On the Impact of Fe Scattering on Integral Benchmarks

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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 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, 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.

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?
- Is it possible to obtained reasonable results with smoothed angular distributions?

Processing of Angular Distributions

The standard release of NJOY99 cannot process the resonance parameters in RML format. NJOY2012 can do so, but the angular distributions can at present only be reconstructed with an additional patch available from the author. This extended version of NJOY was used for the calculations.

The starting point was the ^{56}Fe evaluation from the ENDF/B-VII.1 library. The file received from ORNL (labelled "ornl4") was complete in this respect.

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 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 distribution (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 with 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 be resolution-broadened in the same way.

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

e71	Reference ENDF/B-VII.1 file,
fe56v00	"e71" template, “ornl4” resonance parameters,
fe56v01	"fe56v00" with “ornl4” resonance parameters and angular distributions,
fe56v02	"fe56v01" same as fe56v01, but with thinned angular distributions.

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 or on the scattering moments. 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.

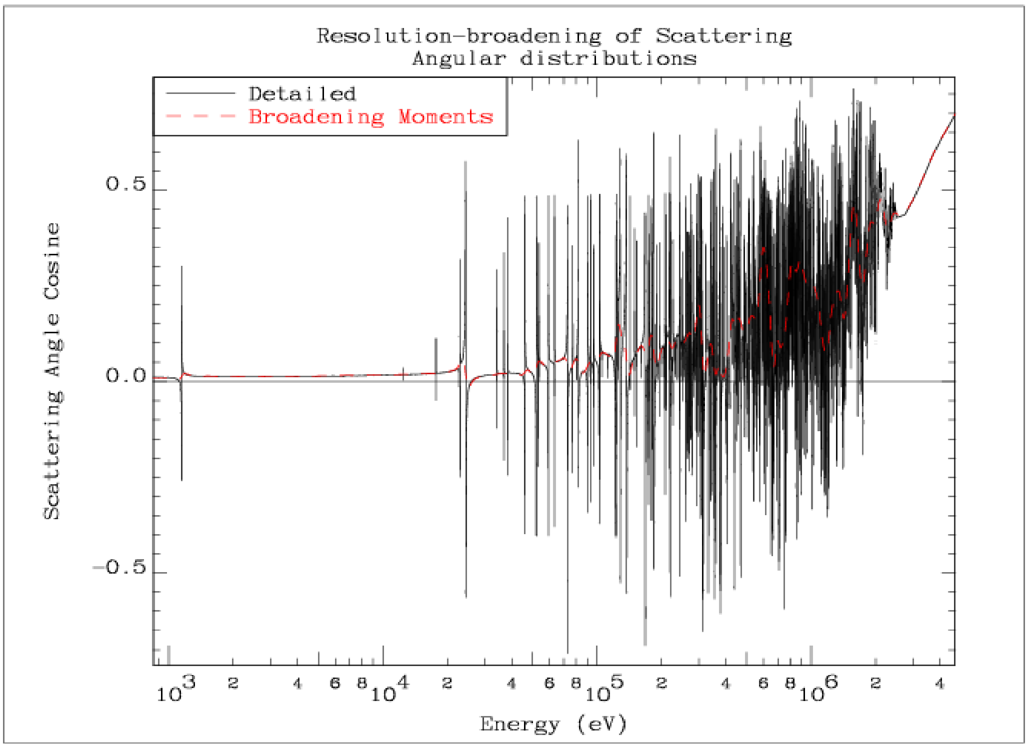

Figure 1: Comparison of the detailed mu-bar and the resolution-broadened values.

