

REPORT ON THE MEETING OF SUBGROUP-I  
OF THE NEACRP/NEANDC EVALUATION COOPERATION:  
INTERCOMPARISON OF CROSS SECTIONS FOR <sup>52</sup>Cr, <sup>56</sup>Fe, AND <sup>58</sup>Ni  
IN THE JENDL-3, JEF-2/EFF-2, AND ENDF/B-VI EVALUATIONS

held at the NEA Data Bank  
on December 3, 1990

PARTICIPANTS:

- C. Y. Fu: ORNL-USA (chairman)
- H. Gruppelaar: ECN-Petten (secretary)
- M. Kawai: Toshiba-Japan
- A. Hogenbirk: ECN-Petten
- L. Petrizzi: ENEA-Frascati
- S. Tagesen: IRK-Vienna
- J. Kopecky: ECN-Petten
- K. Shibata: NEA Data Bank
- G. C. Panini: ENEA-Bologna

ABSENT BUT CONTRIBUTED DOCUMENTS AND/OR GRAPHS:

- N. Yamamuro: DEI-Japan
- T. Asami: JAERI-Japan
- H. Vonach: IRK-Vienna
- D. Hetrick: ORNL-USA
- D. Larson: ORNL-USA (Task Force Monitor for Subgroup-I)
- C. Dunford: BNL-USA
- D. Zhou: CNDC-China

The purpose of the meeting is to examine the large number of graphs prepared by this subgroup overlaying the cross sections, energy and angular distributions in the JENDL-3, JEF-2/EFF-2, and ENDF/B-VI evaluations for <sup>52</sup>Cr, <sup>56</sup>Fe, and <sup>58</sup>Ni, to understand the reasons for the observed discrepancies among the three evaluations, and to come up with recommendations for improvements.

The meeting progressed while the plots were being copied by the Data Bank and made available for each participant so that all participants were looking at the same graph at the same time. The following minutes of the meeting reflects the flow of the discussions.

## CROSS SECTIONS OF $(n, \alpha)$ REACTIONS:

There are large discrepancies among the evaluations for the  $(n, \alpha)$  cross sections. In general, there are two different shapes. Below 14 MeV, EFF-2 is relatively low and ENDF/V-VI is relatively high. Possible reasons:

- . competition of other channels
- . alpha-particle optical model
- . level density
- . preformation factors in pre-equilibrium model

The last point seems most relevant, because it is known that there are large differences among various models. The "best" theory at present is perhaps the description of Zhang (CNDC-China) based on the Harada model. It was concluded that the evaluators should specify exactly which method was used for calculating the  $(n, \alpha)$  cross sections, in preparation for further work on this problem.

Note that for  $^{52}\text{Cr}$  the recent calculations of Yamamuro confirm EFF-2 and there are also data points in favor of it.

It is recommended that more experimental data be taken at energies between 8 and 10 MeV.

## ANGULAR DISTRIBUTIONS FOR ELASTIC SCATTERING

The  $a_1, a_2,$  and  $a_3$  Legendre coefficients for elastic scattering as a function of incident neutron energy show very good agreement. However, the angular distributions plotted at selected energies show some disagreement in the depth of the first minima and at 14 MeV, suggesting discrepancies among the evaluations in the higher-order Legendre coefficients. Since the low-order Legendre coefficients are more important in neutron transport calculations, it is concluded that the angular distributions for elastic scattering are satisfactory in general.

## TOTAL CROSS SECTIONS

There is generally good agreement among the evaluations. For EFF-2, no structure is included because the total cross sections were calculated from the optical model. It was questioned whether fluctuating cross sections based on measured data should be used or whether unresolved resonance parameters should be given. For MCNP calculations, the first option seems to be preferred for deep penetration problems. For  $^{56}\text{Fe}$  in EFF-2, the evaluation plotted has been lowered at energies near 1 MeV in order to follow the smoothed experimental data (warning: even with the dispersion relations, the optical model still does not work well enough near the 1-MeV minima in the total cross sections). Further work on use of the dispersion relation in optical model calculations should be pursued.

