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Low-energy electron dose-point kernels and radial dose distributions around gold nanoparticles: Comparison between MCNP6.1, PENELOPE2014 and Geant4-DNA

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ABSTRACT

With emerging interests in subcellular and nano-scale energy deposition of low-energy electrons, new cross-sectional models for the low-energy electron transport have been integrated into recent releases of Monte Carlo (MC) codes. MCNP6.1 has been released which included extended cross-sections for low-energy electron interactions based on the Evaluated Electron Data Library (EEDL). Moreover, a single-event electron transport method was introduced down to 10 eV. In this study, MCNP6.1 has been benchmarked against early versions of PENELOPE2014 and Geant4-DNA by comparing dose-point kernels (DPKs) of electrons of 100 eV, 1 keV and 10 keV. In addition, radial dose distributions around a 2 or 15 nm-diameter gold nanoparticle (GNP) irradiated by 50 kVp X-rays were calculated for comparison. For all electron energies, the DPKs calculated by MCNP6.1 reached the maximum values at shorter distances and then were decreased more rapidly than those calculated by the other codes. Radial doses within 2 nm from the surface of the GNPs calculated by MCNP6.1 were 1.04 – 1.89 times and 1.13 – 1.58 times higher than those calculated by Geant4-DNA and PENELOPE2014, respectively. These differences would stem from the fact that inelastic cross-sections of MCNP6.1 for low-energy electrons are higher than those of the other codes. At this moment, it is difficult to judge which of the codes is more accurate for nano-scale dose calculations than the others. Depending on the geometrical configuration of the electron source (herein GNPs) and the target (e.g., DNA), the difference in the interaction data for low-energy electron transport, especially below 10 keV, would result in significant differences in calculation of radio-biological effects on the target. It can be concluded that one should pay attention to the interaction data as well as the transport parameters used for MC low-energy radiation transport in a nano- and micro-scale.

1. Introduction

Gold nanoparticles (GNPs) have been emerging as a radiosensitization agent over the last decade [1]. It has been demonstrated that a production of low-energy electrons from GNPs and their local energy-deposition in a subcellular or DNA level could induce the radiosensitization effect [1–4]. Accordingly, there has been a high demand for low-energy electron microdosimetry. Due to the experimental difficulties to measure low-energy electron doses in a nano- or micrometer-scale, several Monte Carlo (MC) codes offer cross-sectional models to describe a step-by-step low-energy electron transport down to a few tens eV [2,4–6]. In particular, a dose-point kernel (DPK) has been used to evaluate the accuracy of MC codes and to assess the differences among them [2,4,7]. Comparison of electron DPKs using different MC codes such as Geant4-DNA, EGSnrc, PENELOPE, CPA100, FLUKA, ETRAN and MCNPX has been reported [2,4,7]. On the other hand, Geant4-DNA and PENLEOPE have been often used to calculate nano-scale radial dose distributions around GNPs [3,8–11].

Previous versions of MCNP such as MCNPX and MCNP5 use the condensed history algorithm or the ITS (Integrated Tiger Series) algorithm for electron transport down to 1 keV [2,12,13]. Therefore, these MCNP codes are of limited use in the nano- or micrometer-scale transport. Recently, MCNP6.1 has been released with an inclusion of extended cross-sections for low-energy electrons and photons down to 10 eV and 1 eV, respectively [12,13]. Furthermore, a single-event electron transport method has been developed in this new version

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which provides a more accurate approach to low-energy electron interactions [12,13]. In order to use MCNP6.1 to calculate doses on the nano- or micrometer-scale, a comparative study of low-energy electron transport of aforementioned codes is necessary. The purpose of this paper is to benchmark MCNP6.1 for low-energy electron interactions in liquid water through the comparison of electron DPKs with PENELOPE2014 and Geant4-DNA. Furthermore, nano-scale radial dose distributions around GNPs irradiated by a polychromatic X-ray were also calculated for a comparison with the two MC codes.

2. Materials and methods

2.1. Monte Carlo codes

In the following sections, MCNP6.1 and the two codes used in the benchmarking are briefly described.

2.1.1. MCNP6.1

The new physics library of MCNP6.1, eprdata12, is based on the Evaluated Nuclear Data File/B-VI.8 (ENDF/B-VI.8) [13]. It includes photon cross-section data for coherent and incoherent scattering, and photoelectric absorption down to 1 eV [13]. In addition, it has subshell photoelectric cross-sections based on the Evaluated Photon Data Library 97 (EPDL97) and enhanced atomic relaxation data based on the Evaluated Atomic Data Library (EADL) [13–15]. The low-energy atomic relaxation of gold was validated by our previous work [16]. For the electron transport, tabulations of cross-sections based on the Evaluated Electron Data Library (EEDL) for electro-atomic transport processes which include atomic excitation, electron elastic scattering, subshell electro-ionization, and bremsstrahlung, are given for energies down to 10 eV [13,17]. In order to use these data for the low-energy electron transport, a new single-event method has been developed to replace the condensed history method [13].

