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TITLE

EVALUATION OF THE ^{7}Li(n,n't)^{4}He CROSS SECTION FOR ENDF/B-VI AND APPLICATION TO UNCERTAINTY ANALYSIS

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EVALUATION OF THE ^{7}Li(n,n't)^{4}He CROSS SECTION FOR ENDF/B-VI AND APPLICATION TO UNCERTAINTY ANALYSIS

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ABSTRACT

A new covariance analysis of n+^{7}Li cross section data has been completed for Version VI of ENDF/B. The analysis updates our 1981 work for ENDF/B-V.2 to include new data that has become available since that time and to incorporate cross correlations between different experiments. The bulk of the new measured data consists of some 10 new (or newly revised) tritium-production measurements involving about 70 new data points. The new analysis results in only small changes in the previous evaluation of the tritium-production cross section but significantly reduces the magnitudes of uncertainties due to the more extensive and accurate data base that was used. A two-dimensional sensitivity and uncertainty analysis of the Lithium Blanket Module experiments at the LOTUS facility was performed in order to assess the effects of the new ^{7}Li cross sections on tritium breeding uncertainty in a realistic system.

INTRODUCTION

The major interest in ^{7}Li for fusion energy applications results from its potential use as a breeding material for tritium.[1] Additionally, because large amounts of ^{7}Li will be required in fusion blankets for this purpose, it is important to accurately describe all neutron-producing reactions for neutronic calculations, as well as charged-particle- and γ-ray-producing reactions for energy deposition studies. Therefore, while the discussion in this paper is focussed on the ^{7}Li(n,n't) reaction, the other major n+^{7}Li reaction channels are also considered.

In 1981 a major re-analysis of ^{7}Li data was completed for Revision 2 of ENDF/B-V.[2] That analysis resulted in a major change in the ^{7}Li(n,n't) cross section near 14 MeV, namely, the cross section was decreased ~9% relative to the previous ENDF/B-V evaluation. Since that time, a number of new measurements, mainly of tritium-production cross sections, elastic scattering angular distributions, and neutron emission spectra, have been completed. Consequently, a new evaluation of n+^{7}Li cross section and covariance data has been performed for Version VI of ENDF/B to reflect the new information in the experimental data base.

A two-dimensional sensitivity and uncertainty analysis was performed in order to assess the effects of the new ^{7}Li cross sections on a calculational analysis of tritium breeding in a realistic system. The Lithium Blanket Module (LBM) experiments at the LOTUS facility[3] were selected for this analysis, primarily because the experiments are well characterized and representative of fusion reactor blanket concepts. This analysis only includes the effect of changes in the cross sections and associated covariances, because the final evaluation of energy-angle correlated neutron emission data for ^{7}Li is not yet complete for ENDF/B-VI. We expect, however, that incorporation of the final Version VI emission spectra will only slightly modify the present results.

NUCLEAR DATA EVALUATION

Analysis Description

As was the case with the ENDF/B-V.2 evaluation, covariance analyses have been performed of each of the major n + ^{7}Li cross-section types for which experimental data exist. The GLUCS code system[4] was utilized to determine evaluated energy-dependent cross sections and covariances for each reaction type from inputted experimental cross sections with their associated uncertainties and correlations. In addition to energy-dependent correlations within individual experiments, cross correlations between different measurements from common flux standards and half life in tritium-counting experiments were included. The results of the GLUCS analysis were combined using the ALVIN code,[5] under the constraint that all partial reactions sum to the total cross section, with full account being taken of all covariances from the GLUCS analysis.

Using a constant 49-point energy grid, independent covariance analyses were carried out with GLUCS for the following four reactions or combinations of reactions:

1. total cross section;
2. elastic plus (n,n_1') cross section to the first excited state of ^{7}Li;
3. (n,n't) tritium-production cross section;
4. (n,2n) plus (n,2nd) plus (n,3np) plus (n,d) cross sections.

Reactions (1)-(4) include all the partial reaction and scattering cross sections that must sum to reaction (1), the total cross section. The data adjustment code, ALVIN, was then used to combine the cross sections and covariances from the independent GLUCS analyses, under the constraint that $\sigma_1 = \sigma_2 + \sigma_3 + \sigma_4$. The results on the 49 point energy grid were smoothed, where necessary, and fit with spline curves for the final evaluated results.

In addition to the above combined analysis, the individual ^{7}Li(n,n') cross sections to the first and second excited states of ^{7}Li were obtained from separate GLUCS analyses of the individual reactions. Because the 0.478-MeV first excited state of ^{7}Li is bound, the experimental data base for the ^{7}Li(n,n_1) reaction consists mainly of (n,n'γ) measurements. The second excited state at E_x = 4.63 MeV is unbound by 2.16 MeV, and direct measurements of inelastic neutrons are available for the (n,n_2) reaction.

