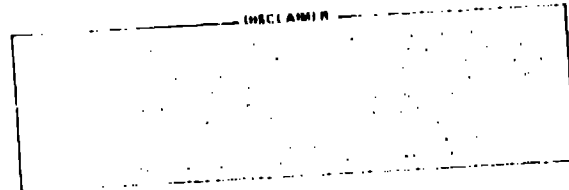TITLE: REVIEW OF NEW DEVELOPMENTS IN FUSION REACTOR NUCLEONICS

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REVIEW OF NEW DEVELOPMENTS IN FUSION REACTOR NUCLEONICS

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ABSTRACT

A review is presented of recent developments in nuclear data, computational methods, and computer codes, especially as pertains to fusion reactor nucleonics. Important nuclear data measurements, evaluations, nuclear model codes and processing codes are discussed. Progress in solution acceleration and deterministic streaming methods for discrete-ordinates codes is covered, along with comments on recent Monte Carlo developments. Finally, sensitivity and uncertainty analysis methods are reviewed.

INTRODUCTION

Two main paths of development have occurred for fusion reactor nucleonics — nuclear data and neutron/gamma-ray transport methods. Each path has included basic foundations which were laid down in the past for other nuclear programs. With a few notable exceptions, the data, methods and codes in use today for fusion reactor nuclear analysis are adapted from those programs. The present review is confined primarily to recent developments in direct support of the U.S. fusion reactor technology program, previous work in other programs already having been extensively reviewed [1-5] for its applicability to fusion reactors.

Over the past several years, considerable effort has gone into identifying deficiencies in nuclear data that impact fusion reactor designs. Problems that have been emphasized include evaluation format deficiencies,[6] lack of energy balance in ENDF/B-V evaluations,[7] gaps in the availability of particular types of data,[8,9] and inadequate accuracy in certain evaluated data as identified in specific sensitivity/covariance analyses.[10] A fusion energy data request list[11] has evolved and has served to focus certain differential data measurement programs on fusion data needs. Progress has been made in several important areas, including new data on tritium production and other neutron reactions with ^6Li and ^7Li, neutron reactions with W isotopes, charged-

particle data, emission spectra for secondary radiation, nuclear model codes, and new evaluated cross sections and covariance data files.

Processing codes have been expanded to accomodate new ENDF/B formats and to generally provide increased information. General purpose data libraries such as ENDF/B·V, GAMDAT78,[12] and series 1-7 of the MATXS library[13] are now available at the National Magnetic Fusion Energy Computing Center (NMFECC). In addition, the TRANSX[13] and NJOY[14] processing code systems as well as the GAMMON activation library[15] are operational at the NMFECC. The GAMMON library, which is specifically designed for fusion reactor applications, contains multigroup cross sections (100 energy groups) for 420 neutron-induced reactions, multigroup gamma-ray spectra (25 energy groups) for 107 unique daughter products, maximum permissible concentrations (MPC's) for 200 reaction products, and absorbable decay energy (sensible heat) for 85 products.

Because of the breadth of data needs, we will restrict our discussion to a few of the more visible problems and will emphasize the measurement, calculation, and evaluation efforts for these cases. A more complete review of fusion data activities was recently given by Haight.[16]

Specific areas of development in transport methods and codes during recent years have included new one-dimensional (1-D) and 2-D discrete-ordinates codes, with features specifically designed for and/or applicable to fusion reactor design. The principal new features in 1-D have included greatly improved efficiency (i.e., reduced computation times) by diffusion synthetic acceleration, a completely new and mnemonic-oriented free-field input format, and evolutionary improvements in hierarchical storage strategies, output and edit features, etc. The ONEDANT code[17], incorporating these features, is now generally available on the NMFECC along with multigroup data libraries. Similarly, the

2-D triangular-mesh code, TRIDENT-CTR,[18] is available on the NMFECC for fusion reactor blanket/shield analysis. Research is presently underway to incorporate deterministic streaming methods into TRIDENT-CTR, with the ultimate goal of achieving accurate discrete-ordinates solutions in the vicinity of large void regions such as vacuum ducts, plasma chambers, etc.

