Chronology of moving from “ib15s” to “e80b2” in Fe-56 (Rev.2)

A. Trkov

International Atomic Energy Agency, Vienna, Austria

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Changes in the document revisions

Rev.1 Added Summary table of file perturbation studies.

Rev.2 Added the net impact of the background in the resonance region.

Introduction

Last-minute changes were made to the ^{56}Fe evaluated data file before the release of “beta2” candidates for the ENDF/B-VIII library. Such changes are potentially dangerous. The results presented by M. Herman at the ND2016 Conference leave several loose ends regarding the impact of ^{56}Fe on integral benchmarks, especially since several changes were made at the same time. Some results for incremental changes were presented, but they seem inconclusive, so a more detailed analysis was performed. In the following, “e80b2” refers to the full ENDF/B-VIII.b2 library and CIELO20160818 refers to the IAEA-CIELO collection of evaluations as of 18 August 2016, with ENDF/B-VII.1 data for the remaining nuclides.

Below is a summary table of the perturbations to the evaluated data file that were investigated in the present report.

Fe56ib17s	Empire calculation ib17, resonance parameters IRSN.v2 up to 850 keV, adjusted capture background, angular distributions reconstructed from resonance parameters and resolution-broadened, increased P2 and P4 Legendre coefficients of elastic scattering in the range 0.5-1.5 MeV (adopted for e80b2)
fe56ib17c	Detailed angular distributions reconstructed from resonance parameters in the resonance range (<850 keV) by NJOY (in the ACE file only, no adjustment of the P2 and P4 coefficients)
fe56ib17d	Same as fe56ib17c but with resolution-broadened angular distributions in the resonance range.
Fe56ib17f	Same as fe56ib17f but including the correction to the P2 and P4 Legendre coefficients; this file should be equivalent to fe56ib17s.
fe56ib17h	Same as fe56ib17f, but first discrete level angular distributions reconstructed from the resonance parameters up to 1.41 MeV and resolution-broadened.
Fe56ib17i	Same as fe56ib17f, but with P1 Legendre coefficient of elastic scattering shifted up by 0.08 in the range 500-850 keV.
Fe56ib17j	Same as fe56ib17i, but with P1 Legendre coefficient of elastic scattering shifted down by -0.1, starting at 850 keV and decreasing linearly to zero at 2.5 MeV.
Fe56ib17m	Same as fe56ib17f, but without background in the resonance region.

Comparison of CIELO20160818 v.s. e80b2

The first observation is that the e80b2 results differ significantly from CIELO20160818 benchmark results, as shown in Figure 1. This could be due to several reasons:

- Data for the updated structural materials, which are not included in CIELO20160818.
- Difference in the fast cross sections, which originate from "ib17" Empire calculation in e80b2 and "ib15" in CIELO20160818.
- Resonance parameters, which were replaced by IRSN.v2 in e80b2 instead of JENDL-4.0.
- Angular distributions, which were reconstructed from the IRSN.v2 resonance parameters with resolution broadening in e80b2.
- Resolution-broadening procedure.

In Figure 1 the net effect of changing ^{56}Fe data only from CIELO20160818 to e80b2 is also shown. From the plot one can conclude that most of the differences come from ^{56}Fe, but the effect of the minor nuclides is important in some cases, particularly the ZPR-9/34 and the Pu-reflected benchmarks.

