NCSD 2013

SESSION: ANALYSIS & EXPERIMENTS I

Validation of 108 MOX powder applications for ANS and ISO standards

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OVERVIEW

- Results and conclusions
- MOX powder – Needs for support
- ISO and ANS standards
- Application systems
- Benchmarks
- Correlated benchmark error sources
- SCALE/TSUNAMI tools
- K_{eff} calculation methods
- Weighted benchmarks
- Biases
- Bias-corrected results
- Observations

RESULTS AND RECOMMENDATIONS

- There is still a lack of high-quality benchmarks
- Accounting for correlations in the U.S.?
- Only one benchmark from correlated set
- Weighting based on uncertainty and C_k value
- Accounting for positive bias not less conservative
- C_k values may not apply to other methods
- Thermal scattering matrix not in C_k
- Basic cross-section data not the major error source
- Bias-correction works with reliable benchmarks
- New critical experiments? Cover range of H/Pu!

MOX POWDER - NEEDS

- Fuel fabrication in France, UK, Japan and U.S.A.
- Transport and other operations
- Validation efforts strong for 20 years (Smolen, etc.)
- Damp MOX powder most challenging
- ISO started development of standard around 1998
- Wide initial range of MOX compositions narrowed
- ANS 8.12 decided to build on ISO work
- OECD supported critical experiments 2004-2005
- Current priority of U.S. MOX fabrication lowered

ISO AND ANS STANDARDS

- ISO criticality safety group very active last 15 years
- MOX standard published in 2011
  - Specifications based on actual experience in fuel fabrication in France and UK
  - Many calculations during almost 15 years
  - No formal validation required
  - Estimates of critical values based on minimum calculated value of any credible method
- ANS 8.12 revision waited for ISO standard specs
  - Validation required
  - Subcritical values expected as main information

108 APPLICATION SYSTEMS

- Homogeneous and uniform materials
- Three geometry shapes: Sphere, cylinder and slab
- Two dimensions:
  - Geometry (Sphere radius, Cylinder diameter and Slab thickness)
  - Mass (Sphere mass, cylinder linear density, slab surface density)
- Two Pu fractions (Pu/(U+Pu) with a maximum Pu density constraint for 35 wt.%: but not for 12.5 wt.%.
- Three Pu isotope distributions: Pu(100,0,0,0), Pu(95,5,0,0) and Pu($65^{15}/_{17}$,20,$12^{16}/_{17}$,$1^{3}/_{17}$)
- Two moderations: Max. 3.0 wt.% water and optimum water
- Two reflections: 30 cm water and 2.5 cm water
- The factors above (3, 2, 2, 3, 2 and 2) lead to 144 reference values
- The 36 low-moderated systems for geometry control are identical to the 36 low-moderated systems for mass control – Total 108 systems

108 SYSTEMS - IDENTIFICATION

MOX			Pu(100,0,0,0)						Pu(95,5,0,0)						Pu($65^{15}/_{17}$,20,$12^{16}/_{17}$,$1^{3}/_{17}$)					
H_2O	Dim	Pu_f (%)	30 cm H_2O			2.5 cm H_2O			30 cm H_2O			2.5 cm H_2O			30 cm H_2O			2.5 cm H_2O		
			Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab
Low (3.0)	Geom & Mass	35[1]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	**18**
		12.5	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36
Opt	Geom	35[1]	**37**	38	39	40	41	42	43	44	45	46	47	48	**49**	50	51	52	53	54
		12.5	55	56	**57**	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72
	Mass	35[1]	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90
		12.5	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108

[1] The MOX density is restricted to maximum 3.5 g/cm^3.

BENCHMARKS

- Selected from ICSBEP Handbook
- Uncertainties not always reliable
- Error correlation between benchmarks
- Similarity between application and benchmark
- Input data for benchmarks
- Possibility of new critical experiments
- Accounting for a positive bias allowed (not less conservative than accounting for a negative bias)

CORRELATED BENCHMARK ERRORS

- What does a correlated error source mean?
  - Identical fissile material (fuel rods, solution, etc.)
  - Identical neutron absorbers, moderators, reflectors
  - Identical methods to determine specifications such as solution properties, room-return, etc.
  - Modification of fuel rod array rather than full reassembly
- Thousands of benchmarks in ICSBEP Handbook
- Many have correlated error sources
- Different ICSBEP evaluations are also correlated
- ICSBEP has not specified the correlations
- An error source correlation is important information
- Correlations can increase or reduce uncertainties

