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AUTHOR(S): A. D. Carlson, NBS
W. P. Poenitz, Argonne-West
G. M. Hale, T-2
R. W. Peelle, ORNL

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Los Alamos Los Alamos National Laboratory
Los Alamos, New Mexico 87545

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THE NEUTRON CROSS SECTION STANDARDS EVALUATIONS FOR ENDF/B-VI

A. D. CARLSON
National Bureau of Standards, Gaithersburg, MD 20899, U.S.A

W. P. POENITZ
Argonne National Laboratory, Argonne-West,
Idaho Falls, ID 83403-2528, U.S.A.

G. M. HALE
Los Alamos National Laboratory, Los Alamos, NM 87545, U.S.A

R. W. PEELLE
Oak Ridge National Laboratory, Oak Ridge, TN 37830, U.S.A

Abstract The neutron cross section standards are now being evaluated as the initial phase in the development of the new ENDF/B-VI file. These standards evaluations are following a somewhat different process compared with that used for earlier versions of ENDF. The primary effort is concentrated on a simultaneous evaluation using a generalized least squares program, R-matrix evaluations, and a procedure for combining the results of these evaluations. The ENDF/B-VI standards evaluation procedure is outlined, and preliminary simultaneous evaluation and R-matrix results are presented.

INTRODUCTION

The Cross Section Evaluation Working Group (CSEWG) is now developing a new version of its Evaluated Nuclear Data File, ENDF/B-VI. As a first step in this process, the neutron cross section standards are being evaluated by the Standards Subcommittee of CSEWG. It was recognized that many evaluations have involved a procedure of qualitatively or semi-quantitatively combining different kinds of data sets by drawing a smooth curve through the existing data. Such evaluations are difficult to document and it is not clear how to determine meaningful uncertainties and covariance information.

In previous standards evaluations for ENDF/B, a hierarchical approach was followed. The order was generally the following: H(n,n) was considered the best known standard and was evaluated first and independently of the other standards. This standard is considered to be so well-known that measurements relative to the hydrogen standard are often called absolute measurements. The ^{6}Li(n,t) cross section evaluation was then performed. The only ^{6}Li(n,t) data which were used were absolute measurements or those measured relative to the H(n,n) which were converted to cross sections using the adopted hydrogen evaluation. Then the ^{10}B+n standard cross sections were evaluated. The only ^{10}B(n,α_1) and ^{10}B(n,α) data used were absolute measurements and those relative to H(n,n) or ^{6}Li(n,t) which were converted using the new hydrogen and lithium evaluations. This process was continued for all the standards. This method for using ratio measurements does not use all the information available. For example, a ratio of the ^{10}B(n,α) to ^{6}Li(n,t) cross sections would be used in the ^{10}B(n,α) cross section evaluation but not in the ^{6}Li(n,t) evaluation. For the new ENDF standards evaluation it was felt that a simultaneous evaluation should be performed to assure proper use of the available information. Thus ratio measurements of standard cross sections will have an impact on the evaluation of each of the standard cross sections in the ratio. Correlations among the experimental data should also be taken into account in the simultaneous evaluation.

To the extent that good quality absolute data on a given cross section are available in addition to measurements of that cross section relative to standards, the evaluation of that cross section (though it is not recognized as a "standard") should be performed simultaneously with the standards evaluation since it in principle will affect the values of the evaluated standard cross sections and their uncertainties. As a practical matter this combination of data from many nuclides can become a very immense problem though it can be handled. Very few cross sections would have any appreciable impact on the determination of a standard cross section other than other standards. Including data on ^{238}U(n,γ), ^{238}U(n,f), and ^{239}Pu(n,f) could improve the quality of the standards evaluations since precise absolute measurements exist and many ratio measurements to the standards are available. There is, of course, the benefit that evaluations of these important fuel cross sections will be obtained.

