

Comparison of GEANT4 Simulations with Experimental Data for Thick Al Absorbers

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Abstract. Proton beams in medical applications deal with relatively thick targets like the human head or trunk. Therefore, relatively small differences in the total proton stopping power given, for example, by the different models provided by GEANT4 can lead to significant disagreements in the final proton energy spectra when integrated along lengthy proton trajectories. This work presents proton energy spectra obtained by GEANT4.8.2 simulations using ICRU49, Ziegler1985 and Ziegler2000 models for 19.68MeV protons passing through a number of Al absorbers with various thicknesses. The spectra were compared with the experimental data, with TRIM/SRIM2008 and MCNPX2.4.0 simulations, and with the Payne analytical solution for the transport equation in the Fokker-Plank approximation. It is shown that the MCNPX simulations reasonably reproduce well all experimental spectra. For the relatively thin targets all the methods give practically identical results but this is not the same for the thick absorbers. It should be noted that all the spectra were measured at the proton energies significantly above 2MeV, i.e., in the so-called “Bethe-Bloch region”. Therefore the observed disagreements in GEANT4 results, simulated with different models, are somewhat unexpected. Further studies are necessary for better understanding and definitive conclusions.

Keywords: Proton beams, Energy measurement, Monte Carlo methods.

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INTRODUCTION

The GEANT4 [1,2] simulations are essential for the development of complex systems like particle detectors for LHC at CERN, or proton computerized tomography (pCT) for medical applications [3-8]. In the last case, however, a proton beam passes through relatively thick targets like the human head or trunk. Although GEANT4 has been validated by the USA National Institute of Standards and Technology - NIST PSTAR stopping powers (SP) for protons [9], the small differences in SP given by the different models provided by GEANT4 may lead to significant disagreements in the final proton energy spectra when integrated along proton trajectories.

At least, our previous simulations [10-14] have shown that there are notable differences between the spectra, simulated by GEANT4 (in the standard execution mode) and the results of simulation by TRIM/SRIM2003 [15] and MCNPX [16]. These differences in the mean final proton energy are observed for H₂O and Al absorbers at any thickness, but for relatively thin (less than ~50% of the full range of protons with the same energy in the same material) targets are less than it could be resolved in a real experiment. For the thickest targets, however, these differences overcame the typical energy resolution.

In addition, it has been observed that there is an obvious scale effect: all the spectra simulated for the pairs of initial proton energies 25MeV - 250MeV [11-13], and 23MeV - 230MeV [14], could be scaled one to the other by applying a factor 10 to the energy scale. It should be noted that the spectra were simulated for target thicknesses equal to 10% to 90% of the corresponded full projected range from NIST PSTAR. Consequently, the ~0.5MeV difference in simulated spectra for the thickest (90%) water target at initial energy 23MeV, for example, corresponds to ~5MeV difference at 230MeV, etc.

This work presents proton energy spectra obtained by GEANT4.8.2 simulations using ICRU49, Ziegler1985 and Ziegler2000 models for 19.68MeV protons passing through Al absorbers with various thicknesses. The spectra were compared with the experimental data [17], with TRIM/SRIM2008 and MCNPX2.4.0 simulations, and with the Payne analytical solution for the Boltzmann transport equation in the Fokker-Plank approximation [18].

METHODOLOGY

The experimental data used in this work as reference were taken from the paper by Tschalär and Maccabee [17], where the spectra of 19.68MeV protons after passing through 0.099, 0.2675, 0.398 and 0.497g/cm² of Al were published as well as for other Al absorbers thicknesses. These data were chosen since they contain the most complete set of experimental spectra for protons passing through the biggest variety of thicknesses of Al targets in relation to full absorption range (see Table 1).

The NIST PSTAR and SRIM2008 values for the mean final proton energy after passing through a layer were extracted from correspondent reference tables using a cubic spline interpolation. The CSDA values were calculated based on the same form of Bethe-Bloch equation as it had been published in [10, 11]. The calculations of proton energy spectra using Payne's theory [18] were based at the equations which could be found in [10, 11] also.

MCNPX is a general-purpose Monte Carlo radiation transport code developed at Los Alamos National Laboratory [16]. We were interested in this code because its applications include, among others, proton therapy. The simulation was done using the MCNPX version 2.4.0.

TRIM is historically one of the first Monte Carlo codes for ion transportation, actually with the friendliest interface [15]. In this work, we used the TRIM code from the SRIM2008 version 04 package.

GEANT4 [1, 2] is actually the most general framework for handling the motion of particles through matter. Its ability to work with very complex geometry and tracking

is essential to the pCT development [10-14]. The simulations were made with the version GEANT4.8.2 by adjusting the parameters for the Hadrontherapy toolkit, as it is discussed in [19]. The simulations were performed using ICRU49, Ziegler1985 and Ziegler2000 models from the Low Energy Extension Pack following the results and discussion at [9].

All the Monte Carlo simulations were done in the narrow pencil beam and wide detector approach. In order to make a correct comparison of the spectra with different number of simulated protons, all the spectra were reduced to the discrete Probability Density Functions (PDF).

