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Monte Carlo Calculated Stopping Power and Range of Alpha Particles in Water

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Abstract— Alpha particles have a wide range of industrial and medical applications. This study investigates stopping power and range of alpha particles in water medium using Monte Carlo simulations. A point source emitting mono-energetic pencil beam of alpha particles irradiatied a 1 cm radius water cylinder placed in vacuum. Disk-shaped thin detectors (r=0.1 cm) were placed inside the cylinder to obtain average absorbed dose and flux at different distances within the phantom. MCNP6 was used to yield average flux and absorbed dose in each detector cell to later compute the value of the stopping power for water at incoming alpha energy. The results obtained in this study are compared with the data from the NIST compilation.

Index Terms— Monte Carlo, stopping power, range, alpha particles.

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1 INTRODUCTION

Interaction of charged particles with absorbing materials involve mostly Coulomb interactions with orbital electrons along with nuclear collisions and thus the energy loss mechanism of such radiation is usually quantified by the concept of stopping power. When charged particles travel a unit distance in an absorber of density ρ, this quantity is typically taken as a measure of the rate of energy lost and is denoted as $-dE/\rho dx$. It depends heavily on the energy of the incoming particle as well as various properties of the absorber, such as ρ and Z and is considered significant in deriving charged particle's range and the amount of absorber thickness necessary for shielding a radiation beam.

A charged particle beam penetrating an absorbing material experiences various types of interactions which determine the track it will follow. Through elastic and inelastic scatterings, the particles in the beam transfer all of their kinetic energy to atomic electrons or nuclei. Consequently, the total stopping power $(-dE/dx)_{total}$ for charged particles is made up of two distinct components: [1]

$$(-dE/dx)_{tot}=(-dE/dx)_{col}+(-dE/dx)_{rad}. \quad (1)$$

In this equation, the first term $(-dE/dx)_{col}$ is known as the collisional stopping power and is a result of Coulomb interactions between the charged particle and the atomic electrons of the absorber. The second term $(-dE/dx)_{rad}$, on the other hand, is defined as the radiative stopping power and leads to emission bremsstrahlung radiation which is usually neglected for heavy charged particles such protons, alpha particles, etc. as compared to the collisional stopping power. Accordingly, a heavy charged particle traversing an absorber transfers most of its energy through collisions with atomic electrons.

Traditionally, stopping power for any type of charged particle is employed as mass stopping power in units of MeV cm^2/g and is given theoretically by the Bethe formula, derived from the quantum mechanical and relativistic derivations. In addition, data tables (from NIST) or computer codes (such as SRIM) are available for essentially obtaining the stopping powers and ranges of charged particles. [2, 3] Figure 1 portrays for water, and for most materials as well, that the electronic stopping power is the sole contributor to the mass stopping power in a wide range of proton energies. Figure 2 shows, for protons, alphas and electrons in water, that mass

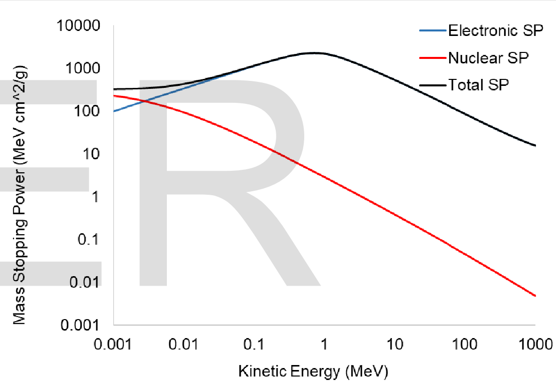

Fig. 1. Comnponents of mass SP versus alpha energy in water.

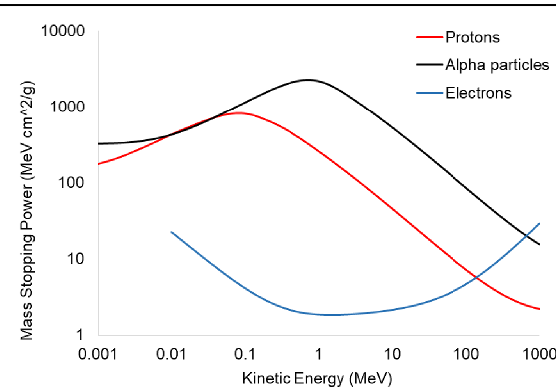

Fig. 2. Mass stopping power versus alpha particle energy in water for electrons, protons, and alpha particles.

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stopping power of heavy charged particles depends heavily on the charge of the particle for most of the energy range and follows a different trend for electrons.

