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Assessment of the ^3H(n,2n) Reaction for NIF-relevant Simulations

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We examine the status of three nuclear data evaluations for the (n,2n) reaction proceeding on ^{3}H, hereafter referred to as T(n,2n)D, that are currently available in the ENDL database at LLNL. The most recent update to this reaction, based upon a new evaluation by G. Hale, suggests a much lower peak cross section than the previous two evaluations. We examined these evaluations to gauge their impact on ICF simulations of nuclear diagnostics at NIF and determined that, although the latest evaluation has a fairly small effect on the total emergent neutron spectrum, it does play a significant role in ^{197}Au activation that could influence the interpretation of solid radiochemical recovery products on NIF. We conclude that a reversion to the original T(n,2n)D evaluation as given by ENDF-B/VI.8 and ENDF-B/VII.1 is warranted.

I. EVALUATIONS

There are three evaluations available for the reaction T(n,2n)D shown in Fig. 1. Two of these cross sections peak around 50 mb at 12-13 MeV, while the third is about five times lower, rising to 10 mb by 20 MeV. Only one direct measurement exists at 14 MeV in the available databases[1]. So any estimate of energy dependence must be made based on theory. Past evaluations for this (n,2n) reaction have used R-matrix fits to the elastic and total neutron cross sections. The (n,2n) cross section is derived as the remainder of these two cross sections, essentially a difference of two large and nearly equal numbers.

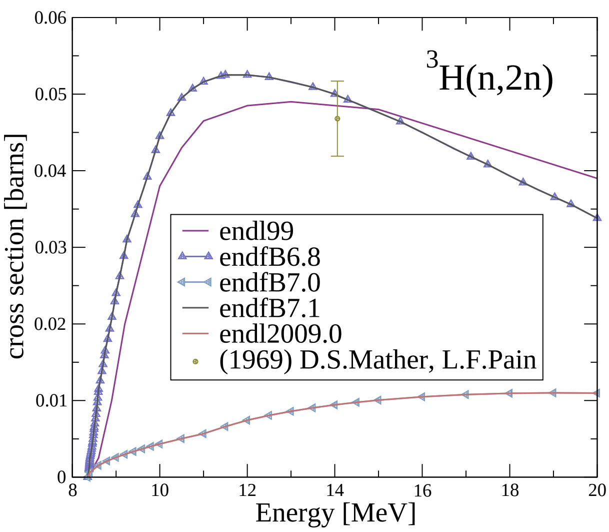

FIG. 1. Cross sections available at LLNL for ^3H(n,2n)^{2}H. The olive point with error bars is the single available direct measurement [1].

The earliest evaluation was introduced in ENDL-94/99 which was based upon an ancient fit from Los Alamos [2]. This first evaluation was updated with new measurements in ENDF-B/VI.8. Recently ENDF-B/VII.0 introduced a completely new evaluation [18] which has been used by all modern ENDL releases (i.e. ENDL2008.2, ENDL2009.0, and ENDL2011.0). This evaluation is in conflict with the single experimental point for T(n,2n)D[1]. ENDF-B/VII.1 restored the (high) (n,2n) cross section of the previous database but retained the new cross sections for total and elastic scattering.

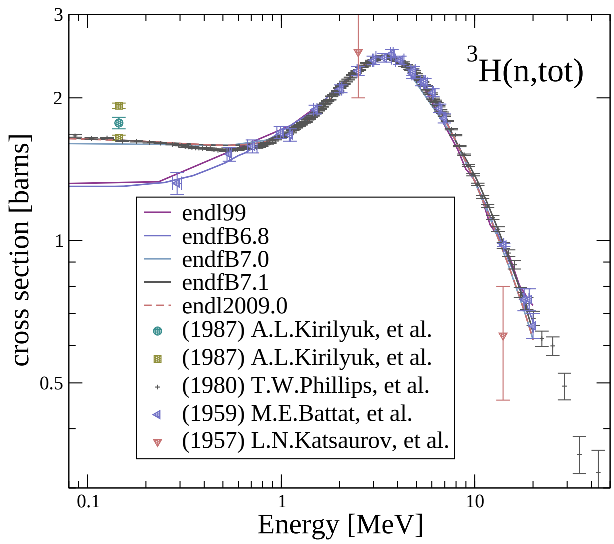

FIG. 2. Evaluations and exfor data for the total neutron cross sections on ^{3}H.

Evaluations up through ENDF-B/VI.8 were based on systematics and the p-^{3}He mirror reaction studies of references [3] and [4]. Total and elastic cross sections, for both n-^{3}H and its isomeric mirror p-^{3}He, were measured extensively up to 1970 [5–17].

