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Title: Using Whisper to Support Nuclear Criticality Safety Validation ANSI/ANS-8.24 Requirements and Recommendations

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Using Whisper to Support Nuclear Criticality Safety Validation ANSI/ANS-8.24 Requirements and Recommendations

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NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

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EST. 1943

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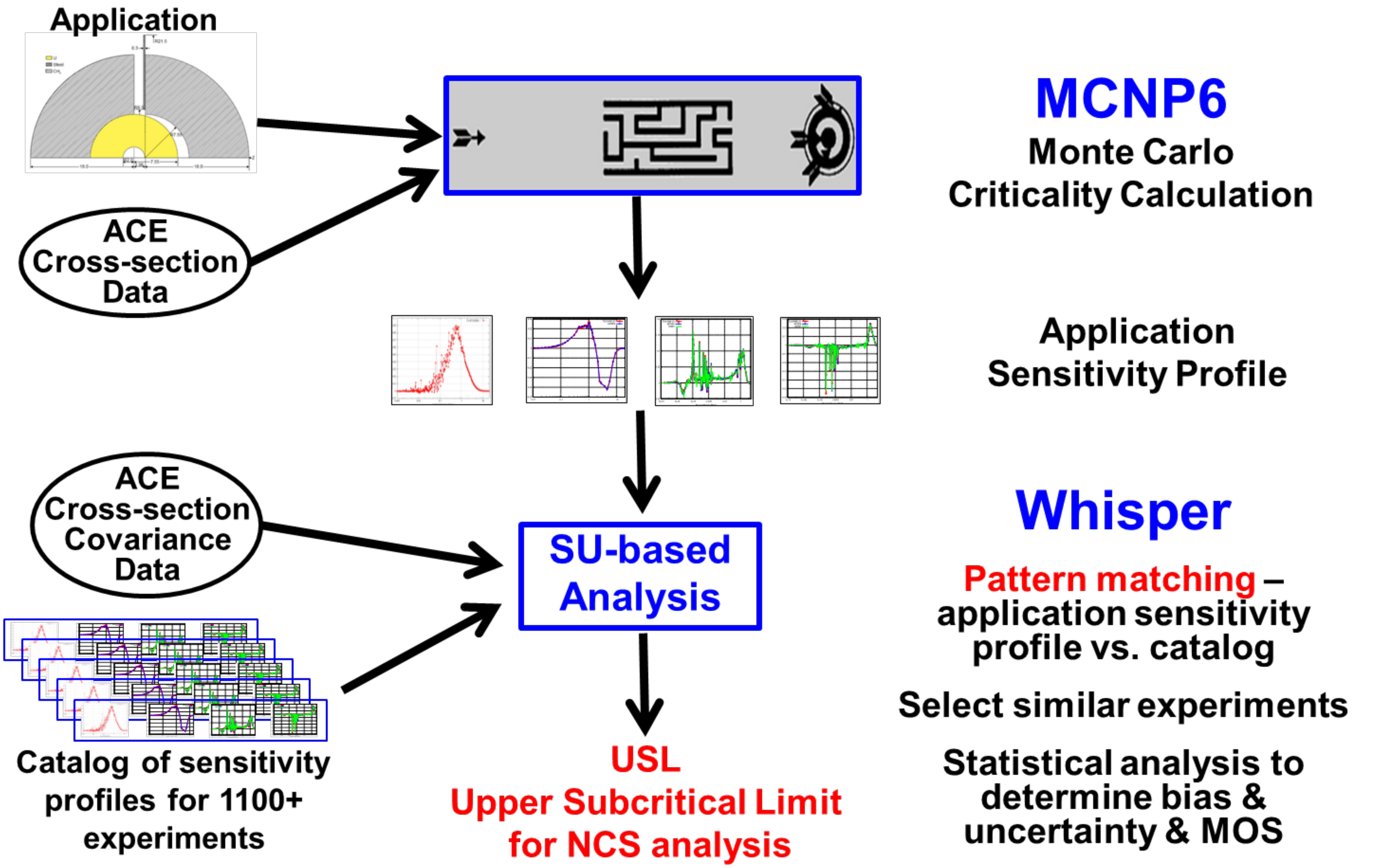
Monte Carlo Methods, Codes & Applications Group
X Computational Physics Division

Whisper Support for Validation

- **Whisper Methodology**
  - Calculational Margin
  - Margin of Subcriticality (Portions)
- **ANSI/ANS-8.24 Requirements/Recommendations**
  - Documented basis for MOS
- **Case Studies**
  - Vault, Array of Pu in Water, Pu Critical Mass Curve, CSE
- **Future Work**
  - Continue Collaboration
  - Incorporate feedback from user community
  - Better Covariance Data
  - Add Benchmarks to Whisper Library
  - Add Benchmark Correlations

Whisper Support for Validation



Whisper Methodology

- **Statistical Analysis code to determine baseline USLs**
- **Uses sensitivity profiles from continuous-energy MCNP6**
- **Uses covariance data from nuclear cross-sections**

1. **automated, physics-based selection of benchmarks neutronically similar to the application, ranked and weighted**
   - Energy bins
   - Reactions [elastic scattering, inelastic scattering, fission, capture, fission total ν, and fission χ]
   - Isotopes
2. **Bias + Bias uncertainty**
   - Extreme Value Theory
3. **Margin for Nuclear data uncertainty**
   - GLLS method

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Computer Code System	Whisper-1.1
Verification prior to validation (document)	Developers run verification suites and document results. Users must verify installation and operation prior to validation.
Configuration Control	Users must manage configuration.
Changes evaluated to determine effect on validation	Recommend running validation_criticality frequently (daily) to look for changes. If changes, complete new sensitivity profiles for Whisper benchmark library.

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Selection and Modeling of Benchmarks	Whisper-1.1
Appropriate process parameters correlate experiment to application	Whisper selects benchmark experiments that are most similar to the application using sensitivity profiles to characterize the neutronics of each application and benchmark for each isotope, reaction and energy.
Identify normal and credible abnormal conditions when determining parameters and values (benchmarks should encompass range)	
Use the same methods and analysis to analyze benchmark and application	Whisper uses same methods and analysis for both.
Review benchmarks prior to use (should be consistent with modeling capabilities of method; drawn from multiple series; evaluated by organization performing validation)	Benchmark models consistent with MCNP6 capabilities; drawn from multiple series; modeled by experienced MCNP6 users; must be reviewed and evaluated by organization performing validation.
Experienced users responsible for modeling benchmarks	

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Establishment of Bias, Bias Uncertainty, Margins	Whisper-1.1
Justify positive bias	Does not use positive bias.
Base trending parameters on application	Establishes USL for each application.
Rejection of outliers based on physical behavior or established statistical rejection methods	Rejection based on GLLS with iterative-diagonal χ^2 rejection technique.
Calculational margin consistent with quality and quantity of benchmarks	Selects similar (quality) benchmarks to conduct valid statistical analysis (quantity).
Method consistent with intended use	Consistent
Bias uncertainty allowance for measurement uncertainties; limitations in representations, statistical and convergence uncertainties	Uses experimental and cross-section uncertainties; statistical and convergence uncertainties; parameter studies used for limitations in geometric, material.
Trends used for extrapolation/wide interpolation based on cause	Application-specific USL, possible to trend with output information or parameter study.

