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A comparison of DNA damages in an E. Coli bacterium induced by low-energy X-ray and electron beam, using Geant4-DNA

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Abstract

Irradiation of food by ionizing radiations is one of the best ways to eliminate pathogenic microorganisms that are mostly present on the surface of the food. Therefore, choosing the right type and energy for surface irradiation of food is of great importance. In this study, a Monte Carlo simulation was performed using Geant4 toolkit to compare the DNA damage yields induced by low-energy electron beams and X-rays in a simplified model of Escherichia coli bacterium. Several initial energies were considered for electrons and X-rays. The results indicated that low-energy electrons caused more damage to the DNA than low-energy X-rays. Therefore, electrons are more effective radiation for the disinfection of microorganisms, specially for surface decontamination.

Keywords: Food irradiation, Escherichia coli, DNA damage, Monte Carlo, Geant4

Introduction

Escherichia coli O157:H7 (E.coli) is a well-known microorganism which can contaminate our food and fruits. Several processing techniques including irradiation (with ionizing and non-ionizing radiations), thermal methods hot air, hot water, and steam), and using chemical agents have used for microorganism elimination on the foods' surface [1,2]. Using ionizing radiation is an effective way to eliminate pathogenic microorganisms and to improve food safety. Several experimental studies investigate the possibility of E. Coli inactivation in foods and fruits, by gamma rays [3], low-energy x-rays [4], and electron beams [5]. Low-energy X-ray and electrons are more interesting than high-energy gamma irradiation for surface decontamination, due to the need for less shielding and the economic benefits. All these experimental studies were limited in the type and the energy of the radiation source. Due to the limitations of laboratory facilities, the simulation method can be used as a good alternative to study and compare different irradiation conditions. In this study, the yield of DNA damages in terms of single strand breaks (SSBs), double strand breaks (DSB), and cluster damage sites (CDS), induced by low energy X-rays and electron beams were obtained using Geant4 Monte Carlo toolkit [6].

Materials and Methods

The Geant4-DNA [7], the extension of Geant4 Monte Carlo toolkit (version 10.7), was used to simulate the interactions of primary and secondary particles in water. This is an appropriate tool to model biological damage induced by ionizing radiation at the scale of the DNA structure. The default DNA physics-list class, “G4EmDNAPhysics_option2”, which is recommended for cellular and sub-cellular scale simulations was implemented in this simulation [7]. It includes several physics models that cover interactions needed for particle transport in a water medium. A simplified E.Coli bacterial cell was simulated as an ellipsoid volume of water with a long axis of 3 µm and two short axes of 2 µm (See Figure 1). The E.coli genome length is about 4.6 mega base pairs (Mbps) [8]. Therefore, 21436 linear DNA segments with a length of 216 bp (73.44 nm), were randomly distributed in the ellipsoid volume. Each DNA bp is represented as a simple cylinder with 0.5 nm in radius and 0.34 nm in length. For modeling sugar and phosphate of DNA, a quarter cylinder was simulated with inner and outer radius of 0.5 nm and 1.185 nm, respectively. Two quarter cylinders on opposite sides were rotated by 36 degrees on each subsequent bp to represent the helical shape of two DNA strands.

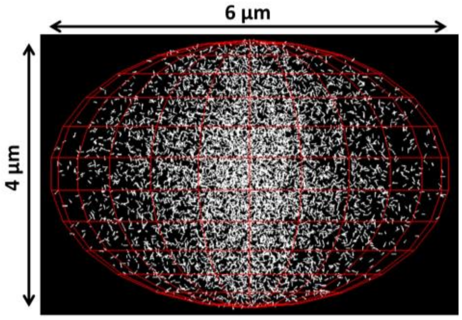

Figure 1. Geometrical model of E.coli bacterium in Geant4. Only 3000 DNA segments with a length of 216 bp are shown for a better visualization.

Mono-energetic electrons of 50 keV, 100 keV, and 150 keV and X-rays of 50 keV and 100 keV energy were determined as the radiation sources. These energies were obtained from literature [4-5, 9]. Primary particles were emitted from the inner surface of an ellipsoid of the same dimensions with the simulated E.coli geometry toward the center of the ellipsoid. The number of primary particles was 2×10^6 and 2.1×10^9 for electrons and photons, respectively. For measuring the DNA damage yields, the positions and the energy depositions of all particles were obtained in each DNA bp (sugar and phosphate backbone). Two thresholds for energy and distance were considered in this algorithm. If the energy deposited in a sugar or phosphate volume was larger 17.5 eV [10], one strand break is assumed to occur. It would be assigned as an SSB, provided that no other energy deposition greater than the 17.5 eV threshold occurs on the opposite strand at a distance less than 10 bp or 3.4 nm. Hence, if the distance of two subsequent SSBs in opposite strands was less than the distance threshold (10 bp) one DSB would be counted A CDS is refer to a region that contain both SSBs and DSBs in a length of 3.4 nm. According to Charlton et al. [9], any damage yield may be obtained by:

$$\text{(1)}\quad \text{Damage yield } (\text{Gy}^{-1}\text{Mbp}^{-1}) = N_{break}/(D\times N_{bp}),$$

in which N_{break} is the number of breaks, D is the total absorbed dose (Gy) to the bacterium, and N_{bp} (Mbp) is the total number of bps.