The principal recent developments for Monte Carlo codes have consisted of evolutionary improvements in geometry routines, output of physically significant particle history data, variance reduction guidance for the user, and general code architecture. Adaptations for fusion technology applications have been made to the MCNP code,[19] which is being used on the NMFECC for nucleonic analyses of the Fusion Materials Irradiation Test (FMIT) facility and several fusion reactor concepts (e.g., EBTR, LINUS, Fast Liner Reactor, Reverse Field Pinch Reactor). Of particular interest is the increased use of both deterministic and stochastic transport codes for analyzing neutral atom distributions in plasma, limiter and divertor regions.[20,21]

NUCLEAR DATA

Neutron Reactions on ^{6}Li and ^{7}Li

Extremely important processes for a D-T fusion reactor economy are the tritium production reactions for ^{6}Li and ^{7}Li. While the ^{6}Li(n,t) cross section is thought to be reasonably well known in the region of importance, serious questions have been raised about the accuracy of the ^{7}Li(n,n't) reaction cross section that is currently in the ENDF/B-V evaluated data file. The over-prediction of tritium production in integral experiments suggests that the ENDF/B tritium production cross section for ^{7}Li might be from 10 to 35% too high near 14 MeV.[22-24] The new differential data from Swinhoe and Uttley[25] and Smith et al.,[26] which are illustrated in another paper at this meeting,[27] indicate the ENDF/B data should be lowered from 15 to 25%. Other new tritium production data at 6 and 10 MeV (inferred from the neutron emission results of Lisowski at al.[28]) tend to support the existing ENDF/B values, but with relatively large uncertainties. To summarize, these new results are all consistent with a lowering of the ENDF/B-V tritium production cross section, but there is disagreement on the magnitude of the corrections. An additional differential measurement is in progress at Geel, which should help clarify the situation.

Other new differential data have become available recently that should indirectly aid in determining the ^{7}Li(n,n't) cross section,

as well as in generally improving ^{6}Li and ^{7}Li neutronics data. These results include new total cross section measurements[29,30] between 0.1 and 50 MeV, differential elastic angular distributions[31,32] between 4 and 14 MeV, measurements of neutron emission spectra[28] at 6 and 10 MeV, and several new measurements[33-35] of the ^{7}Li(n,n'γ) cross section that cover the energy range from threshold to 20 MeV. Of particular importance for fusion applications are the differential elastic and neutron emission spectrum measurements between 9 and 14 MeV. The elastic angular distributions measured by Hogue at al.[32] between 10 and 14 MeV are compared to the ENDF/B-V evaluation in Fig. 1. Significant differences between experiment and evaluation are seen at some angles. New evaluations for ^{6}Li and ^{7}Li that consider both old and new experimental data are currently in progress at Los Alamos Scientific Laboratory (LASL) by one of the authors (Young).

Neutron Reactions on Tungsten

One of the conclusions of a recent uncertainty analysis by Gerstl et al.[10] is that both the cross sections and neutron emission spectra for tungsten are probably inadequate for fusion reactor designs that employ significant amounts of tungsten for shielding. Similarly, as shown in another paper at this meeting,[2] measurements from the Livermore Pulsed Sphere program also indicate that the ENDF/B-V tungsten isotope evaluations lead to seriously deficient neutron emission spectra for 14-MeV incident neutrons.

As a result of these problems, a new evaluation of the neutron-induced data for tungsten isotopes is in progress.[36] The new evaluation couples recent total, elastic scattering, and (n,2n) cross-section measurements with a modern nuclear theory analysis that should significantly improve tungsten data in the 0.1-20 MeV region. The use of nuclear-model calculations will remove the discrepancies between neutron and gamma-ray emission spectra that have led to the serious energy balance problems evident in the ENDF/B-V evaluations.[7] The calculated neutron emission spectrum for 14.6-MeV incident neutrons is compared in Fig. 2 to both ENDF/B-V and to a measurement by Hermsdorf et al.[37] Note that the discrepancy between ENDF/B and the measurements between 5 and 11 MeV is greatly reduced by the new calculations, although not entirely removed.

