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On the Analysis of Benchmarks with ^{233}U fuel and Be or Polyethylene reflectors

(ICSBEP – U233-SOL-THERM-015)

(ICSBEP-U233-SOL-INTER-001)

Andrej Trkov

Jožef Stefan Institute, Ljubljana, Slovenia

and

R. Capote

International Atomic Energy Agency, Vienna, Austria

January 2021

IAEA Nuclear Data Section
Vienna International Centre, P.O. Box 100, 1400 Vienna, Austria

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre
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Austria

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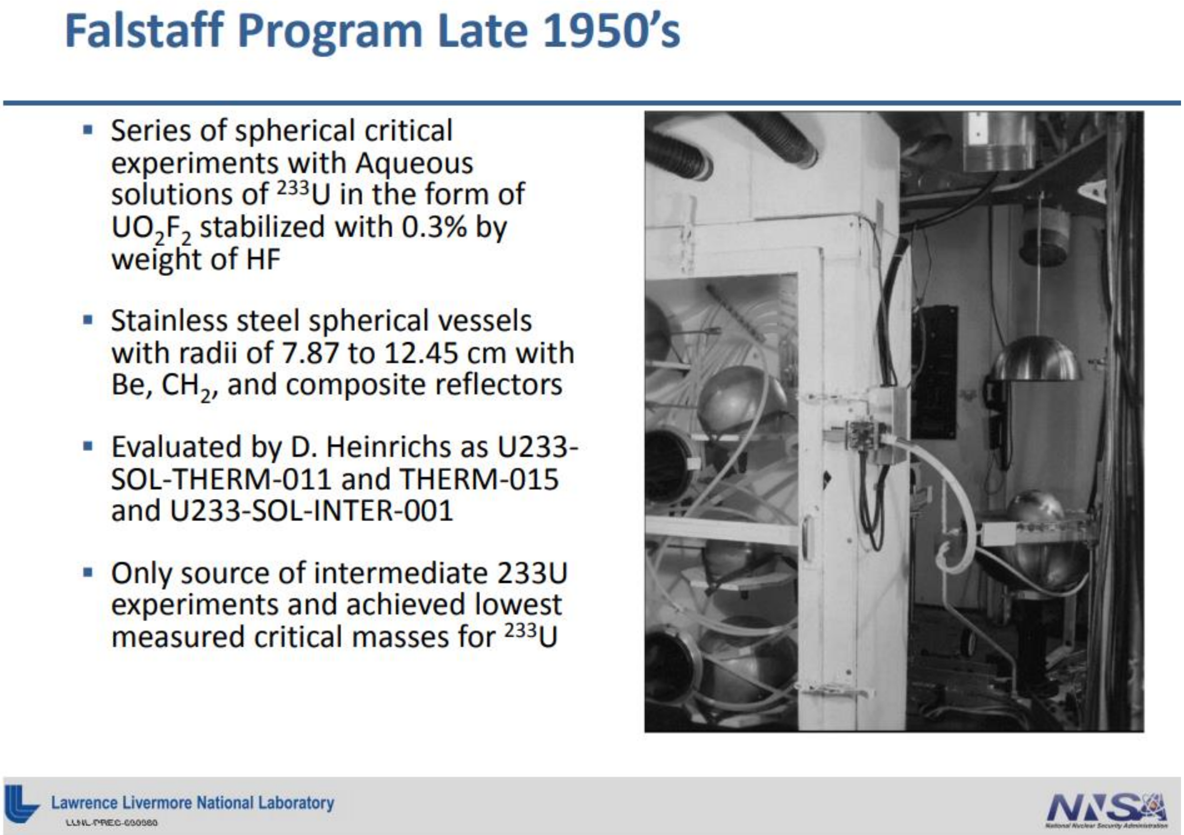
Background

