EVALUATION METHODS FOR NEUTRON CROSS SECTION STANDARDS*

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ABSTRACT

Methods used to evaluate the neutron cross section standards are reviewed and their relative merits assessed. These include phase shift analysis, R-matrix fit and a number of other methods by Poenitz, Bhat, Kon'shin and the Bayesian or generalized least-squares procedures. The problems involved in adopting these methods for future cross section standards evaluations are considered and the prospects for their use discussed.

INTRODUCTION

Methods used to evaluate the neutron cross section standards are discussed in this review and their relative merits assessed. The commonly accepted neutron reactions and the useful energy ranges as standards as given in ENDF/B-V are: $^{1}H(n,n)^{1}H$ (scattering cross section 1 keV-20 MeV; MAT = 1301), $^{6}Li(n,t)^{4}He$ (thermal to 100 keV; MAT = 1303), $^{10}B(n,\alpha_0)^{7}Li$, $^{10}B(n,\alpha_1)^{7}Li^*$ (thermal to 100 keV; MAT = 1305), C(n,n) (carbon elastic scattering angular distribution up to 1.8 MeV; MAT = 1306), $^{3}He(n,p)t$ (thermal to 50 keV; MAT = 1146), $^{197}Au(n,\gamma)$ (200 keV - 3.5 MeV; MAT = 1379) and $^{235}U(n,f)$ (at thermal energy and from 100 keV-20 MeV; MAT = 1395) [1]. The different evaluation procedures used with these may be divided into three broad categories. They are: (A) phase shift analysis for $^{1}H(n,n)^{1}H$; (B) R-matrix fit for $^{6}Li(n,t)^{4}He$, $^{10}B(n,\alpha_0)^{7}Li$, $^{10}B(n,\alpha_1)^{7}Li^*$ and C(n,n); and (C) a miscellany of methods used with $^{3}He(n,p)t$, $^{197}Au(n,\gamma)$ and $^{235}U(n,f)$. A discussion of these methods may be further subdivided into:

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(i) The physical model used,
(ii) types of data,
(iii) statistical model and evaluation procedure and,
(iv) comments and problems.

Use of a physical model to fit a set of data is preferred as opposed to an arbitrary functional or polynomial fit. Apart from providing a physical insight into the nuclear reaction under consideration, a physical model makes credible interpolation or extrapolation of the evaluation to energy regions where there are no data. The physical model, because of its unitarity and other constraints, could also help in identifying discrepant data sets. It can point out inconsistencies in the results of an evaluation such as for example the negative value of ε_1, the $^3S_1 - {}^3D_1$, mixing parameter in $^1H(n,n)^1H$ scattering. This inconsistency is ascribed to lack of completeness of input data and further studies using sensitivity analysis point out new types of measurments which could clear up these problems. If the evaluation process is thought of as a type of data reduction, in which a large amount of data are expressed more succinctly in terms of a fewer number of parameters, a physical model is helpful in identifying the parameters to be determined from the data as opposed to energy, mass and other variations governed by the physics of the reaction. Further studies of the systematics of these parameters could lead to greater understanding of the reaction under study. An example of this is the determination of the resolved resonance parameters and the strength function and other systematics derived from it. However, it should be noted that the physical model chosen must be flexible with enough adjustable parameters so that a good fit to the measured data may be obtained consistent with their assigned errors.

Since this review is mainly concerned with evaluation methods, different data sets for the standards and any of the problems associated with them will not be discussed. Instead, broad categories of data will be mentioned with an indication as to the physical parameters they help to determine.

The statistical model (which has nothing to do with nuclear reaction theories with the same name) and the evaluation procedure are the particular concern of this Workshop and will be discussed in detail with particiuar emphasis on the methods used for the ENDF/B-V standards [1]. Possible shortcomings in these methods and any suggestions for improvements will also be mentioned. As stated earlier, if the evaluation is thought of as a data reduction process, it should be carried out with a minimum loss of information contained in the original data. This information pertains to the data as well as their statistical and systematic errors and any correlations amongst them. Hence, the need for the use of a full variance-covariance matrix of the input data as has been emphasized by Perey [2], Peelle [3,4] and others.

A discussion of the evaluation methods is followed by mention of the problems of neutron cross section standards evaluation and the future outlook for this activity. The problems of implementing some of the recent improvements in the evaluation techniques are also mentioned ending with a brief summary of this review.

Some aspects of the standards evaluation not discussed here deal with (1) evaluation of thermal data and (2) numerical procedures. Because of their high precision, thermal data are used to normalize cross sections in the higher energy region and form an integral part of the analysis. These methods will be discussed by Mughabghab [5] in this Workshop. Numerical procedures enable one to implement the various evaluation methods and deal with different problems such as having to work with a computer with a finite word size, ill conditioned matrices and using numerically stable algorithms. A number of recent advances made in this field are given in Ref. 6-9 and will not be discussed here.

EVALUATION METHODS

A. Phase Shift Analysis

In the energy region from 1 keV-20 MeV the neutron scattering cross section of hydrogen is smooth, large and without any structure-essential qualities needed in a cross section standard. The evaluation in ENDF/B-V is by L. Stewart et al. [10,11] and is based on the work of Hopkins and Breit [12] derived from the Yale phase shift analyses. The variance-covariance files for this evaluation were generated by Foster and Young [13] and give uncertainty information for total, scattering and capture cross sections. In implementing neutron scattering from hydrogen as a standard, it is essential to know the elastic differential scattering for use in recoil telescope detectors [14].

(1) Physical Model

The physical model used for the evaluation is to make a phenomenological phase shift analysis of the different types of data needed to determine the (n,p) scattering matrix. Details of such analysis have been given by Wilson [15], Arndt and MacGregor [16] and Breit and Haracz [17] and a number of other papers. In this analysis, conservation of the total angular momentum J, parity, the isospin T and time-reversal invariance are assumed. With the assumption of charge independence, both the p-p scattering data corresponding to T=1 and the n-p scattering data with T=0, 1 are used in the analysis. Further, because of the tensor force between nucleons, there is a mixing of L states which differ by two units of angular momentum. The nucleon-nucleon scattering phases are denoted by $\delta(^{2S+1}L_J)$ where S is the total spin, J the total angular momentum and L stands for S,P,D,F,G,H corresponding to L=0,1,2,3,4,5 in the usual spectroscopic notation. The mixing parameters which mix states with L=J+1 for the same total J are denoted by ε_J. The relationship between the phase shifts and the measured quantities such as the angular distribution and the different polarization parameters have been given by Stapp [18]. The evaluation consists in forming a χ^2 using experimental observables,

errors and their theoretical expressions in terms of phase shifts and determining the unknown parameters by minimization. In this procedure, it is difficult to make a clear-cut separation between the physical model and the details of the evaluation procedure as the behaviour of the parameters are determined by an appeal to theory. Thus, in this particular case there is much greater intrusion of theory in the evaluation method and this will be made clear wherever possible.

(2) Types of Data

The input data used in the evaluation fall into two broad groups viz., the low energy data usually of high precision and the scattering and polarization data at higher energies. They are listed in Table I together with their estimated precision. Their current best values are not shown as they vary from one compilation to another.

The binding energy of the deuteron B=2.224628±0.00003 MeV is taken from Wapstra and Bos [19]. The uncertainty estimates of the remaining low energy data in Table I are from Koester [20], Lomon and Wilson [21], and Sher et al. [22] for the p-p scattering parameters a_{pp} and r_{opp}. These are supposed to give the order of magnitude of the data uncertainties and vary from one compilation to another. The deuteron radius R is derived from the binding energy B [15]. The free atom n-p scattering cross sections at low energies have been carefully measured by Houk [23], Dilg [24] and others. This cross section σ_0 depends on the weighted sum of the squares of the triplet and singlet scattering lengths a_t and a_s. To determine a_t and a_s, additional data on the coherent scattering length f are used as it depends linearly on a_t and a_s. The coherent scattering length f is most accuractely determined at present using the gravity spectrometer as described by Koester [20]. The low energy n-p scattering phase shift δ is expressed in terms of the scattering length a, the effective range r_0 and the wave number k in the shape independent approximation as [25].

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2} k^2 r_0 \qquad (1)$$

From a_t and the deuteron binding energy, the triplet effective range r_{ot} is calculated. Similarly, from low energy scattering data and a_s one may extract the singlet effective range r_{os}. Proton-proton scattering data below 30 MeV were analyzed by Sher et al. [22] and after applying corrections to the observed data corresponding to a number of physical effects they arrived at the singlet scattering length and effective range for proton-proton scattering. It is found that in doing phase shift analysis, by adding the requirement that S-wave phases extrapolate to the scattering length and the effective range expansion at low energies, excellent fits could be obtained to low energy data [26-29].

Since nucleon-nucleon interaction is spin dependent, a

complete specification of the scattering matrix requires a number of experiments. These have been discussed by Wilson [15] and Moravcsik [30] who list some five different types of experimental data which should be measured over 0^0-90^0 scattering angles for p-p and 0^0-180^0 for (n,p) scattering to specify the scattering matrix for each isospin state. These experiments include angular distributions, polarization, polarization transfer and spin correlation experiments for (n,p) and (p,p) scattering. For (n,p) interaction, one can measure in addition, the total cross section. The available data for (p,p) and (n,p) scattering and their uncertainties have been listed in a number of papers [27,28,29,31,32] and vary from about one percent to several percent depending on the difficulty of the data measurement. In general, the data on (p,p) scattering are much more complete than the (n-p) data. Because of this fact, (p,p) scattering is analyzed to determine the T=1 scattering phase shifts first and assuming charge independence, they are used along with the (n,p) data to extract the T=0 phase shifts. As is seen later on, large uncertainties in the evaluated parameters, multiple solutions and in some cases problems with the sign of the final value are caused by this less than complete data base and of course the experimental errors.

