Monte Carlo Study of Nuclear Fragmentation in Water Irradiated with Protons and $^{12}$C Ions for Particle Therapy Applications

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Abstract. In this study, the nuclear fragmentation of the secondary particles produced when water is irradiated with protons and carbons were investigated. Proton beams with varying incident energies of 100 MeV, 130 MeV, 150 MeV and 160 MeV were used with corresponding $^{12}$C ion beams of about 187.50 MeV/u, 241.67 MeV/u, 285.42 MeV/u and 308.33 MeV/u respectively. The kinetic energy distribution and energy deposition of primary and secondary particles were studied via Monte Carlo simulation with the aid of GATE v.8.0 via GEANT4 simulation toolkit version 10.3.2 with $1 \times 10^6$ incident beams. The physics list used was QGSP_BIC (Quark Gluon String Pre-compound Binary Cascade). When the primary $^{12}$C ion and proton beams interact with water, secondary light-charged and heavy-charged particles are produced with atomic number $Z > 2$. In general, it was shown that the incident $^{12}$C ions are less scattered as they traverse matter compared to the incident protons. Thus, the energy deposition of $^{12}$C ions is well-defined and is better in terms of conformation.

1. Introduction
Nowadays, there are two major modalities used in radiotherapy, namely light-ions (conventional radiotherapy) which utilize photons and electrons and heavy-ions (hadron therapy) such as protons, carbons and oxygen. The major physical advantage of heavy-charged particles over light-ions is their unique characteristic, i.e. depth-dose profile known as the Bragg curve or Bragg peak, a feature that allows high dose deposition to a locally restricted volume (Fig. 1(a)). Their physical depth-dose distribution in tissue is characterized by a small entrance dose, sharp increase of dose in a well-defined depth and the rapid dose fall-off beyond the maximum dose deposition at the distal edge. The well-defined range and small lateral beam spread make it possible to deliver the dose up to millimeter precision [1-2].
Protons and $^{12}$C ions slow down and deposit energy along their tracks within the material and this mechanism determines the distribution of absorbed dose. During the slowing down process, excitation and ionization of the atoms of the material take place. The Bragg peak is a consequence of the interaction mechanism of the particles as described by the Bethe-Bloch formula, which describes the rate of energy loss of the incident particle, which shows a $1/\beta^2$ dependence of the specific energy loss, where $\beta^2$ is the atomic transitions correction. The interaction of the projectiles or ions with the absorbing medium is governed by the elastic and inelastic collisions with the atomic electrons with the absorber material.

![Figure 1. (a) Normalized depth-dose profiles of proton and $^{12}$C ion beams at varying incident energies. (b) Number of secondary particles versus depth of deposition. The position of the Bragg peak is found at 154.29 mm when water is irradiated with 285.42 MeV/u $^{12}$C ion beams.](image)

Particles penetrating or traversing matter do not just loose energy through inelastic collisions with the target electrons, they might be involved in nuclear reactions and undergo nuclear fragmentation. At energies of several hundred MeV/u which are required for applications of heavy-ion beams in deep-seated tumor treatments, the radiation field is significantly affected by nuclear fragmentation processes with increasing penetration depths [3]. Nuclear fragments contribute to the dose deposition and are responsible for the dose tail observed after the distal edge of the Bragg peak [4-5]. Because of geometrical reasons, the most frequent nuclear interactions are peripheral collisions where the particles may lose one or several nucleons. A nuclear interaction model known as the abrasion-ablation model uses this idealization with two-step processes [6]. Projectile and target nucleons which overlap in the collision process are called participants while the remaining parts of the projectile and the target nucleus are called spectators. In the first step of peripheral collisions, the incident beam particle may lose one or several nucleons along the penetration depth and the nucleons in the overlapping zone of the target nuclei are abraded, resulting in the formation of a hot zone or fireball. Here, the outer nucleons or spectators are slightly affected. In the next step, the fireball breaks into single nucleons and small complex and the spectator evaporates nucleons until the excitation energy falls below the binding energy. The produced projectile-fragments continue traveling with nearly the same velocity and direction which contribute to the dose deposition until they are completely slowed down. Nuclear fragmentation reactions lead to the attenuation of the primary beam flux and a build-up of lower-Z fragments with increasing penetration depth. As the range of the particles at same velocity scales with $A/Z^2$, the depth-dose profile of heavy-ion beams shows a characteristic fragment tail beyond the Bragg peak [2-3].

2. Materials and Methods
In this study, the nuclear fragmentation of the secondary particles produced when water is irradiated with protons and $^{12}$C ions at varying incident energies were investigated using the open source software GEANT4 version 10.3.2 via GATE v.8.0. Proton beams with varying incident energies of 100 MeV, 130 MeV, 150 MeV and 160 MeV were used with corresponding $^{12}$C ion beam’s energy of about 187.50 MeV/u, 241.67 MeV/u, 285.42 MeV/u and 308.33 MeV/u. In addition, the kinetic energy distribution and energy deposition of primary and secondary particles were studied.
2.1. *GATE and GEANT4 Simulation Toolkit*

GATE (GEANT4 Application for Tomography Emission) is an open source Monte Carlo simulation application enabling the modeling of emission tomography, transmission tomography and radiation tomography. GATE is based on the GEANT4 tool package. GEANT4 (Geometry And Tracking) is an object oriented toolkit for the simulation of particle interactions with matter and provides advanced functionality for all domains typical of detector simulation: geometry and material modeling, description of particle properties, physical processes, tracking, event and run management, detector response modeling, user interface and visualization. Its advanced geometry modeling capabilities to describe materials provide powerful tools for the representation of the human body and its wide physics coverage allows accurate studies of the radiation effects in anthropomorphic phantoms over an extended energy range. The physics processes offered cover a comprehensive range, including electromagnetic, hadronic and optical processes, a large set of long-lived particles, materials and elements, over a wide energy range starting, in some cases, from 250 eV and extending in others to the TeV energy range [7-9].

