

# IMPROVEMENTS IN ENDF/B-VI IRON AND POSSIBLE IMPACTS ON PRESSURE VESSEL SURVEILLANCE DOSIMETRY

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## ABSTRACT

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The ENDF/B-VI cross-section evaluations for the four iron isotopes are summarized, emphasizing the major improvements over ENDF/B-V. The evaluations were mostly based on a preliminary file generated in 1986 for natural iron that has been used for re-calculating several neutron-transport experiments, all of which showed improved agreement. These re-analyses, including those for pressure-vessel surveillance dosimetry, are also discussed.

## INTRODUCTION

The results (Ref. 1 and references therein) from combining integral, differential, and calculated dosimetry data in the pressure vessels of several existing power reactors, using ENDF/B-V nuclear data, indicated that the iron inelastic scattering cross section in ENDF/B-V is about 8% too large from 3 to 8 MeV. This indication was confirmed by newly available  $(n, n'\gamma)$  data<sup>2</sup> and a new model calculation for <sup>56</sup>Fe using an improved nuclear model code<sup>3</sup> to fit all of the available  $(n, n')$  data and other relevant cross sections. All neutron-producing reaction cross sections above 3 MeV in the ENDF/B-V iron evaluation were revised using the new model fits, resulting in a preliminary file<sup>4</sup> for ENDF/B-VI. In this preliminary file, the energy-angle correlations for the inelastically scattered neutrons in the continuum were also introduced. The processed cross-section set<sup>5</sup> in the Vitamin-E group structure<sup>6</sup> has been collapsed to various broad-group structures for the re-analyses of several neutron-transport experiments,<sup>7-11</sup> including the surveillance dosimetry mentioned above, all with improved agreement. The re-analysis<sup>7</sup> of the neutron leakage spectrum of a thick iron-sphere experiment<sup>12</sup> with a central 14-MeV source showed that about half of the 100% increase in the leakage spectrum between 3 and 10 MeV is due to the lowered inelastic scattering cross section in the new evaluation and the other half is due to the forward-peaked angular distributions introduced for the inelastically scattered neutrons in the continuum.

The test results from using the preliminary ENDF/B-VI evaluation for iron are summarized first. Other major improvements to be discussed are: (1) the separation of the evaluation into four isotopic files, (2) the use of the new File-6 format for better representation of correlated energy-angle distributions of the outgoing neutrons and for introducing the energy distributions of the charged-particle and recoil spectra, and (3) the extension of the resonance parameter region of each isotope to higher neutron energy and the application of measured angular distributions for elastically scattered neutrons to determine the spins and parities of the resonances.

## TEST OF THE PRELIMINARY EVALUATION

The preliminary ENDF/B-VI file for iron was intended to remove several outstanding discrepancies between integral data and calculations which occurred with the ENDF/B-V iron evaluation.

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For a 14-MeV source, the  $(n, n')$  cross section for the continuum (threshold = 4.5 MeV) is important for any neutron transport problem. It is well known<sup>13</sup> that inelastically scattered neutrons in the continuum are forward-peaked. Forward-peaked neutrons are more penetrating, hence the isotropic assumption for the inelastically scattered neutrons in the continuum in ENDF/B-V iron is no doubt a source of error for thick-shield analysis involving fusion sources.<sup>12</sup>

In the cases of fission problems, analyses of three integral measurements consistently indicated that the  $\text{Fe}(n, n')$  cross section in ENDF/B-V above 3 MeV was too large. The three problems are: (1) the pressure vessel surveillance dosimetry for several existing power reactors,<sup>1,8</sup> (2) the source terms for the Hiroshima and Nagasaki dosimetry reevaluation program,<sup>10</sup> and (3) the Tower Shielding Facility deep penetration measurements.<sup>11</sup>

New  $\text{Fe}(n, n'\gamma)$  data for the 846-keV level<sup>2</sup> and the new TNG code<sup>3</sup> capable of calculating angular distributions for continuum neutrons were used for addressing the above two types (fission and fusion) of problems and generating the preliminary file. The corresponding multigroup cross-section set<sup>6</sup> was applied to the four experiments mentioned above, all showing improved agreement with the data.<sup>7-11</sup> Smaller discrepancies remain, but they are rather difficult to resolve. For example, Maerker<sup>8,9</sup> suggested that the  $\text{Fe}(n, n')$  cross section below 3 MeV is still a few percent too large but we don't have any new experimental data or theoretical means (because the cross section below 3 MeV is structured) to answer this question at present. Additional high-resolution (5 keV) and/or high-accuracy (2%) measurement in this energy region are needed.

The ENDF/B-VI iron evaluation retains the basic features of the preliminary file. Figure 1 compares the  $\text{Fe}(n, n')$  cross sections between ENDF/B-VI and -V. The newly available data of Larson<sup>2</sup> are also shown. The ENDF/B-VI results shown are abundance-averages of the isotopic evaluations and closely resemble those shown for the preliminary file,<sup>4</sup> where older data were also plotted.

Figure 2 illustrates the calculated and experimental<sup>13-15</sup> double differential  $\text{Fe}(n, xn)$  cross sections for 14.5-MeV incident neutrons and several secondary energy ranges. Equally good agreement between calculation and experiment has been shown<sup>4</sup> for the incident energy of 26 MeV, suggesting reliability of the model used for the calculation. The ENDF/B-V data, if plotted in Fig. 2, would appear as horizontal lines.