On the other hand, the Standards Subcommittee felt that it is important to include R-matrix analyses in the evaluation of the light element standards. Such analyses provide coupling to reaction theory and give a smooth meaningful analytical expression for the energy dependence of the cross sections. The accurate determination of the R-matrix level parameters does require a large data base. This method had been used successfully in earlier versions of ENDF/B in the evaluation[1-2] of the ^{6}Li and ^{10}B standard neutron cross sections. Data in addition to angle integrated neutron cross sections such as differential cross sections, polarizations, and charged particle measurements involving the same compound nucleus were shown[3] in these analyses to have a significant impact on the standard cross sections. In the R-matrix analysis, different reactions leading to the same compound nucleus are linked by unitarity to the standard cross section. This condition imposes constraints on the standard cross section which are particularly strong near resonances. Work[4] is underway to include particle exhange effects in the ^{7}Li R-matrix analysis.

The R-matrix and simultaneous evaluation methods should be less sensitive to systematic uncertainties assuming these uncertainties are uncorrelated among the different kinds of data sets.

The ENDF/B-VI standards evaluation will, therefore, involve a simultaneous evaluation and R-matrix analyses. This approach will take advantage of the strengths of the two different analysis modes which make use of different classes of experimental information to impact on the evaluation of the standard cross sections. Independent data bases will be used for the two methods of evaluation. It will then be necessary to combine the information obtained from these analyses in a proper way to form the final evaluation and its variance-covariance matrix.

EVALUATION PROCEDURE

The evaluation as outlined above will require a simultaneous evaluation using generalized least squares, R-matrix evaluations for the ^{6}Li+n and ^{10}B+n systems and a procedure for combining the results of these evaluations.

It was decided that the hydrogen scattering cross section used in this evaluation would be fixed since it is known quite well. The new evaluation[5] by Dodder and Hale has been accepted as the new hydrogen standard for ENDF/B-VI. This evaluation is a result of the analysis of n-p and p-p data using the R-matrix formalism. In Fig. 1 the ENDF/B-VI evaluation and high accuracy total neutron cross section measurements are compared with ENDF/B-V. The evaluation is in somewhat better agreement with measurements than the ENDF/B-V (Hopkins-Breit)[6] results. There is also a reduction in the reported uncertainty of the hydrogen cross section for the new evaluation, compared with that of ENDF/B-V.

The thermal cross sections recommended by Holden[7] for Au(n,γ) and by Divadeenam and Stehn[8] for ^{235}U(n,f), and ^{239}Pu(n,f) have been used as input data for the evaluations, though they have not yet been officially accepted as ENDF/B-VI data.

Measurements of the fission cross sections of ^{235}U and ^{239}Pu averaged over the ^{252}Cf spontaneous fission neutron spectrum are also to be included in the data base. These data can be obtained with high accuracy and are only weakly dependent on the uncertainties in the ^{252}Cf spontaneous fission neutron spectrum.

The simultaneous evaluation[9-10] is being performed with the generalized least squares program GMA. The cross sections being evaluated are ^{6}Li(n,t), ^{6}Li(n,n), ^{10}B(n,α_0), ^{10}B(n,α_1), ^{10}B(n,n), ^{197}Au(n,γ), ^{235}U(n,f), ^{238}U(n,f), ^{238}U(n,γ), and ^{239}Pu(n,f). This evaluation uses a large data base file being assembled at Argonne National Laboratory. The data base includes both shape and absolute measurements of these cross sections and their ratios.

