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Coupled Proton/Neutron Transport Calculations Using the S_N and Monte Carlo Methods

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INTRODUCTION

Coupled charged/neutral particle transport calculations are most often carried out using the Monte Carlo technique. For example, the ITS[1], EGS[2], and MCNP (Version 4)[3] codes are used extensively for electron/photon transport calculations while HETC[4] models the transport of protons, neutrons and heavy ions.

In recent years there has been considerable progress in deterministic models of electron transport,[5-10] and many of these models are applicable to protons.[11] However, even with these new models (and the well established models for neutron transport) deterministic coupled neutron/proton transport calculations have not been feasible for most problems of interest, due to a lack of coupled multigroup neutron/proton cross section sets. Such cross section sets are now being developed at Los Alamos. Using these cross sections we have carried out coupled proton/neutron transport calculations using both the S_N and Monte Carlo methods. The S_N calculations used a code called SMARTEPANTS (simulating many accumulative Rutherford trajectories, electron, proton and neutral transport solver), while the Monte Carlo calculations are done with the multigroup option of the MCNP[12] code. Both SMARTEPANTS and MCNP require standard multigroup cross section libraries. HETC on the other hand, avoids the need for precalculated nuclear cross sections by modeling individual nucleon collisions as the transporting neutrons and protons interact with nuclei.

S_N ALGORITHM

The SMARTEPANTS code uses a combination of the multigroup method and the continuous slowing down approximation (CSDA). The fraction of the problem solved in the CSDA mode is controlled by the cross-sections. The total neutron and proton cross sections are expressed as

$$\sigma_p (E' \to E, \hat{\Omega}' \to \hat{\Omega}) \simeq \sigma_p (E', \hat{\Omega}' \to \hat{\Omega}) \, \delta(E-E')$$
$$+ \sigma_p (E' \to E) \, \delta(\hat{\Omega} - \hat{\Omega}')$$
$$+ \sigma_{p\to p} (E' \to E, \hat{\Omega}' \to \hat{\Omega})$$
$$+ \sigma_{p\to n} (E' \to E, \hat{\Omega}' \to \hat{\Omega}) \,, \qquad (1)$$

and

$$\sigma_n (E' \to E, \hat{\Omega}' \to \hat{\Omega}) = \sigma_{n\to n} (E' \to E, \hat{\Omega}' \to \hat{\Omega})$$
$$+ \sigma_{n\to p} (E' \to E, \hat{\Omega}' \to \hat{\Omega}) \qquad (2)$$

where p denotes protons and n denotes neutrons. The first term on the right hand side of Eq. (1) represent collisions such as nuclear coulomb scattering that cause (normally very small) angular deflections, but virtually no energy loss. The second term represents reactions such as proton/electron scattering that cause small energy losses but virtually no angular deflections. The cross section $\sigma_{b\to c}$ $(E' \to E, \hat{\Omega}' \to \hat{\Omega})$ represent the production of particle c, c = n, p due to nuclear collisions of particle b, b = n, p. Due to the relatively large angular and energy changes caused by nuclear collisions, the $\sigma_{b\to c}$ $(E' \to E, \hat{\Omega}' \to \hat{\Omega})$ are more amenable to a multigroup treatment than are the coulomb cross sections.

The small energy losses associated with σ_p $(E' \to E)$ are modeled using the CSDA. The resultant proton Spencer-Lewis equation, along with a suitable neutron transport equation can be given as

$$\left[\frac{\partial}{\partial s} + \hat{\Omega}\cdot\nabla + \sigma_b \right] \phi_b(s,\mathbf{r},\hat{\Omega}) = \int d\Omega' \sigma_b(s, \hat{\Omega}' \to \hat{\Omega}) \, \phi_b(s,\mathbf{r},\hat{\Omega}')$$
$$+ \sum_{c=p,n} \int ds' \int d\hat{\Omega}' \sigma_{c\to b} (s' \to s, \hat{\Omega}' \to \hat{\Omega}) \, \phi_c(s',\mathbf{r},\hat{\Omega}')$$
$$+ Q_b (s,\mathbf{r},\hat{\Omega}) \,, \quad b = p,n \,, \qquad (3)$$

where Q_b is the fixed souce for particle b. The pathlength s is related to energy through the CSDA stopping power, $\left|\frac{dE}{ds}\right|_b$,

$$s(E) = \int_E^{E_0} \frac{dE}{\left|\frac{dE}{ds}\right|_b} \quad . \tag{4}$$

For protons

$$\left|\frac{dE}{ds}\right|_p = \int_0^E (E-E')\, \sigma_p\, (E \rightarrow E')\, dE' \quad . \tag{5}$$

