

Evaluation of neutron induced reactions on ^{56}Fe with CONRAD

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Abstract. The evaluation of the ^{56}Fe neutron induced reactions is currently ongoing at the CEA-Cadarache using the code CONRAD, with the goal to cover the whole energy range from the Resolved Resonance Region to the continuum and estimate the corresponding uncertainties and covariance matrices. Some first results and issues occurred from this work are presented and discussed here, more specifically on the analysed transmission and capture data in the Resolved Resonance Region, as well as the optical and statistical model calculations in the fast neutron energy range.

1 Introduction

Iron is one of the most commonly used structural material in nuclear technology applications, thus the proper evaluation of all the reaction cross sections for this isotope is fundamental for the accurate modelisation of the reactors. However, various issues were found at the existing evaluations which lead to the inclusion of this isotope in the Collaborative International Evaluated Library Organization (CIELO) project [1]. The complexity of the evaluation of this isotope lies into two factors. Firstly, it is strongly dependent on the evaluation of the minor isotopes (^{54}Fe , ^{57}Fe , ^{58}Fe). Secondly, there is a strong fluctuating behavior of the cross section data persisting up to several MeV, which neither the present Resolved Resonance Range (RRR) evaluation methodology nor the continuum models are able to properly describe.

A new evaluation of ^{56}Fe is in progress at the CEA - Cadarache with the code CONRAD [2, 3] in order to solve problems identified in the RRR and in the “continuum” part of the neutron induced cross sections. Some first results from this work are presented in this contribution, more specifically from the evaluation of the transmission and capture measurements in the resolved resonance range and from the optical model and statistical model calculations in the continuum range.

2 Evaluation in the Resolved Resonances Range

The current RRR limit for the ^{56}Fe is 850 keV. In the present work, the initial RRR parameters of JEFF 3.1.1 [4] have been used as a starting point, originating from the Froehner evaluation [5] by manually editing the parameters from Kafala et al. [6].

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2.1 Transmission measurements

There is a large number of experimental data from transmission measurements available in the international EXFOR database, using natural and enriched samples. The datasets selected for the evaluation are of high resolution and contain a sufficient number of points in order to properly describe the s-, p- and d-wave resonances. For each experimental dataset the specific characteristics needed for the RRR analysis were determined (contaminations, resolution function, normalisation factor, etc). In general, the Resolved Resonance (RR) parameters from JEFF 3.1.1 have been confirmed, even for resonances of $\ell > 0$. Some small issues have been identified and are currently under investigation.

Furthermore, the reproduction of the total cross section minima (i.e. transmission maxima) of natural Fe transmission experiment datasets was investigated, using the JEFF 3.1.1 RR parameters. For each dataset, only the normalisation factor and the time offset were fitted and the reproduction of the minima was checked. These regions are mainly sensitive to the elastic cross section of ^{56}Fe and of the minor isotopes. It has already been proposed that the elastic cross section of iron should be increased (for example with the integral measurement described in [7]). When dealing with data from microscopic total cross section measurements the statistics in the minima is generally poor. Nevertheless, high-resolution microscopic data from a very thick target are available in the EXFOR database, from Harvey (1975, EXFOR entry 13765001), which were very useful for this work. An example of the reproduction of these datasets is shown in Fig.1.

A total cross section “correction” was estimated by the difference of the evaluated and the experimental value in the minima up to 850 keV, from all the datasets, and the weighted average value was obtained as the final result. The results are still under analysis, but overall, an increase of 100-200mb seems to be needed in the total cross section of natural iron at the minima, as shown in Fig. 2.

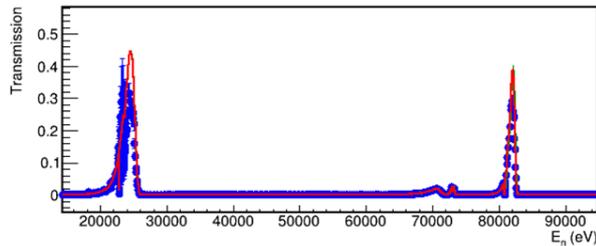


Figure 1. The reproduction of a transmission measurement with a thick target of 2.3 at/b, from Harvey (1975, EXFOR entry 13765001), useful for probing into the total cross section minima. The red line corresponds to the CONRAD result, using the RR parameters from JEFF 3.1.1.