To perform the above analyses, it was necessary to obtain covariance matrices for each experimental data measurement. In many cases, sufficient information was available to infer the correlations in the experimental data, and occasionally the correlation matrices were even provided directly by the experimenters. For several measurements, however, it was necessary to make simple generic assumptions regarding the correlations present in different types of experiments. For example, modern total cross-section measurements were generally assumed to have a normalization uncertainty of the order of 0.3-0.5% due to sample thickness and composition uncertainty. Greater normalization uncertainty was assumed for older measurements. The final GLUCS/ALVIN cross sections were not found to be highly sensitive to the exact assumptions made, although it was observed that significant overestimates of correlations can distort results, especially in energy regions where measured data were scarce.

A simple error-doubling procedure was followed for measurements that differed by more than two standard deviations from trial results from GLUCS. That is, if the results from a particular experiment differed from the GLUCS combination of all other experiments such that χ^2/point was greater than 4, then the uncertainties on all the data from that experiment were doubled. Such a procedure was necessary for some 10 experiments out of the 50 used in the analysis. It should be noted that some 7 of the 10 experiments with doubled errors were reported prior to 1965. The uncertainties on more recent measurements were generally found to be more self consistent.

Experimental Data

All available experimental data for which reasonable error estimates were feasible were included in the GLUCS analyses. A total of some 3400 experimental data points were considered, although the initial 3200 total cross section points were averaged down to about 500 points in order to simplify the analysis. The new experimental data on tritium production,[6-14] completed or revised since the previous ENDF/B-V.2 analysis, are summarized in Table 1. Other new experimental data included in the analysis were the elastic cross section results of Chiba et al.,[12] Shen et al.,[15] Altimenkov et al.,[16] and Drosg et al.,[17] a new 14 MeV (n,2n) data point from the work of Chiba et al., and new results on the (n,n_2) cross section from Chiba et al., Drosg et al., Schmidt et al.,[18] and Dekempeneer and Liskien.[19]

The only experimental data available in the energy range 16-20 MeV are the total and (n,n'γ) cross sections. Therefore, in order to permit an accurate separation of the partial cross sections at these energies, an optical model analysis was performed covering the energy range 10-20 MeV. The elastic angular distribution measurements of Hogue et al.[20] and Shen et al.,[15] together with an average of the total cross section measurements[21] from 10-20 MeV were fit using the SCATOPT spherical optical model code.[22] The results were used to compute elastic cross sections from 15-20 MeV for inclusion in the GLUCS/ALVIN analysis.

Evaluation Results

The total cross section that resulted from the analysis is compared in Fig. 1 with white neutron source measurements[21] between 2 and 18 MeV. The evaluated curve was obtained by passing a spline curve directly through the ALVIN results on the 49-point energy grid. The resulting curve is virtually indistinguishable from our earlier ENDF/B-V.2 evaluation, which is not surprising as the same total cross section data base was used in both analyses.

The (n,n't) cross sections that resulted from the ALVIN analysis were not as smooth as the total cross section, primarily because of the smaller and less consistent experimental data base that went into the (n,n't) analysis, so some smoothing of those results was necessary. The smoothed results are compared in the left half of Fig. 2 to the experimental (n,n't) data[6-14] that have been obtained since the ENDF/B-V.2 analysis, as well as to the older measurements[23] (right half of the figure) and to the earlier ENDF/B-V.2 analysis[2] (dashed curves). Clearly the tritium-production cross section from the present analysis differs only slightly from the 1981 evaluation. The new results lie higher than the earlier analysis between 6 and 10 MeV, fall somewhat lower above 15 MeV, and are within ~1% near 14 MeV. It should be noted, however, that the covariance matrix for the (n,n't) reaction is changed substantially. In particular, the standard deviations are significantly reduced because of the additional data in the analysis. A total uncertainty of about ±2.1% is obtained for the 14-15 MeV region as compared to ~4% for ENDF/B-V.2.

The results for the elastic cross section are compared in Fig. 3 to the available experimental data base[23], and to the ENDF/B-V.2 evaluation. The new analysis represents the experimental data quite well and differs only slightly from the earlier evaluation.

Finally, the ^{7}Li(n,n_1) and ^{7}Li(n,n_2) cross sections that result from the independent GLUCS analyses are compared to experimental data and to ENDF/B-V.2 in Figs. 4 and 5, respectively. The new (n,n_1) results are identical with the earlier evaluation because the same experimental data base was used. The new (n,n_2) evaluation lies higher than ENDF/B-V.2 at neutron energies below 10 MeV and falls lower at higher neutron energies, primarily reflecting the influence of the new Dekempeneer and Liskien[19] data and the fact that a covariance analysis was not used for the (n,n_2) reaction in ENDF/B-V.2 .