For neutrons we normally define a negligibly small stopping power $\left|\frac{dE}{ds}\right|_n \simeq 0$ (so that the Spencer-Lewis solution algorithm can be applied to both particles), and set $\sigma_n\ (s, \hat{\Omega}' \rightarrow \hat{\Omega}) = 0$. However, for very energetic neutrons it can be an advantage to apply the CSDA and SMART scattering theory to the more anisotropic components of the neutron scattering kernel[13] and then both $\left|\frac{dE}{ds}\right|_n$ and $\sigma_n\ (s, \hat{\Omega}' \rightarrow \hat{\Omega})$ would be significant.

Equation (3) is solved using the standard S_N multigroup method with diamond differencing in all variables, x, y, z and s, except that for the proton case (b=p) the first integral is modeled with SMART scattering matrices. Thus, the extremely anisotropic proton coulomb scattering can be treated with a relatively coarse (typically S_4 to S_8) quadrature sets.

MONTE CARLO ALGORITHM

MCNP is a three-dimensional, generalized-geometry, time-dependent Monte Carlo code for coupled neutron/photon/electron transport. The code has traditionally made use of detailed continuous-energy cross sections; a recent version allows multigroup cross-sections data to be used for the first time.[14] MCNP has a rich collection of source options, variance-reduction techniques, and tally features that allow efficient Monte Carlo simulation of problems in areas such as reactor design, radiation shielding, dosimetry, criticality, safeguards, material activation, radiation damage, and physics experiments.

The standard MCNP multigroup option is appropriate for neutral-particle transport. In addition, a hybrid multigroup/continuous-energy method for charged-particle transport has been implemented in MCNP.[15] The hybrid nature of the technique is a result of modifying the multigroup method to accommodate particles with continuously varying energies. Small energy loss processes are modeled with a continuous slowing down operator, and large energy loss processes are modeled with the standard Boltzmann multigroup approximation. An advantage of this technique is that the same multigroup cross-section data generated for deterministic codes is appropriate for the hybrid multigroup/continuous-energy Monte Carlo code.

The MCNP hybrid technique has been applied predominantly to coupled electron/photon problems. In this paper, we apply the method to coupled proton/neutron problems.

CROSS SECTIONS

To define a scattering medium it is necessary to specify $\left|\frac{dE}{ds}\right|_p$, $\sigma_p(E,\hat{\Omega}'\cdot\hat{\Omega})$ and the $\sigma_{b\to c}(E'\to E, \hat{\Omega}'\to\hat{\Omega})$, b,c, = p,n. We use the computer code SPAR[16] for the stopping powers and the Rutherford scattering formula with Moliere[17] screening for $\sigma_p(E,\hat{\Omega}'\cdot\hat{\Omega})$. As mentioned earlier, a limitation in the past for neutron/proton calculations has been the lack of appropriate evaluated data libraries. An effort in the Applied Nuclear Science Group at Los Alamos has partially remedied this problem. Transport libraries have been completed for proton- and neutron-induced reactions on nine materials (^{1}H, Be, C, O, Al, Si, Fe, W, and ^{238}U), with the incident energy range extending to 100 MeV[18]. The major steps involved in the effort have been: (1) extension and validation of low-energy nuclear physics theoretical models for applicability up to 100 MeV; (2) development of evaluated (ENDF/B) data formats appropriate for higher energies; (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. For purposes of the test problem described in the next paragraph, evaluated data for aluminum have been processed by NJOY[19] into a coupled P_4 library with 52 neutron groups and 32 proton groups.

