REPORT OF SUBGROUP 1 OF THE NEANSC WORKING PARTY ON INTERNATIONAL EVALUATION COOPERATION

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ABSTRACT

The purpose of Subgroup 1 is to graphically compare the cross sections, and energy and angular distributions in the JEF-2/EFF-2, ENDF/B-VI, and JENDL-3 evaluations for $^{52}$Cr, $^{56}$Fe, and $^{58}$Ni, to understand the reasons for the observed discrepancies among the three evaluations, and to come up with recommendations for improvements. The goal has been met and this report summarizes the results. The differences most difficult to understand are the ones among the evaluated $^{58}\text{Ni}(n, \alpha)$ cross sections. This part of the work is described in detail and has led to the formation of a new Subgroup on level densities for structural materials.

1. INTRODUCTION

The purpose of Subgroup 1 is to compare graphically all of the evaluated data for $^{52}$Cr, $^{56}$Fe, and $^{58}$Ni commonly present in ENDF/B-VI, JEF-2/EFF-2, and JENDL-3 and to resolve any observed differences. The first subgroup meeting was held in December 1990 at the NEA Data Bank and reviewed the graphical comparisons, parts of which were provided from outside the Subgroup by C. L. Dunford of Brookhaven National Laboratory, USA, and by S. Tagesen of Vienna University, Austria. It was found that the differences among the evaluated $^{58}\text{Ni}(n, \alpha)$ cross sections are the largest; ENDF/B-VI is a factor of 2 larger than EFF-2 near 8 MeV. This comparison is shown in Fig. 1. It is seen that, beside the large differences in magnitudes, EFF-2 also shows a rise-flatten-rise shape not seen in the other two. A second problem that could not be understood during the meeting was the secondary neutron energy distribution from $^{58}\text{Ni}(n, xn)$ for an incident neutron energy of 11 MeV. This distribution is shown in Fig. 2. There were many other problems, though none serious or difficult to understand. A paper summarizing the observations and recommendations of this meeting was presented at the Julich conference in May 1991.
The meeting minutes contain more details and are attached as Appendix 1.

One of the recommendations of the first meeting was to understand the two large differences mentioned above. Both had been determined to be related to model calculations. An item of action was to compare the level densities of $^{58}$Ni used in model calculations for the three evaluations. J. Kopecky and K. Shibata were asked to provide this information for EFF-2 and JENDL-3 respectively, and send them to C. Y. Fu for comparison. This comparison, given in Table 1, was presented at the second working group meeting at Petten in May 1991. The level densities have very large differences; at an excitation energy of 8 MeV, the level density of $^{58}$Ni used for ENDF/B-VI is a factor of 3 lower than those used for EFF-2 and JENDL-3. H. Vonach pointed out that the smallest level density in the neutron channel, as used for ENDF/B-VI, could have led to the largest $(n, \alpha)$ cross section near 8 MeV. This is because that at 8 MeV, the secondary neutrons can see the differences in the level densities but the outgoing alpha particles decay mostly to the discrete levels. Following the meeting, Vonach sent Fu evidence that the level density of $^{58}$Ni used for ENDF/B-VI is too low at 4 MeV. The evidence is that the number of known discrete levels between 3.5 and 4.5 MeV is 19 while the level density used for ENDF/B-VI for this interval is 8. However, from Table 1, it is seen that the level densities in this interval for EFF-2 and JENDL-3 are also low - 11 and 13 respectively. The big problem appears to be at higher energies where the differences in level densities are increasingly larger. The work related to these problems is described in Sections 2-4 below. In Section 5, the problem of the neutron emission spectrum from $^{58}$Ni$(n, x\alpha)$ is explained. The proposal for a new subgroup on level densities for structural materials is given in Section 6. The recommendations supplemental to those given in App. 1 and Reference 1 are given in Section 7.

2. DIFFICULTIES IN THE EVALUATIONS FOR $^{58}$Ni$(n, \alpha)$

The calculations (and evaluation) for the $^{58}$Ni$(n, \alpha)$ cross sections have some intrinsic difficulties not always present in model calculations for other targets or reactions. These difficulties are described in this Section.

