Final Technical Report

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March 31, 2006

Project Title: "Neutron-Deuterium Cross Section Evaluation"
AECL Purchase Order 217739

SUMMARY AND RECOMMENDATIONS

In general, the overall agreement between the ENDF/B-VI.8 and JENDL 3.3 elastic scattering differential cross sections, except at the extreme backward angles is consistently good, in spite of them being obtained from two distinctly different quantum mechanical formalisms. The agreement between the ENDF and JENDL cross section predictions and the experimental data, however, was inconsistent. This is not completely surprising since the consistency among experimental data sets was also often lacking. In general, the experimental cross sections tend to favor larger differential cross section values at back angles and the trend is for the cross sections to rise more steeply as $\mu \rightarrow -1$ than either ENDF/B-VI.8 or JENDL 3.3 provide.

Because of the paucity of data sets and their age (most were published at least 40 years ago) and inconsistencies, measurements of additional, newer, more precise data are necessary if one is to resolve the questions raised by the recently-reported reactivity sensitivity studies [1].

Therefore, it is recommended that measurements of elastic scattering differential cross sections at incident neutron energies from 200 keV through 3 MeV be made. To ensure adequate coverage, neutron energies of 0.2, 0.5, 1, 1.5, 2, and 3 MeV, as a minimum, are suggested. The angular distributions should be measured from CM scattering angles from 0 to π, with particular attention to back angles (values of μ = -1, -0.9, -0.8, -0.7, -0.5, -0.25, 0, 0,25, 0.5, 0.75 and 0.9 or 1 if possible). These data would then be used to either validate an existing data compilation, or to provide input data for a nuclear data file re-evaluation.

BACKGROUND

During post-release testing of Release 8 of Version VI of the Evaluated Nuclear Data File (ENDF/B-VI.8), it was noted that calculated eigenvalues for a set of heavy-water solution benchmarks had decreased substantially compared to earlier versions of ENDF/B-VI [1]. The main source of the change in the reactivity was determined to be revisions to the elastic scattering angular distributions between the ENDF/B-VI.8 and the earlier version promulgated in ENDF/B-VI.4. In particular, changes in the angular distributions for neutron energies below 3.2 MeV, which were made to improve agreement with laboratory measurements, were determined to be the major cause of the changes in the reactivity calculations for the heavy water benchmarks. These angular distribution revisions were particularly significant for back angles (cosine of the center-of-mass scattering angle < 0) at neutron kinetic energies between 500 and 1000 keV. It was also noted that the angular distributions were slightly more forward peaked in the ENDF/B-VI.8 data than in the ENDF/B-VI.4 data. Hence, the effects on calculated leakage of fast and thermal neutrons using these two data sets differed. For the high neutron leakage heavy-water solution benchmarks the use of ENDF/B-VI.8 resulted in increased leakage and a concomitant reduction in calculated k_{eff} over the values obtained using ENDF/B-VI.4.

In order to help understand these findings, it was proposed to investigate the revised values promulgated in ENDF/B-VI.8 and to evaluate their correctness/validity. To accomplish this investigation, four tasks were proposed to AECL:

1.) Obtain existing neutron-deuterium nuclear cross section data, relevant to fission reactions, from the National Nuclear Data Center at Brookhaven National Laboratory and from the Japan Evaluated Nuclear Data Library at JAERI. (Estimate 10 hours)

2.) Search the published literature for other experimental neutron-nucleus nuclear cross section data at energies relevant to fission reactions. (Estimate 10 hours)

3.) Review the existing neutron-deuterium nuclear cross section data (i.e. ENDF/B-VI.8, JENDL-3.3, etc.), particularly the angular scattering distributions at MeV and sub-MeV energies of relevance to fission reactions, with a view to assessing their reliability and accuracy. In particular, attempt to determine how the ENDF/B-VI data were generated (i.e. fits to actual measured data (which ones?) or calculations using a computer model or code) and assess their validity. (Estimate 25 hours)

4.) Provide final report with recommended course of action to AECL. (Estimate 15 hours)

ANALYSIS AND RESULTS

Task 1

Compilations of data for the ENDF/B-VI.4, ENDF/B-VI.8, JENDL 3.3, and JEFF 3.1 evaluations were obtained from the website maintained by the U. S. National Nuclear Data Center (NNDC) at Brookhaven National Laboratory. Compilations of total, elastic and angular distribution cross sections were obtained for neutron-deuterium (ND) collisions over energies ranging from sub-MeV to tens of MeV.

Experimental data for neutron-deuterium cross section measurements in the keV to ~10 MeV range were obtained from the CINDA database at NNDC. Data were downloaded in the EXFOR output format. Electronic copies of the original papers for most of the relevant experimental datasets were obtained from various libraries.

Task 2

Searches for other experimental angular distribution data sets for neutron-deuterium scattering at energies below ~10 MeV using various Internet search engines found no additional published data relevant to this investigation.

Task 3

A review of the evaluated nuclear data files for the ENDF/B-VI.8, JENDL 3.3 and JEFF 3.1 compilations revealed that the elastic scattering angular distribution probabilities and total elastic cross sections for ND scattering were identical in the ENDF and JEFF compilations down to energies as low as 1 keV. The elastic scattering cross sections in the JENDL compilation were only slightly (< 1%) different than those in the other two compilations. Hence, any differences in the angular distribution probabilities in the different compilations at energies ranging up to ~10 MeV are not due to differences in the elastic scattering cross sections. Since the ENDF/B-VI.8 and JEFF 3.1 datasets appear to be the same for ND scattering, no further consideration was given to the JEFF 3.1 compilation.

Comparisons of elastic scattering angular distribution probabilities from the ENDF and JENDL compilations revealed significant differences at various neutron energies and center of mass scattering angles, especially for back angles. Typically, the ENDF/B-VI.8 probabilities tended to be the smallest at back angles and the largest at forward angles in the center of mass system, although the differences between them at forward angles were generally small.

