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AN Expanded Criticality Validation Suite for MCNP

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Monte Carlo Codes, LANL

Nuclear Criticality Safety Program

Comments

- If you don’t validate your computer tools,
your results are worthless

- If you don’t document your V&V work,
your results are worthless

- If you don’t document your work,
you are worthless

- V&V work is absolutely necessary,
but not glamorous or fun

- Well-known codes (MCNP, SCALE, …)
must still be validated for your work

Computer Code Verification & Validation (1)

Criticality safety practitioners are required to validate the computational tools used in their work

Criticality Safety practitioners:

- **Identify a set of experimental benchmarks similar to the problem of interest**
- Analyze the benchmark problems with the code
- Assess the accuracy of computed results vs. benchmark measurements
- Focus:
  Determine whether a general-purpose tool performs adequately for a specific problem of interest

Code developers:

- **Identify a set of experimental benchmarks that span all types of problems that users may run**
- Analyze the benchmark problems with the code
- Assess the accuracy of computed results vs. benchmark measurements
- Focus:
  Determine whether the code performs properly for a wide range of problems

Computer Code Verification & Validation (2)

- **Verification**
  - Does the code faithfully solve the equations & physical models it was designed to solve?
  - Testing with a series of calculations & comparison to other codes, to analytic benchmarks, or to experiments.

- **Validation**
  - Does the the code faithfully reproduce reality for a particular range of applications of interest?
  - May involve assessing that verification problems bound end-user applications, comparing calculations to relevant experiments, or performing scoping studies to ensure that parameter changes produce expected changes in results.

- **While code developers can thoroughly verify their codes, validation is problematic because of the very wide range of different problems and different code options**

- **Validation performed by code developers must necessarily be general, involving suites of problems chosen to broadly represent and span the range of possible applications**

MCNP V&V Suites (1)

- **MCNP code developers have assembled over a dozen verification/validation suites for testing general classes of problems, including**
  - Regression / installation
  - Criticality calculations
  - Shielding / dose
  - Electrons
  - Photons
  - Reactor kinetics parameters
  - Variance reduction
  - etc.
- The suites provide a general indication of the overall performance of MCNP with a given cross-section library, and can alert the user to unexpected or unintended consequences resulting from changes to nuclear data
- **This paper focuses on verification/validation of MCNP5 for criticality safety and reactor applications**

MCNP V&V Suites (2)

Monte Carlo Codes
XCP-3, LANL

- **Standard Testing + V&V Suites for MCNP5**

```
REGRESSION               - 66 installation / regression tests
VALIDATION_SHIELDING     - 19 shielding/dose experiments
KOBAYASHI                - void & duct streaming, point detectors

VALIDATION_CRITICALITY   - 31 ICSBEP Handbook cases
VERIFICATION_KEFF        - 75 analytic problems, exact results
POINT_KINETICS   [new]   - adjoint weighted  Rossi-α, β_eff, Λ_eff

Recent additions:
VALIDATION_CRIT_EXPANDED - 119 ICSBEP Handbook experimentss
ROSSI_ALPHA              - 12 benchmark experiments
VALIDATION_LANL_SB-CS    - 194 ICSBEP Handbook experiments
```

MCNP V&V Suites (3)

- **MCNP Criticality V&V Suites -- Focus**
  - **Physics-based V&V**
  - **Compare to experiment or exact analytic results**
  - Part of MCNP permanent code repository & RSICC distribution
  - Automated, easy execution & collection of results vs experiment

- **Some background**
  - Previously, both Nuclear Data and Monte Carlo teams had their own sets of V&V benchmarks
  - **Data Team V&V sets:**
    - Data testing, ICSBEP, CSWEG, other (?)
    - **No** lattices, intermediate spectra, or low LEU cases
    - Not readily available to others
  - **Monte Carlo Team V&V sets**
    - ICSBEP Handbook, but only 31 cases
    - Wide representation of fissile materials, reflector materials, and spectra
    - Unreflected, heavy reflector, light reflector, lattices, solutions, …

Expanded Criticality Validation Suite (1)

- **An expanded criticality validation suite has been created**
  - Incorporates many of the benchmarks in the older Data & MC Team suites
  - Eliminates overlaps, resolves inconsistencies, fills some of the gaps that neither of older suite addressed

- **119 problems taken from ICSBEP Handbook**

- **Well-documented**

  R.D. Mosteller, "An Expanded Criticality Validation Suite for MCNP", LA-UR-10-06230 (227 pages including MCNP inputs) (available from mcnp.lanl.gov)