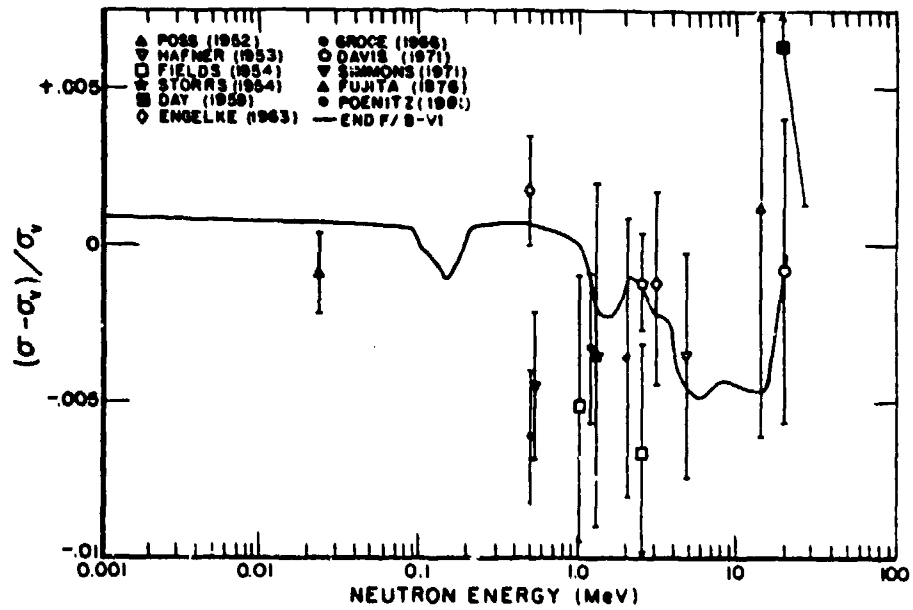

Fig. 1. Comparison of high accuracy measurements of the hydrogen total neutron cross section and the ENDF/B-VI evaluation with the ENDF/B-V evaluation. References for the experimental data are given in Ref. 14.

In addition, total cross section measurements for ^{6}Li and ^{10}B are contained in the data base since the scattering and reaction data are interrelated to these measurements. Considerable effort has been expended in examining the various experiments looking for corrections, etc. which have not been fully documented in the published papers. Ratio measurements other than those to the hydrogen standard which have been converted to cross section values are reinstated to the originally measured quantities. Measurements relative to hydrogen have been converted using the new ENDF/B-VI evaluation. Perhaps the most difficult part of this work has been the determination for each experiment of the uncertainties and correlations in that experiment and correlations with other experiments. This information is used to form covariance matrices for the measurements so that a full covariance analysis can be performed for the evaluation. An energy grid is defined for the evaluation which is the same for all cross sections involved in the evaluation and the fitting parameters are the values of the cross sections at these grid points.

The R-matrix fits[11] are being done at Los Alamos National Laboratory with the program EDA. In these analyses the experimental data are used as measured with weighting normally based on the quoted uncertainties. It is assumed that no correlations other than the overall normalization are present among the data from a particular experiment. The code uses automated search routines to minimize X^2 of the fits to the input data. In addition to the R-matrix parameters, derivatives of fitted cross sections with respect to these parameters and the covariance matrix are available as output. Following the fitting process, the cross sections will be calculated for the same energy grid as is used for the simultaneous evaluation to permit the combination of the results. The ^{6}Li+n and ^{10}B+n analyses are each being done separately with this code. For the ^{7}Li system the data base includes ^{6}Li total, ^{6}Li(n,n) integrated, ^{6}Li(n,n) differential, ^{6}Li(n,n) polarization, ^{6}Li(n,t) integrated, ^{6}Li(n,t) differential, ^{4}He(t,t) differential, and ^{4}He(t,t) polarization data. For the ^{11}B system the data base includes ^{10}B total, ^{10}B(n,n) integrated, ^{10}B(n,n) differential, ^{10}B(n,n) polarization, ^{10}B(n,α_0) integrated, ^{10}B(n,α_0) differential, ^{10}B(n,α_1) integrated, ^{10}B(n,α_1) differential, ^{7}Li(α,α_0) differential, ^{7}Li(α,α_1) differential, and ^{7}Li(α,n) differential data.

