NEA/WPEC-1

International Evaluation Co-operation

VOLUME 1

COMPARISON OF EVALUATED DATA FOR CHROMIUM-52, IRON-56 AND NICKEL-58

A report by the Working Party
on International Evaluation Co-operation
of the NEA Nuclear Science Committee

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NUCLEAR ENERGY AGENCY
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FOREWORD

A Working Party on International Evaluation Co-operation was established under the sponsorship of the OECD/NEA Nuclear Science Committee (NSC) to promote the exchange of information on nuclear data evaluations, validation, and related topics. Its aim is also to provide a framework for co-operative activities between members of the major nuclear data evaluation projects. This includes the possible exchange of scientists in order to encourage co-operation. Requirements for experimental data resulting from this activity are compiled. The Working Party determines common criteria for evaluated nuclear data files with a view to assessing and improving the quality and completeness of evaluated data.

The Parties to the project are: ENDF (United States), JEF/EFF (NEA Data Bank Member countries), and JENDL (Japan). Co-operation with evaluation projects of non-OECD countries are organised through the Nuclear Data Section of the International Atomic Energy Agency (IAEA).

The following report is issued by a Subgroup investigating discrepancies in different evaluations of the major structural materials. The isotopes selected are Chromium-52, Iron-56 and Nickel-58. Graphical overlay comparisons between cross-sections, and also energy-angle correlated particle distributions, in different evaluated libraries was performed. Benefits from these comparisons include information useful for improving structural material evaluations in individual data libraries, for assessing differences associated with present-day evaluation techniques and for development of techniques for graphical representation of the energy-angle correlated data.

The opinions expressed in this report are those of the authors only and do not represent the position of any Member country or international organisation. This report is published on the responsibility of the Secretary-General of the OECD.

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SUMMARY

The purpose of Subgroup 1 is to graphically compare the cross-sections, and the energy and angular distributions in 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 summarises the results. The differences most difficult to understand are the ones among the evaluated ^{58}Ni(n,α) 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*.

COMPARISON OF EVALUATED DATA FOR CHROMIUM-52, IRON-56 AND NICKEL-58

1. Introduction

The purpose of Subgroup 1 is to graphically compare all 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, held in December 1990 at the NEA Data Bank, 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}Ni (n,α) 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 Figure 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}Ni $(n,\times n)$ for an incident neutron energy of 11 MeV. This distribution is shown in Figure 2. There were many other problems, though none serious or difficult to understand. A paper summarising the observations and recommendations of this meeting was presented at the Jülich conference in May 1991 [1]. The meeting minutes contain more details and are attached as Appendix A.

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 to send it to C.Y. Fu for comparison. This comparison was presented at the second working group meeting at Petten in May 1991. 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 (see Table-1). 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,α)

cross-section near 8 MeV. This is because, at 8 MeV, the secondary neutrons can see the differences in the level densities but the outgoing α particles decay mostly to the discrete levels. Following the meeting, H. Vonach sent to C.Y. 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 to 4 below. In Section 5, the problem of the neutron emission spectrum from ^{58}Ni *(n,xn)* is explained. The proposal for a new *Subgroup on Level Densities for Structural Materials* is given in Section 6. The recommendations supplementary to those given in Appendix A and Reference [1] are given in Section 7.

Table 1. Number of levels per MeV used for ^{58}Ni in ENDF/B-IV, EFF-2 and JENDL-3 calculations

E (MeV)	ENDF/B-VI	JENDL-3	E (MeV)	EFF-2
1*	1.2	1.3	0-1	0
2	2.3	2.7	1-2	1
3	4.3	5.9	2-3	4
4	8.0	13	3-4	9
5	15	27	4-5	13
6	28	59	5-6	48
7	52	127	6-7	101
8	96	275	7-8	205
9	179	592	8-9	388
10	333	1188	9-10	747
11	621	2500	10-11	1360
12	1110	5090	11-12	2500
13	1990	10070	12-13	4340
14	3510	19400	13-14	7550

* Midpoint of 1-MeV energy bin.

2. Difficulties in the evaluations for ^{58}Ni *(n,α)*

The calculations (and evaluations) for ^{58}Ni *(n,α)* 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 ^{58}Ni *(n,α)* 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. D.M. Hetrick used the data of Qaim, *et al.* [2,3] and Grimes, *et al.* [4] but not those of Graham, *et al.* [5]. On the other hand, M. Uhl did not know of either the Qaim or Graham data, all he had was the measurement of Grimes, *et al.* [4] 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 Figure 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 Figure 1 because the 14.5-MeV value of Grimes was the only datum used by M. Uhl for EFF-2 and because the data of Graham, *et al.* were quoted at the first Subgroup meeting to support the EFF-2 evaluation. 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,α)* 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,α)* cross-sections show large differences, particularly so near 8 MeV, a fact to be quantified in Section 4.

The reason why 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 it is the case for ^{58}Ni. In other words, if the *(n,n′)* cross-sections were much larger than the *(n,p)* cross-sections, 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,α)* cross-sections would have been less serious. The fact that the observed *(n,α)* 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′)* than *(n,p)* cross-sections help constrain the level densities.

For the above reasons, the calculation for the ^{58}Ni *(n,α)* 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 a 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-IV ^{58}Ni (n,α) 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,α)* cross-sections calculated by D.M. Hetrick [6] were larger than the evaluated values shown in Figure 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 Figure 1 as the open triangles) to obtain the evaluated values. The original calculated results by D.M. Hetrick are shown as TNG-H in Figure 3. This means that the calculated results between M. Uhl (EFF-2) and D.M. Hetrick (ENDF/B-VI) were worse than shown in Figure 1.

