BENCHMARKING OF THE PENELOPE/PENH AND PHITS CODES FOR CALCULATION OF BEAM QUALITY CORRECTION FACTORS IN THERAPEUTIC PROTON BEAMS

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Abstract

This work benchmarks the PENELOPE/PENH (2021 version) and PHITS Monte Carlo codes to calculate the beam quality correction factor (k_Q) in therapeutic proton beams. The latest PENH extension to PENELOPE enables proton transport simulation, including an approximate description of nuclear reactions and neutron production. PHITS, conversely, is an established multi-particle transport code covering protons, neutrons, and electron-gamma showers. The study compares simulated absorbed doses and k_Q factors by modeling two configurations: a thin reference water cavity and a plane-parallel air cavity representing a typical ionization chamber. To determine the k_Q factors, simulations involve a 1.25 MeV photon reference beam (Cobalt-60) and a 150 MeV monoenergetic proton beam. This comparison assesses the suitability and consistency of the PENELOPE/PENH and PHITS codes for accurate clinical proton beam dosimetry.

INTRODUCTION

The radiation therapy dosimetry protocols (see for example [1]) are based on absorbed dose in photon or proton beams to water in reference conditions. It is determined by measurements with air-filled ionization chambers and using the so-called beam quality correction factor k_Q which takes into account the difference between the reference beam quality Q_0 used for chamber calibration (e.g. MV photons) and the user beam quality (e.g. high-energy protons).

Following the approach introduced in Ref. [2] we consider beam quality correction factor defined as

$$k_Q = \frac{f_Q}{f_{Q_0}} \frac{W_{air,Q}}{W_{air,Q_0}} . \tag{1}$$

Here $W_{air,Q}$ and W_{air,Q_0} are the mean energies required to create an ion pair in air for the beam qualities Q and Q_0, respectively. The factor f_Q is calculated as the ratio

$$f_Q = \frac{D_{w,Q}}{D_{a,Q}} , \tag{2}$$

where $D_{w,Q}$ is the absorbed dose to water in a water-filled reference volume and $D_{a,Q}$ is the absorbed dose to air in an air-filled volume representing the cavity of an ionization chamber.

The direct way to determine k_Q factors is to measure them with one of ionization chambers for a user beam quality Q. However, this method requires quite complicated laboratory equipment, especially in the case of proton and ion beams, which is not available for most of the laboratories.

An efficient alternative is to perform Monte Carlo (MC) simulations using one of the existing codes, such as PENELOPE/PENH/penEASY or PHITS. There are numerous publications on this approach, see, for example, [3] and references therein.

In article [4] the beam quality correction factors in monoenergetic proton beams were calculated by detailed MC simulation of ionization chambers. In the present paper the absorbed doses and f_{Q_0} and f_Q ratios are calculated for simplified beam settings and simplified geometry representing the cavity of an ionization chamber.

The ratio of W_{air,Q_0} and $W_{air,Q}$ is determined experimentally, as described in the ICRU report 90 [5]. Here we will use the values $W_{air,Q_0} = 34.44$ eV, $W_{air,Q} = 33.97$ eV and $W_{air,Q}/W_{air,Q0} = 1.014(4)$ reported in Ref [4].

The aim of the paper is to benchmark the latest version of the MC code PENELOPE/PENH/penEASY [6, 7] that includes electromagnetic interactions, as an extension of the PENELOPE [8], and also nuclear reactions and neutron production. The penEASY (2024 version) provides a convenient interface to launch simulations.

The benchmark will be done by comparing results of simulations of absorbed doses to the reference water volume and an air-filled volume for two beam qualities, a photon beam and a proton beam, with the PENH and PHITS codes. PHITS [9–11] is a general purpose MC code that allows to simulate the transport of all main particles and nucleus over a wide energy ranges using several nuclear reaction models and nuclear data libraries.

We would like to mention a study that includes MC simulations of the absorbed doses and f_Q/f_{Q_0} ratios using several codes, namely the first version of PENH, FLUKA and GEANT4/TOPAS, and comparison of the obtained results [3]. Here we complete this work with the values obtained with the latest version of PENH and PHITS.

BEAM SETTINGS AND GEOMETRIES

The simulations of absorbed dose to water-filled and air-filled volumes were performed with the MC codes PENH and PHITS in the geometries and beam settings described in this section.

