Use of Sensitivity and Uncertainty Methods in the Analysis of Validation Outliers

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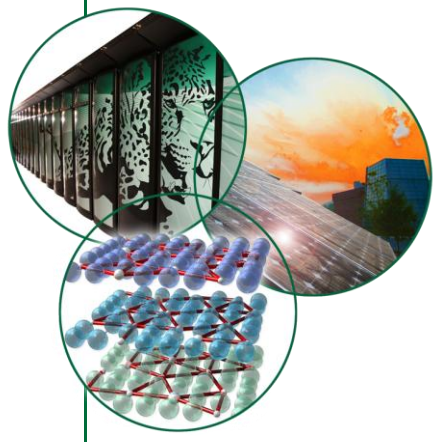

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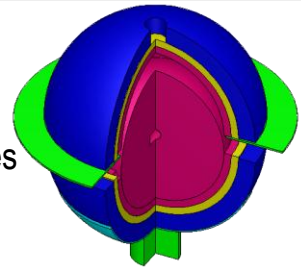
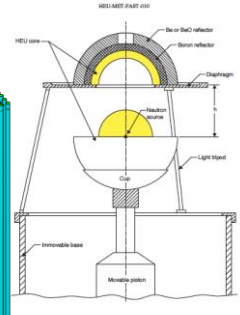
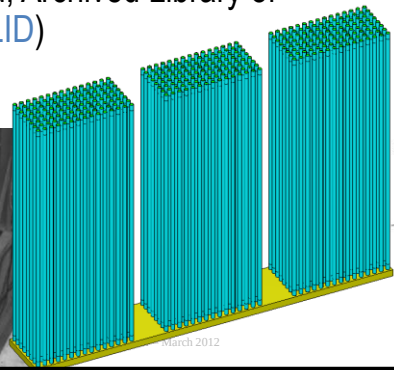
ICSBEP Sensitivity Data

- Over 4000 experiments in ICSBEP
- Under DOE and NRC support, ORNL provides quality-assured SCALE inputs and sensitivity data files for distribution with the ICSBEP
- Files are developed according the SCALE procedure for Verified, Archived Library of Inputs and Data (VALID)

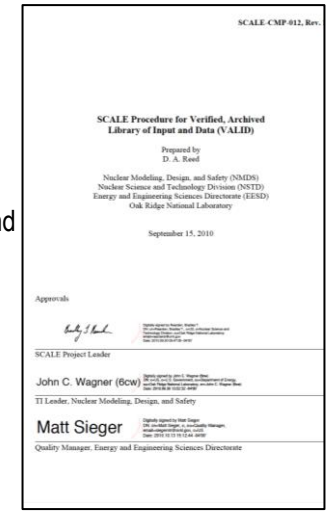






Verified, Archived Library of Inputs and Data (VALID)

- SCALE procedure for preparing, peer-reviewing, and controlling models and data files
- Ensure the models and data are correctly generated using appropriate references with documented checks and peer reviews
- Configuration control to prevent inadvertent modification of the models and data or inclusion of models that have not gone through rigorous checks and review
- Models developed from evaluation using benchmark definitions
  - No direct comparison to sample inputs provided by evaluators
- SCALE KENO-V.a or KENO-VI models
  - Multigroup – 238-group ENDF/B-VII.0
  - All parameters for verified sensitivity data included in TSUNAMI-3D input files
  - Continuous-energy mode models created by user


SCALE-CMP-012, Rev.

SCALE Procedure for Verified, Archived Library of Input and Data (VALID)

Prepared by
D. A. Reed

Nuclear Modeling, Design, and Safety (NMDS)
Nuclear Science and Technology Division (NSTD)
Energy and Engineering Sciences Directorate (EESD)
Oak Ridge National Laboratory

September 15, 2010

Approvals

SCALE Project Leader

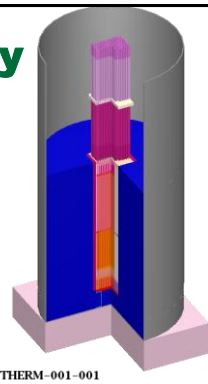
John C. Wagner (6cw)