Charged-Particle Reactions

While very thorough R-matrix analyses[38] have been performed for the most important fusion reactions, the results are still dependent on the accuracy of the experimental

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data base used in the analyses. The experimental data for certain key reactions, such as D(t,n)⁴He, D(d,n)³He, D(d,p)T, and T(t,2n) ⁴He, mainly consist of measurements performed 25 years ago, and the accuracy of these data is subject to some question.[39,40] As a result, a program to measure these cross sections down to as low an energy as possible is in progress at LASL.[40] The energy range for the new measurements is 10-120 keV, which corresponds to plasma ion temperatures of 2-20 keV. The desired accuracy is ±5% or less, which is as much as an order of magnitude better than existing knowledge at the lower end of the energy range The experimental approach consists of using a source of negative hydrogen ions to bombard a windowless, cryogenically pumped gas target. The beam intensity is determined by calorimetric means, and the crucial beam-energy measurement is to be facilitated by a planned laser-photodetachment, time-of-flight technique. The target density is calibrated during the experiment by using scattering or reactions of known cross sections induced by 10-15 MeV particles from a tandem Van de Graaff accelerator.

To avoid tritium contamination problems until the equipment is thoroughly developed, the initial experiments involve only the D + D reactions. Preliminary data have been obtained for the D(d,p)T reactions between 40 and 118 keV. It is expected that during 1981 final data on the D + D reactions will be obtained and work on the D(t,n)⁴He reaction will begin. The T(t,2n)⁴He measurements will be performed last because of their relatively greater difficulty.

Neutron, Charged-Particle, and Gamma-Ray Emission Data

The need for more accurate emission data for secondary neutrons, gamma-rays, and charged-particles has become increasingly evident with improvements in methods and codes for neutron transport, heating, and radiation damage calculations. Experimental facilities have been developed at LASL and at the Triangle Universities Nuclear Laboratory (TUNL) for measuring neutron emission spectra induced by neutrons in the MeV energy region. Thus far, measurements have been made for 6-, 10-, and 14-MeV incident neutrons at LASL[9,40,41] for ⁶Li, ⁷Li, ⁹Be, ¹⁰B, and ¹¹B, and at several energies between 8 and 14 MeV at TUNL[42] for Fe, Cu, Ni, and Pb. Similarly, neutron spectrum measurements have been made at the Oak Ridge Electron Linac Accelerator (ORELA)[43] for ⁷Li, Al, Ti, Cu, and Nb An example of a neutron emission spectrum measurement for ⁹Be is shown in Fig. 3. These data have been incorporated into an evaluation[6] that differs significantly from ENDF/B-V.

An extensive set of measurements of gamma-ray emission spectra using the ORELA white neutron source has been carried out at Oak Ridge.[43] These results generally span the incident neutron energy range from 1 to 20 MeV and have been performed for most of the common materials. In addition, a series of gamma-ray spectrum measurements for monoenergetic 14-MeV neutrons has been carried out at LASL[44] for a variety of materials. These measurements have been very useful for gamma-ray production evaluations, although some discrepancies are known to exist between the two sets of data.

The information on charged-particle emission cross sections and spectra is decidedly less abundant than for gamma rays. Two experimental programs that deserve special mention are recent helium production cross-section measurements that utilize high sensitivity mass spectrometry[45] and charged-particle emission spectrum measurements made with magnetic quadrupole spectrometers.[46] These programs have provided data for several materials of interest at E ≅ 15 MeV and should be very useful in the future as more energies and elements are covered.