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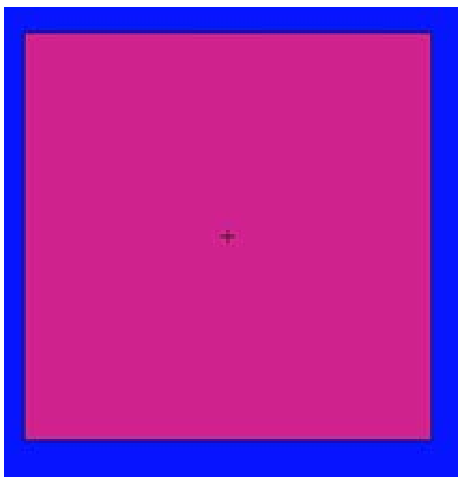
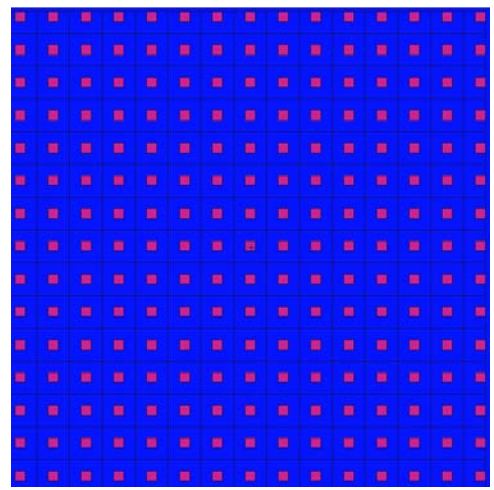
Establishment of Bias, Bias Uncertainty, and Margins Margin of Subcriticality (MOS)	
Sufficiently large to ensure calculated conditions will actually be subcritical	MOS_{data} based on sensitivity profiles and nuclear data covariances, MOS_{code} 0.005 based on MCNP developer expert judgment, $MOS_{application}$ must be applied by NCS analyst.
Take into account sensitivity of application to variations in fissile form, geometry, characteristics. Single trend might not be appropriate over entire validation applicability.	Application-specific, see case study for cubic array of metal pieces.

Whisper Case Study-Cubic Array

- LA-UR-07-0160, *Practical Application of the Single-Parameter Subcritical Mass Limit for Plutonium*: When do plutonium metal and water mixtures cease to appear as “metal” systems and begin to appear more like “solution” systems?
- ^{239}Pu metal cubes in water was performed using MCNP6 and Whisper