The suggestion of H. 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 D.M. Hetrick (TNG-H in Figure 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 [7] for ^{58}Ni and ^{58}Co, and Kocher [8] for ^{55}Fe. The level schemes used for ^{55}Fe, unchanged from those used by D.M. Hetrick, are also given in order to be compared with those of M. Uhl's, which are 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 [9] were used. In this formalism, the high excitation energy

Table 2. Level schemes used in TNG-H and TNG-FU calculations

(TNG-FU used additional levels in parentheses)

Ni-58			Co-58			Fe-55		
J		E(keV)	J		E(keV)	J		E(keV)
0	+	0	2	+	0	1.5	-	0
2	+	1454	5	+	25	0.5	-	412
4	+	2459	4	+	53	2.5	-	931
2	+	2776	3	+	111	3.5	-	1317
1	+	2903	3	+	366	3.5	-	1419
0	+	2943	5	+	374	0.5	-	1919
2	+	3038	4	+	458	1.5	-	2052
2	+	3265	4	+	886	2.5	-	2144
3	+	3421	3	+	1040	4.5	-	2212
(4	+	3525)	(2	+	1044)	2.5	-	2256
(0	+	3531)	(5	+	1050)	4.5	-	2300
(4	+	3558)	(6	+	1076)	1.5	-	2400
(1	+	3593)	(5	+	1185)	5.5	-	2539
(4	+	3620)	(2	+	1237)	2.5	-	2578
(3	+	3774)	(2	+	1352)	6.5	-	2813
(4	+	3870)	(3	+	1354)	2.5	-	2871
(2	+	3898)	(4	+	1369)	3.5	-	2938
(5	+	3934)	(1	+	1377)	5.5	-	2983
(0	+	4020)	(2	+	1414)	4.5	-	2984
(2	+	4108)	(3	+	1425)	1.5	-	3027
(2	+	4261)	(1	+	1436)	5.5	-	3072
(4	+	4299)	(2	+	1512)			
(5	+	4347)	(3	+	1523)			
(4	+	4350)	(4	+	1550)			
(5	+	4379)	(2	+	1555)			
(4	+	4405)						
(2	+	4450)						
3	-	4470						

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 cut-off 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,n′)* and *(n,p)* results than D.M. Hetrick's [6]. To compensate, the Fermi-gas parameter a was changed from 5.438 to 5.400 for

^{58}Ni and from 7.062 to 6.200 for ^{58}Co. Note that in the present calculation the spin cut-off parameters were changed with a according to the formula of Facchini and Saetta-Menichella [10] and the parameters for the constant temperature part were calculated automatically. Therefore, the only adjustment of level density parameters required in TNG is a if the relation used between a and the spin cut-off parameter is pre-determined. The combined changes in discrete levels and Fermi-gas parameters gave slightly better agreement of the calculated *(n,n′)* and *(n,p)* cross-sections with the available data than obtained by D.M. Hetrick. The *(n,α)* cross-sections resulting from this new calculation are shown as TNG-FU in Figure 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 [2] and at 14.5 MeV [3]. *Note that Figure 3 has the same scale as Figure 1.*

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

For TNG-H, TNG-FU, and TNG-MC calculations, the neutron optical model parameters are from Wilmore and Hodgson [13] and the proton from Becchetti and Greenlees [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 binary-channel parameters used by M. Uhl in MAURINA for EFF-2 in order to attempt to reproduce his results. The information sent by M. Uhl is attached as Appendix B. 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 α-particle channels were given in detail in a paper [15] presented at the 1991 Jülich conference. The idea of using Uhl's parameters in TNG was not considered earlier because the work required was 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 [9] to the back-shifted Fermi gas [16]. 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 M. Uhl's results for energies above the tertiary thresholds about 11 MeV.

The starting point is TNG-MC, which is shown in Figure 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 M. Uhl for EFF-2 were adopted. Lower discrete energy cutoffs were used by M. Uhl, hence fewer discrete levels (see Table 2 and Appendix B). 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,α)* channels.

Then M. Uhl's optical model parameters for the n, p and α channels were introduced, one at a time in that order. The three results, shown in Figure 4, are labelled *n*, *np* and *npα*. The changes in cross-sections from each addition of M. 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 three calculations. It is now obvious that the explanation for the rise-flatten-rise shape of EFF-2 comes from the differences in level densities.

M. Uhl's level densities for the *n*, *p* and α channels were then added, one at a time in that order. The resulting cross-sections, shown in Figure 5, are labelled *n*, *np* and *npα*. With the new level densities in the neutron channels, the calculated *(n,α)* cross-sections (labelled n in Figure 5) drop sharply from the results labelled *npα* of Figure 4 for energies above 6 MeV. This drop is due to the large increase of level densities in the neutron channels, which enhances neutron emission. The ratios of M. Uhl's level densities to those of TNG-FU for the three binary channels are shown in Figure 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,α)* cross-sections between the *npα* results of Figure 4 and the *n* results of Figure 5. For the same reason, after M. Uhl's level densities in the proton channels were added, the calculated *(n,α)* cross-sections (labelled *npα* in Figure 5) dropped even more. However, after M. Uhl's level densities for α-channels were included, the *(n,α)* cross-sections (labelled *npα* in Figure 5) increased with energy for energies above 6 MeV. This energy range is where large level densities in the α-channel start to come into play.