SENSITIVITY AND UNCERTAINTY ANALYSIS FOR THE LBM/LOTUS EXPERIMENTS

The Lithium Blanket Module (LBM) was constructed for testing on the Tokamak Fusion Test Reactor (TFTR).[24] With a delay in undertaking D-T operation of TFTR, it was decided that the LOTUS facility at the Ecole Polytechnique Federale de Lausanne in Switzerland (EPFL) could provide an extremely valuable resolution of basic technological uncertainties in fusion reactor blanket physics.[25] The source for the LOTUS experiments has well defined spatial and spectral distributions with a potential for high accuracy analysis. The LBM has both realistic fusion blanket materials and a realistic blanket configuration. It has been designed for detailed experimental analysis of tritium breeding and neutron flux spatial/spectral distributions. It is approximately a cube with 80-cm sides, and the breeding material is Li_2O. Li_2O pellets are placed in the leading 60 cm of stainless-steel rods (the back 20 cm of each rod is solid stainless steel) which are are arranged in an hexagonal array.

A collaborative Los Alamos/Paul Scherrer Institut (Switzerland) effort is underway to analyze the LOTUS/LBM experiments being performed by EPFL. The goals of the analysis are first, to investigate the accuracy of the most recent nuclear data on the part of the U.S. (ENDF/B, versions V and VI) and the European Community (JEF-1/EFF); and second, the adequacy of the common 1-, 2- and 3-D neutron transport and 1- and 2-D sensitivity and uncertainty methods.[3] As part of this effort, a detailed cross-section sensitivity and uncertainty analysis has been performed for experiments using the Haefely Neutron Generator (HNG) with the LBM, both bare and preceded with lead and beryllium multiplier plates.[26] In the work reported here, the sensitivity and and uncertainty analysis was repeated for the bare LBM using only the new ^{7}Li cross-section evaluation.

Table 1. Summary of new ^{7}Li(n,n') cross section measurements since completion of the 1981 ENDF/B-V.2 evaluation.

Reference	No. Points	Energy Range (MeV)	First Author and Laboratory	Covariance Information
6	26	4.99-16.03	Liskien, Geel	Correlations inferred
7	1	14.9	Maekawa, JAERI	- --
8	1	14.74	D.L. Smith, ANL	Correlations with 1981 measurements supplied
9a	6	13.31-14.88	Maekawa, FNS(JAERI)	Correlations estimated
9b	6	13.40-14.79	Maekawa, Tokyo Univ.	Correlations estimated
10	12	13.35-14.83	Takahashi, Osaka Univ.	Correlations estimated
11	1	14.94	Goldberg, LLNL	----
12	3	5.40-14.2	Chiba, Tohoku Univ.	Correlations inferred
13	8	4.57-14.1	Swinhoe, Harwell	Revision of '79 measurements & covariances
14	6	7.945-10.48	Qaim, Jülich	Correlations inferred

