On the Impact of Fe Scattering on Integral Benchmarks (Rev.1)

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May 2015

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 in simulating integral experiments. In the present work the analysis of the effects of elastic scattering angular distributions is addressed.

A new set of resonance parameters has been submitted to CIELO from the Oak Ridge National Laboratory (ORNL), labelled "ornl4". The resonance data set is stored in the so-called RML format in ENDF, which offers more flexibility in defining output channels. It also allows the possibility to reconstruct the angular distributions from the resonance parameters. The angular distributions vary strongly across a resonance. Since the resonance range extends up to 2 MeV, the angular distribution data are very detailed and result in large application libraries such as the ACE formatted files for MCNP.

A new evaluation of the cross sections above the resonance range has been performed at the Brookhaven National Laboratory (BNL) in collaboration with the International Atomic Energy Agency (IAEA). The data were combined with the ORNL resonance evaluation. The resulting file is labelled "fe56ib04x", where suffix "x" denotes various perturbations with respect to the basis.

The objectives of the investigation were to answer the following questions:

- Are the angular distributions reconstructed from the resonance parameters in agreement with the measured data?
- What is the impact of such detailed representation on integral benchmarks?
- What is the impact of the combined effect of the new resonance and fast cross section data?
- Is it possible to obtain reasonable results with smoothed angular distributions?

Processing of Cross Sections and Angular Distributions

The standard release of NJOY99 cannot process the resonance parameters in RML format. NJOY2012 can do so to make an ACE file. It can also reconstruct the angular distributions from the resonance parameters, but to transfer the reconstructed angular distributions into the basic ENDF file requires additional utilities available from the author on request.

By default, NJOY performs Doppler broadening only up to the lowest threshold energy of reactions with a negative Q-value. This is unacceptable for processing ^{56}Fe, since the inelastic channel opens at 850 keV, but the resonances extend to 2 MeV. A patch for NJOY2012 was prepared that can override the default limitation. However, the Doppler broadening of the inelastic channel below 2 MeV remains a problem because there is an issue with the treatment of the cross sections below the nominal threshold. NJOY2012 does not Doppler-broaden the inelastic channel.

The extended NJOY2012 code is capable of assembling an ACE file including detailed angular distributions reconstructed from resonance parameters. The resulting file is about 100 Mb long and it can be processed with the MCNP-6.1 Monte Carlo code. However, for other kinds of testing it was necessary to split the processing steps and use additional local codes operating on ENDF files:

MF4MRG – merges angular distribution data in a specified energy range from one ENDF file into another file.

MF4THN – inserts parts of an ENDF File-4 into another file and performs data thinning. The code assumes that the normalised angular distributions are given in the form of normalised Legendre expansion (zero-order coefficient equals one by definition). The thinning criterion ε implies that the mesh must be dense enough so that the first order Legendre coefficient or the full angular distributions (reconstructed at 200 points in angle) are linearly interpolable to within the prescribed tolerance.

MU_RSL – resolution-broadens cross sections or angular distributions with a Gaussian resolution function. The resolution function f at a pivot point E_0 is given in terms $f(E\text{-}E_0)$ and the width is expressed in terms of percent of E_0. Resolution-broadening of the cross sections is straightforward. Resolution-broadening of angular distributions can be done directly on the Legendre coefficients, or on the Legendre moments, defined as the product of the cross section and the Legendre coefficient; in the latter case it is obvious that the normalizing cross section must also be resolution-broadened in the same way when Legendre coefficients are recovered from the resolution-broadened moments.

The following ENDF files (and the corresponding ACE files) were produced:

e71	Reference ENDF/B-VII.1 file,
fe56ib04	BNL cross sections, “ornl4” resonance parameters,
fe56ib04r	"fe56ib04" with reconstructed angular distributions explicitly included in the ENDF file,
fe56ib04r1	"fe56ib04r" with reconstructed angular distributions thinned to 10 % tolerance,
fe56ib04r2	"fe56ib04r" with reconstructed angular distributions thinned to 2 % tolerance,
fe56ib04s	"fe56ib04r" with resolution-broadened Legendre coefficients, thinned to 10 % tolerance,

fe56ib04t	"fe56ib04r" with resolution-broadened Legendre scattering moments, thinned to 10 % tolerance.

