SCALE TSUNAMI Analysis of Critical Experiments for Validation of ^{233}U Systems

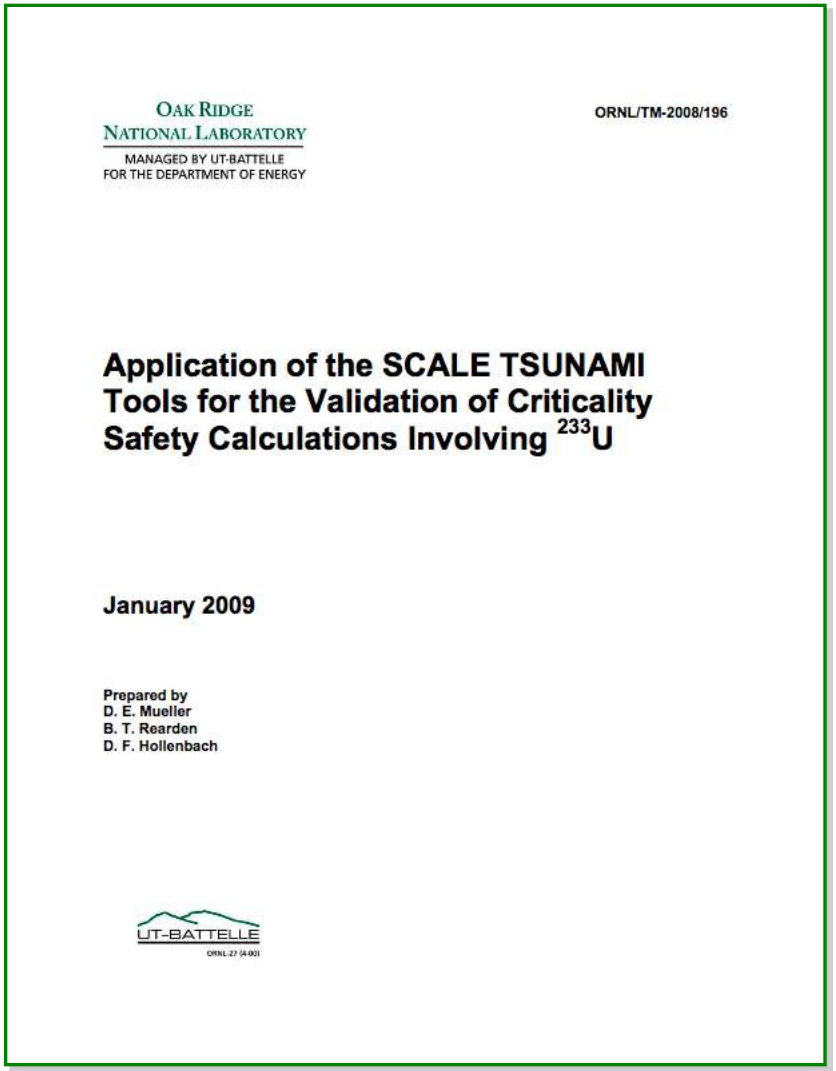
Don Mueller and Brad Rearden

^{233}U Downblending at ORNL

- ISOTEK, LLC designing operations to downblend materials stored at Radiochemical Development Facility (RDF)
  - Highly-enriched ^{233}U downblended with ^{238}U
- Aqueous process will be used
- K. R. ELAM, L. L. GILPIN, and B. W. STARNES, "Integrating Criticality Safety in Design of ^{233}U Downblending Process," *Trans. Am. Nucl.Soc.*, **100**, 343-344 (2009).

SCALE TSUNAMI Analysis

- ORNL staff used the SCALE TSUNAMI tools to provide a demonstration evaluation of critical experiments considered for use in validation of current and anticipated operations involving ^{233}U at the RDF.
- Reported in ORNL/TM-2008/196 issued in January 2009.
- Today we present the analysis of two representative safety analysis models provided by RDF staff and one model that was not considered in the final report.



