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An Analysis of the HEU-MET-FAST-035 Problem Using CENTRM and SCALE

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Abstract

An U/Fe benchmark, designated as HEU-MET-FAST-035, has been approved for inclusion in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. The SCALE code and cross sections performed poorly in calculating this critical experiment. Deficiencies in both the ENDF/B-V representation of the resonance region for Fe and in the Nordheim integral treatment when applied to Fe were identified. The combination of these deficiencies led to an almost 10% over-prediction of k_{eff}.

Problems involving a large percentage of Fe and intermediate-energy spectrums present special cross-section processing difficulties for SCALE. In ENDF/B-V, resonance data for Fe only go to 400 keV, although resonances are present well above 1 MeV. Significant resonance data are stored as file 3 data instead of as resonance parameters. The Nordheim Integral Treatment used in NITAWL to process cross sections assume: resonances are widely spaced and all relevant information is contained in the resonance parameters (file 3 data is not processed). These limitations and assumptions result in poor solutions for this class of problems.

Initial Calculations of Fe Problem

Several limitations in the SCALE processing methodology used to process Fe cross sections were discovered while examining the HEU-MET-Fast-035 benchmark problem [1]. The benchmark is a simplified representation of an experiment performed at the Argonne National Laboratory (ANL) ZPR-9 facility in 1979, designated as ZPR-9/34, loading 303. The problem consists of U/Fe assemblies in a cylindrical arrangement with a depleted U/Fe reflector. Table 1 compares the evaluated benchmark results with the results using three independent codes and ENDF/B-V cross-section data.

Table 1. HEU-MET-FAST-035 Benchmark Calculation Results

Code	k_{eff} ($\pm\ \sigma$)
Evaluated Benchmark	0.9966 ± 0.0020
MCNP	0.9919 ± 0.0003
VIM	0.9883 ± 0.0004
SCALE / KENO-V.a	1.0915 ± 0.0020

Source: reference 1.

MCNP and VIM, which used continuous-energy ENDF/B-V cross sections, are 2 and 4 standard deviations (σ) lower than the evaluated benchmark. The KENO V.a results, which used the 238-group ENDF/B-V cross-section set, are about 10% higher than the evaluated benchmark. The problem with the KENO V.a results is not in KENO V.a but in the method used to self-shield the group cross sections. In SCALE, the cross sections are resonance-processed using NITAWL, which uses the Nordheim Integral Treatment to self-shield the resonances.

Previous Work on Fe Problem

Problems associated with ^{235}U/Fe were previously identified in an article in the winter 1993 issue of the Criticality Safety Quarterly entitled "k_∞ for Certain Metals Mixed with ^{235}U." This article lead to an investigation of the ENDF data and SCALE system [2,3]. Several weaknesses in the ENDF/B-V data were identified: poor Al capture cross sections, nuclides having significant resonance structure but no resonance data, and resonance data above resonance cutoff energies. Deficiencies in the methods used in SCALE to process resonances were also identified and corrected. Corrections to these deficiencies included: modifying NITAWL to enhance the processing of *p*- and *d*-wave resonances and adding *p*- and *d*-wave resonance data to the SCALE master libraries.

This previous work concentrated on infinite systems composed of fissile material and metal. The geometry effects present in a finite system were not considered. Although the present work examines similar material compositions, different problems involving neutron transport and leakage effects are responsible for the differences seen between the codes.

NITAWL Limitations

NITAWL uses the Nordheim Integral Treatment to process the resolved resonance data, producing a problem-dependent working library. This method contains limitations and assumptions that are not valid for the U/Fe problem.