The angular distribution probabilities below 3.2 MeV in the ENDF compilation were obtained using a coupled channels R-matrix formulation and first promulgated in the ENDF/B-VI Mod 4 (1997). Previously, the elastic scattering angular distributions were based upon an analysis originally published by Stewart and Horsley in LA-3271in 1968. The elastic scattering angular distribution probabilities in the JENDL compilations are obtained using a Faddeev three-body scattering formalism.

Since the ENDF and JENDL compilations use different quantum mechanical scattering methods to generate their elastic scattering angular distributions, it was decided to compare their predictions at neutron energies between ~200 keV and 3 MeV with available experimental data. To carry out these comparisons it was necessary to convert the tabulated probabilities [f(μ, E)] into differential cross sections σ(μ, E) in units of mb/sr using

$$\sigma(\mu,E)=\frac{\sigma_S(E)}{2\pi}\,f(\mu,E)$$

where $\sigma_s(E)$ is the elastic scattering cross section. The differential cross sections obtained using the ENDF/B-VI.8 and JENDL 3.3 elastic scattering angular distribution probabilities are displayed in Figures 1 through 9. Also displayed are relevant experimental cross sections [2-6]. Error bars, if quoted in the experimental data and if larger than the symbols used to display the data, are also shown. Data were obtained from the CINDA database. The energies displayed were selected based upon the availability of the experimental data for comparisons.

220 keV Results

Figure 1 displays the results obtained at a neutron energy of 220 keV. Both evaluated data sets are peaked at back angles and decrease monotonically as the cosine of the scattering angle (μ) increases. The ENDF curve has a smaller slope than the JENDL curve. Neither fits the experimental data very well, especially at back angles. The experimental data from Adair [2] suggest that the cross section may be isotropic in the CM system, although the error bars are large (~15%). Since these data are very old (published more than 50 years ago) and have large error bars, the reliability of these data may be suspect.

500 keV Results

Figure 2 displays the results for 500 keV neutron scattering. Here the differences between the ENDF and JENDL results are fairly small, except at back angles where the JENDL cross sections are increasing more rapidly than the ENDF ones as μ decreases. Also plotted are data from the Adair [2] and Elwyn [3] experiments. Note that the Elwyn data (published in 1962) have a much steeper slope than the Adair data as μ increases. The error bars on the Elwyn data are also much smaller (~5%) than the Adair data error bars (~15%). At back angles the Elwyn data are significantly larger than either the JENDL or ENDF evaluations, although both calculations agree fairly well with the Elwyn data at forward angles. The Adair data, however, fall well below the Elwyn data and below both evaluated data sets at back angles. The Adair data also have a much smaller slope with increasing μ than both evaluated data compilations and the Elwyn data set. Adair also provides additional data for neutron energies above 500 keV but these data were not plotted since the trends appear to be the same as with the lower energy data and the error bars are still fairly large.

1 MeV

The 1 MeV elastic scattering differential cross sections are plotted in Figure 3 for ENDF, JENDL, and the Elwyn data [3]. Except at the back angles (μ ~ -1), the two compilations and the experimental data agree fairly well. Again, the JENDL cross sections are larger than the ENDF ones as μ decreases, and both are smaller than the measured value reported by Elwyn. Note also that the cross sections are now increasing as μ increases for the forward angles.

1.2 MeV

Figure 4 displays results for 1.2 MeV neutrons. Again the ENDF and JENDL results are fairly close except at back angles. Their agreement with the data of Vendrenne [4], published in 1966, is poor. Neither data compilation agrees with the experimental data. The compilations and experiments only agree for CM angles near 90° and 180°. The minimum cross sections for the Vendrenne data appear to occur for values of μ ~ 0, whereas the minima in the JENDL and ENDF curves appear to occur for μ ~ 0.3-0.4.

1.71 MeV

Figure 5 displays results for neutrons at 1.71 MeV. The two evaluated data compilations agree fairly well except for extreme back and forward angles. Neither compilation agrees with the Vendrenne experimental data. The experimental cross sections are smaller and flatter than the evaluated data compilations.

2 MeV

Figure 6 displays curves from the ENDF and JENDL calculations, and data from the Elwyn [3] and Weber [5] experiments. The experimental data from Weber (published in 1981) are only for values of $\mu < 0$. Except for the extreme back angles ($\mu \sim -1$), the agreement between compilations and data is good. Both experimental data sets tend to favor larger cross sections at the back angles.

2.22 MeV

Figure 7 displays curves from the ENDF and JENDL calculations, and experimental data from Vendrenne [4]. As was the case for scattering at 1.2 and 1.71 MeV neutron energies, the agreement between the compilations and the experimental data is poor, especially at back angles. Although the experimental cross sections are smaller at all angles, the calculated cross sections from the compilations appear to have flatter distributions than the experimental data.

2.4 MeV

Figure 8 displays curves from the ENDF and JENDL calculations, and experimental data from Chatelain [6], which were published in 1979. The agreement between the predictions of the compilations and the measurements of Chatelain is fairly good at forward angles ($\mu > 0$) and at extreme back angles ($\mu \sim -1$), but is generally poor in between, especially in the range of $\mu \sim -0.5$ to $- 0.75$ where differences exceeding 50 % are noted. It is interesting to note that the Weber data [5] at 2 MeV appear to be part of a follow-on series of measurements to the Chatelain experiment [6].

3.2 MeV

Figure 9 displays results for 3.2 MeV neutrons. Curves from the ENDF and JENDL calculations are displayed with data taken from Vendrenne [4]. Although there is improved agreement between compilations and experiment for values of $\mu \sim -0.7$ to $+0.5$, there is clear disagreement at the extreme forward and backward angles. The substantial disagreement between these data and the compilation predictions at all energies tested, and the differences in the shapes of the calculated distributions and experimental measurements, lead me to question the accuracy and reliability of these data.

