On the Compensating Effects Due to Different Evaluations on Integral Benchmarks

Andrej Trkov

International Atomic Energy Agency, Vienna, Austria

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Introduction

The Working Party on Evaluation Cooperation of the OECD set up a subgroup WPEC-SG40 (alias CIELO) to focus on the evaluated nuclear data of the major nuclides in reactor technology, namely ^{1}H, ^{16}O, ^{56}Fe, ^{235}U, ^{238}U and ^{239}Pu. Different research groups in various parts of the world are working on improved evaluated nuclear data and their uncertainties for these nuclides; the ultimate test of improvement is the performance of the data in simulating integral experiments.

Validation of the capture cross sections of ^{238}U in the unresolved resonance region is one of the topics of interest. A new evaluation of the unresolved resonance parameters has been prepared at IRMM (P. Schillebeeckx, I.Sirakov), with two options for the boundary between the resolved and the unresolved region, namely 20 keV and 10 kev, respectively.

An option has been incorporated into the DICE package for ICSBEP (I.Hill, O.Cabellos) to search the data-base for benchmarks with the highest sensitivity to particular reaction cross sections in a given energy range. As an example, a list was produced for the sensitivities to the ^{238}U capture cross sections in the energy range 10 keV – 20 keV, which can be found in document [8] on the U^{238} tab of https://www-nds.iaea.org/CIELO/.

Scope

MCNP inputs for six cases from the list were available, namely ZPR-3/53, ZPR-6/6A, ZPR-6/7, ZPR-9/31, ZPPR-2 and BSF-31-4. For correspondence with the ICSBEP designations see the Appendix. ACE libraries for the following cases were also available:

E71	Reference ENDF/B-VII.1 library supplied with the MCNP-6.1 package.
U238ib36	IAEA starter file for ^{238}U version “ib36” (https://www-nds.iaea.org/CIELO/)
U238ib36ur	Same as above, with unresolved resonance parameters from IRMM down to 20 keV.
U238ib36ur10	Same as above but with unresolved resonance parameters extending down to 10 keV.
U235g6	ENDF/B-VII.1 data for ^{235}U with prompt fission spectra (PFNS) from thermal to 2 MeV replaced with the GANDR fit prepared at the IAEA.

U235g6nj Same as above, with inelastic data taken from JENDL-4.0.

O16halead The Hale ^{16}O evaluation with missing sections taken from ENDF/B-VII.1 (available from https://www-nds.iaea.org/CIELO/)

O16lealad The Leal ^{16}O evaluation (available from https://www-nds.iaea.org/CIELO/)

Results

The impact of using different data sets for ^{238}U, ^{235}U and ^{16}O are shown in Figures 1 – 3. Generally, the new unresolved resonance data increase the reactivity. The PFNS spectra with a lower average energy affect mainly the ZPR-6/6A benchmark. The oxygen data have some effect on the ZPR-6/6A and ZPR-6/7 benchmarks.

The present combination of data libraries and benchmarks is rather small and can be managed manually, but with increasing number of options it is useful to have a more objective selection criterion to identify the optimal combination of data options. For this purpose the ICSBEP_EVL code was developed, which reads list files that contain the results for different data sets, as shown in the Appendix. The first data set is taken as reference. Differences from the reference for each benchmark for each evaluated data set are calculated. Allowing only one case evaluation for each material and sum over all materials, an estimate for the compensating effects for one benchmark can be made. The root-mean-square (rms) of the deviations for all benchmarks is collected and sorted to find the optimal combination. The results are listed below.

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ICSBEP_EVL - Evaluating Perturbations
=====================================


Top 12 sorted combinations out of    36
   Mat/Case  rms(k_eff) Mx.Df. Outlier
  Reference         605 -1254    6  MIX-MISC-FAST-001   BFS-31-4
      40203         464  -735    6  MIX-MISC-FAST-001   BFS-31-4
      40102         465   729    1  MIX-MET-INTER-004   ZPR-3/53
      40202         467  -735    6  MIX-MISC-FAST-001   BFS-31-4
      30203         470   744    1  MIX-MET-INTER-004   ZPR-3/53
      30102         470   750    1  MIX-MET-INTER-004   ZPR-3/53
      40303         472  -737    6  MIX-MISC-FAST-001   BFS-31-4
      40103         473  -728    6  MIX-MISC-FAST-001   BFS-31-4
      30202         473   746    1  MIX-MET-INTER-004   ZPR-3/53
      40302         475  -737    6  MIX-MISC-FAST-001   BFS-31-4
      40201         475  -735    6  MIX-MISC-FAST-001   BFS-31-4
      30103         477   748    1  MIX-MET-INTER-004   ZPR-3/53
      30303         479   741    1  MIX-MET-INTER-004   ZPR-3/53
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The results suggest that the best combination is option 4 (U238ib36ur10) for ^{238}U, option 2 (U235g6) for ^{235}U and option 3 (O16lealad) for ^{16}O, but the differences are small.