OAK RIDGE NATIONAL LABORATORY
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FOR THE DEPARTMENT OF ENERGY

ORNL/TM-2008/196

Application of the SCALE TSUNAMI Tools for the Validation of Criticality Safety Calculations Involving ^{233}U

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Application Models

- Application 1
  - 12.2 cm radius sphere of 220 g U per liter uranyl nitrate solution
  - U is 100 wt % ^{233}U
  - Reflector – 0.25 cm thick Type 304 stainless steel tank and 2 cm of water.
  - EALF is 0.282 eV
  - k_{eff} calculated for this system is 1.0028 ± 0.0002.
- Application 3
  - 53.0 cm radius sphere of 600 g U per liter uranyl nitrate solution, 80° C
  - U is 3 wt % ^{233}U, 0.2 wt % ^{235}U, and 96.8 wt % ^{238}U.
  - Reflector – 0.25 cm thick Type 304 stainless steel tank and 2 cm of water
  - EALF is 0.0631 eV
  - k_{eff} calculated for this system is 0.9690 ± 0.0002.
- A variant of Application 1 considered in preliminary studies
  - Infinite medium of 220 g U per liter uranyl nitrate solution with 9.5 M excess acid
  - U is 98 wt % ^{233}U, 1 wt % ^{235}U, and 1 wt% ^{238}U
  - EALF is 0.446 eV
  - k_{eff} calculated for this system is 2.055.

