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A joint effort between the Applied Nuclear Science and Radiation Transport groups at Los Alamos has begun to develop and implement proton, neutron, and photon transport libraries for incident energies up to 100 MeV. The major steps involved in this effort are: (1) development of evaluated (ENDF/B) data formats appropriate for higher energies; (2) extension of low-energy nuclear physics theoretical models for applicability up to 100 MeV; (3) calculation and evaluation of nuclear data in ENDF/B-VI format for appropriate materials up to 100 MeV; (4) development of processing code capabilities to handle the higher energy data; and (5) development of the appropriate interfaces and code patches for use of the data in transport codes such as MCNP. In this paper we mainly discuss the development of the basic transport data library, items (2) and (3) above, and summarize the remaining activities.

The motivation for this effort is principally the need to incorporate better nuclear physics data in applied calculations with appreciable sensitivity to proton, neutron, and photon energies below 100 MeV. Presently, a common technique in such calculations is to utilize intranuclear-cascade-evaporation (ICE) models[1,2] to generate nuclear data at all incident energies in the case of protons, and above 20 MeV in the case of neutrons (20 MeV is the maximum incident neutron energy included in ENDF/B-V libraries). Because the physical assumptions embodied in ICE models are most applicable above a few hundred MeV, the use of sucn models below ~100 MeV is questionable. To circumvent this problem, we are constructing evaluated data libraries for proton and neutron energies to 100 MeV using theoretical models (and experimental data) that have been developed and tested in the range of several tens of MeV, in much the same way that the national ENDF/B data library[3] has been developed for neutron energies up to 20 MeV but including less detail.

In the case of ^{1}H, R-matrix and phase shift analyses of the available experimental data base were utilized to obtain the incident proton and neutron transport data libraries. For all other libraries, the GNASH statistical/preequilibrium theory computer code[4] was widely used to calculate the required data. Spherical or coupled-channel deformed optical model analyses were employed to obtain elastic cross sections and angular distributions, and to provide the necessary particle transmission coefficients for the GNASH calculations. New spherical optical model parameterizations valid for nucleon-nucleus reactions in the energy range 50-500 MeV were developed for the calculations.[5] Two new versions of GNASH (in addition to our standard low-energy version) were developed to allow a choice of Hauser-Feshbach, s-wave approximation, or evaporation models, depending on the particular target and incident energies involved.[6] One-step preequilibrium corrections were applied in all GNASH calculations, and multistage preequilibrium contributions were included when the s-wave and evaporation approximations were used.[6] A new model and code module were developed and implemented to permit reliable calculation of neutron and photon spectra from fission reactions, including an extensive sampling of fission fragments.[7]

All the evaluated transport data libraries are provided in ENDF/B-VI format and include extensive use of the new ENDF/B File 6 format[8] and Kalbach-Mann systematics,[9] which permits accurate specification of energy-angle correlations in emission spectra. Extensive experimental data were incorporated into the analyses used to produce the proton and neutron evaluated data for the lighter targets. The libraries for heavier materials, especially at higher energies, rely mainly upon the theoretical calculations, although all the optical model potentials reasonably represent measured elastic and reaction data, and comparisons with differential data from thin and thick target measurements have been made to verify the models.[6]

To date, incident proton data libraries have been completed to 100 MeV for ^{1}H, Be, C, O, Al, Si, Fe, W, ^{238}U. Data libraries for incident neutrons have been completed for this same list of targets plus Ca. The neutron libraries were joined at or below 20 MeV to existing ENDF/B-V libraries, depending on the extent of outgoing charged-particle data in the ENDF/B-V files. In all cases emission data are included for outgoing neutrons, protons, and photons. For targets lighter than W, emission data are also provided for deuterons and alpha particles, and the Be libraries include outgoing triton data as well. Although all libraries include data for emitted photons, photo-nuclear reactions are not yet included for incident photons.

To summarize the status of the complete system, an initial transport data library is now complete for incident proton and neutron energies to 100 MeV for nine materials ranging from A = 1 to 238. Various modules of the NJOY processing code system[10] have been enhanced to permit processing of the ENDF/B-VI formatted evaluations into both continuous-energy and multigroup format. Similarly, the MCNP Monte Carlo transport code[11] has been modified to properly handle the new libraries. Currently, a patched version of MCNP3A is capable of continuous-energy neutron/photon calculations using the 100-MeV libraries. A second version, MCNP3B, includes both a multigroup cross-section option and a hybrid continuous-energy/multigroup Boltzmann-Fokker-Planck option for the transport of charged particles.[12] As a result, the coupled neutron/proton/photon multigroup library derived from the 100-MeV evaluations for nine materials is now suitable for use in MCNP. Testing of both the continuous-energy and multigroup methods and libraries is in progress. A limited set of calculations of benchmark experiments is described in Refs. 13 and 14.

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