The new evaluation introduced in ENDF-B/VII.0 was also based upon an R-matrix analysis of p-^{3}He scattering[18]. This evaluation agreed well with new mea-

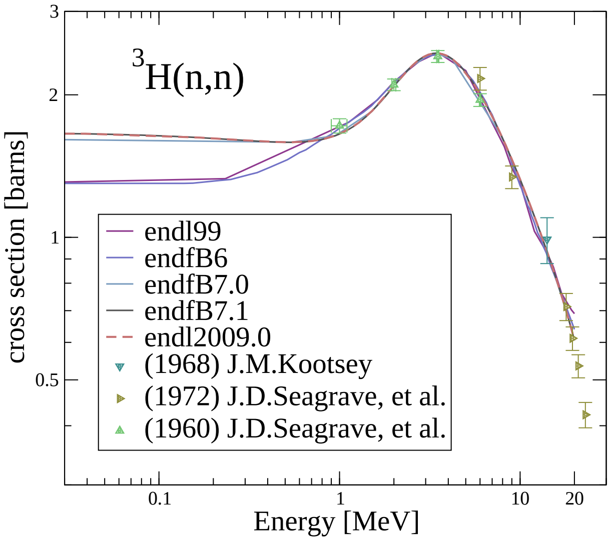

FIG. 3. Evaluations and exfor data for the elastic neutron cross section.

surements of the total neutron cross section [19] and the scattering length [20]. In this evaluation, the resultant ^{4}Li (p-^{3}He) system was translated to the ^{4}H (n-^{3}H) system by shifting all eigenenergies downward by a coulomb shift of 0.86 MeV. The R-matrix parameters were then used to predict the total cross sections and angular distributions of the reaction. The (n,2n) calculation included couplings between the n-n-d and n-t channels though the authors state these may have been underestimated.

The ENDF-B/VII.0 evaluations for the total and elastic scattering neutron cross sections exhibited an apparent improvement at low energies over previous evaluations (se Figs. 2 and 3). Here the new evaluation agrees more closely with the majority of available data and contradicts the older data set of Ref. [5]. However, the difference between the total and elastic, and thus the size of the (n,2n) cross section, is much smaller than the previous result and in conflict with the lone (n,2n) data point.

Recently, in ENDF-B/VII.1, the new (low) result for (n,2n) was retracted in favor of the old (high) one with very little explanation: "(n,2n) replaced by ENDF/B-VI.8, total adjusted (NNDC/2010/06)". The total and elastic contributions were effectively retained as in ENDF-B/VII.0 but the total was altered so that the subtraction of total and elastic would fit the old (n,2n) cross section of ENDF-B/VI.8. This subtraction would still be consistent with the error band on the total and elastic R-matrix fit. Thus ENDF-B/VII.1 contains the apparent best available choice for each channel.

II. EXPERIMENTS

The data of Ref. [5] (blue triangles in Fig. 2) appears to have an outlying data point at the lowest energy since it is inconsistent with the rest of the datasets in that region. The new experiments in Ref. [19] quote uncertainties of the order 2% at energies above the threshold of 8.6 MeV but also agree with previous measurements of thermal-energy cross sections. The inelastic cross section is itself no more than about 2% of the total cross section. So, in terms of experimental error, the (n,2n) cross section is undetermined by these measurments.

Only a single direct measurement of the T(n,2n)D reaction is referenced by the various evaluations in ENDF [1]. This reference comes from an unpublished AWE internal report. This report was obtained and a representative from AWE was consulted for verification. Unfortunately, institutional memory of the details of this measurement are fragmentary at best.

Our own experimental analysis of this report is mixed. The basic method is difficult, but they seemed to be conscientious of the various errors and necessary corrections. They measured reactions on several isotopes with the same setup, notably ^{238}U and ^{239}Pu. The former agrees well with other measurements and the latter is suspect because it is a subtraction of two large values with a small difference. Ultimately, we find this experimental point for T(n,2n)D acceptable, but more statistics are needed to make a definitive statement.

During our investigation, an additional direct measurment was discovered [21] that requires further analysis to provide a comparable data point. Also, recent and future upgrades to neutron time of flight (NTOF) capabilities at NIF might enable additional measurements that could corroborate either of these measurements.

III. SIMULATION

To test the sensitivity of an ICF simulation to the differences in the available T(n,2n)D cross sections, we created an ENDL database file with the the ENDF-B7.1 neutron-triton cross sections swapped into a standard endl2009.0 database, exchanging the newer (low) T(n,2n)D cross section for the older (high) one. With this database S. Sepke and C. Cerjan ran a NIF simulation based upon a three-dimensional fit to the experimental data for a specific implosion experiment, N120321. [22] The resulting density and temperature distributions are used in a HYDRA simulation to produce high fidelity nuclear signatures which are subsequently used to deduce implosion performance. The N120321 shot irradiated a modified Rev 5 capsule that had roughly twice the Si dopant in layers 2, 3, and 4 with the objective of studying mix through measurement of the yield performance of a 2xSi capsule. The NIF laser system delivered a 327 TW no coast pulse shape with $\delta\lambda_{30} = 7.3\AA$ and $\delta\lambda_{23.5} = 8.5\AA$. Performance characteristics were Laser power: 1.51 MJ, Yield: $3.8 \pm 0.9 \times 10^{14}$ (db), NTOF $T_i = 3.0 \pm 0.15$ keV, Bangtime(ns): X=22.904, N=22.835, with $N_{burn} = 153$ ps (GRH).