First-order impression of the anisotropy of the angular distributions can be obtained by observing the so-called mu-bar value, which is effectively the average cosine of the elastic scattering angle. The comparison of the detailed and the resolution-broadened mu-bar are shown in Figure 1. An expanded view of the same comparison is shown in Figure 2. The number of points to represent the angular distributions after resolution broadening is reduced from about 80 000 to less than 500.

As mentioned earlier, resolution-broadening of the angular distributions can be done directly on the Legendre coefficients (label “fe56ib04s”) or on the scattering moments (label “fe56ib04t”). The comparison of the mu-bar obtained by two methods is shown in Figures 3-5. The original ENDF/B-VII.1 values are also shown in the same figures. Resolution-broadening of the scattering moments results in slightly lower and smoother values, but the differences are relatively small. The fluctuations in the ENDF/B-VII.1 library are based on measured data and show much stronger structure. Going to higher energies, it is seen from Figure 5 that the resolution-broadening of scattering moments induces structure in the shape because the relatively higher cross sections at lower energies propagate the lower mu-bar value to higher energies, which is unreasonable. The lesson learned is that the resolution-broadening of scattering moments is only valid across strongly fluctuating cross sections; it should not be used above the resonance range.

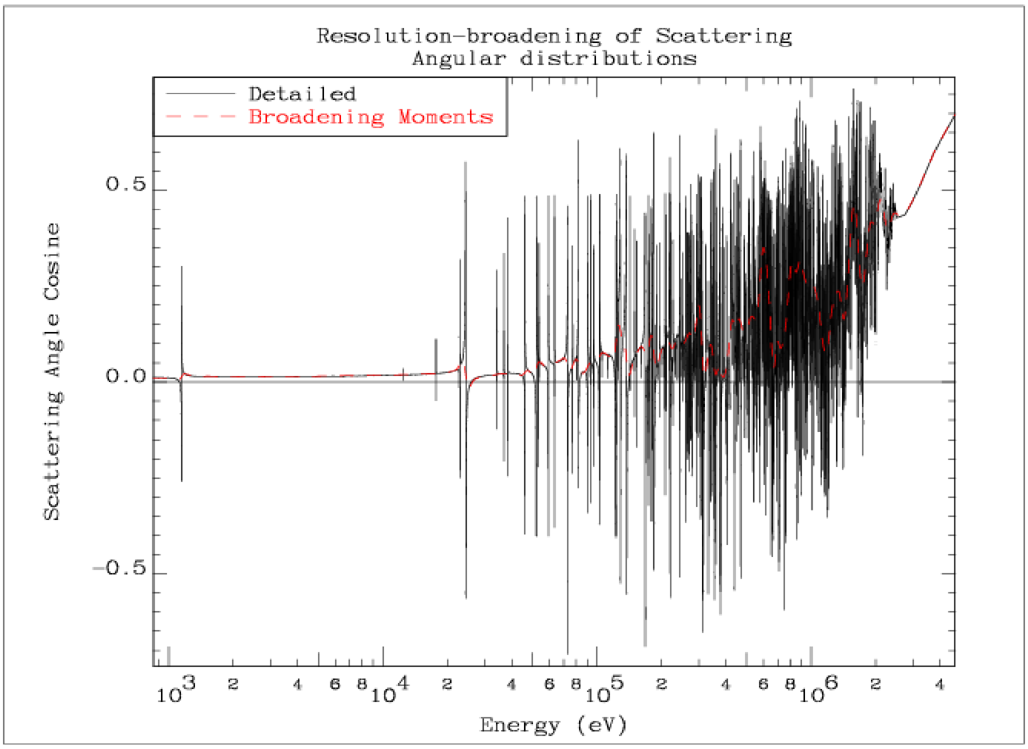

Figure 1: Comparison of the detailed mu-bar and the resolution-broadened values.