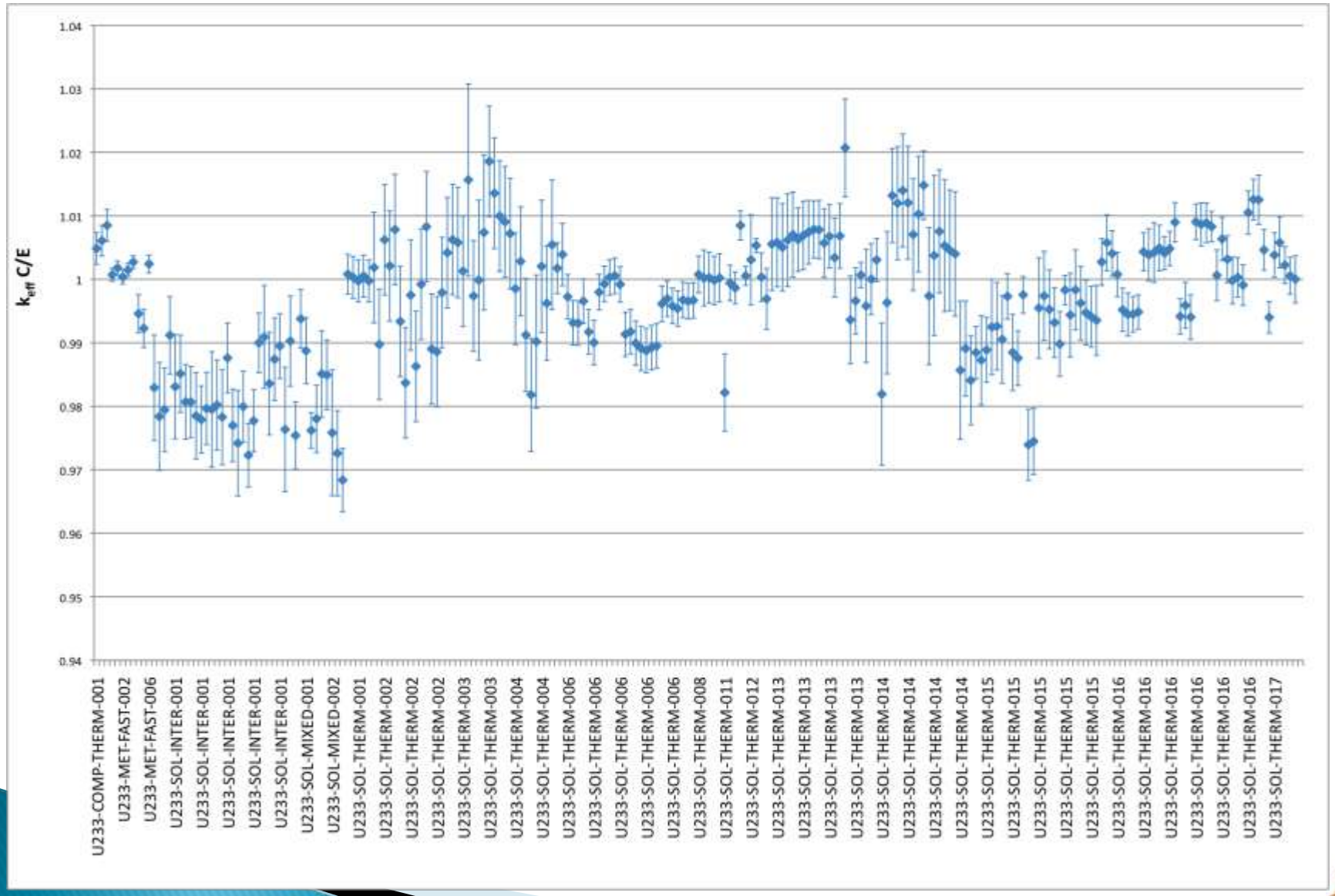
Analysis Methods

- SCALE 5.1 TSUNAMI tools TSUNAMI-3D, TSUNAMI-1D were used to generate k_{eff} sensitivity data for the applications and 672 critical experiments from 101 ICSBEP evaluations
  - 232 ^{233}U configurations
  - 28 mixed U/Pu configurations
  - 153 high uranium enrichment configurations
  - 255 low uranium enrichment configurations
- TSUNAMI-IP used to compare each application with each critical experiment.
- Example upper subcritical limits (USLs) were generated for Application 1 based on trending of the TSUNAMI similarity parameters.

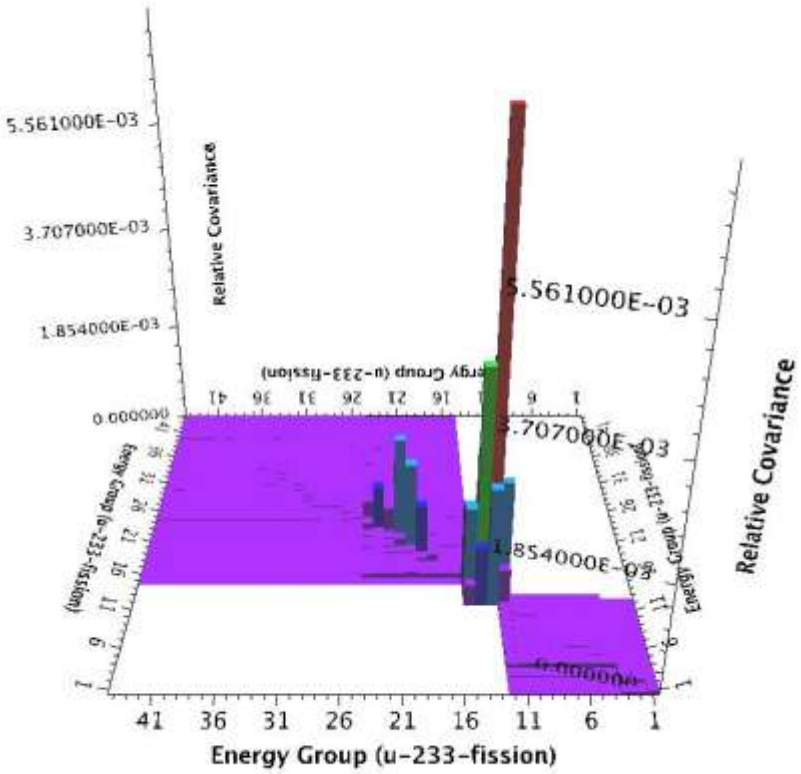
TSUNAMI Validation

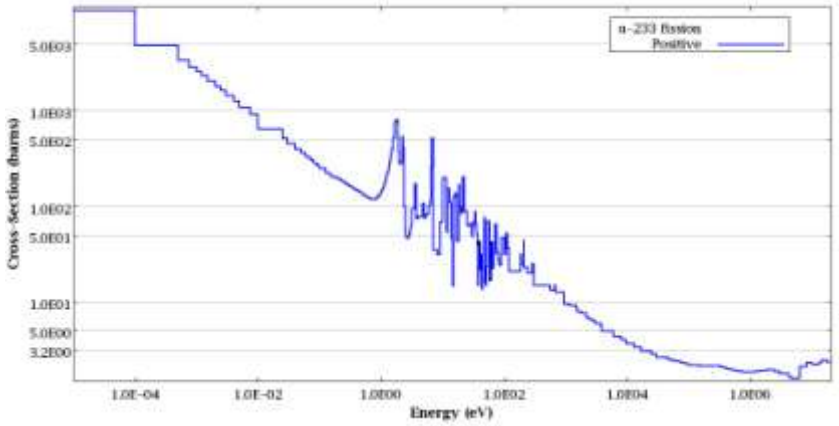
- Computational biases are primarily caused by errors in the cross-section data
- Errors are bounded by uncertainties on cross sections quantified with cross-section-covariance data
- Quantification of uncertainty in k_{eff} due covariance data should bound computational bias