- **Included as standard part of MCNP future RSICC releases**
  - Automated execution & collection of results
  - Can run with ENDF/B-VI, T16+ENDF/B-VI, ENDF/B-VII.0 data
  - 5M neutrons/case - 600 cycles, discard first 100, 10K neutrons/cycle
  - 7.75 hr on 8-core Mac Pro - 714 M total neutron histories

Expanded Criticality Validation Suite (2)

- 119 ICBEP Handbook experiments - Spectral Distribution

Fuel	Fast	Intermed	Thermal	Total
U-233	10	1	7	18
HEU	29	5	6	40
IEU	10	1	6	17
LEU	-	-	8	8
Pu	21	1	14	36
Total	70	8	41	119

Examples

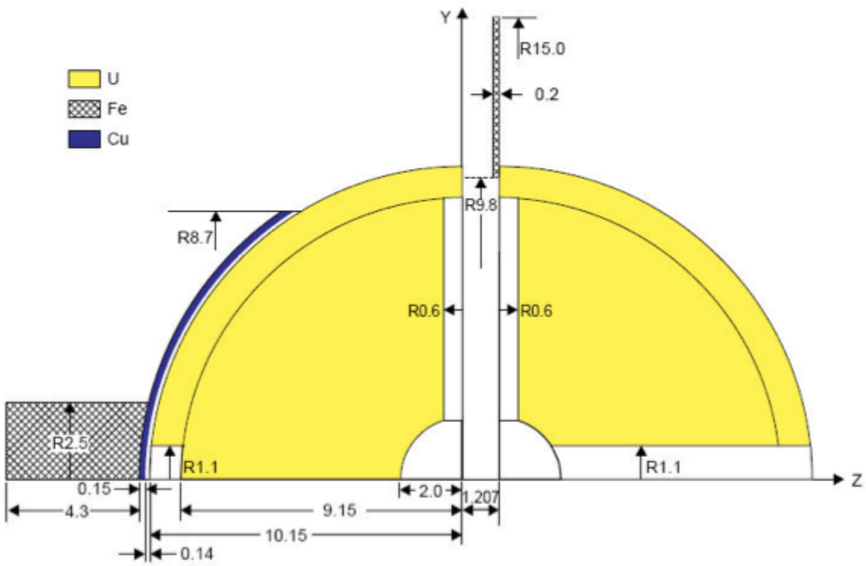


Figure 1. Unreflected HEU Sphere, heu-met-fast-008

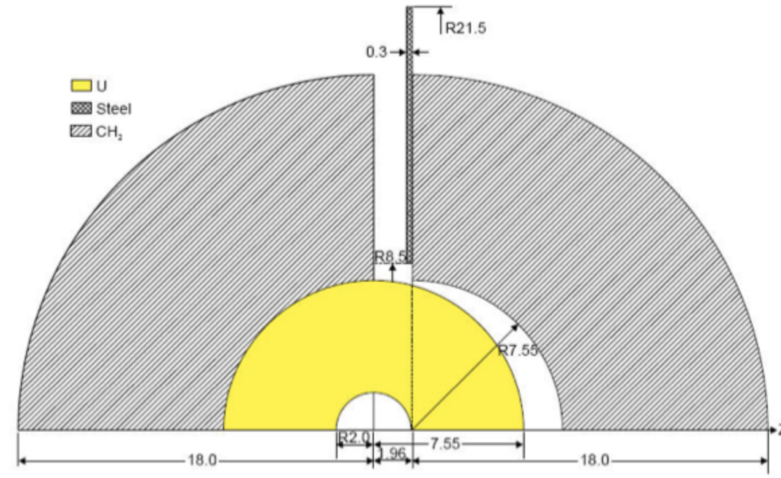


Figure 4. HEU Sphere Reflected by Polyethylene, heu-met-fast-011

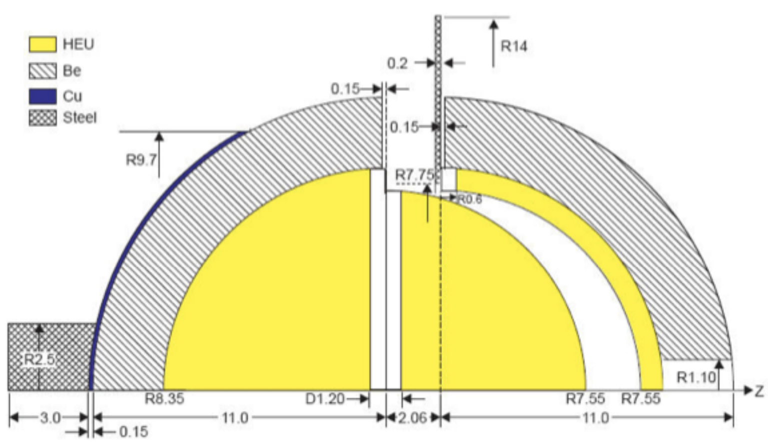
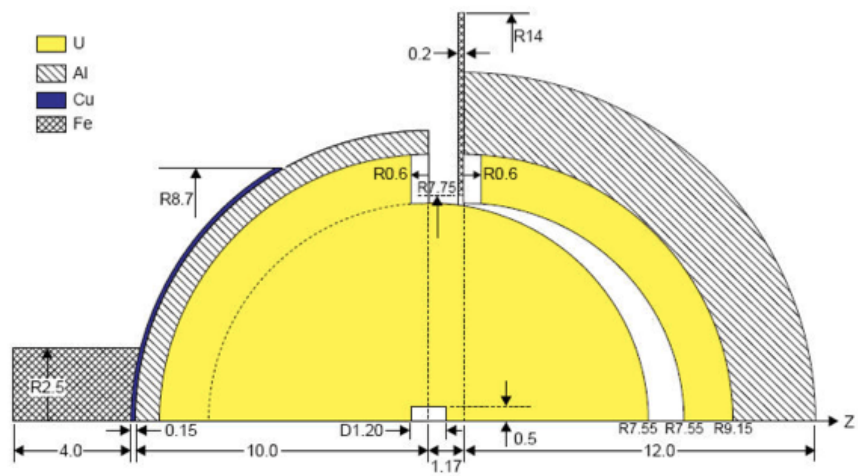
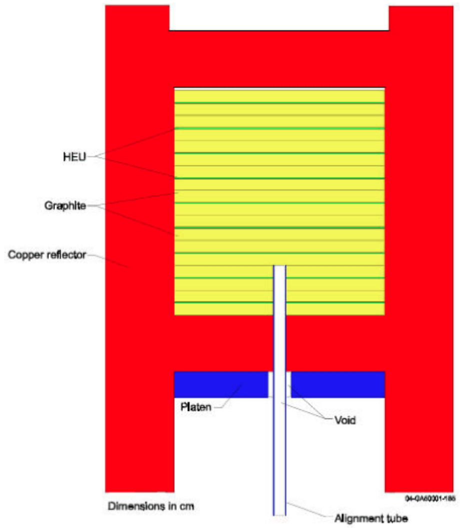