A re-evaluation of the nuclear data for ^{233}U is in progress at the Oak Ridge National Laboratory (ORNL) and the International Atomic Energy Agency (IAEA). Benchmarking is an integral part of the evaluation process. For testing purposes, the current new evaluation available from the INDEN webpage at https://www-nds.iaea.org/INDEN/ labelled "e80u3a3" differs from ENDF/B-VIII.0 (labelled "e80" for short) only in the slightly tuned resonance widths of the bound levels to match the thermal constants from Standards-2017 and the prompt fission neutron spectrum (PFNS): namely, spectrum from the IAEA work on Standards [1,2], where thermal neutron induced PFNS of ^{233}U was evaluated together with other PFNS, and the PFNS at higher incident neutron energies from the IAEA Coordinated research project on the PFNS of actinides, contributed by M. Rising and P. Talou from the Los Alamos National Laboratory [3,4]. Based on the experience with ^{235}U, benchmarks with solutions of uranyl nitrate were analyzed to check for trends in reactivity as a function of the above-thermal fission fraction.

The Falstaff program was carried out at the Lawrence Livermore Laboratory in 1950's with beryllium and polyethylene reflected solutions in spherical vessels of different sizes (see http://ncsd.ans.org/wp-content/uploads/2017/Summer/Presentations/PioneersWedPM/LLNL-Crit-Experiments-Jun-2017-Panel-Final.pdf).



The Falstaff experiments were evaluated as benchmarks into the ICSBP Handbook by D. Heinrichs as U233-SOL-INTER-001 and U233-SOL-THERM-015 (U233-SOL-THERM-011 is documented together with U233-SOL-INTER-001 in the Handbook). These are the only sources of intermediate spectra ^{233}U experiments. Unfortunately, only ^{233}U fuel was used, so no direct comparison with similar HEU solutions is possible. The analysis of these benchmarks was reported in the document describing the ENDF/B-VIII.0 library [5]. From Figure 165 of Ref.[5] a strong negative gradient as a function of above-thermal fission fraction (ATFF) is observed. The aim of the present analysis is to check the reliability of the trend, and whether it is caused by ^{233}U or some other material present in the benchmarks.

Analysis

The Falstaff-I thermal solutions with beryllium and polyethylene reflectors are denoted in the ICSBEP Handbook as U233-SOL-INTER-001 (USI001 for short), which includes cases that are formally labelled as U233-SOL-THERM-011. The complementary campaign Falstaff-II are denoted in the Handbook as U233-SOL-THERM-015 (UST015 for short). There are 33 and 31 cases in the two campaigns, respectively. The assemblies constitute nitrate solutions of different concentration, different sphere diameters and reflector thicknesses. The libraries ENDF/B-VII.1 [6], ENDF/B-VIII.0 [5] and JEFF-3.3 [7] were considered in benchmark calculations, in addition to the trial evaluation “u233a3”.

Results

The benchmark computational models for MCNP were provided by A.C. Kahler (private communication). Predicted reactivity compared to benchmark values is shown in Figure 1. Plotting the same results as a function of the above-thermal fission fraction is shown in Figure 2. The abscissa label FEPIT means the “epithermal fission fraction” and is exactly equivalent to the Above Thermal Fission Fraction parameter (ATFF). The trend of strongly decreasing reactivity with increasing FEPIT is reproduced. The results with ENDF/B-VII.1, ENDF/B-VIII.0 and JEFF-3.3 libraries are rather similar. The reactivity with the “e80u3a3” library (containing ^{233}U evaluation labeled “u233a3”) is systematically shifted in the positive direction (increased) due to the softer PFNS, but the shape is practically the same. However, when the same data are plotted as a function of beryllium reflector thickness, a different picture appears, as shown in Figure 3:

- Benchmarks with only polyethylene reflector do not show any significant gradient (Cases 7, 10, 17 and 25), the results with “u233a3” being practically within the uncertainty band which represents an improvement compared to previous evaluations.
- Only the cases with thin beryllium reflectors seem to strongly under-predict reactivity (Cases 6, 8, 9, 18,19). The case with a comparatively thin polyethylene reflector (Case 10) does not show such anomaly.
- Thin beryllium reflectors with additional polyethylene layers on the outside also do not show a strong trend.
- Most of the other cases are in fair agreement with the reference benchmark values, “u233a3” results being the closest.