2.1.2. PENELOPE2014

PENELOPE2014 (PENetration and Energy Loss Of Positrons and Electrons) performs MC simulations of coupled electron/photon transport. PENELOPE2014 can simulate event-by-event electron transport down to 50 eV, corresponding to ranges of 2–4 nm in water [7]. Elastic scattering cross-sections for electrons are derived from ELSEPA, which is the FORTRAN 77 code system for performing Dirac partial-wave calculation of elastic scattering of electrons and positrons [7,18]. Inelastic collisions are modeled by using the generalized oscillator strength (GOS) model [7,18]. Bremsstrahlung events are based on energy-loss cross-sections from Berger and Seltzer [7,18,19].

2.1.3. Geant4-DNA

Geant4-DNA is a general purpose Geant4 Monte Carlo simulation toolkit, which simulates track structures of electrons, hydrogen and helium atoms as well as C^{6+}, N^{7+}, O^{8+}, and Fe^{26+} ions in liquid water [4,6]. Cross-section models allow the transport of electrons down to about 10 eV. Ionization, electronic excitation, vibrational excitation, dissociative electron attachment and elastic scattering processes are taken into account. The elastic scattering model uses a partial wave approximation for “default” models while one can alternatively choose analytic forms of cross-section with Uehara’s screening parameters for “option 4” models [4]. The “default” ionization and excitation model in Geant4-DNA is based on the first Born approximation using optical data with semi-empirical corrections for low energies described by Emfietzoglou and Nikjoo [4,20]. Compared with the “default” models, the “option 4” used an improved optical data model and several revised corrections [4,20]. These improvements increase the excitation cross-section, while they decrease the ionization cross-section [4,20].

2.2. Simulations

In this work, MC simulations were conducted using the three codes mentioned above for the same source/geometry configuration. In the following sections, the geometry, source, and parameters adopted in the MC codes are described.

2.2.1. DPK generations

The dose-point kernels (DPKs) for monoenergetic electrons of 100 eV, 1 keV, and 10 keV were calculated by simulating 1×10^6 histories in liquid water. The electrons were isotropically emitted from a point source placed at the center of a water sphere. Energy depositions were scored in spherical shells centered on the source. For 100 eV and 1 keV electrons, the radius of the innermost sphere and the thickness of the outer spherical shells were both 1 nm while for 10 keV electrons, they were 100 nm. The DPKs in this study were given in units of deposited energy per distance as described in the literature [4]. The cutoff-energy was set to 50 eV for all codes. The electrons below this cutoff-energy locally deposit all their remaining kinetic energies. The relative difference in DPKs, $\Delta(r)$ in %, between Geant4-DNA “option 4” as a reference and another Monte Carlo code, Y, at a distance r was derived from Eq. (1) [4], where $\delta E_Y(r)$ and $\delta E_{Geant4-DNA\,option4}(r)$ represent the energy deposition in a shell at a distance r from the source, acquired by a code, Y and Geant4-DNA “option 4” , respectively. The denominator represents the maximum value of the energy depositions calculated by the two codes.

$$\Delta(r) = \frac{|\delta E_Y(r) - \delta E_{Geant4-DNA\,option4}(r)|}{\max(\delta E_{Geant4-DNA\,option4}; \delta E_Y)} \times 100 \quad (1)$$

2.2.2. Radial dose distribution around GNP

The radial dose distributions around a GNP (2 or 15 nm diameter) irradiated by 50 kVp polychromatic X-rays were calculated in a nano-scale (see Fig. 1) [21]. With 1×10^9 photon histories for each

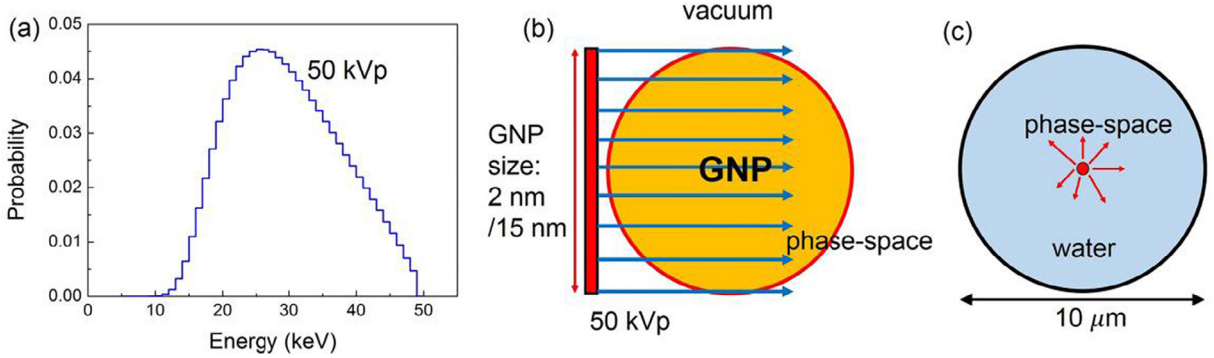

Fig. 1. (a) Energy spectrum of incident 50 kVp X-rays. (b) The phase-space file of secondary electrons was recorded on the surface of GNP (2 or 15 nm diameter). (c) The phase-space file was used as a source in the center of a 10-μm-diameter water sphere.