LA-UR-09-07224

Data Testing at LANL

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CSEWG Meeting

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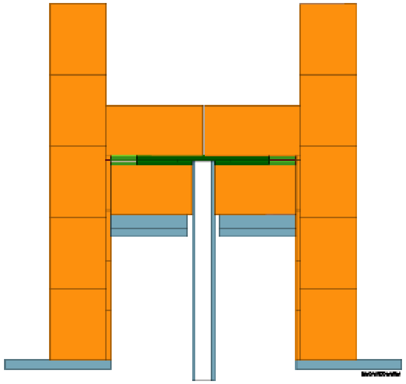
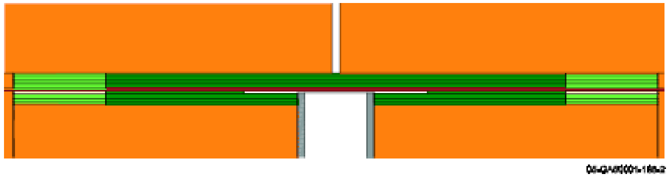
Data Testing Overview

- CENDL-3 / JENDL-4 Copper – Russ.
- Revised ^{113}Cd – Russ.
- Revised ^{9}Be – Skip (Gerry Hale support).
- ^{239}Pu Thermal Solution Criticals – Skip.
- LANL Actinide Evaluations and Reaction Rates – Skip (with encouragement from Mark Chadwick and files produced by Phil Young, Toshihiko Kawano and Patrick Talou).

CENDL-3 / JENDL-4 Isotopic Copper

Unmoderated Zeus Benchmark
("Zeus-5")





The unmoderated Zeus benchmark contains cylindrical platters of HEU enclosed in copper

Previous Zeus benchmarks contained cylindrical platters of graphite interspersed with the fuel platters

CENDL-3 / JENDL-4 Isotopic Copper

MCNP5 RESULTS FOR THE UNMODERATED ZEUS BENCHMARK

Copper cross section	Benchmark k_{eff}	Calculated k_{eff}			
		ENDF/B-VII.0	ENDF/B-VI	JEFF-3.1	JENDFL-3.3
As stated	1.0004± 0.0016	1.0115 ± 0.0003	1.0077 ± 0.0003	1.0084 ± 0.0003	1.0241 ± 0.0003
ENDF/B-V		0.9998 ± 0.0003	0.9971 ± 0.0003	0.9974 ± 0.0003	1.0000 ± 0.0003
CENDL-3.1		1.0049 ± 0.0003			

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $|\Delta k| > 4\sigma$

ENDF/B-V copper cross sections significantly improve the results

CENDL-3.1 copper cross sections also improve the results, but not as much as ENDF/B-V

CENDL-3 / JENDL-4 Isotopic Copper

MCNP5 RESULTS FOR ZEUS BENCHMARKS

Case	E-VII.0 Intermed Fission (%)	Benchmark k_{eff}	Calculated k_{eff}			
			Nuclear Data for Cu from			
			ENDF/B-VII.0	ENDF/B-V*	JENDL-4*	CENDL-3.1*
Zeus-1	72.51	0.9977 ± 0.0008	0.9932 ± 0.0003	0.9925 ± 0.0003	0.9920 ± 0.0003	0.9913 ± 0.0003
Zeus-2	69.29	1.0001 ± 0.0008	0.9970 ± 0.0003	0.9974 ± 0.0003	0.9961 ± 0.0003	0.9949 ± 0.0003
Zeus-3	62.94	1.0015 ± 0.0009	1.0007 ± 0.0003	1.0016 ± 0.0003	1.0003 ± 0.0003	0.9984 ± 0.0003
Zeus-4	49.40	1.0016 ± 0.0008	1.0076 ± 0.0003	1.0079 ± 0.0003	1.0075 ± 0.0003	1.0040 ± 0.0003
Zeus-5	16.23	1.0004 ± 0.0016	1.0115 ± 0.0003	0.9998 ± 0.0003	1.0110 ± 0.0003	1.0049 ± 0.0003

* All other nuclear data from ENDF/B-VII.0

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k| \leq 4\sigma$ $|\Delta k| > 4\sigma$

CENDL-3 / JENDL-4 Isotopic Copper

OBSERVATIONS ON CU CROSS SECTIONS

ENDF/B-V and JENDL-4 copper cross sections have little impact on k_{eff} for Zeus-1 through Zeus-4

