9920	0.8482
pu-met-fast-029-001.i	0.9901	0.8101
pu-met-fast-025-001.i	0.9897	0.8013
pu-met-fast-009-001.i	0.9892	0.7923
pu-met-fast-044-003.i	0.9864	0.7356
pu-met-fast-044-005.i	0.9862	0.7316
pu-met-fast-030-001.i	0.9840	0.6859
pu-met-fast-044-004.i	0.9832	0.6686
pu-met-fast-044-002.i	0.9829	0.6625
pu-met-fast-021-001.i	0.9794	0.5926
pu-met-fast-021-002.i	0.9785	0.5739
pu-met-fast-031-001.i	0.9776	0.5548
pu-met-fast-042-004.i	0.9725	0.4515
pu-met-fast-042-006.i	0.9723	0.4476
pu-met-fast-042-007.i	0.9717	0.4349
pu-met-fast-018-001.i	0.9714	0.4299
pu-met-fast-042-009.i	0.9714	0.4282
mix-met-fast-007-022.i	0.9713	0.4268
pu-met-fast-042-008.i	0.9709	0.4195
pu-met-fast-042-012.i	0.9709	0.4186
pu-met-fast-044-001.i	0.9708	0.4173
pu-met-fast-042-010.i	0.9705	0.4105
pu-met-fast-042-003.i	0.9705	0.4104
pu-met-fast-042-005.i	0.9701	0.4034
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pu-met-fast-042-015.i	0.9700	0.4010
pu-met-fast-011-001.i	0.9698	0.3964
pu-met-fast-042-013.i	0.9697	0.3947
pu-met-fast-042-014.i	0.9695	0.3895
mix-met-fast-007-023.i	0.9689	0.3791
pu-met-fast-042-002.i	0.9683	0.3657
pu-met-fast-003-103.i	0.9677	0.3540
mix-met-fast-001-001.i	0.9664	0.3281
pu-met-fast-027-001.i	0.9631	0.2590
pu-met-fast-042-001.i	0.9618	0.2343
pu-met-fast-045-005.i	0.9618	0.2336
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pu-met-fast-040-001.i	0.9606	0.2089
pu-met-fast-008-001.i	0.9601	0.1984
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pu-met-fast-026-001.i	0.9542	0.0795
mix-met-fast-003-001.i	0.9521	0.0350
mix-met-fast-007-019.i	0.9514	0.0211

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