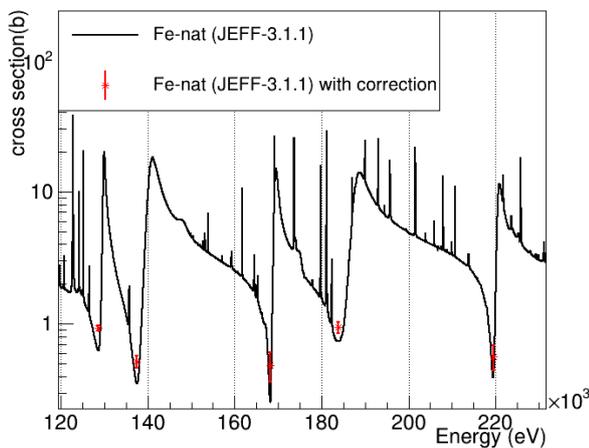


Figure 2. The cross section of the Fe-nat(n,tot) reaction, calculated with the RR parameters from JEFF 3.1.1 (black line) and the “corrected” values at the minima (red points). The error bars correspond to the standard deviation of the values obtained from the analysis of the different datasets.

This increase could be attributed to the elastic channel of ^{56}Fe and/or the minor isotopes which have a strong contribution in the total cross section minima and this possibility will be further studied.

2.2 Capture measurements

Two high resolution capture measurements were used for the evaluation process, one found in EXFOR from Borella et al. at GELINA - 59 m flight path (2005, EXFOR entry 22909001), and one by P. Mutti et al. at GELINA - 30m flight path, provided via private communication.

The normalisation factor was obtained from the fitting of the well known resonance at 1.15 keV. The capture width of the resonance at 28 keV had to be increased, in order to match the transmission experimental data and a better reproduction of the capture data was achieved, as can be seen in Fig 3.

Another issue pointed out within the CIELO project [1] was that the capture cross section is unphysically low and an artificial background had to be added in order to

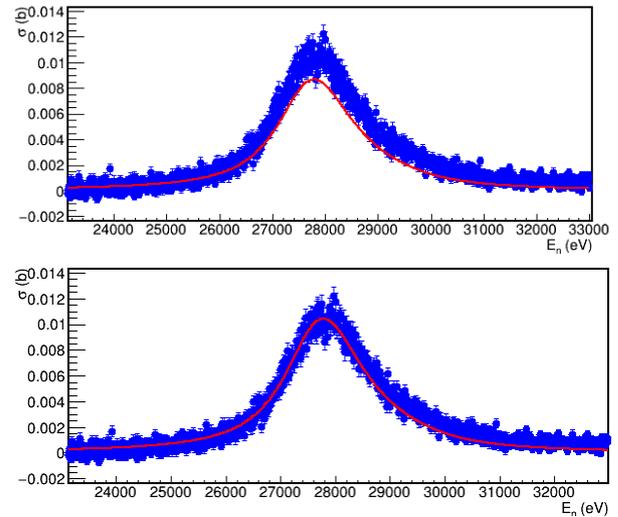


Figure 3. (Upper figure) The comparison of the evaluated resonance at 28 keV with the RR parameters of JEFF 3.1.1, compared to the data of Mutti at GELINA - private communication. (Lower figure) The reproduction of the same resonance with the new set of parameters obtained from this work.

better reproduce a criticality experiment [1]. In the context of the present work, the addition of such a background, potentially coming from a direct capture component, was checked with data from the integral measurement PERLE, performed at the EOLE reactor of CEA, Cadarache. The experiment was designed to validate nuclear data on iron and is described in [8]. A thick stainless steel reflector of 22 cm was used, hosting metallic activation foils (“dosimeters”) and miniature fission chambers at different distances from the core centre. Each dosimeter/detector is mostly sensitive to a different neutron energy range. In the present work, the data from the ^{55}Mn dosimeter was analysed, because the reaction $^{55}\text{Mn}(n,\gamma)^{56}\text{Mn}$ gives an epithermal response, with 75% of the total reaction rate under 600 eV. Thus, it is a good candidate to check whether this integral measurement is sensitive to the change in the $^{56}\text{Fe}(n,\gamma)$.