Table 1: Falstaff UST015 cases identified by the solution number and sphere number, giving the radius of the solution R_sol, steel vessel thickness d_ss, beryllium reflector thickness d_Be and polyethylene thickness d_PE, as applicable. The big outliers in calculations are shaded red.

Case No	Solution No.	Sphere No.	R_sol [cm]	d_ss [cm]	d_Be [cm]	d_PE [cm]
1	4	1	7.8726	0.0483	9.1700	
2	4	2	8.5152	0.0483	6.5800	
3	4	3	9.0079	0.0483	5.2700	
4	4	3	9.0079	0.0483	1.1400	4.8800
5	4	4	9.6633	0.0483	3.8900	
6	4	5	10.1625	0.0482	2.9000	
7	4	5	10.1625	0.0482		3.5700
8	4	6	10.7992	0.0483	1.9900	
9	4	7	11.4152	0.0483	1.2400	
10	4	7	11.4152	0.0483		1.6800
11	5	1	7.8726	0.0483	9.7300	
12	5	2	8.5152	0.0483	7.0900	
13	5	3	9.0079	0.0483	5.5900	
14	5	3	9.0079	0.0483	1.1400	6.2000
15	5	4	9.6633	0.0483	4.0900	
16	5	5	10.1625	0.0482	3.2000	
17	5	5	10.1625	0.0482		4.0400
18	5	6	10.7992	0.0483	2.0800	
19	5	7	11.4152	0.0483	1.3700	
20	6	1	7.8726	0.0483	11.9100	
21	6	2	8.5152	0.0483	8.5300	
22	6	3	9.0079	0.0483	6.6800	
23	6	4	9.6633	0.0483	4.9000	
24	6	5	10.1625	0.0482	3.8200	
25	6	5	10.1625	0.0482		5.5100
26	7	3	9.0079	0.0483	10.0800	
27	7	4	9.6633	0.0483	7.4900	
28	7	5	10.1625	0.0482	5.9200	
29	7	6	10.7992	0.0483	4.4200	
30	7	7	11.4152	0.0483	3.3000	
31	7	8	12.4564	0.0483	1.8400	

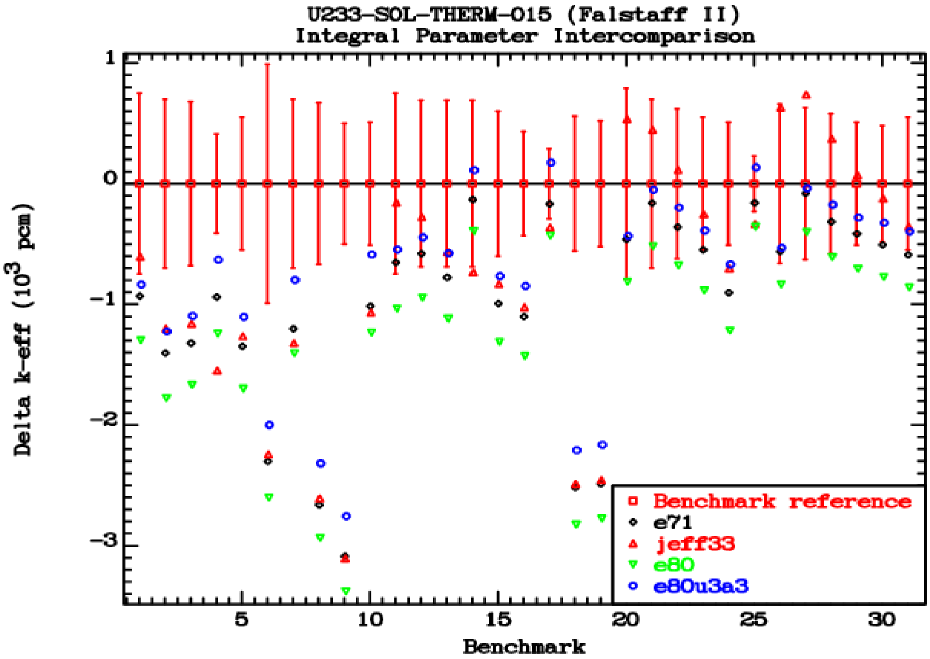


Figure 1 Differences in predicted reactivity from the reference benchmark value by case number.