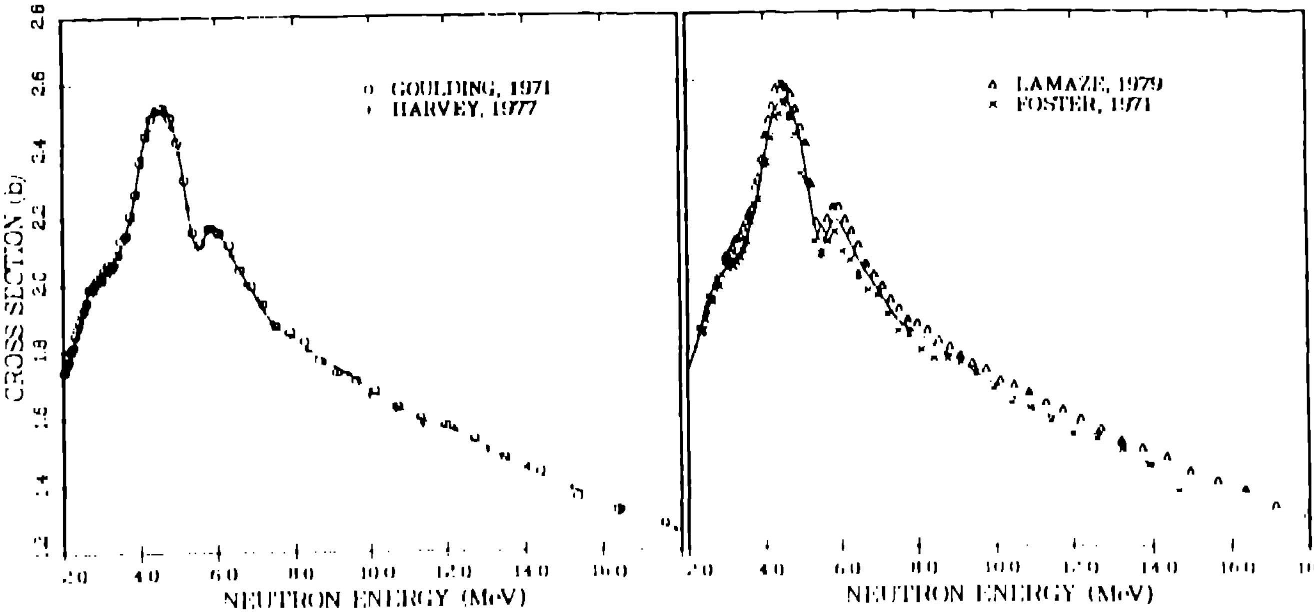

Figure 1. Neutron total cross section of ^{7}Li. The solid curves are from the present covariance analysis, the points are experimental data.[21]

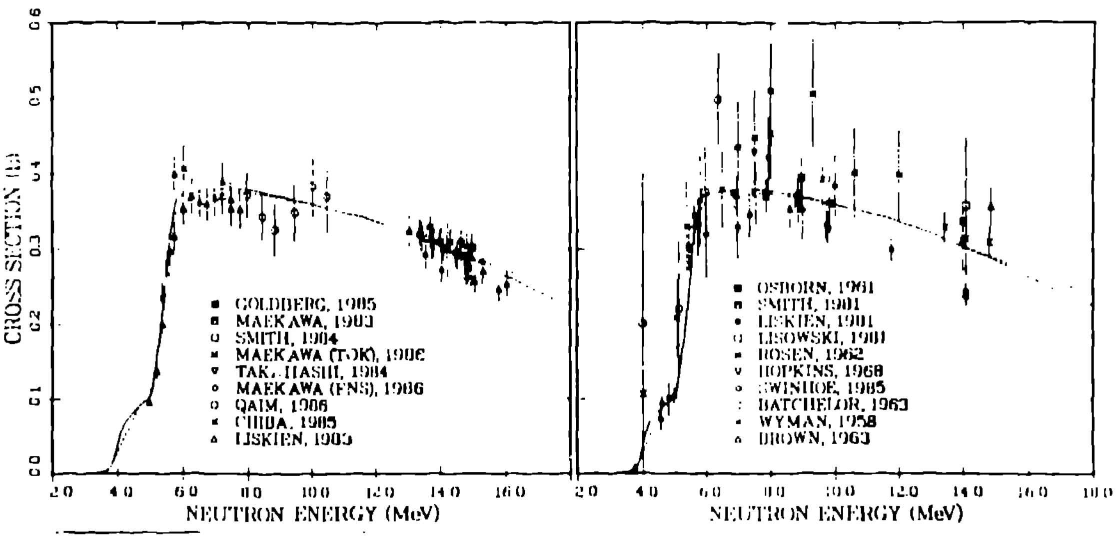

Figure 2. The ^{7}Li(n,n't) cross section. The solid curves are from the present analysis and the dashed curves are ENDF/B-V.2. The experimental data in the right half[23] of the figure were available for the ENDF/V-V.2 analysis; the experimental data in the left half[6-14] became available after the ENDF/B-V.2 analysis.