TI Leader, Nuclear Modeling, Design, and Safety

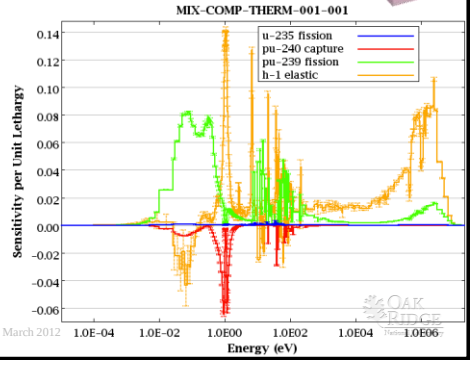
Matt Sieger

Quality Manager, Energy and Engineering Sciences Directorate

2010 ICSBEP TSUNAMI Sensitivity Data: 494 Benchmarks*



- HEU-MET-FAST
  - 33 cases
- HEU-SOL-THERM
  - 52 cases
- IEU-MET-FAST
  - 10 cases
- LEU-COMP-THERM
  - 56 cases
- LEU-SOL-THERM
  - 19 cases
- MIX-COMP-FAST
  - 1 case
- MIX-COMP-THERM
  - 21 cases
- PU-MET-FAST
  - 10 cases
- PU-SOL-THERM
  - 62 cases
- U233-COMP-THERM
  - 3 cases
- U233-MET-FAST
  - 8 cases
- U233-SOL-INTER
  - 29 cases
- U233-SOL-MIXED
  - 8 cases
- U233-SOL-THERM
  - 182 cases



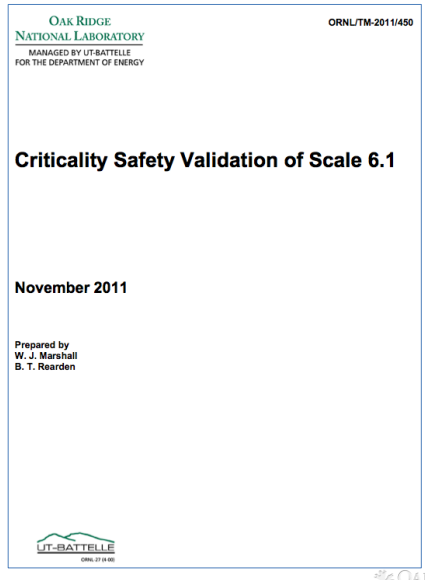
*255 from VALID
249 from ORNL/TM-2008-196

Data on ICSBEP Distribution

- VALID SCALE input files for KENO and TSUNAMI
  - `Dice/data/ornl/inputs`
- Energy-dependent, nuclide-reaction specific sensitivity data files (SDF)
  - `Dice/data/ornl/TSUNAMI-1D`
  - `Dice/data/ornl/TSUNAMI-3D`

Criticality Safety Validation of SCALE 6.1

- Under NCSP support, a validation document was developed for SCALE 6.1
- Used all ICSBEP cases currently in VALID
- SCALE 6.1
  - KENO V.a
  - KENO-VI
- ENDF/B-VII.0
  - Continuous energy
  - Multigroup
- Sensitivity and uncertainty data
- Outlier cases carefully examined to identify areas for improvement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ORNL/TM-2011/450