The evaluations for the $^{58}$Ni$(n, \alpha)$ cross sections for the three files were all completed in 1987, at which time few experimental data were available. Therefore, the evaluations were mainly based on model calculations fitting to whatever data were known to the individual evaluator. For $^{58}$Ni, EFF-2 was evaluated by M. Uhl using the MAURINA code, ENDF/B-VI by D. M. Hetrick using TNG, and JENDL-3 by S. Iijima using PEGASA. Hetrick had the data of Qaim et al. and Grimes et al. but not those of Graham et al. On the other hand, Uhl did not know of either the Qaim or Graham data, all he had was the measurement of Grimes et al. at 14.5 MeV. Iijima deceased in November 1990, so it was not possible to find out what data he knew at the time of his evaluation.

The original plot shown in Fig. 1, contributed by C. L. Dunford, did not have the data of Graham et al. below 12 MeV or Grimes at 14.5 MeV. These data were added to Fig. 1 because the 14.5-MeV value of Grimes was the only datum used by Uhl for EFF-2 and because the data of Graham et al. were quoted at the first Subgroup meeting to support EFF-2. However, the present concern is not to determine which evaluation is better but to find out why evaluations based on model calculations can be so different in
both magnitude and shape. The findings could be important for nuclear model parameter developments for structural materials.

Both the $^{58}$Ni$(n,n')$ and $(n,p)$ cross sections are a factor of six larger than the $(n,\alpha)$ cross section at 8 MeV. These two cross sections, being nearly equal, are sensitive to the ratios of the level densities of their respective residual nuclides but are not very sensitive to their absolute magnitudes. Reasonably good agreement with the available experimental $(n,n')$ and $(n,p)$ data are possible with a factor of 3 changes in the same direction for the level densities of all residual nuclides. However, the resulting $(n,\alpha)$ cross sections show large differences, particularly so near 8 MeV, a fact to be quantified in Section 4.

The reason the level densities (see Table 1) used in the three evaluations differ so much is that there is no level density information for $^{58}$Ni and $^{58}$Co, the residual nuclides of the $(n,n')$ and $(n,p)$ reactions, except for the discrete energy region. The extrapolation from the discrete energy region to higher excitation energies may have a rather large uncertainty. The uncertainty may escape the attention of the evaluator if $(n,n')$ and $(n,p)$ cross sections have similar magnitudes, as the case for $^{58}$Ni. In other words, if the $(n,n')$ cross section were much larger than the $(n,p)$ cross section, then the wrong level density in the $(n,n')$ channel would have hurt the calculated $(n,p)$ cross sections. The evaluator would have noticed the problem from the available cross section data for these two reactions, and the problem in the calculated $(n,\alpha)$ cross sections would have been less serious. The fact that the observed $(n,\alpha)$ cross section differences in the $^{52}$Cr and $^{56}$Fe evaluations are much smaller than those for $^{58}$Ni seems to confirm the explanation that larger $(n,n')$ cross section than $(n,p)$ cross section helps to constrain the level densities.

For the above reasons, the calculation for the $^{58}$Ni$(n,\alpha)$ cross section is indeed a difficult one. The evaluation process in the present case, such as adjusting the calculated cross sections to experimental data, is not an easy task either since the available experimental data were discrepant and inconsistent between $^{58}$Ni and natural nickel.\(^6\)

3. REVIEW OF THE ENDF/B-VI $^{58}$Ni$(n,\alpha)$ CROSS SECTION

A discussion of this problem with M. Uhl, who evaluated the EFF-2 $^{58}$Ni using his model code MAURINA, led to the conclusion that the first step is to concentrate at the energies near 8 MeV where the difference between EFF-2 and ENDF/B-VI is the largest. This simplifies the problem because at 8 MeV, the complications due to tertiary reactions and pre-equilibrium effects need not be considered. To begin with, the ENDF/B-VI part, evaluated by D. M. Hetrick with the aid of TNG calculations, was reviewed.

It was found that the original TNG results for the $^{58}$Ni$(n,\alpha)$ cross sections calculated by Hetrick\(^6\) were larger than the evaluated values shown in Fig. 1 in the energy range from 6 to 13 MeV. The calculated results in this energy range had been lowered to agree with the data of Qaim et al.\(^2\) (the data shown in Fig. 1 as the open triangles) to obtain the evaluated values. The original calculated results by Hetrick are shown as TNG-H in Fig. 3. This means that the calculated results between Uhl (EFF-2) and Hetrick (ENDF/B-VI) were worse than shown in Fig. 1.