The (p-p) and (n-p) data have been measured over a number of years at different laboratories using experimental techniques of different degrees of sophistication. In addition, to the known and estimated errors, the data are bound to have unknown systematic errors. Hence, if at all possible, some kind of unbiased data selection should be made provided the discrepant data sets could be identified. This process as carried out by the Livermore group [27] may be described as follows. The purpose of this selection is to find out whether or not a particular experiment can be considered to be compatible with other data. One obvious procedure in comparing two identical experiments is to see whether the error bars overlap or not. However, the (p-p) and (n-p) scattering data are of such varied nature differing in type, energy and angle that such direct comparison can be made very rarely. Therefore, as a general criterion of compatibility, it is demanded that they be described by the same phase-shift representation. This procedure is carried out as follows. A subset D of data self-consistent and complete enough to give a set of parameters by χ^2 minimization is chosen; and let the minimum χ^2 be devoted by χ^2_D. If now an experiment E (not included in D) with N_E experimental points is added to this set, and a minimum χ^2_{D+E} is obtained, the change in the χ^2 minimum per additional degree of freedom is defined as

$$f_c = (\chi^2_{D+E} - \chi^2_D)/N_E \qquad (2)$$

This f_c includes not only the χ^2 minimum increase due to the additional points N_E but also their influence on the fit as determined by their compatibility or lack of it with the set D. For a set E compatible with D, it is demanded that f_c be of the order of unity.

As has been emphasized [27] it is important to recognize that f_c is a measure of the compability between the data sets D and E only within the constraints of the model used for the fit. The details of this selection procedure are given in Ref. 27 and 16.

(3) Statistical Model and Evaluation Procedure

The p-p and n-p scattering data have been most extensively analyzed by the Livermore group [16,26-29,31,32,] and the Yale group [17,33,34] for many years. In addition, such analyses have also been done at a number of other institutions. In the case of every group, the evaluation procedures have evolved over a number of years and to do full justice to them, the original papers should be consulted. Though the details of analyses vary from group to group, they have some common features which will be discussed in this review. These are summarized here by discussing the procedures adopted by the Livermore group.

The basic idea of the fitting procedure is to use χ^2 minimization to find the set of parameters which best describe the data. The χ^2 is defined as [16,35]

$$\chi^2 = \sum_{i=1}^{N_D} \left[(\alpha^n \theta^i(p) - \theta^i_{exp})/\Delta\theta^i_{exp} \right]^2 + \sum_{J=1}^{N_\alpha} \left[(\alpha^j - 1)/\Delta\alpha^j_{exp} \right]^2 \quad (3)$$

where $\theta^i(p)$ are the observables predicted by the set of parameters p, θ^i_{exp} are the experimental values of these observables and $\Delta\theta^i_{exp}$ their experimental errors (one standard deviation), i is the index which varies from 1 to N_D where N_D is the number of data points; α^n are the normalization parameters N_α in number, p stands for the set of parameters specifying the phase shifts (N_p in number). The normalization parameters are introduced for sets of data points where the entire set has a correlated uncertainty in the measured values. The minimum is found by varying the parameters and normalization constants (p_j, α^n). There are a number of techniques used to find the minimum of such a χ^2 function and they are described by Arndt and MacGregor [16]. They also discuss the problem of estimating the errors and their correlations for the evaluated parameters and the goodness-of-fit.

One of the problems noted in the earliest computer based phase shift analysis of 310 MeV p-p scattering data by Stapp et al. [13] was the multiplicity of solutions viz. eight that were obtained. Out of these, some three were rejected as their χ^2_{min} values lay between 34.6 and 52.3 for 22 degrees of freedom and it was estimated that the probability of $\chi^2_{min} > 34$ was about 3%. For the remaining solutions, χ^2_{min} varied from 17.9 to 34.2 and a clear cut choice other than that determined by χ^2_{min} could not be made to choose amongst these. The mulitpliicity of solutions was attributed to data errors and the incomplete data base in the sense that though the data were made up of five types of

experiments they did not extend over the whole angular range. Also, in the phase shift analysis, partial waves up to $\ell_{max}=5$ were used with the phase shifts corresponding to the higher partial waves being set equal to zero. It was suggested [36] that an improvement in the phase shift analysis could be made by setting the higher -ℓ phases equal to the one-pion exchange contribution. This reduced the number of solution to two and made a significant improvement in the analysis [37]. This feature of using one-pion exchange potential and other theoretical calculations as adjuncts to the nucleon-nucleon scattering analysis has continued since then.

The phase shift analysis is done using experimental data confined to a narrow range of energies (energy independent analysis) or with data spanning a wider range of a few hundred MeV (energy dependent analysis). In the case of energy independent analysis, the low angular momentum phases are treated as free parameters to be determined by fitting the data and the high angular momentum phases are represented by their one-pion exchange contributions. For the energy dependent analyses, the Livermore group uses the following expression for phase shifts [27]

$$\delta_\ell^{(S,J)}(E) = \delta_{\ell 0}^{(S,J)}(E) + \sum_{i=1}^{N} \alpha_i^{(S,J)} F_{\ell i}(E) \qquad (4)$$

where ℓ is the orbital angular momentum, J and S are total momentum and spin and E is the laboratory kinetic energy. For $\ell=0$, the phase has at its asymptotic lower limit the appropriate effective range expansion [27,29] and for $\ell\neq 0$, $\delta_{\ell 0}^{(S,J)}$ are set equal to the one-pion exchange values. The functions $F_{\ell i}(E)$ are derived from theory and the $\alpha_i^{(S,J)}$ are treated as free parameters to be determined from the fit. The energy-dependent form of the phase shifts are chosen with guidance from theory and with enough free parameters to fit the data. Results of energy-independent analyses at a few energies are compared with those of energy-dependent analyses and if they agree, this is taken as an indication that the energy-dependent fits are not form-limited.

As mentioned earlier, the p-p scattering data base is in general more complete than the n-p scattering data. Because of the incomplete data base and the data uncertainties, the evaluated parameters are not determined uniquely especially at low neutron energies. One of the vexing problems of (n-p) scattering phase shift analysis has been the negative value of ε_1, the $^3S_1$-$^3D_1$ mixing parameter. Because the electric guadruple moment of deuteron is experimentally measured to be positive, it is expected that ε_1 should be positive at very low energies [38]. According to theoretical calculations ε_1 is also expected to be positive at low energies [39]. Also, the phase $\delta(^3P_2)$ as determined from the phase shift analysis, though it has a negative value as given by theory, is found to have a smaller magnitude as compared to theoretical estimates [39]. To get around these problems, the

Livermore group constrained their fit to pass exactly through the Wisconsin data [40] which measured the ratio $\sigma(164^0)/\sigma(89^0) = 1.134 \pm .016$ for (n-p) scattering at 24 MeV. This constrained solution was found to give ε_1 and $\delta(^1P_1)$ values that were in reasonable agreement with those expected from theory. Though the Yale solutions are not constrained by experimental data, as has been pointed out by MacGregor et al. [28] (pages 1294-1299), the reason the Yale solutions do not have the type of problems which the Livermore solutions have and they follow a one-pion exchange contribution type of behaviour at low energies is because they are constrained to do so. These experimental or theoretical constraints are necessary because the low energy (n,p) data are not yet adequate to give a unique solution to the problem.

The ENDF/B-V (n,p) scattering evaluation is based on the Hopkins and Breit analysis [12] which is mainly based on the results obtained by the Yale N-N Interaction group [33,34]. A brief discussion of the Yale and Livermore [29] phase-shift analyses is given in Ref. 12. These authors conclude that the results of these two analyses are in essential agreement; and the differences between the cross sections or polarizations as calculated from the Yale or Livermore phase shifts are less than the uncertainties associated with the experimental data. The Hopkins and Briet evaluation has been confirmed by some measurements done after the evaluation. These are the Davis and Barschall total cross section data from 1.5-27.5 MeV [41], the Masterson differential data at 24 MeV [42], the Burrows data [43] at 24.0 and 27.2 MeV and the Cookson et al. data [44] at 27.3 MeV.

Since the phase shifts are extracted from the experimental data by least-squares minimization, the errors in the evaluated parameters and their correlations are determined from the error matrix. The details may be found in the article by Arndt and MacGregor [16], or other papers [26,35]. The variance -covariance files for the ENDF/B-V evaluation were derived by Foster and Young as described in Ref. 13. These are given for total, scattering and capture cross sections. However, the variance-covariance files, could be obtained from the error matrix originating as part of the evaluation process. As has been emphasized by Stewart and Young [45] use of hydrogen as a cross section standard is limited only by the accuracy with which one measures and knows the differential elastic scattering. Hence, a variance-covariance matrix dealing with the uncertainties in this quantity appears to be more pertinent in the evaluated data files and is not available at present.

(4) Comments and Problems

In this section, a few brief comments on the statistical model used and the problems of the (n-p) data base will be made. First, from the form of the χ^2 used in Eq. (3), it is assumed that the individual data points in the whole data base are independent. This assumption neglects any correlations in the data uncertainties

of quantities measured in the same experiment. There are usually such non-zero correlations. Second, since "the normalization parameters are introduced for sets of data points where the entire set has a correlated uncertainty in the measured values" [16] is considered as a solution to the first problem, normalization parameters cannot allow for energy dependent systematic errors. In addition to assuming that the systematic errors are constant, this also implies that the statistical errors are small compared to the systematic errors — an assumption which may not be true. Though these simplifying assumptions are made in practice, one should carefully examine the data bases to see whether they do indeed hold true for the particular data under consideration. Of course, the correct procedure is to work out the full variance-covariance matrix for the input data and use it in the analysis.