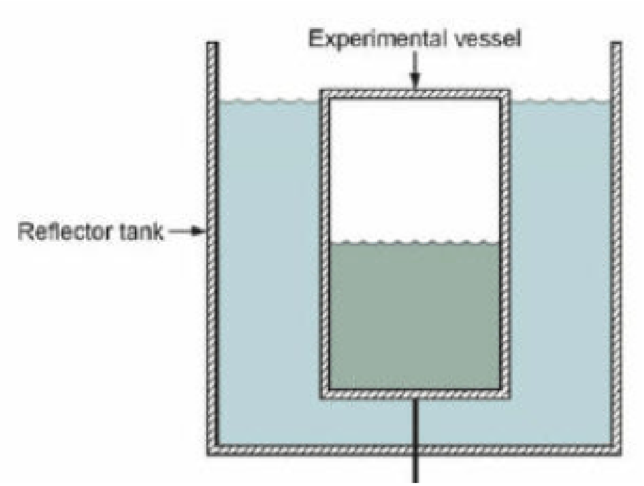
CENDL-3.1 copper cross sections have significant impact on k_{eff} for all five Zeus benchmarks

Judgments about adequacy of copper cross sections are complicated by the fact that the uranium cross sections produce an unquantified energy-dependent bias in k_{eff} for the Zeus benchmarks

Revised ^{113}Cd RR Data

20 benchmarks with highly enriched uranyl nitrate solutions, 18 of them containing Cd

Two different cylindrical stainless-steel vessels containing a highly enriched uranium (HEU) nitrate solution were surrounded by an effectively infinite reflector of water around and beneath it



The nitrate solution contained Cd for 16 of the 20 cases, and the water reflector contained Cd for 9 of them

The height of the reflector was substantially greater than that of the solution in the vessel in all cases

Criticality was obtained by adjusting the height of the solution

Revised ^{113}Cd RR Data

ENDF/B-VI and ENDF/B-VII.0 produce poor results for these benchmarks, even though ENDF/B-V produces reasonable results

Almost all thermal absorption in Cd occurs in a single isotope, ^{113}Cd

Most of the thermal absorption in ^{113}Cd occurs in a single resonance at 0.178 eV

A revised thermal capture cross section for ^{113} Cd was generated by Said Mughabghab at BNL, based on earlier measurements of that resonance

Recently, new measurements of that resonance have been performed at Geel, and a new capture cross section for ^{113}Cd has been generated based on those data

S. Kopecky *et al*, "The Total Cross Section and Resonance Parameters for the 0.178 eV Resonance of ^{113}Cd, Nuclear Instruments and Methods in Physics Research B," **267**(2009)2345.

Revised ^{113}Cd RR Data

MCNP RESULTS FOR THE BENCHMARKS WITH THE SMALLER VESSEL (24.18 cm DIAMETER)

Case	In-Vessel Cd Conc. (mg/g)	Benchmark k_{eff}	Calculated k_{eff}		
			ENDF/B-VII.0	ENDF/B-VII.0 + BNL ^{113}Cd	ENDF/B-VII.0 + Geel ^{113}Cd
1	0	1.0012 ± 0.0026	0.9997 ± 0.0004		
2*	0	1.0012 ± 0.0029	0.9897 ± 0.0004	0.9911 ± 0.0004	0.9894 ± 0.0004
3	1.208	1.0012 ± 0.0026	0.9957 ± 0.0004	0.9982 ± 0.0004	0.9978 ± 0.0004
4	2.393	1.0012 ± 0.0025	0.9955 ± 0.0004	0.9998 ± 0.0004	0.9979 ± 0.0004
5	3.897	1.0012 ± 0.0025	0.9974 ± 0.0004	1.0042 ± 0.0004	1.0019 ± 0.0004
6	4.069	1.0012 ± 0.0025	0.9998 ± 0.0004	1.0059 ± 0.0004	1.0034 ± 0.0004
7	4.196	1.0012 ± 0.0024	0.9995 ± 0.0004	1.0070 ± 0.0004	1.0037 ± 0.0004
8	4.271	1.0012 ± 0.0024	0.9983 ± 0.0004	1.0049 ± 0.0004	1.0025 ± 0.0004

* Reflector contains Cd

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

Revised ^{113}Cd RR Data

MCNP RESULTS FOR THE BENCHMARKS WITH THE LARGER VESSEL (29.16 cm DIAMETER)