Results are summarized in Fig. 4 which shows the total time-integrated neutron flux as a function of energy for this specific shot. The blue curve represents the emergent neutron spectra using the newer [18] (low) (n,2n) cross section while the red curve used the older (high) cross section, resulting in a 10% difference in the integrated spectrum below the 6 MeV threshold for these kinematics. This effect is quite modest given a difference of a factor of five between the two cross section choices, and thus demonstrates a small fractional contribution to the total emergent neutron spectrum. Increasing the T(n,2n)D cross section from the new (low) ENDL 2009.0 model to the higher ENDF-B.VI.8 model increases the total number of neutrons that escape from a typical layered deuterium-tritium (DT) ICF capsule by roughly 0.5%.

Three NTOF diagnostic signatures are potentially affected: the D-neutron backscattering peak near 2 MeV, the T-neutron backscattering peak near 4 MeV, and the measurement of the DD fusion peak centered at 2.45 MeV. The primary effect in all three cases would be an increase in the background signal for each measurement. The DD fusion peak is routinely measured and analyzed, so the impact for this measurement is the most important. Sepke and Cerjan also noted a tritium density dependence of this result - $T(T,2n)^4He$ neutrons overwhelm the T(n,2n)D signal at higher tritium densities in the energy range of 1-10 MeV.

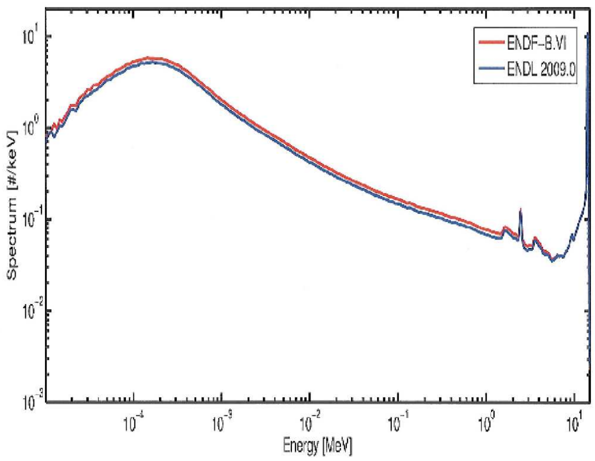

FIG. 4. A NIF capsule simulation showing the relative effect on the emergent spectrum of the old (high - red) and new (low - blue) T(n,2n)D cross sections.

However, the effect of increasing the T(n,2n)D cross section becomes much more pronounced when examining the impact of an increased number of neutrons with energies below 1 MeV. Figures 6 and 5 show the spectrum of neutrons escaping from the layered DT capsule implosion N120321 (in black) as well as the portion of this spectrum coming from each of the six most significant neutron contributing reactions. In each case, the predominant contributions to the spectrum below 1 MeV are from the $T(D,n)^4He$ and $D(n,2n)^1H$ reactions. When using the new (smaller) T(n,2n)D cross section, that reaction is the smallest contributor of the six comprising only ∼3% of the total number of neutrons. When using the old (larger) ENDF-B.VI.8 evaluation, however, the T(n,2n) reaction contributes ∼14% of the total below 1 MeV, and is now the fourth most important. In fact, the total number of neutrons in this range increases by ∼12.5%.

The neutron energy spectrum below 1 MeV is very important in simulations of the solid radiochemistry (SRC) experiments at the National Ignition Facility (NIF). In these experiments, neutrons escaping the imploding capsule activate a known mass of material — typically gold — and this material is collected and counted to determine the relative number of (n,γ) to (n,2n) reactions. This provides a measure of the capsule areal density immediately following burn and the low energy spectrum itself. As an example, consider ^{197}Au activation. The $^{197}Au(n,2n)^{196}Au$ activation only changes by about half a percent in a typical activation calculation when changing this cross section since this reaction is only sensitive to neutrons with energy greater than 11 MeV. The $^{197}Au(n,\gamma)^{198}Au$ activation, however, increases by over 11.5% when using the old (larger) ENDF-B.VI.8 T(n,2n)D cross section since the capture cross section is dominated by resonances in the 100 eV - 10 keV energy range.