Results and discussion

The SSB, DSB and CDS yields normalized to the total dose deposited in the DNA molecules per total number of bps for electron beams are shown in Figure 1. The same yields for incident X-rays are shown in Figure 2.

The total number of DNA damage (SSB+DSB) per particle normalized to that of of 50 keV electron beam as well as the normalized deposited dose (Gy/particle) in the bacterium are tabulated in table 1, for electrons and X-rays of different energies.

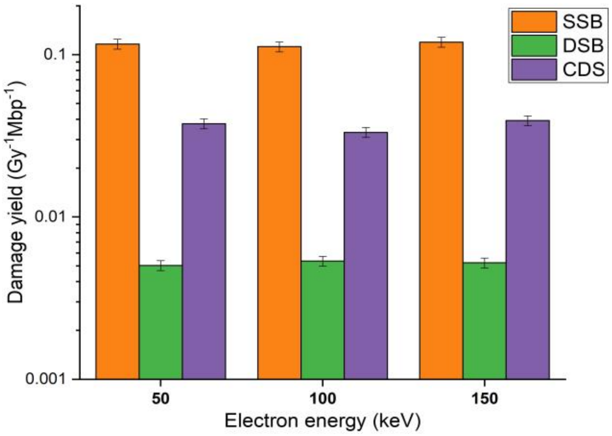

Figure 2. Normalized DNA Damage yields obtained by equation 1 for electrons of three different energies.

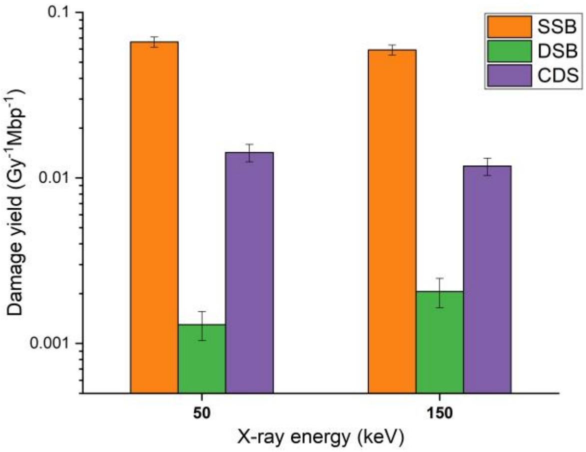

Figure 3. Normalized DNA Damage yields obtained by equation 1 for X-rays of two different energies.

Table 1. The total number of DNA damage normalized to the electrons of 50 keV, and the total deposited dose per particle in the bacterium.

Radiation	Energy (keV)	Deposited dose (Gy/particle)	Range in water	Normalized total damages (%)
Electron	50	9.02E-3	42.4 μm	100
Electron	100	5.45E-3	142 μm	58.4
Electron	150	4.15E-3	280 μm	47.3
X-ray	50	1.01E-6	4.41 cm	6.19E-3
X-ray	150	6.87E-7	6.65 cm	3.83E-3

As shown in Table 1, by increasing the initial energy of electron beam, the deposited dose per particle, and also the total number of damages per particle are decreasing. However, the normalized damage yields ($\text{Gy}^{-1}\text{Mbp}^{-1}$) induced by electrons of 50, 100, and 150 keV energy are nearly the same, according to Figure 1. The fact that the damage yields are almost constant with increasing energy of incident electrons, is consistent with the results of Lampe et al. [11]. Nevertheless, the discrepancy in yield values reaches up to 40%, quantitatively. It is because of the differences in the implemented physics-lists (Option 2 vs Option 4) as well as the geometrical modelling (simple randomize positioning vs fractal geometry using Hilbert curve). The same trend is observed for X-rays. The small increase in DSBs for 150 keV X-rays may be due to the statistical errors, because the probability of interations (i.e., the cross-sections) for photons are much less than those of electrons. As DSBs and CDSs are less reparable and thus more critical than SSBs, low-energy electrons are more effective radiation than X-rays for microorganism elimination. It can be infered by comparing Figures 1 and 2. For a depth of up to 280 μm, electron beams will be the radiation of choice due to their shorter range and greater deposited dose than X-rays, according to Table 1. Since this is a simulation study to compare different radiation fields, we ignore modelling of DNA repair mechanisms in this study.

Conclusions

In this simulation study, we showed the advantagous of electron beams over X-rays for surface decontamination of E.coli bacteria. There is no significant superiority in damage yield for various energies of electrons in the range of 50-150 keV, and therefore the choice of energy depends on the depth of the irradiated surface. In future, we will add some experimental evaluations.

Acknowledgments

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