Both the magnitude and the rise-flatten-rise shape of the EFF-2 *(n,α)* cross-sections are now closely reproduced when all parameters used by M. Uhl for EFF-2 were introduced in TNG. The major reason for this difference in shape is the much larger level densities used by M. 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 α-particles emit predominantly to the discrete levels, so the *(n,α)* cross-section is smaller in M. Uhl's work. As incident

energies go higher, the outgoing α-particles can reach the larger level densities of M. Uhl shown in Figure 6, and the calculated *(n,α)* 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}Cr and ^{56}Fe) are not known experimentally, hence all existing tabulations have large uncertainties. The case for ^{58}Ni is worse because the level density information for the *(n,p)* channel ^{58}Co, the cross-sections of which are large too, is also absent.

The second problem is that the ratios shown in Figure 6 are not linear with energy but peak between 7 and 12 MeV, which is 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 both approaches are adjusted to yield the same value at a given energy, the shape difference will remain. For instance, if both level densities in the proton channels are made the same at 10 MeV by adjusting the Fermi gas parameter a, the ratio will become 1.09 at 7 MeV and 0.85 at 14 MeV. 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,α)* cross-sections. Such differences should be quantified and fully understood for important structural materials.

5. Neutron emission spectra from ^{58}Ni (n,xn)

The differences in the neutron emission spectra for ^{58}Ni *(n,xn)* for an incident neutron energy of 11 MeV, shown in Figure 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 the two components were summed for EFF-2. 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 Figure 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 re-normalising the weighted distribution using the same discrete energy cutoff as in Figure 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 normalised to a common discrete energy cut-off), contributed by D.M. Hetrick. Both 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 co-ordinator 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,α)* cross-sections of ^{58}Ni shown in this report, the new Subgroup will initially study the level densities of ^{58}Ni, ^{58}Co and ^{55}Fe, and 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}Ni *(n,n')*, *(n,p)* and *(n,α)* 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}Ni (for level density of ^{59}Ni).

7) Comparison of the above and final deduction.

Parts of the above work should include ^{52}Cr and ^{56}Fe and the related residual nuclides. For example, Item 6 should include at least ^{56}Fe simultaneously.

Members will include scientists interested in working on one or more of the above items. 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 Appendix A) and the paper by the Subgroup presented at Jülich [1]. A complete set of comparison graphs could be obtained from the following people who attended the first meeting: H. Gruppelaar, J. Kopecky, K. Shibata, S. Tagesen, M. Kawai, G.C. Panini, L. Petrizzi, A. Hogenbirk, and C.Y. Fu.

H. Vonach, *et al.* [17] have evaluated, based on Bayes theorem, the available experimental data at 14 MeV for ^{52}Cr, ^{56}Fe, ^{58}Ni, and ^{60}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 H. Vonach's. It is recommended that future evaluations or revisions of existing evaluations carefully consider H. Vonach's results.

Any near-term revision for ^{58}Ni (n,α) should consider all measured data, including older data shown in Figure 1 and recent data by Wattecamps [18] and Vonach [19]. The evaluator should consider ^{60}Ni (n,α) 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.

Acknowledgements

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 US part of this international collaboration was sponsored by the Office of Energy Research, Division of Nuclear Physics, US Department of Energy, under contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

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Figure 1. ^{58}Ni (n,α) cross sections available in three evaluations: ENDF/B-VI of the USA, JENDL-3 of Japan, and JEF-2/EFF-2 of Europe

The comparison was prepared by C.L. Dunford. The data of Grimes [4] and Graham [5] are added to aid in discussions presented in the text.

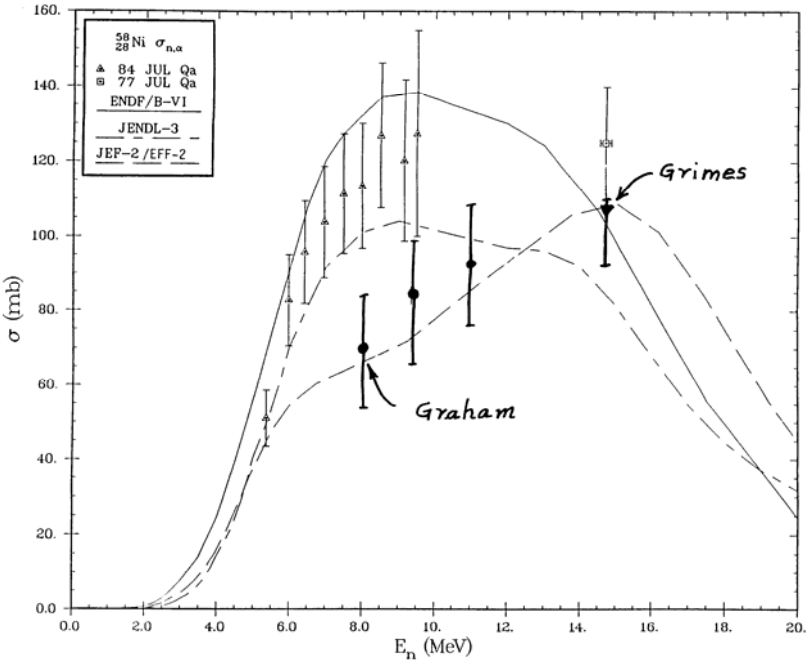


Figure 2. Secondary energy distributions from ^{58}Ni (n,xn) for an incident neutron energy of 11 MeV available in the ENDF/B-VI, JEF-2/EFF-2 and JENDL-3 evaluations. Differences among the three evaluations shown here and in Figure 1 are resolved in this report.