The suggestion of Vonach that the 19 observed discrete levels in $^{58}$Ni between 3.5 and 4.5 MeV should be included as a constraint for level densities led to a review of all discrete levels. As a result, the discrete energy region of $^{58}$Ni used by Hetrick (TNG-H in Fig. 3)
was increased from 3.5 to 4.5 MeV and that of $^{58}$Co from 1.04 to 1.55 MeV. These two level schemes are given in Table 2 where the added levels are shown in parentheses. These schemes are based on Kocher and Auble\textsuperscript{7} for $^{58}$Ni and $^{58}$Co, and Kocher\textsuperscript{8} for $^{58}$Fe. The level schemes used for $^{58}$Fe, not changed from those used by Hetrick, are also given in order to compare with those of Uhl’s to be given below in Section 4.

The number of discrete levels cannot be changed without a corresponding modification in level densities. In TNG, the composite level-density formulas of Gilbert and Cameron\textsuperscript{9} were used. In this formalism, the high excitation energy formula is Fermi gas and the low excitation energy formula is constant temperature. The low energy formula is required to agree with cumulative discrete levels at the discrete energy cutoff and be tangent to the high energy part. So, changing the number of discrete levels or their energy range leads to a change in the low-energy level densities only. The resulting shape changes in the level densities yielded worse $(n \, \rho)$ and $(n', \rho)$ results than Hetrick’s\textsuperscript{6}. To compensate, the Fermi-gas parameter $a$ was changed from 5.438 to 5.400 for $^{58}$Ni and from 7.002 to 6.200 for $^{58}$Co. Note that in the present calculation the spin cutoff parameters were changed with $a$ according to the formula of Facchini and Saetta-Menichella\textsuperscript{10} and the parameters for the constant temperature part were calculated automatically. Therefore, the only adjustment of level density density parameters required in TNG is $a$ if the relation used between $a$ and the spin cutoff parameter is predetermined. The combined changes in discrete levels and Fermi-gas parameters gave slightly better agreement of the calculated $(n, \rho)$ and $(n', \rho)$ cross sections with the available data than obtained by Hetrick. The $(n, \alpha)$ cross sections resulting from this new calculation are shown as TNG-FU in Fig. 3. These cross sections are smaller than those of TNG-H below 12 MeV and larger above and are in good agreement with Qaim’s data below 10 MeV (Ref. 2) and at 14.5 MeV (Ref. 3). Note Fig. 3 has the same scale as Fig. 1.

Maintaining all parameters as TNG-FU above but changing the alpha-particle optical model parameters from Huizenga and Igo\textsuperscript{11} to McFadden and Satchler\textsuperscript{12}, we obtained TNG-MC shown in Fig. 3. The new $(n, \alpha)$ cross sections are now in reasonable agreement with all data shown in Fig. 1. However, the rise-flatten-rise shape of EFF-2 was not reproduced.

For the TNG-H, TNG-FU, and TNG-MC calculations, the neutron optical model parameters are from Wilmore and Hodgson\textsuperscript{13} and the proton from Becchetti and Greenlees\textsuperscript{14}. This information is given so that tests of optical model parameters given below will have some significance.

4. MAURINA PARAMETERS IN TNG

It was finally decided to test in TNG all of the binary-channel parameters used by Uhl in MAURINA for EFF-2 to attempt to reproduce his results. The information sent by Uhl is attached as App. 2. It contains the optical model parameters for the proton channels, the discrete levels used, and the level density parameters. The optical model parameters for the neutron and $\alpha$-particle channels have been given in detail in a paper\textsuperscript{15} presented at the 1991 Juelich conference. The idea of using Uhl’s parameters in TNG was not considered earlier because the work required is substantial: TNG had to be modified to handle energy-dependent radius and diffuseness terms in the optical model parameters.
and to change the level density formulas from Gilbert and Cameron\textsuperscript{9} to the back-shifted Fermi gas\textsuperscript{10}. A temporary version of TNG was created to accommodate these differences in the binary channel only, so the calculated results shown below should not be compared with Uhl’s results for energies above the tertiary thresholds, about 11 MeV.