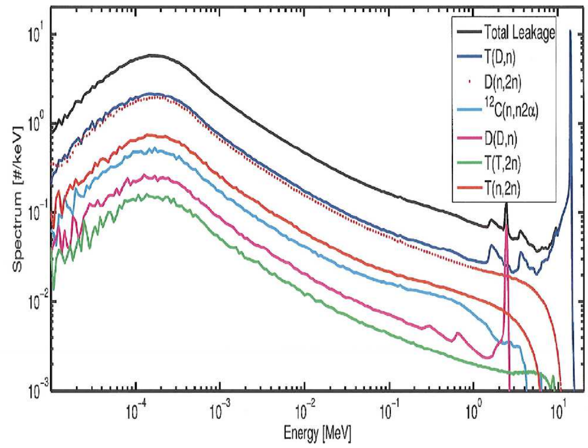

FIG. 5. A NIF capsule simulation showing the total leakage neutron spectrum and the contributions to it from the six most important (n,xn) reactions. This panel illustrates the inclusion of the old (large) T(n,2n) cross section.

IV. THEORY

We have also explored some additional theoretical considerations of the n+T reaction. Ref. [23] presents calculations of the elastic cross section for n-T scattering and uses the optical theorem to compute the total and thus, by subtraction, the difference between the two. This evaluation for T(n,2n)D comes in about half way between our two existing evaluations. Correspondence with the au-

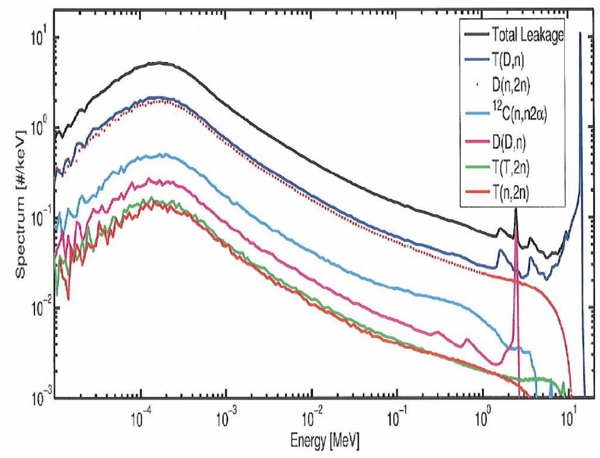

FIG. 6. Same as Figure 6 but using the new (low) T(n,2n)D cross section.

thors revealed that they see a discrepancy between the experimental values for the total and elastic contributions and therefore suspect some unrecognized systematic errors, particularly for the total. Calculations with the same methods have yielded better agreement with (and correlation between) experiments in other reaction cases. In particular p-^3He is much easier to measure experimentally. The capabilities of their codes do not yet include the use of full three-nucleon interactions and we suggested collaboration to provide these matrix elements. New work and publication in this area is imminent.

LLNL also has its own light ion reaction theory program under the direction of S. Quaglioni. As their work progresses, we will eventually be able to calculate three-body breakup reations *ab initio* with the most complete description of the nuclear interactions currently available. This approach will enable more accurate correlations between disparate experimental results for many different light-ion reactions.

V. CONCLUSIONS

In this investigation of the data and evaluations for neutron-Triton reactions we arrive at the following conclusion:

Given that this evaluation is based on the subtraction of two nearly equal large numbers, we choose to revert to the older (higher) T(n,2n)D cross section that agrees with the one existing experimental measurment, following both ENDF-B/VII.1 and AWE. We encourage a modern experimental effort.

We also note that:

- Sensitivity of the total emergent neutron spectrum in a NIF simulation is fairly insensitive to the factor of 5 difference in available cross sections at the less than 10% level, and not sensitive at all for incident neutron energies above 6 MeV.
- However, in light of the large sensititivy to Gold activation due to the larger low-energy leakage spectrum exhibited in a “typical” implosion calculation (the (n,γ) activation of ^{197}Au increased by 11.6% with the increased cross section) means that the uncertainty in the cross section choice is relevant in the analysis of experimental data, confusing the comparison of simulation to data.
- New updates to the LLNL nuclear data libraries, endl2011.1 and endl2009.1 will include this revision. To be clear, we are reverting to the (old) higher T(n,2n)D cross section.

We look forward to several developments that will affect this and other light-ion reaction science items:

- NTOF measurements at NIF which could validate or eliminate some of the various evaluations.
- Improved reaction calculations by A.Deltuva through the use of full χEFT potentials with three-body forces (once his codes can take them).
- RGM-NCSM (Resonating Group Method - No Core Shell Model) calculations by S.Quaglioni and collaborators will incorporate the full three-body breakup physics necessary to compute T(n,2n)D accurately.

ACKNOWLEDGMENTS

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