Conclusions

A scheme for performing a scoping study of the compensating effects from different evaluations on integral benchmarks, which allows the identification of possible optimal combinations of evaluated data sets that minimise the overall discrepancy over a selected set of benchmark experiments. The method is based on the linear assumption.

For the present series of benchmarks the optimal choice has been identified as U238ib36ur10 for ^{238}U, U235g6 for ^{235}U and O16lealad for ^{16}O. The maximum deviation in k-eff is reduced from -1254 pcm to 735 pcm and the rms deviation is reduced from 605 pcm to 464 pcm. However, the reader is warned that the method should not be used blindly because it could easily converge on a wrong combination if genuine outliers in the integral benchmarks are present. The next step would be to repeat the calculations with a combined selection of the data to confirm the results and eliminate non-linearities.

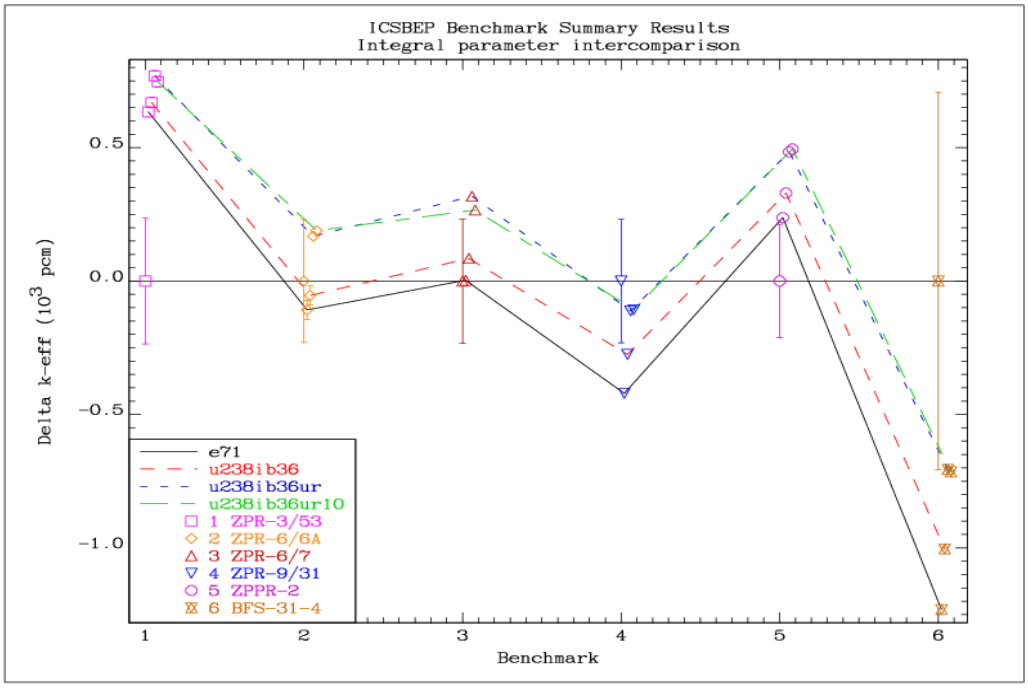

Figure 1: Benchmark results using different cases of ^{238}U evaluation.