One limitation is that NITAWL only processes resonance parameters; it does not use the ENDF file 3 data when processing resonances. For ENDF/B-V, the natural iron evaluation uses the Multi-Level Breit-Wigner (MLBW) resonance formalism. It appears the resonance fits were done using the Reich-Moore (RM) formalism, then converted to MLBW. Since the RM and MLBW formalisms do not give the same calculated elastic scattering cross sections, a file 3 background was added to the MLBW data. This resulted in a very large file 3 background that is negative in some regions. In the MLBW formalism, the absorption peak is normally at the resonance E, with the scattering peak shifted a fraction of the total width from E. The energy mesh algorithm must be able to represent the structure of the shifted peak.

An assumption is that resonances are widely spaced, so resonance overlap is unimportant. The Northam Integral Treatment processes one resonance at a time, thus assuming resonance overlap is unimportant. The resonance overlap above ~300 keV is significant for the ^{235}U/Fe sphere. Consideration of resonance overlap is important, for problems where significant events occur in the resonance region,

Problem Analysis

The discrepancies in the ZPR-9/34 (HEU-MET-FAST-035) benchmark problem were analyzed by first simplifying the problem to a 90-cm-radius ^{235}U/Fe sphere. Calculations showed that the simplified system had substantially the same characteristics as the ZPR benchmark. Namely, SCALE over predicted k_{eff} by 14%. The ^{235}U/Fe sphere was analyzed using the CENTRM Sequence being developed by ORNL [4].

This sequence generates a problem-dependent point-wise flux that is used to produce group cross sections. CENTRM produced the same results as those produced by NITAWL.

An ultra-fine set of multigroup cross sections was created to study the problem. The SCALE master library has an upper limit of 999 groups. A 996 group ENDF/B-V cross-section set was made using XLACS. The energy group widths were small enough over the resolved resonance range so that no resonance self-shielding was required for the *s*-wave resonances. The results for the simplified system are shown in Table 2.

Table 2. 90-cm Radius ^{235}U/Fe Sphere Calculations (ENDF/B-V)

Code/Cross Sections	k_{eff} (± σ)
MCNP / Continuous	0.8669 ± 0.0018
CSAS / 238 Group	0.9898
CENTRM / 238 Group	1.0349
XLACS / 996 Group	0.9094
NJOY / 727 Group*	0.9034

* *Source*: reference 5.

The differences in the MCNP and CSAS results are caused by inadequacies in NITAWL and the overlapping resonances above 300 keV. Figures 1 and 2 are plots of the total cross section versus energy for ^{56}Fe. Figure 1 shows each resonance explicitly as processed by NITAWL. The overlapping resonances are readily apparent above 300 keV. Figure 2 shows *s*-wave cross-section structure when reconstructed using SLBW. The cross sections in Figures 1and 2 differ dramatically between 300 and 500 keV. The results using the 996- and 727-group cross sections are more consistent with those from MCNP. The differences between the MCNP and CENTRM results show that the flux is not the appropriate weighting function for collapsing group cross sections for this problem.

Problem Solution

Flux collapsing the 996-group cross sections to 238-group cross sections produced poor results, similar to those using NITAWL. After discussions with personnel at ANL, we decided to try current weighting the cross sections. Current collapsing the 996-group cross sections to 238-group cross sections produced results similar to MCNP. Similar results were obtained using CENTRM with the 238-group library and processing the cross sections using the flux and current weighting; Table 3 contains these results. Flux collapsing conserves reaction rates; current collapsing conserves transport and leakage.

Better understanding of the problem can be achieved by examining the 996-group cross sections, flux, and current and the 238-group CENTRM flux and current for the 90-cm-radius ^{235}U/Fe sphere. Figure 3 is a plot of the ^{56}Fe 996-group scattering cross section versus Energy. Figure 4 is a plot of the flux and current versus energy of the 996-group ^{235}U/Fe sphere. In the energy range between 3×10^3 and 3×10^5 eV the peaks and dips are much more pronounced in the current than the flux, but the overall shape is very similar. Figure 3 turned upside down strongly resembles Figure 4 in this energy range. Figure 5 is a plot of the flux and current generated by CENTRM for the ^{235}U/Fe sphere. It is similar to the 996-group flux and currents. For this problem, the current weighting seems to be more appropriate than flux weighting.