## ENERGY DISTRIBUTIONS

The continuum inelastic cross sections in the three evaluations have different thresholds due to different number of discrete levels used. For comparing the total neutron emission spectra in the continuum range, Dr. Tagesen truncated the continuum inelastic distributions in all evaluations to simulate a common threshold, and renormalized the resulting distributions. Large differences were found at energies below 14 MeV, in particular for  $^{58}\text{Ni}$  at 11 MeV. For  $^{58}\text{Ni}$  at 11 MeV, the  $(n, np)$  channel may lead to difficulties because the  $(n, 2n)$  channel is not open so the calculated neutron emission is a result of photon emission in competition with proton emission. Another possibility is that the level density, which governs the shape of the evaporation spectrum, is different in different evaluations. It was therefore recommended to ask the evaluators to specify the total number of levels per MeV for  $^{58}\text{Ni}$  for each MeV up to 14 MeV to allow further study of the problem. Furthermore, more experimental DDX measurements for iron at energies below 14 MeV are strongly encouraged.

## GAS PRODUCTION CROSS SECTIONS

The hydrogen production cross sections are in good agreement below 14 MeV due to the availability of abundant experimental data for the  $(n, p)$  cross sections. However, they diverge above 14 MeV because of the  $(n, np)$  contributions which were essentially based on calculations. Note the plotted ENDF/B-VI  $^{60}\text{Ni}(n, p)$  and hydrogen-production cross sections have already been lowered to agree with the newly available data.

The helium production data show a rather large spread due to the above-mentioned problems with the  $(n, \alpha)$  cross sections and they disagree even more above 14 MeV where the  $(n, n\alpha)$  cross sections begin to dominate.

## TOTAL PHOTON-PRODUCTION CROSS SECTIONS

Total photon-production cross sections as a function of incident neutron energy in the three evaluations were found to be in substantial disagreement: from 4 to 10 MeV for  $^{52}\text{Cr}$ , above 8 MeV for  $^{56}\text{Fe}$ , and above 4 MeV for  $^{58}\text{Ni}$ . The discussion was centered on  $^{56}\text{Fe}$ . There were two suggested reasons for the discrepancies.

The two major measurements for natural iron, one by J. K. Dickens and the other by G. T. Chapman, have large discrepancies. The data by Dickens is lower than Chapman's by nearly a factor of 2 near 8 MeV and 14 MeV. Even though Chapman's measurement was newer, it may not be better around 14 MeV. This may have caused some confusion.

The second possibility has to do with a 3.5% spread in the evaluated nonelastic cross sections near 14 MeV for  $^{56}\text{Fe}$ . Due to a photon multiplicity of approximately 3, the spread in the nonelastic cross section at 14 MeV can produce a 10% discrepancy in the

total photon-production cross sections. This correlation was confirmed by inspecting the relevant plots.

Vonach has provided an independent evaluation for the 14-MeV cross sections based solely on experimental data. Comparison of the ENDF/B-VI  $^{56}\text{Fe}$  evaluation with Vonach's showed agreement for all partial reaction cross sections to within 1%. Yet the ENDF/B-VI  $^{56}\text{Fe}$  cross section for the nonelastic, summed from the partials, is 3.5% low. This suggests discrepancies in the experimental data used in Vonach's evaluation, which needs to be adjusted by least squares. However, it was recommended that all evaluators consider Vonach's evaluation (distributed during the meeting) for the 14-MeV data in their future revisions.

It is also recommended that similar graphs be made for the natural elements and compared with experimental data. Further resolution of the discrepancies in the total photon-production data will await the completion of plots for the photon energy distributions.

### $(n, \gamma)$ CROSS SECTIONS

There are large differences above 1 MeV, but the cross sections are quite small. For JENDL-3, the direct/semi-direct component is lacking.