Case	In-Vessel Cd Conc. (mg/g)	Benchmark k_{eff}	Calculated k_{eff}		
			ENDF/B-VII.0	ENDF/B-VII.0 + BNL ^{113}Cd	ENDF/B-VII.0 + Geel ^{113}Cd
9	0	1.0012 ± 0.0020	0.9980 ± 0.0004		
10*	0	1.0012 ± 0.0024	0.9892 ± 0.0004	0.9900 ± 0.0004	0.9884 ± 0.0004
11*	1.240	1.0012 ± 0.0022	0.9895 ± 0.0004	0.9923 ± 0.0004	0.9910 ± 0.0004
12*	2.250	1.0012 ± 0.0021	0.9920 ± 0.0004	0.9970 ± 0.0004	0.9949 ± 0.0004
13*	3.362	1.0012 ± 0.0021	0.9915 ± 0.0004	0.9981 ± 0.0004	0.9955 ± 0.0004
14*	4.189	1.0012 ± 0.0020	0.9919 ± 0.0004	0.9994 ± 0.0004	0.9964 ± 0.0004
15*	4.577	1.0012 ± 0.0021	0.9943 ± 0.0004	1.0014 ± 0.0004	0.9978 ± 0.0004
16*	4.897	1.0012 ± 0.0020	0.9920 ± 0.0004	1.0004 ± 0.0004	0.9965 ± 0.0004
17*	5.047	1.0012 ± 0.0021	0.9909 ± 0.0004	0.9993 ± 0.0004	0.9961 ± 0.0004
18	5.032	1.0012 ± 0.0020	0.9933 ± 0.0004	1.0014 ± 0.0004	0.9981 ± 0.0004
19	5.937	1.0012 ± 0.0020	0.9936 ± 0.0004	1.0024 ± 0.0004	0.9980 ± 0.0004
20	6.626	1.0012 ± 0.0019	0.9913 ± 0.0004	1.0005 ± 0.0004	0.9970 ± 0.0004

* Reflector contains Cd $\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

Revised ^{113}Cd RR Data

OBSERVATIONS ON ^{113}CD CAPTURE CROSS SECTION

Cases 2 , 10 ,and 11 produce anomalously low values for k_{eff} even though they contain relatively low concentrations of Cd; consequently, they probably should be omitted from the set of cases upon which decisions are based

Both the BNL and the Geel cross sections produce better agreement with benchmark values for k_{eff} than ENDF/B-VII.0 does

For the 15 "reliable" cases with Cd present, the BNL cross section produces $|\Delta k| > 2\sigma$ for just 1 case, while the GEEL cross section does so for 6 cases

On the other hand, if the calculated k_{eff}'s for the no-Cd cases (1 for the smaller vessel and 9 for the larger one) are taken as the baselines, then the Geel cross section produces better agreement than the BNL cross section

Revised ^{9}Be, Including RPI Data

- **Inclusion of recent RPI total cross section data moves the data set back toward ENDF/B-VI, per Gerry Hale, and confirmed by limited eigenvalue testing.**

- **HEU-MET-FAST-041, cases 1 & 2**
  - Spherical HEU with Be reflector (~4.7 cm thick Be in case 1; ~11.8 cm thick Be in case 2).
    - Case 1 **ENDF/B-VI.8**, **ENDF/B-VII.0** and **new** calculated eigenvalues are **1.00561(9)**, **1.00279(9)** and **1.00691(9)**
    - Case 2 ENDF/B-VI.8, **ENDF/B-VII.0** and **new** calculated eigenvalues are **1.00513(11)**, **1.00024(11)** and **1.00532(10)**

- **Still more evaluation work to be done (e.g. angular distributions).**

^{239}Pu Thermal Solution Criticals

- **Critical eigenvalues calculations were performed for a suite of >100 Pu-SOL-THERM critical experiments during ENDF/B-VII beta testing.**
- **The average eigenvalue was ~1.0045; a result consistent with the greater than unity bias seen in historical plutonium solution eigenvalue calculations.**
  - When correlated against common parameters such as Above-Thermal Leakage Fraction (ATLF), Above-Thermal Fission Fraction (ATFF), atom percent ^{239}Pu or grams Pu per liter no trend in calculated eigenvalue is observed.
- **Recent results from the JEFF community suggest that the revised evaluation currently in JEFF-3.1.1 has significantly reduced this bias.**
- **ORNL submitted a revised evaluation to ENDF/A more than one year ago.**
  - Preliminary testing at ANL suggests that the calculated eigenvalue bias is little changed when this evaluation is used.

^{239}Pu Thermal Solution Criticals

- **A set of seven Pu-SOL-THERM benchmarks have been extracted from the larger set.**
  - PST1.4 & PST12.13 span the ATLF space;
  - PST12.10 & PST34.15 span the ATFF space;
  - PST4.1 & PST18.6 span the ^{239}Pu atom percent space;
  - PST12.10 & PST34.3 span the g Pu per liter space.