ACCOUNTING FOR CORRELATIONS

- U.S. safety reports lack consideration of problem
- ANSI/ANS 8.24 Validation standard (2007)
  - A recommendation to account for correlations
  - Appendix does not account for evident correlations
- NRC FCSS ISG-10 (2006) has recommendation
- MOX Fuel Fabrication Facility?
  - Submitted 59 benchmarks (59 is magical number …)
  - NRC accepted 38 benchmarks – All correlated!
  - No account for correlations made
  - All 38 accepted by ICSBEP but still controversial
  - MOX FFF made application before ANSI/ANS 8.24

EMS practice – Only one benchmark from correlated set

SCALE/TSUNAMI TOOLS

- The TSUNAMI tools in SCALE are established
- Sensitivity results very informative
- Uncertainties from cross-section covariances? OK
- C_k value from TSUNAMI IP
  - Correlation of physics (not of general error sources)
  - Demonstrated to be useful
  - Grading usefulness of benchmark to C_k is complicated
- The TSURFER tool is very promising: Established?
- All information with reliable uncertainties is useful, not only critical experiments

K_{EFF} CALCULATION METHODS

Participants in the ISO and ANS MOX standard WG:

- CRISTAL, MCNP, MONK, SCALE, etc.
  - ENDF/B-IV, -V, VI and VII.0, JEF 2.2, JEFF 3.1.1, JENDL 3.2, -3.3 and 4.0

The methods discussed here (EMS):

- SCALE 6.1.2 (CSAS5, CSAS6, TSUNAMI tools, TSURFER)
  - ENDF/B-VI and VII.0 continuous energy, ENDF/B-V and VII.0 238-groups
- MCNP5-1.60
  - ENDF/B-V, -VI and VII.0, JENDL-3.2, -3.3 and -4.0, JEF 2.2, JEFF-3.1.1

WEIGHTED BENCHMARKS

- Expert judgment is the primary tool for validation
- Benchmark quality weighting:
  - Value and reliability of uncertainty need accounting for
  - Weight each benchmark by inverse square of uncertainty (not necessarily ICSBEP estimate)
  - Weight each benchmark as a function of C_k value.

$$1/W_{b,i} = \sigma_b^2 * 10000 + (C_0 - C_{b,i})^2 * N_0$$

- Where $W_{b,i}$ is weight for benchmark b and application i,
- σ_b is benchmark uncertainty,
- C_0 is an arbitrary value (1.01 in this evaluation),
- $C_{b,i}$ is C_k value for benchmark b and application I, and
- N_0 is an arbitrary value (9 in this evaluation)

C_K VALUES FOR APPLICATIONS

Cases with $C_k > 0.90$ & $C_k > 0.80$ for appl. 1-36 and only $C_k > 0.90$ for rest

MOX			Pu(100,0,0,0)						Pu(95,5,0,0)						Pu($65^{15}/_{17}$,20,$12^{16}/_{17}$,$1^{3}/_{17}$)					
			30 cm H_2O			2.5 cm H_2O			30 cm H_2O			2.5 cm H_2O			30 cm H_2O			2.5 cm H_2O		
H_2O	Dim	Pu_f (%)	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab	Sph	Cyl	Slab
Low (3.0)	Geom & Mass	35[1]	2&7	2&8	4&12	2&3	2&3	2&3	2&4	2&4	2&6	1&2	1&2	1&2	1&2	1&2	1&2	1&2	1&2	**1&1**
		12.5	1&7	1&9	3&14	0&2	0&2	2&2	1&6	2&7	2&13	0&2	1&2	2&2	1&2	1&7	2&9	0&2	0&2	1&2
Opt	Geom	35[1]	**11**	12	12	11	11	12	12	12	12	12	12	12	**12**	12	12	12	12	12
		12.5	10	11	**13**	9	10	11	11	12	12	10	11	12	12	12	12	11	12	12
	Mass	35[1]	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12
		12.5	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12	12

32 SELECTED BENCHMARKS

	ICSBEPevaluation id.	Case no(s)	Total in evaluation
1.	MIX-COMP-MIXED-001	2, 10 or 13	19
2.	MIX-MISC-MIXED-001	4 or 11	11
3.	MIX-COMP-THERM-001	1, 2 or 4	4
4.	MIX-COMP-THERM-002	2 or 5	6
5.	MIX-COMP-THERM-005	1, 4, 5 or 6	7
6.	MIX-COMP-THERM-007	1, 3 or 5	27
7.	MIX-COMP-THERM -011	4	6
8.	MIX-MISC-THERM-001	8 or 11	11
9.	MIX-MISC-THERM-004	1 or 6	6
10.	MIX-SOL-THERM-001	5, 6 or 10	13
11.	MIX-SOL-THERM-002	1	3
12.	MIX-SOL-THERM-004	2, 5 or 7	9
13.	MIX-SOL-THERM-006	1	6
14.	MIX-SOL-THERM-007	1	7
15.	PU-SOL-THERM-001	1	6