The key component of the effort described in the previous paragraph is the extensive model code development required to provide the 100-MeV libraries. Prior to the present effort, the methods and models that we routinely utilized in our analyses (mainly at energies below 30 MeV) included R-matrix and phase shift analyses, spherical and coupled-channel optical models, various level density models involving energy-independent level density parameters, distorted-wave Born approximation calculations, and multibarrier fission models. Reliable calculations of higher energy neutron and proton reaction data, however, required development and improvement of these existing models as well as utilization of several new ones. Our development efforts centered upon extension of optical and reaction theories (preequilibrium and statistical models), research into nuclear level densities more appropriate for higher excitation energies, and the development of systematics needed to describe angular distributions associated with continuum particle emission. Most importantly, extensive new development was required in order to address the problem of neutron and γ-ray emission from fission reactions at higher energies, particularly regarding the calculation of fission cross sections at the higher energies and the excitation and deexcitation of fission fragments by neutron and photon emission. All the model improvements were incorporated into the GNASH code system[20], which already included many features useful for the higher energy analyses[21]. Details of our model code development may be found in Reference 18.

RESULTS

To test the algorithms, transmitted and reflected currents due to monodirectional normally incident beams of neutrons and protons were calculated. The beams were incident on aluminum plates measuring 16 cm in the x- and y-directions and 0.5, 1, 2, 3, 3.5, and 4 cm in the z-direction. The results are shown in Figs. 1 and 2. Except for the reflected protons the agreement is excellent.

The major difference between the models is the usual continuous Monte Carlo versus discrete

S_N variables (here we used S_4 quadrature with 9 x- and y-mesh cells and 6 or 8 z-mesh cells). In addition, narrow angle coulomb deflections were neglected in the Monte Carlo calculations but modeled using SMART scattering theory in the S_N code. This could explain the slightly larger proton range predicted by the Monte Carlo method (see Fig. 2).