A procedure[12] for combining the simultaneous and R-matrix evaluations has been defined. It is based on the observation that the individual fitting processes described above include computation of sums that can be combined to produce the same overall output parameters as would have been obtained from a global least squares fit of all the input data in terms of R-matrix parameters for the ^{6}Li+n and ^{10}B+n systems and pointwise values for the other cross sections. A program for performing the combination is being written at Oak Ridge National Laboratory. This procedure requires that the boron and lithium experimental data be separated into two uncorrelated groups, one to be used in the simultaneous evaluation and the other in the R-matrix analyses. All ratio measurements other than those to the hydrogen standard are used in the simultaneous evaluation. The combining procedure makes use of the variance-covariance matrices from the separate fits as well as the derivatives with respect to the evaluation parameters of the fitted values corresponding to the input data elements. The output will be adjusted R-matrix parameters for the ^{6}Li+n and ^{10}B+n systems and final point cross sections for the remaining reactions, by taking into account in a consistent manner all the input data sets. If the procedure succeeds, the adjusted R-matrix parameters will be used to calculate the ^{6}Li+n and ^{10}B+n cross sections for ENDF/B-VI. It is expected that the procedure will work if the underlying data base does not contain serious inconsistencies.

PRELIMINARY RESULTS OF THE EVALUATION

As a first step in the evaluation process, the R-matrix and simultaneous evaluations have each been performed using the best data base for their respective analyses. Some common lithium and boron data sets have been used in the evaluations. These will be referred to as the partially overlapping data base analyses. Data base differences are thus reduced for these analyses and better consistency should be obtained. This also represents a baseline to be compared with the results obtained with the non-overlapping data base analyses. The degree of change in the cross sections for the different data bases will indicate the sensitivity to data base changes.

Analyses have also been done with a first attempt at grouping to provide non-overlapping data bases. It should be noted that the deletion of common data sets in forming non-overlapping data bases results in a poorer data base for each of the separate evaluations. Some preliminary results obtained with both the non-overlapping and partially overlapping data bases are shown in subsequent figures. It must be emphasized that any conclusions given here are based on the assumption that the results will not change significantly with the final grouping of the data and the use of the combination procedure.

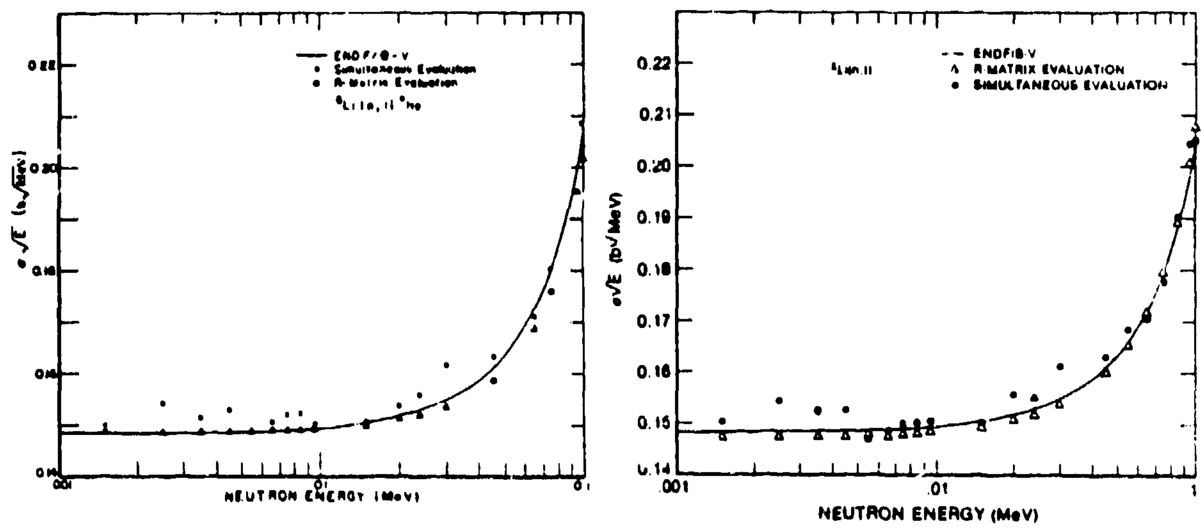

Fig. 2. Preliminary results of the simultaneous and R-matrix evaluations for the ^{6}Li(n,t) cross section for neutron energies from 0.001-0.1 MeV compared with the ENDF/B-V evaluation. The data on the left part of the figure are from the partially overlapping data base analyses. Those on the right are from the non-overlapping data base analyses.