BIASES FOR APPLICATIONS 1-36

Estimated k_{eff} biases for applications 1-18 and each method (pcm)												
App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	VII.0	VI	VII.0	V	VII.0	VI	V	3.1.1	2.2	4.0	3.3	3.2
1	-260	-674	305	-183	72	-359	-834	-75	-246	172	-111	-221
2	-422	-776	104	-265	-3	-394	-808	-133	-276	97	-140	-221
3	-536	-821	39	-153	-61	-408	-595	-210	-239	58	-109	-138
4	-108	-467	443	-194	42	-246	-752	-96	-331	122	-194	-342
5	-86	-441	446	-195	46	-235	-752	-95	-322	128	-197	-342
6	-226	-536	326	-211	68	-208	-636	-99	-264	117	-162	-278
7	-212	-521	332	-209	66	-207	-641	-102	-264	117	-167	-283
8	-219	-528	332	-203	63	-211	-636	-105	-264	115	-167	-282
9	-329	-601	166	-199	-73	-343	-729	-226	-341	21	-236	-303
10	-121	-409	302	-334	96	-130	-722	-77	-251	140	-175	-311
11	-110	-399	309	-329	95	-130	-724	-78	-251	141	-177	-313
12	-88	-379	323	-319	94	-129	-728	-79	-249	144	-183	-316
13	-106	-396	311	-328	95	-129	-724	-78	-250	142	-178	-313
14	-110	-399	309	-329	95	-130	-724	-78	-251	141	-177	-313
15	-126	-414	299	-337	96	-130	-721	-77	-251	139	-174	-310
16	-86	-377	324	-319	94	-129	-728	-79	-249	144	-183	-317
17	-81	-373	327	-316	94	-129	-729	-80	-249	145	-184	-317
18	-130	-352	88	-328	-198	-272	-966	-521	-713	-161	-492	-505

Estimated k_{eff} biases for applications 19-36 and each method (pcm)												
App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	VII.0	VI	VII.0	V	VII.0	VI	V	3.1.1	2.2	4.0	3.3	3.2
19	-372	-800	222	-235	72	-412	-817	-71	-237	179	-74	-191
20	-488	-849	175	-162	17	-419	-658	-144	-233	135	-86	-149
21	-658	-918	-59	-164	-107	-464	-484	-264	-219	35	-104	-116
22	-281	-582	292	-430	-34	-291	-907	-163	-424	20	-229	-438
23	-232	-535	312	-405	-20	-271	-890	-154	-402	38	-229	-428
24	-123	-428	357	-349	12	-226	-852	-135	-352	79	-230	-405
25	-349	-749	273	-245	38	-392	-706	-106	-275	145	-122	-259
26	-315	-726	256	-224	68	-380	-799	-79	-241	172	-97	-213
27	-584	-843	-3	-170	-84	-415	-525	-240	-234	38	-117	-138
28	-216	-518	319	-396	-15	-264	-884	-151	-394	45	-229	-424
29	-179	-482	334	-377	-4	-249	-872	-145	-377	58	-229	-417
30	-67	-374	380	-321	29	-203	-833	-125	-326	100	-230	-393
31	-250	-552	305	-414	-25	-278	-896	-157	-410	32	-229	-432
32	-328	-748	253	-223	68	-389	-833	-75	-246	171	-92	-209
33	-501	-830	50	-251	-32	-423	-724	-171	-275	82	-137	-195
34	-283	-584	291	-431	-35	-292	-908	-163	-425	19	-229	-438
35	-231	-533	313	-404	-20	-270	-890	-154	-401	39	-229	-427
36	-107	-413	363	-341	17	-220	-847	-132	-345	85	-230	-402

BIASES FOR APPLICATIONS 37-72

Estimated k_{eff} biases for applications 37-54 and each method (pcm)