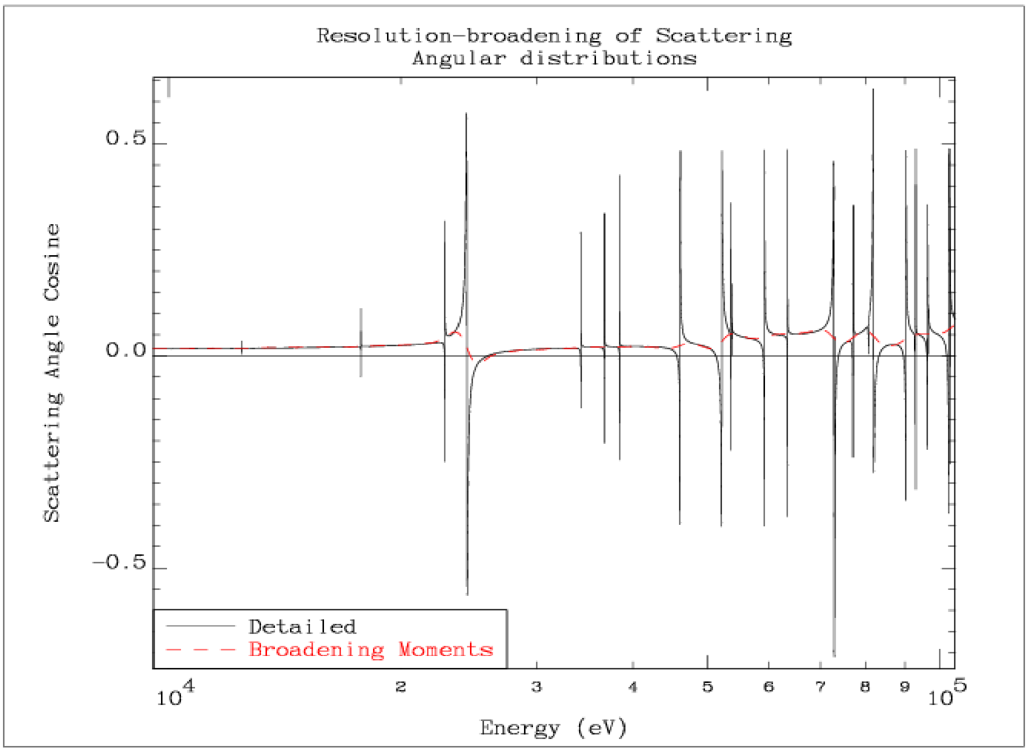

Figure 2: Expanded view of the detailed mu-bar and the resolution-broadened values.