The status of the hydrogen scattering cross section and the problems of data discrepancies has recently been reviewed by Stewart and Young [45] and Uttley [46]. One of the phase shift analyses of p-p and n-p scattering data was done by Arndt et al. after the Hopkins and Breit work and dealt with the data near 50 MeV [47]. They found that the allowed range of values for ε_1 (the $^3S_1$-$^3D_1$ mixing parameter) varied from about -10^0 to $+3^0$, though theoretical calculations predicted about $+2.78^0$. The χ^2 vs ε_1 plot indicated that the χ^2 surface was essentially flat between -10^0 and $+3^0$. To obtain a unique solution, even when ε_1 was constrained to $+2.78^0$, $\delta(^1P_1) = -3.52+1.04^0$, was obtained which was estimated to be 4.5 standard deviations above the predictions of theoretical models. As a result of this study, one of the conclusions reached by these authors was that existing n-p data on total, differential elastic and polarization cross sections could not remove this ambiguity in ε_1 as these data were not sensitive to changes in ε_1. In order to understand these problems with ε_1 and $\delta(^1P_1)$ better, Binstock and Bryan [48] carried out a detailed sensitivity analysis of the various n-p scattering observables to the phase parameters near 50 MeV. This confirmed their earlier conclusion that ε_1 was not sensitive to the σ_{tot}, $d\sigma/d\Omega$ or polarization data; however, they observed that it was sensitive to a number of polarization transfer or spin correlation parameters. These in order of decreasing sensitivity are A_{zz}, C_{00}, A'_t, C_{kk}, A_t, D_t, C_{nn} and A_{xx}. Further they observed that the differential cross section is sensitive to $\delta(^1P_1)$ at backward angles and to the triplet-D parameters at both forward and backward angles. Inaccurate $d\sigma/d\Omega$ data, therefore, could vitiate the $\delta(^1P_1)$ evaluation by giving wrong triplet-D phases from the forward data and then giving incorrect contribution at the backward angles. Therefore, these authors emphasize the need for good absolute $d\sigma/d\Omega$ data at both near 0^0 and 180^0. There have been some recent measurements by the UC Davis group of the n-p spin correlation parameter A_{yy} at 50 MeV [49], the (n-p) differential cross section data at 25.3 and 50.0 MeV [50], polarization at 50 MeV [51,52], differential scattering cross section at 53.1 MeV [53] and a remeasurement of $A_{yy}(\theta)$ at 50.0 MeV [54] with several

improvements in the experimental technique. They were able to considerably reduce the normalization uncertainty in Ayy. These new data with the other Davis data [51,50,53,55,49] and the data of Langsford et al. [56] were used for a phase shift analysis at 50 MeV and Fitzgerald et al. obtain $\varepsilon_1 = 3.6^0 \pm 1.0^0$ and $\delta(^1P_1) = -6.4^0 \pm 1.1^0$ [54]. These values are said to be in much better agreement with model-dependent calculations. From the above discussion, it appears that further studies and measurments are needed to get better (n-p) scattering phase shift parameters. It would be interesting to carry out the type of Binstock-Bryan sensitivity analysis at a lower energy of say 25 MeV to identify the data needed to determine ε_1 and $\delta(^1P_1)$. Maybe, they will be the same data singled out at 50 MeV. More measurements of these quantities viz. absolute $d\sigma/d\Omega$ at forward and backward angles and the various polarization transfer and spin correlation parameters are also needed. In addition, a statistical model using the full variance-covariance matrix could be used in the analysis to obtain better phase-shift parameters.

B. R-Matrix Analysis

R-matrix analysis was used to evaluate $^6Li(n,t)^4He$, $^{10}B(n,\alpha_0)^7Li$, and $^{10}B(n,\alpha_1)^7Li^*$ and C(n,n) as standards for ENDF/B-V. The first three reactions were evaluated by G.M. Hale and co-workers [57,58] and he will discuss these at this Workshop [59]. The Carbon scattering was analyzed by Fu and Perey [60]. There will also be a discussion of R-matrix methods by Froehner in this Workshop. Therefore, this discussion of C scattering will be very brief with only a few comments on the (MAT = 1306, ENDF/B-V) evaluation. Fu and Perey have assembled the variance-covariance files for total, scattering, non-elastic, total inelastic, inelastic scattering to discrete states and the continuum, capture, (n,p), (n,d) and (n,α) reactions [1,60] as part of the evaluation process. An earlier evaluation of this reaction by Reynolds et al [61,62] done for ENDF/B-III (MAT = 1165) used coupled-channel analysis and a few comments will be made comparing these two procedures.

(1) The Physical Model

R-matrix theory has been discussed in detail in a number of review articles [63,64] and a few of the characteristics of this physical model will be mentioned.

In R-matrix theory, the configuration space of all the interacting nucleons is divided into an internal region which corresponds to all the interacting nucleons being close together in physical space. This internal region is separated from an external region where the nucleon forces between nucleons do not act. Corresponding to this surface of separation there are channel radii a_c for different reaction channels or interacting particles. Usually, a_c is set equal to the sum of the radii of the interacting particles. Thus, R-matrix theory deals usually with two-body breakup reactions, with three-body breakup being considered as a succession of two-body

reactions [63]. Usually, since data corresponding to only a limited energy region are analyzed in an R-matrix fit, provision should be made to represent the tails of resonances that lie outside the region of fit. Bound levels are represented by a few resonances whose parameters are determined to be consistent with low energy data and the contributions of positive energy resonances at higher energies.

(2) Types of Data Used

In R-matrix analysis, where levels corresponding to a particular compound system are investigated, data for all the reaction channels producing the same compound nuclear system are used. As has been pointed out by Hale [57], experimental data corresponding to all the reaction channels influence the R-matrix parameters through unitarity and other general physical constraints and discrepant experiments may be identified and separated from the main body of data. Thus, a comprehensive multilevel, mulitchannel R-matrix analysis is expected to give a good representation of the data consistent with their errors.

^{13}C occurs in natural carbon with an abundance of 1.11%. Though the measured data are for natural carbon, the evaluations are for ^{12}C [63,66,60]. This problem has been discussed [65,66] and the data indicate that the cross sections for ^{13}C are very close to the corresponding ones for ^{12}C except in the vicinity of the 0.153, 1.751 MeV resonaces of ^{13}C which lie in the standards region of up to 1.8 MeV. Hence, it is felt [66] that the vitiating influence of this isotope, especially in elastic scattering, would not distort the elemental results beyond the current experimental errors except at the ^{13}C resonances. However, an evaluation of the ^{13}C data and its inclusion in the evaluated data file is recommended [65,67].

The data used in the evaluation [60] are for total, differential scattering and for differential polarization cross sections. The total cross section data were smoothed and averaged using the full variance-covariance matrices and a procedure based on Bayes' theorem as described by Fu and Perey [60].

(3) Statistical Model and Evaluation Procedure

As mentioned earlier, a study of natural carbon data involves ^{12}C as the major isotope. Since ^{12}C has zero spin, only one channel spin s=1/2 is involved and for neutron energies below the inelastic threshold at about 4.81 MeV, only elastic scattering is possible. Capture cross section is also negligible below ~2 MeV. Thus, in effect, there is only one open channel below 4.8 MeV and the R-matrix reduces to an R-function. Fu and Perey [60] used the R-function

$$R_{cc'}(E) = \sum_{\lambda} \left[\frac{\gamma^2_{\lambda c}}{E_\lambda - E} \right] \delta_{cc'} + R^{\infty}_{cc'}(E) \qquad (5)$$

where γ_λ^2 and E_λ are the reduced width and the characteristic energy respectively of the λ-th state of given J^π, and $R^\infty_{\ell J}(E)$ is the corresponding background term given by

$$R^\infty_{\ell J}(E) = R_0 + R_1 E + R_2 E^2 \qquad (6)$$

where E is the laboratory energy of the incident neutron in MeV. The corresponding phase shift is

$$\delta_{\ell J}(E) = \tan^{-1}\left[\frac{P_\ell(\rho)\, R_{\ell J}(E)}{1 - \left[S_\ell(\rho) - b_{\ell J}\right] R_{\ell J}(E)}\right] - \phi_\ell(\rho) \qquad (7)$$

where $\rho = ka$, k being the wave number of the incident neutron and a the interaction radius. The interaction radius was set equal to 3.72 fm, a value recommended by Lane et al., [68]. In the above expression, $P_\ell(\rho)$ is the penetration factor, $(S_\ell - b_{\ell J})$ the shift factor for boundary value $b_{\ell J}$ and $\phi_\ell(\rho)$ is the hard sphere phase. The boundary values $b_{\ell J}$ were chosen such that the E_λ fall near the observed resonance energies. All other parameters were determined by fitting the data without any constraints.

The evaluation procedure consists in forming χ^2 corresponding to each of the measured quantities and minimizing them using an interactive graphics program. Only diagonal elements of the data variance-covariance matrices were used in the minimazation [69]. The variance-covariance matrices of the fit were evaluated as part of the evaluation.

(4) Comments and Problems

Since, the evaluation is the result of a χ^2 minimization, the data uncertainty files may be derived from the error matrix as part of the evalution. However, the error estimates and their correlation would be more representative of the true state of affairs if the full variance-covariance matrices for data are used in the evaluation. In addition, it would be useful to have the data uncertainty information for elastic differential scattering in the evaluated data files as it is the standard. Some of these error estimates are given in the evaluation report [60]. As has been mentioned earlier, an independent evaluation of ^{13}C data, if available, could allow for the 1.11% impurity of ^{13}C in natural carbon data.

An alternate physical model was used for carbon to obtain an evaluation for ENDF/B-III (MAT = 1165) [61,62]. The reasons for adopting this procedure are given [61] and include having to vary from one energy region to another reduced widths (considered energy-independent) and the energy of at least one resonance. These authors found the usual description of the background cross section in terms of hard-sphere phase shifts inadequate and had to use potential-well phase shifts in their place. These potential-well parameters had to be changed from one energy region to another. Because of these

reasons and as a means of understanding the underlying physics better, these workers used the coupled channel analysis. However, coupled channel analysis seems to have its own peculiar problems [61,62]. For example, the coupling parameter β which fits the data was very small compared to the experimental value obtained in Coulomb excitation. In addition, the potential well parameters had to be changed so that the different shell model states agreed with experimental data. Though they were able to fit the available data on total, differential and polarization experiments satisfactorily, the coupled channel analysis approach appears to involve much more work than an R-function fit. There appears to be a much greater involvement of theoretical models, some ad hoc procedures and no fewer number of parameters to be adjusted. With a greater intrusion of theoretical models the error estimates of the final results is not simple. The R-function fit for this reaction appears to be the simpler procedure.