In Fig. 2 the ^{6}Li(n,t) results are compared with ENDF/B-V for the energy region from 1-100 keV. This cross section is used as a standard for ENDF/B-V for neutron energies below 100 keV. There is no smoothing of the output from the simultaneous evaluation. Smoothing will not be required for the ^{6}Li+n and ^{10}B+n simultaneous evaluation results since the information from the simultaneous evaluation will be used to help create the adjusted R-matrix parameters. There is general agreement between the simultaneous and

R-matrix results but the simultaneous evaluation results are systematically somewhat higher than those of the R-matrix calculations for both the partially overlapping and non-overlapping data bases. The ENDF/B-V evaluation agrees well with the present results. The version V evaluation is generally between the results of the simultaneous and R-matrix evaluations. In Fig. 3 the ^{6}Li(n,t) results near the ~ 240 keV resonance are compared. The agreement is good among all three sets of data. For the non-overlapping data bases, the cross section at the peak of the resonance determined from the R-matrix analysis agrees well with ENDF/B-V and is ~ 3% higher than that obtained from the simultaneous evaluation. For the partially overlapping data bases, the cross section difference near the peak of the resonance is smaller but the width of the resonance is somewhat wider with larger cross sections in the wings for the simultaneous evaluation compared with the R-matrix results. Further work to be done on the data base for the simultaneous evaluation by shifting the data for some experiments to a common resonance energy should reduce this difference. The small differences between the present R-matrix results and those of ENDF/B-V indicate that the present data base is consistent with that used in the R-matrix analysis for ENDF/B-V. In general for the ^{6}Li(n,t) cross section, though differences exist between the partially overlapping and non-overlapping analyses, they are not so large that problems are expected.

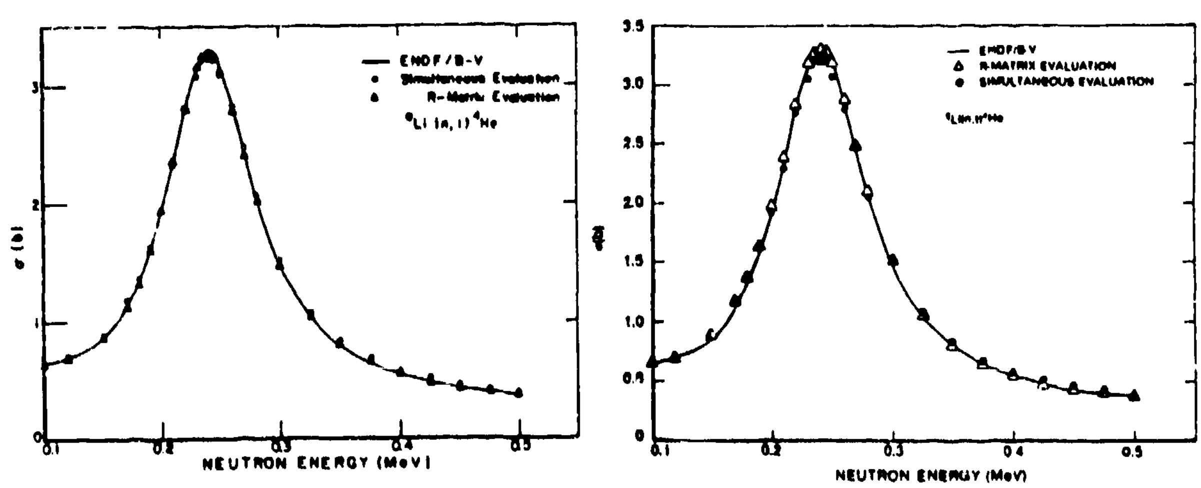

Fig. 3. Preliminary results of the simultaneous and R-matrix evaluations for the ^{6}Li(n,t) cross section for neutron energies from 0.1-0.5 MeV compared with the ENDF/B-V evaluation. The data on the left part of the figure are from the partially overlapping data base analyses. Those on the right are from the non-overlapping data base analyses.