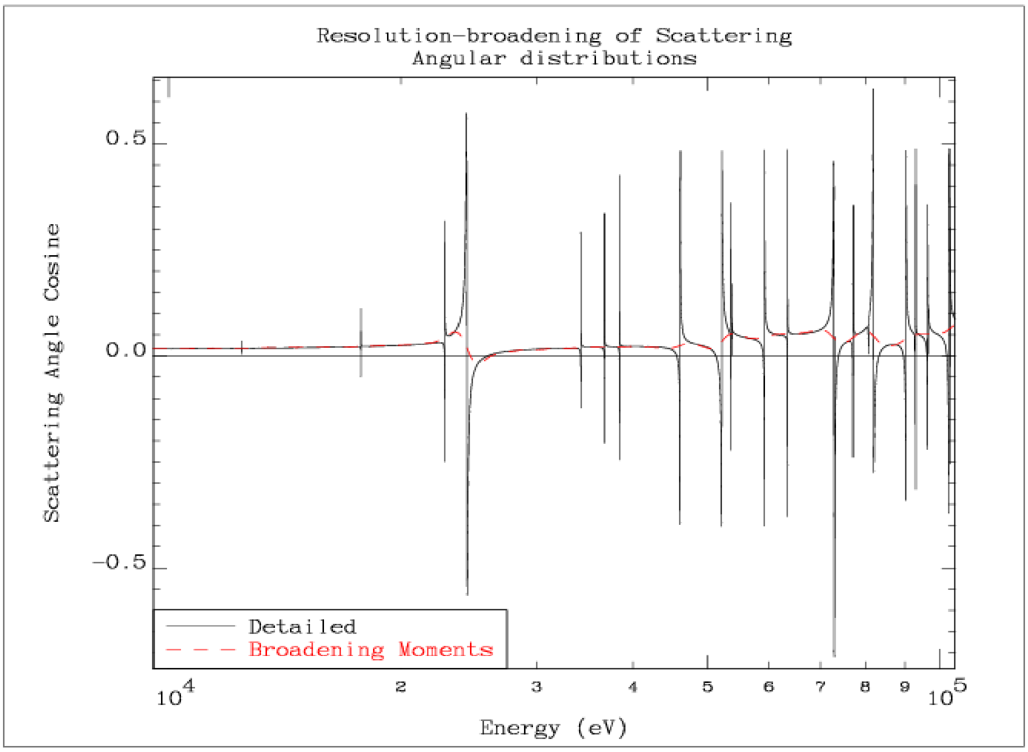

Figure 2: Expanded view of the detailed mu-bar and the resolution-broadened values.

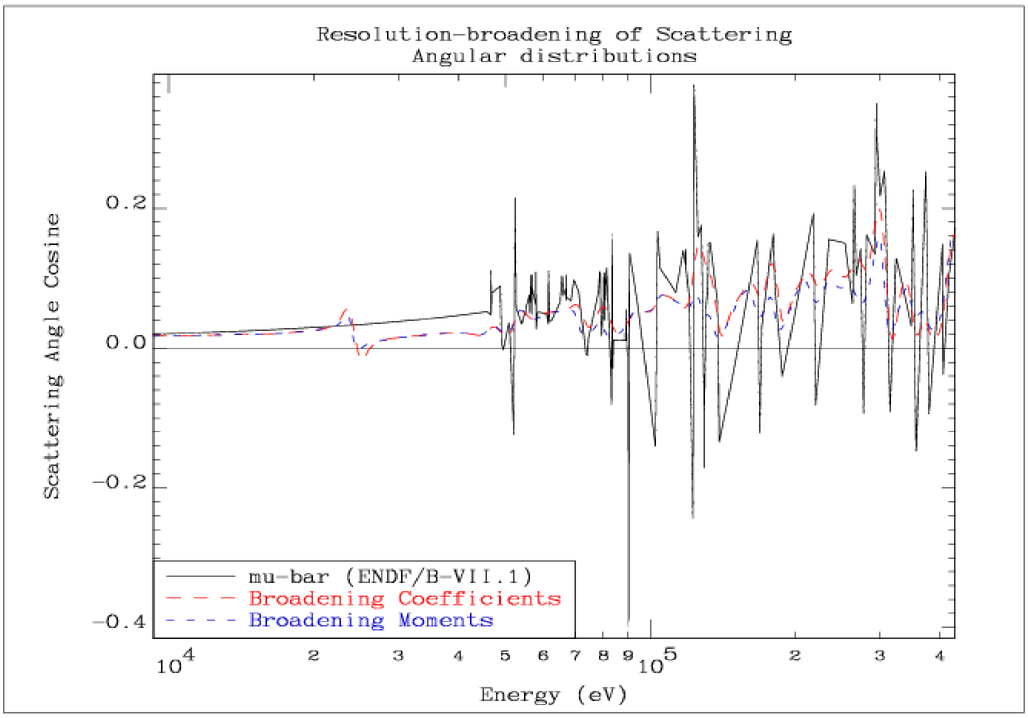

Figure 3: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – lower epithermal energy region.