Criticality Safety Validation of Scale 6.1

November 2011

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UT-BATTELLE

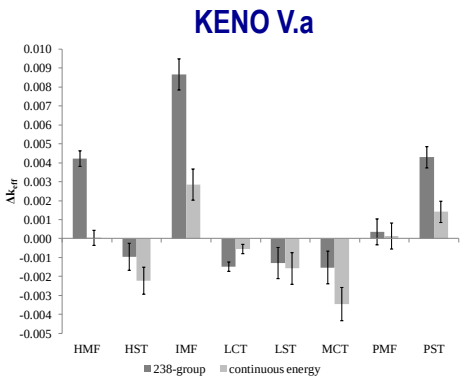
VALID cases used for this study

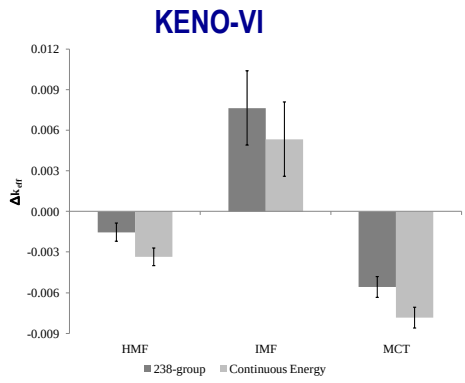
Sequence	Experiment class	IHECSBE case numbers	Number of configurations
CSAS5/KENO V.a	HEU-MET-FAST	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 65	18/22[a]
	HEU-SOL-THERM	1, 13, 14, 16, 28, 29, 30	52
	IEU-MET-FAST	2, 3, 4, 5, 6, 7, 8, 9	8/11[a]
	LEU-COMP-THERM	1, 2, 10, 17, 42, 50	97
	LEU-SOL-THERM	2, 3, 4	19
	MIX-COMP-THERM	1, 2, 4	21
	PU-MET-FAST	1, 2, 5, 6, 8, 10, 18, 22, 23, 24	10
	PU-SOL-THERM	1, 2, 3, 4, 5, 6, 7, 11, 20	81
CSAS6/KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80	15
	IEU-MET-FAST	19	2
	MIX-COMP-THERM	8	28

[a]The larger number includes simplified cases that are duplicate cases for which detailed models are also available in the library.

- **313 KENO V.a cases**
- **45 KENO-VI cases**

General Results

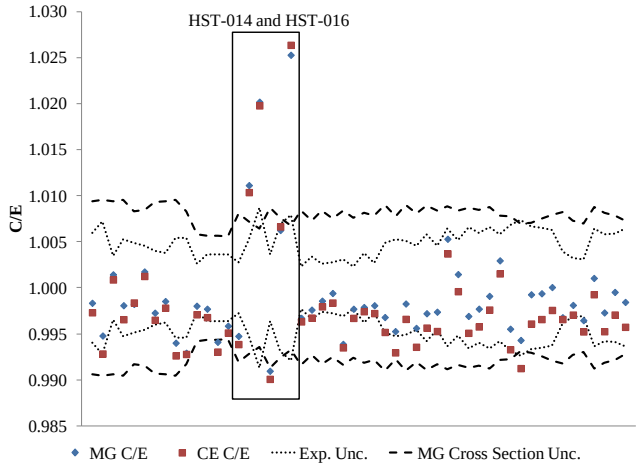




- **Generally acceptable small biases are observed**
- **Users can proceed with confidence under proper validation (e.g., ANS 8.24 guidance)**

HST Systems

- HST-014 and HST-016 cases contain varying concentrations of Gd



ICSBEP Results HST-016

Similar trends observed with other codes and data

Table 14.a. Sample Calculation Results (Russian Federation).

Case No.	MMK (26-Group ABBN-78)
1	0.9936 ± 0.0022
2	1.0097 ± 0.0019
3	1.0249 ± 0.0015

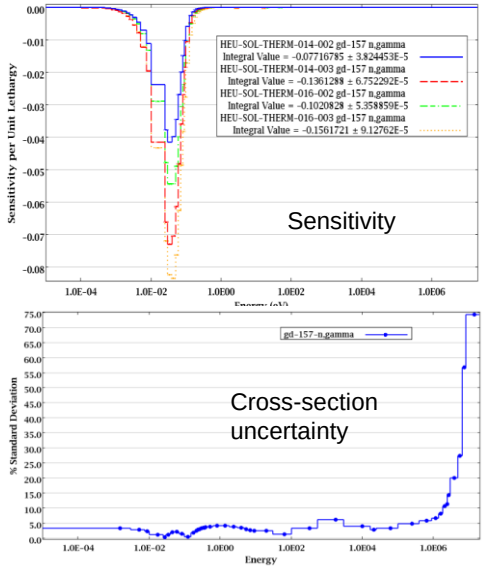
Table 14.b. Sample Calculation Results (United States).[a]

Case No.	KENO (Hansen-Roach)	MCNP (Continuous-Energy ENDF/B-V)
1	0.9744 ± 0.0013	0.9961 ± 0.0010
2	0.9816 ± 0.0012	1.0100 ± 0.0009
3	0.9947 ± 0.0010	1.0280 ± 0.0009

(a) Results supplied by the authors.