App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	-VII.0	-VI	-VII.0	-V	-VII.0	-VI	-V	-3.1.1	-2.2	-4.0	-3.3	-3.2
37	-772	-914	-46	104	-133	-329	29	-312	-21	47	-7	87
38	-786	-927	-52	102	-138	-333	31	-315	-24	42	-8	86
39	-789	-930	-54	107	-139	-338	32	-316	-28	37	-6	86
40	-754	-896	-36	116	-131	-324	32	-313	-16	52	-7	91
41	-772	-914	-45	104	-133	-328	29	-313	-21	47	-8	87
42	-793	-934	-55	101	-140	-337	32	-317	-26	39	-10	84
43	-797	-936	-57	101	-141	-335	37	-316	-25	38	-8	87
44	-807	-946	-62	100	-145	-339	39	-318	-27	34	-9	85
45	-764	-891	-46	165	-114	-318	108	-313	-16	44	27	110
46	-791	-931	-54	101	-140	-333	36	-316	-23	40	-9	86
47	-800	-940	-59	99	-142	-336	37	-317	-25	37	-9	86
48	-813	-951	-64	99	-147	-341	40	-319	-29	31	-10	84
49	-798	-940	-61	99	-141	-336	29	-314	-25	37	-7	85
50	-801	-943	-62	100	-142	-338	30	-314	-27	35	-7	85
51	-727	-847	-43	187	-109	-304	110	-312	-2	50	40	120
52	-787	-929	-57	101	-137	-331	28	-312	-23	41	-6	87
53	-801	-942	-62	98	-142	-336	29	-314	-26	36	-8	85
54	-808	-948	-65	99	-145	-340	31	-316	-28	32	-8	84

Estimated k_{eff} biases for applications 55-72 and each method (pcm)

App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	-VII.0	-VI	-VII.0	-V	-VII.0	-VI	-V	-3.1.1	-2.2	-4.0	-3.3	-3.2
55	-768	-904	-42	112	-136	-324	43	-319	-14	48	-9	91
56	-793	-930	-54	98	-140	-331	39	-319	-21	41	-10	86
57	-749	-918	-44	66	-126	-399	-35	-331	-98	39	-38	29
58	-749	-884	-34	117	-130	-317	38	-317	-11	54	-7	94
59	-764	-900	-40	113	-135	-322	44	-319	-13	49	-8	92
60	-801	-937	-58	97	-144	-334	41	-321	-23	38	-12	85
61	-801	-935	-57	106	-146	-332	51	-322	-19	37	-10	90
62	-819	-953	-66	95	-149	-337	48	-322	-25	32	-11	86
63	-824	-958	-70	98	-151	-342	47	-323	-29	27	-9	85
64	-788	-922	-51	108	-142	-328	49	-321	-17	41	-10	91
65	-801	-935	-57	105	-146	-332	50	-323	-19	37	-11	89
66	-824	-958	-69	94	-151	-340	48	-324	-26	29	-12	84
67	-828	-961	-73	97	-154	-339	50	-324	-22	28	-12	87
68	-822	-957	-71	93	-149	-338	42	-320	-25	30	-10	85
69	-792	-907	-60	160	-121	-313	132	-317	-9	40	28	117
70	-800	-935	-60	104	-145	-330	44	-319	-17	38	-9	89
71	-809	-944	-64	102	-148	-334	45	-321	-20	34	-10	88
72	-832	-966	-76	91	-153	-342	43	-322	-27	27	-12	83

BIASES FOR APPLICATIONS 73-108

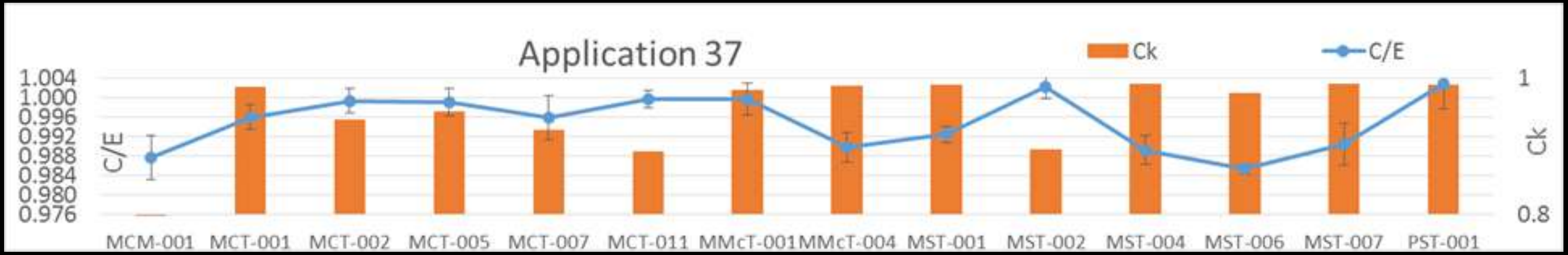
Estimated k_{eff} biases for applications 73-90 and each method (pcm)