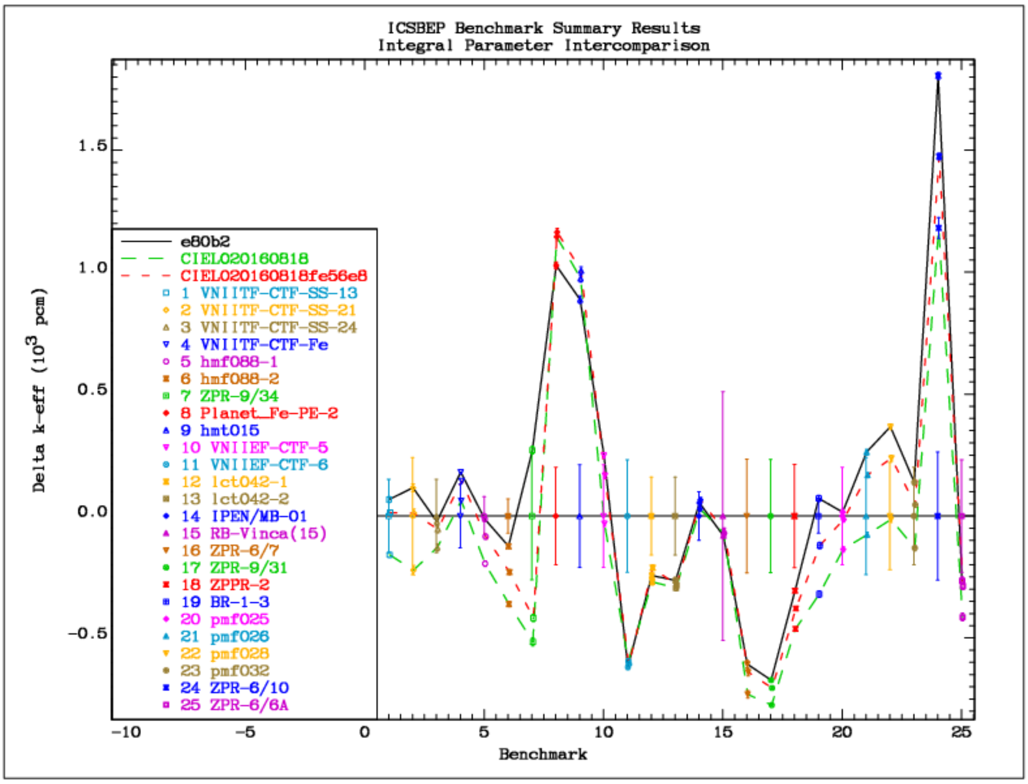

Figure 1: Benchmark results comparison of e80b2, CIELO20160818, and the latter with ^{56}Fe data from e80b2.

Impact of the resonance parameters

The IRSN.v2 resonance parameters look very similar to the ones in the JENDL-4.0 library, which was the previous choice for the CIELO evaluation. The main difference were the adjustments at the upper end of the resolved resonance range, where no background correction was specified; on average the reconstructed cross sections were higher than JENDL-4.0 without the background correction, but lower than CIELO20160818. Background was introduced in File 3 to restore the capture cross section, which was considered good in CIELO20160818: the background near 20 keV remained the same since the capture cross section reconstructed from the new resonance parameters practically did not change. Comparison plots of the capture cross sections in this energy range is shown in Figure 1a.The low-resolution measurements by Allen support the low cross section values of ENDF/B-VII.1 (label “e71”), but integral measurements favour higher values of Ernst. The background correction at the upper end of the resonance range had to be decreased compared to the CIELO20160818 value. Again, the low-resolution measurements by Allen support the high cross section values of ENDF/B-VII.1 (label “e71”), but (unpublished) measurements at RPI favour lower values. Comparison plots of the resolution-broadened capture cross sections in this energy range is shown in Figure 1b. The width of the Gaussian resolution function was 3 % of the central value of the Gaussian.