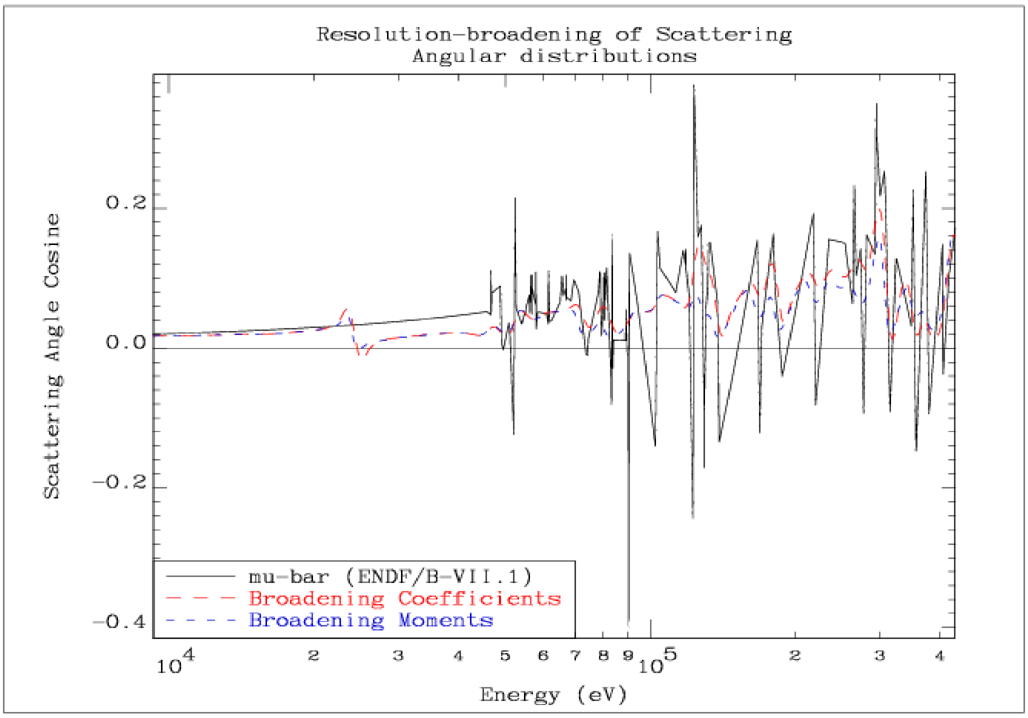

Figure 3: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – lower epithermal energy region.

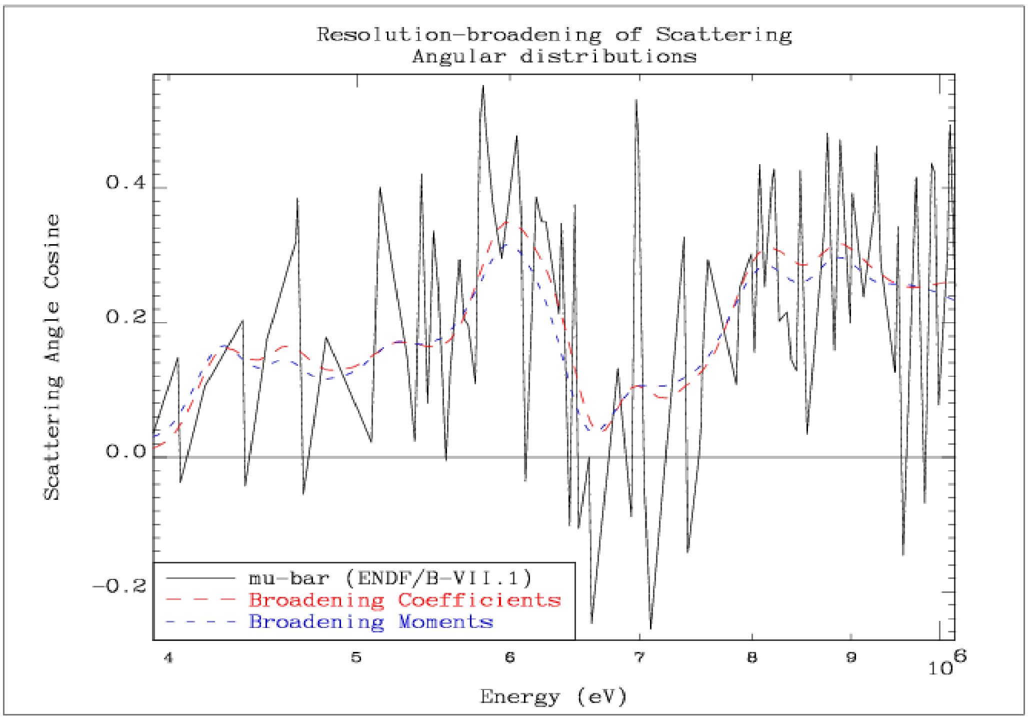

Figure 4: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – upper epithermal energy region.