Nuclear Model Codes and Higher-Energy Data

Considerable progress has been made over the past decade in development of nuclear-model codes for use in complementing experimental data in evaluations and even for predicting unmeasured data (see Refs. 47 and 48 for recent reviews). Of most interest for fusion reactor applications are several new multistep Hauser-Feshbach/preequilibrium model codes that are capable of handling the numerous reaction channels that open in the neutron energy range from 7 to 50 MeV. The codes in most common use in the United States are GNASH,[49] HAUSER-5,[50] STAPRE[51] and TNG.[52] When care is taken to obtain physically meaningful model parameters, these codes have been quite successful in tying together and extrapolating experimental information. Such calculations have the additional advantage that energy conservation is built into the models. It is expected that these models will be a key element in augmenting experimental data in the 10-50 MeV region for the FMIT facility.

Analyses covering the incident neutron energy range from ~3 to 40-50 MeV have recently been carried out for ⁵⁴,⁵⁶Fe, ⁵⁹Co, and ⁵⁸,⁶⁰Ni at LASL using the GNASH code. Neutron, gamma-ray, and proton emission spectra for 14-MeV neutrons incident on iron from a single calculation[53] are compared to experimental data[44,46,54] in Fig. 4. The agreement is reasonable, especially considering that these measurements were not used in determining the model parameters.

Results from the ^{59}Co analysis[55] are compared to measurements of (n,xn) cross sections in Fig. 5, and the full ^{59}Co cross-section predictions to 50 MeV are shown in Fig. 6.

Covariances

A significant expansion of covariance data occurred between ENDF/B Versions IV and V. The number of ENDF/B-V general purpose evaluations containing covariance data is now about 24 and includes many important fusion materials. For the first time, covariances for resonance parameters are given for some materials, although the information is not complete. Materials having covariances include ^{1}H, ^{6}Li, ^{10}B, C, ^{14}N, ^{16}O, ^{27}Al, Si, Cr, Fe, Ni, and Pb. The covariances are mainly for smooth cross sections and the entire energy range is not covered in all cases. Important omissions in the list of materials are ^{7}Li, Cu, and the W isotopes. Additionally, there are no covariances for angular distributions or secondary energy distributions. Simplified, ad hoc analyses of secondary energy distributions have been performed for use in sensitivity analyses,[10] and the need for such data in evaluations is evident.

Summary Comments on Nuclear Data

In the above sections, we have highlighted some of the nuclear-data developments of the past few years. Progress is evident in several important areas, and significant advances have clearly been made. However, we should point out that a number of problem areas remain in the data. For example, there is still significant disagreement among even the new ^{7}Li(n,n't) measurements; between 7 and 14 MeV, there are still large gaps in most of the required data, especially neutron and charged-particle emission spectra; experimental data of any type are very sparse between 15 and 50 MeV; reaction data for neutrons incident on radioactive nuclei are virtually nonexistent; energy imbalance problems are present in many ENDF/B-V evaluations; significant deficiencies still exist in theoretical model codes and improvements are needed; and the covariance data presently available in ENDF/B-V is limited both in quality and in the extent of reactions and materials for which data are provided.

SENSITIVITY AND UNCERTAINTY METHODS

Inextricably entwined with the assessment of nuclear data needs and adequacy is the quantitative methodology known generically as sensitivity analysis, but including both sensitivity and uncertainty calculations. The theory is founded on simple perturbation methods, with wide applications to fission and fusion reactors. A recent exposition[56] gives an excellent summary of numerous applications of ordinary and generalized perturbation theory. Specific fusion reactor applications usually require only the inhomogeneous source case, and have been reviewed extensively.[57,58] An exception to the inhomogeneous source restriction occurs for fusion/fission hybrid reactor analysis.[59,60] Because of the extensive review literature available, the present discussion is confined to (1) the recently released SENSIT code; (2) secondary energy and angle distribution sensitivity; and (3) 2-D sensitivity analysis.

A latest generation sensitivity code, SENSIT,[61] is currently operational on the NMFECC network. The code is specifically tailored for fusion reactor sensitivity and uncertainty analyses, both for cross-section errors and design perturbations. Included in the cross-section category is the capability to compute sensitivities and uncertainties caused by secondary-neutron energy and angle distribution errors.[62] As has been shown in a comprehensive analysis for a fusion reactor,[10] the secondary-energy-distribution (SED) contribution to response uncertainties is generally lower than that from cross-section uncertainties, but not negligible. For the TNS design analyzed in Ref. 10, the overall uncertainties in TF-coil dpa were 72% and 33% (at the 68% confidence level) from cross-section and SED uncertainties, respectively.