- **All benchmark experiments are performed in simple geometry**
  - PST1.4 & PST4.1 are a water-reflected spheres;
  - PST18.6, PST34.3 & PST34.15 are water-reflected cylinders;
  - PST12.10 & PST12.13 are a water-reflected slabs;

^{239}Pu Thermal Solution Criticals

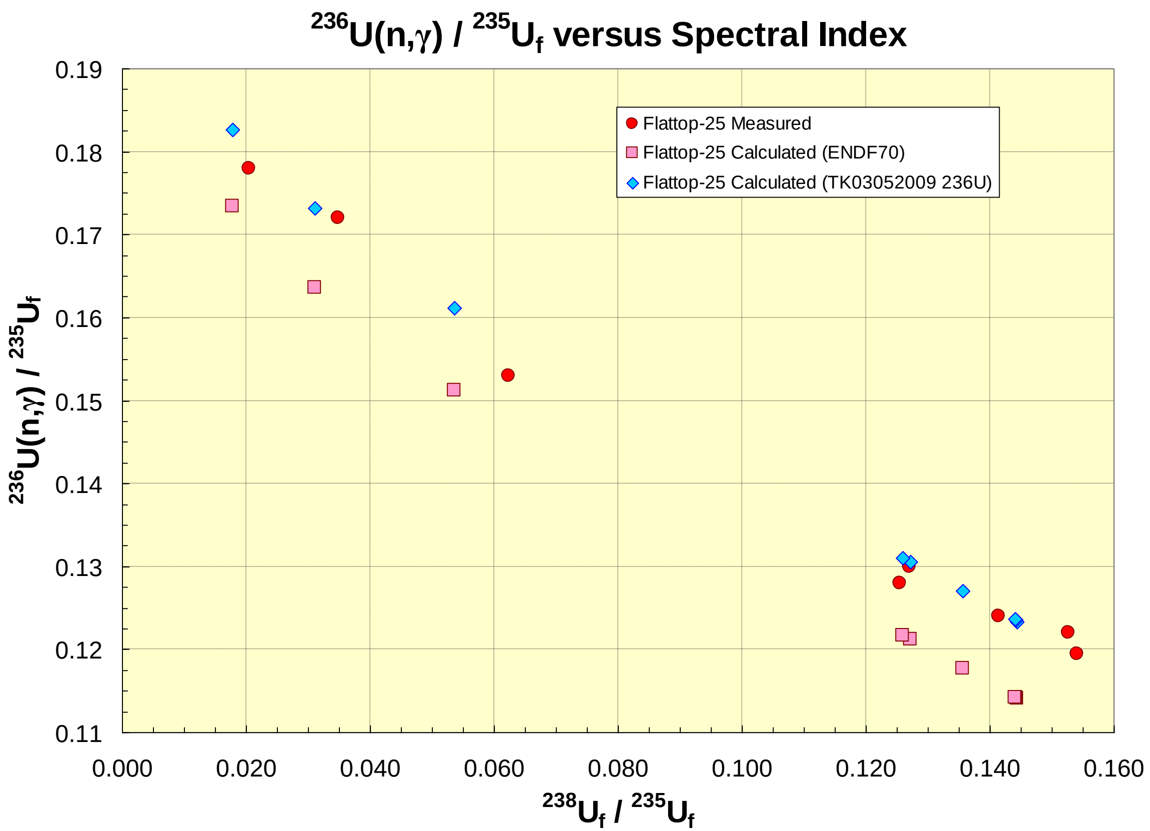
Parameter	Benchmark	ENDF/B-VII.0	"old" ORNL ENDF/A	JEFF-3.1.1
ATLF	PST1.4	1.00484(13)	1.00652(13)	1.00137(13)
	PST12.13	1.00977(6)	1.00954(6)	1.005xx(x)
ATFF	PST12.10	1.00440(10)	1.00431(10)	1.00011(10)
	PST34.15	0.99785(11)	1.00231(11)	0.99606(10)
^{239}Pu atom percent	PST4.1	1.00389(11)	1.00409(11)	0.99899(11)
	PST18.6	1.00502(11)	1.00549(12)	1.00194(11)
g Pu per liter	PST12.10	1.00440(10)	1.00431(10)	1.00011(10)
	PST34.4	1.00240(11)	1.00313(11)	0.99991(11)

- **MCNP results for this subset of benchmarks – new JEFF-3.1.1 gives most accurate results.**