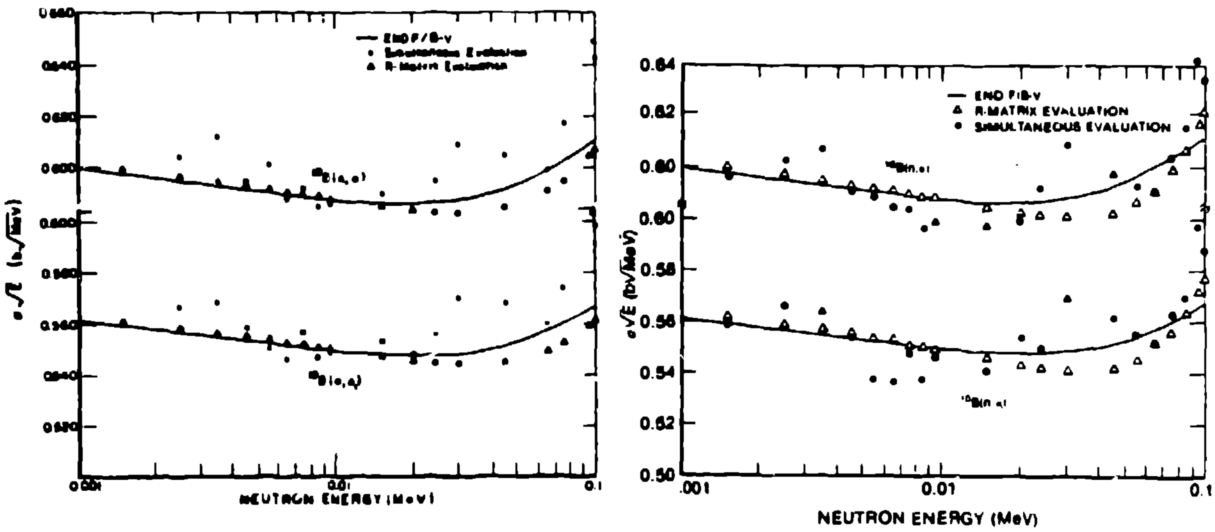

Fig. 4. Preliminary results of the simultaneous and R-matrix evaluations for the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ cross sections for neutron energies from 0.001-0.1 MeV compared with the ENDF/B-V evaluation. The data on the left part of the figure are from the partially overlapping data base analyses. Those on the right are from the non-overlapping data base analyses.

The $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ results are shown in Fig. 4 for neutron energies from 1-100 keV. These cross sections are considered standards below 100 keV. Note the highly expanded scale and suppressed zero. There is agreement among the evaluations except at the higher neutron energies where the simultaneous evaluation results are higher. Differences between the partially overlapping and non-overlapping data-base analyses also appear at the higher energies. These differences are believed to be due to the data bases used. In Fig. 5 the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ results from 0.1-1 MeV obtained from the partially overlapping data bases are shown. Differences are apparent between the R-matrix and simultaneous evaluations. These differences are most pronounced near the resonance structure at ~ 0.2 and ~ 0.5 MeV. Differences between these evaluations and ENDF/B-V are most pronounced for the $^{10}B(n,\alpha)$ cross section near the ~ 0.5 MeV resonance and for both the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ cross sections above ~ 0.5 MeV.