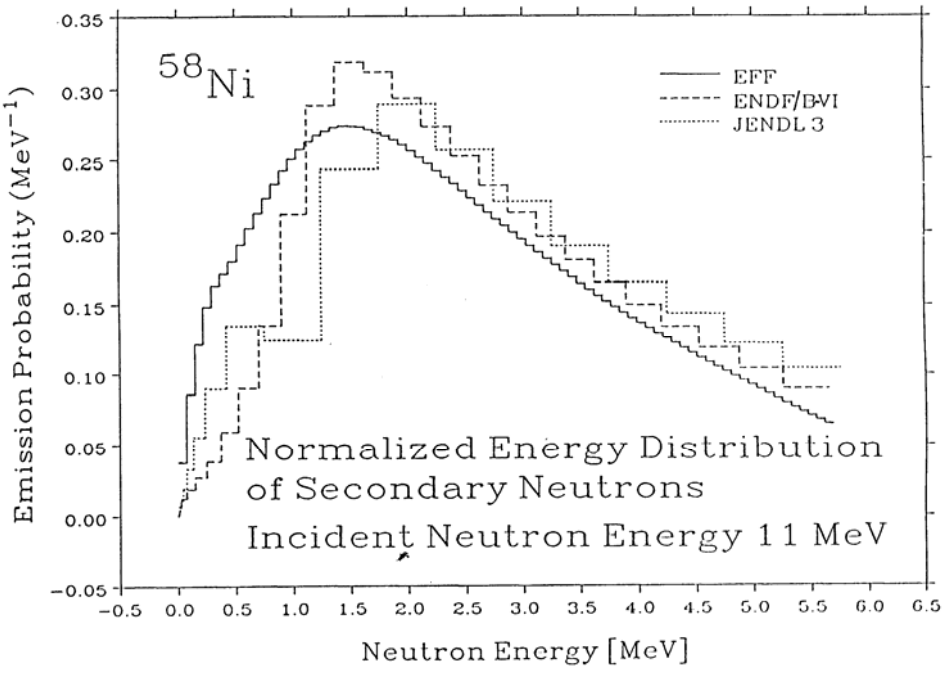


Figure 3. The ^{58}Ni (n,α) cross-section in ENDF/B-VI, evaluated by combining experimental data of Qaim [2,3] and acalculation using the TNG code, is examined to see if the calculation could be reasonably lowered to agree better with the other two sets of evaluated results

The calculated points labelled TNG-H was the original TNG results obtained by Hetrick. TNG-Fu points are obtained by Fu using refined discrete level schemes in the Hetrick's input to TNG. TNG-MC results from replacing the parameters of the alpha optical potential used in TNG-FU by that of McFadden and Satchler. This last result agrees better with the other two evaluations.

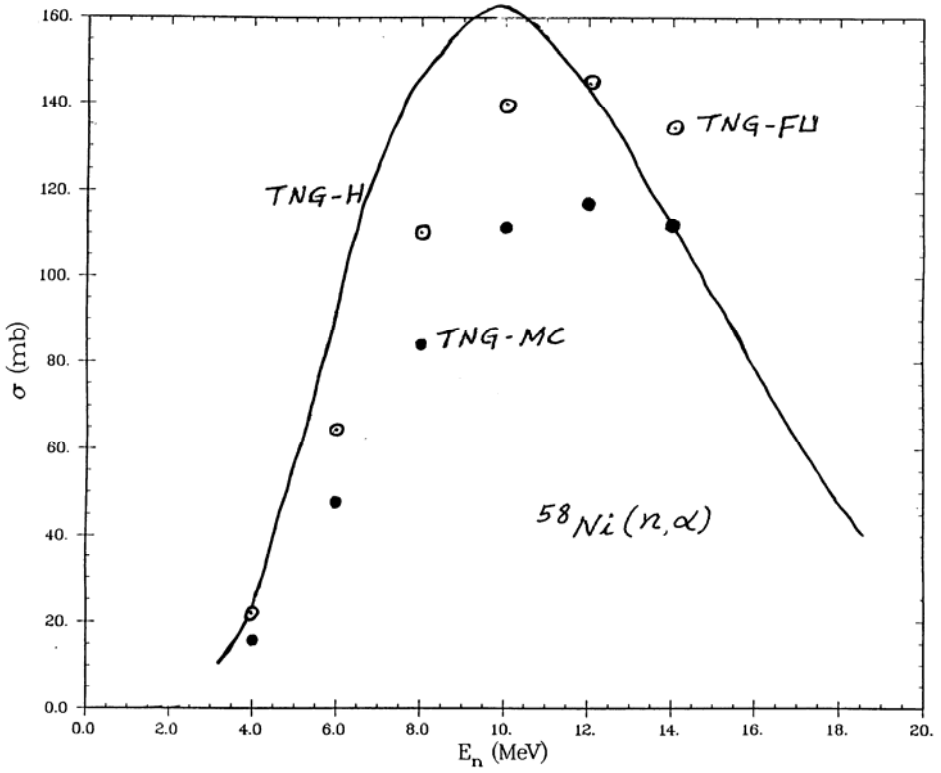


Figure 4. Three TNG calculations using TNG-FU parameters except the optical model parameters of Uhl used for the JEF-2/EFF-2 evaluation

The points labelled "n" had the neutron optical model parameters of Uhl. Those labelled "np" had neutron and proton optical model parameters of Uhl. Similarly, "npα" for n, p and alpha. These results ruled out the optical model parameters as the major problem area for the differences seen in Figure 1.