<u>Overall Assessment of Comparisons Between ENDF/B-VI.8 and JENDL 3.3 with Experimental Data</u>

The overall agreement between the ENDF/B-VI.8 and JENDL 3.3 cross sections, except at the extreme backward angles, is fairly good, in spite of them being obtained from two distinctly different quantum mechanical formalisms. The agreement between the ENDF and JENDL cross section predictions and the experimental data was inconsistent. This is not completely surprising since the consistency between experimental data sets was often lacking. In general, the experimental cross sections tend to favor larger cross section values at back angles and the trend, except for the Adair data at low energies, is for the cross sections to rise more steeply as $\mu \rightarrow -1$.

All of these data sets were published over 25 years ago. Several were over 40 years old. While age of the data, by itself, does not indicate that they are incorrect or not useful, the paucity of data sets in this neutron energy range and the inconsistencies between them suggest that additional, newer, more precise data are needed if one is to resolve the questions raised by the recently-reported reactivity sensitivity studies [1].

There are a larger number of additional data sets available for a variety of neutron energies between 3.2 and 14 MeV in the CINDA database. Several included measurements reported in the mid 1980's to mid 1990's. However, because of time constraints, these were not extensively reviewed and will not be further addressed in this report. Most were at beam energies ~ 7 - 10 MeV.

RECOMMENDATIONS

Measurements of elastic scattering differential cross sections at incident neutron energies from 200 keV through 3 MeV are suggested. To ensure adequate coverage, neutron energies of 0.2, 0.5, 1, 1.5, 2, and 3 MeV, as a minimum, are suggested. The angular distributions should be measured from CM scattering angles from 0 to π, with particular attention to back angles (values of μ = -1, -0.9, -0.8, -0.7, -0.5, -0.25, 0, 0,25, 0.5, 0.75 and 0.9 or 1 if possible). Measurements below 200 keV should also be considered since I was unable to locate any data for energies below 100 keV, and only a single data set (published around 1955) at 100 keV.

As a check on the consistency of any measurements undertaken in response to the above recommendation, and as a further check on the quality of existing experimental data at energies above 3.2 MeV, additional measurements at 2 or 3 energies ranging up to 10 MeV could be made if desired (e.g., neutron energies of 4, 7, and 10 MeV).

REFERENCES

[1] R. D. Mosteller, K. S. Kozier, J. M. Campbell and R. C. Little, “Reactivity Impact of Deuterium Cross Sections for Heavy-Water Benchmarks,” Los Alamos National Laboratory Report LA-UR-05-3992 (2005).

[2] R. K. Adair, A. Okazaki and M. Walt, “Scattering of Neutrons by Deuterons,” Physical Review, Vol. 89, No. 6, (1952), 1165.

[3] A. J. Elwyn, R. O. Lane and A. Langsdorf, Jr., “Polarization and Differential Cross Sections in n-d Scattering,” Physical Review, Vol. 128, No. 2 (1962), 779.

[4] G. Vendrenne, “Neutron Interactions on Deuterium,” Journal de Physique – Colloque, Vol. 27, No. 1 (1966), 71.

[5] J. Weber, ”The nd Differential Elastic Cross Section at 2 MeV,” Helvetica Physica Acta, Vol. 54 (1981), 547.

[6] P. Chatelain, Y. Onel and J. Weber, “The nd Elastic Differential Cross Section at E = 2.48 and 3.28 MeV,” Nuclear Physics A, Vol. 319, No. 1 (1979) 71.