### $(n, p)$ CROSS SECTIONS

It is recommended to adopt the dosimetry cross sections in the IRDF file for  $^{56}\text{Fe}(n, p)$ ,  $^{58,60}\text{Ni}(n, p)$  in all future revisions.

### INELASTIC SCATTERING TO DISCRETE LEVELS

Good agreement was found around the cross-section maxima but not for the tails where the deformation parameters used for the direct components may differ in each evaluation. The overall agreement seems satisfactory, in fact, often better than the agreement among the experimental data. More high quality experimental data for the discrete levels are needed.

### DOUBLE DIFFERENTIAL NEUTRON EMISSION

A comparison of the double differential neutron emission spectra is still lacking. However, this work is currently being performed at CNDC-China by D. Zhou et al. and their results will be requested for consideration by this group through official channels.

## RESOLVED RESONANCE RANGE

Although there are a number of graphs displaying the various evaluations in the energy range below 1 MeV, there was no time for a good discussion. There was, however, some discussion during the JEF-2 meeting on this point. Due to the importance of the resolved resonance range in fission reactor applications it should be covered in detail in the near future. It was suggested to make also a comparison of group constants (3 per decade) in order to find important differences. Such intercomparisons should also be made for the natural elements. In particular it was considered of importance to study the status of the capture cross sections. Recently, new data have become available. At CBNM (Geel) capture data are re-analysed with new detector response functions. It is desirable to check the evaluations against these new data when available.

## EVALUATIONS FOR THE NATURAL ELEMENTS

For ENDF/B-VI and EFF-2, there are presently no evaluations for natural Cr, Fe, or Ni. The understanding is that these evaluations have already taken into account experimental data for the natural elements, hence can be processed into multigroup cross sections and combined for the natural elements on the multigroup level. On the other hand, JENDL-3 has evaluated files for the natural elements. For JENDL-3 users, the evaluations for the natural elements are recommended for transport calculations, while the evaluations for the isotopes were intended for activation applications. Therefore, if there are discrepancies between JENDL-3 and the other evaluations for the isotopes, this is not always serious as the natural elements are the leading evaluations in JENDL-3.

In ENDF/B-VI some total cross sections measured for the natural elements have been used for the isotopic evaluations where the isotopic data are either unavailable or are judged to be inferior, for example  $^{56}\text{Fe}$  above 2 MeV.

In EFF-2, the evaluations above 1 MeV, including the total cross sections, are entirely based upon calculations fitted as well as possible to the available data. For this reason, the distinction among the total cross sections of the isotopes is also entirely based on theory.

## INFORMATION FROM SUBGROUP-II

Some of the conclusions above were based on plots done by Drs. Tagesen and Vonach for the covariances in the EFF-2 evaluations. Their covariance results were in turn largely based on the graphs provided by this subgroup. Conclusions to be made by Subgroup-II will be obtained and distributed for consideration by members of Subgroup-I.

## SUPER EVALUATION?

It was concluded that the main task of this working group is to compare the evaluations, to come up with recommendations for improvements, and to recommend further studies for generic problems, such as the  $(n, \alpha)$  reaction and the level density. Evaluators are encouraged to update their evaluations rather than to try for a super evaluation. It seems likely that the evaluation methods will improve, that the modified evaluations will converge, and that a consensus will be reached in the future.

## REMINDER OF ACTIONS

The evaluators of JENDL-3 and EFF-2 should send to C. Y. Fu immediately: (1) a brief description of the alpha-particle preformation model used in the evaluations, (2) the level density (number of levels per MeV) for each MeV up to 14 MeV for  $^{58}\text{Ni}$ . Responsible persons: K. Shibata for JENDL-3 and J. Kopecky for EFF-2. This information will be examined along with that for ENDF/B-VI and summarized by Fu and distributed to all members and interested parties.

Volunteers are needed to work on comparisons for: (1) the secondary photon energy distributions, (2) the total and capture cross sections in the resonance region in groups of 3/decade with a flat weighting. If you have not contributed anything so far, this is your chance. Please let the coordinator or monitor of the subgroup know of your progress or plans.