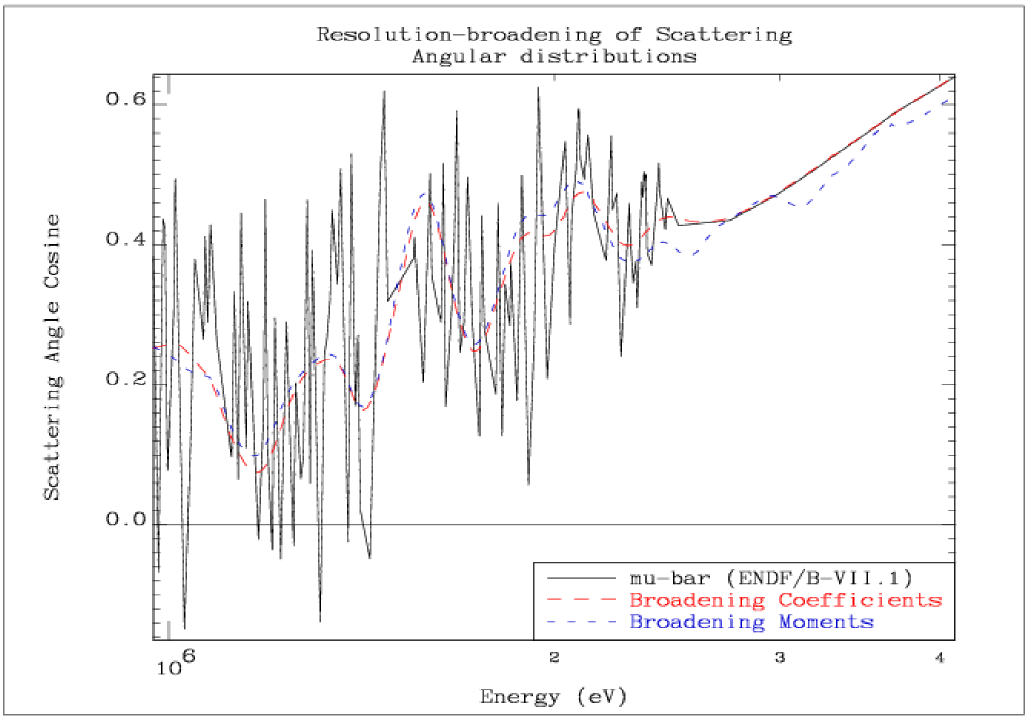

Figure 5: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – fast energy region.

Integral Benchmarks

A set of benchmarks was selected from the ICSBEP compilation that was found to be sensitive to the scattering properties of materials. The list of benchmarks with their ICSBEP name and the common name is given in Table 1. The reference nuclear data for Monte Carlo calculations with the MCNP code were from the ENDF/B-VII.1 library.

Compared to the pure ENDF/B-VII.1 results (label "e71"), the ^{56}Fe file with only resonance cross sections replaced by "ornl4" data (label "fe56v00") produces a trend of an increase in reactivity. When in addition the angular distributions are reconstructed from the resonance parameters (label "fe56v01"), the trend is reversed, meaning that the resonant angular distributions exhibit a negative trend on reactivity, which practically compensates the positive reactivity gained by the cross sections alone. The results are shown in Figure 6. Only the first 20 benchmarks are shown. The ZPR-6/10 assembly (case 21) is a notorious outlier with all evaluated data and shows a relatively small sensitivity to the changes in the resonance cross sections angular distributions of ^{56}Fe, so it was excluded from the plot. The remaining three assemblies (cases 22-24) showed very small sensitivity to the changes in the angular distribution representation and were also excluded.

When the cross sections above the resonance range are replaced by the new BNL evaluation (label "fe56ib04r") a slight bias to higher reactivities is observed in some cases, but mostly the differences are very small.

Figure 7 shows the effects of resolution-broadening of angular distributions. Resolution-broadening of scattering moments (label "fe56ib04t") seems physically reasonable, but may introduce structure in the shape of mu-bar where the nominal value is smooth (e.g. above the resonance range, see Figure 5). Thus it is important to restrict smoothing to the resonance range. Direct smoothing of Legendre coefficients is "safe" in this respect, when the coefficients vary smoothly. Figure 7 suggests that the smoothing of angular distributions in the resonance range introduces an observable effect in some benchmarks, but the effect is smaller than the uncertainties in the integral experiments and is therefore considered acceptable. Smoothing directly the Legendre coefficients as opposed to scattering moments produces changes in reactivity of opposite sign. A slight preference is given to the smoothing of scattering moments.