Actinide Reaction Rate Data Testing

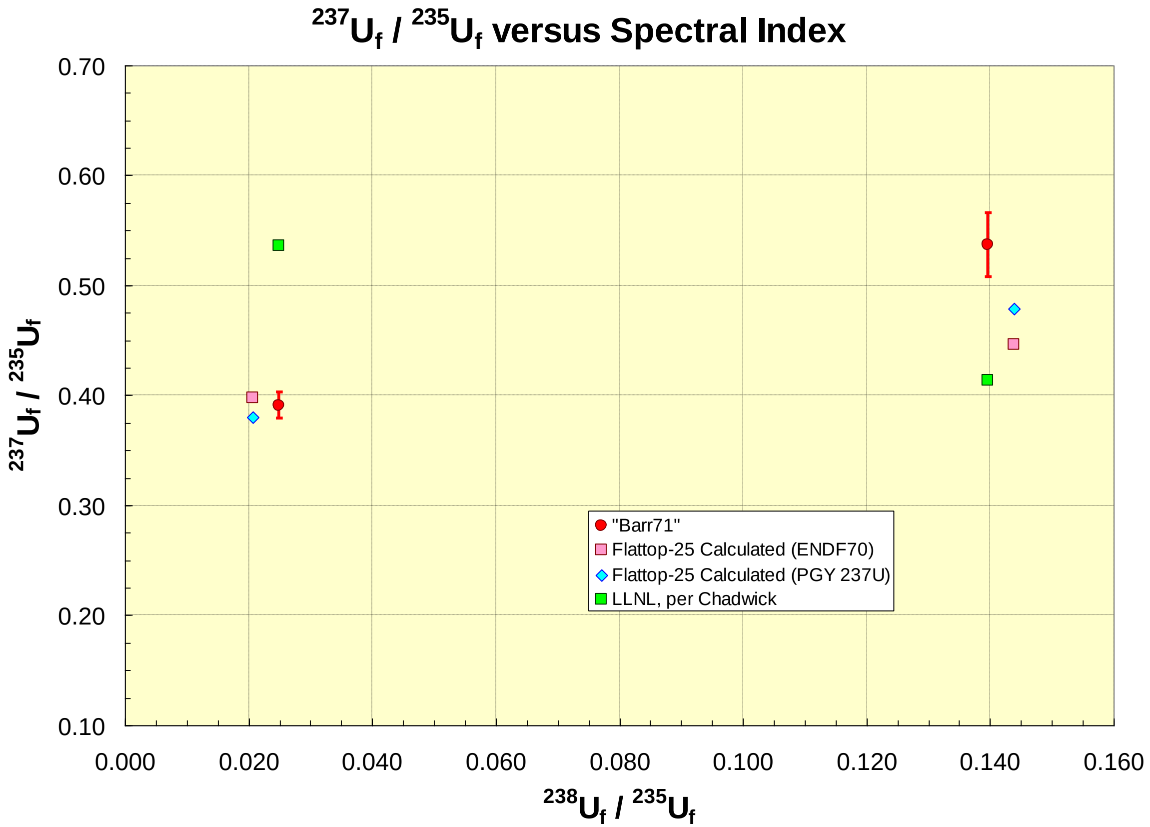
- **A summary of results presented last summer.**
- **LANL Actinide evaluations include ^{236,237}U, ^{240}Pu and ^{241}Am**
- **Reaction rate measurements have been performed in one or more of the LANL fast assemblies – Godiva, Jezebel, Jezebel-40, Flattop-25, Flattop-Pu and Big-10.**
- **New result – reaction rates published for a wide variety of cross sections in FUND-IPPE-FE-MULT-RRR-001.**
  - Accepted for publication in the 2009 edition of the ICSBEP Handbook
  - Model and calculations shown here are derived from the preliminary evaluation approved last Spring.

LANL Actinide Evaluation Revisions – ^{236}U Data Testing



- **Flattop-25: An HEU sphere surrounded by a thick ^{nat}U reflector.**
- **Calculated ^{236}U capture rate is now in better agreement with experiment.**
- **Right-to-left on the abscissa corresponds to increasing radial distance from the center of Flattop-25.**