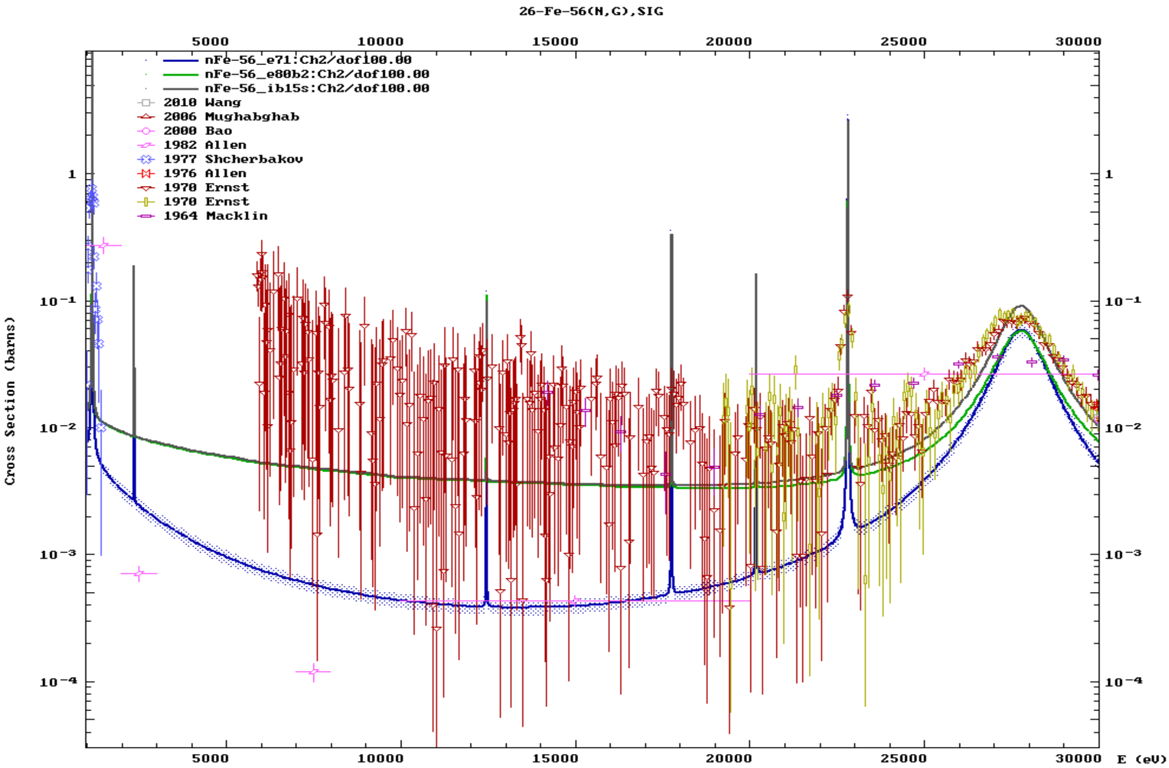

Figure 1a: Comparison of the capture cross sections near 20 keV.

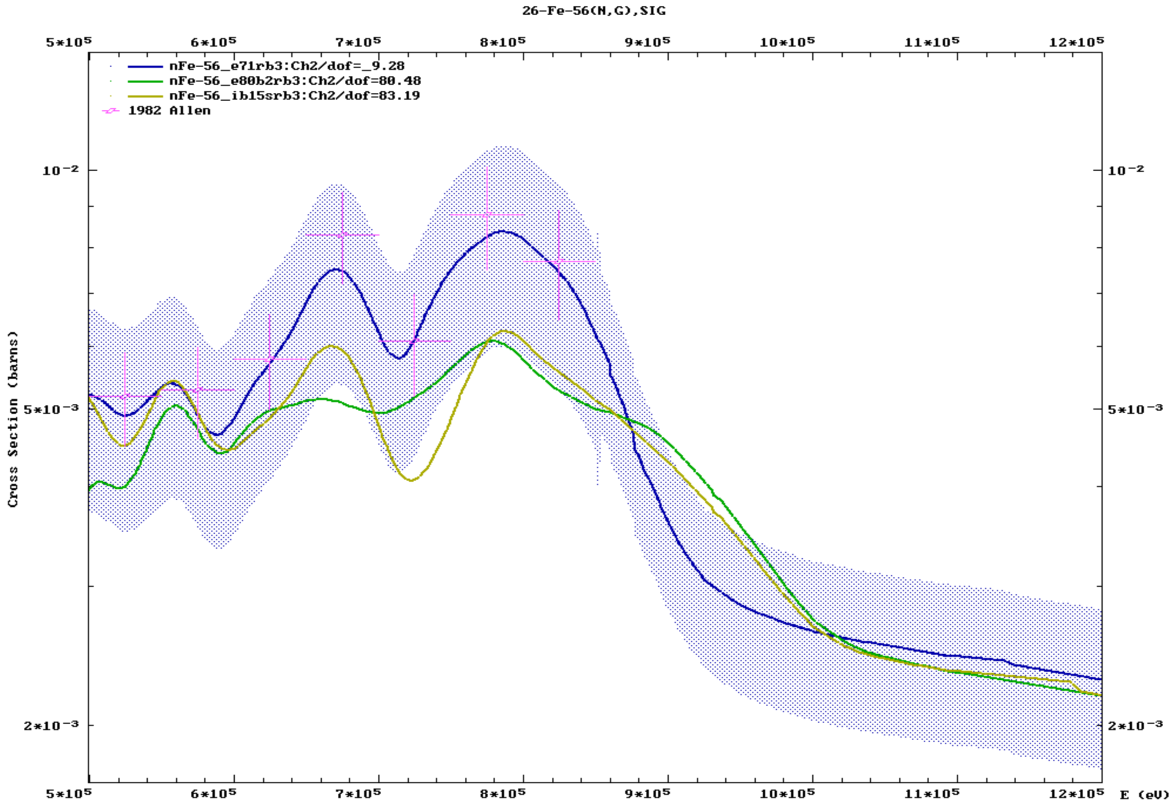

Figure 1b: Comparison of the capture cross sections near 800 keV.

Impact of the resolution-broadening of angular distributions

To study the effects of the changes in the resonance parameters file fe56ib17c was assembled, replacing the JENDL-4.0 resonance parameters with IRSN.v2 up to 850 keV. An ACE file was prepared including the patch by R.E. MacFarlane to reconstruct detailed angular distributions from the resonance parameters and include them in the ACE file. Suffix “fe56c” is appended to the CIELO name. Note that the original file “fe56ib15s” in CIELO20160818 contains scaled P2 and P4 Legendre coefficients to improve the performance in benchmarks with iron and steel reflectors.