Table 1: List of benchmarks for testing the ^{56}Fe evaluated nuclear data

	ICSBEP name	Common name
1	PU-MET-FAST-015	BR-1-3
2	PU-MET-FAST-025	pmf025
3	PU-MET-FAST-026	pmf026
4	PU-MET-FAST-028	pmf028
5	PU-MET-FAST-032	pmf032
6	HEU-MET-FAST-013	VNIITF-CTF-SS-13
7	HEU-MET-FAST-021	VNIITF-CTF-SS-21
8	HEU-MET-FAST-024	VNIITF-CTF-SS-24
9	IEU-MET-FAST-005	VNIITF-CTF-SS-5
10	IEU-MET-FAST-006	VNIITF-CTF-SS-6
11	HEU-MET-FAST-087	VNIITF-CTF-Fe
12	HEU-MET-FAST-088	hmf088-1

13	HEU-MET-FAST-088	hmf088-2
14	LEU-COMP-THERM-042	lct042-1
15	LEU-COMP-THERM-042	lct042-2
16	LEU-COMP-THERM-043	IPEN/MB-01
17	LEU-MET-THERM-015	lmt015
18	HEU-MET-THERM-013	hmt013-2
19	HEU-MET-THERM-015	hmt015
20	HEU-MET-INTER-001	ZPR-9/34
21	PU-MET-INTER-002	ZPR-6/10
22	MIX-COMP-FAST-001	ZPR-6/7
23	MIX-COMP-FAST-005	ZPR-9/31
24	MIX-COMP-FAST-006	ZPPR-2

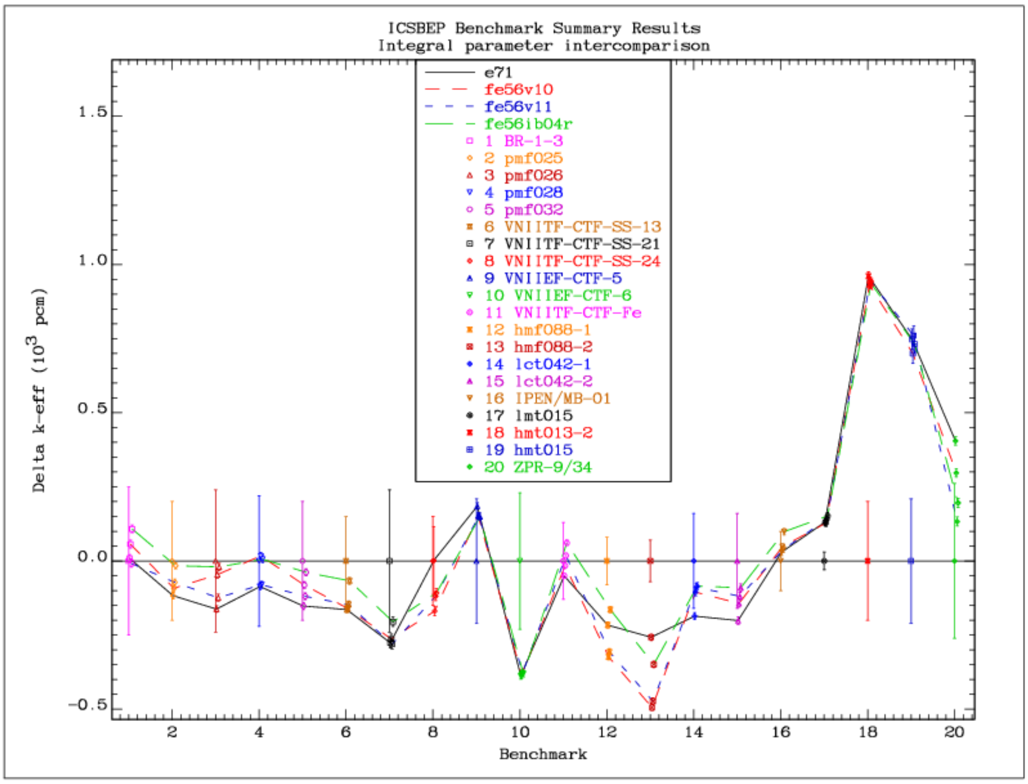

Figure 6: Differences in k_{eff} for a collection of benchmarks based on pure ENDF/B-VII.1 data and ^{56}Fe data updated with “ornl4” resonance parameters (v00=cross sections only, v01=cross sections and angular distributions).