Capabilities for design sensitivity analysis have yet to be exploited extensively. Effects on various nucleonic design parameters (e.g., dpa and kerma) can be easily determined for small perturbations in blanket/shield region dimensions, densities, material compositions, etc. Such analyses with a design sensitivity code could readily be adapted to shield optimization studies.

Two-dimensional sensitivity analyses have not yet been warranted for fusion reactor studies, mostly because of the conceptual nature (and therefore lack of detail) of such designs. However, the ETF project or its sequel (FED) will provide a requirement for such analyses in the next few years, as the shield designs firm. Some capability already exists for 2-D cross-section sensitivity,[56,63] and has been applied to a preanalysis of the ORNL fusion reactor shielding experiments.[64] For this particular application, the adequacy of a 1-D sensitivity study was demonstrated by comparison with the 2-D analysis. As is the case for 1-D, the 2-D methods and codes are readily extendable to design sensitivity and shield optimization when required.

TRANSPORT METHODS AND CODES

Extensive work to improve neutron/gamma-ray transport numerical methods has been per-

formed in the last few years. An adequate review, however, is beyond the scope of this paper. Thus, we will confine ourselves to brief discussions of some major new methods, codes or code versions of particular interest to the fusion community.

One-dimensional discrete-ordinates codes are the workhorses of the routine, but very important, blanket/shield design tradeoff studies. Such codes are long established, but still have been greatly improved in recent years. Some of these improvements have consisted of correcting esoteric anomolies of the solution algorithms, but others have provided more stable and/or accelerated solut.ons to the majority of typical fusion reactor transport applications. In the latter category is the diffusion synthetic acceleration technique employed in the ONEDANT code.[17] This acceleration technique is increasingly effective as a transport problem approaches one amenable to diffusion theory, so its value may be greatest in fusion/fission hybrid reactor analysis. Typical reductions of the solution times, exclusive of input and edit data processing, are a factor of 2 to 5, depending on the problem spectra, source distribution, scattering-to-absorption ratios, etc. Another recent enhancement of ONEDANT, specifically included for neutral-atom transport analysis, is a general albedo boundary condition allowing returning particles in all energy groups.

Reductions in computation time have their greatest payoff in 2-D transport codes, which typically run about two orders of magnitude longer times than 1-D codes. One such 2-D code, TWODANT, is scheduled for release in about a year. Realistic test problems[65] with a preliminary version of the code in use at LASL, TWOTRAN-DA, also have shown reduced computation times by factors of 2 to 5.

Another 2-D discrete-ordinates code of direct interest to the fusion reactor community is TRIDENT-CTR. Although this triangular-mesh code has been available for some time on the NMFECC, it has been continually undergoing 'mprovement as new and challenging fusion reactor nucleonic problems arise (e.g., cf. other papers in this Session dealing with applications of TRIDENT-CTR to ETF and EBTR). For example, the code now allows internal boundary sources (such as the walls of NBI or vacuum ducts) and is linked to a surface source produced by a Monte Carlo code. The required linking to Monte Carlo output illustrates a current shortcoming of all discrete-ordinates codes; viz, the streaming effects problem in large void regions. Development efforts for discrete-ordinates code applications to fusion problems are now directed mainly to this shortcoming. Efforts to ameliorate the numerical streaming effects

are being undertaken in what is called deterministic streaming methods. One such method that shows considerable promise of short-term payoff is being actively pursued[66] for x-y and r-z geometries. Plans are to extend the method from the presently developed orthogonal meshes to triangular meshes, for ultimate incorporation into TRIDENT-CTR. Implementation of deterministic streaming methodology should allow the direct use of discrete ordinates in regular geometries, where Monte Carlo calculations are now required solely for the streaming aspects of problems rather than because of geometric complexity.