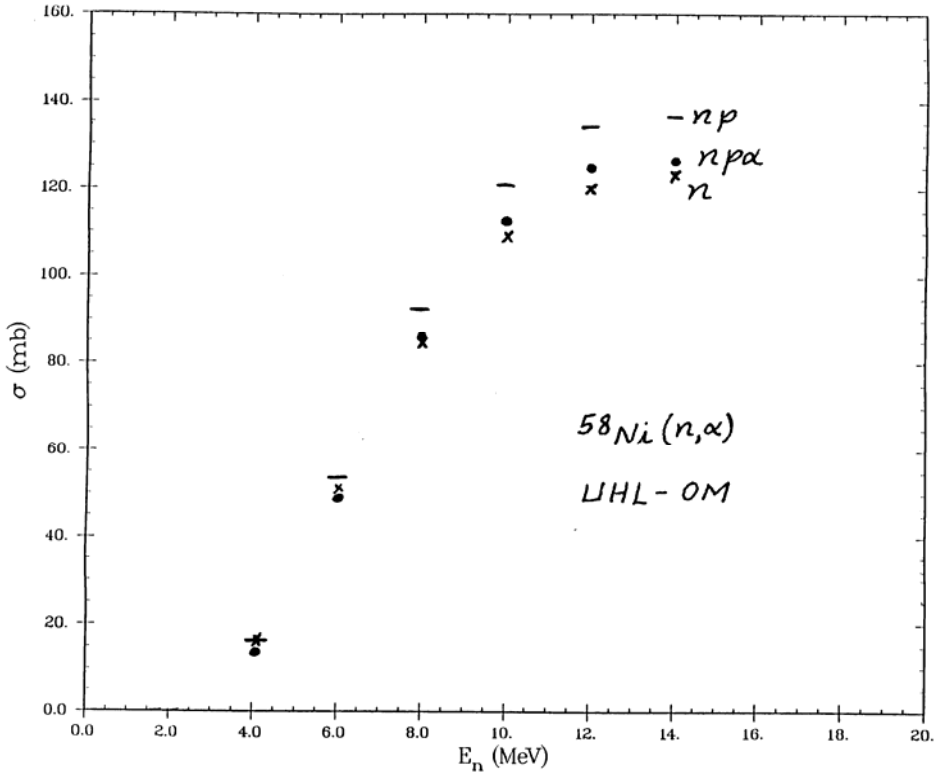


Figure 5. Three TNG calculations using the "npα" parameters of Figure 4 except the binary part of the level densities of Uhl used for the JEF-2/EFF-2 evaluation

The results labelled "n" had the neutron part of the level density parameters of Uhl. Those of "np" had both n and p parts of the level density parameters of Uhl and so on for "npα". The last result nearly reproduced Uhl's results used for JEF-2/EFF-2 but with a different model code and established the level density as the major cause of the ^{58}Ni (n,α) problem.

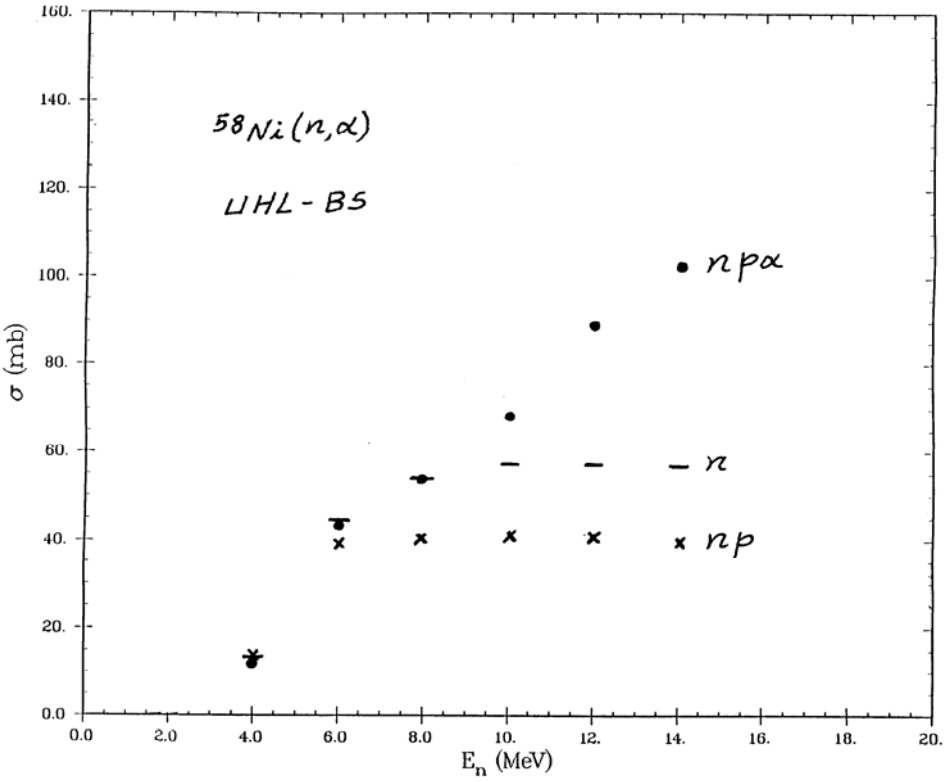


Figure 6. Ratios of level densities used by Uhl for JEF-2/EFF-2 and by Fu slightly refined from that used for ENDF/B-VI

The curves labelled "n", "p" and "α" represent level densities in the n-channel (^{58}Ni), p-channel (^{58}Co) and α-channel (^{55}Fe), respectively.