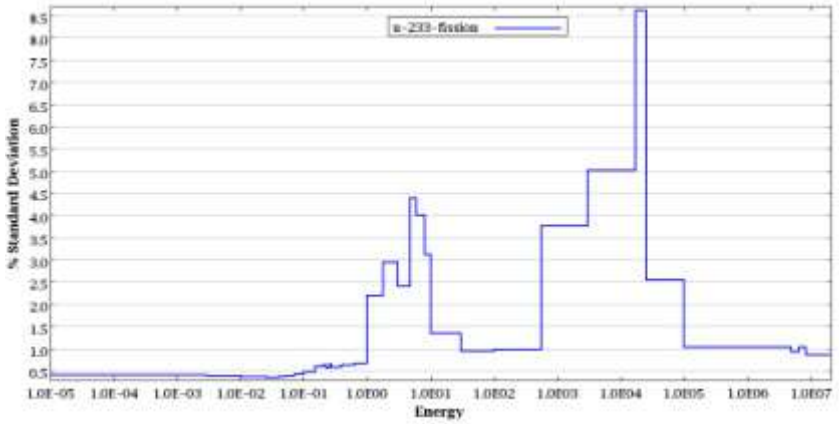
230 ^{233}U Systems from 2009 ICSBEP Handbook Distribution k_{eff} C/E and Experimental Uncertainty