Development of 3-D discrete-ordinates codes has lain dormant for the last two years, since the completion of the THREETRAN and THREETRAN(hex,Z)[67] codes.* However, interest in extending these codes has been shown in the statement of ETF supporting R&D needs,[27] where analysis of divertor coil shields requires such capability. Adaptation of the 3-D codes to the selected specialized fusion applications (which could include neutral-atom transport in divertors or limiters) could probably best be done on an ad hoc basis. However, additional code development would be required beforehand to extend the capabilities to P_3 scattering and increased convergence acceleration.

Recent developments in Monte Carlo methods and codes were discussed extensively at the April 1980 RSIC Monte Carlo Theory and Application Seminar-Workshop, the proceedings of which were published as ORNL/RSIC-44. Most fusion applications have involved MCNP, MORSE or TARTNP. Evolutionary improvements in the first two codes were covered in papers at the abovementioned seminar, and cannot be reviewed in detail within the scope of this paper. However, as a generalization it appears that progress has occurred on two fronts which were recommended by various fusion reactor nucleonics Working Groups. First, more user-oriented input modules (e.g., geometry specifications) and code manuals are appearing; and, second, useful "event" information is being computed and edited to improve the user's understanding of the physics of the problem solution as it progresses. Research has continued on improved biasing techniques and protocols for employing the techniques[19,68,69], but little progress has occurred in automating selection of, for example, exponential-bias or splitting parameters in production codes.

*These codes now provide only the rudimentary capability to generate virtually unaccelerated solutions for P_1 scattering.

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In summary, we have attempted to review recent developments in transport codes, without necessarily commenting on the adequacy of the effort as compared to the needs. Another paper[21] at this meeting addresses the status and needs questions. It is our observation that the present pace of development is inadequate for even the well-defined needs, without accounting for the unpredicted requirements which inevitably evolve as projects such as ETF approach a detailed design stage.

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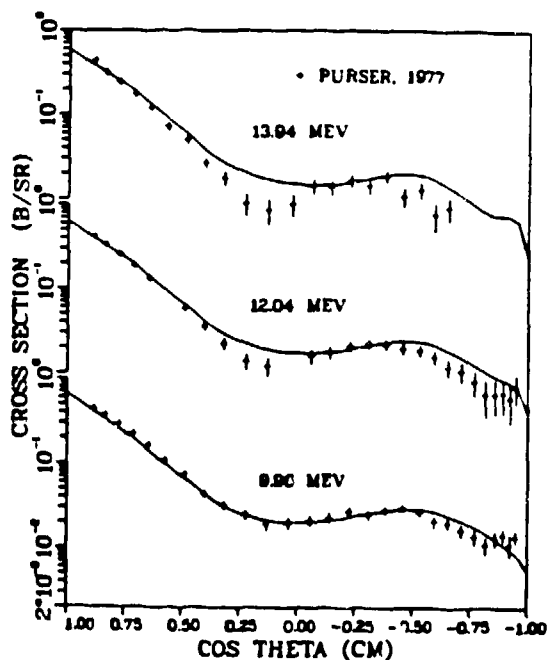
Fig. 1. Elastic scattering angular distribution for n + 6Li. The solid curves are from ENDF/B-V and the experimental points are from Ref. 32.
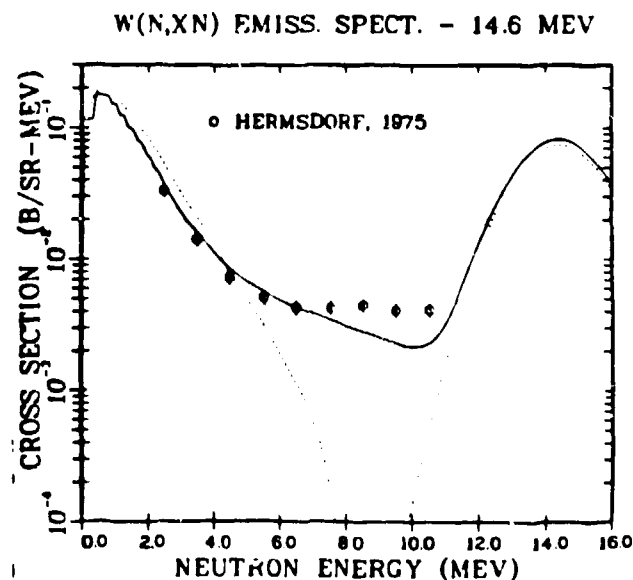
W(N,XN) EMISS. SPECT. — 14.6 MEV