C. Other Evaluation Methods

The cross section standards discussed here are $^{3}He(n,p)t$ (from thermal to 50 KeV), $^{197}Au(n,\gamma)$ (200 keV-3.5 MeV) and $^{235}U(n,f)$ (at thermal energy and 100 keV-20 MeV). One interesting feature of these reactions in the standards region is that they cannot be expressed explicity in a functional form (except for $^{3}He(n,p)t$ in the $1/v$ region) with an energy dependence determined by the physics of the reaction as for example in the Breit-Wigner formula for resonances. If such a functional form was known, it would be a simple matter to write an expression for χ^2, minimize it with respect to the unknown parameters and determine them. Since this is not the case, a number of other evaluation techniques have to be used to arrive at a best representation of the data. These are: (a) Empirical Evaluation, (b) Poenitz, (c) Bhat, (d) Kon'shin, and the (e) Bayesian Methods.

a. Empirical Evaluation Method

$^{3}He(n,p)t$ reactions in ENDF/B-V was evaluated by L. Stewart for ENDF/B-III, used in Versions IV and V without any changes [11,70]. This evaluation continues to be a valid representation of data base as it stands now [71]. There are no variance-covariance files for this evaluation. This and other evaluations of light elements will be further discussed by Stewart at this Workshop [72]. The final evaluated curve is not the result of a χ^2 minimization statistical procedure. Also, explicit use of the variance-covariance information of the input data is not made. However, it should be appreciated that this evaluation uses a number of adjunct data such as inverse and charge-conjugate reactions, elastic scattering of charged particles and other information in arriving at the best representation of the data. Thus, the final evaluation was based on experimental data, quite a bit of auxilary information and the evaluator's experience. It is proposed to call such a procedure — Empirical Evaluation Method (a name suggested by my colleague A. Prince) — to distinguish it from an eyeguide drawn through the experimental points. Empirical as used here means "originating in or based

on observation or experience" [73]. As mentioned before, uncertainty files for the evaluation are not readily obtained as part of the evaluation procedure. However, it may be possible to assemble them using the SUR program approach described by Peelle [4] where the scatter of the input data about the evaluated curve are considered to provide a guide to the uncertainties of the evaluation.

The $^{197}Au(n,\gamma)$ cross section was evaluated by S.F. Mughabghab [74] using the empirical evaluation procedure. The gold capture data were renormalized to the other ENDF/B-V standards and evaluated. Explicit use of the data variance-covariance matrices is not made. The evaluated data uncertainty files give only the diagonal elements as error estimates.

b. Poenitz Method

The thermal energy evaluation of $^{235}U(n,f)$ for ENDF/B-V is by Leonard et al. [75]. The fission cross section from 100 keV-20 MeV was evaluated by Poenitz [76]. His evaluation method is described in this reference [76] with a bibliography of earlier discussions. Changes and improvements made since then have been discussed at this Workshop [77]. Poenitz carried out an evaluation of $^{235}U(n,f)$ using his method and the available data in October 1978 [78]. This evaluation was renormalized upward by multiplying by 1.009 on the recommendation of the Normalization and Standards Subcommittee of the Cross Section Evaluation Working Group (CSWEG) [78] and forms the evaluation in ENDF/B-V. The evaluation method as it was used to derive the ENDF/B-V cross section, did not explicity use the full variance-covariance matrices of input data and it did not produce the uncertainty files for the evaluation. These were generated by Peelle [79]. Subsequent to this work, Poenitz reevaluated $^{235}U(n,f)$ with an updated data base and published it along with discussion of the evaluation [76]: In general, the ENDF/B-V evaluation is 0.1-1.9% higher than the 1979 evaluation.

c. Bhat or Ratio Method

The evaluation procedure developed by the author of the review [80] may be described as follows. It recognizes the fact that the physics of fission does not enable one to give a functional form for the $^{235}U(n,f)$ cross section for 100 keV-20 MeV and that it cannot be readily parameterized uniquely. Use is also made of the fact that the experimental data lie in a rather narrow band about a mean. Therefore, a curve may be drawn to lie evenly amongst the data points and the values of this reference curve read off. The procedure is to work with the ratios of experimental data and their errors divided by the corresponding values read off this curve. This is found to have the following advantages.

(1) It linearizes the $^{235}U(n,f)$ fitting problem since the energy dependence of the cross section is divided out.

(2) Since the experimental data lie within a few percent about a mean; the ratios of the experimental data divided by the

reference curve should lie within a few percent of the straight line y=1.0. Thus, any method of fitting the ratios can make use of the fact that the final curve is anchored about the line y=1.0 with deviations characteristic of an individual data set being of the order of a few percent.

(3) It enables us to obtain a least-squares fit to the experimental data and a best fit corresponding to a minimum of χ^2 defined in the usual way. Also, the variance-covariance matrix for the fit can be calculated.

(4) After having obtained a best fit for all the data, one could analyze each data set by forming ratios. A decomposition of these ratios into orthogonal polynomials having energy dependence corresponding to different powers of the neutron energy can give us useful information on the systematic errors in each data set, thus providing clues to possible corrections to eliminate them.

Details of the Ratio Method

The absolute fission data used (Table II) are plotted on a graph paper and a smooth curve lying evenly amongst the data points is drawn. The values of this reference curve are read off and assembled in the ENDF/B Tab. 1 format with a linear interpolation code. The procedure calls for determing the shape information contained in the relative and absolute data sets and incorporating this shape information into the reference curve. The shape information is obtained by analyzing one data set at a time to preserve the intra-data-set correlations. The next step is to use only the absolute data and renormalize the reference curve with the shape information to include magnitude as well as the inter-data-set shape information contained in them. A code URAN [60] has been developed and tested to carry out this procedure.

Some 17 data sets were used for this purpose and are given in Table III. One starts from a reference curve drawn as mentioned earlier and goes through the following steps (1)-(4) for each data set.

(1) Determine $r(E_i) = \sigma_{exp}(E_i)/\sigma_R(E_i)$; $\Delta r(E_i) = \Delta\sigma_{exp}(E_i)/\sigma_R(E_i)$

for the experimental data $\sigma_{exp}(E_i)$ and their total error $\Delta\sigma_{exp}(E_i)$ at neutron energies E_i using values $\sigma_R(E_i)$ read off from the reference curve.

(2) Fit the ratios $r(E_i)$ with errors $\Delta r(E_i)$ in terms of orthogonal polynomials and using the F-test (see Appendix) and the χ^2_{min}/degrees of freedom determine the maximum degree of polynomial fit. Use of orthogonal polynomials gets around the problem of having to invert an ill-conditioned matrix usually encountered in a polynomial fit of degree of about six or greater.

(3) The fitted curve is interpolated on to a denser energy grid formed by the union of the energy grid of the reference curve and the experimental data points. This energy grid is further thinned by rejecting energy points in the grid which lie less than .5% from one another. The thinning is done only on the energy grid; no

experimental points are thrown out. In interpolating the fitted curve, its value as well as the error of the fit are calculated at the grid points.

(4) The fitted curve for each data set is then shifted along the y-axis (i.e., the curve is moved parallel to itself keeping the x-axis and the same shape) and a weighted average of the shapes of all the data sets is determined.

(5) This weighted average is fitted with orthogonal polynomials (or smoothed) and a smooth curve representing the average shape curve (for the ratios of experimental data to the reference curve) $\ell(E_i)$ and its weights $\omega(E_i)$ are determined.

(6) This curve is shifted along the y axis such that $\sum \ell(E_i)\omega(E_i)=1.0$. This is done to make sure that only the shape of the reference curve and not its magnitude is changed when it is multiplied by $\ell(E_i)$.

(7) The reference curve $\sigma_R(E_i)$ is multiplied by $\ell(E_i)$ to obtain the new reference curve. At this stage, the new reference curve may be plotted, χ^2/degrees of freedom calculated to check the fit. One may then go to step (1) and go through the whole process until it is felt that the reference curve has all the shape information in it and further iterations do not produce any change.

At this stage, the intra-data-set shape information in both the relative and absolute data sets have been built into the reference curve. In addition, by going through steps (8)-(10) inter-data-set shape information or the shape information contained in the relative positioning of the absolute data sets is incorporated into the evaluation.

(8) The 13 absolute data sets (Table II) were merged and energy sorted assuming that the different sets are statistically consistent. The reference curve from step (7) is used and ratios $r(E_i) = \sigma_{exp}(E_i)/\sigma_R(E_i)$ and their errors $\Delta r(E_i) = \Delta\sigma_{exp}(E_i)/\sigma_R(E_i)$ are formed.

(9) These ratios with their errors are fitted using orthogonal polynomials as before. The χ^2/degrees of freedom and the F-test are used to determine the maximum degree of the polynomial fit (see Appendix).

(10) The fitted curve then multiplies the reference curve to give the new reference curve and χ^2/degree of freedom etc., are calculated.

In practice, it is found that a best fit corresponding to a minimum in the χ^2 is found in one iteration and further iterations confirm that one has indeed reached a minimum.

Further tests such as fission spectrum average of the evaluated cross section may be carried out but they have not yet been coded into URAN.

The result of such a fit (solid line) is shown in Figs. 1-4. For comparison are shown the Poenitz evaluation [76] (dashed curve) and the ENDF/B-V evaluation (Δ). The curve obtained from this procedure agrees with the Poenitz evaluation from 100 keV-8 MeV to within ∿1.8% or less. Above 8 MeV, it follows the Kari [81] data and is about 1.0-4.9% higher than the Poenitz evaluation.

In Fig. 5 are shown the ENDF/B-IV and V evaluations with some of the recent experimental data between 0.6-6.6 MeV. It is noted that the trend of the Barton data [82] between 2-6 MeV shows a "tilt" with respect to the ENDF/B-V evaluation. The Poenitz [83] and the Carlson and Patrick data [84] on the other hand show a "concave" shape with respect to the Version V evaluation in the same energy region. If ratios of these data sets are formed with respect to the best representation of all data or the evaluation, and are fitted by orthogonal functions, one can expect to calculate the "tilt" and the "bow" or "concave" shape terms as the coefficients of the second ($\sim x$) and the third degree ($\sim x^2$) orthogonal polynomials (see Appendix). This could provide clues to systematic errors in data due to effects which vary as the first and second powers in energy. Such analyses could provide useful clues in pinpointing and correcting for systematic errors in data.

A number of improvements in this procedure are possible. As it stands now, the method does not use the full variance-covariance matrices of input data. Further, the energy grid of the average shape curve is less than ideal. It is planned to rectify these defects in the near future. It should, however, be pointed out that this method does lead to a least-squares fit to the data and can be applied to any case where the form of the data or cross section as a function of energy is not known.

d. Kon'shin Method

Recently, two reports [85,86] describing a method proposed by Kon'shin et al. to evaluate fission cross section and alpha data have been published. The authors claim to have developed a method of evaluating data and the errors in them with allowance for correlations between partial errors of different experiments. This method has been applied to evaluate σ_f and α for ^{235}U and ^{239}Pu.