## INTRODUCTION OF ISOTOPIC EVALUATIONS

The isotopic evaluations enabled us to make use of additional data measured for the individual isotopes. For example, careful analyses of the inelastic scattering cross sections of the minor isotopes make the values of the inelastic cross section for natural iron between 1.4 and 3.4 MeV about 2% smaller, a change that would not have drawn our attention without evaluating the cross sections of the minor isotopes separately. This reduction in the inelastic scattering cross section of natural iron may result in improved agreement between calculated and measured  $^{237}\text{Np}(n, f)$  responses in the pressure vessels of existing power reactors. However, confirmation of it will await processing of the new evaluation and re-analysis of the surveillance dosimetry data.

The separation of the natural iron evaluation into four isotopic evaluations allows the representation of activation and dosimetry reaction cross sections in the general purpose files. For example, the dosimetry reactions  $^{54}\text{Fe}(n, p)$  and  $^{56}\text{Fe}(n, p)$  are now contained in the respective general purpose files. These two cross sections were updated for ENDF/B-VI primarily by using the ENDF/B-VI  $^{235}\text{U}(n, f)$  and  $^{238}\text{U}(n, f)$  standards in the GLUCS package containing 14 correlated reactions.<sup>16</sup> The evaluation of 37 high-priority dosimetry and activation cross sections available in the general purpose files for which we are responsible has been summarized.<sup>17</sup>

In an evaluated cross-section file for an element containing several isotopes, it is not possible to represent the energies of the reaction products correctly, hence the energy balance cannot be guaranteed. For example, the Q-values for the  $(n, \gamma)$  events for  $^{54}\text{Fe}$  and  $^{56}\text{Fe}$  are, respectively, 9.3 and 7.8 MeV. This difference in the capture gamma-ray energies can be correctly accounted for only in the new isotopic evaluations, ensuring energy balance and more reliable estimates of derived quantities such as Kerma factors. In the area of radiation damage studies, the new File-6 format plays an important role, which is explained below.

## USE OF FILE-6 FORMAT

Correlated energy-angle distributions of outgoing neutrons can now be given efficiently in the new File-6 format in ENDF/B-VI. In the case of the iron isotopes, correlated energy-angle distributions are given for the outgoing neutrons for each neutron-producing reaction, and energy distributions are available for the emitted protons, alpha-particles, heavy recoils, and gamma rays. The incident neutron energy and the sum of the average energies of all reaction products have been checked to be consistent within 1%. The fact that energies are balanced and the fact that energy distributions of heavy recoils are given should have a positive impact on derived quantities such as displacement cross sections for radiation damage studies.

## RESONANCE PARAMETERS

SAMMY,<sup>18</sup> an R-matrix code based on the Reich-Moore formalism and Bayes' Equations, was used for the resonance region of the iron isotopes. For  $^{56}\text{Fe}$ , the analysis was based on measured cross sections for total<sup>19</sup> and capture,<sup>20</sup> and the angular distributions for neutron elastic scattering.<sup>19</sup> The resolved resonance region for all isotopes were extended to higher energy than available in ENDF/B-V. In the case of  $^{56}\text{Fe}$ , the resonance region was increased from 400 to 850 keV. An example is shown in Fig. 3 where the measured transmission data<sup>19</sup> and elastic angular distributions<sup>19</sup> jointly determine the spin and parity assignments of several resonances. The new ENDF/B-VI formats allow the calculation of elastic angular distributions in the resonance region directly from the resonance parameters. It has been shown<sup>19</sup> that resonance parameters evaluated without considering the scattering data often resulted in incorrect spin and parity assignments and hence poor results for the calculated angular distributions. The ENDF/B-V data in the energy region shown in Fig. 3 agree well with the ENDF/B-VI results shown; therefore they are omitted. However, angular distributions for the elastically scattered neutrons, such as shown in the three lower graphs of Fig. 3, cannot be obtained from ENDF/B-V.

## CONCLUDING REMARKS

Five major improvements in the ENDF/B-VI evaluation for iron over Version V have been summarized, namely, (1) the consideration of integral data in a preliminary ENDF/B-VI evaluation, (2) the introduction of energy-angle correlations for the nonelastically scattered neutrons in the continuum, (3) the separation of the evaluation into four isotopic files, (4) the use of the new File-6 format for charged-particle energy distributions and energy balance assurance, and (5) the extension of the resolved resonance parameters to higher energies and the ability to calculate angular distributions for the elastically scattered neutrons in the resonance energy range. The first two have been positively tested,

particularly in the surveillance dosimetry area. The other three improvements are solidly based on advanced model analyses of a rather large data base.

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## FIGURE CAPTIONS

Fig. 1. Comparison of the Fe inelastic cross sections of ENDF/B-VI with ENDF/B-V and with experimental data of Larson.<sup>2</sup>

Fig. 2. Calculated and experimental<sup>13,14,15</sup> double differential Fe( $n, xn$ ) cross sections for 14.5-MeV incident neutrons and several secondary energy ranges.

Fig. 3. In the upper graph the theoretical total cross sections, calculated with the parameters of ENDF/B-VI  $^{56}\text{Fe}$ , are compared with the data.<sup>19</sup> Parentheses are used to indicate uncertain spin and parity assignments. The assignments were made using the differential elastic scattering data<sup>19</sup> shown in the three lower graphs.

# nat-Fe TOTAL INELASTIC SCATTERING CROSS SECTION