LANL Actinide Evaluation Revisions – ^{237}U Data Testing

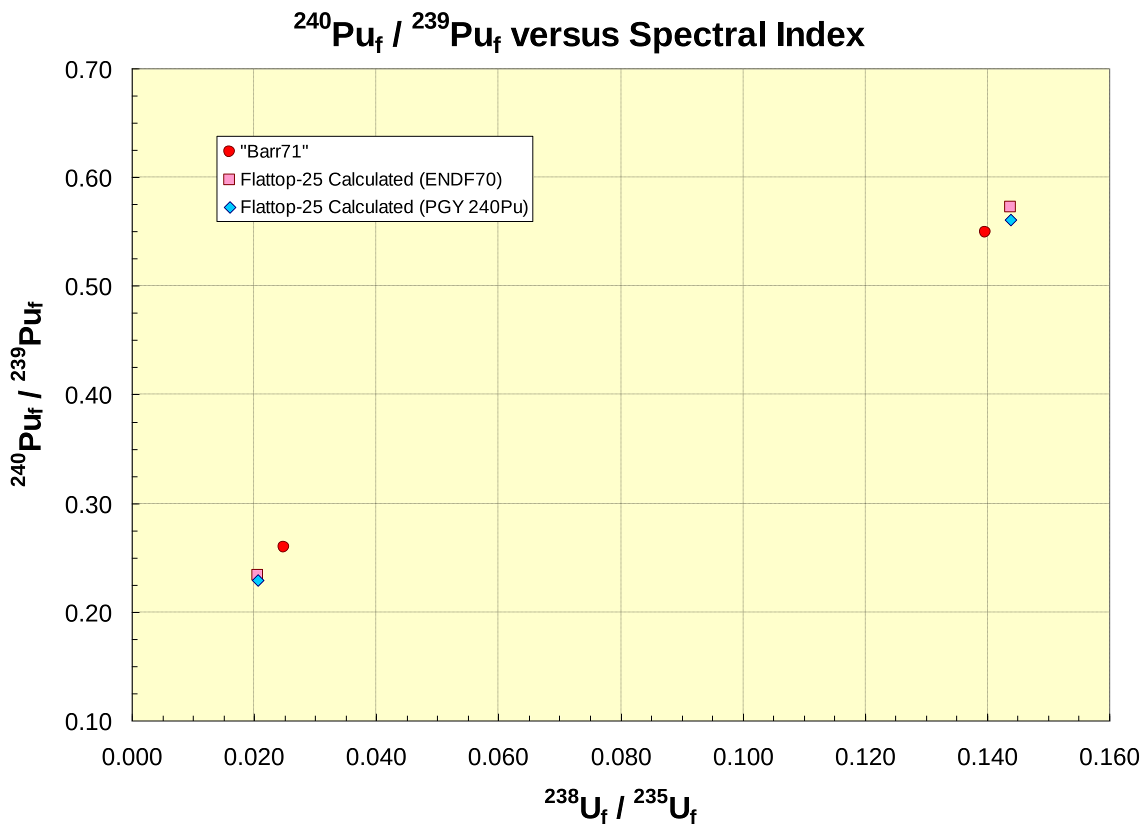


- **Barr71 = Flattop-25 measurements at r=1.11 cm (right) and r=13.97 cm (left).**
- **C/E near the core center is slightly improved with the new (PGY) evaluation, and remains good in the reflector.**