The starting point is TNG-MC shown in Fig. 3. Each calculation described below was changed from the previous one, to isolate the effect of each change.

First the discrete level schemes used by Uhl for EFF-2 were adopted. Lower discrete energy cutoffs were used by Uhl, hence fewer discrete levels (see Table 2 and App.2). The resulting changes in all calculated cross sections were negligibly small, probably due to the fact that the reductions in discrete levels are nearly proportional for the \((n,n')\), \((n,p)\), and \((n,\alpha)\) channels.

Then Uhl’s optical model parameters for the \(n\), \(p\) and \(\alpha\) channels were introduced, one at a time in that order. The three results, shown in Fig. 4, are labeled \(n\), \(np\), and \(n\alpha\). The changes in cross sections from each addition of Uhl’s optical model parameters are significant, but not large enough to explain the difference at 8 MeV. There is no change in the shape from any of the 3 calculations. It is now obvious that the explanation for the rise-flatten-rise shape of EFF-2 has to come from the differences in level densities.

Uhl’s level densities for the \(n\), \(p\), and \(\alpha\) channels were now added, one at a time in that order. The resulting cross sections, shown in Fig. 5, are labeled \(n\), \(np\), and \(n\alpha\). With the new level densities in the neutron channels, the calculated \((n,\alpha)\) cross sections (labeled \(n\) in Fig. 5) drop sharply from the results labeled \(n\alpha\) of Fig. 4 for energies above 6 MeV. This drop is due to the large increase of level densities in the neutron channels which enhance neutron emission. The ratios of Uhl’s level densities to those of TNG-FU for the three binary channels are shown in Fig. 6. For the neutron channels, the ratios increase with increasing excitation energies up to 12 MeV, peaking at 3.6 near 12 MeV. This explains the increasingly larger gap with energy in the \((n,\alpha)\) cross sections between the \(n\alpha\) results of Fig. 4 and the \(n\) results of Fig. 5. For the same reason, after Uhl’s level densities in the proton channels were added, the calculated \((n,\alpha)\) cross sections (labeled \(np\) in Fig. 5) drop even more. However, after Uhl’s level densities for the alpha channels were included, the \((n,\alpha)\) cross sections (labeled \(n\alpha\) in Fig. 5) increase with energy for energies above 6 MeV. This energy is where the large level densities in the alpha channel start to come into play.

Both the magnitude and the rise-flatten-rise shape of the EFF-2 \((n,\alpha)\) cross sections are now closely reproduced when all parameters used by Uhl for EFF-2 were used in TNG. The major reason for this difference in shape is the much larger level densities used by Uhl in all binary channels. In a calculation near 8 MeV, secondary neutrons and protons can sense the large differences in level densities, but outgoing alpha particles emit predominantly to the discrete levels, so the \((n,\alpha)\) cross section is smaller in Uhl’s work. As incident energies go higher, the outgoing alpha particles can reach the larger level densities of Uhl shown in Fig. 6 and the calculated \((n,\alpha)\) cross sections increase again.

Figure 6 suggests two problems. First, the two sets of level densities differ by up to a factor of 3.7. Which set is closer to the truth is a serious problem that should receive wide attention. The basic problem is that level densities in the \((n,n')\) channels for many important targets (including \(^{52}\text{Cr}\) and \(^{56}\text{Fe}\)) are not known experimentally, hence all existing tabulations have large uncertainties. The case for \(^{58}\text{Ni}\) is worse because the
level density information for the \((n,p)\) channel, \(^{58}\text{Co}\), whose cross sections are also large, is absent also.

The second problem is that the ratios shown in Fig. 6. are not linear with energy but peak between 7 and 12 MeV, a result of the differences in energy dependence between the level-density formulas used in MAURINA and TNG. On a log scale, the constant temperature formula, used below about 12 MeV for ENDF/B-VI, is linear in excitation energy while the back-shifted Fermi-gas formula (used for EFF-2) varies with the square root of energy. Even if the parameters in the two approaches are adjusted to yield the same value at a given energy, the shape difference will remain. For instance, if the two level densities in the proton channels are made the same at 10 MeV by adjusting the Fermi gas parameter 'a', the ratio at 7 MeV will become 1.09 and the ratio at 14 MeV will be 0.85. This intrinsic shape difference in the two commonly used level density formulas may lead to differences in the calculated \((n,n')\), \((n,p)\), and \((n,\alpha)\) cross sections. Such differences should be quantified and fully understood for important structural materials.