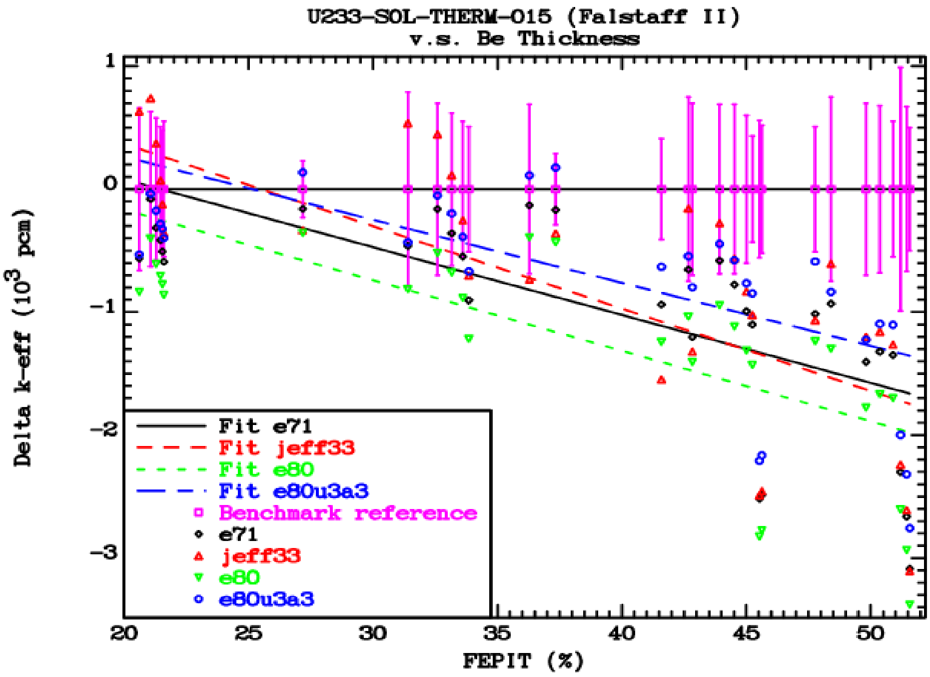


Figure 2 Differences in reactivity from the reference benchmark value as a function of the epithermal fission fraction FEPIT for the U233-SOL-THERM-015 benchmark.