- Trend in results could be due to experiment description, not in models, codes or data

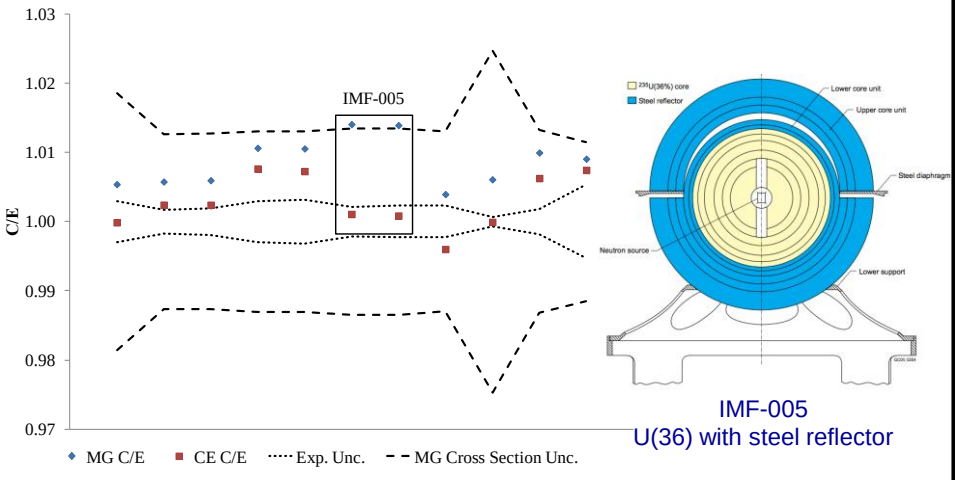
S/U Analysis of HST-016



- HST-016 case 3
  - Bias is approximately 2.5% Δk
  - ^{157}Gd integral sensitivity is ~0.156 (%Δk/k)/(Δσ/σ).
  - Gadolinium cross section would have to be in error by a factor of 16 to explain the observed bias.
  - Uncertainty in the ^{157}Gd cross section is less than 5% in the energy range where the vast majority of the ^{157}Gd sensitivity lies.
  - Discrepant results most likely due to errors in experiment descriptions

IMF Systems

- Good agreement except for IMF-005
- IMF-005 detailed and simplified model show similar results



IMF-005
U(36) with steel reflector

Uncertainty in k_{eff} due to covariance data

- Comparing IMF-005 to similar IMF-003, uncertainties are driven by ^{235}U fission and capture and ^{238}U scattering
- Limited sensitivity/uncertainty due to steel

IMF-003

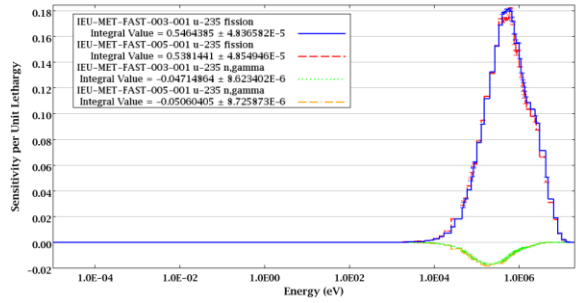
Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U n,gamma	^{235}U n,gamma	1.1151E+00 ± 1.1516E-04
^{238}U elastic	^{238}U n,n'	-4.5765E-01 ± 1.5852E-04
^{238}U elastic	^{238}U elastic	3.6909E-01 ± 1.8811E-05
^{238}U n,n'	^{238}U n,n'	3.5513E-01 ± 3.0403E-04
^{235}U elastic	^{235}U n,gamma	3.0515E-01 ± 1.1863E-05
^{235}U chi	^{235}U chi	2.7049E-01 ± 4.5186E-07
^{235}U n,n'	^{235}U n,n'	2.6154E-01 ± 5.6635E-05
^{235}U elastic	^{235}U n,n'	-2.4297E-01 ± 2.0807E-05
^{235}U fission	^{235}U fission	2.2699E-01 ± 1.7859E-06
^{238}U nubar	^{238}U nubar	1.6996E-01 ± 2.0705E-07