Using CENTRM to do the resonance processing and flux collapsing, the cross sections prior to KENO V.a produces results similar to standard SCALE. When CENTRM collapses the cross sections using the current, the results are very good, within 1 standard deviation of the evaluated benchmark. These results are shown in Table 4.

Table 3. k_{eff} of Flux versus Current Collapsing of Group Cross Sections for the 90-cm Sphere

Cross-sections	Flux Collapsed	Current Collapsed
996 / 238 Group	1.0077	0.8836
CENTRM	1.0349	0.8404

Table 4. HEU-MET-FAST-035 Benchmark Calculation Results Using CENTRM

Collapsing Spectrum	k_{eff} (± σ)
Flux	1.0823 ± 0.0020
Current	0.9986 ± 0.0018

Conclusions

The discrepancies between MCNP and SCALE, illustrated by the 90-cm bare ^{235}U/Fe sphere, are primarily due to the limitations of the Nordheim Integral Treatment used in NITAWL. Additional limitations are imposed on this problem by the large file 3 background in the ENDF/B-V iron data, which NITAWL does not use in processing resonances. There are also inadequacies in the ENDF data caused by the lack of capture resonance data and resonance structure above 400 keV.

Reasonably consistent results with MCNP can be achieved using NITAWL when an ultra-fine group library, consisting of 996-groups, is used. Excellent results are achieved by processing and current weighting the 238-group cross sections using CENTRM.

Additional studies are warranted to understand the implications and proper usage of flux-collapsed versus current-collapsed cross sections.

References

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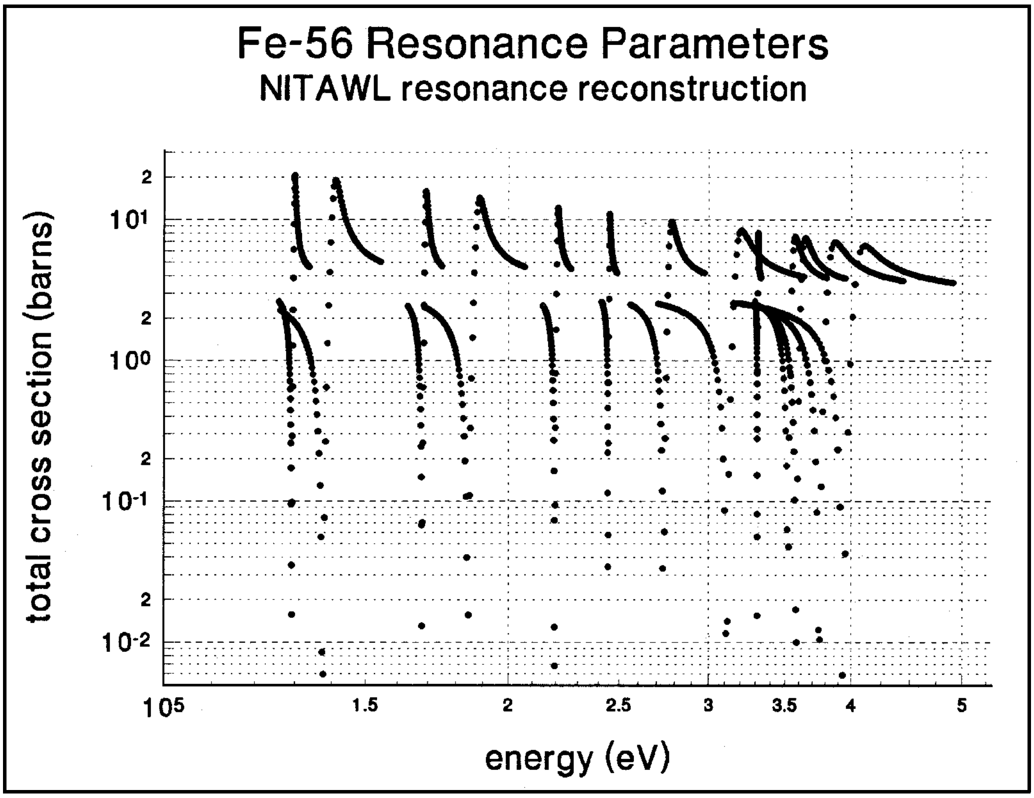