Secondly, the scattering moments of elastic angular distributions were resolution-broadened with a Gaussian resolution function of constant width of 1 keV. The file label is fe56ib17d. Suffix “fe56d” is appended to the CIELO name. Figure 2 shows that resolution-broadening of the angular distributions has a negligible effect on integral benchmark performance. The combined effect of new resonance parameters and angular distributions has practically the same effect as the scaling of the P2 and P4 Legendre coefficients in CIELO20160818.

The question is, how much of the difference between e80b2 and CIELO20160818 comes from ^{56}Fe and how much from the secondary nuclides, particularly the minor isotopes of Fe, which were also changed in e80b2. The answer is evident from Figure 3, in which the Legendre coefficients in fe56ib17d were scaled in the same way as in e80b2 to produce fe56ib17f, which is completely equivalent to content of e80b2. Evidently, much of the differences are due to these changes in the Legendre coefficients, the remainder coming from the other nuclides in e80b2.

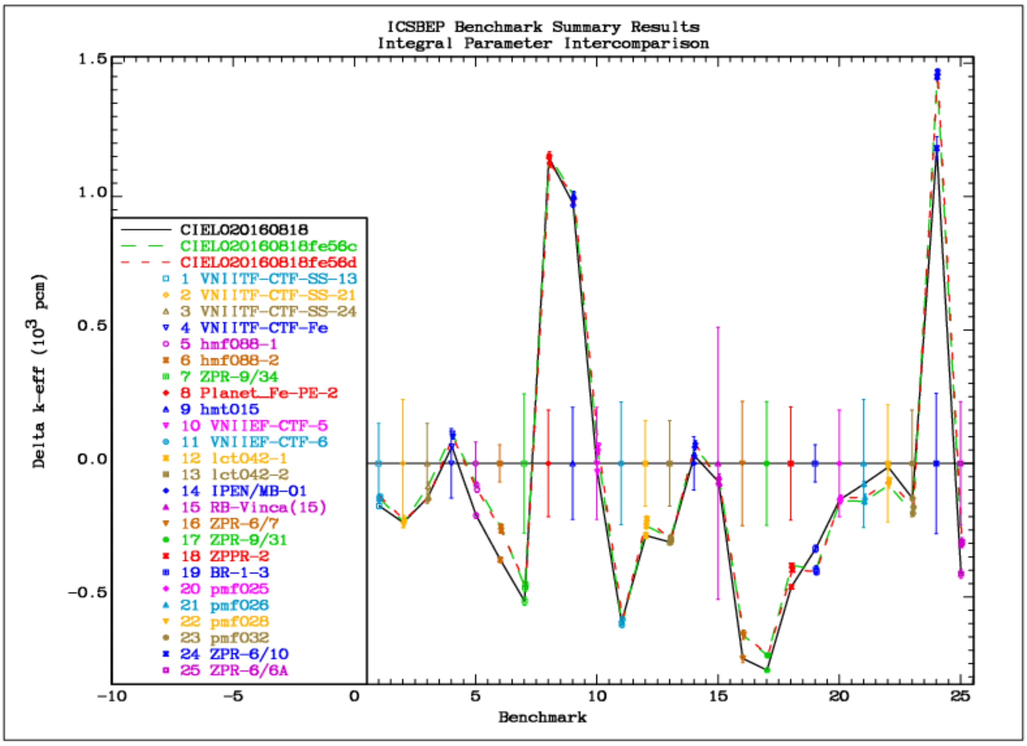

Figure 2: Benchmark results comparison showing the impact of the new resonance data.