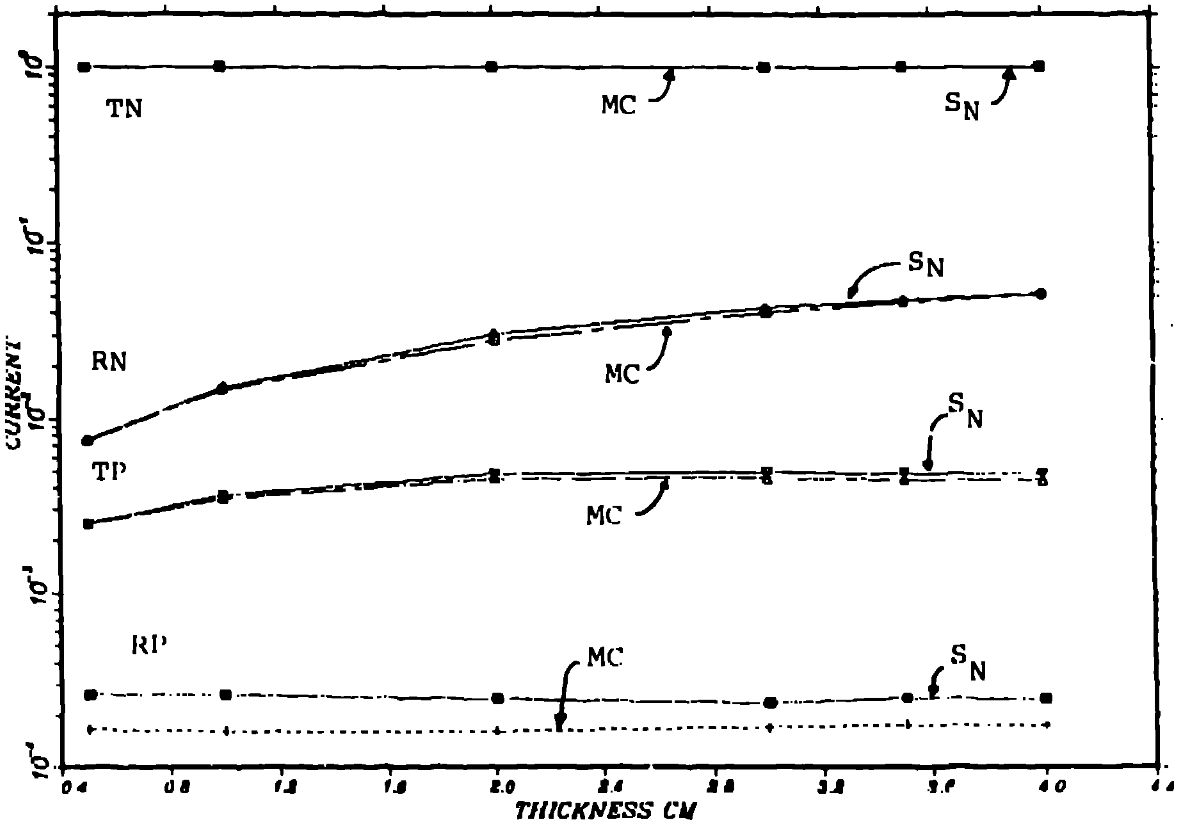
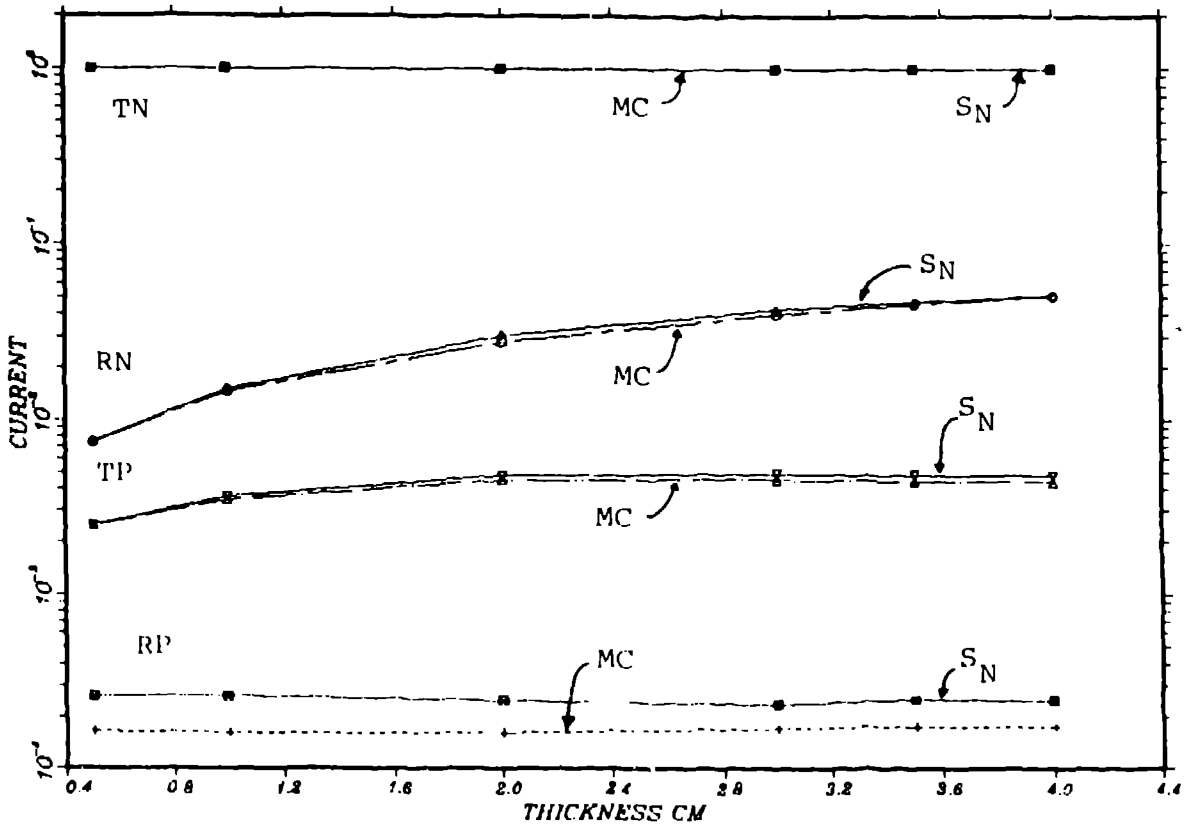


Fig. 1. Transmitted Nuctron (TN), Reflected Nuctron (RN), Transmitted Proton (TP) and Reflected Proton (RP) Currents for Six Slab Thicknesses due to Normally Incident 100 MeV Neutron Beams. Both Monte Carlo (MC) and S_N results are shown.



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