Figure 1. ^{56}Fe Cross Sections versus Energy for Single Resonance Data

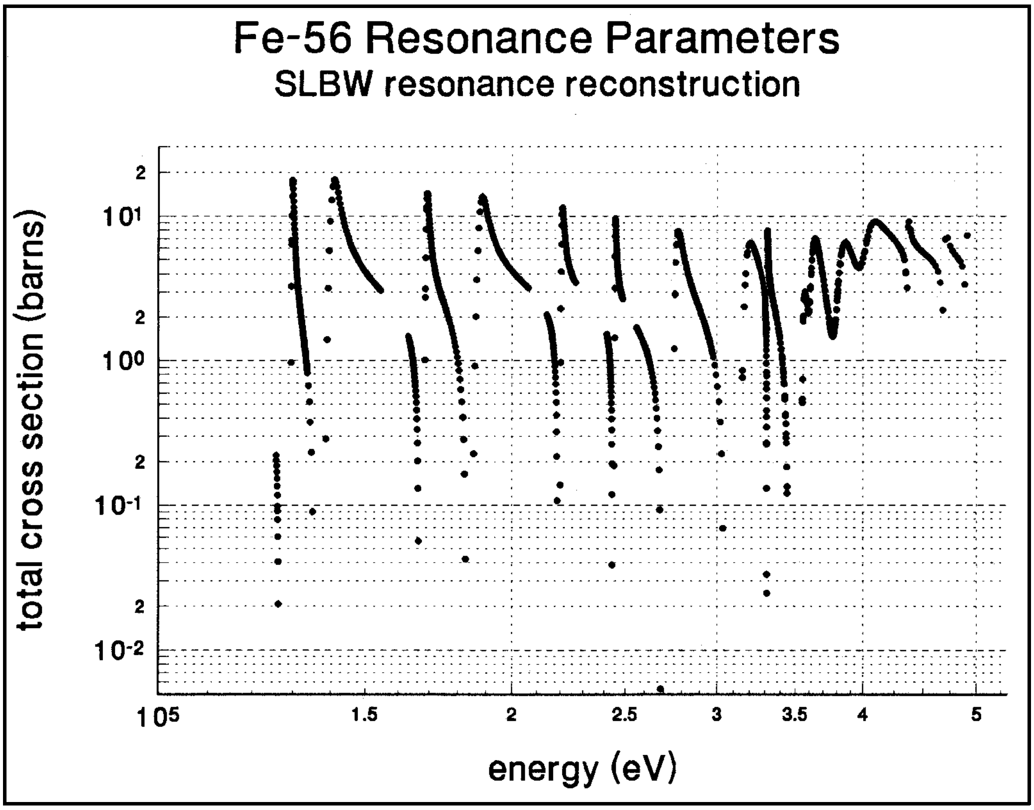

Figure 2. ^{56}Fe Cross Sections versus Energy Produced by Summing Resonance Parameter Data