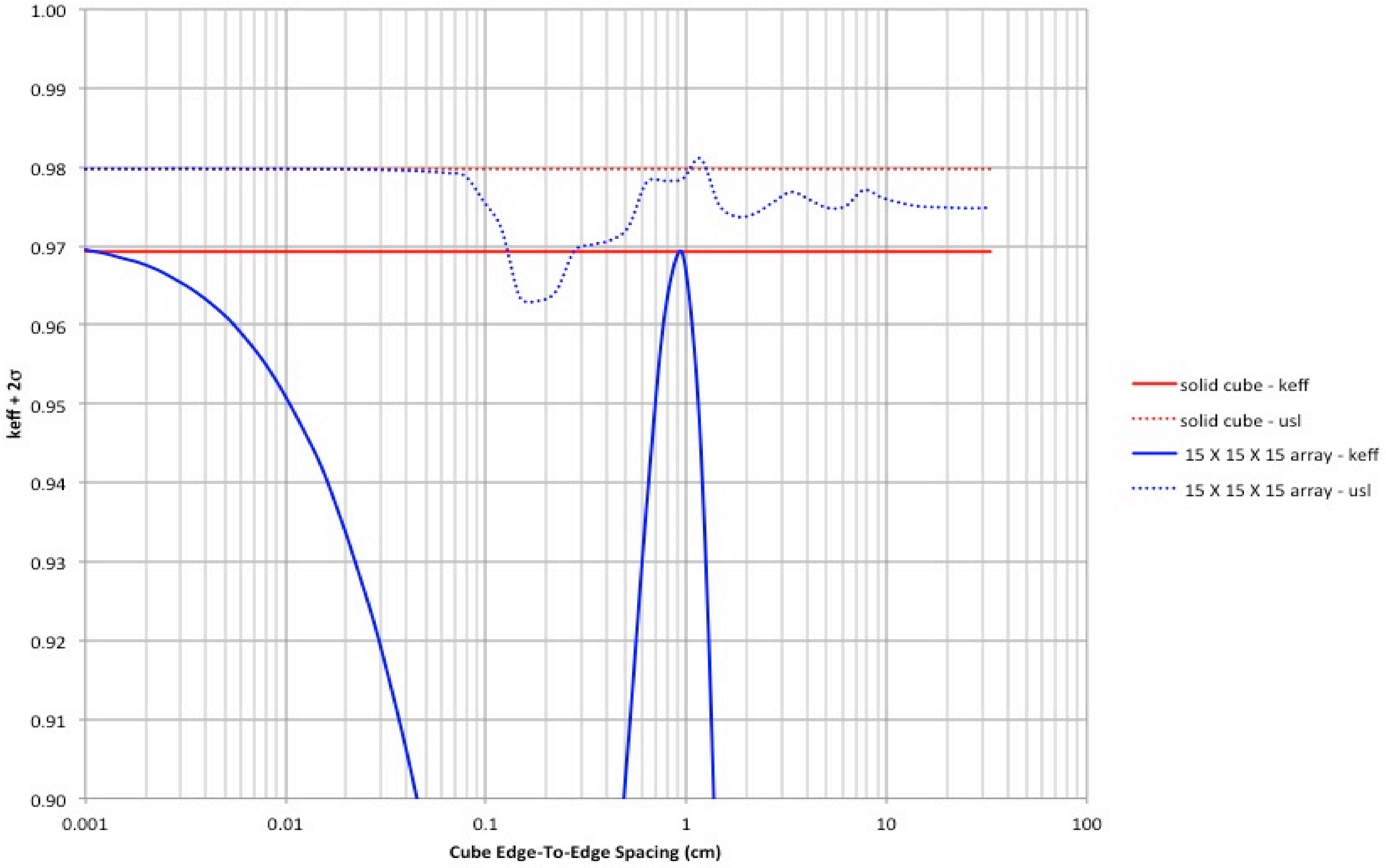


N = 1,Mass Per Cube = 5,000 g



N = 15, Mass Per Cube = ~1.48 g
Spacing = 1 cm

Whisper Case Study-Cubic Array



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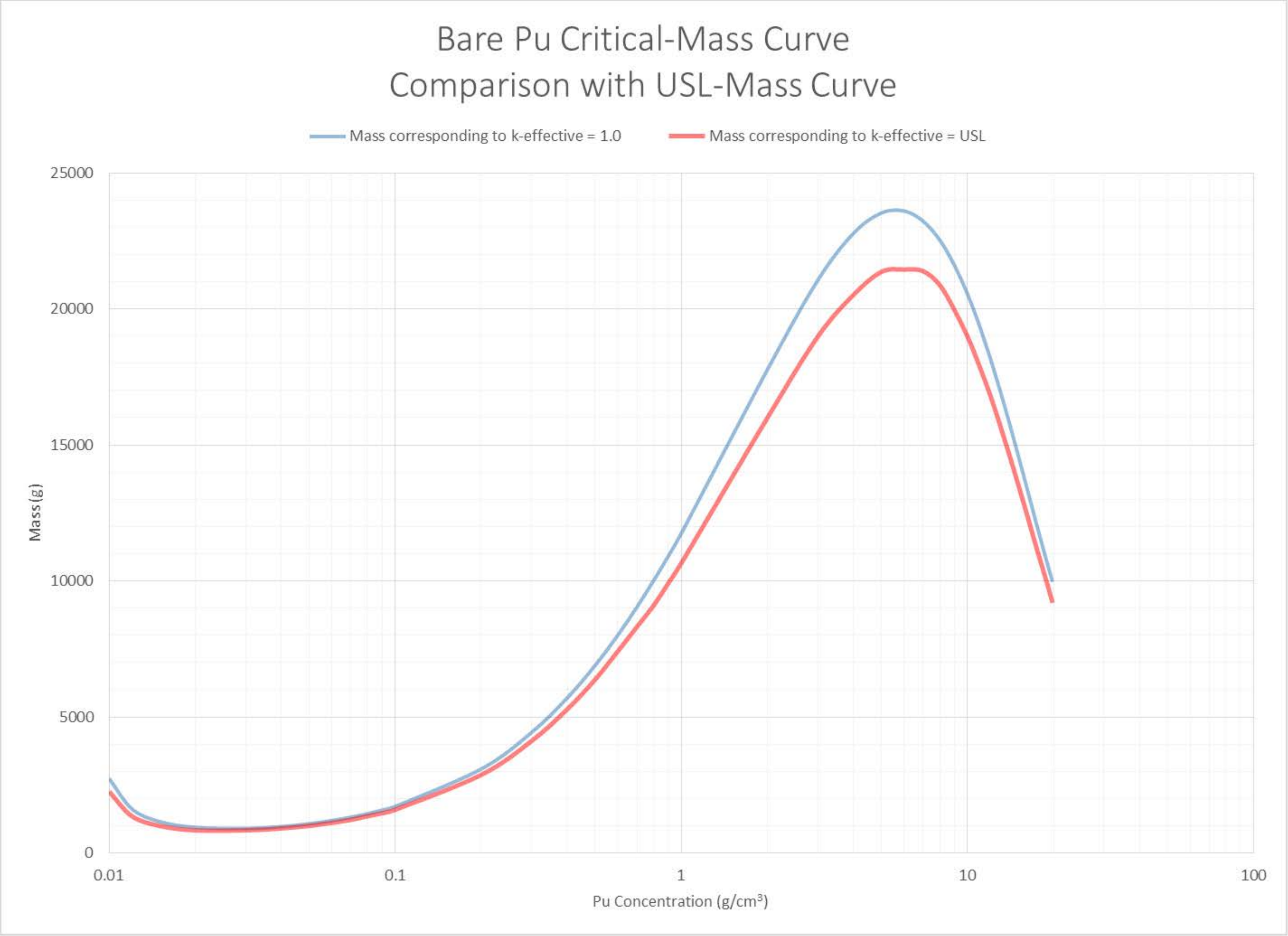
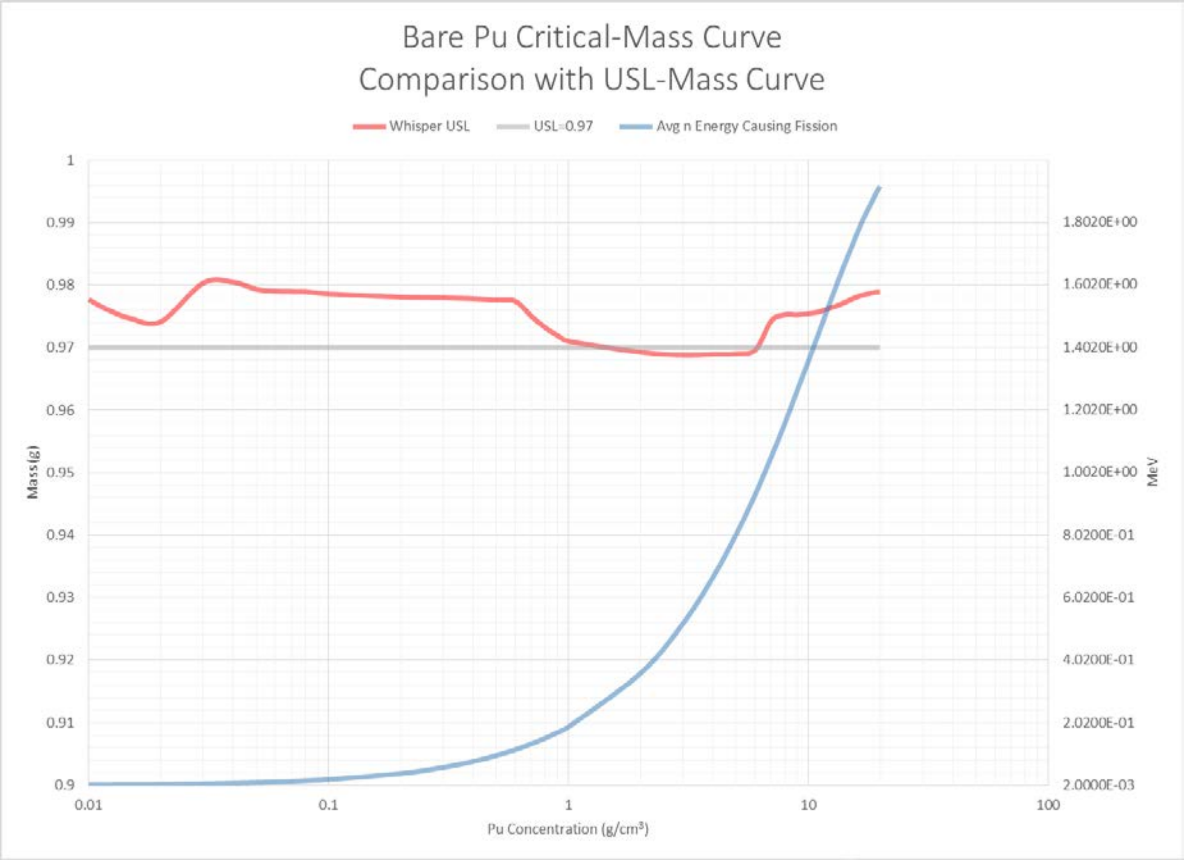
Adequacy of the Validation	
Validation applicability based on benchmark applicability (may be extended)	Sensitivity profiles to select most similar benchmarks, ranked by c_k. Extrapolation/wide interpolation lower c_k; $c_k < 0.8$ requires additional margin based on expert judgment.
USL based on CM and MOS	USL = 1 – CM - MOS
The validation applicability should not be so large that a subset of data with a high degree of similarity to the system or process would produce a higher USL that is lower than that determined for the entire set. Subset of data closely related to application is not nonconservatively masked by benchmarks that do not match the system as well.	Application-specific USL, see Whisper Case Study Critical Mass Curve

