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ARTICLE

Validation of New Geant4 Electromagnetic Physics Models for Ion Therapy Applications

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We have developed simulation codes to handle electromagnetic process in Geant4 in an attempt to improve the accuracy of dose calculations for ion radiotherapy. Geant4 is a Monte Carlo simulation toolkit for simulating the passage of particles through matter, and capable of handling all physics processes including electromagnetic, hadronic and nucleus-nucleus interactions which are indispensable to calculate three-dimensional dose distributions in ion therapy. In this work we report the recent progress for Geant4 models for ions and new validation results, which were obtained for depth-dose distributions of carbon ions incident on water against experimental measurements. We found simulations to reproduce the experimental data fairly well.

KEYWORDS: Monte Carlo simulation, Geant4, carbon ion radiotherapy

I. Introduction

Ion therapy using several 100 MeV/u carbon beams[1,2)] is currently performed at several facilities in the world because of their therapeutic advantages over conventional photon or proton beams. Radiotherapy with beams of heavy ions provides highly localized dose distributions at the end of the range (called Bragg peak). On the other hand, the projectile fragmentation products cause an undesired dose beyond the Bragg peak. Also, fragmentation reactions increase the complexity of ion beam transport modeling and dosimetric calculations.

The Monte Carlo method (MC) is known as the most accurate three-dimensional dose calculation algorithm, in particular for a heterogeneous radiation field. MC is also useful to obtain a quantitative characterization of complicated radiation fields produced as a result of nuclear fragmentation. This information is very important for ion therapy to precisely evaluate relative biological effectiveness.

Geant4[3,4)] is a Monte Carlo simulation toolkit for simulating the passage of particles through matter emerging from the high-energy physics community. It is capable of handling all physics processes including electromagnetic, hadronic and nucleus-nucleus interactions, which are indispensable to calculate three-dimensional dose distributions in ion therapy.

In recent years, new developments[5,6)] were carried out respectively addressing Geant4 electromagnetic (EM) physics models and software infrastructure. Major updates of software for ion transport[7)] are aimed to improve models for energy loss which is the most important factor to determine depth-dose distribution as follows. First of all, numerical tables of stopping powers as a function of energy for all ion-material combinations available in the ICRU 73[8,9)] report are built in Geant4. A spline algorithm for interpolation was introduced to handle EM data: stopping powers, ranges and cross sections, which are essential for ion Bragg peak simulation. Also, a new energy loss fluctuation model was introduced for ions and nuclear stopping model was implemented as a separate Geant4 process (before it was coupled with the ionisation energy loss process).

In summary, these developments allow to obtain precise results for the transport of therapeutic ion beams, which are stable against simulation step length and delta-ray production threshold. These new functions, optimized parameters and a proper choice of physics models are provided with the Geant4 version 9.3.

In this paper, we report validation results demonstrating accuracy and stability of depth-dose distributions against cut values and the verification of depth-dose distributions measured in beams used for patient treatment. We use previously published data,[10)] as well as new data for the dose distribu-

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tion of a 320 MeV/u carbon beam measured at Hyogo Ion Beam Medical Center[11] (HIBMC).

II. Material and Methods

1. Physics Models for Ions in Geant4

In version 9.3 of Geant4, models simulating the energy loss and its fluctuation are implemented in the C++ class *G4hIonisation* for protons, deuterons and tritons, and in the class *G4ionIonisation* for all other ions. By default, stopping power models[12] of the Geant4 'Standard EM Package' are used. For ions below 2 MeV/u, the Helium ion parameterization from the ICRU 49 report[13] is employed. Above 2 MeV/u, the restricted energy loss rate of ions is calculated by using the Bethe-Bloch formula including Barkas, Bloch and Mott corrections. A correction term is applied to enable a smooth transition between these two models. In Geant4 9.3, the mean ionisation potential of liquid water is set to I = 78 eV according to revised version of ICRU 73[9].