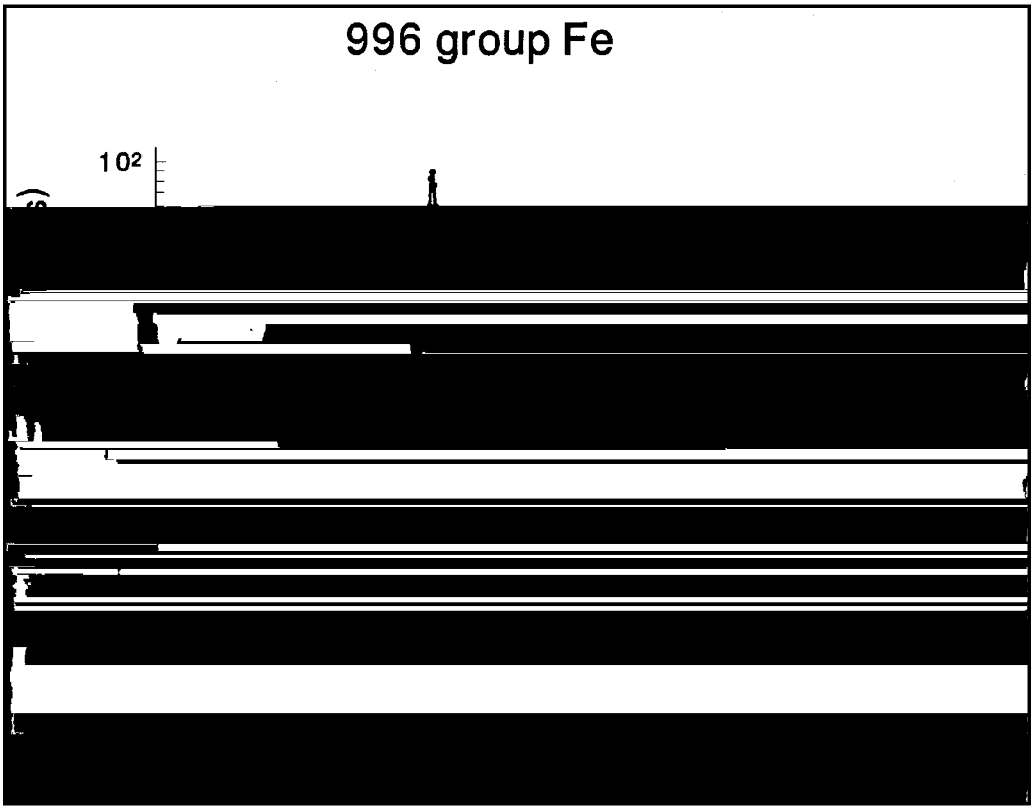

Figure 3. 996-group ^{56}Fe Scattering Cross Sections versus Energy

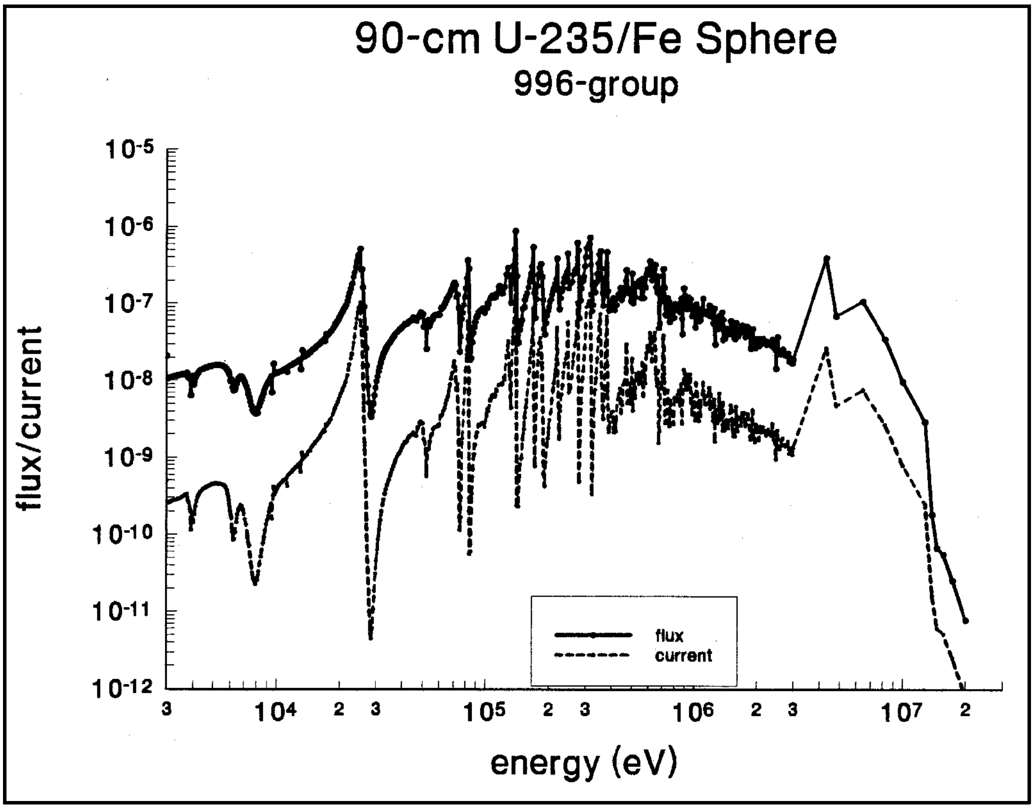

Figure 4. Flux and Current