Whisper Case Study-Critical Mass Curve



Whisper Case Study-Critical Mass Curve

The validation applicability should not be so large that a subset of data with a high degree of similarity to the system or process would produce an upper subcritical limit that is lower than that determined for the entire set. This criterion is recommended to ensure that a subset of data that is closely related to the system or process is not nonconservatively masked by benchmarks that do not match the system as well.



THERMAL

- **Average neutron energy causing fission: 0.00854 MeV**
- **% of fissions caused by neutrons: 96%; 3.5%; 0.5%**
- **Bias+bias uncertainty: 0.01306**
- **Nuclear data uncertainty: 0.00057**
- **USL = 0.98046**

INTERMEDIATE

- **Average neutron energy causing fission: 0.519 MeV**
- **% of fissions caused by neutrons: 18%; 55%; 27%**
- **Bias+bias uncertainty: 0.02197**
- **Nuclear data uncertainty: 0.00162**
- **USL = 0.96881**

FAST

- **Average neutron energy causing fission: 1.92 MeV**
- **% of fissions caused by neutrons: 0%; 2%; 98%**
- **Bias+bias uncertainty: 0.01419**
- **Nuclear data uncertainty: 0.00073**
- **USL = 0.97891**

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- **Documentation and Independent Technical Review**
  - **Trending analysis and technical basis**
  - **Validation applicability**
  - **Differences validation applicability – application**
  - **Limitations**
  - **MOS and its basis**
  - **USL and methods to determine**
  - **Independent technical review**
    - Benchmark applicability
    - Input/output files
    - methodology: CM, MOS
    - Concurrence with validation applicability

Whisper Case Study-Vault CSE Finding

data unc margin	baseline (1-sigma)	k(calc) USL	> USL
0.01471	0.00062	0.97867	-0.01239

Benchmark population = 45
Population weight = 25.88913
Maximum similarity = 0.99111

Bias = 0.00745
Bias uncertainty = 0.00726
Nuc Data uncert margin = 0.00062
Software/method margin = 0.00500
Non-coverage penalty = 0.00000

benchmark	ck	weight
pu-met-fast-003-103.i	0.9911	1.0000
pu-met-fast-025-001.i	0.9903	0.9669
pu-met-fast-030-001.i	0.9882	0.8793
mix-met-fast-009-001.i	0.9882	0.8774
pu-met-fast-044-002.i	0.9881	0.8736
pu-met-fast-023-001.i	0.9875	0.8524
pu-met-fast-042-012.i	0.9872	0.8360
pu-met-fast-042-015.i	0.9872	0.8358
pu-met-fast-042-013.i	0.9871	0.8347
pu-met-fast-021-002.i	0.9871	0.8332
pu-met-fast-042-011.i	0.9869	0.8244
pu-met-fast-042-014.i	0.9868	0.8218

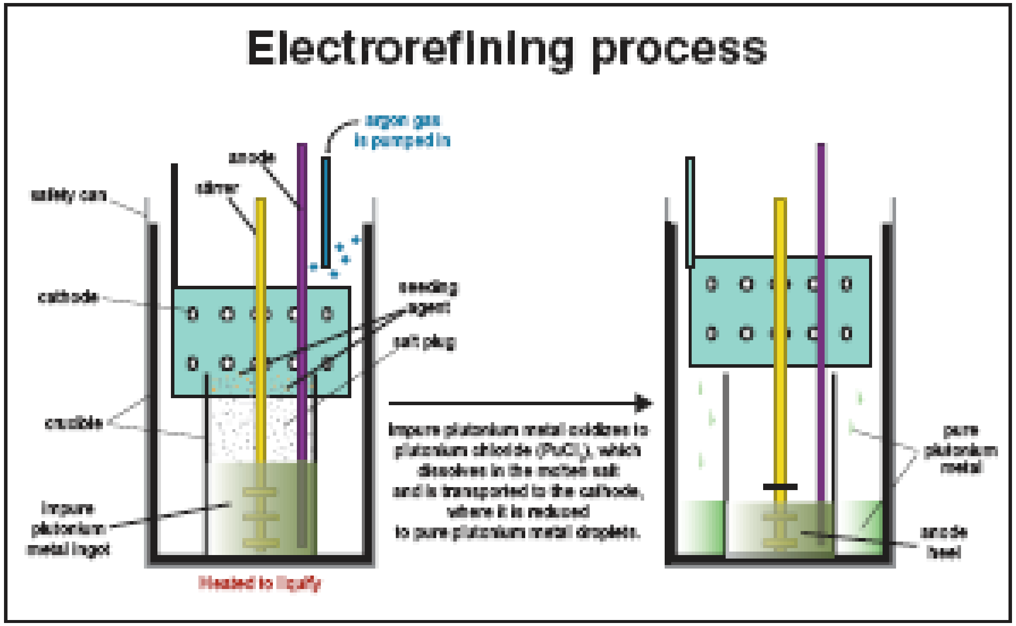
"CSE discusses the validation reports used and concludes that the Area of Applicability (AoA) is met with no AoA adjust met required.

The validation reports were reviewed and the benchmark experiments evaluated do not include experiments of large arrays, mixed energy spectra systems, or metal systems with thermal spectra.

The array in question is a large array with a mixed neutron energy spectra.