Fig. 2. Neutron emission spectra from 14.6-MeV neutron interactions with W. The solid curve is from recent calculations,[44] the dashed curve is from ENDF/B-V, and the points are experimental data from Ref. 37.
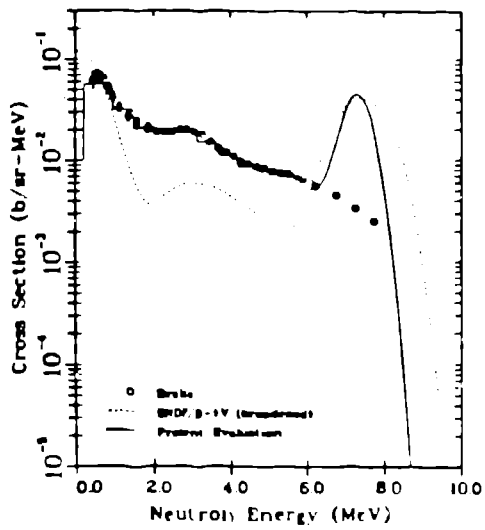
Fig. 3. ^{9}Be neutron emission spectra at 35° induced by 10.1-MeV neutrons. The solid curve is a new evaluation,[4] the dashed curve is ENDF/B-V, and the points are from Ref. 41.
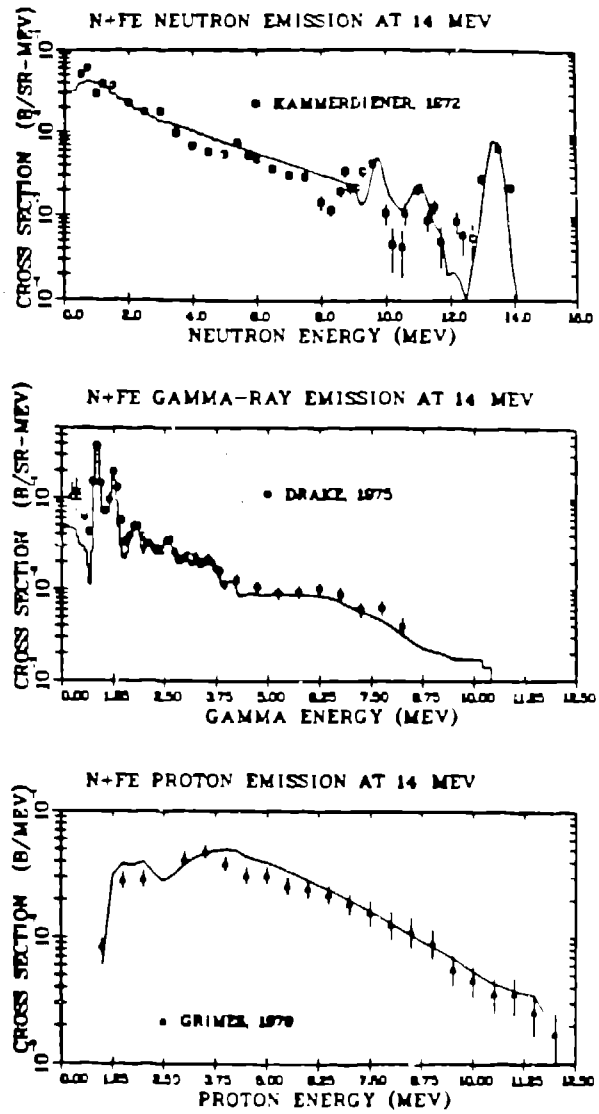