A new energy loss model[7] for ions heavier than Helium, *G4IonParametrisedLossModel*, and corresponding software to handle material data were implemented with focus on Geant4-based ion therapy applications. In the energy range from 25 keV/u to 1 GeV/u, the model uses ICRU 73 stopping powers,[8,9] which covers a variety of combinations of different ion species (Z = 3-18, 26) and absorbers (25 elemental materials and 31 compounds). The energy loss of other ions is determined by means of a scaling method. For compounds not covered by the ICRU 73 report, Bragg's additively rule is applied, i.e. stopping powers are calculated as the weighted sum of individual stopping powers of target components. For atomic targets not included in ICRU 73 tables the standard parameterization from the ICRU 49 report is used. For interpolation of all data the cubic spline interpolation is applied. Delta-electron production above the production threshold is simulated using the standard algorithm.[7]

Energy loss fluctuation of ions is simulated by means of the new *G4IonFluctuations* model using a combined approach. The standard Geant4 model of fluctuations,[14] which samples Vavilov fluctuations, is used for energies $E/u > Z_1 * 10$MeV, where Z_1 is the projectile ion charge. Below this limit Yang's empirical formula[15] is used, which takes into account Bohr's formula[16] and additional fluctuation due to electron exchange between an ion and media. The delta-ray production threshold is taken into account in the model at all energies.

Multiple Coulomb scattering is simulated by using model from Urban;[17] in Geant4 9.3, *G4UrbanMscModel90* is applied for ions.

Two models for simulating inelastic nucleus-nucleus reaction are available in Geant4. The first one is the Binary cascade model,[18] *G4BinaryLightIonReaction* and second is more recent model[19] *G4QMDReaction* based on theory of quantum molecular dynamics.[20] The de-excitation of excited residual nuclei, which are created in the pre-equilibrium stage of the reaction, can be handled by various models[21] including Fermi break-up, generalized evaporation model (GEM) and *G4Evapolation*.

Various formulae of inelastic reaction cross-sections are available. In this study, *G4TripathiCrossSection* and *G4TripathiLightCrossSection* are used for light ions. In these classes parameterisations described by Tripathi *et al.*[22,23] are implemented. They are recommended to be used for ion therapy applications in the current version of Geant4.

The decay of radioactive nuclei resulting from the inelastic nuclear reactions was also simulated.

2. Experimental Depth-Dose Distribution

Geant4-based depth-dose distributions are validated for 290, 320 and 400 MeV/u ^{12}C beams in water. For 290 and 400 MeV/u, previously published data are adopted, which were measured at HIMAC of National Institute of Radiological Sciences (NIRS) in Japan. For 320 MeV/u, new data measured at HIBMC are used for analysis. These two beam-lines are equipped for broad beam irradiation for carbon ion radiotherapy.

They have a pair of dipole magnets (wobbler magnets) to provide radiation over a circular area. A scatterer made of Lead or Tantalum is placed behind the magnets to broaden the beam and to produce a uniform circular dose distribution at the treatment position. These beam lines are equipped with ionisation chambers for monitoring the intensity and profile of the beams.

A water tank is placed at the beam line behind the monitors. The isocenter is in the middle of the water tank, the distance of the water surface to the isocenter was slightly different for HIMAC and HIBMC, it is taken into account in MC geometry. A ridge filter to form spread-out Bragg peak, a range compensator and a collimator can be installed on the beam line, but they are removed from the beam line and a multi-leaf collimator is fully opened when the depth-dose distributions were measured. A detailed description of the beam–line at HIMAC can be found in Reference 10.

The dose absorbed in water was measured by parallel-plate ionisation chambers. The dose distribution along the depth in the water was obtained by sliding the chambers along the beam direction.

3. Geometry and Scoring

This implementation used the class library developed for Geant4 in previous work.[24,25] To obtain depth-dose distributions in water tanks, water was equally sliced along the beam axis and energy deposition of each slice was scored. The slice thickness was set to 0.1 mm. Thus, simulation steps for ions and secondary electrons were forced to be smaller.

III. Results and Discussion

We evaluate the performance of Bragg peak simulations using Geant4 version 9.3 patch-01.