To this purpose, the experiment was interpreted with the Monte Carlo code TRIPOLI-4 [9] and compared to the experimental results as follows: experimentally, for each position i the reaction rate (R_i) for the $^{55}\text{Mn}(n,\gamma)$ dosimeter was determined by measuring a specific gamma ray from this reaction (energy: 0.847 MeV, intensity: 98.9%, half life 2.58 h). In order to avoid the calculation of absolute reaction rates and thus minimise the systematic uncertainties, the reaction rates at the various positions i were normalised to the one at the core center ($i=0$): R_i/R_0 . This ratio was experimentally determined (namely E) and calculated from the Monte Carlo simulation (namely C). The simulation was performed twice, once with the JEFF 3.1.1 library for all the reactions involved and once with the modified $^{56}\text{Fe}(n,\gamma)$ cross section. The results are shown in Fig. 4, where the quantity C/E-1 is plotted as a function of the dosimeter position. It seems that the increasing trend among the dosimeters vanishes with the changed

$^{56}\text{Fe}(n,\gamma)$ cross section, improving the agreement between calculated and experimental results. This gives an indication that the increase in the $^{56}\text{Fe}(n,\gamma)$ cross section goes in the right direction. It has to be further checked with the ^{235}U fission chamber data, which are also sensitive to the epithermal neutron energy region, and eventually with other integral experiments.

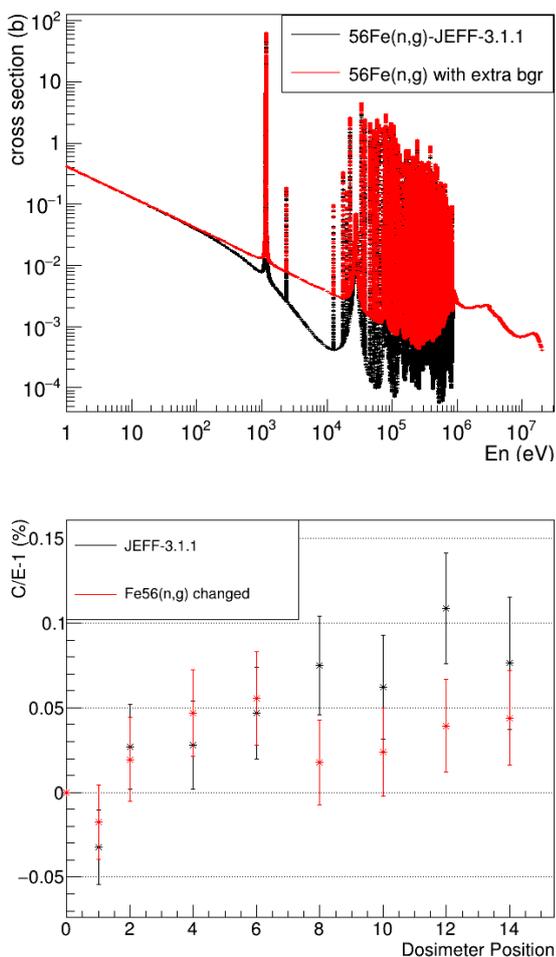


Figure 4. (Upper figure) The evaluated capture cross section of ^{56}Fe from JEFF 3.1.1 (black line) and the increased one (red line) tested with the integral measurement PERLE. (Lower figure) The C/E-1 quantity as a function of the dosimeter position from the analysis of the PERLE integral measurement with the JEFF 3.1.1 library for all the reactions involved (black points) and with the modified $^{56}\text{Fe}(n,\gamma)$ cross section (red points).

3 Fast neutron range

In the present work, the energy range between 862 keV (neutron inelastic scattering threshold) and 20 MeV was treated as continuum and evaluated with optical and statistical models. The models and parameterisation used are explained in [10]. The nuclear reaction code TALYS [11] coupled to the optical model code ECIS [12] was used, as implemented in CONRAD. The sensitivity of the calculation results to various optical model parameters was

analysed. The parameters and the covariance matrices are finally determined to mimic the experimental data.

Some first results and the corresponding uncertainties for various reactions (n,tot), (n,el) and (n,inl) are shown in Fig. 5, along with selected experimental data available in EXFOR and the evaluated libraries JEFF 3.1.1 and the latest ENDF/B-VIII.0 [13]. The first three inelastic levels (not shown in this paper) are also re-evaluated to match data available in EXFOR.