The authors point out the importance of allowing for correlations in errors in experimental data which are used in an evaluation and the correlations in errors of the final result. As an example, in the case of $^{235}U(n,f)$ data, some 12 types of experimental errors are considered followed by a detailed discussion of these errors and their correlations. Such a discussion is useful and should form part of any evaluation effort. The subsequent evaluation procedure, however, is new. An expression is written for the difference between the evaluated values σ_{ev} and σ_0 (the unknown true value of the quantity being measured) squared and averaged over the statistical distribution in terms of the weights a_i^2 and their correlations and partial errors. This expression is minimized with respect to the weights a_i^2 and the corresponding values of these weights are determined. In the words of the authors,

> "..the algorithm described here was used in a computer program which employs the partial errors and the correlations between them as a basis for determining by the iteration method, the "weights" of the experimental data which will minimize the error in the evaluated

value, the errors in the evaluated values at different points and the coefficients of correlation between them" [85].

Thus, it appears as though, having decided on an evaluation, (which is presumably drawn through a set of points, the details are not given), the weights of the data are changed to make the evaluation "look good." The usual procedure is to keep the weights as determined from the precision of the data unchanged and vary the "evaluation" subject to proper statistical criteria. The weights are seldom set to be other than those given by the data measurer and that too for reasons that can be defended and justified. A little reflection shows that one obvious result of this procedure would be to give high weights to those data points which happen to lie close to the evaluation and low weights to others. This is exactly what seems to happen in Table 2.1[85] of one of the reports. In this Table, the column K=0 corresponds to no correlations assumed and the weights = $\frac{1}{\Delta\sigma_i^2}$ = inversly as the variance of data (the usual procedure) and K and K=1 are for ascribed correlations and full correlation. From this Table, in the 2nd and 3rd column (K≠0) non-zero weights are obtained for only a few data sets as a result of minimization procedure described above. Such a procedure which assigns zero weights to more than half the input data sets must be treated with caution. This evaluation procedure is curious and the exact purpose of this interesting exercise is not clear.

e. Bayesian Methods

Use of Bayes' theorem [87] in data evaluation is relatively new and the methods based on it form an interesting group. The essential idea is to use Bayes' theorem to incorporate new knowledge obtained from measurement (likelihood) into the prior knowledge (from previous measurements usually or conjecture sometimes) to obtain updated information or knowledge a posteriori. There are many ways of stating Bayes' theorem; however, for our purpose it is written as:

$$\text{posterior distribution} \propto \text{prior distribution} \times \text{likelihood} \qquad (8)$$

where the prior distribution expresses the state of knowledge of a physical parameter in terms of a distribution, and the above equation states how it gets changed by the knowledge of the same quantity obtained from a new measurement and represented by the likelihood. This equation may be put in more concrete terms if we assume that the prior and likelihood are given by: $N(\mu_1,\sigma_1^2)$ and $N(\mu_2,\sigma_2^2)$ respectively where $N(\mu,\sigma^2)$ stands for a normal distribution with mean μ and variance σ^2. It can be shown that using the above equation (8) one obtains [87] a posterior distribution $N(\mu_3,\sigma_3^2)$ where

$$\frac{1}{\sigma_0^2} + \frac{1}{\sigma_1^2} = \frac{1}{\sigma_2^2} \tag{9}$$

$$\frac{\mu_0}{\sigma_0^2} + \frac{\mu_1}{\sigma_1^2} = \frac{\mu_2}{\sigma_2^2} \tag{10}$$

The above expressions are the same as those used in obtaining weighted average of two quantitites μ_0 and μ_1 with variances σ_0^2 and σ_1^2 and whose weights ω_i are inversely proportional to the variances. The above results may also be obtained by minimizing the expression

$$q^2 = \frac{(\mu-\mu_0)^2}{\sigma_0^2} + \frac{(\mu-\mu_1^2)}{\sigma_1^2} \tag{11}$$

with respect to μ. From Equations (9) and (10) it is evident that the new measurement can make a significant improvement in our knowledge of the mean provided its variance σ_1^2 is significantly smaller than σ_0^2. Otherwise, the prior knowledge given by $N(\mu_0,\sigma_0^2)$ which could have been obtained from previous experiments or a conjecture would remain essentially unchanged. Hence, new data have to be significantly more precise to influence old data.

Extension of these ideas to data adjustment using integral experiments was made by Dragt [88,89]. Dragt showed that if integral experiments are considered to represent new knowledge their effect on differential data may be derived using Bayes' theorem with the assumption of multivariate normal distributions for these quantities or by minimizing an expression corresponding to Equation (11) in the general case. This is also called a generalized least-squares method in that it denotes an extension of the usual least-squares method in using full variance-covariance matrices for input data and the evaluation and also prior information [90]. Let the vector $\bar{T}$ denote a set of n_t nuclear data with a covariance matrix M of order $(n_t \times n_t)$ and having a Gaussian distribution. Let the new knowledge be represented by n_r measured integral quantities written as vector R with a covariance matrix V of order $(n_r \times n_r)$. The same integral quantities calculated from $\bar{T}$ are denoted by $\bar{R}$. Their dependence on $\bar{T}$ is expressed by the sensitivity matrix $G(n_r \times n_t)$ containing partial derivatives of $\bar{R}$ with respect to T so that

$$\delta\bar{R} = G\delta\bar{T} \tag{12}$$

Dragt has shown that by minimizing an expression analogous to (11) viz:

$$q^2 = (T'-\bar{T})^t M^{-1}(T'-\bar{T}) + (\bar{R}'-R)^t V^{-1}(\bar{R}'-R) \tag{13}$$

where T' the adjusted quantities are found by minimizing equation (13) and $\bar{R}'$ are the new values for the integral quantitites belonging to T' and

$$\bar{R}' = \bar{R} + G(T'-T) \tag{14}$$

Here t denotes transpose of the matrices. One obtains T' and the new covariance matrix M' as solutions of

$$(M^{-1} + G^t V^{-1} G)\ (T'-T) = G^t V^{-1}(R-\bar{R}) \tag{15}$$

$$M' = (M^{-1} + G^t V^{-1} G)^{-1} \tag{16}$$

Procedures for sloving these equations have been discussed [89] and this method has been applied by Perey [91,92] to dosimetry problems. Schmittroth has also discussed the generalized least-squares method [90,93] and written a code FERRET [94] to implement it. He has also proposed a finite element representation of cross section data given by a continuous function and illustrated the procedure in the case of $^{54}Fe(n,p)$ cross section from threshold to 20 MeV [95]. Hetrick and Fu have written a code GLUCS [96] which is a generalized least-squares program and used it to evaluate $^{32}S(n,p)$, $^{56}Fe(n,p)$ and $^{65}Cu(n,2n)$ using previous evaluations of these reactions and the new ratio data [97]. As has been mentioned earlier, one important feature of these evaluation methods based on Bayes' theorem or generalized least-squares is that they use the full variance-covariance information for input data and generate such matrices for the evaluation. In addition, they could use prior information in the form of a previous evaluation or a nuclear model calculation. Though these methods have not yet been used for any of the cross section standards, there is no reason why they cannot be. The prior information could also be in the form of a curve drawn through experimental points with a rough uncertainty estimate. This initial estimate could then be refined using this procedure. Schmittroth's finite element representation ensures that smooth prior curves transform into smooth posterior curves. The GLUCS code does not as yet have any specific method to do this and relies on the fact that the experimental data points are densely distributed and hope no unphysical wiggles would appear in the final curve [98]. If there are any problems, some smoothing procedures could be built into it.

As a further aid in understanding the above Equations (15) and (16), it is instructive to establish a one-to-one correspondence between them and the Equations (9) and (10) for the simple one dimensional case. They can be rewritten as:

$$\frac{1}{\sigma_0^2} + \frac{1}{\sigma_1^2} = \frac{1}{\sigma_2^2} \tag{17a}$$

$$M^{-1} + G^t V^{-1} G = M'^{-1} \tag{17b}$$

and

$$\frac{u_0}{\sigma_0^2} + \frac{u_1}{\sigma_1^2} = \frac{u_2}{\sigma_2^2} \tag{18a}$$

$$M^{-1} T + G^t V^{-1} G \left(T + G^{-1}(R-\bar{R})\right) = (M^{-1} + G^t V^{-1} G)T' = M'^{-1} T' \tag{18b}$$

From these equations, one notices that the correspondence between $\frac{1}{\sigma_0^2}$ the inverse of variance of u_0 and M^{-1} the inverse of the variance matrix of the prior data T; $\frac{1}{\sigma_1^2}$ of the new data corresponds to $G^t V^{-1} G$ (the sensitivity matrix occurs here because the new data are integral data R rather than data of the same type as T) and $\frac{1}{\sigma_2^2}$ corresponds to M'^{-1} the inverse of the variance matrix for the posterior distribution. The same correspondence is in Equation (18) where the $(R-\bar{R})$ has an extra factor G^{-1} which converts the difference between the measured values R and the values $\bar{R}$ calculated from T into a correction ΔT to T to give the value of T which corresponds to the integral measurements R.

In addition to this correspondence, these equations may also be interpreted in terms of Fisher's definition of "information" [99]. There are many definitions of "information" in statistics and communication theory and Fisher's definition is one of them. In proposing this definition, Fisher required that [99]

(1) the information in a set of observations should increase with the number of observations,
(2) it should be conditional on what one wants to learn from the experiment, that is, data which are irrelevant to the parameters of interest should contain no information, and
(3) information should be related to precision; the better the precision of the experiment, the greater the information.

With these ideas in mind, Fisher proposed a definition of information which may be written as:

$$\left[I_{\underline{x}}(\underline{\theta})\right]_{ij} = -E\left[\frac{\partial^2}{\partial\theta_i \partial\theta_j} \ln L(\underline{x}|\underline{\theta})\right] \tag{19}$$

where $I_{\underline{x}}(\underline{\theta})$ is an expression for the amount of information given by

an observation $\underline{x}$ about the parameter $\underline{\theta}$ and L is the likelihood function considered as a function of both $\underline{x}$ and $\underline{\theta}$. Thus, if x is normally distributed with variance σ^2 and unknown mean μ, then the information about μ from a single observation is

$$I_1(\mu) = \frac{1}{\sigma^2} \tag{20}$$

and from N independent observations

$$I_N(\mu) = \frac{N}{\sigma^2} \tag{21}$$

From the definition (19) it follows that in the general case of the mulitvariate distribution the information matrix for the vector T is

$$I_T(T) = \frac{1}{M} \tag{22}$$

and similarly

$$I_R(T) = G^t V^{-1} G \text{ provided} \tag{23}$$

$$E\left[G^t V^{-1} G\right] = G^t V^{-1} G \tag{24}$$

In the expression in (23) it should be noticed that we are asking for the information about T from the observed multivariate normal distribution of R. This explains the reason for the presence of the sensitivity matrix G. If the new data are of the same type as T one would get only V^{-1}. The condition (24) may or may not hold; if not, G should be replaced by some mean <G> corresponding to an average over the distribution of R.