Figure 2. Incomplete HEU Sphere Reflected by Beryllium, heu-met-fast-009-case-1

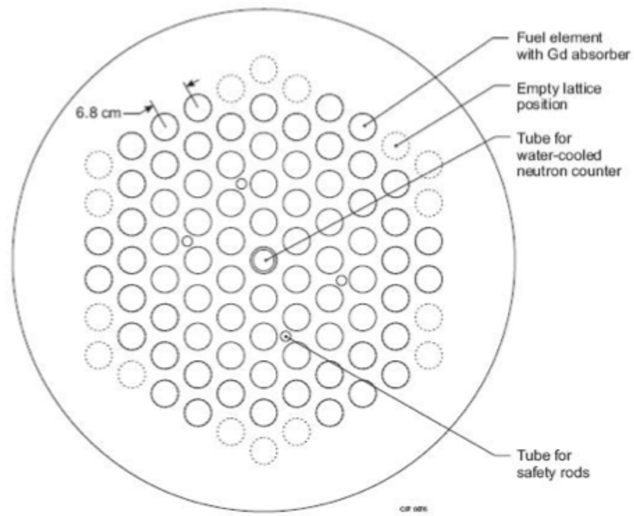


e 5. Incomplete HEU Sphere Reflected by Aluminum, heu-met-fast-012

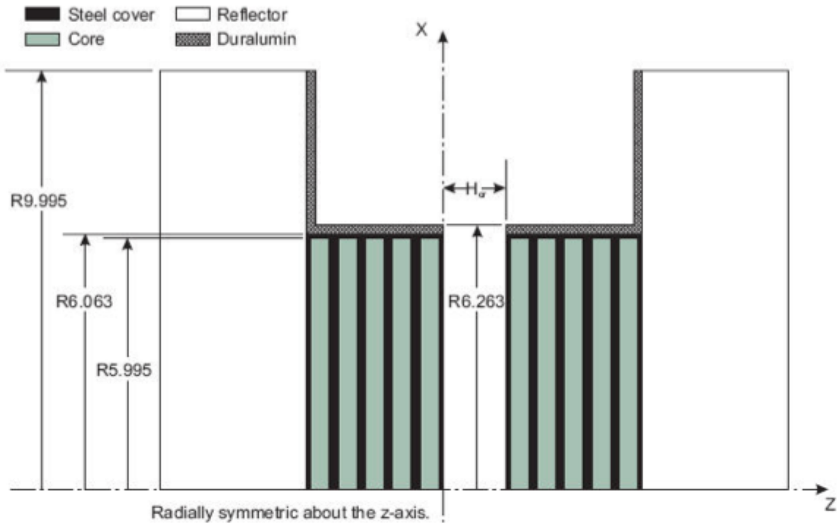
Examples



Vertical Slice through the Center of the Zeus-2 Benchmark, heu-met-inter-006-case-2



rods, ieu-comp-therm-002-case-3



6. Stacked Plutonium Cylinder Reflected by Beryllium or Beryllium Oxide, pu-met-fast-021-case-1 or pu-met-fast-021-case-2

U-233 Benchmark Characteristics

Monte Carlo Codes
XCP-3, LANL

Spectrum	Form	Shape	Moderator and /or Reflector	Benchmark(s)
Fast	Metal	Sphere	Unreflected	u233-met-fast-001
			HEU	u233-met-fast-002-case-1 u233-met-fast-002-case-2
			Normal uranium	u233-met-fast-003-case-1 u233-met-fast-003-case-2 u233-met-fast-006
			Tungsten	u233-met-fast-004-case-1 u233-met-fast-004-case-2
			Beryllium	u233-met-fast-005-case-1 u233-met-fast-005-case-2
Intermediate	Solution	Sphere	Beryllium	u233-sol-inter-001-case-1
Thermal	$UO_2 + ZrO_2$	Lattice	Water	u233-comp-therm-001-case-3
	Solution	Sphere	Unreflected	u233-sol-therm-001-case-1 u233-sol-therm-001-case-2 u233-sol-therm-001-case-3 u233-sol-therm-001-case-4 u233-sol-therm-001-case-5 u233-sol-therm-008

HEU Fast Benchmark Characteristics

Monte Carlo Codes
XCP-3, LANL

Spectrum	Form	Shape	Reflector	Benchmark(s)
Fast	Metal	Sphere	Unreflected	heu-met-fast-001 heu-met-fast-008 heu-met-fast-018-case-2
			Normal uranium	heu-met-fast-003-case-1 heu-met-fast-003-case-2 heu-met-fast-003-case-3 heu-met-fast-003-case-4 heu-met-fast-003-case-5 heu-met-fast-003-case-6 heu-met-fast-003-case-7 heu-met-fast-028
			Depleted uranium	heu-met-fast-014
			Tungsten carbide	heu-met-fast-003-case-8 heu-met-fast-003-case-9 heu-met-fast-003-case-10 heu-met-fast-003-case-11
			Nickel	heu-met-fast-003-case-12
			Steel	heu-met-fast-013 heu-met-fast-021-case-2
			Duralumin	heu-met-fast-022-case-2
			Aluminum	heu-met-fast-012
			Graphite	heu-met-fast-019-case-2
			Beryllium oxide	heu-met-fast-009-case-2
			Beryllium	heu-met-fast-009-case-1
			Polyethylene	heu-met-fast-011 heu-met-fast-020-case-2
			Water	heu-met-fast-004-case-1
		Cylinder	Unreflected	heu-met-fast-015
		Lattice	Paraffin	heu-met-fast-026-case-c-11

HEU Intermediate & Thermal Characteristics

Spectrum	Form	Shape	Reflector, Moderator and/or Buffer	Benchmark(s)
Intermediate	UH_3	Cylinders	Natural uranium	heu-comp-inter-003, case-6
	Metal	Cylinders	Graphite, copper	heu-met-inter-006-case-1 heu-met-inter-006-case-2 heu-met-inter-006-case-3 heu-met-inter-006-case-4
Thermal	$UO_2 + ZrO_2$	Lattice	Water, ThO_2	u233-comp-inter-001-case-6
	Solution	Sphere	Unreflected	heu-sol-therm-013-case-1 heu-sol-therm-013-case-2 heu-sol-therm-013-case-3 heu-sol-therm-013-case-4 heu-sol-therm-032