Fig. 1 - 220 keV nd Angular Distribution

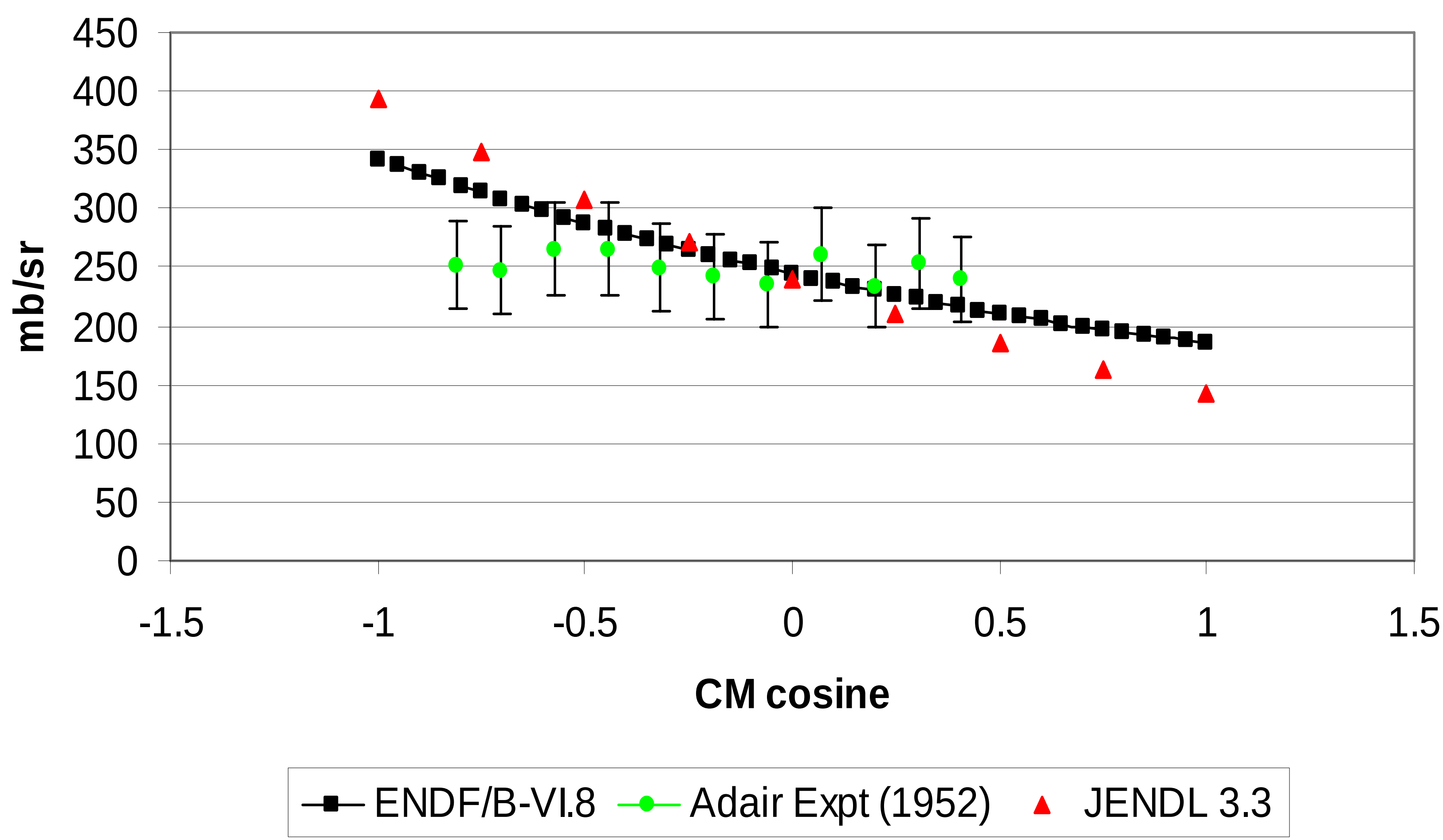
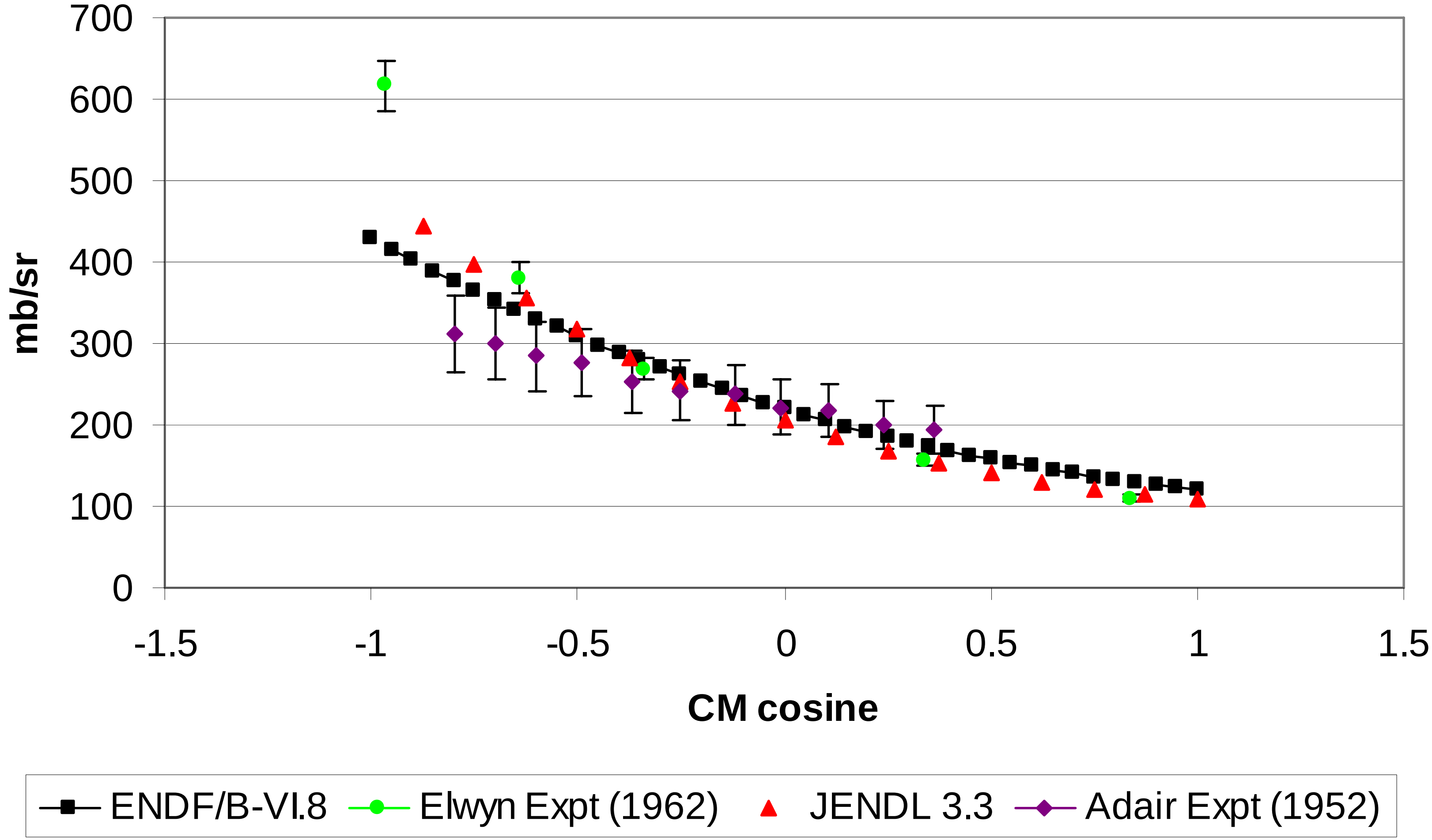