With this interpretation in mind, Equation (17a) corresponds to the information about the prior mean ($1/\sigma_0^2$) being added to the information about the mean of the new data ($1/\sigma_1^2$) to give the information about the mean of the posterior distribution ($1/\sigma_2^2$). The same interpretation holds for Equation (17b) were we have information matrices. Equation (18) shows how the means are weighted by the corresponding "information" to give the posterior mean weighted by its information.

From the above expressions the following observations may be made:

(1) the transfer of information about the mean of a quantity is full and faithful only when the new data are of the same type as the prior data i.e., G=1.0

(2) the amount of information transferred to the prior is $G^t V^{-1} G$ and depends on where G is evaluated i.e., T or the prior mean and its energy dependence.

From the above equations it is also noticed that in one iteration, the amount of information contained in the new data has been transferred to the prior. Hence, iterations using the same data over again are not justified. Hence, so long as the above equations based on linear approximation are valid, one should not iterate though the values obtained will depend on T or where G's are calculated. This supports a statement made by Perey [91] justifying only one iteration in this method.

PROBLEMS AND PROSPECTS

From the above discussion of evaluation methods, it is apparent that future evaluations will have to make explicit use of the full variance-covariance information about the input data. Unfortunately, this information is not available in most cases. Hence, the first task of the evaluator or any specialized committees convened to coordinate an evaluation would be to sift through the available information and construct the covariance matrices. Perey [91] and Peelle [3,4] have discussed this problem and endorsed it as an extremely useful endeavor worthy of being published. Of course, the ideal thing would be for the measurer to come up with the covariance information. If such data uncertainty information becomes available it should be stored in the neutron data files like CSISRS (Cross Section Information Storage and Retrieval System) to facilitate data exchange. If in a measurement involving ratios with respect to a standard, the standard evaluation used to convert these ratios into cross sections and the covariance files will have to be stored in the data files. All these extra data will involve format changes and additional effort on the part of the Data Centers. Perhaps the changes should be tried out with a few of the cross section standards and then extended to dosimetry and other reactions where the data usage and analysis have become sophisticated enough to make use of this additional information.

One of the favorite complaints professional statisticians have against physicists is that the statisticians are consulted after an experiment is done and not before. While it is true that the physics experiments need not be "designed" with the same care as in the life sciences because of greater control over the experimental conditions, there is some virtue in thinking through the possible systematic and statistical errors and their correlations before doing an experiment. Such an in depth error analysis in the planning phase of an experiment could reveal unexpected correlations and dependence of the new data on other measurements. This would also be helpful in working out the covariance data for the experiment after it is done.

Future data evaluations, at least for standards, are expected to use

(1) full covariance information for input data,
(2) objective evaluation procedure based on a well-defined statistical model,
(3) produce variance-covariance information for the evaluation and have,
(4) full and complete documentation of the evaluation procedure and the data base used.

A consistent evaluation of the neutron cross section standards has been advocated by Poenitz [100] and others for a number of years. This is because the standards are related by a number of ratio data and any correlations brought about by the process of measurement.

After each of the standards has been analyzed to understand its problems and discrepancies, a consistent analysis of all of them by an objective procedure and full error information would be a worthwhile objective.

SUMMARY

Evaluation methods used with the neutron cross section standards have been reviewed in this article. In addition to the methods used for those reactions where the functional form of the cross sections are known, a number of new procedures have been proposed for cases where this is not so. Hence, it is now possible to use objective evaluation methods for all the standards reactions. The need to use the full covariance information of the input data has been stressed. It is hoped that the data measurers would cooperate to provide this information for their data. It is also obligatory to obtain full uncertainty files for the evaluations as part of the evaluation process. A consistent evaluation of the primary cross section standards should also be carried out.

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APPENDIX

Orthogonal Polynomials and the F-test

The method used to generate the orthogonal polynomials follows closely the work of Forsythe [101], with modifications suggested by Martin [102].

If there are n data points $y_1 \ldots\ldots y_n$ with errors $\Delta y_1 \ldots\ldots \Delta y_n$ measured at $x_1 \ldots\ldots x_n$; the weight matrix is assumed to be diagonal with elements,

$$W_j = \frac{1}{(\Delta y_j)^2} \tag{A.1}$$

and the orthogonal polynomials ϕ_k are defined to be orthogonal if

$$\sum_{j=1}^{n} W_j \, \phi_k(x_j)\phi_\ell(x_j) = 0 \text{ for } k \neq \ell \tag{A.2}$$

To construct the polynomials of high orders with a computer with a finite word size, the x_j are normalized to lie within the interval [-1,+1] and the three term recurrence relations used are as follows:

$$\phi_1(x) = 1/2$$

$$\phi_2(x) = (2x+\beta_1)\phi_1(x)$$

and for $k \geq 2$

$$\phi_{k+1}(x) = (2x+\beta_k)\phi_k(x) + \gamma_{k-1} \, \phi_{k-1}(x) \tag{A.3}$$

where

$$\beta_k = -2\sum_{j=1}^{n} W_j x_j \phi_k^2(x_j) / \sum_{j=1}^{n} W_j \phi_k^2(x_j) \tag{A.4}$$

$$k=1,2,3....$$

and

$$\gamma_{k-1} = -\sum_{j=1}^{n} W_j \phi_k^2(x_j) / \sum_{j=1}^{n} W_j \phi_{k-1}^2(x_j)$$

$$k=2,3,4.... \qquad (A.5)$$

If the observations y_j are fitted by a number of p parameters as

$$f_j = \sum_{k=1}^{p} \theta_k \phi_k(x_j) \qquad (A.6)$$

the least-squares estimates of the parameters are:

$$\theta_k = \sum_{j=1}^{n} W_j y_j \phi_k(x_j) / \sum_{j=1}^{n} W_j \phi_k^2(x_j)$$

$$k=1,2....p. \qquad (A.7)$$

From the three-term recurrence relationship (A.3, A.4) it is noticed that the orthogonal polynomials

$$\phi_k(x) \sim x^{k-1} \qquad (A.8)$$

hence, the various coefficients have the following simple interpretation. Because $\phi_1(x) = 1/2$; $\theta_1/2$, gives a normalization for the curve as a whole; $\theta_2 \sim x$ a tilt term and $\theta_3 \sim x^2$ a "bow" term and so on. This simple visualization is helpful in understanding how the function obtained by fitting the ratios of experimental data to the reference curve affects the reference curve when it is multiplied by it to obtain a new reference curve.

If one uses p orthogonal polynomials to obtain a least squares fit, the sum of squared residuals at the minimum is given as

$$S_p = \sum_{j=1}^{n} W_j \left[y_j^2 - \sum_{k=1}^{p} \theta_k^2 \phi_k^2(x_j) \right] \qquad (A.9)$$

To test whether the p-th coefficient is statistically significant one calculates [103],

$$\frac{\left(S_{p-1} - S_p\right)(n-p)}{S_p} \qquad (A.10)$$

and if this is greater than F(1,(n-p)) at the 1% confidence level, the coefficient θ_p is considered to be non-zero. In addition, one should also look at the $\chi^2/(n-p)$ for the p-coefficient fit and in running the program in addition to the F-test, the number of parameters was chosen such that $\chi^2/(n-p)$ was between 2.0 and 0.2. Another criterion to use would be to look at a visual display of the fit on a screen for various values of p. This has not been implemented yet.

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TABLE I

Types of Data Used in $^{2}H(n,n)^{2}H$ Phase Shift Analysis

Data Type	Approximate Precision
Deuteron Binding Energy B	0.001%
Deuteron Radius R (from B)	0.002%
Epithermal Scattering Cross Section σ_o	0.07%
Coherent Scattering Length f	0.03%
a_t (from σ_o and f)	0.06%
a_s (from σ_o and f)	0.03%
r_{ot} (from a_t and B)	0.3%
r_{os} (from a_s and low energy scattering)	2%
a_{pp}	0.05%
r_{opp}	0.6%
Total, differential elastic scattering, polarization, spin transfer and spin correlation (n,p) data	1-several %
Differential elastic scattering, polarization spin transfer and spin correlation (p,p) data	1-several %

TABLE II

Absolute Data Used in Shape/Magnitude Fit

No.	Author	Ref.	Energy Range (keV)	AN/SAN	Comments
1	Barton, et al.	82	3.0+3	10000/1	
2	Poenitz	83	1.93+2 - 8.275+3	45000/71	Black Det.
3	Poenitz	104	3.99+2 - 3.5+3	13000/2	Black Det.
4	Poenitz	104	4.98+2	40000/2	VSO_4 Bath
5	Poenitz	104	4.48+2 - 6.44+2	40000/2	Assoc. Activ.
6	Kari	81	1.0+3 - 2.031+4	45000/4	
7	Cance & Grenier	105	1.39+4 , 1.46+4	40000/2	
8	White	106	6.7+1 - 1.41+4	18000/1	
9	Wasson & Meier	107	2.54+2 - 1.217+3	31000/1	Preliminary
10	Szabo, et al.	108	5.1+1 - 5.53+3	17000/1	non-White Counter
11	Davis, et al.	109	1.4+2 - 9.64+2	36000/1	
12	Wasson	110	5.5+1 - 7.5+2	45000/10	
13	Arit	111	1.47+4	40000/2	