As a general remark, the average trend of the experimental data and the chosen evaluations is successfully reproduced. The estimated uncertainties for the total cross section are of the order of 5% (above 4 MeV), which corresponds to the discrepancy among experimental data. The 5% uncertainty is more reasonable than the 0.5% proposed in JEFF 3.1.1. The structures that appear in the experimental data up to 6 MeV and are adopted by the evaluations cannot be reproduced by the optical and statistical model calculations. An effort is ongoing so as to be treated within the R-matrix theory. Nevertheless, the calculated average cross sections and uncertainties are useful for nuclear energy applications, such as uncertainty quantification of the neutron fluence in reactor pressure vessels and neutron-induced irradiation damage of materials containing ^{56}Fe [14, 15].

4 Conclusions

The first results of the evaluation on the ^{56}Fe reaction cross section with CONRAD are presented in this contribution. Overall, the resonance parameters in JEFF 3.1.1 nicely reproduce the experimental data of the transmission and capture measurements, apart from few issues that have been identified and need to be further studied. For example, it seems that the total cross section minima should be increased and this could be attributed to the elastic cross section of the iron isotopes. Furthermore, the need of increase of the capture cross section on ^{56}Fe , already pointed out by the CIELO project, was checked with data from the integral measurement PERLE (CEA Cadarache) and found to be in the right direction. Finally, optical model and statistical model calculations were performed in the energy region 860 keV - 20 MeV. The results above 4 MeV are in good agreement with the average experimental data and evaluated libraries and an estimation of the uncertainties and covariance matrices was obtained.

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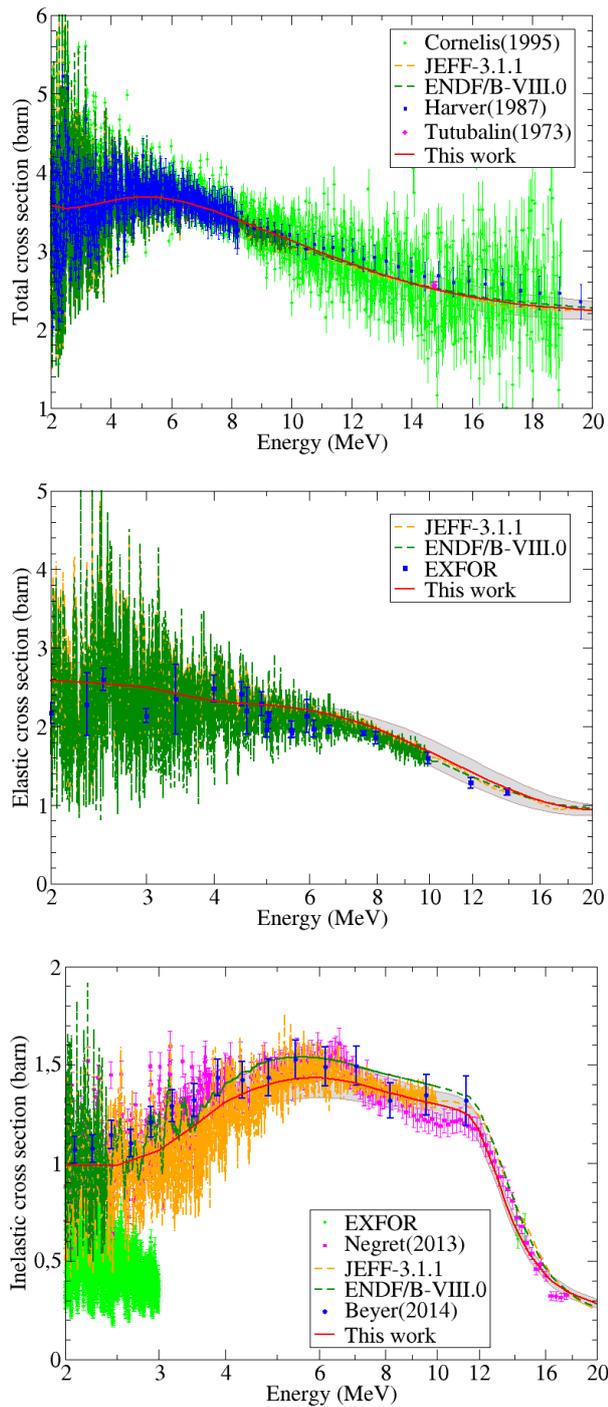


Figure 5. The results of the adjusted optical and statistical model calculations (red line) in comparison with selected experimental data and evaluations for the $^{56}\text{Fe}(n,\text{tot})$ -upper figure, $^{56}\text{Fe}(n,\text{el})$ -middle figure and $^{56}\text{Fe}(n,\text{inl})$ -lower figure.

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