Fig. 2 - 500 keV nd Angular Distribution



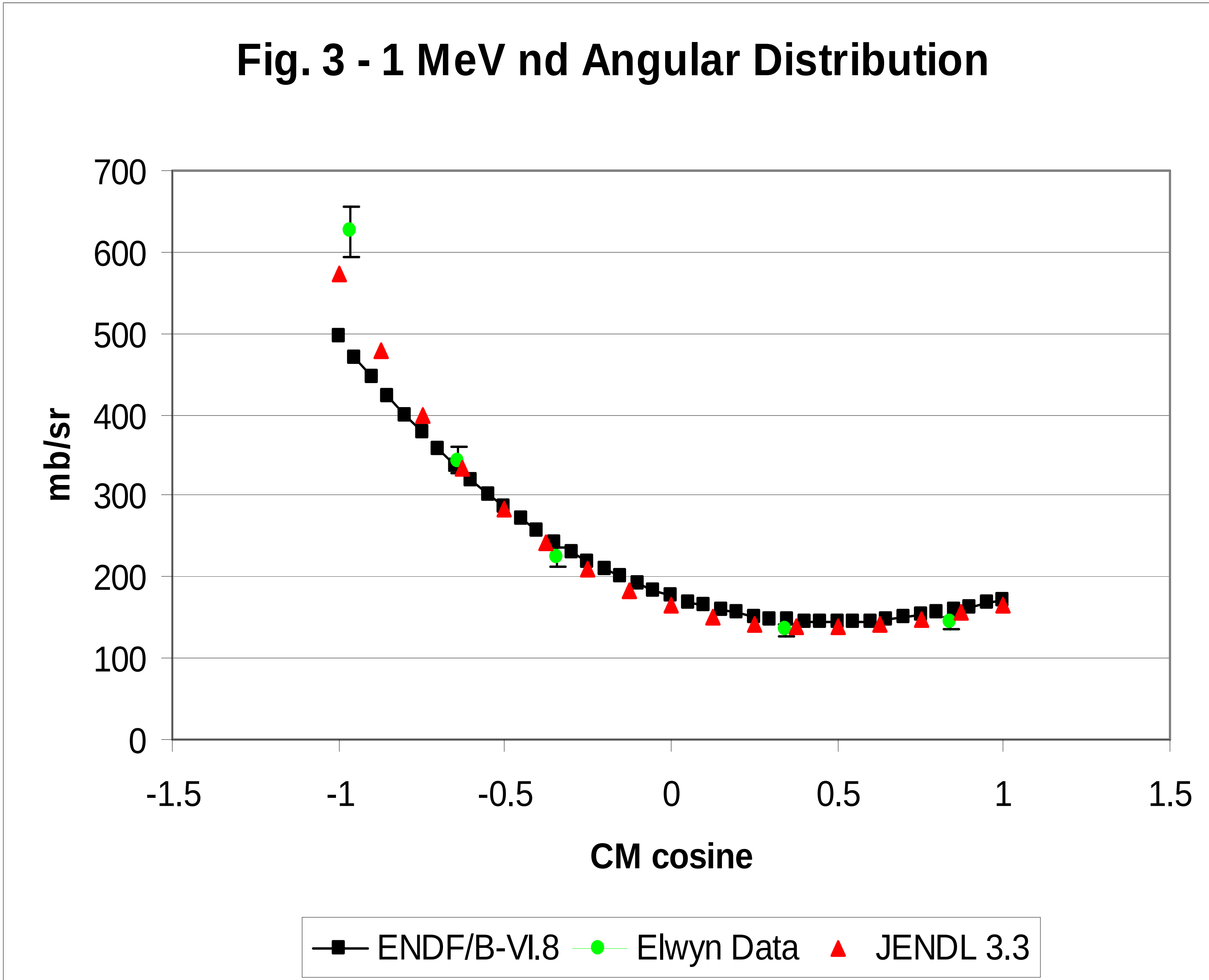


Fig. 3 - 1 MeV nd Angular Distribution
mb/sr
700
600
500
400
300
200
100
0
-1.5
-1
-0.5
0
0.5
1
1.5
CM cosine
ENDF/B-VI.8
Elwyn Data
JENDL 3.3