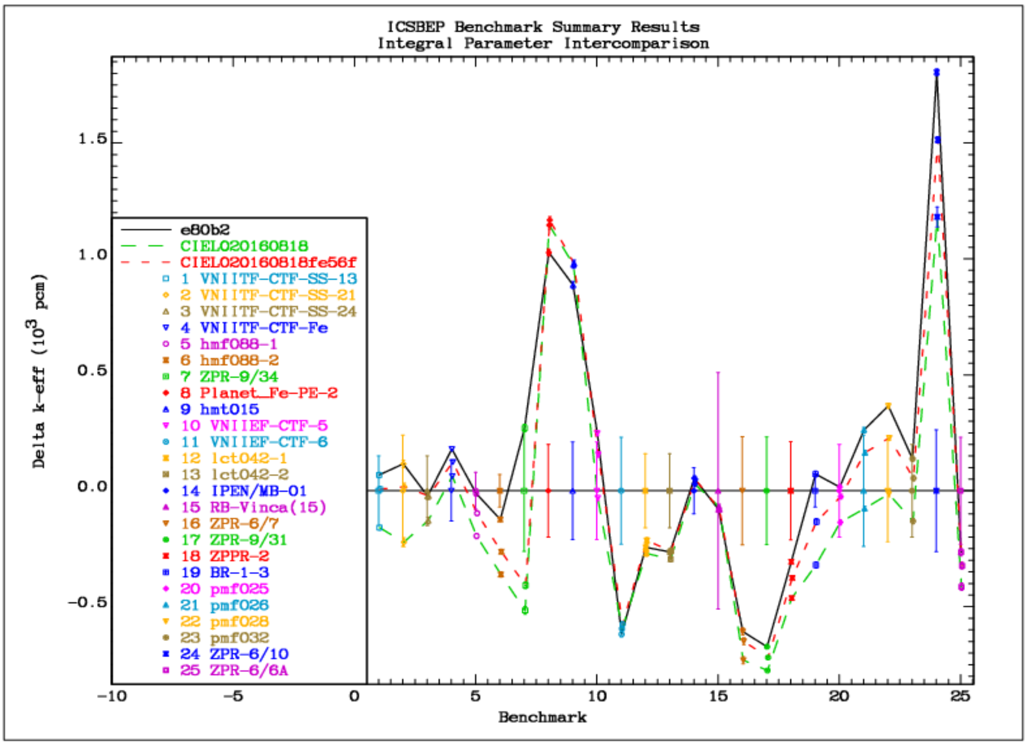

Figure 3: Benchmark results comparison, showing the impact of scaling the P2 and P4 Legendre coefficients of elastic angular distributions.

The impact of angular distributions

In the ND2016 presentation M. Herman reported that the elastic and the inelastic angular distributions could have a big effect on the ZPR-6/7 and ZPR-9/31 benchmarks, the reactivity of which is significantly under-predicted with e80b2.

High-resolution measurements of angular distributions by Perrey (EXFOR#13511504) and by Kinney (EXFOR#10571502) are available in the EXFOR database. The derived average cosines of scattering *mu-bar* in the laboratory system are shown in Figure 4. The label f32rb03 denotes JEFF-3.2 data, which have a low-resolution shape in the resonance region below 850 keV, but follow closely the Kinney data above. The fe56ib15s evaluation has a similarly low resolution in the resonance range, but slightly lower values; above 850 keV it coincides with JEFF-3.2. The file fe56ib17g was assembled in which all elastic scattering angular distributions up to 1.41 MeV were reconstructed from the resonance parameters and resolution-broadened with a resolution function of fixed width 1 keV. The plot of the average cosines shows that above 850 keV the resulting shape disagrees significantly from the measured values and is considered unacceptable for any further consideration.