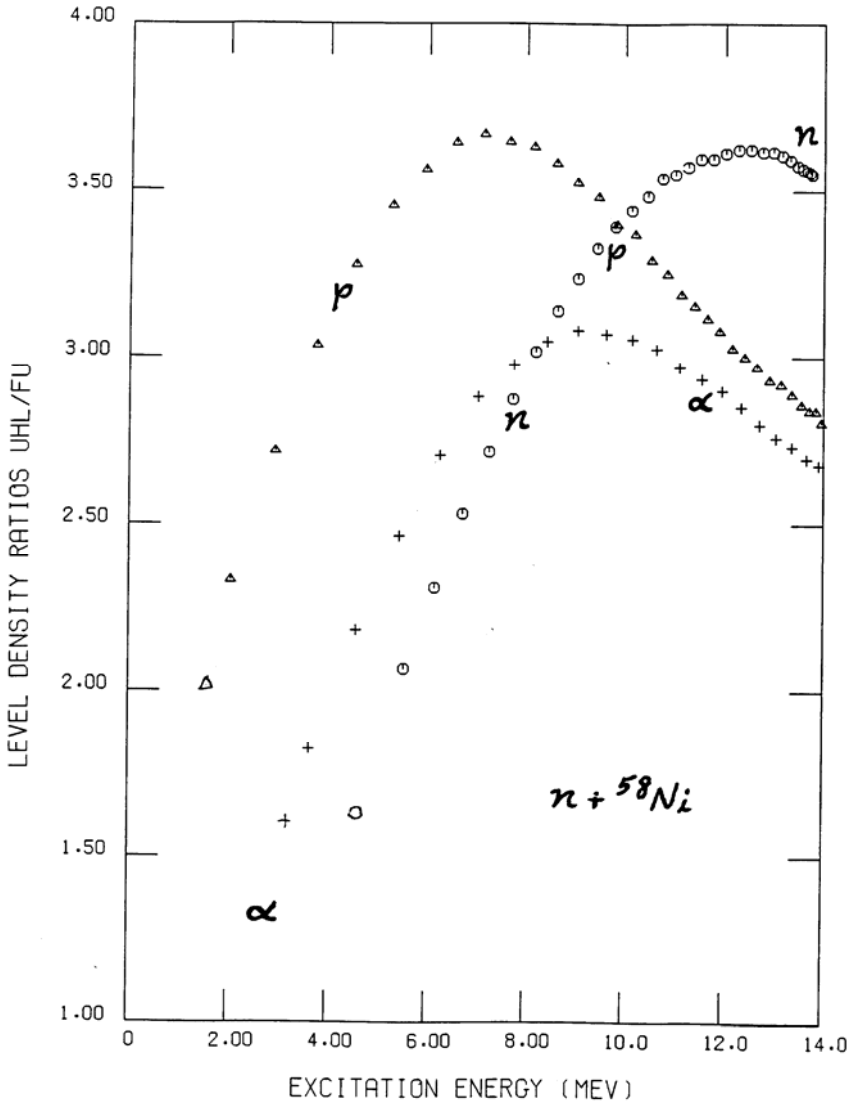


Figure 7. Secondary neutron distributions from ^{58}Ni (n,xn) reproduced from Figure 2 with added data points

These added data result from adding the (n,pn) contribution to the dashed curve labelled ENDF/B-VI that contains only the (n,n') contribution. The newly added data are the true ENDF/B-VI that agree with the solid curve labelled EFF.