2.2. *Simulation setup*

The monoenergetic pencil beam source is placed 11 cm away from the target which is a water phantom and is directed towards the $+x$ axis. The dimensions of the water phantom are 20 cm $\times$ 20 cm $\times$ 20 cm. The physics list Quark Gluon String Pre-compound Binary Cascade (QGSP_BIC) is utilized. A $1 \times 10^6$ events or primaries were simulated in order to obtain an adequate statistics. The secondary particles produced by the interaction of the $^{12}$C ions and protons with the water phantom are recorded via the PhaseSpace Actor. The results of the simulations (i.e. kinetic energy and the energy deposition) are recorded in ROOT files and analysis were done using ROOT data analysis.

3. *Results and Discussion*

3.1. *Contributions of Secondary Fragments*

Some of the secondary fragments that were produced are electron, proton, gamma, alpha, hydrogen fragments (deuteron and triton) as well as fragments with atomic number $Z > 2$ such as secondary carbons ($^{11}$C, $^{10}$C, $^{13}$C), lithium, beryllium, boron, nitrogen and oxygen ions, etc. The energy deposition contributions deriving from incident $^{12}$C ions and proton beams of both primary and secondary fragments are shown in Fig. 2 – Fig. 5. These nuclear fragments contribute to the dose deposition and are observed after the distal edge of the Bragg peak specifically for $^{12}$C ions as shown in Fig. 2(c), Fig. 3(c) and Fig. 5. No fragments can be observed beyond the distal edge of the Bragg peak for proton beams (see Fig. 2(d), Fig. 3(d) and Fig. 5). These secondary particles caused the dose tail which is deposited via ionization process caused by fragments of nuclear matter and neutrons.

It can be observed also that the lower-Z fragments like hydrogen, helium (He) and lithium (Li) have longer ranges than the primary particles. While the heavy ion beams have characteristic fragment tail beyond the Bragg peak region.

3.2. *Kinetic Energy Distribution and Energy Deposition of Primary and Secondary Fragments*

Because the energy loss is inversely proportional to the square of the velocity of the particle, this means that upon entering the target material, which in this case water, the incident particles both protons and $^{12}$C ions have maximum energy and therefore have maximum velocity. As these particles traverse matter and interact with the atomic electrons, they lose energy and decrease with their velocity. As a result, these particles deposit more and more dose as they slow down until they reach their range and deposit the maximum dose at this depth. It is evident that heavy ions penetrate matter at very high speed and hence leave a very small portion of its energy at shallower depths. Consequently, the dose deposited near the surface of the target is relatively low.
Figure 2. 2D histograms of the kinetic energy distribution of (a) primary $^{12}$C ion beams at 187.50 MeV/u, (b) of primary proton beams at 100 MeV, (c) of secondary particles of $^{12}$C ion beams at 187.50 MeV/u and (d) of secondary particles in water phantom irradiated with proton beams at 100 MeV.

Figure 3. 2D histograms of the energy deposits of (a) primary $^{12}$C ion beams at 285.42 MeV/u, (b) of primary proton beams at 100 MeV, (c) of secondary particles of $^{12}$C ion beams at 285.42 MeV/u and (d) of secondary particles in water phantom irradiated with proton beams at 100 MeV.
Figure 4. 2D histograms of the energy deposits of the secondary fragments when water is irradiated with 285.42 MeV/u $^{12}$C ion beams.

Figure 5. 2D histograms of the energy deposits of the secondary fragments when water is irradiated with 150MeV proton beams.

In summary, as shown in Fig. 2 to Fig. 5, secondary light-charged particles and heavy-charged particles with $Z > 2$ are produced when the primary $^{12}$C ion and proton beams interact with water. In addition, it can be observed that the lighter ions undergo greater lateral scattering and therefore deposit more energy out of the primary radiation field, while the heavier nuclear fragments contribute more
substantially to the energy deposition at the distal edge of the Bragg peak. The fragment tail clearly is indicative that the largest fraction of fragmentation reactions results in a smaller number of nucleons from either the target being ejected in ablation-abrasion reactions [10-12].

4. Conclusion
In general, it was shown that the incident $^{12}$C ions are less scattered as they traverse matter compared to the incident protons. As a result, the energy deposition of incident carbon ions is well-defined and is better in terms of conformation. However, due to the huge amount of scattered secondary particles, the energy deposition using incident carbon ions exhibit fragment tail, i.e. dose tail in the depth-dose profile of carbon ions. Therefore, in order to have an accurate dose calculations, nuclear fragmentation of secondary particles are to be taken into consideration for organs at risks may be located in this region.

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