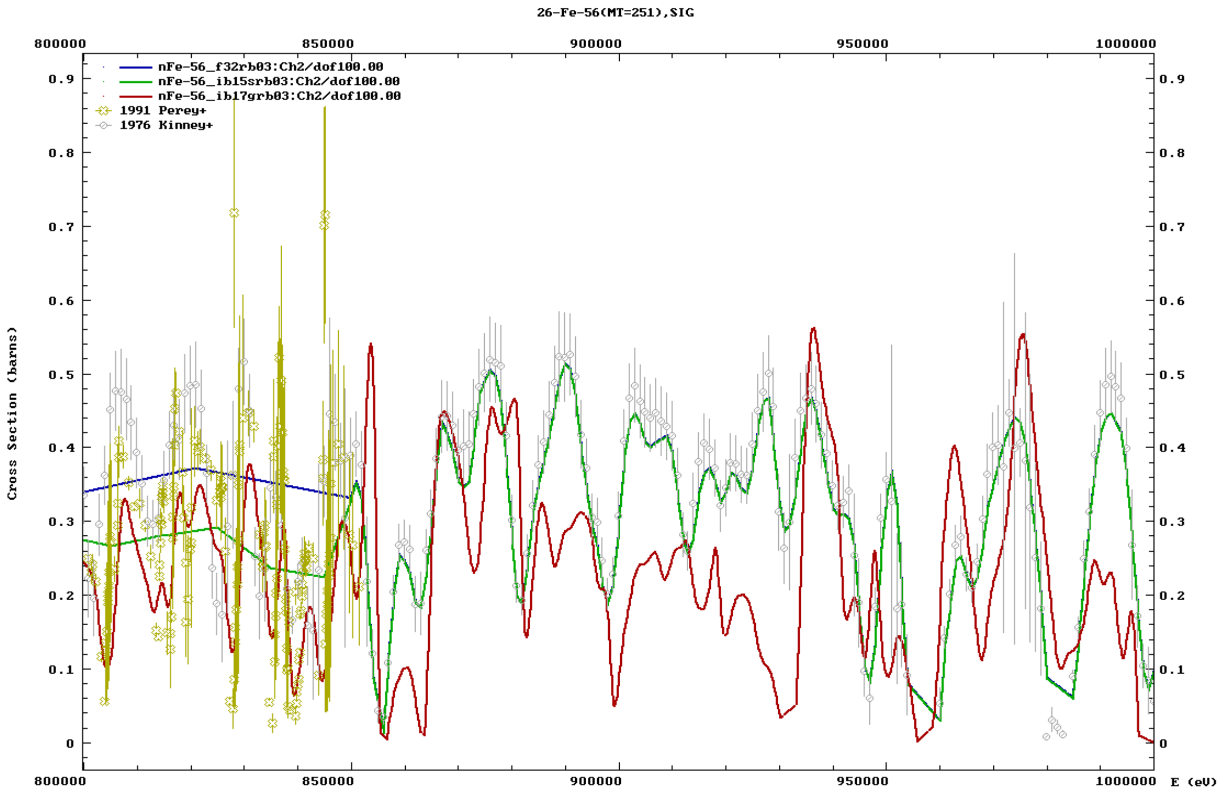

Figure 4: Comparison of the average cosine of scattering in the laboratory system from different evaluated data files with measured values.

Another file fe56ib17h was assembled in which the angular distributions of the first discrete-level inelastic cross section in the range 0.85 – 1.41 MeV were replaced by resolution-broadened angular distributions reconstructed from the resonance parameters. The results are shown in Figure 5. The hypothesis of M. Herman that using reconstructed angular distributions improves benchmark performance cannot be confirmed. There is a small effect on the Pu-reflected benchmarks, but it is too small to be significant.

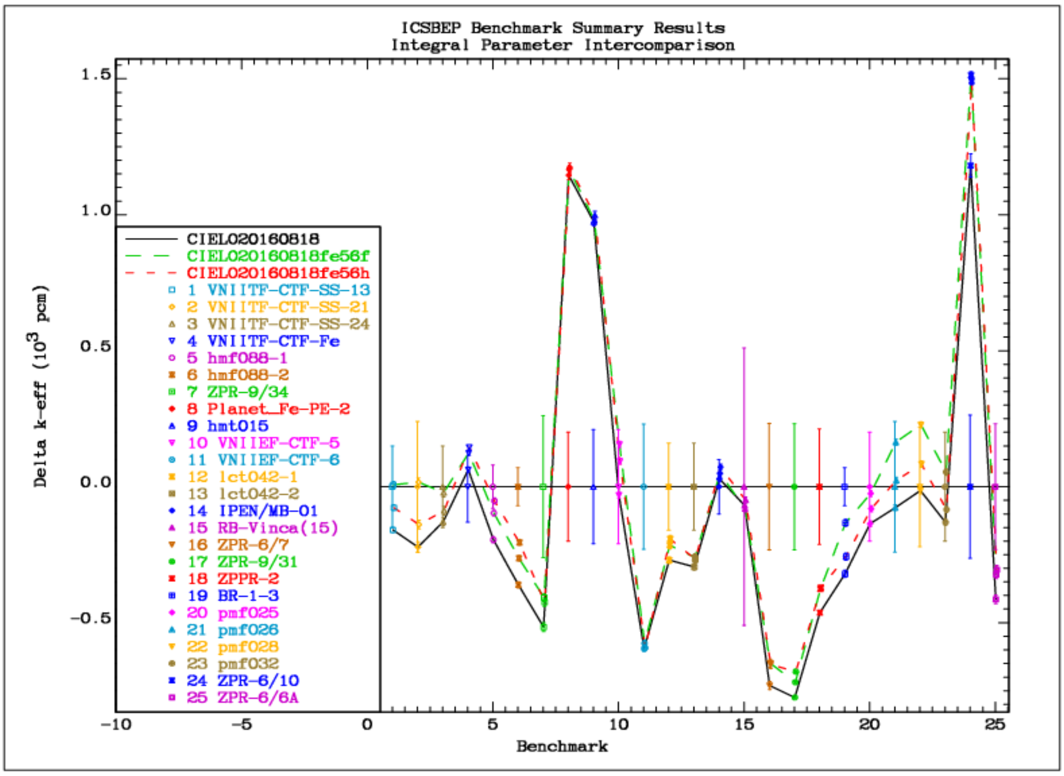

Figure 5: Benchmark results comparison, showing the impact of inelastic angular distributions above 850 keV.