TABLE III

Data Sets Used in Shape Fit

No.	Author	Ref.	Energy Range (keV)	AN/SAN	Comments
1	Barton et al.	82	1.0+3 - 6.0+3	10000/1	
2	Czirr & Sidhu	112	7.54+2 - 2.01+4	11000/1	
3	Poenitz	104	6.8+1 - 3.5+3	13000/1	grey det. data
4	Poentiz	104	3.99+2 - 3.5+3	13000/2	black det. data
5	Smith, et al.	113	2.22+3 - 2.05+4	16000/1	
6	Szabo, et al	108	5.1+1 - 5.53+3	17000/1	non-white counter
7	White	106	6.7+1 - 1.41+4	18000/1	
8	Kari	81	1.0+3 - 2.031+4	45000/4	
9	Poenitz	83	1.93+2 - 8.275+3	45000/71	black det. data
10	Carlson & Patick	84	1.171+3 - 6.203+3	45000/151	Preliminary
11	Szabo, et al.	108	5.5+1 - 2.1+3	30000/1	White counter
12	Wasson & Meier	107	2.54+2 - 1.217+3	31000/1	Preliminary
13	Davis, et al.	109	1.4+2 - 9.64+2	36000/1	
14	Gayther	114	5.5+1 - 9.5+2	45000/8	
15	Wasson	110	5.5+1 - 7.5+2	45000/10	
16	Kaeppeler	115	5.46+2 - 1.175+3	45000/111	
17	Kaeppeler	115	5.13+2 - 1.164+3	45000/112	

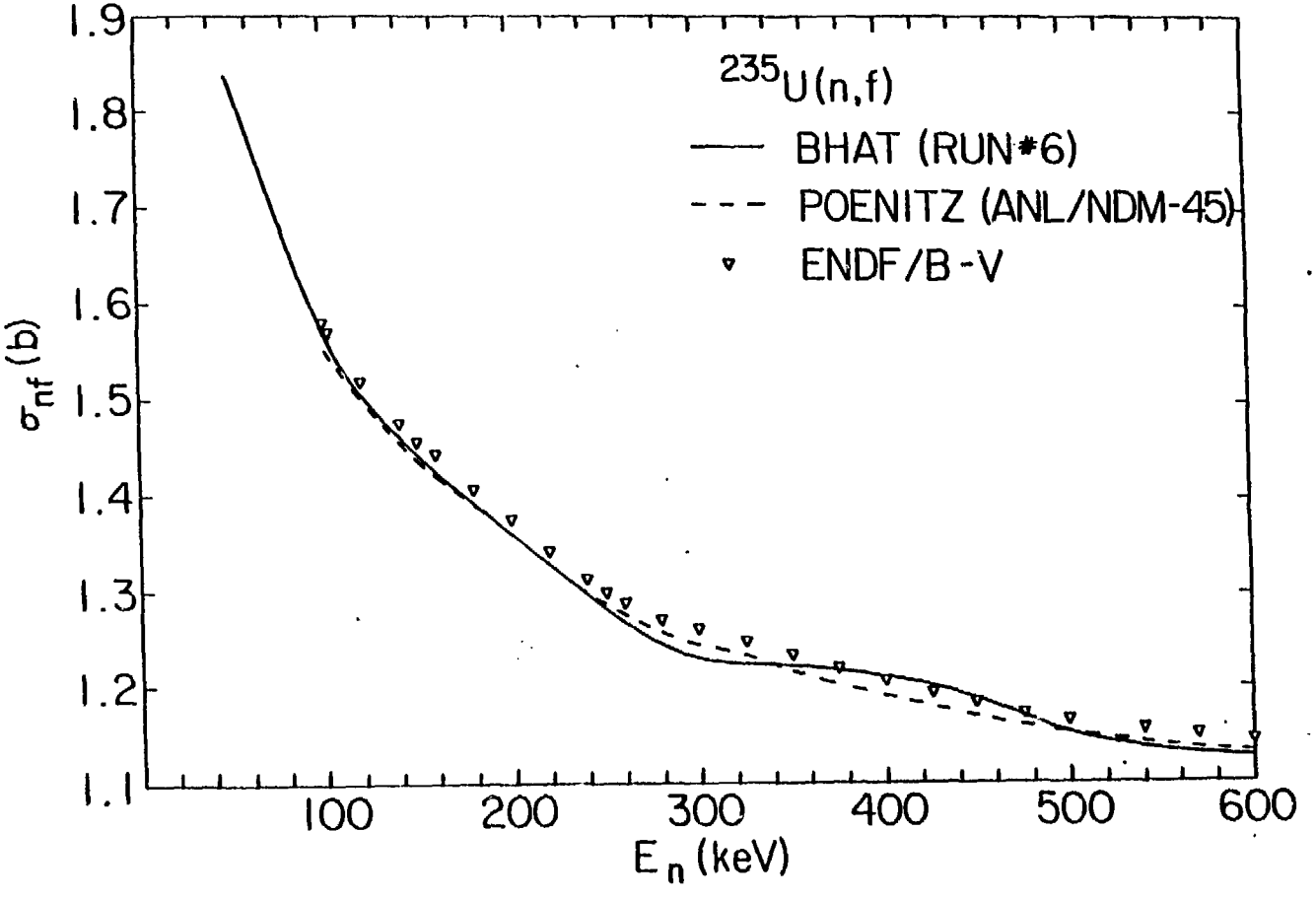

Fig. 1. Comparison of ENDF/B-V, Poenitz and Bhat Evaluations of ^{235}U(n,f) From 100-600 keV.

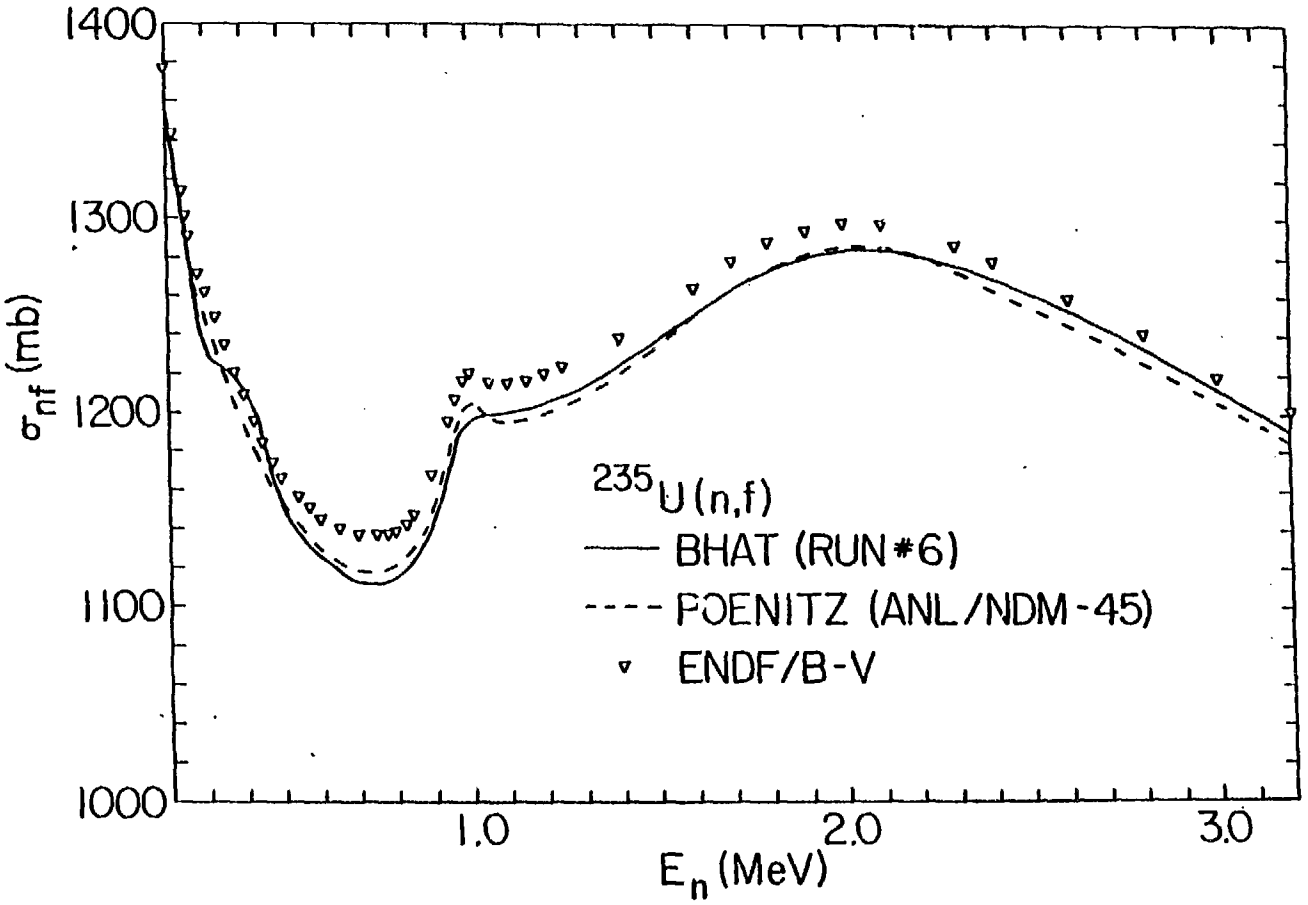

Fig. 2. Comparison of ENDF/B-V, Poentiz and Bhat Evaluations of $^{235}U(n,f)$ From 0.2-3.2 MeV.