The evaluation does not provide a technical justification for no AoA adjustment. (ANSI/ANS 8.1, Section 4.3.6; ANSI/ANS 8.24, Section 7.1)"

Whisper Case Study-CSE



Ref. Actinide Research Quarterly 3rd Quarter 2008

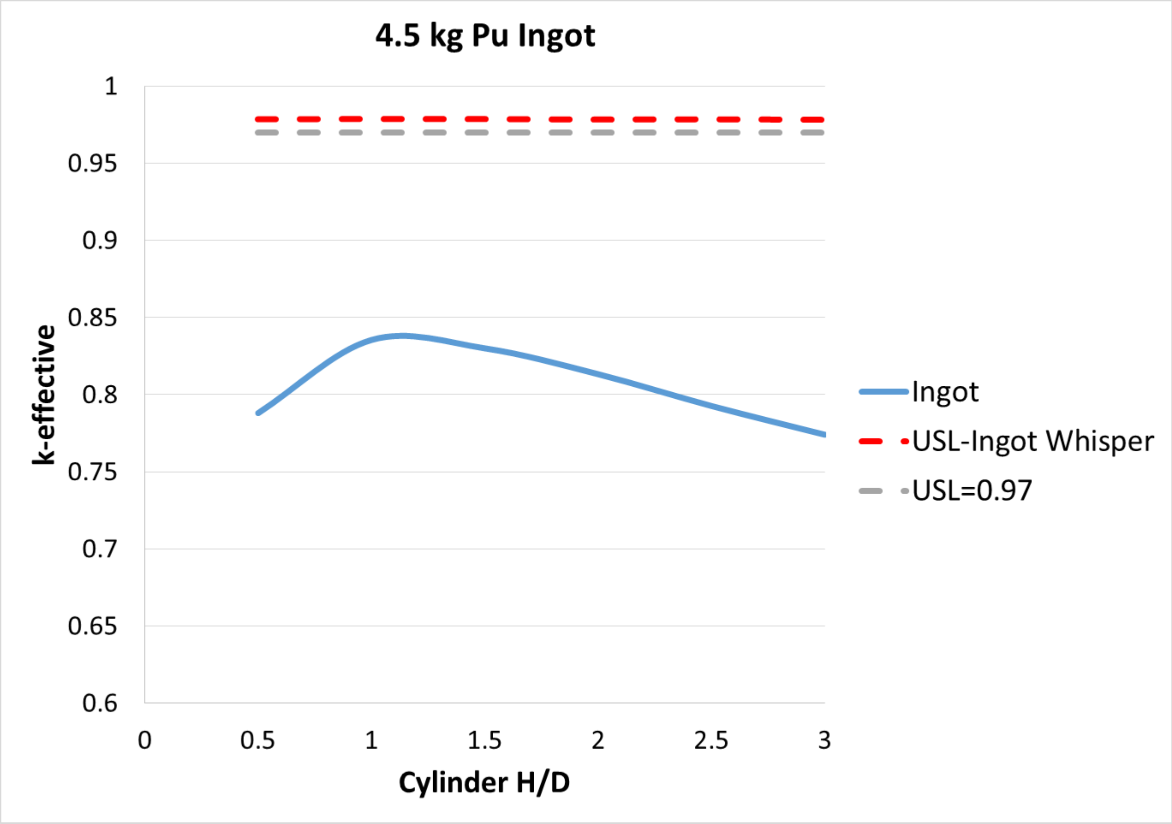
Whisper Case Study-CSE

application	calc margin	data unc (1-sigma)	baseline USL	k(calc) > USL
ingot.txt_1_in	0.01441	0.00076	0.97862	-0.14366

```
Benchmark population   =   44
Population weight      =  25.38028
Maximum similarity     =   0.99621

Bias                   =   0.00858
Bias uncertainty       =   0.00583
Nuc Data uncert margin =   0.00076
Software/method margin =   0.00500
Non-coverage penalty   =   0.00000
```

benchmark	ck	weight
pu-met-fast-036-001.i	0.9962	1.0000
pu-met-fast-022-001.i	0.9957	0.9850
pu-met-fast-024-001.i	0.9956	0.9813
pu-met-fast-001-001.i	0.9940	0.9319
pu-met-fast-023-001.i	0.9937	0.9207
pu-met-fast-039-001.i	0.9932	0.9069
mix-met-fast-009-001.i	0.9923	0.8774
pu-met-fast-044-005.i	0.9917	0.8598
pu-met-fast-035-001.i	0.9913	0.8449
pu-met-fast-025-001.i	0.9902	0.8117
pu-met-fast-009-001.i	0.9898	0.7976
…		
pu-met-fast-003-103.i	0.9714	0.2215
mix-met-fast-007-023.i	0.9709	0.2041
mix-met-fast-001-001.i	0.9675	0.0979
pu-met-fast-045-005.i	0.9668	0.0777
pu-met-fast-032-001.i	0.9644	0.0015



Whisper Case Study-CSE

Parameter	Area of Applicability
Fissile Material	^{239}Pu
Fissile Material Form	Pu Metal, PuO_2, and $Pu(NO_3)_4$
$H/^{239}Pu$	$0 \leq H/^{239}Pu \leq 2807$
Average Neutron Energy Causing Fission (MeV)	$0.003 \leq ANECF \leq 1.935$
^{240}Pu	0 to 42.9 wt% ^{240}Pu
Moderating Materials	none, water, graphite, polystyrene
Reflecting Materials	none, water, steel, oil, Plexiglas, polyethylene, graphite, W, Cu, U, Th, Al, Ni, Fe, Pb, Cd, Mo, Be, BeO
Other Materials	concrete, PVC, Ga, B, Gd, Ta
Geometry	cylinder array, cylinder, slab, sphere, hemisphere, stacked discs, cuboid, annular

5.3 Metallic units

The enrichment subcritical limit for uranium and the mass subcritical limits given in Table 3 apply to a single piece having no concave surfaces.

Table 3 – Single-parameter subcritical limits for metal units

Parameter	Subcritical limits for		
	^{233}U [15]	^{235}U [16]	^{239}Pu [17]
Mass of fissile nuclide (kg)	6.0	20.1	5.0

Benchmark	^{240}Pu wt%	Form	Geometry	Moderator / Reflector	$H/^{239}Pu$	Other Materials
pu-sol-therm-032-001	10.0	Pu(NO3)4	Annular	Water/Water	449.5	Steel
pu-sol-therm-032-002	10.0	Pu(NO3)4	Annular	Water/Water	488.2	Steel
pu-sol-therm-032-003	10.0	Pu(NO3)4	Annular	Water/Water	555.3	Steel
pu-sol-therm-032-004	10.0	Pu(NO3)4	Annular	Water/Water	622.5	Steel
pu-sol-therm-032-005	10.0	Pu(NO3)4	Annular	Water/Water	700.7	Steel
pu-sol-therm-032-006	10.0	Pu(NO3)4	Annular	Water/Water	800.5	Steel
pu-sol-therm-032-007	10.0	Pu(NO3)4	Annular	Water/Water	850.5	Steel
pu-sol-therm-032-008	10.0	Pu(NO3)4	Annular	Water/Water	949.6	Steel
pu-sol-therm-032-009	10.0	Pu(NO3)4	Annular	Water/Water	1021.5	Steel

- **Does SPSL, 5 kg Pu metal, apply to a ring with concave surfaces?**
- **Is annular cylinder validated geometry for this application?**
- **How can this be established; what benchmarks include this geometry? Are these benchmarks similar to the ring?**