LANL Actinide Evaluation Revisions – ^{240}Pu Data Testing

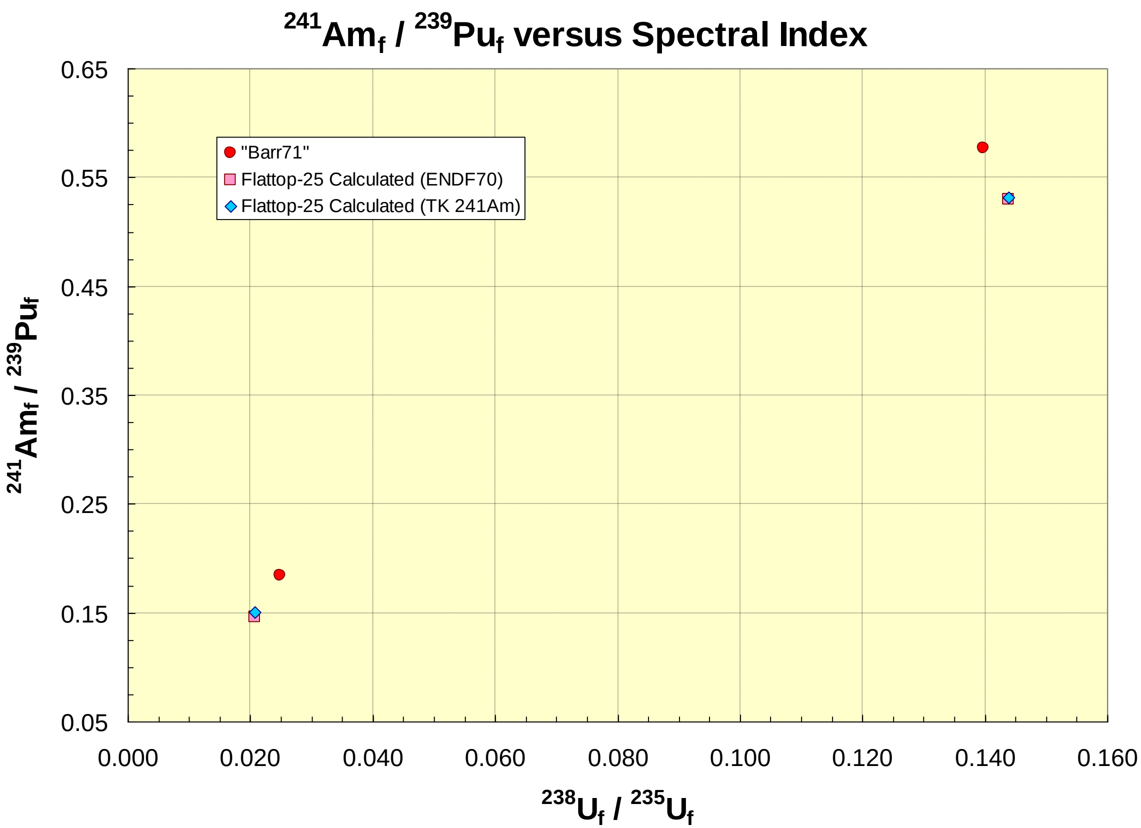
- **Eigenvalue variation with ICSBEP Benchmarks**
  - PMF1: Jezebel (95 a/o ^{239}Pu, 4.5 a/o ^{240}Pu bare sphere)
  - PMF2: “dirty” Jezebel (76 a/o ^{239}Pu, 20 a/o ^{240}Pu bare sphere)
  - PMF22: Russian (98 a/o ^{239}Pu, 2 a/o ^{240}Pu) bare sphere
  - PMF29: Russian (89 a/o ^{239}Pu, 10 a/o ^{240}Pu) bare sphere
  - In all cases, the benchmark model k_{eff} uncertainty is ~0.2%.
- **PMF1 k_{eff}(ENDF/B-VII.0 & E70+new ^{240}Pu): 0.99984(5); 0.99990(6)**
- **PMF2 k_{eff}(ENDF/B-VII.0 & E70+new ^{240}Pu): 0.99992(3); 0.99963(6)**
- **PMF22 k_{eff}(ENDF/B-VII.0 & E70+new ^{240}Pu): 0.99842(3); 0.99851(4)**
- **PMF29 k_{eff}(ENDF/B-VII.0 & E70+new ^{240}Pu): 0.99558(7); 0.99552(3)**
- **Conclusion: Little change in calculated eigenvalues, but underlying ^{240}Pu microscopic cross section data are fundamentally more accurate.**

LANL Actinide Evaluation Revisions – ^{240}Pu Data Testing



- **Barr71 = Flattop-25 measurements at r=1.11 cm (right) and r=13.97 cm (left).**
- **Fission C/E's near the core center and in the reflector are little changed with the new (PGY) evaluation.**

LANL Actinide Evaluation Revisions – ^{241}Am Data Testing



- **Barr71 = Flattop-25 measurements at r=1.11 cm (right) and r=13.97 cm (left).**
- **Fission C/E's near the core center and in the reflector are little changed with the new (TK) evaluation.**
- **In the center of Jezebel, the ^{241}Am(n,γ)^{242g}Am ratio to ^{239}Pu(n,f) C/E was 0.96, it is now 0.99.**

FUND-IPPE-FE-MULT-RRR-001 Reaction Rates

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{232}Th(n,f) / ^{235}U(n,f)	0.03898	0.00002	0.0430	0.0013	0.907	0.027
^{233}U(n,f) / ^{235}U(n,f)	1.55457	0.00068	1.54	0.03	1.009	0.020
^{234}U(n,f) / ^{235}U(n,f)	0.72938	0.00039	0.790	0.024	0.923	0.028
^{236}U(n,f) / ^{235}U(n,f)	0.32151	0.00019	0.333	0.010	0.965	0.029
[^{236}U(n,f) - TK] / ^{235}U(n,f)	0.32157	0.00019	0.333	0.010	0.966	0.029
^{238}U(n,f) / ^{235}U(n,f)	0.16222	0.00011	0.165	0.005	0.983	0.030
^{237}Np(n,f) / ^{235}U(n,f)	0.81346	0.00044	0.771	0.023	1.055	0.031
^{239}Pu(n,f) / ^{235}U(n,f)	1.36031	0.00056	1.33	0.04	1.023	0.031
^{240}Pu(n,f) / ^{235}U(n,f)	0.82336	0.00044	0.877	0.026	0.939	0.028
[^{240}Pu(n,f) - PGY&PT] / ^{235}U(n,f)	0.81106	0.00044	0.877	0.026	0.925	0.027