Using the 996-group Cross Sections for the $^{235}U/Fe$ 90-cm Sphere

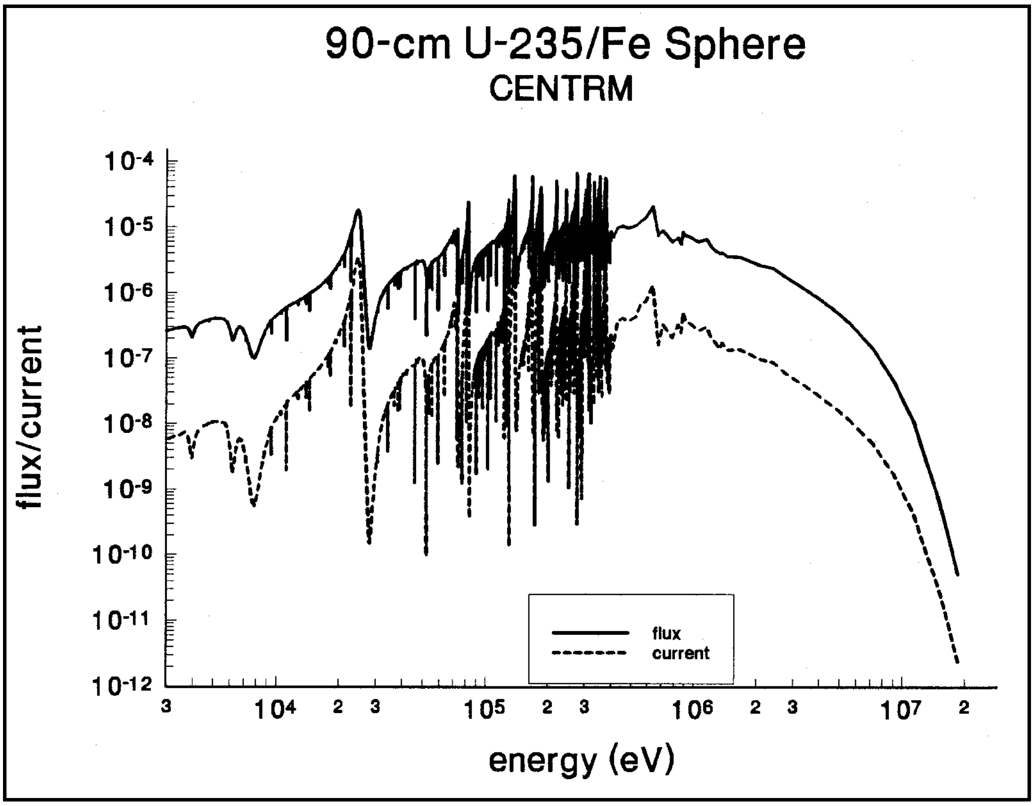

Figure 5. Flux and Current Using CENTRM for the ^{235}U/Fe 90-cm Sphere