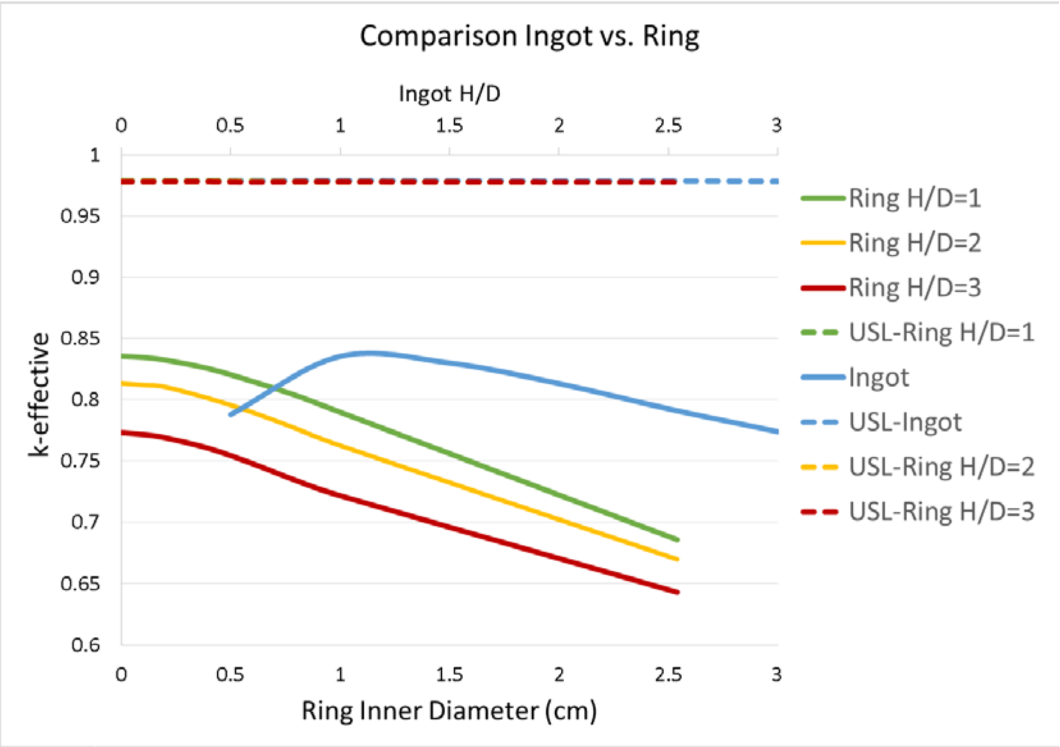
Whisper Case Study-CSE

application	calc margin	data unc (1-sigma)	baseline USL	k(calc) > USL
ringhd2.txt_0.4_in	0.01464	0.00075	0.97840	-0.17760

```
Benchmark population   =   41
Population weight      =  25.47164
Maximum similarity     =   0.99532

Bias                   =   0.00836
Bias uncertainty       =   0.00628
Nuc Data uncert margin =   0.00075
Software/method margin =   0.00500
Non-coverage penalty   =   0.00000
```

benchmark	ck	weight
pu-met-fast-036-001.i	0.9953	1.0000
pu-met-fast-024-001.i	0.9941	0.9608
pu-met-fast-044-005.i	0.9933	0.9360
pu-met-fast-011-001.i	0.9928	0.9196
pu-met-fast-044-004.i	0.9925	0.9117
pu-met-fast-044-003.i	0.9898	0.8275
pu-met-fast-023-001.i	0.9890	0.8020
pu-met-fast-022-001.i	0.9886	0.7898
pu-met-fast-039-001.i	0.9884	0.7823
…		
pu-met-fast-029-001.i	0.9777	0.4468
pu-met-fast-044-001.i	0.9743	0.3409
pu-met-fast-018-001.i	0.9720	0.2678
mix-met-fast-007-022.i	0.9690	0.1754
mix-met-fast-007-023.i	0.9655	0.0635
pu-met-fast-045-005.i	0.9653	0.0586



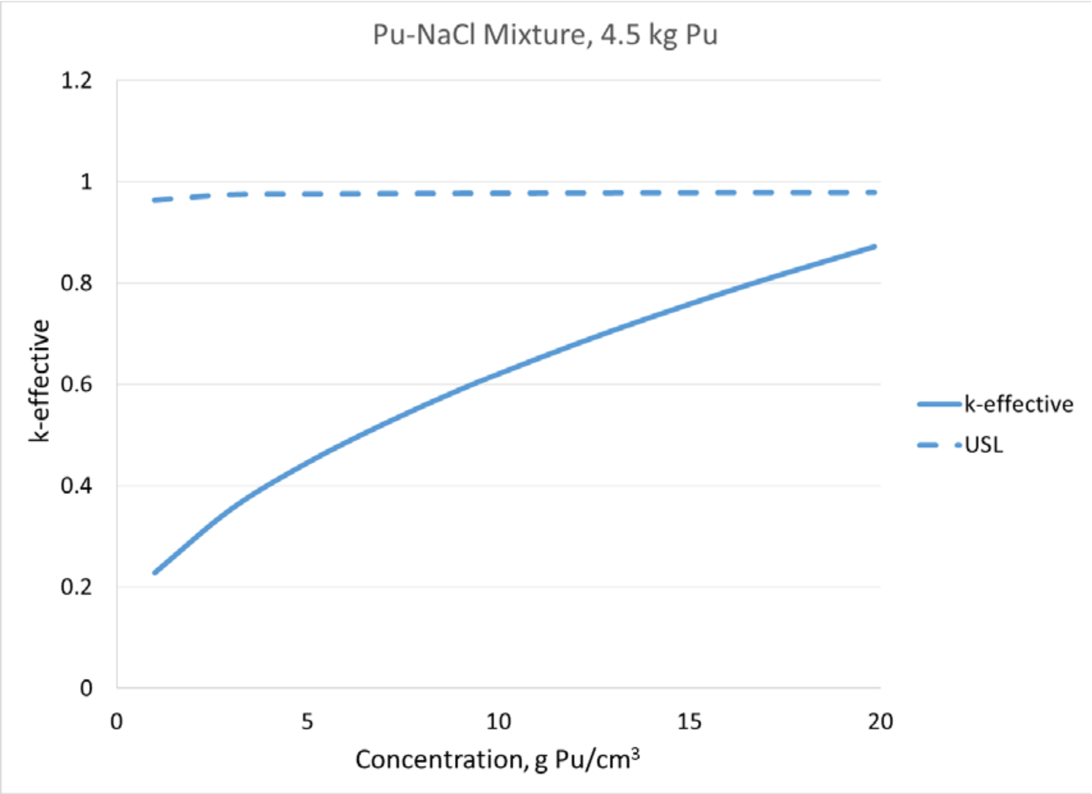
Benchmarks are the same as those for the ingot

