IEC-39

# STATUS REPORT TO THE NEANSC WORKING GROUP ON INTERNATIONAL EVALUATION COOPERATION from Subgroup 1: Comparison of ENDF/B-VI, JEF-2/EFF-2, and JENDL-3 for $^{52}$Cr, $^{56}$Fe, and $^{58}$Ni


C. Y. Fu, Coordinator of Subgroup 1
Oak Ridge National Laboratory
Oak Ridge, TN 37831


## PROGRESS SUMMARY

The subgroup first met in December 1990 at the NEA Data Bank to examine the large number of graphical comparisons. Findings and recommendations of this meeting were reported in the meeting minutes and summarized as a paper at the Juelich conference in May 1991. Further progress was reported to the working group at the Petten meeting following the Juelich conference. The goals recommended by the working group for this subgroup were to resolve the worst discrepancies among the three evaluations, namely, the $^{58}$Ni(n,$\alpha$) cross sections, and the $^{58}$Ni(n,n') neutron emission spectra for $E_n$=11 MeV and $E'_n$ near 1 MeV. The result of this endeavor was thought to be benefitial not just to future improvement of the Cr, Fe, and Ni cross-section evaluations but also to the application of nuclear models for data evaluation in general.

Steady progress has been made to achieve the stated goals. In addition, a general purpose code to plot the double differential neutron emission spectra and gamma-ray production spectra has been completed by D. M. Hetrick. The new JENDL-3 Fusion File completed recently (for Cr, Fe, and Ni) have double differential neutron emission spectra and can now be compared with ENDF/B-VI and EFF-2. Changes in the membership of the subgroup are proposed.

## RESOLUTION OF $^{58}$Ni(n,$\alpha$) DISAGREEMENT

The largest $^{58}$Ni(n,$\alpha$) disagreement is near 8 MeV where the cross section in ENDF/B-VI is a factor of two larger than EFF-2, while that of JENDL-3 lies in between. At the December 1990 meeting, the problem was determined to be a calculational one since all three evaluations for this cross section were based on calculations. While disagreement above 14 MeV is also large, it was decided at Juelich that the lower energy problem should be solved first as it is more important and does not involve the complication of the preequilibrium part of the calculations.

The comparison of the three evaluations for $^{58}$Ni(n,$\alpha$) is attached as Fig. 1 to aid the following discussions.

Examination of the TNG calculations done for ENDF/B-VI $^{58}$Ni showed that the preequilibrium effect is negligible below 12 MeV, thus the discrepancy near 8 MeV can only be the results of different level density and optical model parameters used. By confining our attention to the energy range below 12 MeV, the problem is much simplified as the three calculations used entirely different preequilibrium models and different alpha-particle preformation factors.

For $^{58}$Ni, we encountered several unusual situations that all contributed to the difficulty in the calculations. These are described below.

First of all, both the (n,n') and (n,p) cross sections are a factor of six larger than the (n,$\alpha$) near 8 MeV. So, small variations in either the (n,n') or the (n,p) model parameters can change the calculated (n,$\alpha$) cross section by a larger amount.

Secondly, and much more serious, neither residual nuclide of the (n,n') and (n,p) reactions has level density information except for the discrete level region. Extrapolation of the level densities from the discrete level region upward in energy is uncertain. This uncertainty increases for $^{58}$Ni because the number of discrete levels in $^{58}$Ni from 3.5 to 4.5 MeV has an unusually large jump from lower energies, as pointed out by Vonach. This two factors explains the large differences among the level densities used for the calculatiosn for the three evaluations. For example, at 13 MeV, there are 1990 $^{58}$Ni levels per MeV used for the calculation for ENDF/B-VI, 5900 for EFF-2, and 10070 for JENDL-3. Note that the available experimental data for the (n,n') and (n,p) cross sections do not constrain the level densities of their residual nuclides.