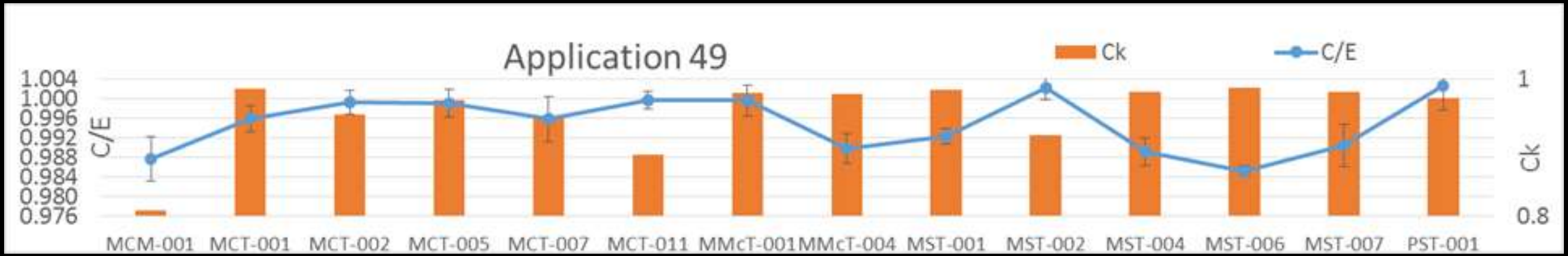
App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	-VII.0	-VI	-VII.0	-V	-VII.0	-VI	-V	-3.1.1	-2.2	-4.0	-3.3	-3.2
73	-689	-782	-24	246	-101	-263	164	-320	17	54	59	156
74	-683	-782	-21	230	-96	-271	155	-319	7	54	58	145
75	-621	-724	-33	231	-115	-285	121	-330	-29	41	46	135
76	-698	-796	-27	227	-104	-276	158	-325	9	51	51	142
77	-679	-778	-20	232	-96	-270	154	-319	7	55	59	145
78	-620	-722	-32	233	-114	-283	123	-329	-28	42	47	136
79	-710	-809	-30	226	-108	-280	161	-324	5	47	51	142
80	-650	-706	-25	229	-79	-153	76	-284	-38	-4	6	53
81	-585	-650	-46	216	-99	-190	-8	-298	-60	0	8	61
82	-708	-806	-30	226	-107	-231	-22	-324	-82	-14	-34	19
83	-693	-792	-25	227	-100	-229	-20	-320	-79	-8	-25	25
84	-590	-655	-47	216	-99	-191	-7	-299	-61	-1	6	60
85	-701	-804	-32	213	-103	-231	-39	-317	-82	-10	-32	16
86	-669	-771	-18	228	-94	-226	-30	-314	-74	0	-19	29
87	-582	-650	-51	204	-100	-191	-29	-295	-63	-1	5	56
88	-705	-807	-32	220	-108	-231	-38	-320	-83	-15	-37	14
89	-671	-773	-19	227	-94	-226	-32	-314	-75	-1	-20	28
90	-570	-628	-47	205	-95	-189	-48	-287	-55	7	10	63

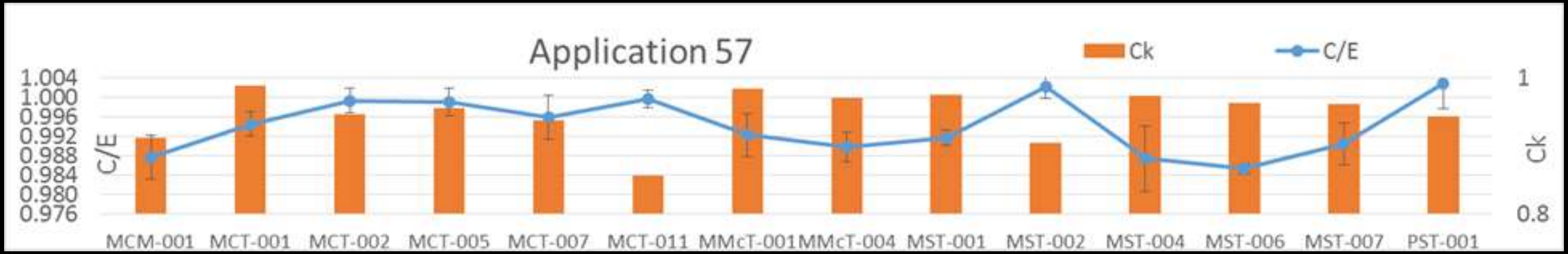
Estimated k_{eff} biases for applications 91-108 and each method (pcm)

