LA-UR- 97-1825

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CONF-970524--8

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AUG 14 1997
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Submitted to: International Conference on Nuclear Data for Science & Technology, May 19-24, 1997, Trieste, Italy

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UTILIZATION OF NEW 150-MEV NEUTRON AND PROTON EVALUATIONS IN MCNP

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MCNP™ and LAHET™ are two of the codes included in the LARAMIE (Los Alamos Radiation Modeling Interactive Environment) code system. Both MCNP [1] and LAHET [2] are three-dimensional continuous-energy Monte Carlo radiation transport codes. MCNP Version 4B simulates the coupled transport of neutrons, photons, and electrons. LAHET Version 2.8 simulates the transport of nucleons, pions, muons, light ions, and antinucleons.

LAHET and MCNP have often been linked for simulations of accelerator applications as follows: protons have been transported from their source energy to termination energy in LAHET; secondary neutrons above 20 MeV have been transported in LAHET; and neutrons that are produced below 20 MeV or are down-scattered to 20 MeV are transported in MCNP. MCNP has also been used to transport secondary photons. In the MCNP energy regime, there has been no secondary charged-particle production.

Transport in LAHET is accomplished via the use of various physics models, including intranuclear cascade, multistage pre-equilibrium, evaporation, Fermi breakup, and fission models. Transport in MCNP, on the other hand, relies on nuclear data contained in cross-section tables. The data in these tables are derived from nuclear data evaluations, such as ENDF/B-VI. [3]

The capabilities of MCNP and LAHET are currently being merged into one code for the Accelerator Production of Tritium (APT) program at Los Alamos National Laboratory. Concurrently, a significant effort is underway to improve the accuracy of the physics in the merged code. In particular, full nuclear-data evaluations (in ENDF6 format [4]) for many materials of importance to APT are being produced for incident neutrons and protons up to an energy of 150-MeV. [5] After processing, [6] cross-section tables based on these new evaluations will be available for use in the merged code.

In order to utilize these new cross-section tables, significant enhancements are required for the merged code. Neutron cross-section tables for MCNP currently specify secondary emission data for neutrons and photons only; the new evaluations also include complete neutron-induced data for protons, deuterons, tritons, and alphas. In addition, no provision in either MCNP or LAHET currently exists for the use of incident charged-particle tables other than for electrons.

To accommodate the new neutron-induced data, it was first necessary to expand the format definition of an MCNP neutron cross-section table. This was done to allow for an arbitrary number of additional secondary particles. Data specified in the expanded tables for each secondary particle include: total particle-production cross sections; total energy carried away by the particle; multiplicities for each reaction that produces the particle; and differential spectra (energy, angle, energy/angle) for each reaction that produces the particle. All quantities are a function of incident neutron energy.

We have prepared a 150-MeV neutron cross-section library in this expanded format for 15 nuclides (H-2, C-12, O-16, Al-27, Fe-54,56,57,58, W-182,183,184,186, and Pb-206,207,208). The average increase in size of an MCNP data table that includes charged-particle production data compared to one without such data is 30 percent.

Modifications to MCNP have been implemented so that this expanded neutron library can be utilized. At every neutron collision, the expected weight of a particular secondary charged particle i is WGT * sigma $_{cp,i}$ (E) / sigma $_{tot}$ (E), where WGT is the weight of the incident neutron, sigma $_{cp,i}$ is the total particle-production cross section for particle i, sigma $_{tot}$ is the total neutron-interaction cross section, and E is the incident neutron energy. The number of charged particles produced is an integer (possibly 0) determined by analog sampling; each is produced with weight WGT.

If the code determines that a charged particle will be produced, it then samples the reaction responsible for that particle. There is no correlation between the reactions sampled as being responsible for the various secondary particles that may be produced as a result of a single neutron collision.

Several ENDF6 representations of scattered energy-angle distributions are supported in the modified version of MCNP. To be specific, the following representations for neutron-induced charged particles are allowed: tabular energy distributions; angular distributions via equally-probable cosine bins; Kalbach systematics for correlated energy-angle distributions; discrete two-body scattering; and n-body phase-space energy distributions. In all cases where necessary, kinematics algorithms currently incorporated in MCNP that are specific for neutron-in, neutron-out physics have been generalized to be appropriate for neutrons in and charged particles out. In addition, a general center-of-mass to laboratory conversion technique has been incorporated. As is currently the case for neutron production, all such conversions are based on the assumption of two-body kinematics, which is clearly only an approximation for many high-energy neutron reactions of current interest.

A prototype version of the merged MCNP-LAHET code called MCNPX, has been issued. [7] Fully coupled proton-neutron transport over the entire energy range of interest may be achieved in a single integrated MCNPX simulation. Protons are still transported from their source energy to their termination energy using the physics models of LAHET. Any neutrons with energies greater than the upper boundary of the evaluated data (now 150 MeV) are also transported using the physics model of LAHET. Neutrons below 150 MeV are transported using the new cross-section library described above. All relevant secondary particles are produced by all nuclear interactions, whether simulated by LAHET models or by evaluated cross sections.

Several calculations have been performed with MCNPX to verify that the new physics capabilities associated with utilization of the 150-MeV neutron evaluations have been correctly implemented. Total neutron-induced charged-particle production rates have been calculated with MCNPX and compared with an alternative means of calculation. Charged-particle spectra resulting from monoenergetic neutrons have been calculated with MCNPX and compared with the original evaluation. All comparisons indicate correct implementations.

In addition, preliminary calculations of an integral experiment have been performed with MCNPX and the new cross-section library. We have chosen to simulate a recent measurement of the transmission of quasi-monoenergetic neutrons generated by 68-MeV protons through 70 cm of iron. [8] An MCNP model of the experiment had been previously generated [9] to benchmark LAHET 2.8. We recalculated the configuration using MCNPX. Results are in better qualitative agreement with the measurement than are the results from LAHET 2.8.

Remaining work will focus on completing the implementation of proton cross-section tables in MCNPX. The tables will provide cross sections for proton-incident reactions as well as spectral data for secondary particles. MCNPX will ultimately use table-based nuclear data in the energy range that it exists for any combination of incident particle and target material. This will result in a general, coupled-particle, Monte Carlo transport capability based on state-of-the-art nuclear data and physics models.

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