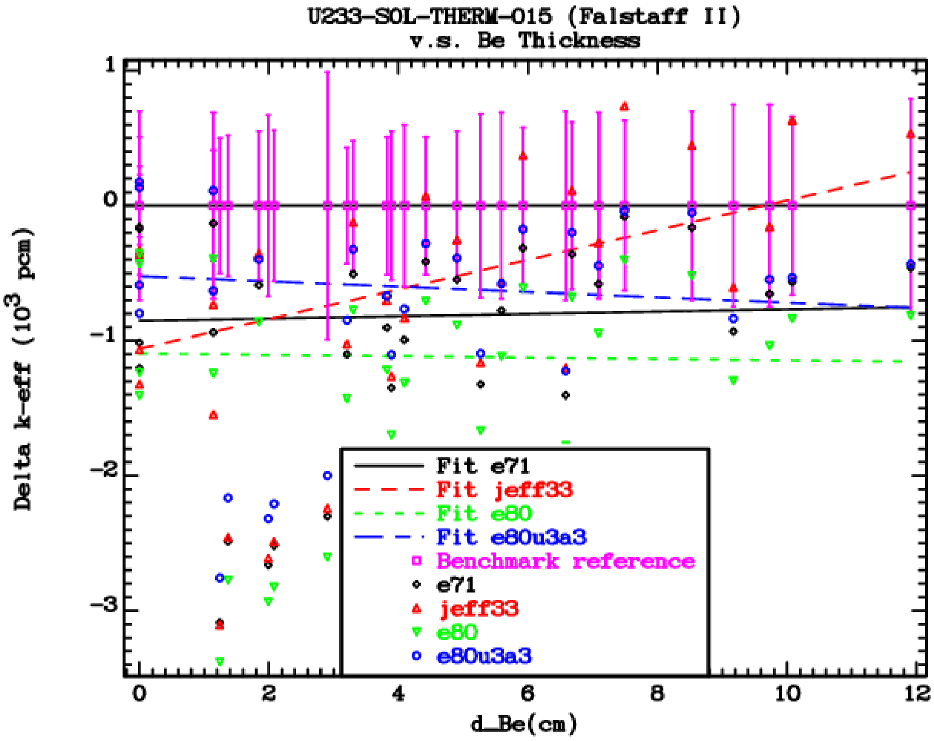


Figure 3 Differences in predicted reactivity from the reference benchmark value as a function of the beryllium reflector thickness d_Be for the U233-SOL-THERM-015 benchmark.

A similar analysis of the intermediate spectrum benchmarks U233-SOL-INTER-001 was performed. The plot as a function of beryllium reflector thickness is shown in Figure 4. It reveals significant scatter of the data, but no distinct outliers. The predicted reactivity for UST001 benchmarks is lower than measured by about 1-1.3% but the new evaluation is still the closest to data. The plot as a function of the epithermal fission fraction FEPIT is shown in Figure 5. It extends the range of FEPIT to over 70 %. Note that the calculations with the JEFF-3.3 library are incomplete.

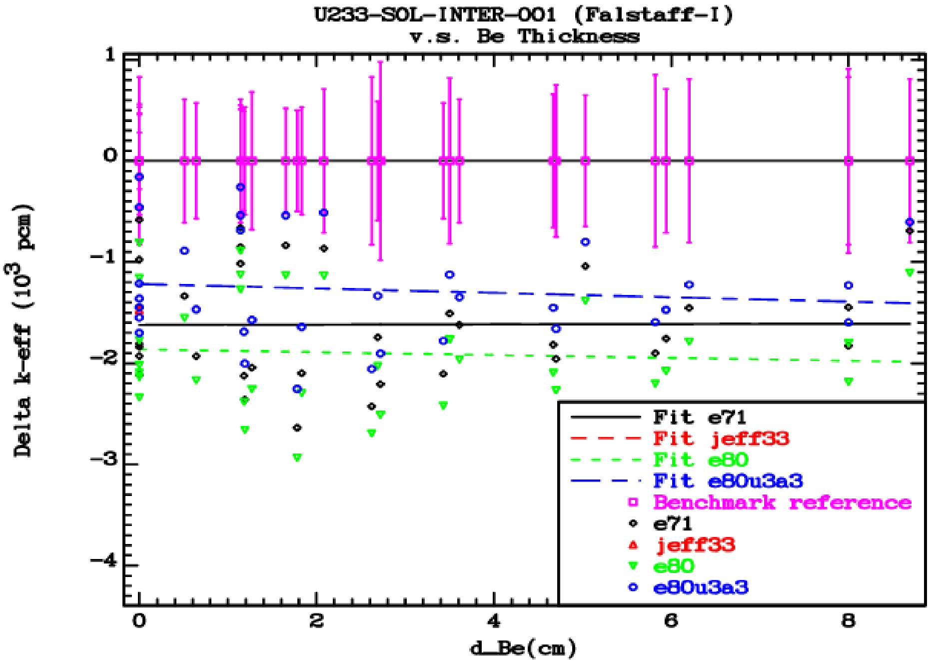


Figure 4 Differences in predicted reactivity from the reference benchmark value as a function of the beryllium reflector thickness d_Be for the U233-SOL-INTER-001 benchmark.