5. NEUTRON EMISSION SPECTRA FROM \(^{58}\text{Ni}(n,xn)\)

The differences in the neutron emission spectra for \(^{58}\text{Ni}(n,xn)\) for an incident neutron energy of 11 MeV, shown in Fig. 2, turned out to be due to an error in interpreting the ENDF-6 formats in the plotting program. For ENDF/B-VI and JENDL-3, the \((n,np)\) component is given separately from the \((n,n')\) while for EFF-2, the two components were summed. The plotting program of S. Tagesen was written for EFF-2 and when applied to ENDF/B-VI and JENDL-3, only the \((n,n')\) component was included.

A graph showing a corrected result for ENDF/B-VI is given in Fig. 7. This result was obtained by generating separate energy distributions for the secondary neutrons from \((n,n')\) and \((n,np)\), weighting them by the respective cross sections, and then renormalizing the weighted distribution using the same discrete energy cutoff as used for Fig. 2. This new result is in much better agreement with that of EFF-2.

Figure 8 shows a comparison between EFF-2 and ENDF/B-VI of the secondary neutron emission spectra (instead of distributions normalized to a common discrete energy cutoff), contributed by D. M. Hetrick. The two are in good agreement for the continuum region.

6. PROPOSAL FOR NEW SUBGROUP ON LEVEL DENSITIES

A proposal to form a new subgroup to study the level densities of the major isotopes in stainless steel has been approved by the Working Party as Subgroup 16. C. Y. Fu and D. C. Larson are the coordinator and monitor, respectively, for this subgroup. In view of the large differences in the level densities used for the calculation of \((n,n')\), \((n,p)\) and \((n,\alpha)\) cross sections of \(^{58}\text{Ni}\) shown in this report, the new subgroup will initially study the level densities of \(^{58}\text{Ni}\), \(^{58}\text{Co}\), and \(^{55}\text{Fe}\), the residual nuclides of these three reactions. The specific steps may include the following:

(1) Sensitivities of particle emission cross sections and spectra to differences in level-density formulas such as the back-shifted Fermi-gas formula and the Gilbert-Cameron formula.

(2) Level densities deduced from the calculational fits to the evaluated cross sections
of $^{58}\text{Ni}(n, n')$, $(n, p)$, and $(n, \alpha)$ up to 14 MeV. The evaluation will include newly available experimental data.

(3) Level densities deduced from averages of existing ones used in calculations and/or evaluations.

(4) Level densities from existing tabulations based on empiricism and/or extrapolation.

(5) Level densities deduced from theoretical approaches, including moments method, combinatorial method based on shell model states, and pure shell model calculations.

(6) Level density parameters deduced from updating existing systematics such as Gilbert-Cameron by using the much improved neutron resonance information for $^{58}\text{Ni}$ (for level density of $^{59}\text{Ni}$).

(7) Comparison of the above and final deduction.

Parts of the above work should include $^{52}\text{Cr}$ and $^{56}\text{Fe}$ and the related residual nuclides. For example, item (6) should include at least $^{56}\text{Fe}$ simultaneously.

Members will include scientists interested in working on one or more of the above. Interests have been expressed by H. Vonach, S. Grimes, G. Reffo, S. Chiba, D. C. Larson and C. Y. Fu. Existing members of Subgroup 1 will be asked to stay on as members of Subgroup 16.

7. RECOMMENDATIONS FROM SUBGROUP 1

Most of the recommendations from Subgroup 1 can be found in the minutes of its first meeting at the NEA Data Bank in December 1990 (see App. 1) and the paper by the Subgroup presented at Julich$^1$. A complete set of comparison graphs could be obtained from the following people attending the first meeting: H. Gruppelaar, J. Kopecky, K. Shibata, S. Tagesen, M. Kawai, G. C. Panini, L. Petrizzi, A. Hegenbirk, and C. Y. Fu.