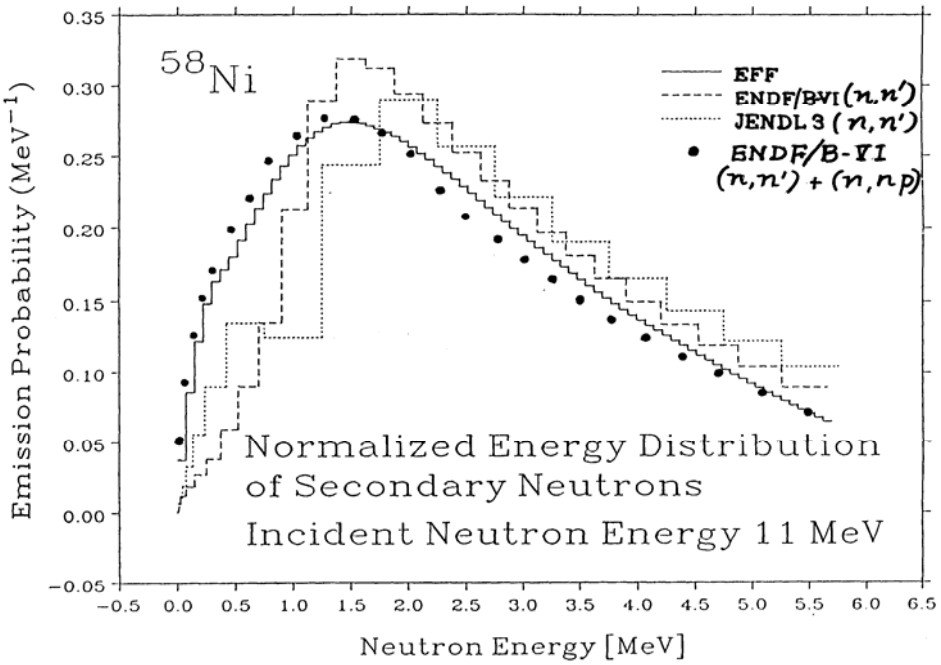
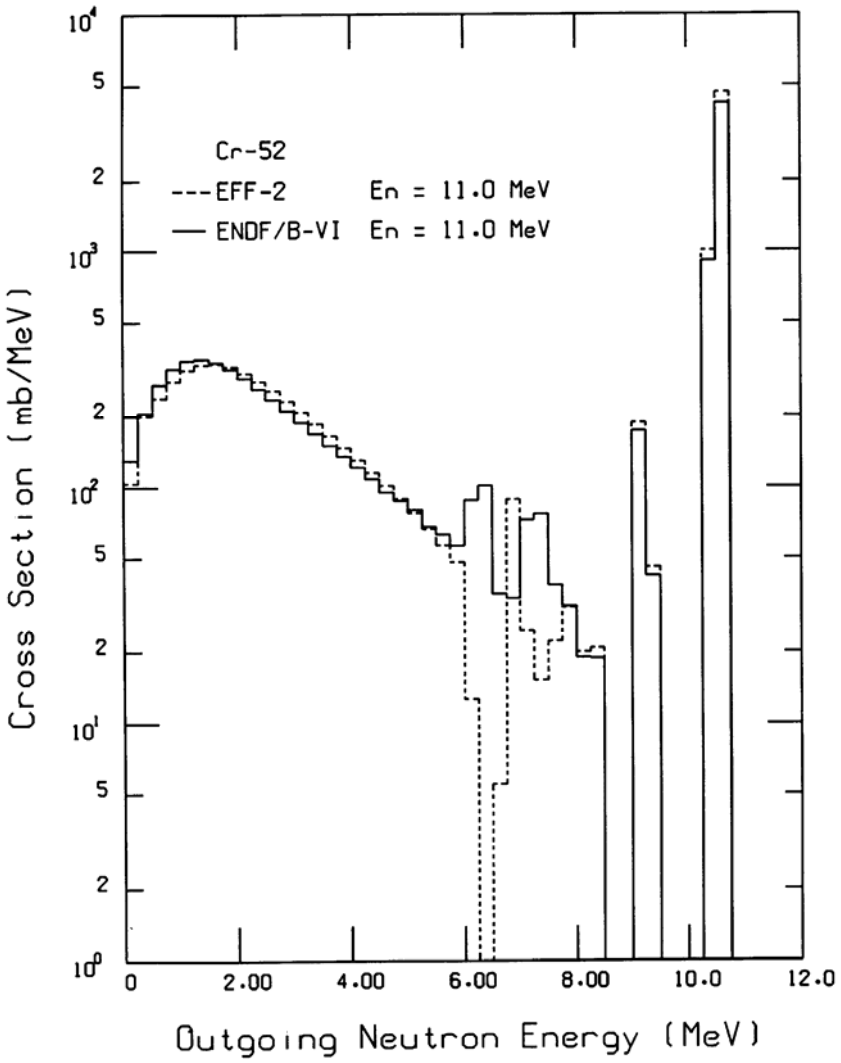


Figure 8. Comparison of ^{52}Cr (n,xn) neutron spectra of EFF-2 and ENDF/B-VI for an incident neutron energy of 11 MeV

Some problems exist in the discrete energy region due to the use of discrepant level schemes in the calculations performed for the two evaluated files.



Appendix A

Report on the Meeting of Subgroup-1
of the NEACRP/NEANDC Evaluation Co-operation:
Intercomparison of Cross-sections For ^{52}Cr, ^{56}Fe. and ^{58}Ni
in the JENDL-3, JEF-2, and ENDF/B-VI Evaluations

held at the NEA Data Bank
on 3 December 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 Subgroup 2 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 ^{81}Ni, to understand the reasons for the observed discrepancies among the three evaluations, and to come up with recommendations for improvement.

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

Cross-sections of *(n,α)* reactions

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

- 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,α)* cross-sections, in preparation for further work on this problem.

Note that for ^{57}Cr the recent calculations of N. Yamamuro confirm EFF-2 and there are also data points in favour of it.

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

Angular distribution 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}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 the 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 the different numbers 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 re-normalised the resulting distributions. Large differences were found at energies below 14 MeV, in particular for ^{58}Ni at 11 MeV. For ^{58}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}Ni for each MeV up to 14 MeV in order 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 that the plotted ENDF/B-VI ^{60}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,p)* cross-sections and they disagree even more above 14 MeV where the *(n,nα)* 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}Cr, above 8 MeV for ^{56}Fe, and above 4 MeV for ^{58}Ni. The discussion was centred on ^{56}Fe. There were two suggested reasons for these discrepancies.

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

The second possibility has to do with a 3.5%-spread in the evaluated non-elastic cross-sections near 14 MeV for ^{56}Fe. Due to a photon multiplicity of approximately 3, the spread in the non-elastic cross-section at 14 MeV can produced a 10%-discrepancy in the total photon-production cross-sections This correlation was confirmed by inspecting the relevant plots.