Another unusual factor is that the evaluation for ENDF/B-VI $^{58}$Ni was completed (report ORNL/TM-10219 published in June 1987) before the low values of the Graham et al. (n,$\alpha$) data were published. The ENDF/B-VI evaluators were not aware of these data until the first subgroup meeting in December 1990. So ENDF/B-VI evaluators had only the high values of Qaim's data below 12 MeV for consideration while EFF-2 and JENDL-3 evaluations, completed later than ENDF/B-VI, had considered also the lower values of Graham et al. Besides large differences in magnitude, the two data sets also have different shape.

The original TNG results for $^{58}$Ni(n,$\alpha$) were larger than shown for the evaluation. The original calculated cross section is shown in Fig. 2, as TNG-1. This calculated result was lowered to agree with Qaim's data shown in Fig. 1 for the ENDF/B-VI evaluation. Two examples of many new TNG calculations, performed to understand the discrepancy and explained below, are also shown in Fig. 2.

By increasing the number of discrete levels (as suggested by Vonach) and changing the level densities used for the (n,n') and (n,p) reactions while maintaining good fits for these two cross sections, the (n,$\alpha$) cross section near 8 MeV was reduced. An example is shown in Fig. 2 as TNG-2. This result was obtained by extending the discrete energy region used for TNG-1 above (3.5 MeV) to 4.5 MeV for $^{58}$Ni and from 1.04 to 1.55 MeV for $^{58}$Co, and by changing the Fermi gas parameters $a$ from 5.438 to 5.400 for $^{58}$Ni and from 7.062 to 6.200 for $^{58}$Co. In between the Fermi gas part of the level density and the discrete region, the constant temperature formula of Gilbert and Cameron was used and the fit for its parameters was obtained automatically by the TNG code.

Maintaining all parameters as in TNG-2 above but changing the alpha-particle optical model parameters from Huisenga and Igo to Mcfadden and Satchler, we obtained TNG-3 shown in Fig. 2. This new (n,$\alpha$) cross section is now in better agreement with all data as well as with EFF-2 and JENDL-3. However, the shape difference between EFF-2 and the other two evaluations remains.

We have obtained all the optical model parameters used for EFF-2 from Mario Uhl and plan to use them in TNG while maintaining all other parameters as used for TNG-3 above to isolate the effects of the optical model parameters. Uhl's optical model parameters for the (n,n'), (n,p), and (n,$\alpha$) channels will be used, one at a time for each channel. Hopefully, this will shed some light on the unresolved shape difference noted above.

## STUDY FOR THE $^{58}$Ni(n,n') SPECTRA

The $^{58}$Ni(n,n') spectra of the three evaluations at $E_n$=11 MeV and $E'_n$=1 MeV show large deviations as shown in Fig. 3. At the first subgroup meeting, it was agreed that the level densities used for $^{58}$Ni should be examined first. K. Shibata, J. Kopecky, and D. Hetrick provided the level densities shown in Table 1.

It is well known that the steeper the level density rises with energy, the softer the calculated (n,n') spectra at low outgoing energies. For $E_n$=11 MeV and $E'_n$=1 MeV, one should examine the slope of the level density at an excitation energy of 10 MeV. However, checking the level densities given in Table 1 against the spectra of Fig. 3, the expected correlation is not found. Both the ENDF/B-VI and JENDL-3 level densities have a steeper rise with energy at 10 MeV than that of EFF-2, yet the ENDF/B-VI and JENDL-3 spectra at low $E'_n$ are harder than that of EFF-2. Besides the soltness or hardness in the spectra at low outgoing energies, there is a remarkable difference in the shape of the spectra near $E'_n$=0.5 MeV. Therefore, explanations other than level densities have to be sought.