H. Vonach et al.$^{17}$ has evaluated, based on Bayes theorem, the available experimental data at 14 MeV for $^{52}\text{Cr}$, $^{56}\text{Fe}$, $^{58}\text{Ni}$, and $^{60}\text{Ni}$. The evaluated values contain uncertainties and have been adjusted so the partial cross sections sum to the total. It has been found from comparisons made by this subgroup that most evaluated values at 14 MeV disagree with Vonach's. It is recommended that future evaluations or revisions of existing evaluations consider carefully Vonach's results.

Any near term revision for $^{58}\text{Ni}(n, \alpha)$ should consider all measured data, including older data shown in Fig. 1 and recent data by Wattecamps$^{18}$ and Vonach$^{19}$. The evaluator should consider $^{60}\text{Ni}(n, \alpha)$ simultaneously so that new data for natural nickel by Wattecamps$^{18}$ and Chiba$^{20}$ can be used. A new calculation fitting all other cross sections and data will be needed. This could be achieved by the new Subgroup on level densities.

ACKNOWLEDGMENTS

The contributions of graphs, documents, or advice by C. L. Dunford, H. Gruppelaar, S. Tagesen, M. Uhl, and K. Shibata, who are not members of Subgroup 1, are gratefully acknowledged. The U. S. part of this international collaboration was sponsored by Office of Energy Research, Division of Nuclear Physics, U. S. Department of Energy, under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.
REFERENCES


17. H. Vonach, S. Tagesen, M. Wagner, and A. Pavlik, "Uncertainty Estimates for the Fast Neutron Cross Sections of the European Fusion File EFF for $^{52}\text{Cr}$, $^{56}\text{Fe}$, $^{58}\text{Ni}$, and $^{60}\text{Ni}$ and Evaluation of the 14-MeV Cross Sections of these Isotopes from the Existing Experimental Data Base," Institute of Radiation and Nuclear Physics, Vienna University, Austria, EFF-DOC-85 (1991), and private communication (1992).


TABLE 1. Number of Levels per MeV Used for Ni-58 in ENDF/B-VI, EFF-2, and JENDL-3 Calculations

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Normalised Energy Distribution of Secondary Neutrons

Incident Neutron Energy: 11 MeV

$^{58}$Ni

Fig. 2

Emission Probability (MeV$^{-1}$) vs. Neutron Energy [MeV]

- EFF
- ENDF/B-VI
- JENDL 3
$58_{\text{Ni}} (n, \alpha)$

UHL - OM

Fig. 4
$^{58}\text{Ni}(n,\alpha)$

$UHL-BS$

$\sigma$ (mb)

$E_n$ (MeV)

Fig. 5.
Fig. S.

LEVEL DENSITY RATIOS UHL/FU

EXCITATION ENERGY (MEV)

n
ρ
α

(n + 58Ni)
Incident Neutron Energy 1 MeV

Normalized Energy Distribution

Emission Probability (MeV⁻¹)

Fig. 7
\textbf{Fig. 8}

\begin{enumerate}
\item \textbf{Cr-52}
\item \textit{---EFF-2 \quad En = 11.0 \, MeV}
\item \textit{--- ENDF/B-VI \quad En = 11.0 \, MeV}
\end{enumerate}

\begin{center}
\begin{tabular}{c}
\textbf{Cross Section (mb/MeV)}
\end{tabular}
\end{center}

\begin{center}
\begin{tabular}{c}
\textbf{Outgoing Neutron Energy (MeV)}
\end{tabular}
\end{center}
Appendix 1  Report of Subgroup-I

REPORT ON THE MEETING OF SUBGROUP-I
OF THE NEACRP/NEANDC EVALUATION COOPERATION:
INTERCOMPARISON OF CROSS SECTIONS FOR $^{52}$Cr, $^{56}$Fe, AND $^{59}$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 $^{52}$Cr, $^{56}$Fe, and $^{59}$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 Yamamura 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 $^{56}$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 $^{56}$Fe evaluation with Vonach's showed agreement for all partial reaction cross sections to within 1%. Yet the ENDF/B-VI $^{56}$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 $^{56}$Fe$(n, p)$, $^{58,60}$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 \(^{58}\)Ni. Responsible persons: K. Shibata for JENDL-3 and J. Kopecy 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.
INSTITUT FUER RADIUMFORSCHUNG
UND KERNPHYSIK
der Universität Wien
A-1090 WIEN, Boltzmannsgasse 3
Telefon 346650,342630
Bitnet: A251DAA at AWIUNI11