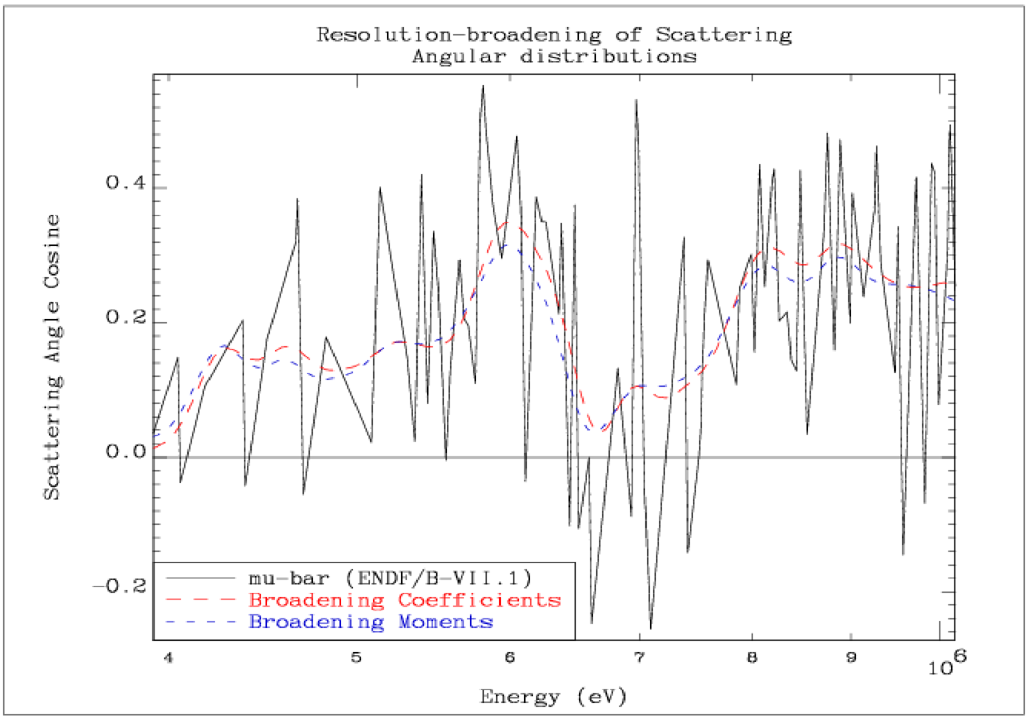

Figure 4: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – upper epithermal energy region.