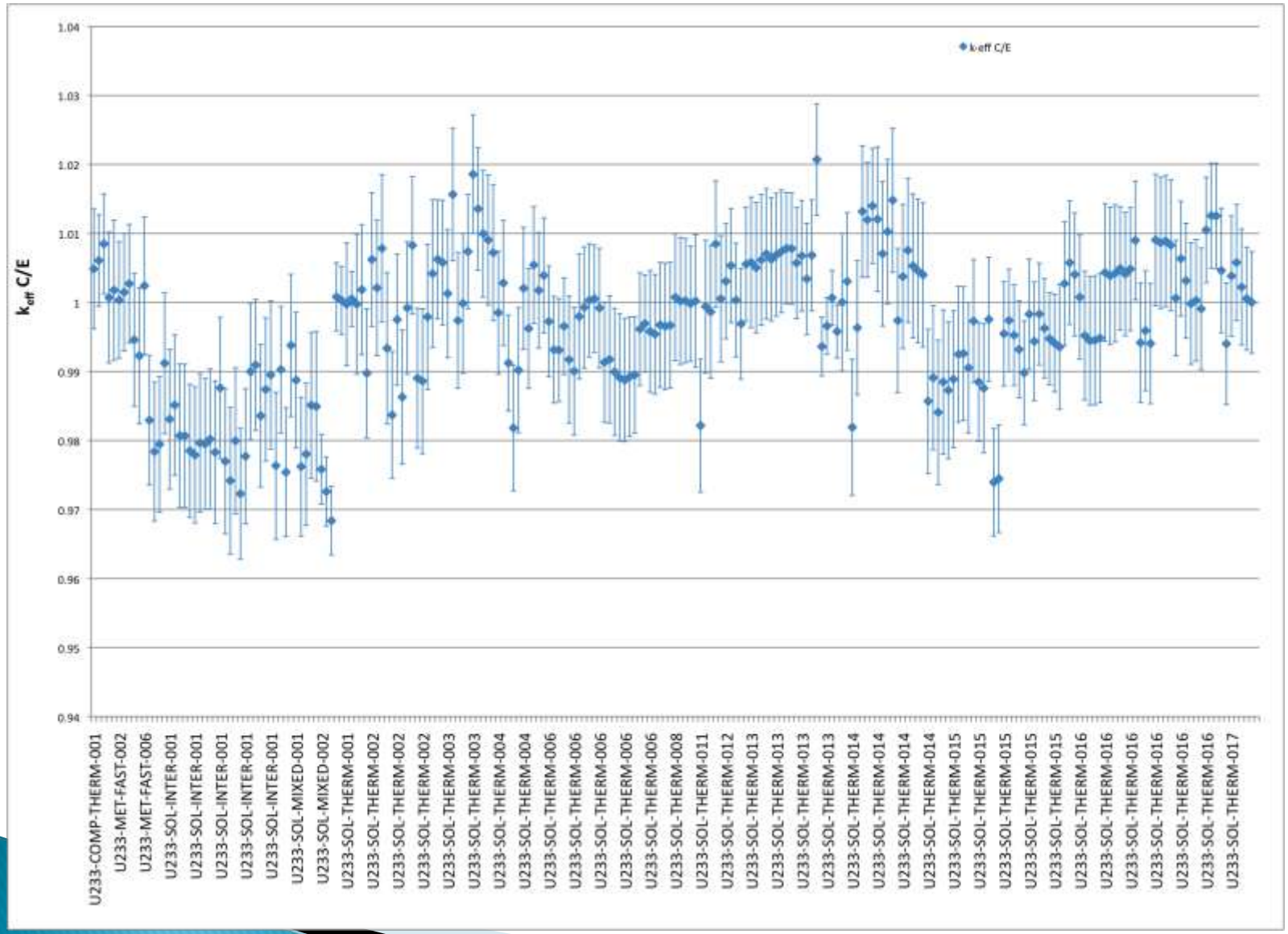
Covariance Data – ^{233}U Fission



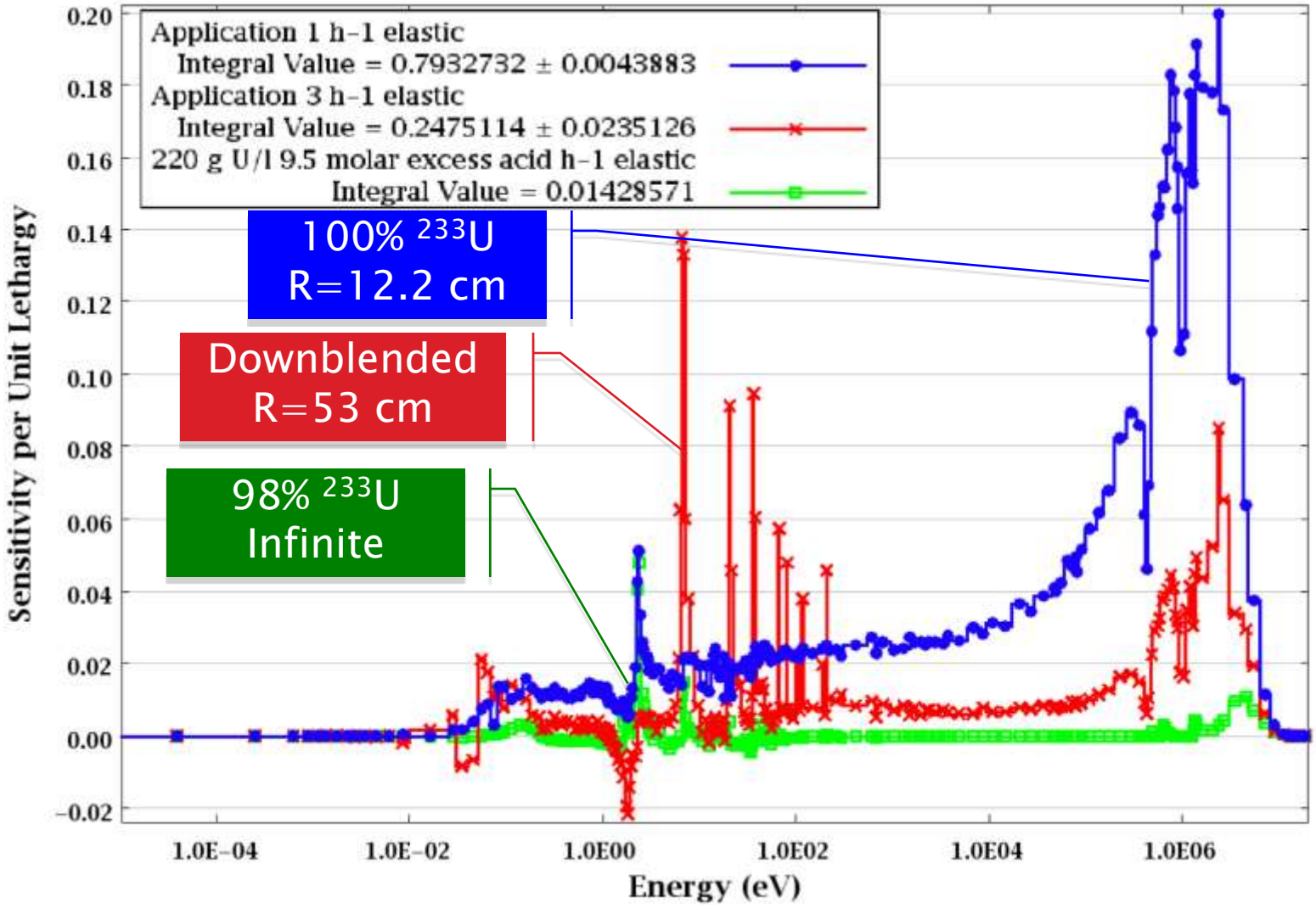