The beams are of square cross section of 10×10 cm^2 impinging on a surface of a water phantom. The photon beam is of energy 1.25 MeV modeling a ^{60}Co source, and the 150 MeV proton beam represents a radiotherapeutic irradiation. Both beams are monoenergetic, monodirectional and perpendicular to the water phantom surface.

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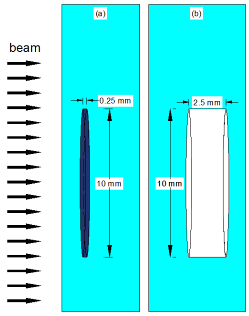

Figure 1: Geometries used for the simulations.

The geometries are shown in Fig. 1. The reference volume is a disc with a diameter of 10 mm and a thickness in beam direction of 0.25 mm filled with water, see Fig. 1 (a). The volume for scoring the absorbed dose in air is a disc cavity with a diameter of 10 mm and a thickness of 2.5 mm in the beam direction, Fig. 1 (b).

The volumes are placed in a water phantom of 20 × 20 × 15 cm^3 size for the photon beam and 20 × 20 × 10 cm^3 for the proton beam so that the plane facing the beam is the 20 × 20 cm^2 square. The center of each scoring volume is positioned in the center of the beam at a depth of 5 cm in the water phantom for photons and at a depth of 2 cm for protons.

The average absorbed dose to water scored in the reference volume approximates the absorbed dose to water in a point, see Ref. [2]. The air-filled volume models an ionization chamber.

In what follows the beam qualities Q_0 and Q stand for the photon and proton beams defined here, respectively.

MONTE CARLO SIMULATIONS

Since the source and geometries defined above have planar symmetry in the plane orthogonal to the beam direction, the simulations were performed in the reciprocal configuration making use of the reciprocity theorem, see for example Refs. [12, 13]. The theorem states that the dose absorbed in the cavity of interest, normalized to the number of histories, is the same as that obtained in a reciprocal setting in which the source and the detector have interchanged their respective sections. Thus, in the case of the reference volume irradiated with the photon beam the reciprocal volume is a plane-parallel cavity of 10 × 10 × 0.025 cm^3 size with the plane 10 × 10 cm^2 facing the beam and thickness of 0.25 mm in the beam direction placed inside the same phantom as in the initial geometry, so that its center is at the depth of 5 cm. The source is a monoenergetic pencil beam of the radius 5 mm perpendicular to the water phantom surface, see Fig. 2. For the air-filled volume the reciprocal configuration is defined in a similar way. By using this approach the CPU simulation time was drastically reduced.

In the simulations with PENH, for each scoring volume an additional region around it, called "skin", was defined with more conservative transport parameters to ensure that the multiple scattering models used in the mixed simulation (see Ref. [8]) do not introduce significant alterations, see Fig. 2.

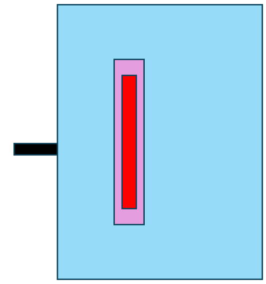

Figure 2: Reciprocal configuration used for the simulations. The phantom is shown in blue color, reference volume in red, "skin" in pink and beam in black color.

The idea of introducing the "skin" around the scoring volume is have the option to set low enough absorption energies for electrons and protons in these two volumes only and define higher absorption energies in the rest of the phantom. The concrete values are given below.

PENH

The libraries used for the description of electron-gamma showers and proton transport physics were PENELOPE (v.2018) [8] and PENH (v.2021) [7], respectively. The steering main program penEasy (v.2024-03-13) was used to define the source model and the tally, which scored the energy deposited in the detection volume, either water or air.

The thickness of the "skin" region around the scoring volumes were determined on the basis of the values of the CSDA ranges of electrons and protons in water and the radiation yield of electrons, resulting in 0.9 cm for 1.25 MeV photons and 0.15 cm for 150 MeV protons.

The absorption energy for photons was set to 1 keV in all regions. The absorption energy for electrons and positions in the scoring volume and "skin" was set to $E_{\mathrm{abs}}(e^-) = E_{\mathrm{abs}}(e^+) = 100$ keV in the dose to reference volume simulations and to 10 keV in the dose to air cavity simulations. In the simulations with the proton beam $E_{\mathrm{abs}}(p) = 4$ MeV in the dose to reference volume simulations and $E_{\mathrm{abs}}(p) = 150$ keV in the dose to air cavity simulations. The absorption energy for neutrons was set to 100 keV in both cases.