Mario Uhl

Wien, January 21st, 1992

Dr. C. Y. Fu
Oak Ridge National Laboratory
Building 6010 MS o356
Oak Ridge, Tennessee 37831
USA

Dear Peter,

thank you very much for your recent letter. Also I was glad to meet you at Juelich after so long time. The Mani parameters read as follows (conventional notation):

\[-U(r,E) = - V_s(E) \frac{1}{1 + e^{(r-A_s)/\sigma_s}} + W_s(E) e^{-(r-R_s)/\sigma_s} - 2.0 \psi_{so}(E) \frac{1}{r} \frac{d}{dr} \left[ \frac{1}{1 + e^{(r-R_{so})/\sigma_{so}}} \right]^2 \cdot \sigma_s.\]

The reduced radii \(R_{sr}, R_{so}\) and \(R_{so}\) are all 1.25 fm. For the reduced Coulomb radius I used 1.3 fm.
The diffuseness parameters \(\sigma_s, \sigma_s, \text{ and } \sigma_{so}\) are 0.65, 1.2 and 0.65 fm, respectively.

The depths (MeV) of the components are given by:

\[-V_s(E) = 49.66 - 0.424E - 0.0042E^2,\]

\[-W_s(E) = 0.5293 \text{ for } E \leq 0.8 \text{ MeV,} \]

\[-W_s(E) = 0.5293 + 4.35 \ln \frac{E}{0.8} \text{ for } E \geq 0.8 \text{ MeV,} \]

\[V_{so}(E) = 12.1 - 1.79 \ln E.\]

I made a small change in the depth of the surface potential. The original prescription was: \(W_s(E) = 1.5 + 4.35 \ln E\)

I hope that this information will be useful. With the best wishes for a good and successful 1992, yours sincerely

\[\frac{\text{Mario}}{}\]
Dr. C. Y. Fu  
Oak Ridge National Laboratory  
Building 6010 MS o356  
Oak Ridge, Tennessee 37831  
USA

Dear Peter,

thank you very much for your letter and the interesting status report. I am sorry that you still have these problems with the $^{58}$Ni$(n, \alpha)$ reaction.

I did the calculations which are the base for EFF-2 essentially in 1986. Therefore I did not know the results of Graham et al.. The only data which I used for adjusting model parameters were those of Grimes at 15 MeV. I was lucky not to be aware even of Qaim's data and so I did not notice the problems with the $(n, \alpha)$ reaction.

In the following I send you the requested information:

**Level density parameters**

I used for all nuclei the rigid body moment of inertia to define the spin cutoff parameter: $\sigma^2 = 0.0150A^{5/3}t$. For the temperature I used a slightly more complicated formula than you, namely the relation resulting from Eq.(3) in Nucl. Phys. A217, 269 (1973). However, I believe that your formula is a good approximation. I used the back-shifted Fermi gas model in the whole continuum region, without a constant temperature portion. This might have some impact on the results. The level density parameters $a$ and the backshifts $\Delta$ employed for the residual nuclei populated by first chance particle emission read:

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**Levels**

Tables with excitation energy $E$, spin $S$ and parity of the levels employed for Ni-58, Co-58 and Fe-55 follow.
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Continuum Edge: 4.8000(MeV)

Co-58

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Continuum Edge: 1.0920(MeV)
Fe-55

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CONTINUUM EDGE: 2.8000(MEV)

Width-fluctuation correction (WFC)

For the levels I used the formulation of Moldauer, presented in Nucl. Phys. A344, 195(1980). The continuum was represented by a group channel. I do not expect a significant influence of the WFC on the present \((n, x)\) cross sections. As an indirect proof I regard the fact that STAPRE (Avrigeanu's results) and MAURINA with different WFC formulations yield similar shapes for the \(^{58}\text{Ni}(n, x)\) excitation function.

I hope that all these numbers will be useful.

With best regards,

Mario

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