For the particular grouping of the boron experimental data base which was chosen in forming the non-overlapping data groups, important data sets were removed from the R-matrix data base. The effect of removing these data from the relatively small data base which contains inconsistencies has caused significant changes in the R-matrix results above 100 keV. The largest change is ~ 10% near 200 keV for both the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ cross sections. Some of the problems with the boron data base are discussed in Ref. 13 and 14. Other partitioning of the boron data base for

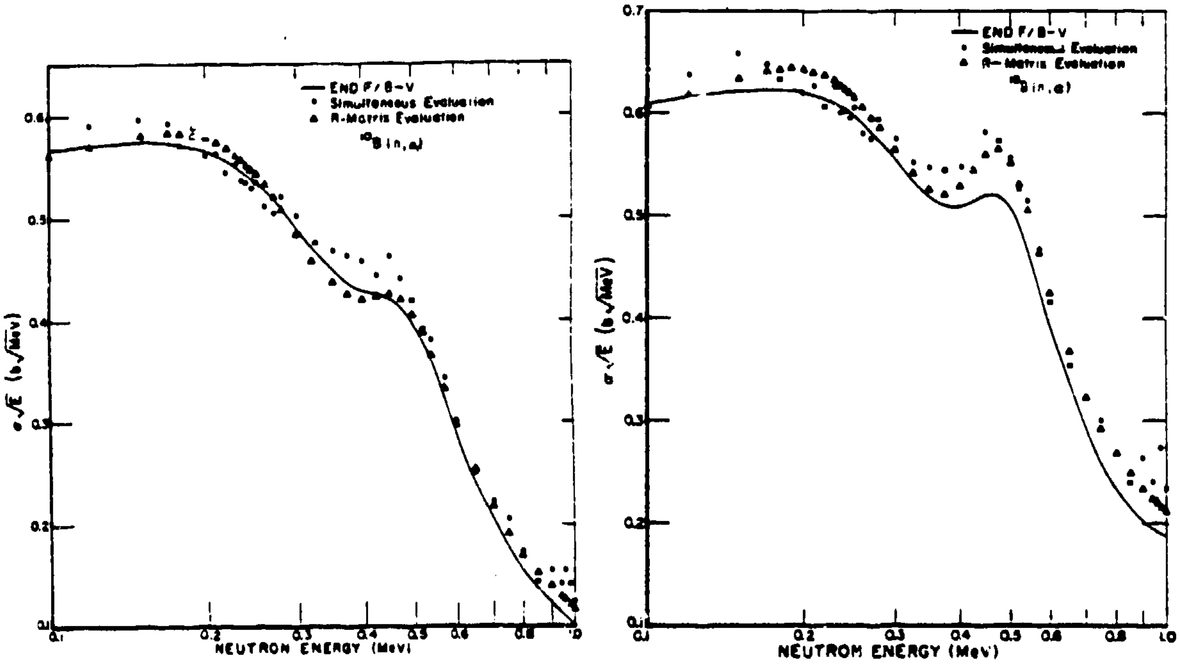

Fig. 5. Preliminary results of the simultaneous and R-matrix evaluations for the $^{10}B(n,\alpha_1)$ and $^{10}B(n,\alpha)$ cross sections for neutron energies from 0.1-1 MeV compared with the ENDF/B-V evaluation. The data are from the partially overlapping data base analyses.

these analyses is now underway. Concerning the combination procedure it should be noted that the individual fitted results using non-overlapping data bases in the R-matrix and simultaneous evaluations need not be obtained in developing the final combination fit. However it will be convenient if the overall data base can be partitioned so the separate fits to the partitions yield parameters (cross sections) not much different from the final values to be obtained from the combination fit.

In Fig. 6 the results of the gold capture cross section from the simultaneous evaluation are shown. This cross section is considered a standard for ENDF/B-V for neutron energies from 0.2-3.5 MeV though it is often used as a standard at lower neutron energies. Below ~ 300 keV structure[15,16] in the cross section is present in the new evaluation. This structure is a result of competition with inelastic scattering, fluctuations in the spacings and neutron widths of the compound nucleus levels and to some extent data inconsistencies. The new evaluation is somewhat lower than ENDF/B-V, in the regions from ~ 0.5 to 0.8 MeV and above 1.3 MeV. Some type of smoothing or fitting to a model is being considered for removing non-physical structure in this evaluation.

