Implementation of Whisper-based Validation at the Hanford Tank Farms





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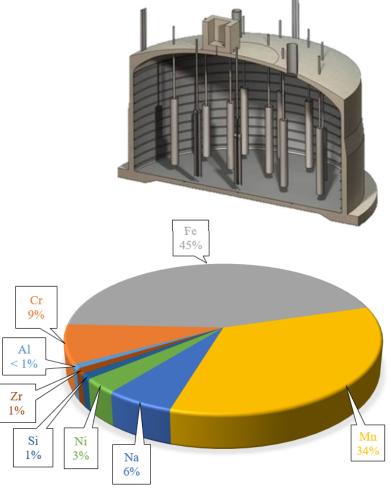
June 2020 ANS Summer Meeting

HANFORD TANK WASTE

- Product of 50 years of plutonium production
 - Many distinct waste streams and compositions
- 56 million gallons of waste in 177 tanks, including:
 - Various metals
 - **Fission products** ۲
 - Uranium (~600 metric tons)
 - Plutonium (670 kg)

• NCS analysis mainly based on presence of:

- o Aluminum
- o Chromium o Silicon
- o Iron
- o Manganese
- o Nickel
- o Sodium
- o Zirconium





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CRITICALITY SAFETY CALCULATIONS

- Current NCS evaluation is based on <u>Pu-to-absorber ratios</u>:
 - Infinite, homogenous mixtures of Pu, water, and one absorber metal oxide
 - Absorbers combined proportionally (iron-equivalent mass)
- Future evaluations will include direct calculation of waste compositions

... How similar are benchmark experiments to these models?

Previous recommendations to use sensitivity/uncertainty validation methods



VALIDATION CALCULATIONS

- MCNP6.2 with Whisper-1.1
 - ENDF/B-VII.1 cross-sections
- 1,223 total benchmark experiments:
 - 1,101 distributed with Whisper
 - + 122 added locally
 - Added:
 - ✓ Many MIX benchmarks
 - \checkmark Available thermal Pu benchmarks with absorbers of interest

• USL calculations using:

- Each absorber over full H-to-X range
- 'Real' tank compositions [~400 total solids layers], at optimal moderation



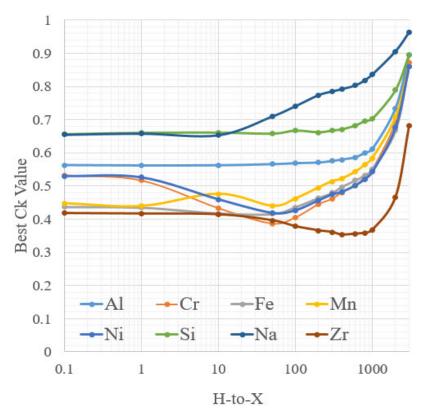
INITIAL WHISPER CALCULATIONS



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BENCHMARK SIMILARITY

- Using standard Whisper calculation flow:
 - Best c_k value typically between 0.4 and 0.6
 - [Good match is $c_k > 0.9$]
- Minimal presence of most absorbers in benchmarks:
 - Structural materials, cladding, or trace contaminants
 - No significant sensitivity in k_{eff}
- (n, γ) sensitivity in calcs often 100+ times any benchmark



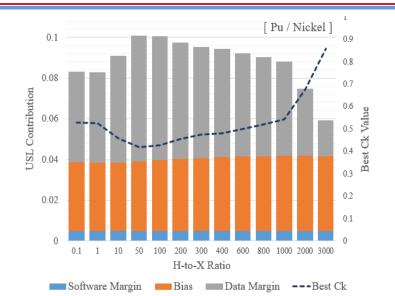


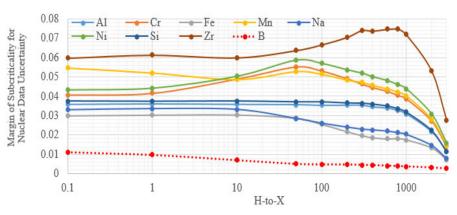
IMPACT ON WHISPER USL

 $USL = 1 - Bias - MOS_{nuclear data} - MOS_{software}$

For initial calculations:

- Bias large and near-constant
 - Low $c_k = little variation across H-to-X or elements$
 - Near maximum possible for benchmark set
- *MOS_{data}* largest component of calculated USL
 - Little uncertainty reduction (~few comparison points)
- Produced USLs around <u>0.87</u> to <u>0.90</u>







MODIFIED CALCULATION & RESULTS



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SPLITTING USL CALCULATION

"[It] is possible to bound the computational bias introduced by a particular nuclide, for which little experimental data are available, by examining the keff uncertainties introduced by the uncertainties in that nuclide's nuclear data. ... The additional margin should be at least as large as the keff uncertainties introduced by the uncertainties in that nuclide's nuclear data (at the one sigma level."