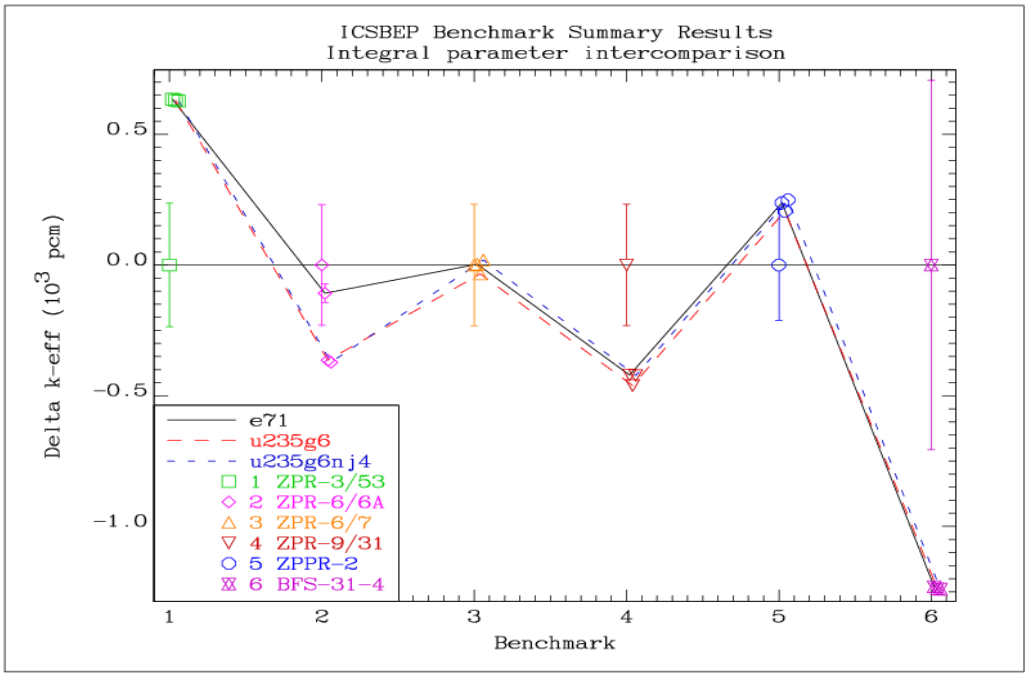

Figure 2: Benchmark results using different cases of ^{235}U evaluation.

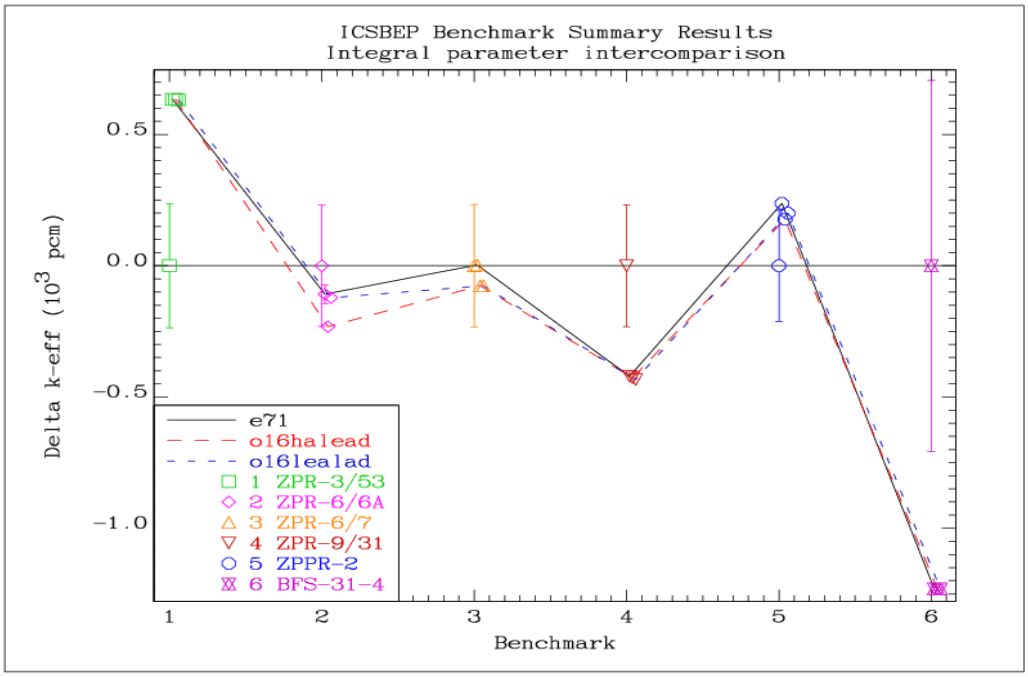

Figure 3: Benchmark results using different cases of ^{16}O evaluation.