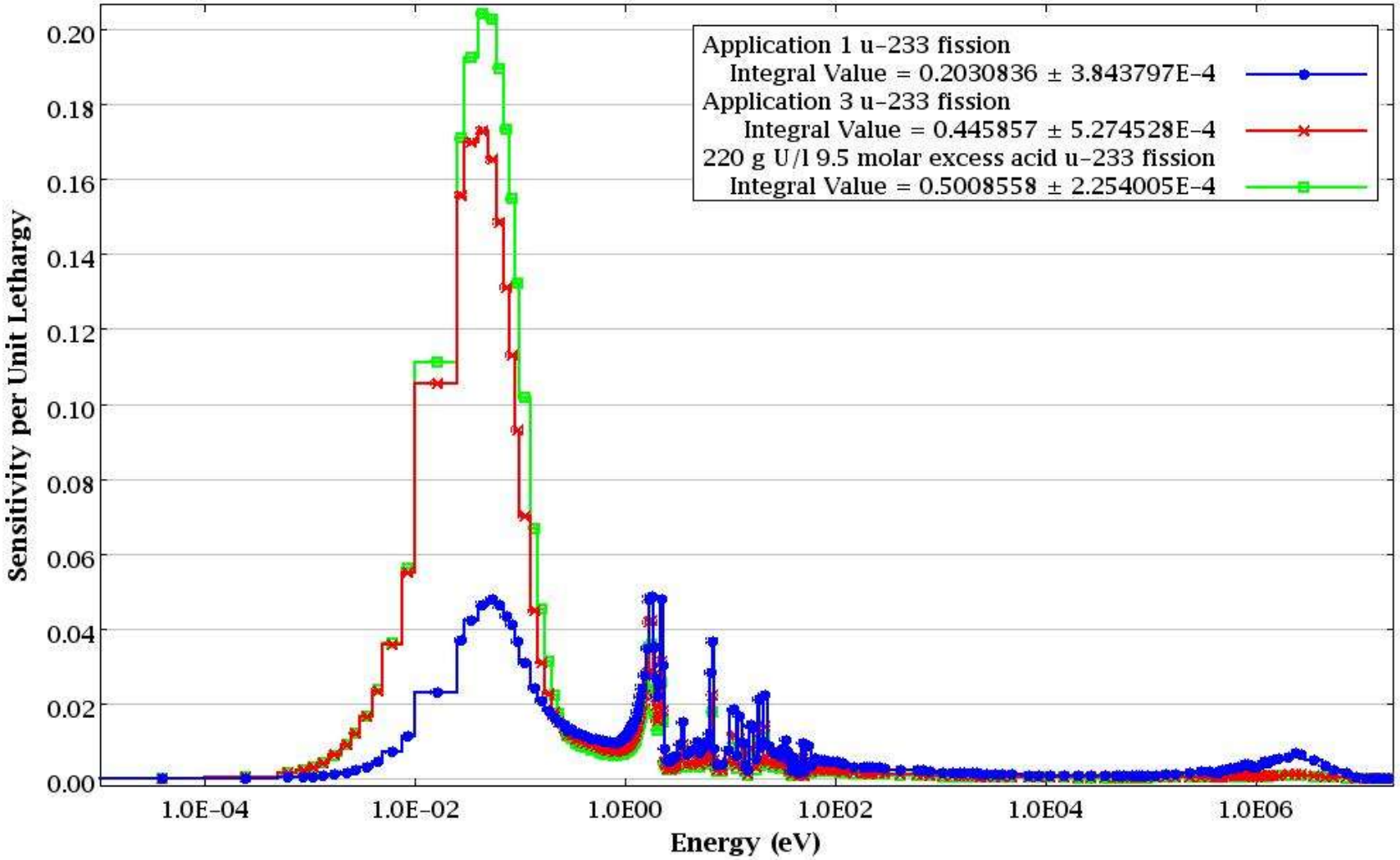
230 ^{233}U Systems from 2009 ICSBEP Handbook Distribution k_{eff} C/E and Cross-Section Uncertainty



