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**NEUTRON- AND PROTON-INDUCED NUCLEAR DATA LIBRARIES TO 150
MEV FOR ACCELERATOR-DRIVEN APPLICATIONS**

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ABSTRACT

A program is underway at Los Alamos National Laboratory to develop nuclear data libraries for incident neutrons and protons to 150 MeV for accelerator-driven applications. These libraries will be used initially for design of an accelerator-based facility to produce tritium, including analysis of system performance, induced radiation doses, material activation, heating, damage, and shielding requirements. The libraries are based primarily on nuclear model calculations with the GNASH reaction theory code, including thorough benchmarking of the model calculations against experimental data. All evaluations include specification of production cross sections for light particles, gamma rays, and heavy recoil particles, energy-angle correlated spectra for secondary light particles, and energy spectra for gamma rays and heavy recoil nuclei. The neutron evaluations are combined with ENDF/B-VI evaluations below 20 MeV. To date, neutron and proton evaluations have been completed for ^2H , ^{12}C , ^{16}O , ^{27}Al , $^{28,29,30}\text{Si}$, ^{40}Ca , $^{54,56,57,58}\text{Fe}$, $^{182,183,184,186}\text{W}$, and $^{206,207,208}\text{Pb}$.

INTRODUCTION

Progress in high-power accelerator technology, materials separations, and ability to model the neutronics of large, complicated systems has motivated the design of new accelerator-based systems that can impact important problem areas. Several systems are currently being investigated at Los Alamos National Laboratory (LANL). These include tritium production, plutonium disposition, destruction of long-lived components of nuclear waste, and ultimately long-term energy supply requirements. In this paper we describe a LANL program directed at improving the nuclear data base and methods for design of an accelerator-based system for producing tritium (APT) being carried out with participation by scientists from Lawrence Livermore and Brookhaven National Laboratories.

The current APT design is driven by an intense proton beam of energy 1.7 GeV which is stopped in a thick W-Pb target/blanket assembly. Neutrons are produced through (p,xn) and (n,xn) reactions, thermalized in heavy and light water, and then captured in (n,p) reactions on ^3He to produce tritium. Design of this system requires information on nuclear interactions by protons and neutrons from essentially zero energy up to the primary beam energy with target materials, coolants, cladding, structural materials, moderator and blanket materials. Preconceptual design of the system has been carried out using the LAHET Code System (LCS).¹ With the current system intranuclear cascade (INC) plus evaporation / Fermi-breakup calculations are used to model the nuclear interactions as well as the radiation transport above 20 MeV (and below 20 MeV for incident charged particles). Below 20 MeV, the nuclear interactions and the transport of neutral particles are handled by the MCNP code² which uses ENDF/B-VI evaluated nuclear data libraries. The INC models in LAHET are most accurate above 150 MeV where semiclassical approximations become applicable. Below 150 MeV, however, nuclear interactions become more sensitive to specific details of nuclear structure along

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with quantum effects in the scattering. For this reason, we are extending the evaluated nuclear data libraries for both incident neutrons and protons up to 150 MeV using the GNASH nuclear reaction model code³ along with experimental data, as summarized below. The GNASH code makes use of direct, preequilibrium, and Hauser-Feshbach evaporation theories. In a recent code comparison it was shown to be one of the most accurate codes available for modeling nuclear reactions below 150 MeV.⁴

NUCLEAR MODELS / NEUTRON AND PROTON LIBRARIES

The neutron and proton data libraries to 150 MeV were developed using experimental data and the GNASH nuclear model code. This code calculates nuclear reaction cross sections using equilibrium and preequilibrium theories, and makes use of predetermined direct reaction cross sections calculated with codes such as ECIS and DWUCK. A capability exists to use either the exciton model or the Feshbach-Kerman-Koonin (FKK) quantum theory for preequilibrium emission. However, for generating APT data libraries, the exciton model was used because of the shorter computational time needed, and FKK calculations were performed only for a selection of reactions to help validate the exciton model results. Sequential equilibrium emission is accounted for by using the Hauser-Feshbach theory with a full conservation of angular momentum and parity. All reaction chains are included providing their cross sections exceed 0.1 mb, which usually required calculating the decay of approximately 100 excited nuclides for a typical target nucleus. Full details of the nuclear reaction theories included in the GNASH code are described elsewhere.³ Improvements and developments required to extend the validity of the models to higher energies are described in Ref. 5.

The evaluated data libraries include production cross sections and double differential energy/angular distributions for emission neutrons and light charged particles. Production cross sections and angle-integrated energy distributions are given for gamma rays and heavy recoil nuclei. The energy spectra of heavy recoils are calculated using a newly developed model.⁶ The libraries for incident neutrons are combined at 20 MeV with existing ENDF/B-VI evaluations usually without smoothing the juncture at 20 MeV. The proton libraries cover the energy range down to an energy where the cross sections become negligibly small due to Coulomb suppression. To date, we have completed neutron and proton evaluations to 150 MeV for targets of ²H, ¹²C, ¹⁶O, ²⁷Al, ^{28,29,30}Si, Ca, ^{54,56,57,58}Fe, ^{182,183,184,186}W, and ^{206,207,208}Pb. The ²H evaluation is based mainly on experimental data; all other evaluations relied on the GNASH analyses.

In order to validate these libraries, the evaluated data have been extensively benchmarked against measured data. Examples are shown in Fig. 1, as well as in Ref. 8 where comparisons of calculated heating with kerma measurements are given. The importance of using evaluated data libraries is illustrated in the upper left corner, where the evaluated tungsten proton nonelastic cross section is compared with LAHET calculations using the Bertini model and with measured data.⁷ In fact, only one tungsten measurement exists; the other nonelastic experimental values are shown from nearby elements (tantalum) and from systematics of measurements on other targets. It is evident that LAHET agrees well with measurements above a few hundred MeV but underestimates the nonelastic cross section at lower energies. The evaluated data library is based on an optical model calculation and agrees well with the limited experimental data.

The upper right hand corner of Fig. 1 compares our calculations with the 26-MeV ¹⁸⁴W(n,xn) measurements by Marcinkowski et al.⁹ Our calculated angle-integrated spectrum agrees well with the measured data, and demonstrates the importance of collective giant isoscalar resonance excitation mechanisms at high energies. The peaks at the highest energies are due to collective excitation of the low-lying rotational levels.

The lower half of Fig. 1 shows benchmark comparisons of the evaluated cross sections for lead for incident protons and neutrons. The lower left figure shows the calculated neutron production spectra for incident protons at various angles compared with the Meier et al. (1989) 113-MeV measurements.¹⁰ Agreement is good, except at 150 degrees, though the discrepancies here have minimal practical importance since the back-angle cross sections are very small. In the lower right of Fig. 1, angle-integrated neutron and proton emission spectra are shown for 90-MeV protons incident on lead. No

experimental data exist for lead at this energy, so the calculated results are compared with data on bismuth,⁷ which would be expected to be similar. This figure demonstrates that the GNASH calculation correctly account for the relative neutron and proton emission.

SUMMARY

To summarize, we have completed and benchmarked evaluations of neutron and proton reactions to 150 MeV for a total of 19 target isotopes. These data are available for general use on the T-2 Nuclear Information Service Web site (<http://t2.lanl.gov>), including documentation and benchmark validation. We plan to complete similar evaluations for ^{14}N , $^{50,52,53,54}\text{Cr}$, $^{58,60,62}\text{Ni}$, $^{63,65}\text{Cu}$, Mg, Mn, He, H, and other nuclides in the future.

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Fig. 1. Comparison of measured and calculated data for W and Pb targets. See text.

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