H. Vonach has provided an independent evaluation for the 14-MeV cross-sections solely based on experimental data. Comparison of the ENDF/B-VI ^{56}Fe evaluation with that of H. Vonach showed agreement for all partial reaction cross-sections to within 1%. Yet the ENDF/B-VI ^{56}Fe cross-section for the non-elastic, summed from the partials, is 3.5% low. This suggests discrepancies in the experimental data used in H. Vonach's evaluation, which needs to be adjusted by least squares. However, it was recommended that all evaluators consider H. 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 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,γ) 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 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 Subgroup through official channels.

Resolved resonance range

Although there are a large 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 on this point during the JEF-2 meeting. 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 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 at present no evaluations for natural Cr, Fe or Ni. The understanding is, that these evaluations have already taken into account experimental data for natural elements, hence they can be processed into multi-group cross-sections and combined for the natural elements on the multi-group level. On the other hand, JENDL-3 has evaluated files for natural elements. For JENDL-3 users, the evaluations for 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 natural elements represent 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}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 2

Some of the conclusions mentioned 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-2 will be obtained and distributed for consideration by members of Subgroup-1.

One single evaluation

It was concluded that the main tasks of this Subgroup were to compare the evaluations, to come up with recommendations for improvements, and to

recommend further studies for generic problems, such as the *(n,α)* reaction and the level density. Evaluators are encouraged to update their evaluations rather than creating one single evaluation at this stage. 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 α-particle pre-formation 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. Kopecky for EFF-2. This information will be examined along with that for ENDF/B-VI and summarised 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 per decade with a flat weighting. If you have not contributed anything so far, this is your chance. Please let the co-ordinator or monitor of the Subgroup know of your progress or plans.

Appendix B

M. Uhl's letters

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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 paramerters read as follows (conventional notation):

$$-U(r,E) = V_r(E)\frac{1}{1+e^{(r-R_r)/a_r}} + W_s(E)e^{-((r-R_s)/a_s)^2} - 2.00V_{so}(E)\frac{1}{r}\frac{d}{dr}\left[\frac{1}{1+e^{(r-R_{so})/a_{so}}}\right]\vec{\ell}\cdot\vec{\sigma}.$$

The reduced radii R_{0r}, R_{0s} and R_{0so} are all 1.25 fm. For the reduced Coulomb radius I used 1.3 fm.
The diffuseness parameters a_r, a_s and a_{so} are 0.65, 1.2 and 0.65 fm, respectively.

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

$$\begin{aligned} V_r(E) &= 49.66 - 0.424E - 0.0042E^2 , \\ W_s(E) &= 0.5293 \qquad\qquad\qquad \text{for } E \le 0.8 \text{ MeV} , \\ &= 0.5293 + 4.35 \ln\frac{E}{0.8} \qquad \text{for } E \ge 0.8 \text{ MeV} , \\ V_{so}(E) &= 12. - 1.79 \ln E . \end{aligned}$$

I made a small change in the depth of the surface potential. The original presription 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

Mario

Mario Uhl

Wien, August 7th, 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 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, α) 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, namly 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, whithout a contant 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:

	a(1/MeV)	Delta(MeV)
Ni-58	5.517	0.104
Co-58	6.061	-2.571
Fe-55	5.821	-0.700

Levels

Tables with excitation energy E, spin S and parity of the levels employed for Ni-58, Co-58 and Fe-55 follow.

Ni-58

No	E(MeV)	S	P
1.	0.0000	0.0	1
2.	1.4500	2.0	1
3.	2.4600	4.0	1
4.	2.7800	2.0	1
5.	2.9000	1.0	1
6.	2.9400	0.0	1
7.	3.0380	2.0	1
8.	3.2630	2.0	1
9.	3.4200	3.0	1
10.	3.5240	4.0	1
11.	3.5300	0.0	1
12.	3.5930	1.0	1
13.	3.6200	4.0	1
14.	3.7740	3.0	1
15.	3.8930	2.0	1
16.	4.1070	2.0	1
17.	4.2990	2.0	1
18.	4.3470	3.0	1
19.	4.4050	4.0	1
20.	4.4750	3.0-1	
21.	4.5380	2.0	1
22.	4.7550	4.0	1

CONTINUUM EDGE: 4.8000(MEV)

Co-58

1.	0.0000	2.0	1
2.	0.0250	5.0	1
3.	0.0530	4.0	1
4.	0.1120	3.0	1
5.	0.3660	3.0	1
6.	0.3740	5.0	1
7.	0.4570	5.0	1
8.	0.8860	3.0	1
9.	1.0400	3.0	1

CONTINUUM EDGE: 1.0920(MEV)

Fe-55

No	E(MeV)	S	P
1.	0.0000	1.5	-1
2.	0.4110	0.5	-1
3.	0.9310	2.5	-1
4.	1.3160	3.5	-1
5.	1.4080	3.5	-1
6.	1.9180	0.5	-1
7.	2.0520	1.5	-1
8.	2.1440	2.5	-1
9.	2.2120	4.5	-1
10.	2.2560	5.5	-1
11.	2.3010	4.5	-1
12.	2.4700	1.5	-1
13.	2.5390	5.5	-1
14.	2.5780	2.5	-1

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, α) 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 $^{58}Ni(n, \alpha)$ excitation function.

I hope that all these numbers will be useful.

With best regards,

Mario

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