Empirical adjustment of the anisotropy

From Figure 4 we note that Kinney data tend to be higher than the Perrey data and that the average cosine of scattering reconstructed from the resonance parameters is lower than either of them. To study the impact of possible systematic errors in the angular distributions, empirical increments to the P1 Legendre coefficient were made as follows, with linear interpolation in between:

Energy [MeV]	Increment
0.45	0
0.5	0.08
0.8505	0.08
0.851	-0.1
2.5	0

The impact of these changes below 0.8505 MeV was incorporated into the file fe56ib17i and over the entire range into fe56ib17j. The effect of these changes on benchmarks is shown in Figure 6. Increasing the P1 Legendre coefficients below 850 keV significantly reduces the reactivity of many fast assemblies. Decreasing the P1 Legendre coefficients above 850 keV increases reactivity, but the effect is much smaller. The benchmark assemblies, which are discrepant, are hardly affected.

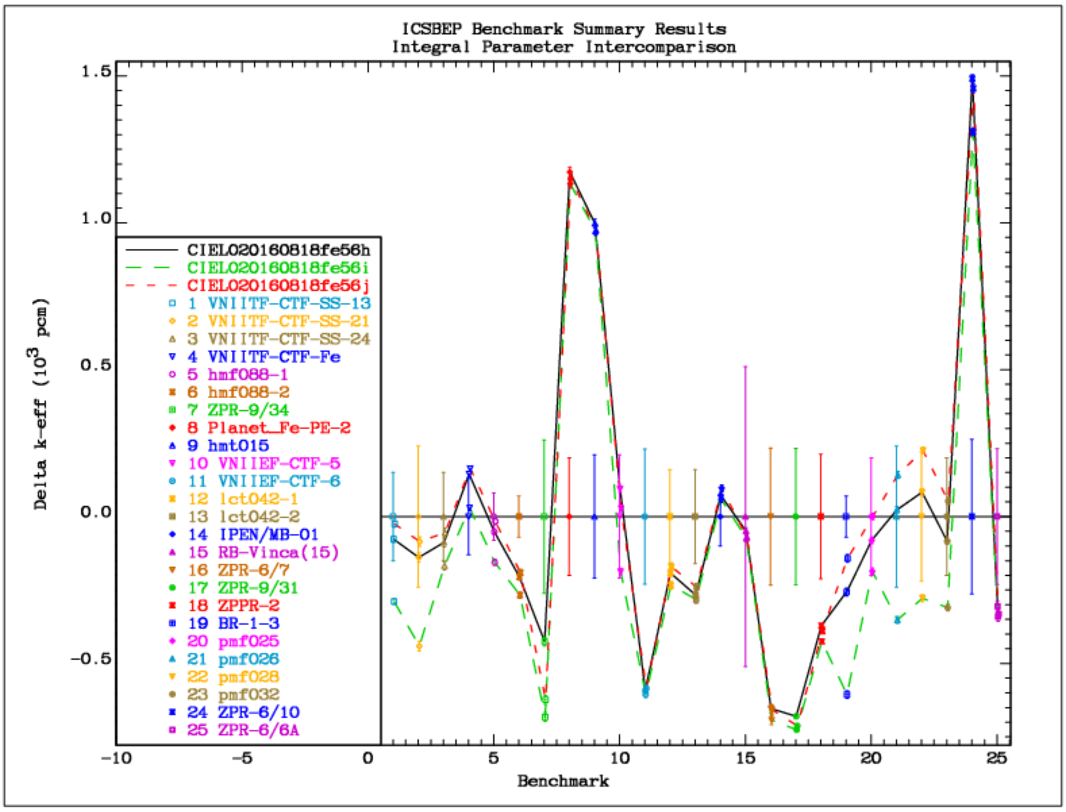

Figure 6: Impact of the empirical adjustment to the anisotropy (P1 Legendre coefficient) in the energy range 0.45 – 2.5 MeV.

Net impact of the background in the resonance region

In his ND2016 presentation M. Herman argued that the use of the IRSN.v2 resonance data greatly improve the agreement with benchmark results. So far, the perturbation studies above included the background correction in the resonance region because it was supported by the measurements at RPI. To check the direct impact of the background the file fe56ib56m was constructed, which differs from fe56ib56f only in the removal of the background. The results in Figure 7 indicate that the background contribution near the upper end of the resonance region is the main component that contributes to the increase of reactivity in the ZPR-6/7, ZPR-9/31 and ZPPR-2 assemblies, and the background near 20 keV is the key contribution that reduces the reactivities of the ZPR-9/34 and ZPR-9/10 assemblies.