Whisper Case Study-CSE

```
                            USL baseline = .979
Benchmark population    =   46
Benchmark weight        =   25.75745
Benchmark similarity    =   0.99245

Bias                    =   0.00796
Bias uncertainty        =   0.00682
Nuc Data                =   0.0012
Software/method margin  =   0.005
Non-coverage penalty    =   0

benchmark   ck          weight
pu-met-fast-011-001.i   0.9924      1
pu-met-fast-044-004.i   0.9842      0.8636
pu-met-fast-042-001.i   0.9831      0.8448
pu-met-fast-042-002.i   0.9828      0.8396
pu-met-fast-044-005.i   0.9827      0.8377
pu-met-fast-027-001.i   0.981       0.8107
pu-met-fast-036-001.i   0.9805      0.8018
pu-met-fast-042-003.i   0.9802      0.7965
pu-met-fast-031-001.i   0.9792      0.7798
pu-met-fast-042-004.i   0.9787      0.7727
pu-met-fast-024-001.i   0.978       0.7604
pu-met-fast-044-003.i   0.9768      0.7401
pu-met-fast-042-005.i   0.9757      0.7213
pu-met-fast-042-006.i   0.9746      0.7039
pu-met-fast-021-002.i   0.9737      0.6893
…
pu-met-fast-019-001.i   0.9421      0.1637
pu-met-fast-038-001.i   0.9384      0.1032
mix-met-fast-001-001.i  0.9374      0.0871
pu-met-fast-040-001.i   0.9355      0.055
pu-met-fast-003-103.i   0.9352      0.0505
```



Whisper Case Study-CSE Validation Weakness

- **Reflection: Ta**

Is Ta validated as a reflector in the AoA?

Parameter	Area of Applicability
Fissile Material	^{239}Pu
Fissile Material Form	Pu Metal, PuO_2, and $Pu(NO_3)_4$
H/^{239}Pu	$0 \leq H/^{239}Pu \leq 2807$
Average Neutron Energy Causing Fission (MeV)	$0.003 \leq ANECF \leq 1.935$
^{240}Pu	0 to 42.9 wt% ^{240}Pu
Moderating Materials	none, water, graphite, polystyrene
Reflecting Materials	none, water, steel, oil, Plexiglas, polyethylene, graphite, W, Cu, U, Th, Al, Ni, Fe, Pb, Cd, Mo, Be, BeO
Other Materials	concrete, PVC, Ga, B, Gd, Ta
Geometry	cylinder array, cylinder, slab, sphere, hemisphere, stacked discs, cuboid, annular

- **CSSG Response on Validation with Limited Benchmark Data:**

"For those situations where a nuclide is determined to be important and limited data exist, validation may still be possible. However, an additional margin should be used to compensate for the limited data. This margin is separate from, and in addition to, any margin needed for extending the benchmark applicability to the validation. Sensitivity and uncertainty tools may be used as part of the technical basis for determining the magnitude of the margin."

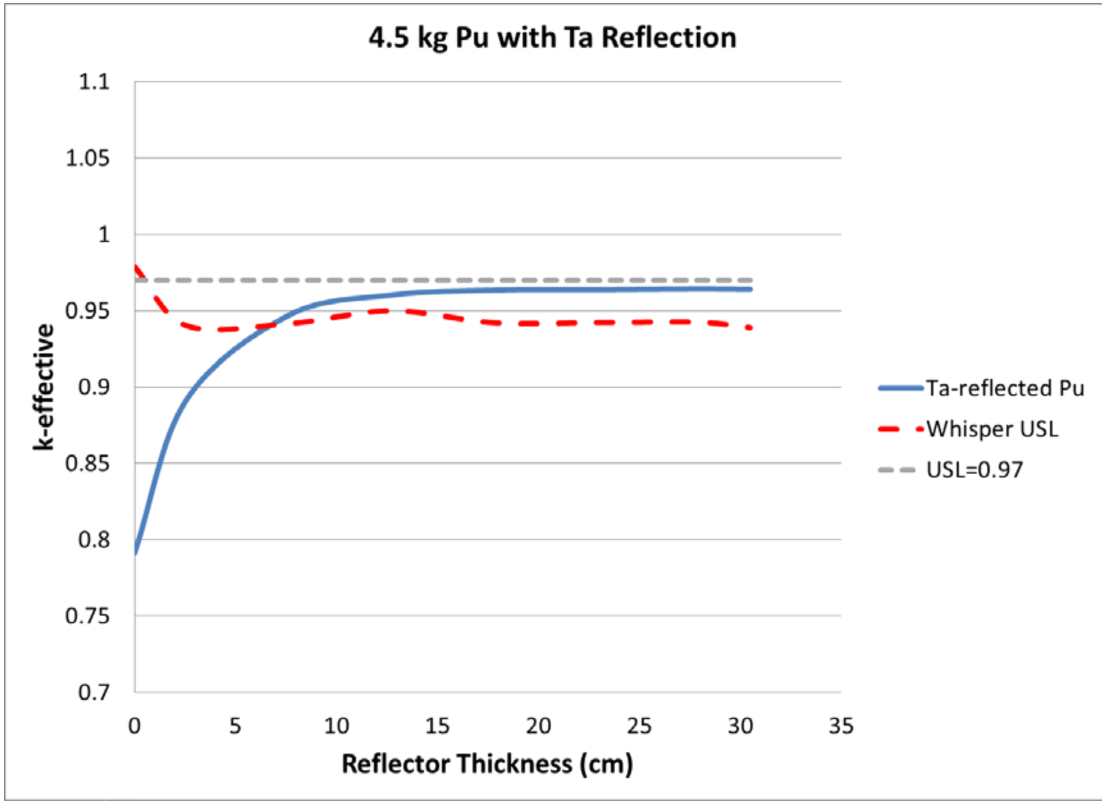
Whisper Case Study - CSE Validation Weakness

application	calc margin	data unc (1-sigma)	baseline USL	k(calc) > USL
tarefl.txt_7.62_in	0.01707	0.01502	0.93889	0.00750

```
Benchmark population    =  119
Population weight       =  60.92464
Maximum similarity      =   0.64075

Bias                    =   0.00912
Bias uncertainty        =   0.00795
Nuc Data uncert margin  =   0.01502
Software/method margin  =   0.00500
Non-coverage penalty    =   0.00000
```

benchmark	ck	weight
pu-met-fast-045-006.i	0.6408	1.0000
pu-met-fast-045-004.i	0.6400	0.9986
pu-met-fast-045-003.i	0.6368	0.9926
pu-met-fast-045-002.i	0.6297	0.9796
pu-met-fast-045-007.i	0.6259	0.9725
pu-met-fast-045-001.i	0.6213	0.9641
pu-met-fast-045-005.i	0.5469	0.8270
pu-met-fast-023-001.i	0.4203	0.5937
pu-met-fast-039-001.i	0.4201	0.5935
…		
pu-met-fast-042-011.i	0.4134	0.5810
pu-met-fast-042-009.i	0.4134	0.5810
pu-met-fast-042-013.i	0.4133	0.5808
pu-met-fast-042-014.i	0.4133	0.5808
pu-met-fast-042-010.i	0.4133	0.5808
pu-met-fast-042-007.i	0.4132	0.5807
pu-met-fast-018-001.i	0.4132	0.5806
pu-met-fast-042-006.i	0.4131	0.5806…