App	SCALE 6.1.2				MCNP5-1.60 Continuous energy cross-sections							
	CE ENDF/B		238 ENDF/B		ENDF/B			JEFF	JEF	JENDL		
	-VII.0	-VI	-VII.0	-V	-VII.0	-VI	-V	-3.1.1	-2.2	-4.0	-3.3	-3.2
91	-696	-792	-27	228	-103	-226	-11	-323	-72	-6	-27	28
92	-674	-770	-16	243	-97	-224	-7	-322	-70	-2	-18	35
93	-597	-662	-48	217	-101	-191	-4	-301	-61	-2	5	59
94	-694	-789	-26	228	-102	-225	-11	-323	-70	-5	-26	28
95	-679	-774	-18	240	-99	-224	-9	-322	-71	-4	-20	33
96	-598	-663	-48	217	-101	-192	-4	-302	-61	-2	5	59
97	-713	-810	-33	224	-108	-231	-20	-325	-81	-15	-35	18
98	-583	-678	21	276	-65	-208	36	-313	-41	36	25	81
99	-599	-664	-49	216	-102	-193	-7	-302	-63	-3	4	58
100	-714	-810	-33	223	-109	-230	-21	-325	-81	-16	-35	17
101	-692	-787	-23	236	-103	-227	-14	-324	-76	-10	-25	27
102	-599	-664	-49	216	-102	-193	-6	-303	-63	-3	4	58
103	-711	-809	-35	218	-109	-229	-35	-322	-81	-16	-37	14
104	-678	-776	-21	235	-100	-225	-26	-319	-74	-5	-23	28
105	-586	-654	-52	207	-102	-192	-26	-299	-63	-2	4	56
106	-709	-807	-35	217	-109	-229	-34	-322	-80	-15	-36	15
107	-568	-667	27	279	-64	-206	20	-306	-34	44	23	82
108	-720	-821	-80	183	-147	-262	-78	-340	-130	-51	-61	-11