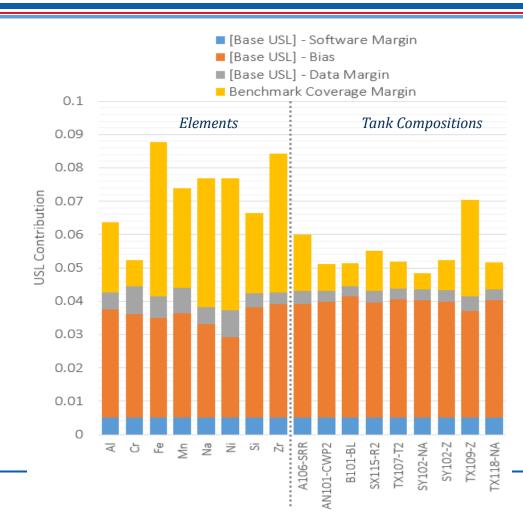
~ CSSG response 2014-02

- Final USLs calculated in 2 parts:
 - A "base USL" calculated with Whisper
 - o Sensitivity calculation limited to Pu, U, H, and O
 - o Same input file; exact match to spectra
 - \circ C_k shows applicability to isotopes that <u>can</u> be matched
 - An additional margin based on CSSG response 2014-02, "Validation with Limited Benchmark Data"
 - o Accounting for absorbers without benchmark representation
 - Based on sensitivities calculated for each isotope, and their crosssection uncertainties



CALCULATED MARGINS

- Calculated bounding singleelement margins for all H-to-X
 - Lowest final USLs for Fe, Zr
- Smaller total margins for tank waste compositions:
 - Absorption in ²³⁸U part of "base USL"
 - 8 different absorber elements



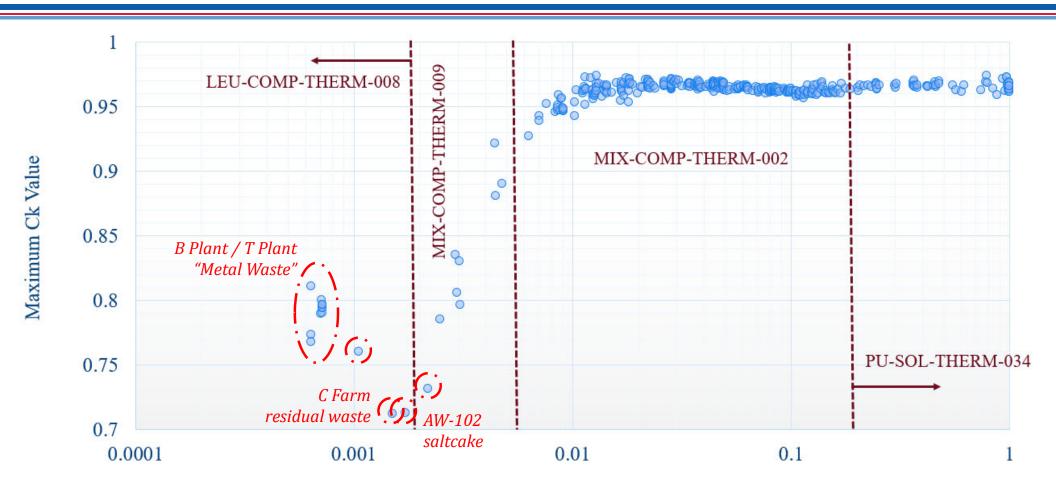


BASE USL – C_{κ} **SIMILARITY VALUES**

- Almost all tank layers had excellent c_k values for base USL calculation [$c_k > 0.95$]
 - Only 3 kg Pu [0.4%] in layers with $c_k < 0.8$
 - 7½ kg Pu [1%] in layers with $c_k < 0.9$
- Clear trends with uranium content
- Highest-ranked benchmark was always one of four experiments:
 - ✓ PU-SOL-THERM-034 plutonium solution containing Gd
 - \checkmark MIX-COMP-THERM-002 Pu and natural UO₂ in borated water
 - ✓ MIX-COMP-THERM-009 Pu and DU in water
 - ✓ LEU-COMP-THERM-008 2.5% enriched UO₂ fuel pins in borated water



HIGHEST-RANKED BENCHMARKS



Pu / (U + Pu)

MARGINS IN LOW-C_K BASE USLS

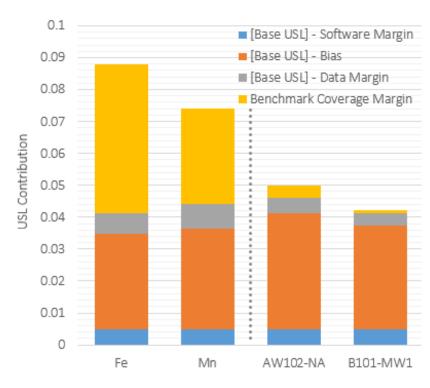
Lowest-c_k layers = highest U content

- Vast majority of absorption in ²³⁸U
- Much less reliant on absorbers like Fe, Mn, etc.
- Smaller benchmark coverage margins for other absorbers
- Future calculations use same USL for all compositions:
 - Bounding, worst-case single element = Fe, 0.913
 - Significant extra margins for high-U, low- c_k waste layers

Majority of low-c_k layers are compositions with lowest NCS concern

- Minimal actual Pu
- Very large absorber masses





CONCLUSIONS & PATH FORWARD



CONCLUSIONS & PATH FORWARD

- Sensitivity / Uncertainty methods implemented for Tank Farms NCS calculations
 - Showed that few highly applicable benchmarks were available
- New MCNP6.2 validation uses variant of standard Whisper method
 - Additional margins to compensate for absorbers
- More use of full tank layer calculations
 - Less reliance on any single absorber element
 - Include absorption from near-natural U in same calculation
- Development of new thermal Pu benchmarks
 - Designed for strong absorption from credited elements
 - Fe & Mn versions of TEX experiment