Fig. 4. Neutron, gamma-ray, and proton emission spectra from 14-MeV neutron interactions with Fe. The curves represent a recent calculation,[54] and the experimental points are from Refs. 44, 46, and 54.
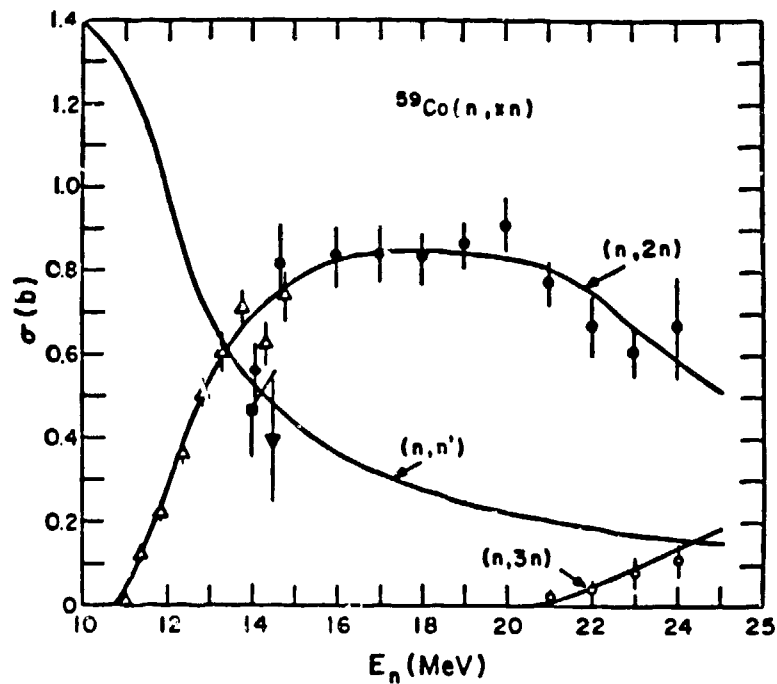
Fig. 5. ^{59}Co(n,xn) cross sections from 10-25 MeV. The solid curves are calculations by Arthur et al.,[55] and the points are experimental data from several sources (see Ref. 55 for details).
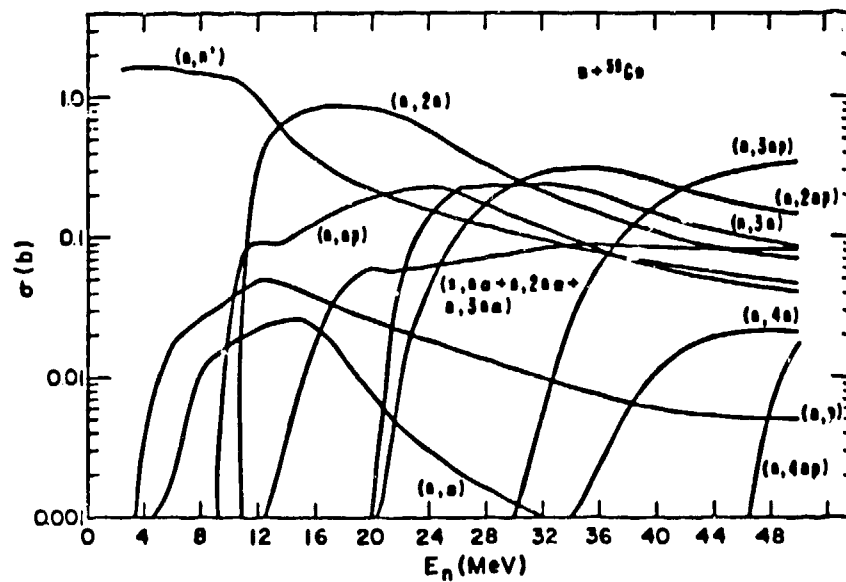

Fig. 6. Cross sections in n + ^{59}Co reactions calculated (Ref. 55) between 3 and 50 MeV.