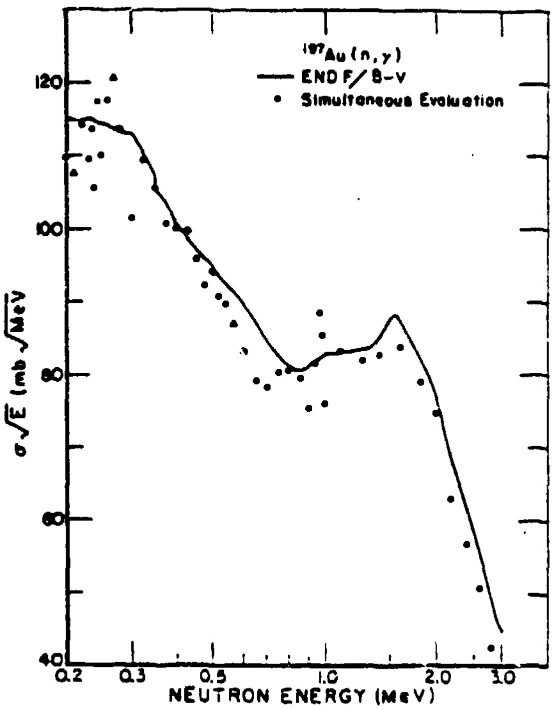

Fig. 6. Preliminary results of the simultaneous evaluation of the Au(n,γ) cross section for neutron energies from 0.2-3 MeV compared with the ENDF/B-V evaluation. The data are from the non-overlapping data base analysis.

In Fig. 7 the simultaneous evaluation results for the ^{235}U fission cross section are shown for neutron energies from 0.1-20 MeV where it is a standard. This evaluation is approximately the same above 4 MeV and 1-2% lower below 4 MeV compared with ENDF/B-V. The results are in excellent agreement with recent high accuracy data at 14 MeV.

An indication of the reduction in the evaluated cross section is given by the calculated average $^{235}U(n,f)$ cross section in a ^{252}Cf spontaneous fission neutron spectrum. This quantity is ~ 1% lower with the new evaluation compared with ENDF/B-V.

CONCLUSIONS

The preliminary results reported here are part of the process of determining the standards for ENDF/B-VI. The comparisons of the simultaneous and R-matrix evaluations are generally encouraging when the presence of inconsistencies in the data base is taken into account. A significant amount of work remains to be done in determining sensitivity to various experiments, the grouping of the lithium and boron data, performing the combining procedure and resolving any inconsistencies.

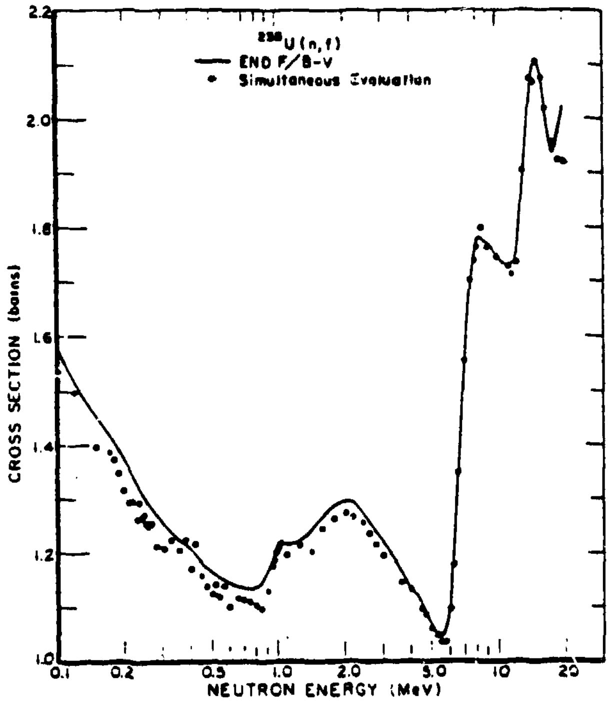

Fig. 7. Preliminary results of the simultaneous evaluation of the $^{235}U(n,f)$ cross section for neutron energies from 0.1-20 MeV compared with the ENDF/B-V evaluation. The data are from the non-overlapping data base analysis.

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