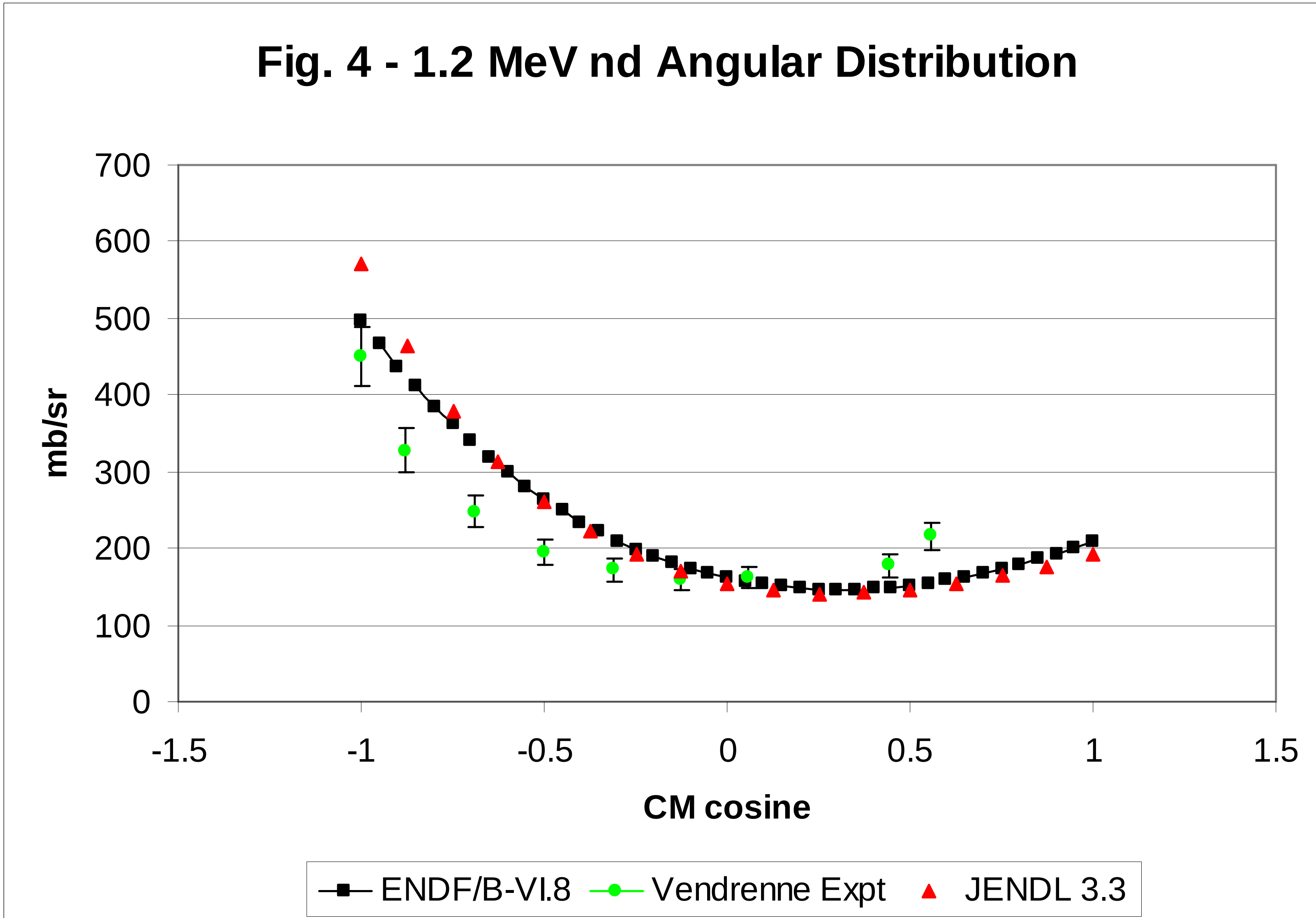


Fig. 4 - 1.2 MeV nd Angular Distribution
mb/sr
700
600
500
400
300
200
100
0
-1.5
-1
-0.5
0
0.5
1
1.5
CM cosine
ENDF/B-VI.8
Vendrenne Expt
JENDL 3.3

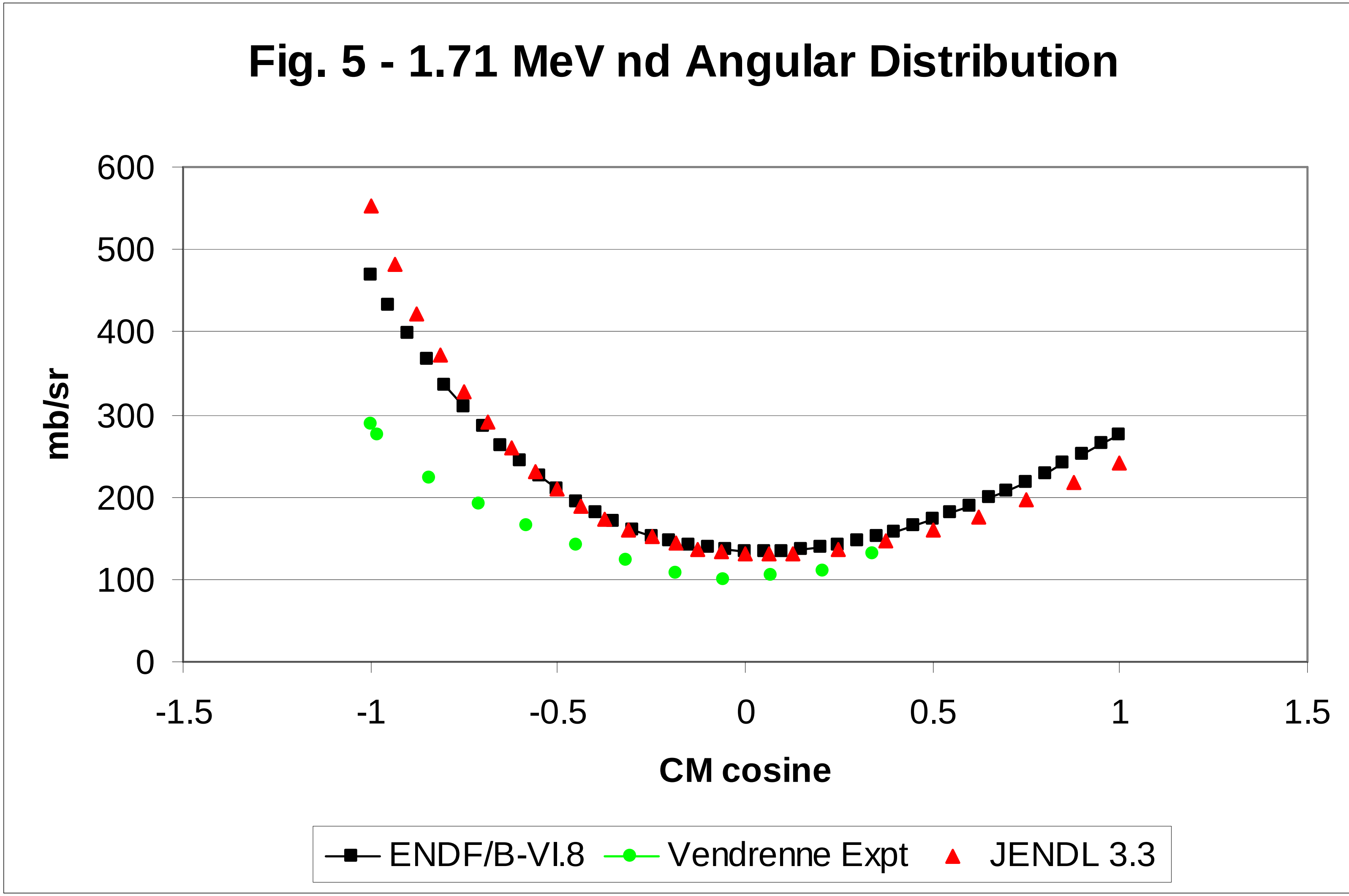


Fig. 5 - 1.71 MeV nd Angular Distribution
mb/sr
600
500
400
300
200
100
0
-1.5
-1
-0.5
0
0.5
1
1.5
CM cosine
ENDF/B-VI.8
Vendrenne Expt
JENDL 3.3