1. Stability against Range Cut

First, we examine the stability of results against Geant4 cut in range with a simple geometry, i.e. only a water phantom is put in the vacuum. The Geant4 cut in range approach[3] allows one to define the spatial precision of the simulation by setting a single parameter according to re-

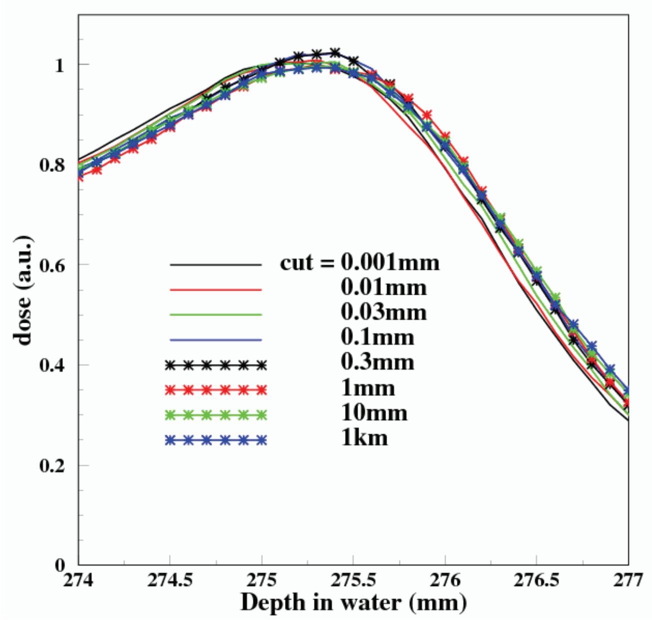

Fig. 1 Zoomed simulated depth-dose curves for various range cuts

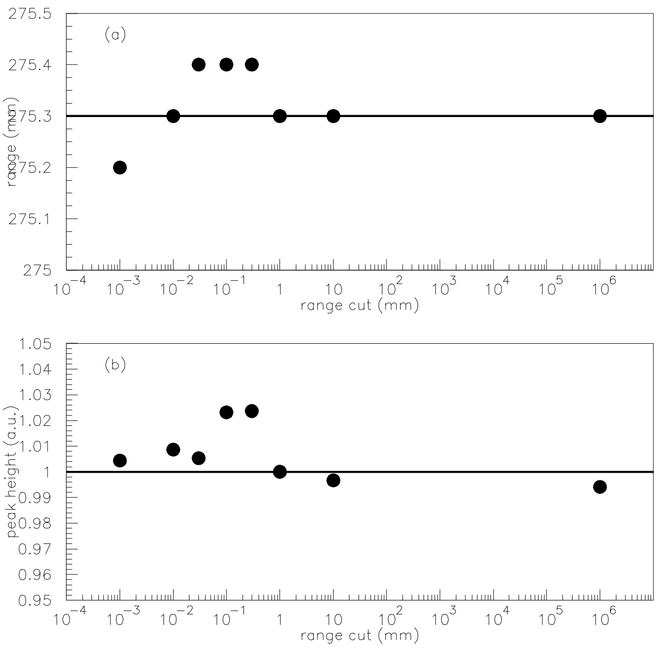

Fig. 2 Stability of simulation versus range cut for (a) range; (b) peak heights (unit for cut = 1 mm)

quirements imposed by a concrete application. At the initialization time of Geant4, the cut in range is converted into production thresholds for delta-electrons and bremsstrahlung photons. Ion therapy application is a very sensitive test of stability against depth-dose profile, because the Bragg peak of ions is very narrow.

For the simulation a standard set of Geant4 processes was used. Electromagnetic physics processes were activated using the Option3 physics constructor[26] which includes the new model[7] of ion ionisation based on ICRU73 data. The Binary cascade model was used to simulate inelastic nuclear reactions of ions, protons and neutrons. The initial beam energy spread was assumed to be zero. We simulated the Bragg peak of 400 MeV/u carbon beam in water with various cut in range values from 0.001 mm to 1 km.

In **Fig. 1** simulated Bragg curves and in **Fig. 2** range and deviation in peak height are shown as functions of range cuts for electrons, positrons and photons. Deviation in peak position is within ± 0.1 mm (0.04%) and in peak height within +2.4% and - 0.6% against default range cut of 1 mm. This stability is achieved mainly because of an introduction of a spline algorithm for interpolation.

2. Bragg Peak in Water

Secondly, we compared measured and simulated Bragg peak in water. We pay particular attention to the ion range. The parameterized energy loss model was used to simulate electronic energy loss. The QMD model with the standard de-excitation module of Geant4 for the de-excitation of excited residual nuclei was used to simulate inelastic nuclear reaction of ions. The Binary cascade model was used to simulate inelastic reactions of protons and neutrons. Other electronic processes were identical to those applied in section III-1. The measured dose profiles considered in this study are associated with a Gaussian energy spectrum, with a standard deviation of approximately 0.07% slightly decreasing with beam energy.