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{241}Pu(n,f) / ^{235}U(n,f)	1.32221	0.00059	1.29	0.04	1.025	0.032
^{242}Pu(n,f) / ^{235}U(n,f)	0.67041	0.00036	0.658	0.020	1.019	0.031
^{241}Am(n,f) / ^{235}U(n,f)	0.78156	0.00044	0.825	0.025	0.947	0.029
^{241}Am(n,f) - TK] / ^{235}U(n,f)	0.78891	0.00044	0.825	0.025	0.956	0.029
^{232}Th(n,g) / ^{235}U(n,f)	0.10194	0.00008	0.109	0.004	0.935	0.034
^{236}U(n,g) / ^{235}U(n,f)	0.11176	0.00015	0.123	0.006	0.909	0.044
[^{236}U(n,g) - TK] / ^{235}U(n,f)	0.12038	0.00016	0.123	0.006	0.979	0.048
^{238}U(n,g) / ^{235}U(n,f)	0.07779	0.00006	0.077	0.003	1.010	0.039
^{237}Np(n,g) / ^{235}U(n,f)	0.30066	0.00030	0.240	0.012	1.253	0.063
^{232}Th(n,2n) / ^{235}U(n,f)	0.01084	0.00006	0.00924	0.00050	1.174	0.064
^{238}U(n,2n) / ^{235}U(n,f)	0.00954	0.00005	0.00916	0.00050	1.041	0.057

FUND-IPPE-FE-MULT-RRR-001 Reaction Rates

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{50}Cr(n,g) / ^{235}U(n,f)	0.005469	0.000023	0.0057	0.0005	0.960	0.084
^{55}Mn(n,g) / ^{235}U(n,f)	0.003855	0.000014	0.00297	0.00015	1.298	0.066
^{58}Fe(n,g) / ^{235}U(n,f)	0.003023	0.000014	0.00228	0.00009	1.326	0.053
^{59}Co(n,g) / ^{235}U(n,f)	0.005853	0.000014	0.0064	0.0003	0.914	0.043
^{64}Ni(n,g) / ^{235}U(n,f)	0.004754	0.000005	0.00185	0.00008	2.570	0.111
^{63}Cu(n,g) / ^{235}U(n,f)	0.012043	0.000024	0.0114	0.0005	1.056	0.046
^{65}Cu(n,g) / ^{235}U(n,f)	0.007464	0.000010	0.0076	0.0006	0.982	0.078
^{94}Zr(n,g) / ^{235}U(n,f)	0.009600	0.000016	0.0064	0.0004	1.500	0.094
^{96}Zr(n,g) / ^{235}U(n,f)	0.004750	0.000100	0.00306	0.00015	1.552	0.083
^{98}Mo(n,g) / ^{235}U(n,f)	0.027100	0.000037	0.0193	0.0008	1.404	0.058
^{197}Au(n,g) / ^{235}U(n,f)	0.100997	0.000179	0.105	0.005	0.962	0.046
^{24}Mg(n,p) / ^{235}U(n,f)	0.001016	0.000005	0.00090	0.00004	1.129	0.051

	Calculated Ratio	Stdev (calculated ratio)	Measured Ratio	Stdev (measured ratio)	C / E	Stdev (C / E)
^{27}Al(n,p) / ^{235}U(n,f)	0.002151	0.000004	0.00221	0.00015	0.973	0.066
^{46}Ti(n,p) / ^{235}U(n,f)	0.007056	0.000013	0.0066	0.0003	1.069	0.049
^{47}Ti(n,p) / ^{235}U(n,f)	0.009284	0.000007	0.0097	0.0005	0.957	0.049
^{48}Ti(n,p) / ^{235}U(n,f)	0.000180	0.000001	0.000180	0.000008	1.002	0.045
^{54}Fe(n,p) / ^{235}U(n,f)	0.041785	0.000043	0.0447	0.0015	0.935	0.031
^{56}Fe(n,p) / ^{235}U(n,f)	0.000616	0.000002	0.00061	0.00002	1.010	0.033
^{59}Co(n,p) / ^{235}U(n,f)	0.000778	0.000002	0.00084	0.00004	0.926	0.044
^{58}Ni(n,p) / ^{235}U(n,f)	0.055214	0.000052	0.055	0.003	1.004	0.055
^{27}Al(n,a) / ^{235}U(n,f)	0.000460	0.000003	0.0004	0.0000	1.069	0.050
^{54}Fe(n,a) / ^{235}U(n,f)	0.000533	0.000002	0.0005	0.0000	1.066	0.043
^{59}Co(n,a) / ^{235}U(n,f)	0.000096	0.000001	0.00010	0.00000	1.014	0.043
^{92}Mo(n,a) / ^{235}U(n,f)	0.000086	0.000000	0.00006	0.00001	1.560	0.142