Discussion of this problem with several members of the subgroup and other experts on model calculations led to the decision that comparison of neutron transmission coefficients near 1 MeV should be made next. It has already been found that none of the optical model parameters used in the three evaluations is capable of reproducing the total cross sections near 1 MeV. The plan is to use the optical model parameters used for EFF-2 in the TNG code (used for ENDF/B-VI) with all other parameters fixed and then examine the differences in the transmission coefficients and the resulting spectra. This work is not quite straight forward as the TNG code needs to be modified to accept the energy-dependent radius and diffuseness parameters used for EFF-2. The modification has been made but the comparison has not been made. The optical model parameters used for JENDL-3 cannot be ascertained since the decease of Dr. S. Iijima, the $^{58}$Ni evaluator for JENDL-3.

## PROPOSED CHANGES IN SUBGROUP MEMBERSHIP

Dr. E. Menapace recommended the addition of Dr. A. Mengoni of Bologna as a new member of subgroup 1 as he is actively involved in the evaluation of Fe for JEF-2 and should benefit from the subgroup's activity.

Since Dr. S. Iijima has passed away and Dr. N. Yamamuro has had a heart attack, JENDL-3 has had no active members for over a year. Dr. Y. Kikuchi has nominated two new subgroup 1 members - Dr. T. Asami and Dr. S. Chiba.

Approval of these three new members of subgroup 1 by members of the working group is hereby requested.

## PROPOSED FUTURE WORK

The attempt to resolve the two largest discrepancies among the three evaluations has turned out to be very challenging. The new TNG calculation, shown in Fig. 2 as TNG-3, almost appears acceptable as an evaluation as far as the available experimental data are concerned. However, it does not show a hint of the shape trend seen in EFF-2. It is hard to brush away this shape difference because two other calculations with different optical model and level density parameters also show a similar shape as EFF-2. These two other calculations were done by Dr. N. Yamamuro and Dr. N. Avrigeanu.

The two sets of experimental data below 12 MeV shown in Fig. 1 also display a similar shape difference in the (n,$\alpha$) cross sections discussed for the calculations above. It is desirable that more accurate measurement be made in the energy range between 6 and 12 MeV. Otherwise, even after we have solved the problems in the calculations, the uncertainty in the evaluated (n,$\alpha$) cross section will remain unacceptably large.

We plan to look for an explanation for the shape difference by detailed calculations using various optical model parameters. This effort will also help in resolving the (n,n') spectral discrepancies.

It has been discovered from the work done so far that the calculation for EFF-2 used a spin cutoff parameter half as large as used for ENDF/B-VI and JENDL-3. The effects of this will also be looked at.

Regardless of the outcome of these efforts, the results will be written up in detail for distribution to members of the subgroup this September. Further work, if needed, will be based on suggestions from the subgroup members upon review of the results distributed this fall.

Approval by members of the working group for continuing the comparison to include at least a few double differential neutron spectra, for example at 9, 11, and 14 MeV, is requested. If approved, the work will be completed by May 1993. This comparison may turn out to be interesting since the JENDL-3 Fusion File is new and may have higher quality than either ENDF/B-VI or EFF-2. Experimental data is presently available at 14 MeV, double differential data is needed at energies below 14 MeV for Cr, Fe, and Ni.