Whisper Case Study – CSE Validation Weakness

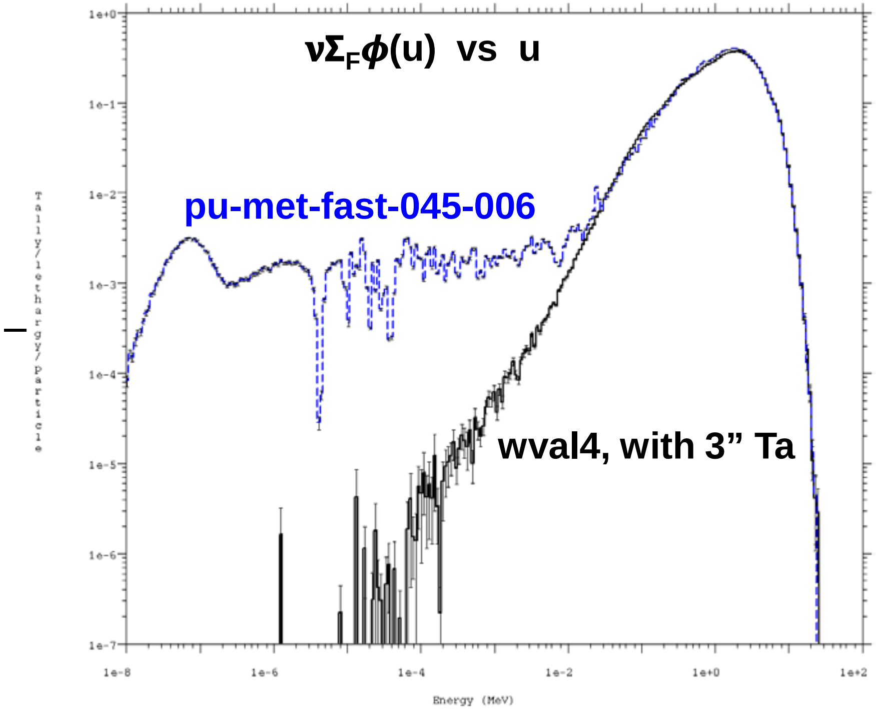
- **None of the benchmarks appear to have the same neutronics as the application**
  - Largest C_k in the Whisper example output is 0.64 – very low
  - Guidance from ORNL Scale/Tsunami developers:

0.95 < C_k	**→**	**great**
0.90 < C_k < 0.95	**→**	**good**
C_k < 0.90	**→**	**not so good**

For C_k's in range 0.9 – 1.0,
at least 5-10 benchmarks needed

For C_k's in range 0.8 – 0.9,
at least 10-20 benchmarks needed

  - If all C_k's are low, there is a need to expand the benchmark suite, add similar benchmarks
  - If no similar benchmarks, need extra analysis, analyst judgment, & margin



- **The current benchmark suite for Whisper was focused on main needs for LANL validation, few benchmarks with Ta**
- **Need to find more benchmarks with Ta reflector & add to Whisper suite, if Ta-reflected applications are expected**

Acknowledgements

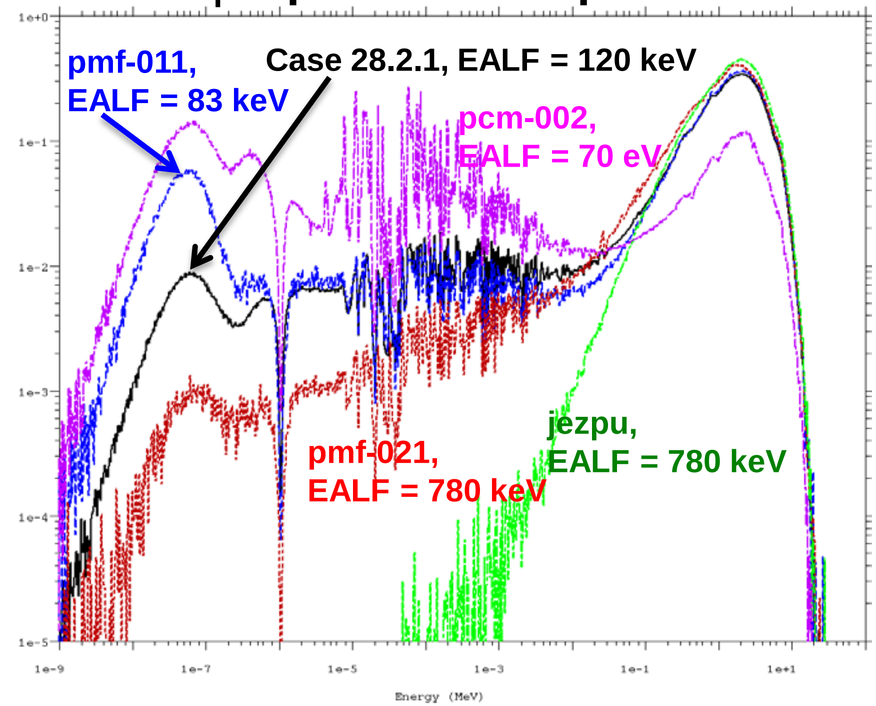
- This work was supported and funded by the US DOE/NNSA Nuclear Criticality Safety Program.
- The original version of Whisper-1.0 was developed by B.C. Kiedrowski, now a professor at the University of Michigan.

Impact of Pu Chemistry in Analysis

Whisper with MCNP6

- Nuclear Criticality Safety analysis requires validation of computational methods
- Neutron spectra are complex functions of geometry, materials, nuclear cross-section, etc.
- **MCNP-WHISPER Methodology:**
- MCNP determines sensitivity profiles to characterize neutronics of an application or benchmark, S(energy, reaction, isotope) S=(dk/k)/(dσ/σ)
- **WHISPER uses:**
  - Sensitivity profile data for application
  - Covariance files for nuclear data
- **To determine**
  - Baseline upper subcritical limit (USL) with bias, bias uncertainty, margin of subcriticality
  - Similar benchmarks from library of 1100+ ICSBEP experiments
- **Can support traditional validation and help determine or support validation weaknesses**

$\nu\Sigma_F\Phi$ production spectrum



Brown, F. E., M. Rising, and J. L. Alwin., *MCNP-WHISPER Methodology for Nuclear Criticality Safety Validation*. LA-UR-16-23757

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