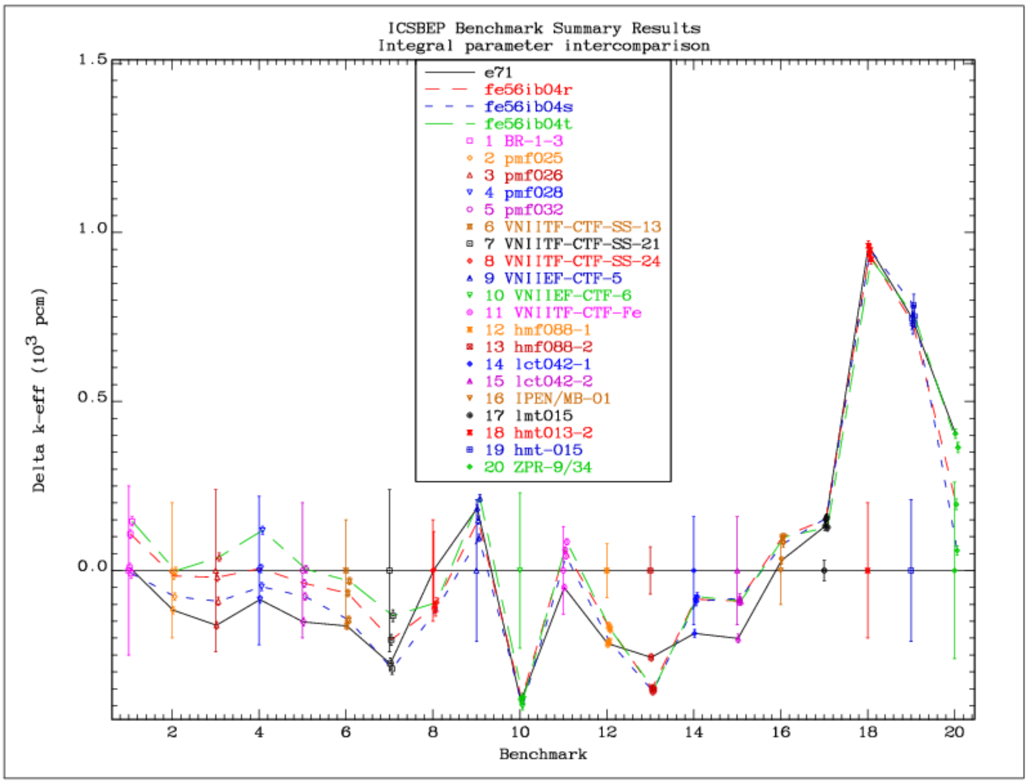

Figure 7: Differences in k_{eff} for a collection of benchmarks based on ^{56}Fe data updated with "ornl4" resonance parameters and detailed angular distributions (v01=detailed angular distributions, v02= resolution-broadened scattering moments, v02a=resolution broadened Legendre coefficients).

Conclusions

The use of detailed angular distributions reconstructed from the resonance parameters was investigated. The influence of resolution-broadening of the angular distributions was analysed. The results for the criticality of benchmark assemblies indicate that replacing the detailed angular distributions with resolution-broadened values has a minimal effect on the results. This greatly reduces the size of the data sets in application libraries, since the number of data points for angular distributions can be reduced from about 80 000 to about 500. It is recommended to include smoothed angular distributions (consistent with the resonance parameters) in the ENDF files; if needed, detailed angular distributions can be reconstructed from the resonance parameters by the processing codes).

Deep penetration problems are not expected to be sensitive to the angular distributions in the resonance range, but the new cross sections in the fast energy range could have an effect. Further analysis is pending.

Resolution-broadening of the scattering moments (as opposed to broadening of the Legendre coefficients directly) seems to be the right approach, but it should be applied only in the resonance range where the angular distributions are reconstructed from the resonance parameters.

The resolution-broadening tool (MU_RSL code) for angular distributions has been developed. It will be used to compare angular distributions reconstructed from the resonance parameters to the measured values, which are usually given with a significantly lower resolution, what makes the comparison difficult. This work is in progress.

Overall, the impact of the new evaluation on the criticality benchmarks is relatively small, which is good news since the ^{56}Fe evaluation was considered to be quite good to start with. The main value of the new evaluation is completeness and internal consistency because it is primarily based on model calculations. This advantage should be reflected in derived quantities such as kerma, heating, etc.

Assembly of the covariance information is the next step to be taken in the evaluation process.