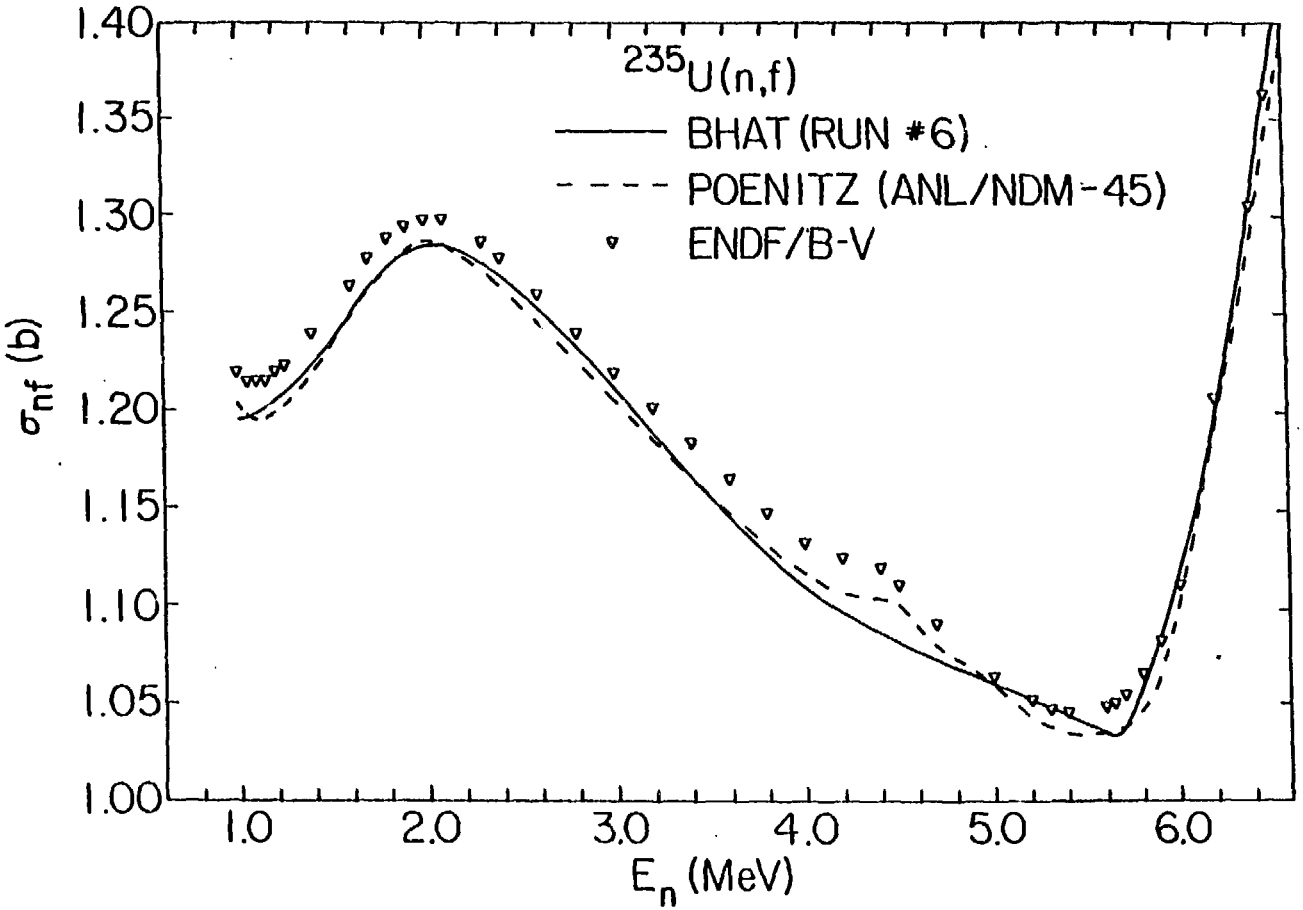

Fig. 3. Comparison of ENDF/B-V, Poenitz and Bhat Evaluations of ^{235}U(n,f) From 1.0-6.6 MeV.

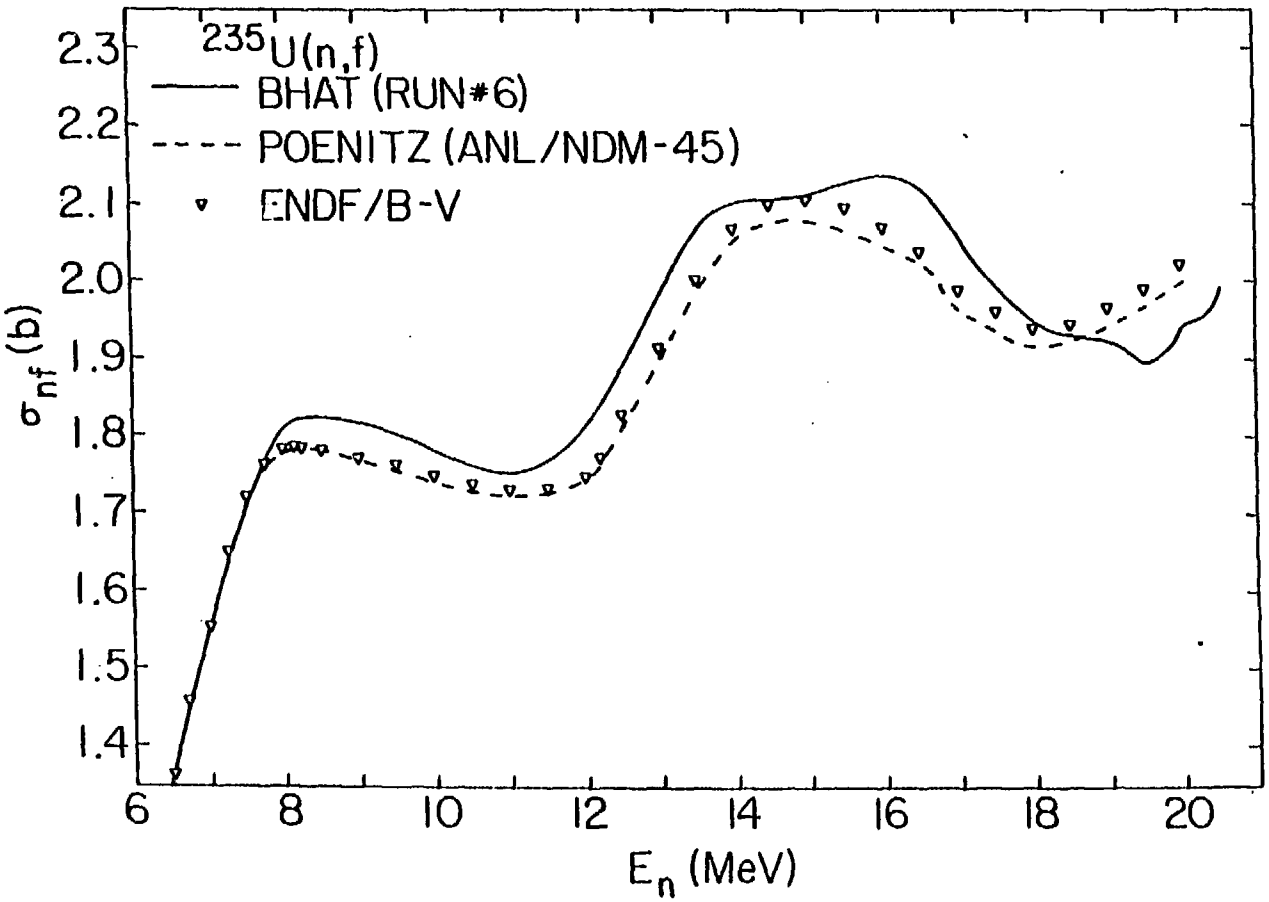

Fig. 4. Comparison of ENDF/B-V, Poenitz and Bhat Evaluations of ^{235}U(n,f) From 6-20 MeV.

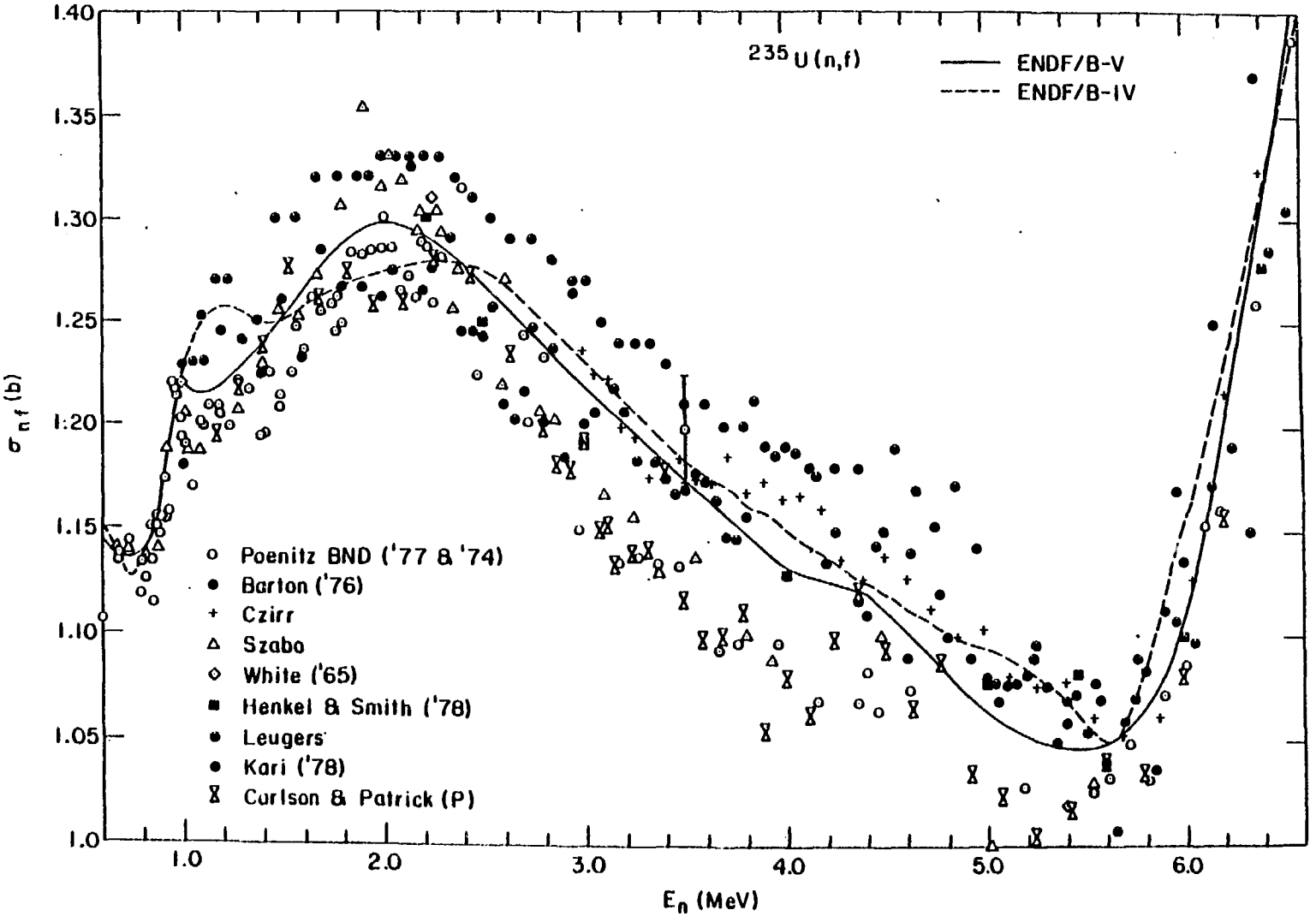

Fig. 5. Experimental ^{235}U(n,f) Data From 0.6-6.6 MeV With ENDF/B-IV, V Evaluations.