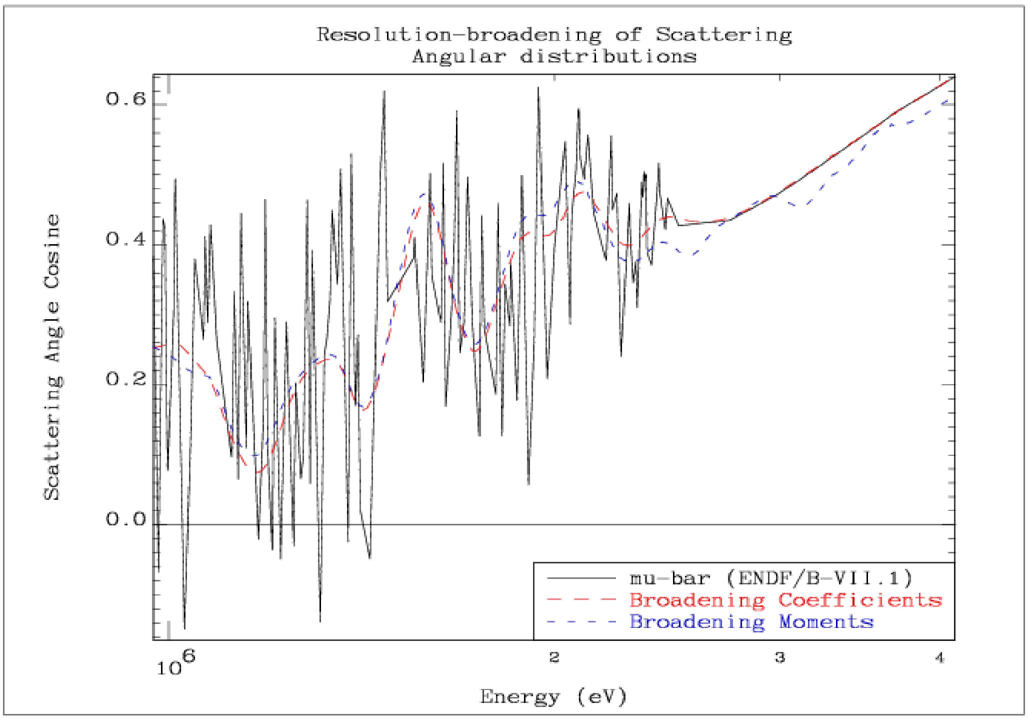

Figure 5: Comparison of mu-bar from ENDF/B-VII.1 and values obtained by resolution-broadening of Legendre coefficients and scattering moments, respectively – fast energy region.

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. Some of the calculations were done with the code version MCNP5-1.6. It was verified that the results with MCNP-6.1 were statistically the same.

Compared to the pure ENDF/B-VII.1 results, the ^{56}Fe file with only resonance cross sections replaced by “ornl4” data produces a trend of an increase in reactivity (label “fe56v00”). When in addition the angular distributions are reconstructed from the resonance parameters, the trend is reversed, meaning that the resonant angular distributions exhibit a negative trend on reactivity, which is stronger than the positive trend due to the cross sections. The results are shown in Figure 6. Only the first 20 benchmarks are shown. The ZPR-6/10 assembly is a notorious outlier and shows a relatively small sensitivity to the changes in the angular distributions. The remaining three assemblies showed very small sensitivity to the changes in the angular distribution representation.

Figure 7 shows the effects of resolution-broadening of angular distributions. Resolution-broadening of scattering moments seems physically reasonable, but introduces structure in the shape of mu-bar where the nominal value is smooth (see Figure 5). This is the main reason for the apparent discrepancy in the results (see label v02a) for the Pu-fuelled fast assemblies with a very hard neutron spectrum. Direct smoothing of Legendre coefficients is “safe” when the coefficients vary smoothly.

Figure 7 suggests that the effect of smoothing angular distributions in the resonance range has a minimal effect on criticality.