Sensitivity of k_{eff} to ^{1}H elastic scattering



Sensitivity of k_{eff} to ^{233}U fission



Uncertainty in Applications due to Covariance Data

System	Standard deviation (%)	Top six contributors and standard deviation (%)	
Application 1	0.937	^{233}U χ to ^{233}U χ	0.819
		^{1}H elastic to ^{1}H elastic	0.320
		^{16}O elastic to ^{16}O elastic	0.194
		^{233}U n,γ to ^{233}U n,γ	0.174
		^{233}U nubar to ^{233}U nubar	0.145
		^{233}U fission to ^{233}U fission	0.117
Application 3	0.515	^{14}N n,p to ^{14}N n,p	0.346
		^{238}U n,γ to ^{238}U n,γ	0.233
		^{233}U fission to ^{233}U fission	0.173
		^{1}H n,γ to ^{1}H n,γ	0.145
		^{233}U χ to ^{233}U χ	0.136
		^{233}U nubar to ^{233}U nubar	0.135
220 g U per liter with 9.5 M excess acid	0.293	^{233}U n,γ to ^{233}U n,γ	0.192
		^{233}U nubar to ^{233}U nubar	0.143
		^{14}N n,p to ^{14}N n,p	0.108
		^{233}U fission to ^{233}U fission	0.081
		^{16}O n,α to ^{16}O n,α	0.070
		^{233}U χ to ^{233}U χ	0.062

Correlation Coefficient (c_k)

(a.k.a. representativity factor)

- Quantifies degree of shared variance in k_{eff} between design application and benchmark experiment.

$$c_k = \frac{\sigma_{ae}^2}{\sigma_a \sigma_e}$$

Covariance between Experiment (e) and Application (a) due to all nuclides and reactions

Standard deviations for Application (a) and Experiment (e) due to all nuclides and reactions