Fig. 6 - 2 MeV nd Angular Distribution

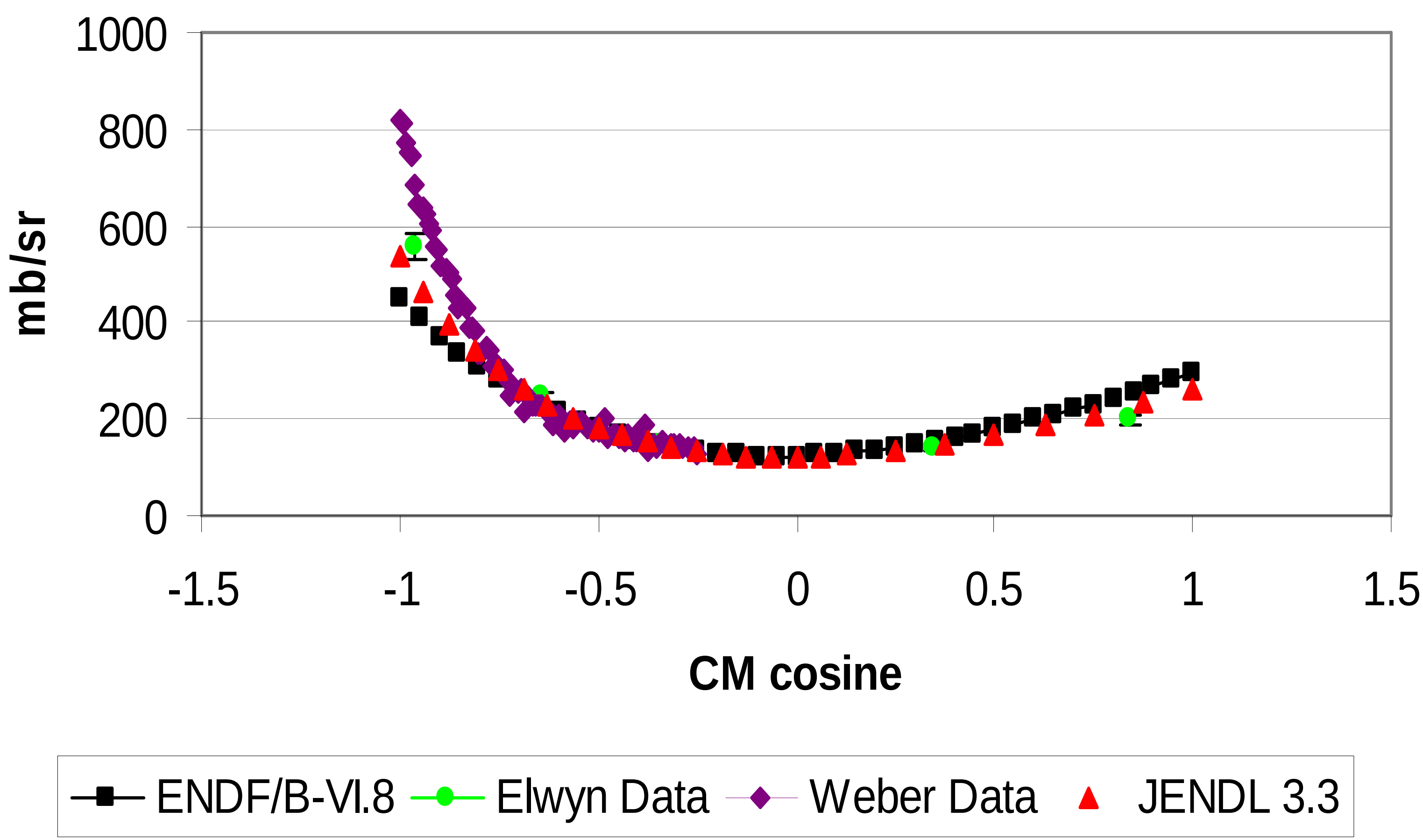


Fig. 7 - 2.22 MeV nd Angular Distribution