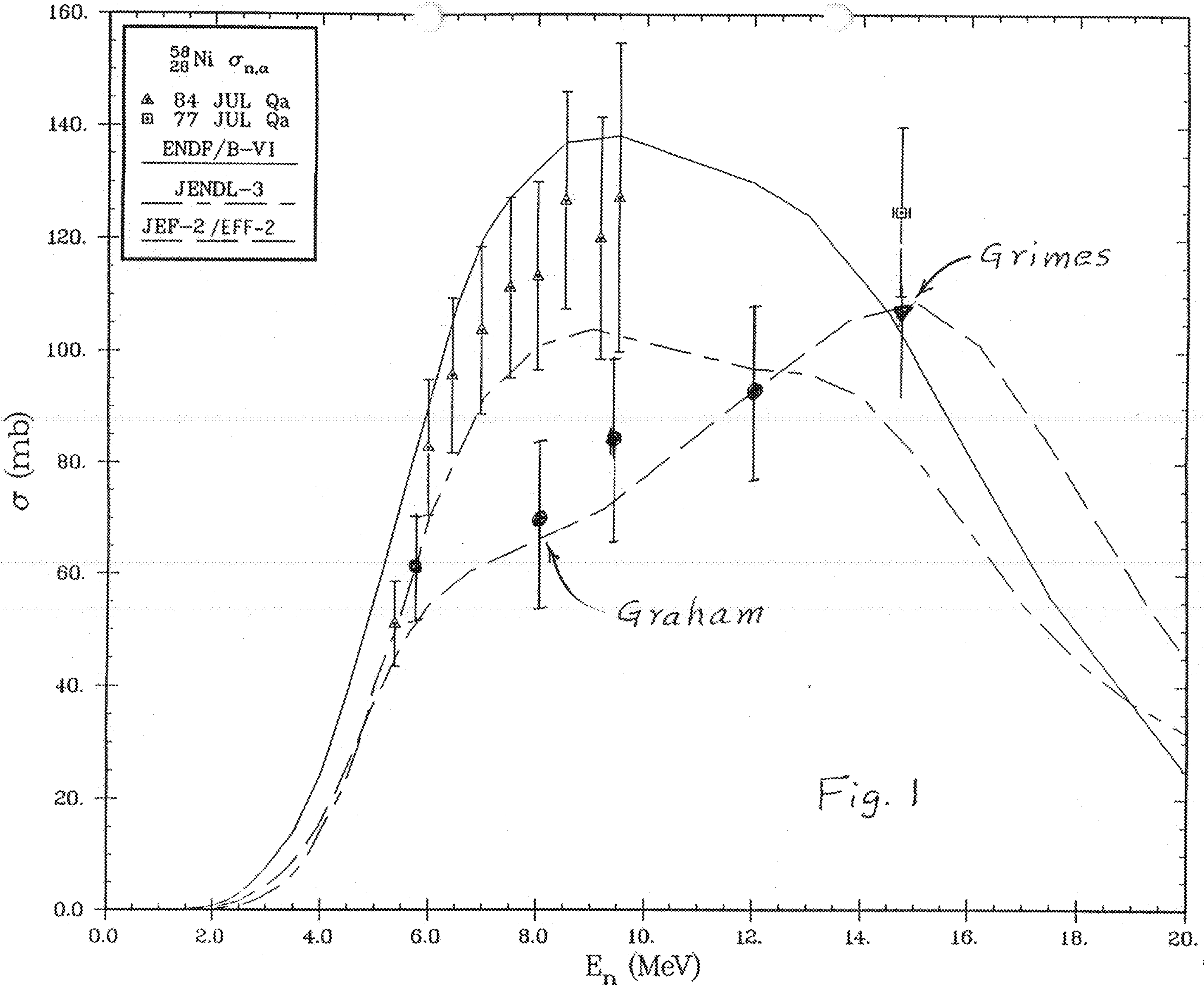
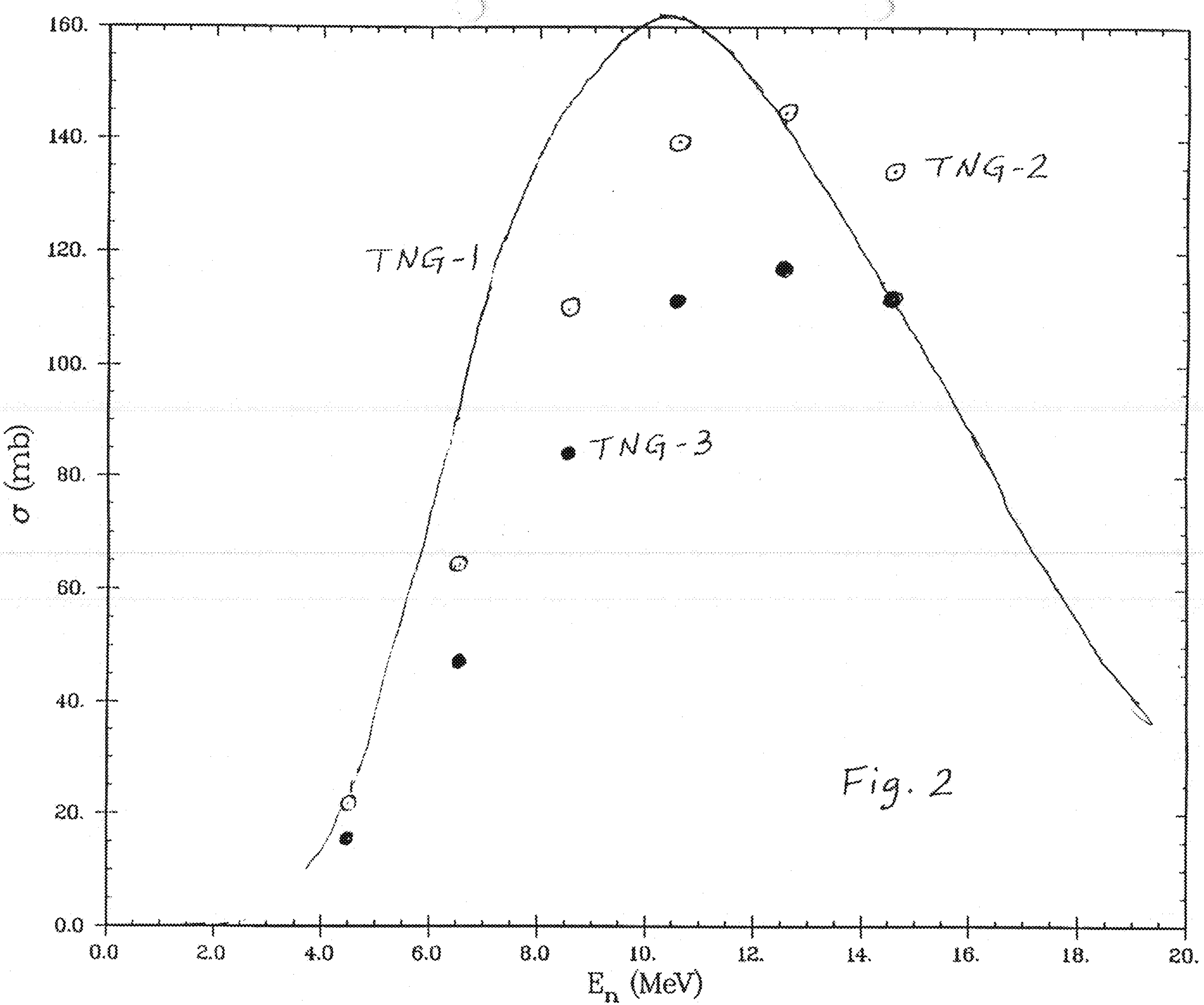
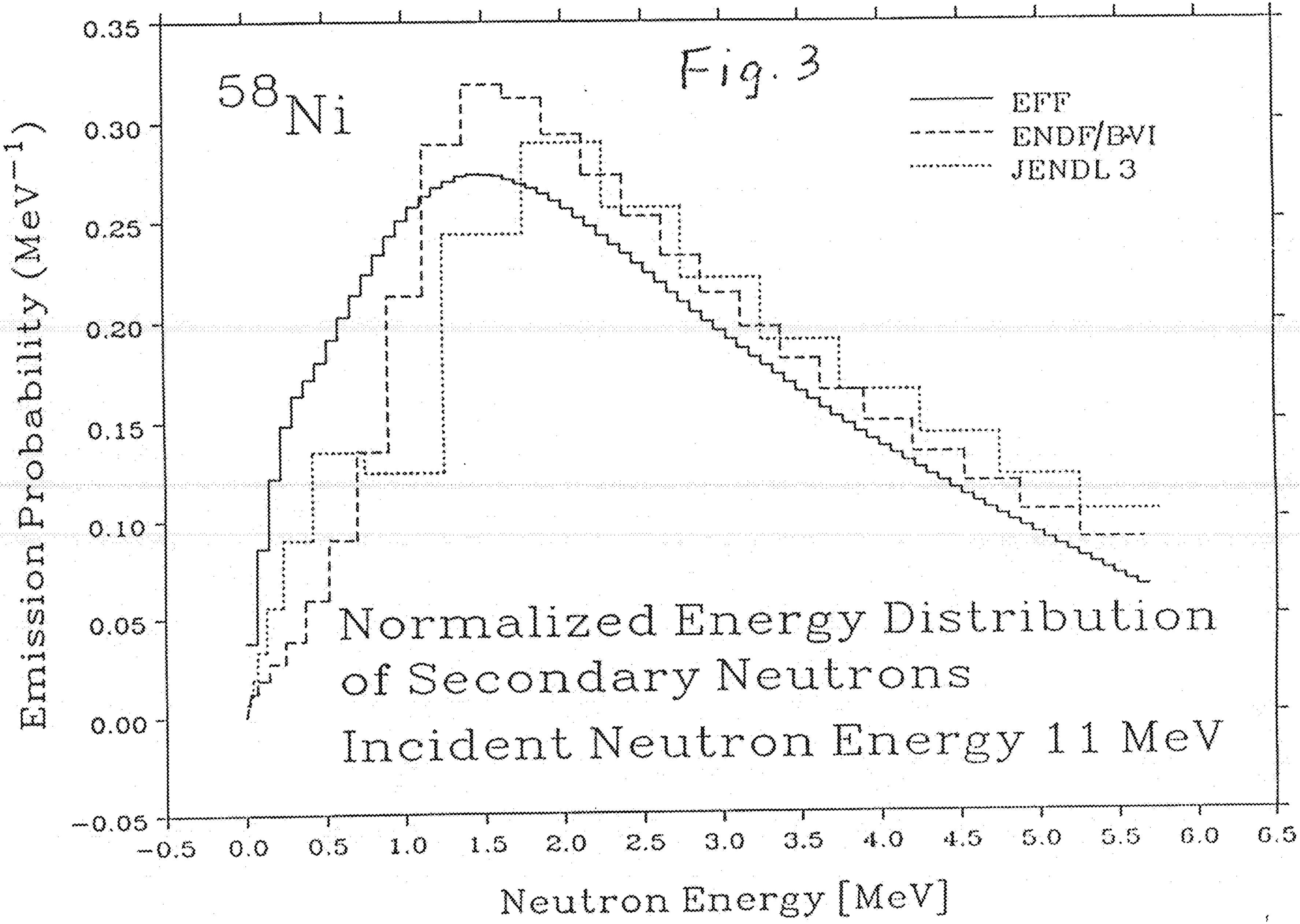

$^{58}_{28}$Ni $\sigma_{n,\alpha}$
84 JUL Qa
77 JUL Qa
ENDF/B-VI
JENDL-3
JEF-2/EFF-2
Grimes
Graham
σ (mb)
160.
140.
120.
100.
80.
60.
40.
20.
0.0
0.0
2.0
4.0
6.0
8.0
10.
12.
14.
16.
18.
20.
$E_n$ (MeV)

Fig. 1



160.
140.
120.
100.
80.
60.
40.
20.
0.0
σ (mb)
0.0
2.0
4.0
6.0
8.0
10.
12.
14.
16.
18.
20.
$E_n$ (MeV)
TNG-1
TNG-2
TNG-3
Fig. 2

Fig. 3



58Ni
EFF
ENDF/B-VI
JENDL 3
Normalized Energy Distribution
of Secondary Neutrons
Incident Neutron Energy 11 MeV
Emission Probability (MeV⁻¹)
Neutron Energy [MeV]

## Table 1

Ni-58: Number of levels per MeV

| 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 |