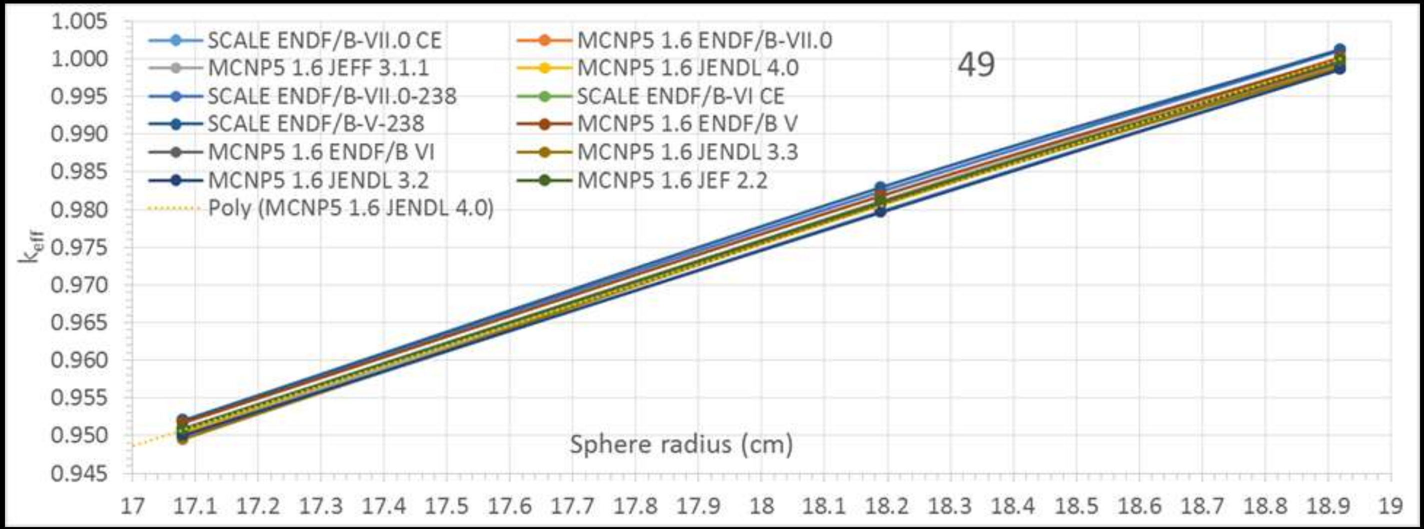
SOME VALIDATION RESULTS

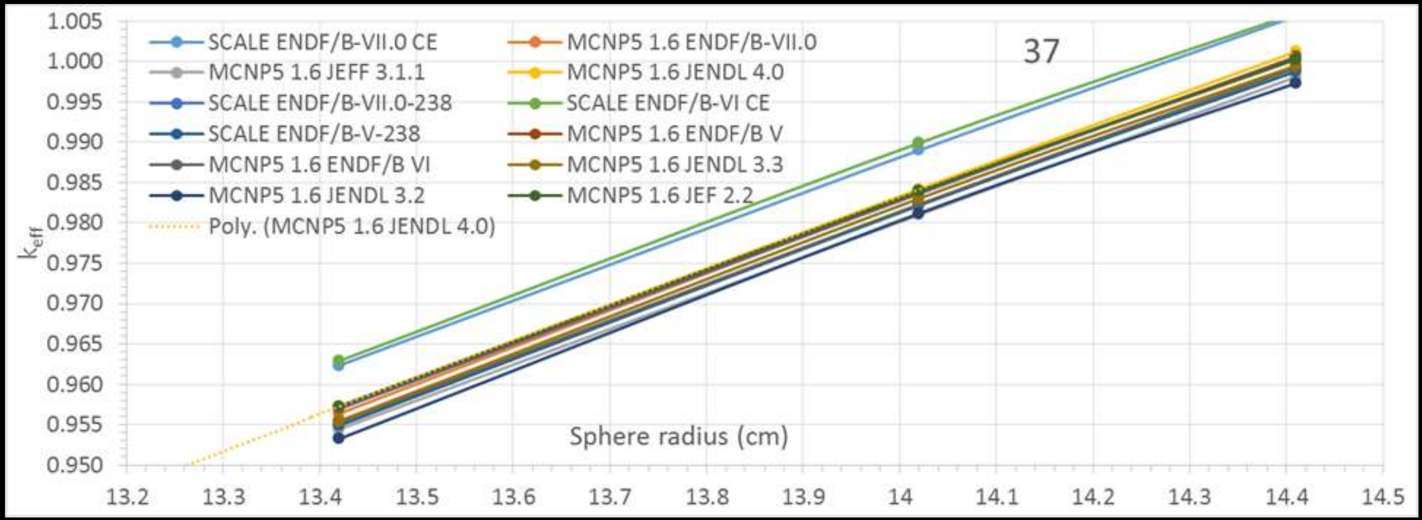




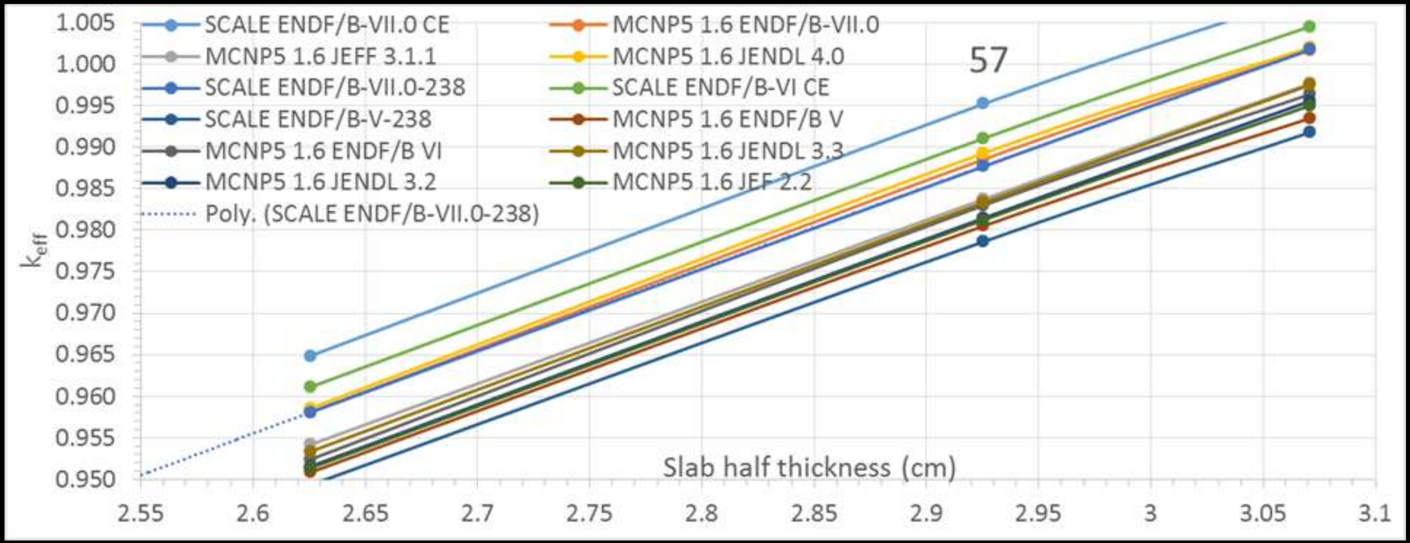


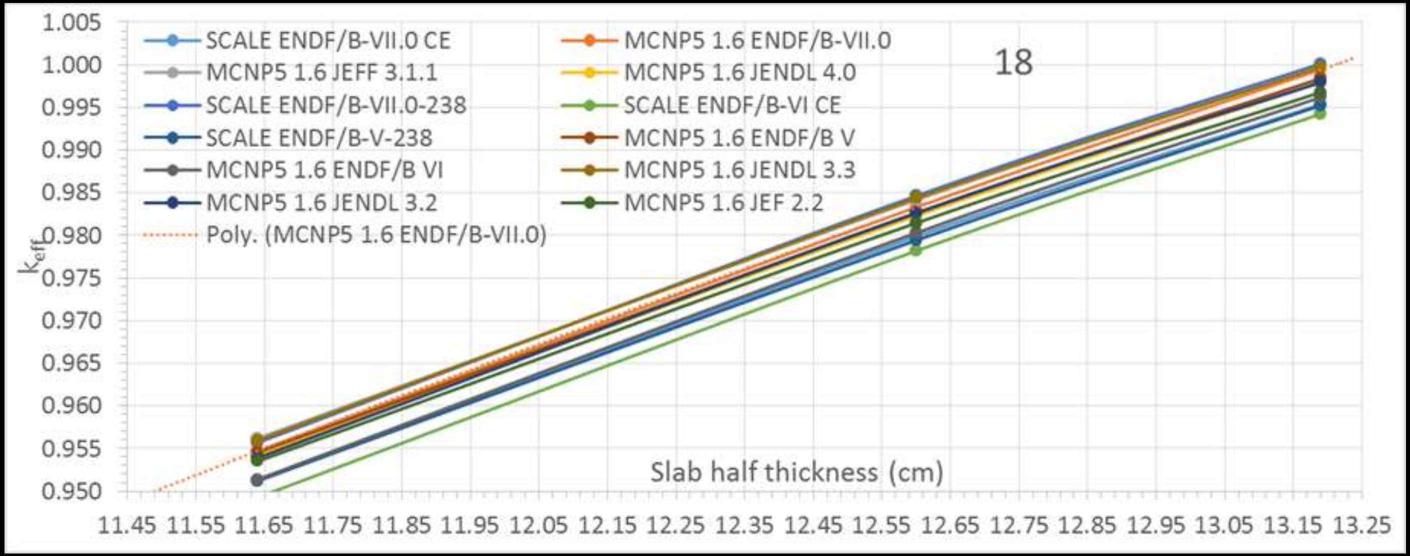
BIAS-CORRECTED RESULTS – 49 & 37





BIAS-CORRECTED RESULTS – 57 & 18





OBSERVATIONS

- SCALE 6.1.2 and earlier with CE cross-sections:
  - Large biases detected during validation for reactor-grade plutonium and applications had the same biases
  - Large biases were detected during validation for weapons-grade Pu but application only had small biases
  - Similarity between reactor-grade Pu benchmark and weapons-grade Pu application applies to 238-group X-section method but not to CE X-section method.
  - ORNL is aware of problem and it is corrected in beta version of SCALE 6.2 (not confirmed in this project)
  - Error source is related to thermal scattering
- Thermal scattering in ENDF/B-VII.0 and JEF 3.1.1 ACE libraries result in significant differences in MCNP5 results.

RESULTS AND RECOMMENDATIONS

- There is still a lack of high-quality benchmarks
- Accounting for correlations in the U.S.?
- Only one benchmark from correlated set
- Weighting based on uncertainty and C_k value
- Accounting for positive bias not less conservative
- C_k values may not apply to other methods
- Thermal scattering matrix not in C_k
- Basic cross-section data not the major error source
- Bias-correction works with reliable benchmarks
- New critical experiments? Cover range of H/Pu!

ACKNOWLEDGEMENTS

- The Swedish Radiation Safety Authority (SSM) has supported some of the speaker's involvement in ISO and ANS standards development.
- The ISO and ANS working groups have provided specifications and constructive discussions.
- The ANS 8.12 working group members Scott Revolinsky and Kermit Bunde have contributed with input data for SCALE and MCNP.