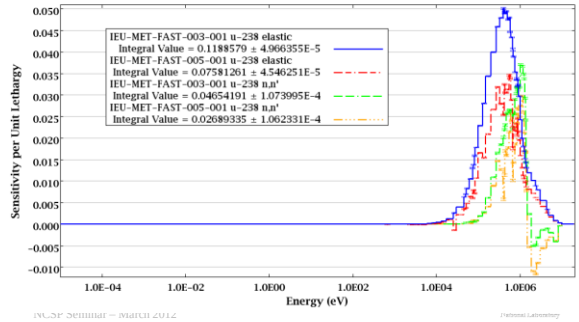
IMF-005

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{235}U n,gamma	^{235}U n,gamma	1.2077E+00 ± 1.1803E-04
^{235}U chi	^{235}U chi	2.6004E-01 ± 4.1739E-07
^{235}U elastic	^{235}U n,gamma	2.4774E-01 ± 1.0598E-05
^{238}U elastic	^{238}U elastic	2.4699E-01 ± 1.0719E-05
^{235}U fission	^{235}U fission	2.2369E-01 ± 1.6854E-06
^{238}U elastic	^{238}U n,n'	-2.0925E-01 ± 9.7319E-05
^{56}Fe elastic	^{56}Fe elastic	2.0083E-01 ± 9.0655E-06
^{235}U n,n'	^{235}U n,n'	1.9520E-01 ± 4.3250E-05
^{238}U n,n'	^{238}U n,n'	1.8882E-01 ± 2.1825E-04
^{235}U elastic	^{235}U n,n'	-1.6855E-01 ± 1.2801E-05

Sensitivity data

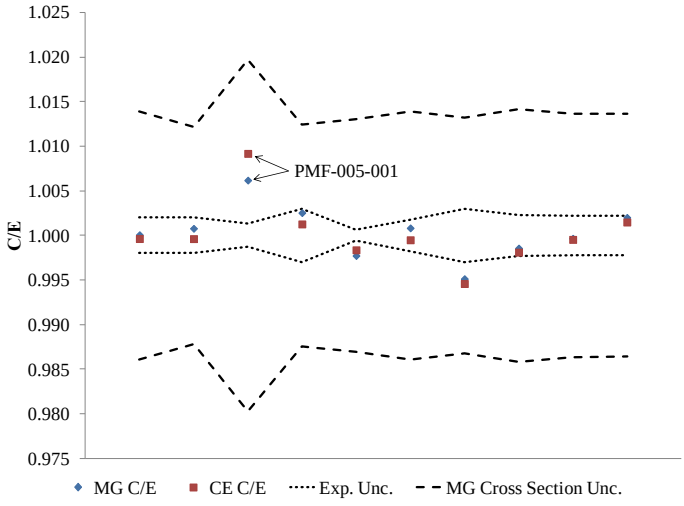
- ^{235}U sensitivities are nearly identical between the two systems
- ^{238}U sensitivities vary
- Differences between CE and MG are likely due to processing differences in libraries for ^{238}U scattering





PMF Systems

- Good agreement except for PMF-005 with W reflector

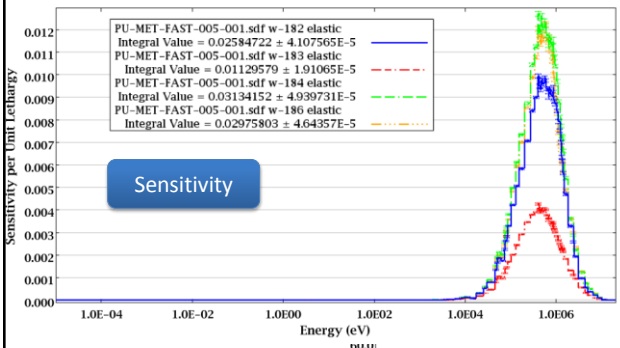


PMF-005 Uncertainties

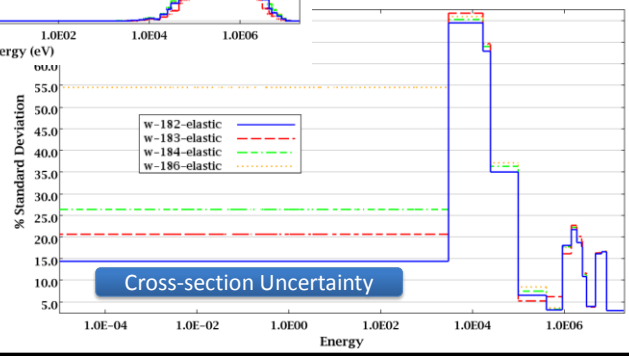
- System is sensitive to ^{239}Pu and W
- Other ^{239}Pu systems do not show a similar bias
- W is likely source of bias