IEU Benchmark Characteristics

Spectrum	Form	Shape	Reflector and/or Buffer	Benchmark(s)
Fast	Metal	Sphere	Unreflected	ieu-met-fast-003-case-2
			Steel	ieu-met-fast-005-case-2
			Duralumin	ieu-met-fast-006-case-2
			Graphite	ieu-met-fast-004-case-2
		Cylinders	Unreflected	ieu-met-fast-001-case-1 ieu-met-fast-001-case-2 ieu-met-fast-001-case-3 ieu-met-fast-001-case-4
			Normal uranium	ieu-met-fast-002
			Depleted uranium	ieu-met-fast-007-case-4
Intermediate	Plate	Lattice	Normal uranium, steel	mix-met-fast-008-case-7
Thermal	UO_2	Lattice	Water	ieu-comp-therm-002-case-3
	Solution	Cylinder	Unreflected	leu-sol-therm-007-case-14 leu-sol-therm-007-case-30 leu-sol-therm-007-case-32 leu-sol-therm-007-case-36 leu-sol-therm-007-case-49

LEU Benchmark Characteristics

Monte Carlo Codes
XCP-3, LANL

Spectrum	Form	Shape	Buffer and/or Reflector	Benchmark(s)
Thermal	UO_2	Lattice	UO_2 Rods, Water	leu-comp-therm-008-case-1 leu-comp-therm-008-case-2 leu-comp-therm-008-case-5 leu-comp-therm-008-case-7 leu-comp-therm-008-case-8 leu-comp-therm-008-case-11
	Solution	Sphere	Water	leu-sol-therm-002-case-1
			Unreflected	leu-sol-therm-002-case-2

Pu Fast Benchmark Characteristics

Monte Carlo Codes
XCP-3, LANL

Spectrum	Form	Shape	Reflector and/or Buffer	Benchmark(s)
Fast	Metal	Sphere	Unreflected	pu-met-fast-001 pu-met-fast-002 pu-met-fast-022-case-2
			HEU	mix-met-fast-001 mix-met-fast-003
			Normal uranium	pu-met-fast-006 pu-met-fast-010
			Depleted uranium	pu-met-fast-020
			Thorium	pu-met-fast-008-case-2
			Tungsten	pu-met-fast-005
			Steel	pu-met-fast-025-case-2 pu-met-fast-026-case-2
			Aluminum	pu-met-fast-009
			Graphite	pu-met-fast-023-case-2
			Beryllium	pu-met-fast-018 pu-met-fast-019
			Polyethylene	pu-met-fast-024-case-2
			Water	pu-met-fast-011
		Cylinders	Beryllium oxide	pu-met-fast-021-case-2
			Beryllium	pu-met-fast-021-case-1
		Lattice	Unreflected	pu-met-fast-003-case-103

Pu Intermediate & Thermal Characteristics

Spectrum	Form	Shape	Reflector and/or Moderator	Benchmark(s)
Intermediate	Mixture	Homogeneous	Hydrogen, graphite	pu-comp-inter-001
Thermal	MOX	Lattice	Water	mix-comp-therm-002-case-pnl-30 mix-comp-therm-002-case-pnl-31 mix-comp-therm-002-case-pnl-32 mix-comp-therm-002-case-pnl-33 mix-comp-therm-002-case-pnl-34 mix-comp-therm-002-case-pnl-35
	Solution	Sphere	Unreflected	pu-sol-therm-009-case-3a pu-sol-therm-011-case-16-5 pu-sol-therm-011-case-18-1 pu-sol-therm-011-case-18-6 pu-sol-therm-021-case-1 pu-sol-therm-021-case-3
		Cylinder	Water	pu-sol-therm-018-case-9 pu-sol-therm-034-case-1

HEU Spheres

Reflector	k_{eff}		
	Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
None	1.0000 ± 0.0010	0.9997 ± 0.0003	0.9994 ± 0.0003
None	1.0000 ± 0.0014	0.9996 ± 0.0003	0.9999 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9947 ± 0.0003	0.9948 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9947 ± 0.0003	0.9945 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9995 ± 0.0003	0.9991 ± 0.0003
Normal U	1.0000 ± 0.0030	0.9974 ± 0.0003	0.9971 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0012 ± 0.0003	1.0008 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0019 ± 0.0003	1.0020 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0018 ± 0.0003	1.0018 ± 0.0003
Depleted U	0.9989 ± 0.0017	0.9976 ± 0.0003	0.9978 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