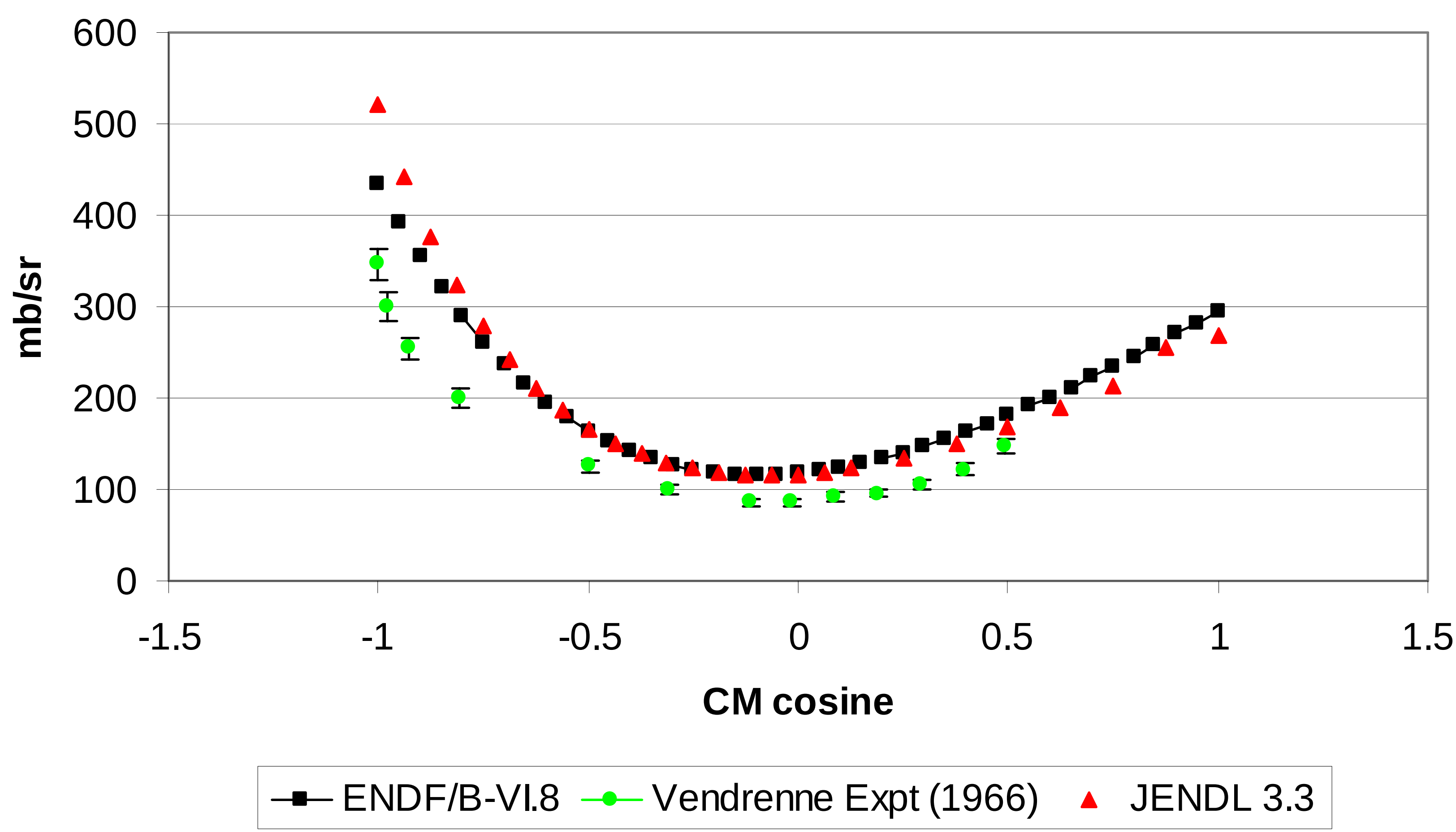


Fig. 8 - 2.4 MeV nd Angular Distribution

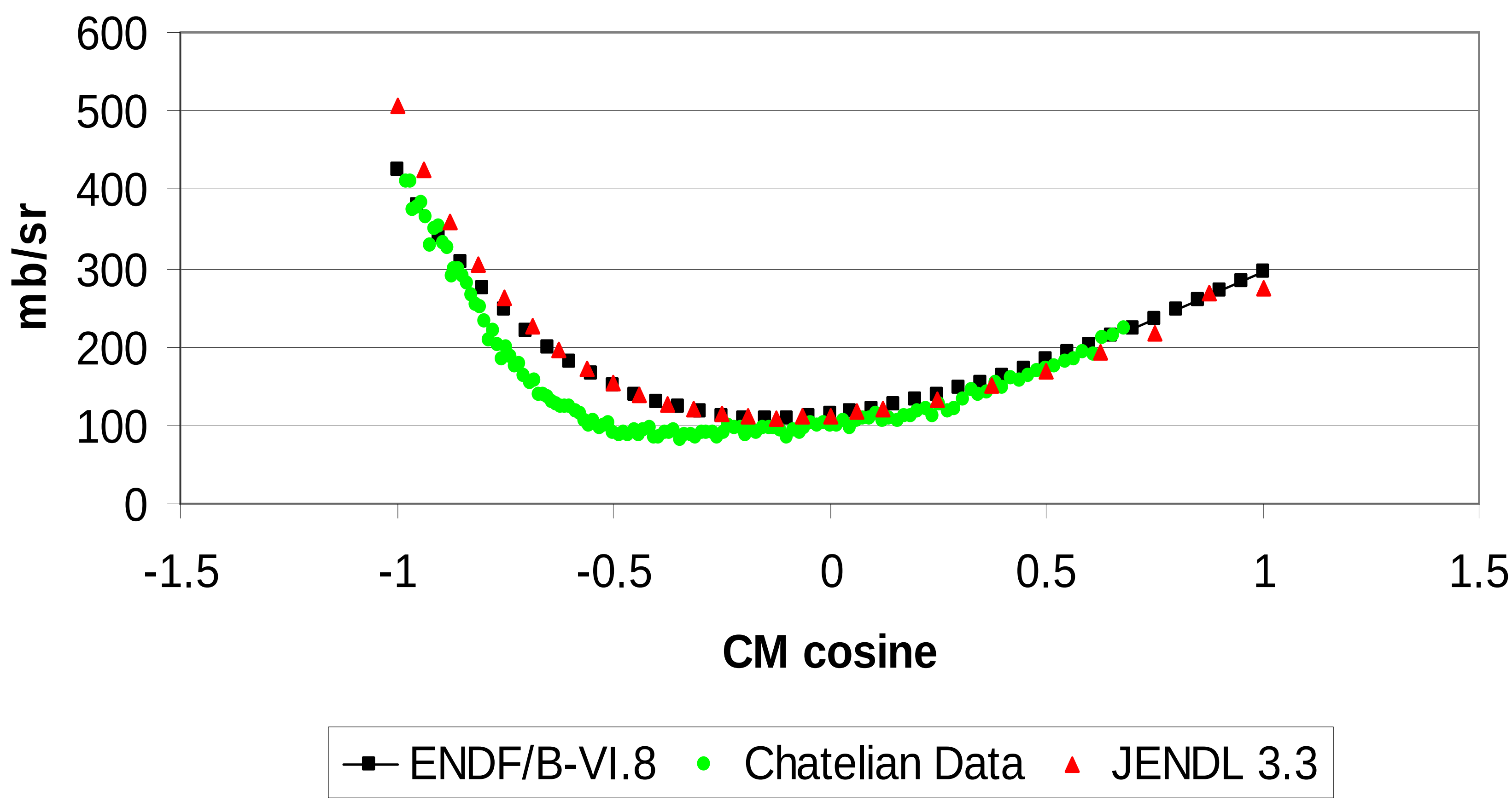


Fig. 9 - 3.2 MeV nd Angular Distribution