Covariance Matrix		Unc. in % dk/k
Nuclide-Reaction	Nuclide-Reaction	Due to this Matrix
^{239}Pu nubar	^{239}Pu nubar	1.1953E+00 ± 1.2703E-05
^{184}W n,n'	^{184}W n,n'	7.8394E-01 ± 5.4380E-04
^{186}W n,n'	^{186}W n,n'	7.2679E-01 ± 4.7947E-04
^{182}W n,n'	^{182}W n,n'	6.7679E-01 ± 3.8972E-04
^{239}Pu n,n'	^{239}Pu n,n'	5.5915E-01 ± 3.3604E-04
^{183}W n,n'	^{183}W n,n'	5.5555E-01 ± 2.3994E-04
^{239}Pu elastic	^{239}Pu n,n'	-5.2229E-01 ± 1.6806E-04
^{184}W elastic	^{184}W elastic	3.2915E-01 ± 4.8450E-05
^{186}W elastic	^{186}W elastic	3.2714E-01 ± 4.5977E-05
^{239}Pu fission	^{239}Pu fission	3.2659E-01 ± 7.9042E-06
^{182}W elastic	^{182}W elastic	2.5963E-01 ± 3.1905E-05

W Sensitivities and Uncertainty

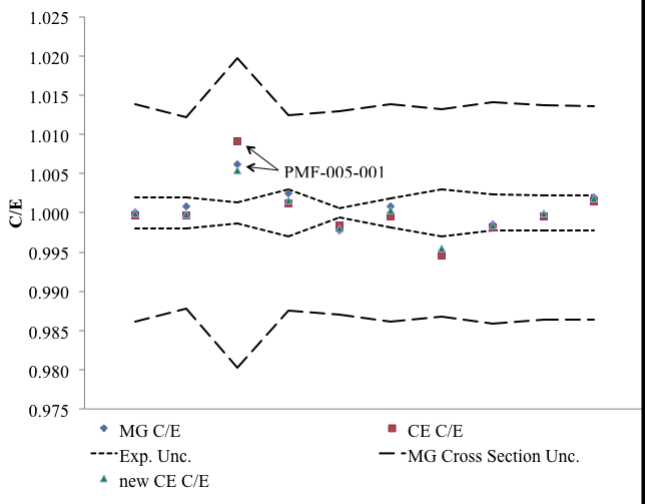


- W isotopes have high uncertainty at same energy as sensitivity in PMF-005



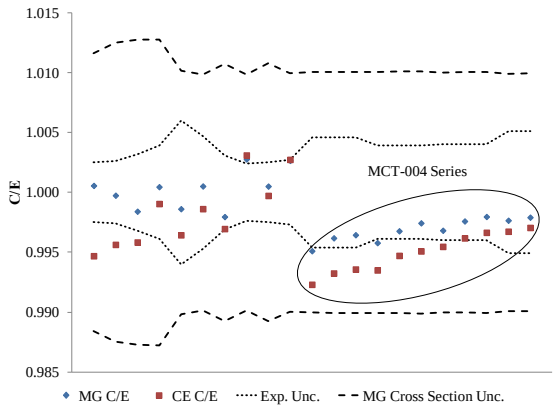
Improved results

- After release of SCALE 6.1, improvements were made in W processing for CE data, resulting in improved agreement
- Improved data will be available in next SCALE release