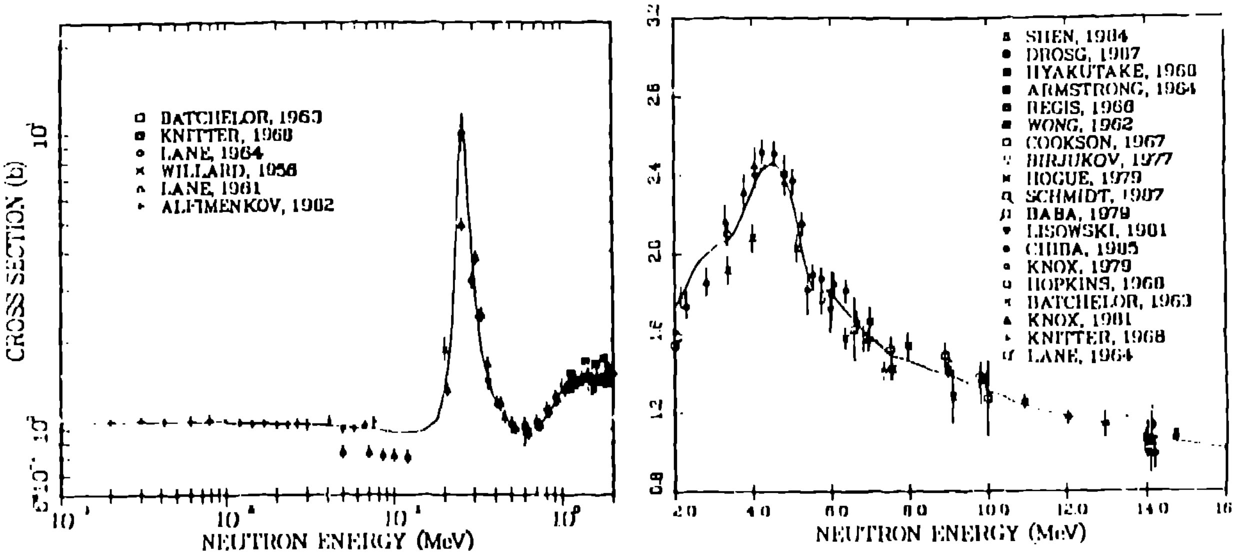

Figure 3. Neutron elastic scattering cross section of ^{7}Li. The solid curve is from the present analysis; the points are experimental data.[23]

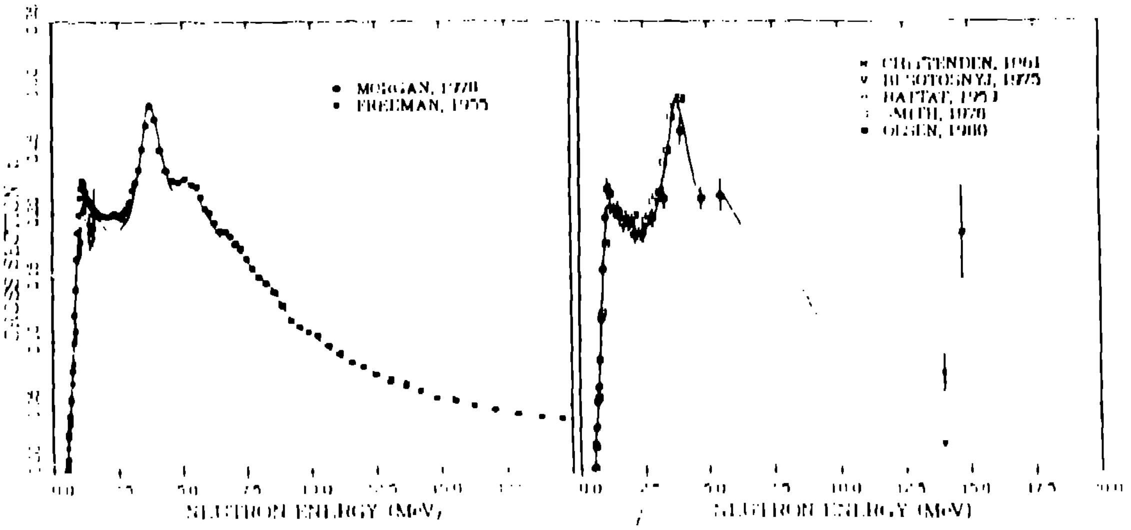

Figure 4. Evaluated and measured[23] cross sections for the ^{7}Li(n,n'γ) reaction, corresponding to the ^{7}Li(n,n') reaction to the 0.478 MeV first excited state of ^{7}Li.

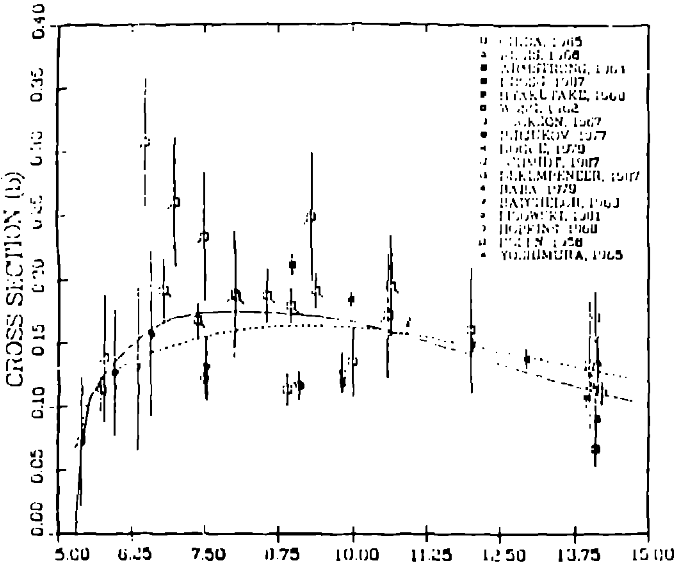

Figure 5. Evaluated and measured[12,18,19,23] cross sections for the $^{7}\mathrm{Li}(n,n_2)$ reaction to the 4.63-MeV second excited state of ^{7}Li. The dashed curve represents the ENDF/B-V.2 evaluation.