Appendix

MIX-MET-INTER-004 ZPR-3/53	Benchmark value		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	0.97570	0.00230	0.98189	0.00020	0.98223	0.00020	0.98320	0.00020	0.98299	0.00020

IEU-COMP-INTER-001 ZPR-6/6A	Benchmark value		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	0.99390	0.00230	0.99283	0.00036	0.99336	0.00036	0.99557	0.00015	0.99578	0.00015

MIX-COMP-FAST-001 ZPR-6/7	Benchmark value Simplified model		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	0.98660	0.00230	0.98663	0.00016	0.98744	0.00016	0.98974	0.00016	0.98922	0.00016

MIX-COMP-FAST-005.s ZPR-9/31	Benchmark value Simplified model		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	0.99130	0.00230	0.98713	0.00007	0.98857	0.00007	0.99019	0.00007	0.99024	0.00007

MIX-COMP-FAST-006 ZPPR-2	Benchmark value Simplified model		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	0.98890	0.00210	0.99125	0.00007	0.99216	0.00007	0.99369	0.00007	0.99380	0.00007

MIX-MISC-FAST-001 BFS-31-4	Benchmark value		e71		u238ib36		u238ib36ur		u238ib36ur10	
k-eff	1.01880	0.00720	1.00626	0.00009	1.00857	0.00009	1.01161	0.00008	1.01152	0.00009

MIX-MET-INTER-004 ZPR-3/53	Benchmark value		e71		u235g6		u235g6nj4	
k-eff	0.97570	0.00230	0.98189	0.00020	0.98185	0.00021	0.98182	0.00020

IEU-COMP-INTER-001 ZPR-6/6A	Benchmark value		e71		u235g6		u235g6nj4	
k-eff	0.99390	0.00230	0.99283	0.00036	0.99028	0.00016	0.99020	0.00016

MIX-COMP-FAST-001 ZPR-6/7	Benchmark value Simplified model		e71		u235g6		u235g6nj4	
k-eff	0.98660	0.00230	0.98663	0.00016	0.98626	0.00017	0.98679	0.00017

MIX-COMP-FAST-005.s ZPR-9/31	Benchmark value Simplified model		e71		u235g6		u235g6nj4	
k-eff	0.99130	0.00230	0.98713	0.00007	0.98673	0.00007	0.98711	0.00007

MIX-COMP-FAST-006 ZPPR-2	Benchmark value Simplified model		e71		u235g6		u235g6nj4	
k-eff	0.98890	0.00210	0.99125	0.00007	0.99094	0.00007	0.99136	0.00007

MIX-MISC-FAST-001 BFS-31-4	Benchmark value		e71		u235g6		u235g6nj4	
k-eff	1.01880	0.00720	1.00626	0.00009	1.00619	0.00008	1.00617	0.00008

MIX-MET-INTER-004 ZPR-3/53	Benchmark value		e71		o16halead		o16lealad	
k-eff	0.97570	0.00230	0.98189	0.00020	0.98189	0.00020	0.98187	0.00021

IEU-COMP-INTER-001 ZPR-6/6A	Benchmark value		e71		o16halead		o16lealad	
k-eff	0.99390	0.00230	0.99283	0.00036	0.99159	0.00016	0.99269	0.00017

MIX-COMP-FAST-001 ZPR-6/7	Benchmark value Simplified model		e71		o16halead		o16lealad	
k-eff	0.98660	0.00230	0.98663	0.00016	0.98585	0.00016	0.98585	0.00016

MIX-COMP-FAST-005.s ZPR-9/31	Benchmark value Simplified model		e71		o16halead		o16lealad	
k-eff	0.99130	0.00230	0.98713	0.00007	0.98707	0.00007	0.98701	0.00007

MIX-COMP-FAST-006 ZPPR-2	Benchmark value Simplified model		e71		o16halead		o16lealad	
k-eff	0.98890	0.00210	0.99125	0.00007	0.99065	0.00007	0.99088	0.00007

MIX-MISC-FAST-001 BFS-31-4	Benchmark value		e71		o16halead		o16lealad	
k-eff	1.01880	0.00720	1.00626	0.00009	1.00626	0.00008	1.00626	0.00008