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INTRODUCTION

Adding the ability to transport protons has been a recent focus in MCNP5 [1] development. The Fortran 90 routines that implement straggling, multiple coulomb scattering, nuclear interactions, and energy loss must be thoroughly tested before integration into MCNP5. The energy loss routines, based on the calculation of stopping power from Bethe's formulas and the Lindhard's [2] (low energy) linear response formula, have been extensively compared to published ICRU data [3] as well as LaRC [4] and Janni [5] calculations. This summary describes the physics implemented in the stopping power routines and the efforts to verify their values.

STOPPING POWER

The stopping power is calculated according to the energy of the particle of interest. If the equivalent proton energy is below 1.31 MeV or above 5.24 MeV, the low or high energy models, respectively, are used. An energy weighted average is used between the two energies.

For the lower energy regime, which uses the same methodology as the SPAR code [6] (as originally used in HETC), the electronic stopping power is calculated using Lindhard's linear response function of a free electron gas to a perturbation. This value is added to the calculated nuclear stopping power.

For higher energies, where nuclear stopping power is negligibly important, the stopping power routines are based on Bethe's electronic stopping power formula, as it appears in equations 1 and 2 below. The constants are defined on page 6 of ICRU Report 49. The variables Z, z, A, I and β have their usual meaning. The summations are a function of the atom fraction, f_i, for each element, i, in the material of interest.

$$\frac{-1}{\rho}\frac{dE}{dx}=\frac{4\pi r_e^2 mc^2}{\beta^2}\frac{1}{u}\frac{\sum_i \mathrm{Z_i f}_i}{\sum_i \mathrm{A_i f}_i}z^2 L(\beta) \qquad (1)$$

$$L(\beta)=\frac{1}{2}\ln\left(\frac{2mc^2\beta^2 W_{\mathrm{m}}}{1-\beta^2}\right)-\beta^2-\frac{\sum_i \mathrm{Z_i f}_i \ln I_i}{\sum_i \mathrm{Z_i f_i}}-\sum_{\mathrm{i}}\frac{\mathrm{C_i f_i}}{\mathrm{Z_i}}-\frac{\delta(\beta,z,I)}{2} \qquad (2)$$

The last two terms in equation 2 are corrections to the stopping power for atom specific shell (or subshell) electron velocities, C_i, and the high-energy density effect, δ, respectively. The atomic shell or subshell corrections can be based on models by Bichsel [7], Janni, Kjandelwal [8] or Walske [9]. For heavier elements, the n, o, or p shell corrections are scaled from the m or l shell correction to agree with experimental data. Based on a comparison of the calculated stopping powers to ICRU published values, Janni's method was selected as the default.

The density effect is calculated with the method developed by Sternheimer [10]. The density correction and the mean excitation energy (I) are both dependant on the phase of the material, which can be specified in the MCNP input deck with the GAS=# option on the material card.

VERIFICATION EFFORTS

ICRU Report 49 [3] discusses the physics underlying stopping power calculations, including density effects, range and energy straggling, chemical binding, and phase effects. More importantly, they state typical methods for calculating these quantities, a few comparisons to experiments, and a large bibliography. The report lists the electronic, nuclear and total stopping powers, CSDA range, detour factor, and mean excitation energies for 25 elements and 48 common materials over the energy range of 1 keV to 10 GeV. The low energy stopping powers are based on experimental data, while the higher energy values are calculated from Bethe's formulas with various corrections. The total stopping powers given for all available elements and 15 of the materials were compared to those calculated with MCNP5. Figure 1 shows that the agreement between MCNP5 and ICRU stopping powers is usually within 3% between 4 MeV and 10 GeV. Agreement for energies between 1 keV and 1 MeV is mostly better than 35%. ICRU 49 states that, "The differences between the various theoretical predictions and measured cross sections are largest at energies where the curve of stopping power vs. energy peaks, and can amount to 20 percent or more." The agreement for materials is similar to their constituent elements at all energies.

The calculated stopping powers were also compared to the results of the LaRC [3] and Janni [4] codes, obtained in the NASA technical paper 3644. This is necessary since the ICRU report only provides values up to 10 GeV, while the NASA document provides calculations for 12 select elements up to 100's of GeV. Agreement between the LaRC and MCNP5 stopping powers between 10 GeV and 100 GeV for is less than ~3%.

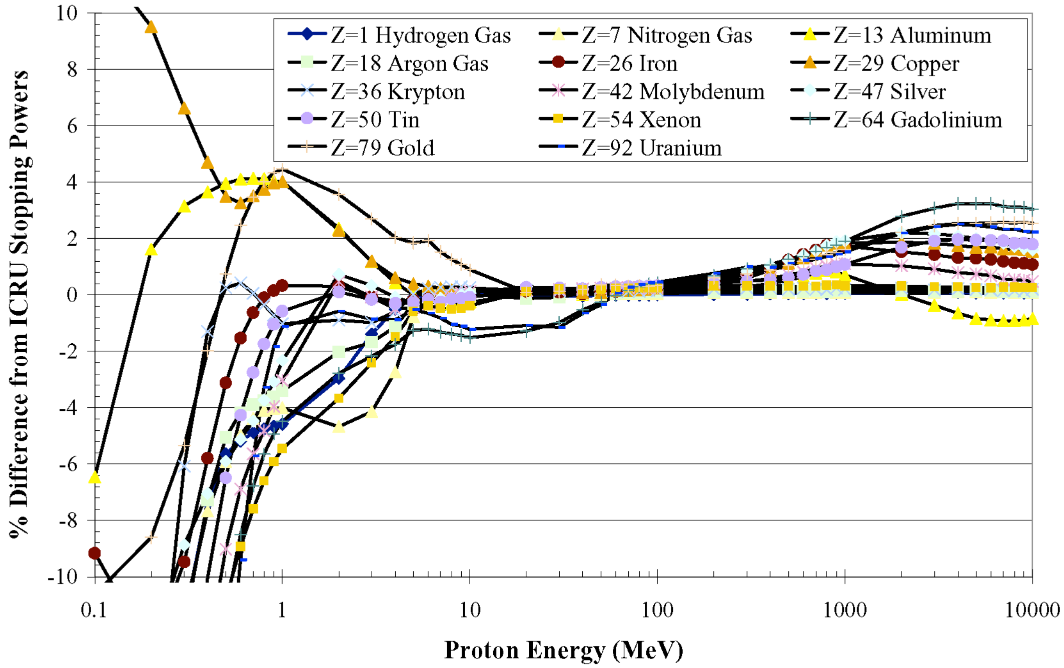

Fig. 1. Comparison of MCNP5 proton stopping powers in various elements to ICRU Report 49.

CONCLUSIONS

The stopping powers calculated by the MCNP5 routines agree well with ICRU and LaRC published values. Future verification efforts will include other phenomenon included in the ICRU report: nuclear stopping power, energy straggling, and detour factors. While the stopping power routines are capable of handling heavy charged particles other than protons, appropriate verification efforts will be to be performed before this capability is implemented.

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