Cross-Section Data Libraries

The final evaluation of energy-angle correlated neutron emission data for ^{7}Li is being performed by Beynon[27] using a sequential breakup model. As that work is not expected to be complete until the end of 1988, an interim version of the ENDF/B-VI ^{7}Li evaluation was constructed for the present sensitivity and uncertainty analysis. In particular, a complete ENDF-formatted file was constructed that fully reflects the new cross section and covariance results described above and that utilizes the same neutron spectrum *shape* as Version V.2. The main difference between this file and the eventual ENDF/B-VI evaluation is that the excitation energy binning technique used for Version V.2 is employed here to describe neutron emission spectra rather than the energy-angle correlation format (File 6) that will be used in the final evaluation.

The transport and reaction cross sections were obtained from libraries in the MATXS8 187-neutron-group format.[28] MATXS8A, a library containing 31 isotopes and MATXS8F, containing 21 isotopes, and based on ENDF/B-V evaluations were used for all materials except the new ^{7}Li evaluation. A special single-nuclide MATXS8 formatted library was prepared for the new ^{7}Li evaluation data.

Neutron spectra (187-group) were calculated for ten regions of a three dimensional model of the LBM using the Monte Carlo code MCNP.[29] The transport and reaction cross-section data was collapsed into the 74-neutron group structure of the COVFILS-2[30,31] covariance data library using the calculated neutron spectra. The generation of the collapsed transport libraries from the MATXS libraries was accomplished with the code TRANSX-CTR.[28]

COVFILS-2 is a library of multigroup neutron cross sections, scattering matrices, and covariances (uncertainties and their correlations). The 14 materials included in the first version of COVFILS-2 are ^{1}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{nat}C, ^{14}N, ^{16}O, ^{23}Na, ^{27}Al, ^{nat}Si, ^{nat}Cr, ^{nat}Fe, ^{nat}Ni, and ^{nat}Pb. COVFILS-2 was produced using various modules of the NJOY nuclear data processing system.[32,33] It is largely based on data evaluations from the ENDF/B-V library, although some minor corrections and improvements are incorporated. In cases where the covariance evaluation is missing (as in the case of Be) or judged to be inadequate, private Los Alamos evaluations[34] are employed. The 74-group structure was chosen for compatibility with the extensive, general-purpose MATXS8 187-group library which was produced including scattering reactions for which covariance evaluations are available. A special single nuclide library (COVFILS-4) containing the covariance data for the new ^{7}Li evaluation was prepared using the NJOY system. This data library was incorporated into COVFILS-2 for the calculations reported here.

Calculational Methods and HNG/LBM Model

Neutron transport calculations were performed with TRISM,[35] a computer program for solving the two-dimensional neutral particle transport equation in rectangular (x-y) and cylindrical (r-z) geometries using triangular finite elements within a general domain having curved or other nonorthogonal boundaries. The code SENSIBL[36] was used to perform the cross-section sensitivity and uncertainty analyses. The algorithms used are based on first-order generalized perturbation theory. SENSIBL is coupled to TRISM and ONEDANT[37] via interface files. The forward and adjoint angular fluxes as well as the geometry from TRISM (or ONEDANT) are transferred as input to SENSIBL on these files.

In the model of the HNG/LBM used for the calculations with TRISM, all of the rectangular geometry of the LBM and HNG was represented by equivalent r-z geometry. The Haefely neutron source was positioned 10 cm from the front of LBM on its axis. The HNG has been modeled for several studies in both two- and three-dimensions;[38,39] the HNG was modeled for TRISM using 44 bands and as many as 11 material regions per band.