Bethe's equation is regarded as a useful technique for calculating stopping power for electronic collisions. Its application, however, is cumbersome for practical applications and involves prior calculation of various parameters. Alternative techniques to this equation for obtaining stopping power data, but for a limited number of materials, is available as tabular data or computer codes. A substitute and novel approach to compute stopping powers and ranges of charged particles is the use of Monte Carlo simulations. This study investigates the use of MCNPX to determine total mass stopping power of alpha particles in water medium over an energy range of 1-100 MeV.

2 Materials and Methods

As a well established statistical method, Monte Carlo is a numerical technique for solving problems that has no practical solution. It offers an alternative way of simulating radiation transport through any material media. A practical application starts with random numbers following certain probability distributions that are employed to search for estimates of particle properties, such as energy, position, direction and path-length of individual particles. These predictions are based on validated libraries interaction cross sections which in turn provide the associated probability of certain reactions that the particles undergo in traversing the materials. This procedure is repeated for a finite number of histories and as a result of Monte Carlo simulations, an average value for the quantity that is being searched is produced. These particle properties can be anything from particle fluence across a surface or a cell to energy deposition in any volume of interest. Thus, as a stochastic method alternative to analytical or deterministic solutions, Monte Carlo provides many advantages in charged particle transport and therefore can be viewed as a well established alternative for the Bethe-Bloche equation. [4]

There are many Monte Carlo packages that are available for treating radiation transport problems. This study employed MCNP6 (version 2.7.0) which was developed at the Los Alamos National Laboratory (LANL, USA) and can be obtained from the Oak Ridge National Laboratory (ORNL). [5] MCNP6 handles transport of charged or uncharged particles in wide energy ranges based on interactions of particles with absorber atoms available in the problem whose geometry can be modeled arbitrarily in three dimensions. The particle interactions are treated either as continuous or discrete energies based on the cross-section data obtained from the ENDF/B data libraries (Evaluated Nuclear Data Files, version B). The code can use many dfferent source distributions, detector combinations and output options in a text formatted input file.

A plot of the problem geometry is given in Figure 3 where a water phantom (cylinder; r=1 cm, h=1 cm) placed in a vacuum sphere (r=5 cm) is tracked with 1000 detector disks (r=0.1 cm) positioned consecutively from the surface. These disk has a fixed thickness for each simulation but vary depending on the source particle's energy, basically a fraction of the range of charged particle at that energy. Alpha particles from the source were mono-energetic and mono-directional created from a point source at one end of the water phantom. Tally types F4 and +F6 were employed in each of 1000 detector cells to record the average cell flux (in units of #/cm^2/source particle) and the absorbed dose (in units of MeV/g/source particle) by all primary and secondary particles, respectively. Secondary particles created following alpha particle interactions were included in the simulations. Each run was carried out for one million particle histories which usually yields about 1% statistical errors. A total of 15 cases were studied, each at a different source energy from 1 MeV to 100 MeV.

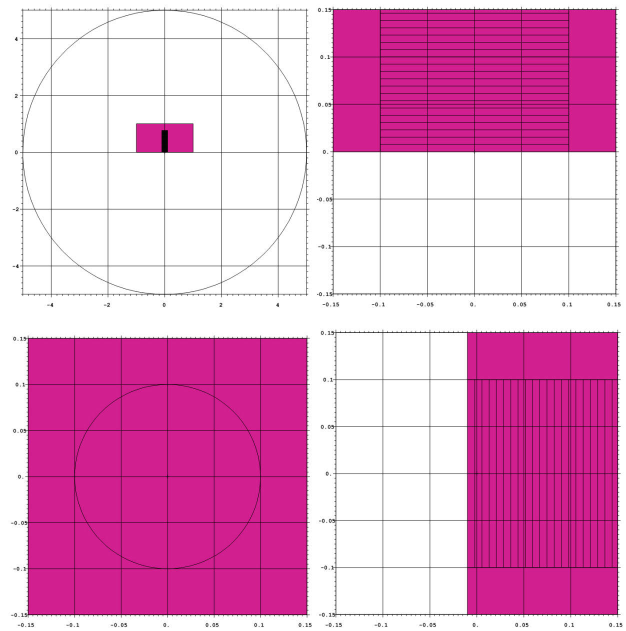

Fig. 3. Plot of the problem from MCNP6's geometry module. (a) Whole geometry, y-z slice at EXT 5. (b) Detector array, y-z slice at EXT 0.1. (c) Detector array, x-y slice at EXT 0.1. (d) Detector array, z-x slice at EXT 0.1.

3 Results

MCNPX was used to compute the absorbed dose and flux at each detector with varying material depths from alpha particle interactions in the energy range of 1-100 MeV.