PHITS

The PHITS code version 3.35 [10] was used for the benchmarking simulations. The absorbed dose was scored with the tally T-deposit, energy deposition in a region mesh. The transport of electrons, positrons and photons was based on the EGS5 algorithm by setting the value of the *negs* parameter to negs = 1. Since PHITS does not have option of setting different values of the cut-off energies in different regions in a direct way, the same conservative cut-off energy for electrons and positrons, emin(12) and emin(13), was defined in all regions of the phantom. These parameters were set to 100 keV for the absorbed dose to water simulations and 10 keV in the case of the air-filled volume. The mean ionization potential for water was set to 78.0 eV (parameter *ih2o*).

In the simulations with the proton beam, the INCL model for nuclear reactions and the JENDL-5 data library were used with the upper energy limit for protons and neutrons equal to 150.0 MeV. Also the options for the Coulomb diffusion and energy straggling were turned on (nspred = 2, nedisp = 1). For both geometries the cut-off energy of protons was set to 1.0 keV whereas for neutrons the default value of 10^{-5} eV was used.

Results

Results of the calculations of the absorbed doses, f_{Q0}, f_Q factors, f_Q/f_{Q0} ratio and the beam quality correction factor are given in Tables 1 - 4.

The simulations with the PENH code were performed at a computer with the 11th Gen Intel(R) Core(TM) i7-11850H (2.50 GHz), 8 Cores(s) processor. Simulations carried out in PENH were not configured to run in parallel. Between 2×10^8 and 8.5×10^8 histories were simulated depending on the case. With the PHITS code, the simulations were carried out at a computer with the 13th Gen Intel(R) Core(TM) i7-1355U (1.70 GHz), 12 Core(s) processor and were fully parallelized. The number of simulated particles was 3×10^7 for the photon beam and 3.75×10^6 for the proton one.

Table 1: Absorbed Dose to the Reference Volume in eV/g per History

MC code	$\mathbf{D}_{w,Q_0}$	$\mathbf{D}_{w,Q}$
PENH	333.97(11)	6.1401(18)×10^4
PHITS	333.7(9)	6.1458(43)×10^4

Table 2: Absorbed Dose to the Air-filled Volume in eV/g per History

MC code	$\mathbf{D}_{a,Q_0}$	$\mathbf{D}_{a,Q}$
PENH	293.5(11)	5.386(21) ×10^4
PHITS	289.4(14)	5.380(16) ×10^4

Table 3: f_{Q_0}, f_Q Ratios

MC code	$\mathbf{f}_{Q_0}$	$\mathbf{f}_Q$
PENH	1.1380(43)	1.1401(43)
PHITS	1.1530(64)	1.1424(35)

Table 4: f_Q/f_{Q_0} Ratio and the Beam Quality Correction Factor

MC code	$\mathbf{f_Q/f_{Q_0}}$	$\mathbf{k}_Q$
PENH	1.0018(53)	1.019(4)
PHITS	0.9908(64)	1.004(8)

DISCUSSION AND CONCLUSION

The absorbed doses to the reference water volume and to air-filled parallel-plane disc volume for the irradiation with 1.25 MeV photons and 150.0 MeV protons are calculated using the Monte Carlo codes PENH (2021 version) and PHITS (v. 3.35). From the results given in Tables 1 - 4 we conclude that the mean values of the absorbed doses per primary particle (history) agree within 1.4 % or better for the photon beam and within 0.8 % or better for the proton one.

From the analysis of results of simulations of the absorbed doses and calculation of the f_{Q0}, f_Q and f_Q/f_{Q0} factors performed using the FLUKA, GEANT4 and PENH (2013 version) codes reported in Ref. [3] we can conclude that the same level of agreement with the PENH (2021 version) and PHITS takes place. The obtained results establish the consistency of the PENELOPE/PENH/penEasy and PHITS codes for accurate clinical proton beam dosimetry.

Further benchmarks of the PENH and PHITS, and other Monte Carlo codes are of interest. These future studies may include MC simulations for other geometries of air-filled volumes or calculation of spectral fluences, electronic, nuclear buildup, and stopping power. The benchmarking of the PENH and PHITS codes by simulating the integrated depth dose curves is reported in Ref. [14].

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