The LBM was subdivided along the axis into 28 bands, one in the grill plate, 22 in the Li_2O breeding zone and 5 in the reflector. In the radial direction the zones are Li_2O, cladding, the cooling channel, one zone with homogenized Li_2O and cladding, and one zone with homogenized Li_2O, cladding and cooling channels. The Plexiglas surrounding the the LBM was omitted for simplicity. In the axial direction the zones were subdivided into regions between 0.23 to 30.73 and 30.73 to 60.23 cm for the precalculation of weighting spectra with MCNP. All TRISM forward and adjoint calculations were performed in the 74-neutron-group structure with a P_3S_8 approximation and converged to within 10^{-3}. The forward source was distributed in the copper region of the Haefely generator using a Gaussian shape on the copper surface representing the target area. A calculated source spectrum[40] was distributed into the appropriate (nine highest) energy groups. The adjoint sources for the five detector regions were specified as the macroscopic tritium production cross section for lithium in the Li_2O detector volumes. The LBM calculational model is shown schematically in Fig 6. The zone designations are as follows: 1 and 2, Li_2O; 3 and 4, stainless steel cladding; 5 and 6, homogenized Li_2O and cladding; 7 and 8, homogenized Li_2O, cladding, and void; 9, grill plate stainless steel; 10, reflector steel; and 11, reflector steel with void.

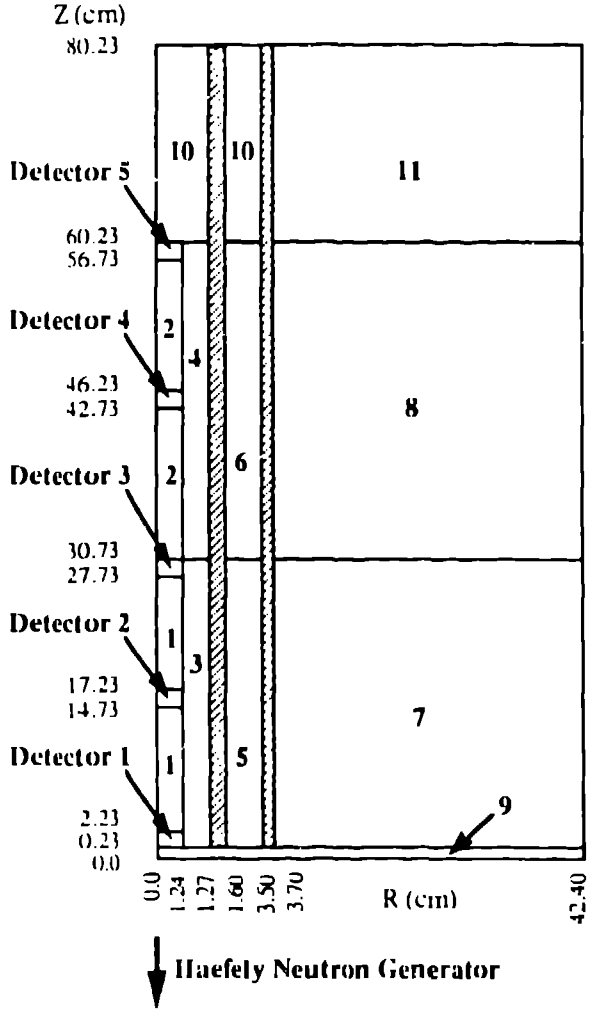

Figure 6. Material divisions and detector regions specified in the TRISM geometry model for the LBM.

Sensitivity and Uncertainty Calculations

The goal of the cross-section sensitivity and uncertainty analysis is to determine the uncertainties of a calculated response function, tritium production per source neutron from lithium. In the analysis reported here, the uncertainties in the calculated tritium production at five different positions along the central Li_2O rod in the LBM (see Fig. 6) were computed using SENSIBL. The detector region mid points are at 1.0, 15.75, 29.0, 44.25, and 58.25 cm along the central rod from the rear of the grill plate.

For each of five investigated positions mentioned above, an adjoint calculation with TRISM was performed using the macroscopic tritium production cross section as the adjoint source. To check the consistency of the forward and adjoint calculations, a comparison was made between the tritium production per source neutron computed in the forward mode for the detector region $<\Phi,R>$ and the corresponding value computed as an integral over the HNG source region of the product of the forward source and the adjoint flux for that detector $<S,\Phi^*>$. Perturbation theory predicts that the inner product relationship $<\Phi,R> = <S,\Phi^*>$ should hold. The results of this comparison are given in Table 2.

Table 2. Comparison of the inner products of the forward $<\Phi,R>$ and adjoint $<S,\Phi^*>$ calculations for each LBM detector region.

LBM Detector Region	Relative difference between inner products (%)	
	^{7}Li(v5.2)	^{7}Li(v6)
1	0.593	0.588
2	0.344	0.342
3	0.022	0.021
4	0.093	0.098
5	0.070	0.066

A total of ten SENSIBL calculations were required for the sensitivity and uncertainty analysis; five for the ^{7}Li(v5.2) calculations and five for the ^{7}Li(v6) calculations. These calculations required as input the forward (two sets) and adjoint (ten sets) angular fluxes calculated by TRISM. In the calculations for ^{7}Li(v5.2), the MAT number 1397 was specified for this nuclide in COFVILS-2 while the number 3007 was specified for ^{7}Li(v6). The response input was the macroscopic tritium production cross section for natural lithium in Li_2O collapsed from 187 to 74 groups using the weighting spectra calculated for the region in which the detector volume was located and including the appropriate ^{7}Li cross section.