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

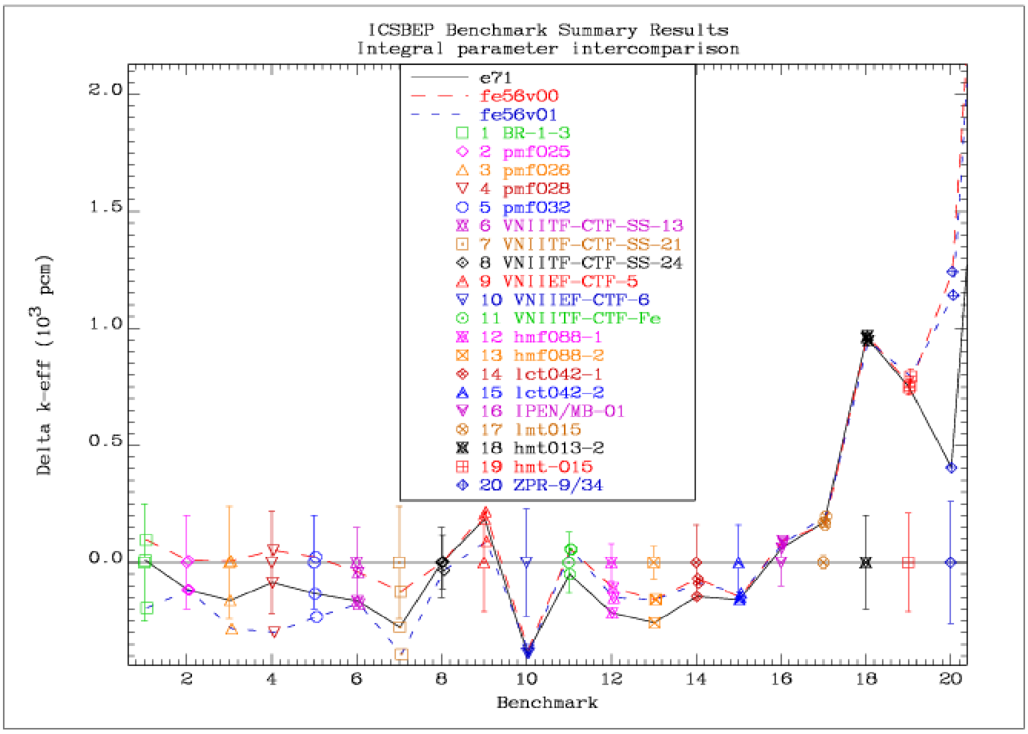

Figure 6: Differences in k_{eff} for a collection of benchmarks based on pure ENDF/B-VII.1 data and ^{56}Fe data updated with "ornl4" resonance parameters (v00=cross sections only, v01=cross sections and angular distributions).

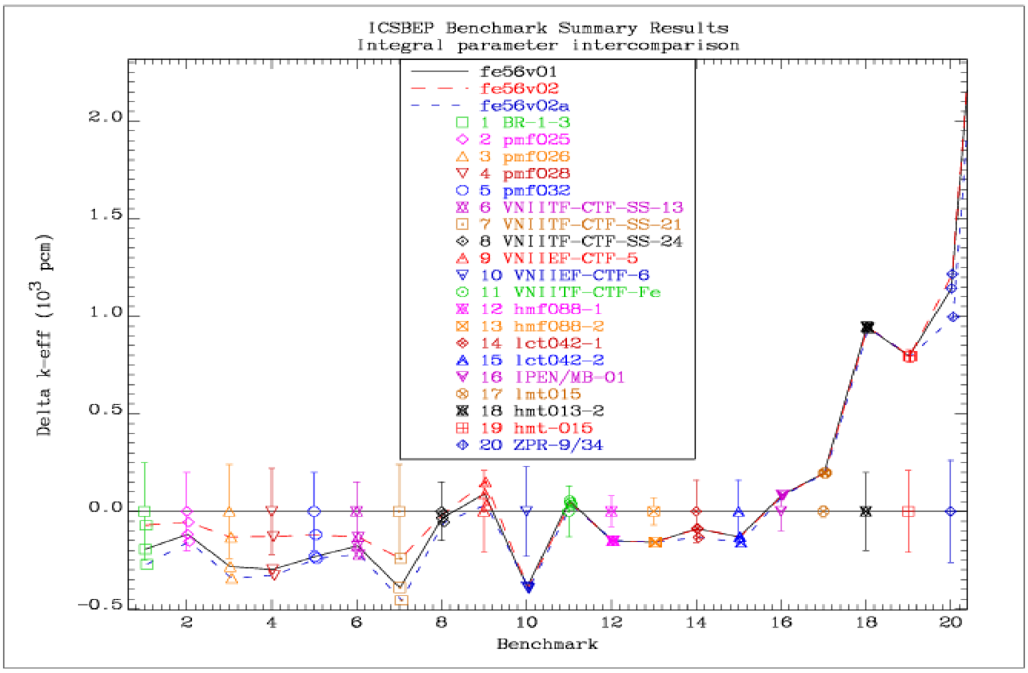

Figure 7: Differences in k_{eff} for a collection of benchmarks based on ^{56}Fe data updated with "ornl4" resonance parameters and detailed angular distributions (v01=detailed angular distributions, v02= resolution-broadened scattering moments, v02a=resolution broadened Legendre coefficients).

Conclusions

The use of detailed angular distributions reconstructed from the resonance parameters was demonstrated. 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 needs to be verified if the same conclusions are valid for deep penetration problems.

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 tools for angular distributions will be useful to compare angular distributions reconstructed from the resonance parameters to measured values, which are usually given with a significantly lower resolution, what makes the comparison difficult. This work will be performed when an updated set of resonance parameters of ^{56}Fe is released from the ORNL.