Summary of Similarity Results

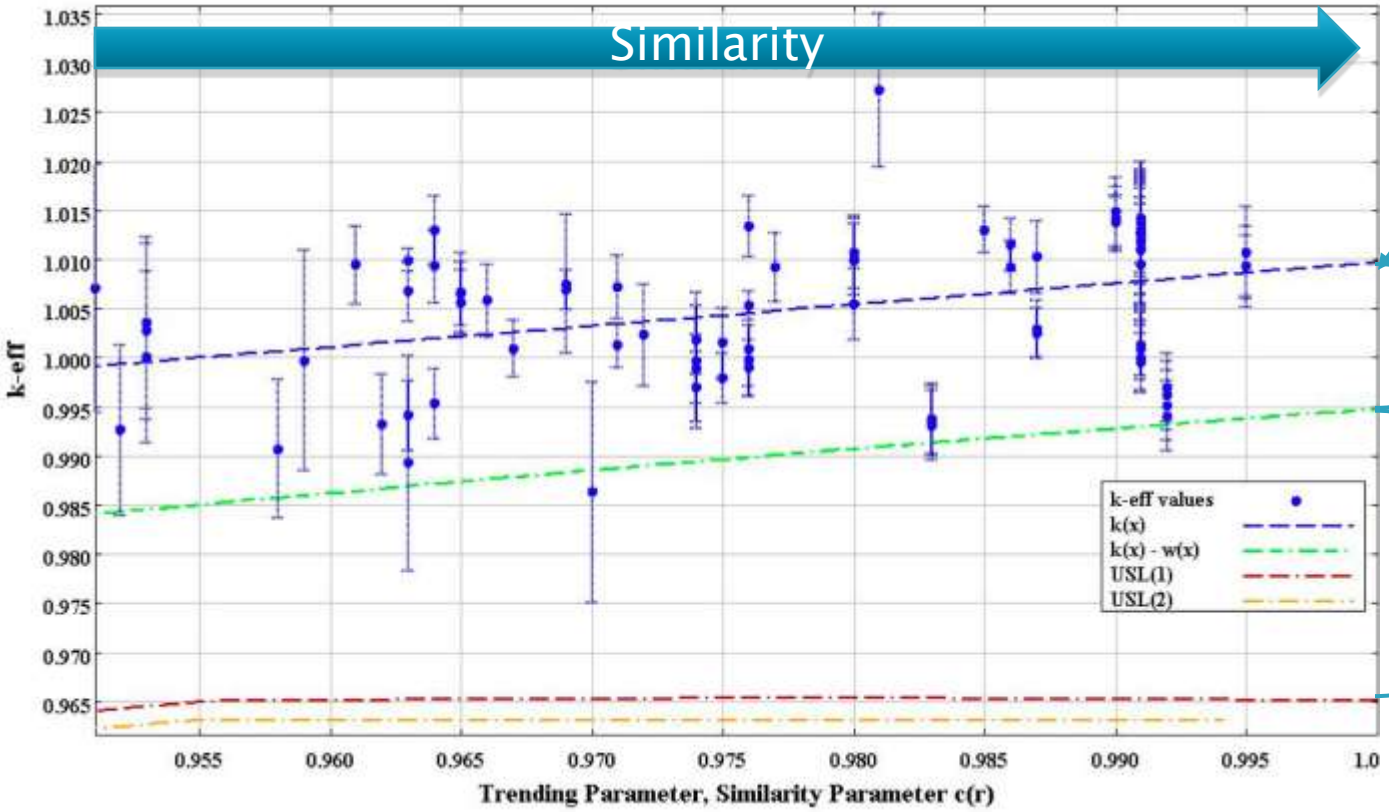
- Analysis used c_r, a reduced version of c_k that excludes fission spectra (χ) data

Similarity index range	Similarity	Application		
		1	3	220 g U per liter with 9.5 M excess acid
		Number of experiments in each category		
$c_r < 0.1$	Low	43	54	367
$0.1 \leq c_r < 0.2$	Low	80	124	15
$0.2 \leq c_r < 0.3$	Low	136	141	89
$0.3 \leq c_r < 0.4$	Low	140	176	14
$0.4 \leq c_r < 0.5$	Low	63	79	25
$0.5 \leq c_r < 0.6$	Low	30	68	101
$0.6 \leq c_r < 0.7$	Low	14	30	50
$0.7 \leq c_r < 0.8$	Low	7	0	10
$0.8 \leq c_r < 0.9$	Marginal	17	0	0
$0.9 \leq c_r < 0.95$	Acceptable	60	0	0
$0.95 \leq c_r < 1.0$	High	82	0	0

Comments on Similarity

- 82 ^{233}U thermal solutions provided excellent match to Application 1 in terms of common sources of uncertainty
- No single experiment was similar to Application 3 due to mixture of ^{233}U and depleted U
  - Could benefit from advanced Generalized Linear Least Squares analysis (TSURFER) to combine bias from different types of experiments – ^{233}U and LEU solutions
- No single experiment was similar to the infinite model with $k_{eff} > 2.0$
  - Similar materials as available experiments
  - Simple, but non-realistic geometry leads to elimination of leakage and very different sensitivities
  - Realism must be considered

USLSTATS Trend for Application 1



Biased k_{eff} for Application
(bias is this intercept - 1.0)

Confidence band
(uncertainty in bias)

Positive Bias Adjustment and Administrative Margin

Computational bias, β = 1.0 %Δk/k
Uncertainty in the bias, Δβ = 1.5% Δk/k
USL1 (disallowing positive bias) = 0.965

Addressing Validation Gaps

- No critical experiments were identified that are adequately similar to Application 3
  - Locate additional experiments similar to application
  - Modify safety model to not take credit for certain materials – Could ^{14}N be omitted as conservative approximation?
- Quantification of additional margin with uncertainty analysis using uncertainties due to cross-section covariance data
- Additional means of bias and bias uncertainty assessment using generalized linear least square techniques are available in the SCALE 6 code TSURFER.
  - See ORNL/TM-2008/196 for example TSURFER calculations.

Questions?

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