A possible large source of uncertainty in the calculated response is the cross sections for the copper in the HNG. Because this material is not available in COVFILS-2 and since aluminum is not a HNG/LBM material, ^{27}Al was substituted for ^{nat}Cu in the SENSIBL calculations. With some knowledge of the relative covariance data for ^{nat}Cu and ^{27}Al cross sections, an estimate can be made of the contribution to the uncertainty in the calculated response from copper cross sections.

The contributions to the uncertainty in the calculated tritium production in the five LBM detector volumes calculated with SENSIBL are given in Table 3 for all of the materials present which have data in COVFILS-2. Materials used in the calculation which did not have data on COVFILS-2 are ^{10}B, ^{11}B, ^{nat}K, ^{55}Mn, ^{nat}Cu, ^{64}Zn, ^{nat}Zr, and ^{nat}Mo; in all cases except copper, these are trace constituents. The effect of the new ^{7}Li evaluation is to substantially reduce the contribution to tritium production uncertainty from ^{7}Li data in the inner-most zones. The overall tritium production uncertainty is reduced by 0.4% in the two inner zones, and ^{7}Li is no longer the dominant source of uncertainty in those zones.

Table 3. Contributions to the Uncertainty in the Calculated Tritium Production per Source Neutron Using ^{7}Li(v5.2) and ^{7}Li(v6) Cross-Section Evaluations.

		LBM detector region				
		1	2	3	4	5
Material	^{7}Li Cross Section	Relative standard deviation (%)				
^{1}H	^{7}Li-V.2	.22	.04	.02	.01	.02
	^{7}Li-VI	.22	.04	.02	.01	.02
^{6}Li	^{7}Li-V.2	.31	.28	.15	.06	.13
	^{7}Li-VI	.31	.28	.15	.06	.13
^{7}Li	^{7}Li-V.2	1.15	1.09	.87	.74	.80
	^{7}Li-VI	.22	.51	.68	.67	.79
^{nat}C	^{7}Li-V.2	.07	.03	.02	.01	.01
	^{7}Li-VI	.07	.03	.02	.01	.01
^{16}O	^{7}Li-V.2	.29	.90	1.14	1.30	1.35
	^{7}Li-VI	.29	.89	1.14	1.29	1.35
^{nat}Cu (^{27}Al)	^{7}Li-V.2	.87	.27	.18	.13	.13
	^{7}Li-VI	.87	.27	.18	.13	.13
^{nat}Cr	^{7}Li-V.2	.08	.16	.18	.23	1.03
	^{7}Li-VI	.08	.16	.18	.22	1.02
^{nat}Fe	^{7}Li-V.2	.85	.35	.31	.30	.55
	^{7}Li-VI	.85	.35	.31	.30	.55
^{nat}Ni	^{7}Li-V.2	.04	.11	.12	.13	.14
	^{7}Li-VI	.04	.11	.12	.13	.14
Total	^{7}Li V.2	1.74	1.52	1.51	1.55	1.97
	^{7}Li VI	1.33	1.17	1.40	1.52	1.97

SUMMARY

The ^{7}Li cross sections and covariances for the ENDF/B-VI evaluated data file have been improved over the previous evaluation by consideration of new experimental data since 1981 in a covariance analysis. The usefulness of this type analysis is highlighted by the fact that the resulting ^{7}Li(n,n't) cross section differs little from that of the previous covariance analysis, despite the availability of much more accurate and consistent data. The major impact of the new measurements on the evaluation is to significantly reduce uncertainties in the evaluated data and to improve the associated covariances.

The effects of the new ^{7}Li evaluation were assessed by performing a detailed sensitivity and uncertainty analysis of a HNG/LBM model, first using the prior ENDF/B-V.2 evaluation and then substituting the new interim ENDF/B-VI evaluation into the analysis. The main result of the new evaluation is to significantly reduce the uncertainty in tritium production due to ^{7}Li data in the inner most zones of the calculations. Because of the reduction in uncertainty from the ^{7}Li data, the need for improved accuracy in data for other materials such as ^{16}O, ^{nat}Cu, and ^{nat}Fe is apparent.

ENDF/B-VI evaluations for other fusion materials are described in another paper at this conference.[41]

ACKNOWLEDGMENTS

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