Conclusions

Various aspects of the ^{56}Fe evaluation moving from CIELO20160818 to e80b2 were analysed.

- The cross sections reconstructed from the IRSN.v2 resonance parameters below 850 keV remain practically the same when the adjusted background is included.
- Angular distributions reconstructed from the resonance parameters below 850 keV increase reactivity in a similar way as the adjustments to the P2 and P4 Legendre coefficients in CIELO20160818. This adjustment could be reduced in e80b2, if needed.

- Resolution-broadening of the angular distributions has negligible impact on the benchmark performance. It is recommended to keep the resolution-broadened angular distributions in the evaluated data file; the user still has the option to reconstruct them from the resonance parameters, if needed.
- The average cosines of elastic scattering above 850 keV reconstructed from the resonance parameters differ significantly from the measured values, indicating that angular distributions are poor and should not be used in evaluated data files.
- Angular distributions of the first discrete inelastic scattering cross sections have a small impact on benchmark performance.
- Considering that the resonance parameters do not capture all the trends of experimentally measured observables above 850 keV, it is recommended to limit the range in which resonance parameters are used to 850 keV.
- The background contribution near 20 keV is needed to fix the overprediction of reactivity of the ZPR-9/35 and ZPR-6/10 assemblies. Better agreement in the predicted reactivities in the ZPR-6/7, ZPR-9/31 and ZPPR-2 assemblies, reported by M. Herman at the ND2016 Conference is mainly due to the background near 850 keV, and partly due to the differences in the capture and inelastic cross sections and angular distributions between 850 keV and 1.41 MeV. However, these cross sections and angular distributions cannot be supported by the differential measurements.

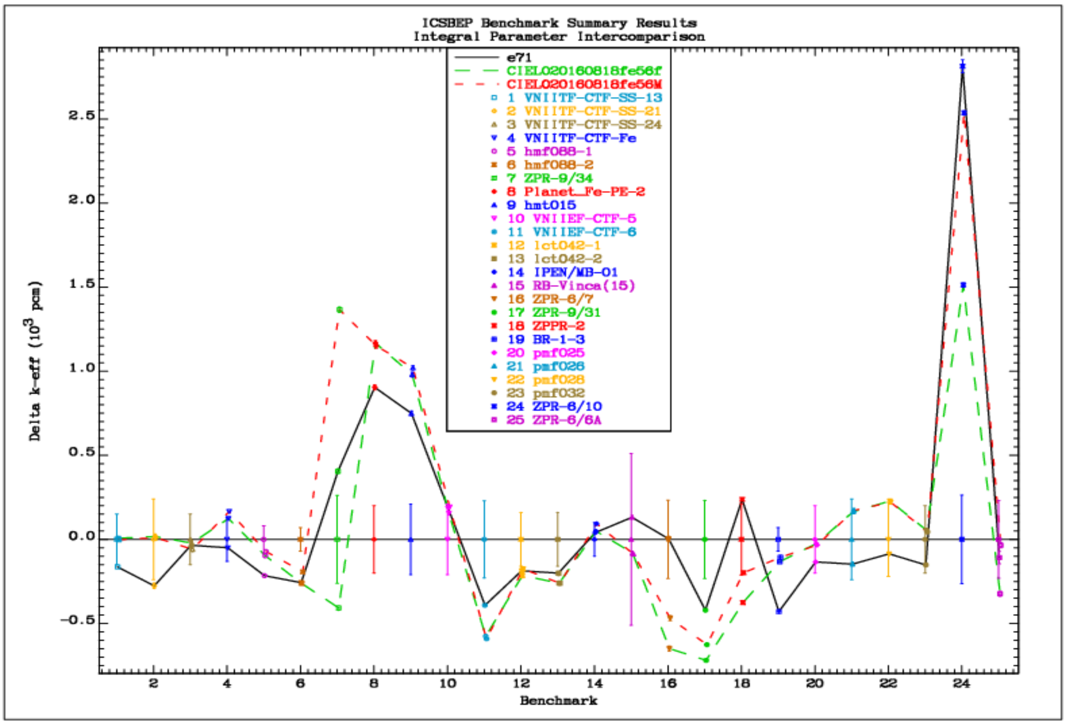

Figure 7: Impact of the background in the resolved resonance region.