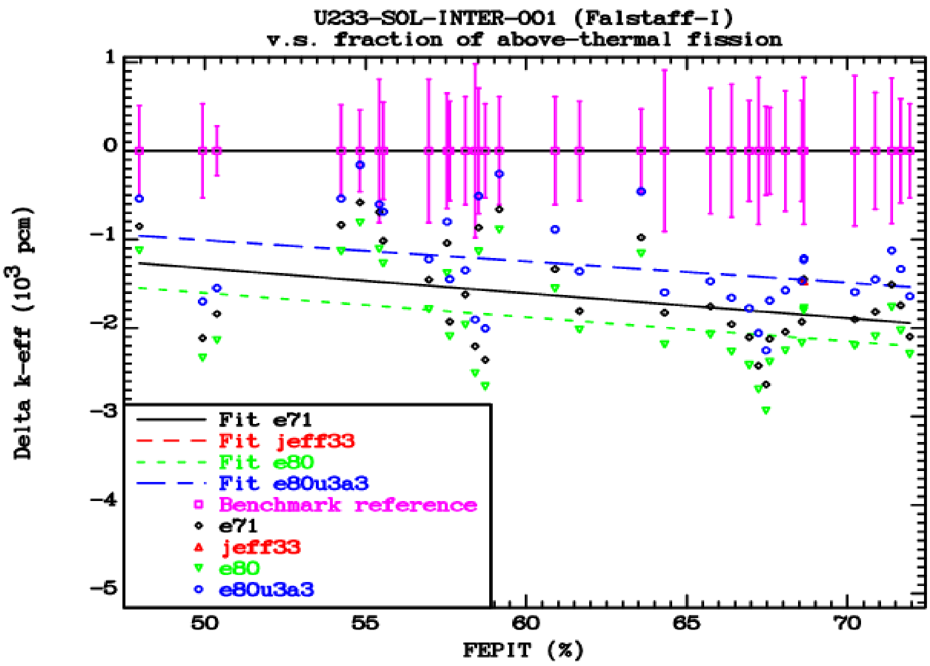


Figure 5 Differences in reactivity from the reference benchmark value as a function of the epithermal fission fraction FEPIT for the U233-SOL-INTER-001 benchmark.

Discussion

The problem of reactivity under-prediction in U233-SOL-THERM-015 benchmarks seems to be strongly emphasized in assemblies with thin beryllium reflectors. Thin polyethylene reflectors do not exhibit a similar trend; neither is such strong trend observed with thicker reflectors, nor with cases that have an additional polyethylene layer on the outside. That means that a potential problem in assemblies with thin beryllium reflectors (UST015, cases 6,8,9,18,19) is identified, likely related to benchmark specifications or to beryllium nuclear data. Those benchmarks (outliers) cannot be used to assess the quality of ^{233}U data until the problem is solved.

However, even after eliminating the big outliers (identified above) from the analysis does not solve the ^{233}U wrong trend with FEPIT, as shown in Figures 6, in which UST015 benchmarks are combined with USI001. The gradient in reactivity as a function of FEPIT is still present. The trend-lines represent a quadratic fit over all points. For FEPIT<40% no trend is observed and good agreement is achieved using the newly evaluated PFNS (u233a3). However, a marked decrease in reactivity appears when FEPIT exceeds about 40 %. The analysis indicates that the problem is very likely caused by the ^{233}U cross sections, in particular the energy dependence of alpha (capture to fission cross-section ratio) and/or the energy dependence of the average number of neutrons per fission (nubar) in the epithermal region.

Looking at the results calculated with the ENDF/B-VIII.0 ^{233}U evaluation "e80" in comparison with "e80u3a3" with updated thermal constants and PFNS, it is clear that the new PFNS has a big positive impact on the increase of reactivity. However, the reactivity gradient for FEPIT greater or equal to 40% is almost independent of the PFNS.