Total mass stopping power (in MeV cm^2/g) for each alpha energy was computed at the first detector of the array from the ratio of the absorbed dose from +F6 tally (in MeV/g/source particle) and the flux from F4 tally (in #/cm^2/source particle). Table 1 presents the total mass stopping power of water for alpha particles along with the corresponding NIST data. The data from the Monte Carlo simulations and the NIST database agree reasonably well, the discrepancy being at most 6% as depicted by Figure 4.

Later, for each source energy (for each simulation), the depth of the detector cell at which absorbed dose falls below 1% of the Bragg peak was determined and chosen as the range of the incoming protons at that particular energy. The protone ranges obtained by this approach for bone, soft tissue

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and water are given in Table 2 along with the NIST data for comparison purposes. As shown in Figures 3d-f, the Monte Carlo approach provides data that are in good agreement with those of the NIST database. Again, both data follow the same trend and the deviate at no more than 4%.

Table 1. Monte Carlo calculated total mass stopping power (in $MeV\ cm^2/g$) of alpha particles in water and comparison with NIST values.

E (MeV)	MCNPX	NIST	% Diff
1	2146	2193	-2.2%
2	1637	1625	0.7%
3	1284	1257	2.2%
4	1086	1035	4.9%
5	905.8	885.5	2.3%
6	796.4	777.7	2.4%
8	652.3	630.6	3.4%
10	532.4	534.4	-0.4%
20	309.3	314.6	-1.7%
30	235.5	228.6	3.0%
40	178.6	181.6	-1.7%
50	155.4	151.7	2.4%
60	135.2	130.9	3.3%
80	102.3	103.7	-1.4%
100	88.90	86.49	2.8%

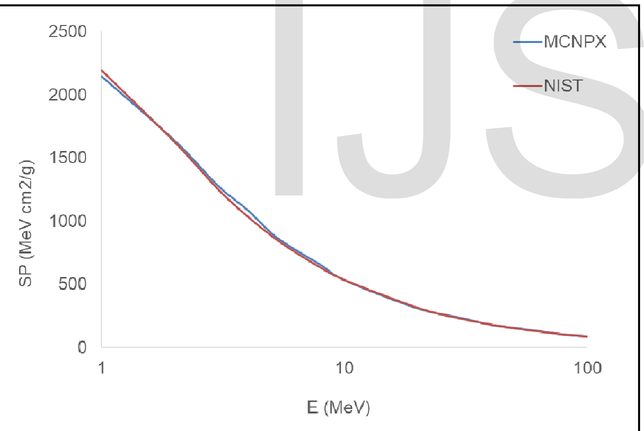

Fig. 4. Comparison of SPs from MCNP and NIST for water.

A similar trend is observed in alpha particle ranges as seen in Table 2 and Figure 5.

4 Conclusions

In this study, Monte Carlo approach was applied to determine stopping power and range data for alpha particles of 1-100 MeV energy. MCNPX simulations provide results that confirm to tabular data. This methodlogy is promising for other charged particles, different materials, and wider energy range.

Table 2. Monte Carlo calculated range (in *cm*) of alpha particles in water and comparison with NIST values.

E (MeV)	MCNPX	NIST	% Diff
1	0.0004935	0.0005702	-13.5%
2	0.001043	0.001099	-5.1%
3	0.001749	0.001804	-3.0%
4	0.0025905	0.002686	-3.6%
5	0.0036225	0.003733	-3.0%
6	0.00483	0.004941	-2.2%
8	0.007661	0.007813	-1.9%
10	0.01113	0.01127	-1.2%
20	0.03674	0.03664	0.3%
30	0.07515	0.07446	0.9%
40	0.12525	0.1239	1.1%
50	0.18745	0.1844	1.7%
60	0.25885	0.2555	1.3%
80	0.43605	0.4285	1.8%
100	0.65065	0.6406	1.6%

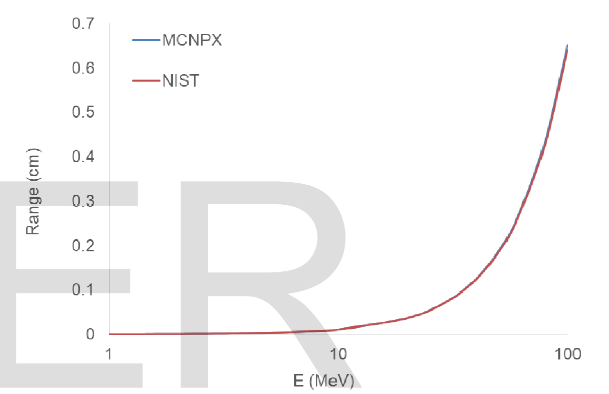

Fig. 5. Comparison of ranges from MCNP and NIST for water.

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