Figure 3 shows simulated depth-dose distributions along with experimental measurements. We normalized the simulation results such that they coincide with the measurement at the phantom entrance. We have not applied any correction such as scaling or shifting in the horizontal axis in order to be able to compare the absolute range.

As a whole, we found very good agreement between measurements and MC in range (**Fig. 4**). Maximum deviation of 1.2 mm (0.5%) is found at 400 MeV/u. The satisfactory agreement of Geant4 simulations with experimental values confirms the accuracy of energy loss algorithms invoked at each particle step in the simulation, and also demonstrates the precision of the cubic spline interpolation algorithm. In addition, good agreement between measurements and MC is also found in the dose distributions beyond the Bragg peak. This means that the dose coming from fragmentation products are precisely simulated by using the QMD model.

On the other hand, the MC simulations overestimate the peak/plateau ratio by up to 20%. Possible experimental reasons of this are underestimation of the initial energy spread, heterogeneity of the effective thickness of materials installed in the beam line, for example, scatterer and electrode in the monitors, and some systematic uncertainty due to the ionisation chamber measurements. For practical applications, these factors should be considered carefully. However, MC simulations may be also responsible for the discrepancies. The sensitive components of Geant4 simulation are energy dependence of stopping power in water and air, model of fluctuations of energy loss of ions, and model of ion nuclear fragmentation. The method of normalization chosen for this work maximally emphasizes the difference in the peak/plateau ratio. Because ridge filters and range compen-

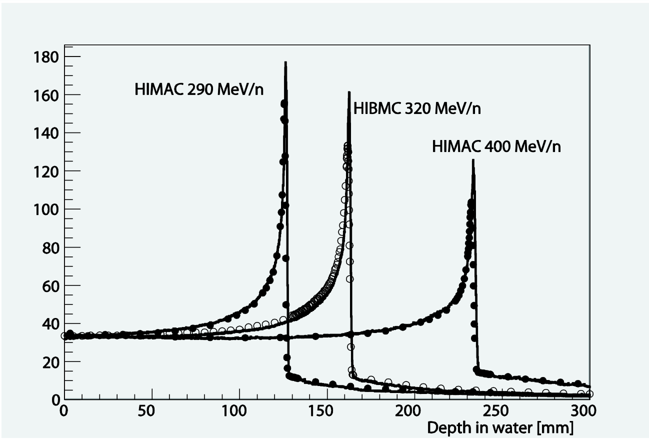

Fig. 3 Simulated depth-dose curves along with published data[10] for HIMAC 290 and 400 MeV/u and new data for HIBMC beam 320 MeV/u

sators are used for practical applications, the observed difference significantly reduces.

IV. Conclusion

We have developed simulation codes to handle electromagnetic processes in Geant4 in an attempt to improve the accuracy of dose calculations for radiotherapy using ions. Recent major developments are aimed to improve the stability against range cut or simulation steps and the models for energy loss which is the most important factor to determine range. We validated simulated depth-dose distributions of therapeutic carbon ions incident on water against published and new experimental results performed at practical broad beam irradiation systems for carbon ion radiotherapy. We found the simulation to be well stabilized against range cut and able to reproduce the measured ranges fairly well.

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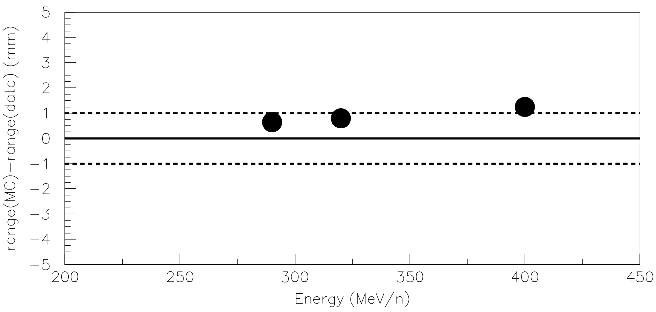

Fig. 4 Differences between simulated ranges and measurements

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