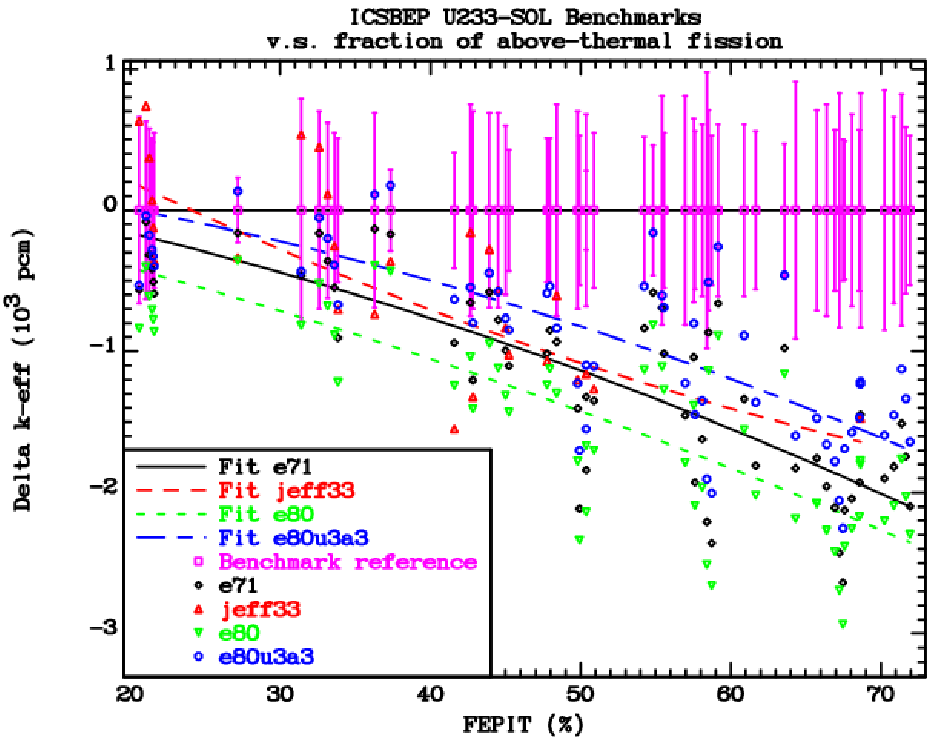


Figure 6 Differences in predicted reactivity from the reference benchmark value as a function of the epithermal fission fraction FEPIT, without the big outliers.

Conclusions

A discrepancy between calculations and measured benchmark values is identified in assemblies with thin beryllium reflectors (UST-015, cases 6,8,9,18,19). The discrepant results are likely related to issues in beryllium nuclear data. The discrepancy diminishes when an extra polyethylene layer is placed on the outside, which makes the flux in beryllium less anisotropic.

This could be a hint that:

- Angular distributions of emitted neutrons from neutron interactions with beryllium should be looked at.
- One should check the room-return effect for the cases with thin reflectors.
- There could be some other structural feature of the relevant benchmarks that is not properly considered in the benchmark specifications.

The outlying (UST-015, cases 6,8,9,18,19) benchmarks cannot be used to assess the quality of ^{233}U data.

However, there remains the overall negative gradient in reactivity with increasing spectrum hardness expressed by the above-thermal fission fraction FEPIT, which is observed even when the strong abovementioned outliers are eliminated. This could be an indication of problems with the ^{233}U evaluation that need to be identified and corrected. Most likely, changes in the ^{233}U capture-to-fission ratio and/or the average number of neutrons per fission energy dependences in the epithermal region are required.

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Nuclear Data Section
International Atomic Energy Agency
Vienna International Centre, P.O. Box 100
A-1400 Vienna, Austria

E-mail: nds.contact-point@iaea.org
Fax: (43-1) 26007
Telephone: (43-1) 2600 21725
Web: http://www-nds.iaea.org