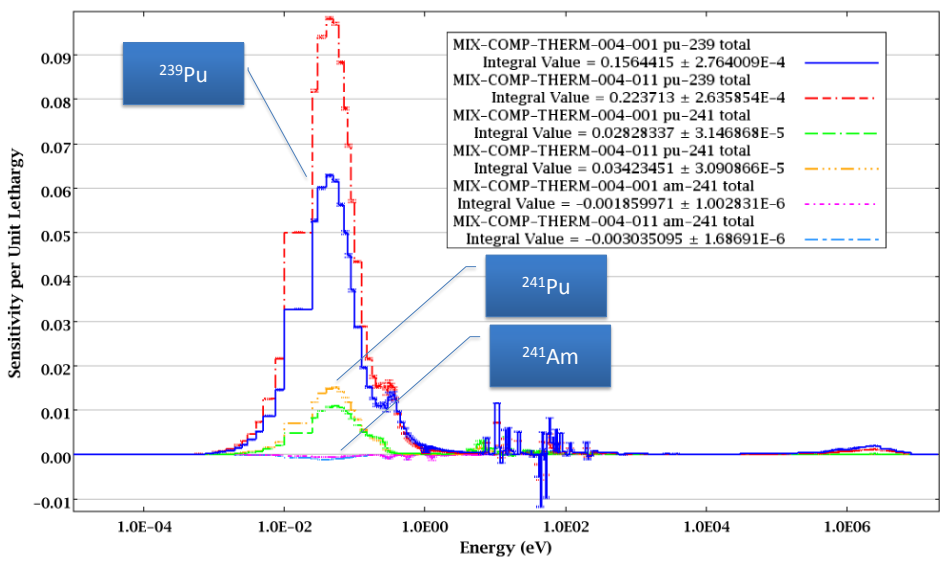
MIXED-COMP-THERM

- MCT-004 is water-moderated lattice
- Varying pitch
  - 1.825 cm for case 1
  - 2.474 for case 11
- Performed over significant time scale such that ^{241}Pu transition to ^{241}Am must be modeled
- CE to MG differences
  - 0.28 %Δk for case 1
  - 0.09 %Δk for case 11



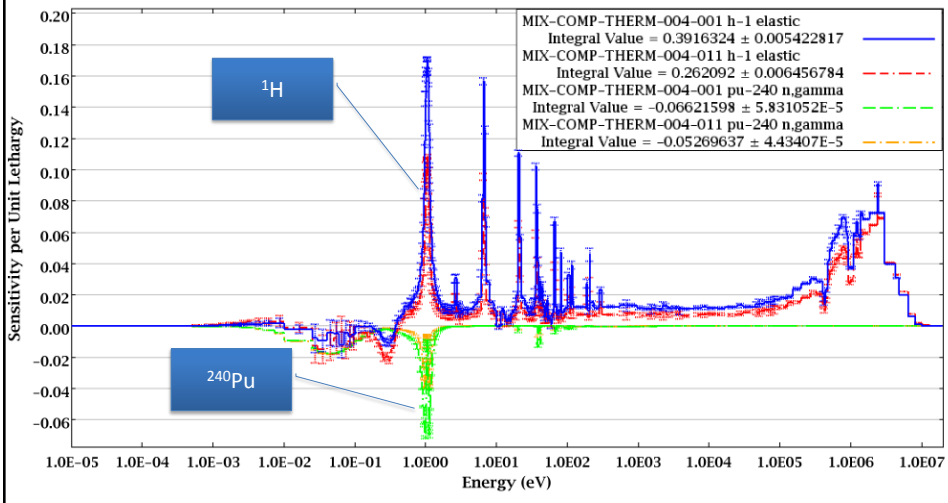
^{239}Pu, ^{241}Pu, ^{241}Am

- ^{241}Am sensitivity is insignificant and not likely source of bias



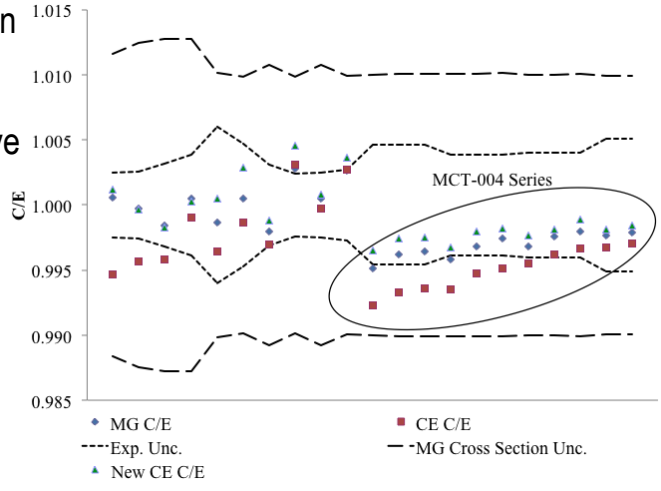
^{1}H and ^{240}Pu

- Impact of ^{1}H in H_2O S(α,β) is important for 1 eV resonance of ^{240}Pu



Improved results with post SCALE 6.1 CE data

- CE data generation in AMPX was improved to more accurately preserve strongly peaked kinematics data
- Improved data will be available with next SCALE release



Conclusions

- SCALE 6.1 has been validated with ~300 ICSBEP benchmark models that were generated under the SCALE/VALID procedure
- Sensitivity and uncertainty data were generated for each model
- Overall, low bias results were obtained for a wide range of systems, with results generally with 1 σ or less of the cross section uncertainty
- Specific outliers were subjected to further investigation using sensitivity and uncertainty analysis methods
- Several improvements were made to the CE data generation procedures in AMPX to correct some outlier cases
- Investigations into MG data processing are continuing
- Updated testing and validation strategies will continue to improve the performance of SCALE using AMPX data