Metal Spheres with Tungsten or Tungsten-carbide Reflector

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
			Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
^{233}U	5.0444	2.4384	1.0000 ± 0.0007	0.9987 ± 0.0003	1.0049 ± 0.0003
^{233}U	4.5999	5.7912	1.0000 ± 0.0008	0.9954 ± 0.0003	1.0052 ± 0.0003
HEU	6.6020	4.8260*	1.0000 ± 0.0050	1.0014 ± 0.0003	1.0082 ± 0.0003
HEU	6.2527	7.3660*	1.0000 ± 0.0050	1.0014 ± 0.0003	1.0095 ± 0.0003
HEU	6.0509	11.4300*	1.0000 ± 0.0050	1.0050 ± 0.0003	1.0129 ± 0.0003
HEU	6.0159	16.5100*	1.0000 ± 0.0050	1.0099 ± 0.0003	1.0166 ± 0.0003
Pu	5.0419	4.6990	1.0000 ± 0.0013	1.0011 ± 0.0003	1.0093 ± 0.0003

* Tungsten carbide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

Metal Spheres with Be or Be-oxide Reflector

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
			Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
^{233}U	5.0444	2.0447	1.0000 ± 0.0030	0.9963 ± 0.0003	0.9941 ± 0.0003
^{233}U	4.5999	4.1961	1.0000 ± 0.0030	0.9956 ± 0.0003	0.9924 ± 0.0003
HEU	8.3500	2.6500	0.9992 ± 0.0015	0.9976 ± 0.0003	0.9949 ± 0.0003
HEU	8.3500*	2.6500**	0.9992 ± 0.0015	0.9967 ± 0.0003	0.9955 ± 0.0003
Pu	5.0419	3.6881	1.0000 ± 0.0030	0.9993 ± 0.0003	0.9964 ± 0.0003
Pu	5.3500*	5.6500	0.9992 ± 0.0015	1.0009 ± 0.0003	0.9976 ± 0.0003
Pu	3.7938	8.4938	0.9983 ± 0.0019	1.0000 ± 0.0003	0.9965 ± 0.0003

* Inner radius 1.4 cm
** Beryllium oxide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$

HEU Solutions with Cadmium (small vessel)

Case	In-Vessel Cd Conc. (mg/g)	Benchmark k_{eff}	Calculated k_{eff}	
			ENDF/B-VII.1β3	ENDF/B-VII.0
1	0	1.0012 ± 0.0026	0.9986 ± 0.0004	0.9997 ± 0.0004
2*	0	1.0012 ± 0.0029	0.9906 ± 0.0004	0.9897 ± 0.0004
3	1.208	1.0012 ± 0.0026	0.9979 ± 0.0004	0.9957 ± 0.0004
4	2.393	1.0012 ± 0.0025	0.9987 ± 0.0004	0.9955 ± 0.0004
5	3.897	1.0012 ± 0.0025	1.0037 ± 0.0004	0.9974 ± 0.0004
6	4.069	1.0012 ± 0.0025	1.0047 ± 0.0004	0.9998 ± 0.0004
7	4.196	1.0012 ± 0.0024	1.0047 ± 0.0004	0.9995 ± 0.0004
8	4.271	1.0012 ± 0.0024	1.0038 ± 0.0004	0.9983 ± 0.0004

* Reflector contains Cd

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

Current Application - ENDF/B-VII.1β3 Testing (5)

Preliminary results summary for ENDF/B-VII.1β3

- **Produces results that are in very close agreement with results from ENDF/B-VII.0 & ENDF/B-VII.1**
- **Produces substantially improved results for cases with tungsten, beryllium, or cadmium**
- **Further improvement is needed for cases with beryllium**
- **A number of previously identified problems still remain, including**
  - **Unresolved resonance range for 235U**
  - **Thermal range for 239Pu**
  - **Fast range for 237Np**
  - **Fast range for copper**

Conclusions

- The Expanded Validation Suite provides a significant advance in the quality assurance and verification/ validation of MCNP for criticality problems.
- The careful selection of Handbook benchmark problems that span the expected application space provides the required broad coverage of code applicability.
- For validation purposes, it is expected that the suite will be used with different cross- section libraries, e.g., ENDF/B-VII.1, to broadly assess the impact of library improvements.
- For practitioners, the suite may also serve as a starting point for validating MCNP and its data libraries for their specific applications.

Questions ?