The standard analysis of statistical errors was done. The values of mean energies extracted from all simulated spectra are shown in **TABLE 1** with the same number of significant digits as the exact results in the first 4 rows. However, the margin of statistical error in these values should be understood to be one-half the value of the pre last significant place, i.e. 0.005MeV.

As for the values in **TABLE 1**, extracted from experimental data [17], the margin of total error is estimated to be less than approximately 0.02 - 0.03MeV.

RESULTS AND DISCUSSION

The mean protons energies from simulated spectra are presented at **TABLE 1**:

TABLE 1. Mean energies of 19.68MeV protons after Al absorbers (in MeV).

Absorber Thicknesses (part of PSTAR Projected Range, [%])	0.099g/cm² (17.79%)	0.2675g/cm² (48.07%)	0.398g/cm² (71.52%)	0.497g/cm² (89.31%)
NIST PSTAR	17.614	13.566	9.616	5.440
SRIM2008	17.622	13.574	9.583	5.347
CSDA	17.603	13.522	9.515	5.198
Payne's Theory	17.964	13.522	9.512	5.185
MCNPX 2.4.0	17.637	13.602	9.667	5.514
TRIM/SRIM2008	17.611	13.557	9.587	5.378
GEANT4.8.2 (ICRU49)	17.619	13.522	9.558	5.297
GEANT4.8.2 (Ziegler1985)	17.664	13.694	9.867	5.832
GEANT4.8.2 (Ziegler2000)	17.606	13.482	9.468	5.113
Experiment	17.632	13.602	9.722	5.558

It is evident that in the case of thin, 0.099g/cm² absorber all the results are very similar. That is why, to visualize the differences, only the spectra simulated for the thickest, 0.497g/cm² target are shown in **FIGURE 1**.

As seen from the values from **TABLE 1**, however, there is a similarity in results obtained for all absorber thicknesses. The GEANT spectra, simulated with Zigler1985 model, are always more energetic than the experimental data. The MCNPX spectra are in the best agreement with the experiment. The TRIM spectra are also close to the experimental ones, but always have a little bit lower energy. The use of the ICRU49 model always leads to a less overestimation of proton energy loss than the Ziegler2000 model, but still gives the mean energies below the TRIM results. At the same time, the theory predicts mean proton energies between the GEANT results with these two models. It should be noted that a special correction procedure has been applied to the

theoretical results in [17] to arrange the coincidence with experimental data. The results of present simulations are presented in Table 1 without any adjustment.

It should be also noted that all proton spectra were obtained at the energy region significantly above 0.5MeV, i.e., in the so-called “Bethe-Bloch region” [9]. Therefore the observed disagreements in GEANT4 results, simulated with different models, are somewhat unexpected.

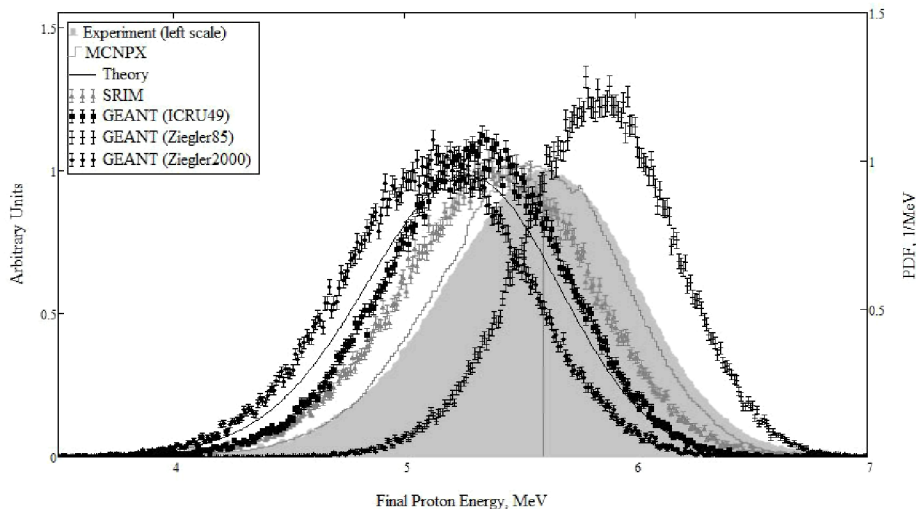


FIGURE 1. Simulated proton energy spectra for the 19.68MeV protons after 0.497g/cm² of Al absorber.

Another interesting result is that NIST PSTAR always overestimates the proton energy loss: in the case of 0.497g/cm² target the experimental spectrum has the mean energy 120keV greater. This obviously overcomes the energy resolution. For the SRIM and CSDA calculations the effect is even greater.

CONCLUSIONS

It was detected that in the case of thick Al target, the execution of GEANT4 code with various models from Low Energy Extension Pack leads to notable different spectra at the Bethe-Bloch domain. The results of present simulations show very clear some sort of proton energy loss overestimation in calculations performed at the base of NIST PSTAR, SRIM and CSDA models.

The comparison with only one set of experimental spectra was not helpful to make a definitive choice for the most adequate way to use GEANT4 for pCT simulations. Thus, we are planning to continue this work involving other experimental data.

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