

Dose Point Kernels and Cellular S-values of Radionuclides for Positron Emission Tomography using a Monte Carlo method

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***Keywords :** dose point kernel, s-value, positron emission tomography, Monte Carlo simulation

1. Introduction

Positron emission tomography (PET) is widely used for diagnostic imaging with various radionuclides having different physical decay characteristics. PET radionuclides exhibit differences in decay schemes, emission spectra, and particle energies, which determine the range of emitted particles and the spatial distribution of energy deposited in biological media. Consequently, even among radionuclides used for the same imaging modality, their absorbed-dose distributions may differ depending on their radionuclide-specific decay characteristics. Quantitative characterization of these differences is therefore important for understanding and comparing the dosimetric characteristics of PET radionuclides.

Dose point kernels (DPKs) provide information on the spatial distribution of absorbed dose around a radioactive source and can be used to characterize differences in energy deposition associated with the emission characteristics of individual radionuclides. However, the biological relevance of energy deposition at microscopic scales also depends on the dimensions of cellular structures and the spatial relationship between the radioactive source and the target region. Cellular S-values provide a means of evaluating absorbed dose to cellular targets while accounting for these geometric and source-target relationships. Therefore, the combined evaluation of DPKs and cellular S-values is useful for comparing radionuclide-specific energy deposition from its spatial distribution in a medium to absorbed dose at the cellular scale. In this study, DPKs and cellular S-values for various PET radionuclides were evaluated using Monte Carlo simulations to compare their radionuclide-specific dosimetric characteristics.

2. Materials and Methods

2.1 Overview

Both DPKs and cellular S-values were calculated based on Geant4 version 11.3.2, while the DPK was actually derived using TOPAS (TOOl for PArticle Simulation) [1,2] version 4.2.1, a wrapper of Geant4.

The physics constructors G4EmLivermorePhysics, G4RadioactiveDecayPhysics, and G4DecayPhysics, along with the corresponding modules in TOPAS, were used to account for the full decay spectra of the PET radionuclides, including positrons, Auger electrons, and internal conversion electrons, along with secondary particles. A total of one million decay events were simulated for each radionuclide (⁴⁴Sc, ⁶⁴Cu, ⁶⁸Ga, and ¹²⁴I). Tracking cut was set to 10 eV. Decay properties of each radionuclide are shown in Table I.

Table I: Properties of radionuclides used in this study.

	Half-life	$E_{\beta^+}^{\text{average}}$ (keV)	$I_{\beta^+}^{\text{average}}$ (%)
⁴⁴ Sc	3.97 h	632	94.3
⁶⁴ Cu	12.7 h	278	17.6
⁶⁸ Ga	67.8 min	830	88.9
¹²⁴ I	4.18 days	820	22.7

2.2 Dose Point Kernel

The DPK represents the radial distribution of energy imparted to a uniform medium by radiation emitted from a point-like radioactive source. In this study, the DPKs of PET radionuclides were obtained by scoring the deposited energy in concentric spherical shells within a water sphere surrounding the source. The resulting energy deposition was normalized to the number of simulated nuclear decays to enable comparison among radionuclides. The DPKs were calculated at 2 μm intervals up to a radial distance of 100 μm .

2.3 Cellular S-value

The cellular S-value was calculated as the energy imparted to a specified cellular target per nuclear decay occurring within a designated source compartment in Geant4-DNA [3–7]. The cellular S-value was calculated as the mean energy deposited in the target region per decay divided by the target mass:

$$(1) \quad S(T \leftarrow S) = \frac{1}{m_T N} \sum_{j=1}^N E_{dep,T}^{(j)}$$

where $E_{dep,T}^{(j)}$, is the energy deposited in the target region for the j -th simulated decay, m_T is the target mass, and N is the number of simulated decays.

Radionuclides were randomly distributed within the cytoplasm, which was defined as the source region, and S-values for the nucleus and cytoplasm were evaluated. A simplified cellular geometry was modeled using two concentric spheres, with radii of 10 μm for the cell and 5 μm for the nucleus. The region between the nuclear and cellular boundaries was defined as the cytoplasm.

3. Results

3.1 Dose Point Kernel

Fig. 1 shows the DPKs derived with one million decays for each radionuclide. As the distance increases, all radionuclides exhibit exponential decrease while ^{124}I shows a distinct change compared to other radionuclides. This could be attributed to multiple factors such as the ranges of positrons they emit, the numbers and energies of Auger and internal conversion electrons. Although not shown in this abstract, the relative uncertainties were below 10 % for all radionuclides.

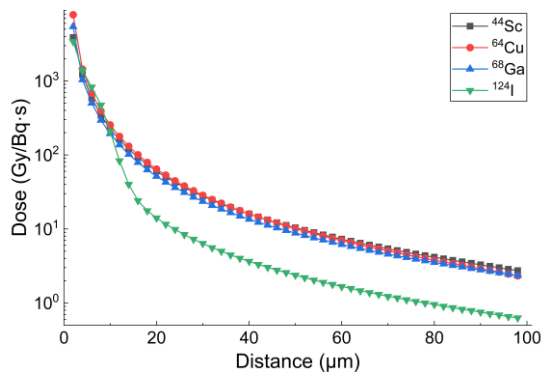


Fig. 1. Dose point kernels of each radionuclide with an interval of 2 μm up to 100 μm .

3.2 Cellular S-value

Table II shows the cellular S-values within the considered geometry. Since cytoplasm was the source, the S-values were higher for the cytoplasm than the nucleus. The differences between (Cy $\leftarrow$ Cy) and (N $\leftarrow$ Cy) were bigger for ^{64}Cu and ^{124}I . This could be attributed to aforementioned factors owing to the properties of decay from each radionuclide.

Table II: Cellular S-values for ^{44}Sc , ^{64}Cu , ^{68}Ga , and ^{124}I .

	S (N $\leftarrow$ Cy) (Gy / Bq.s)	S (Cy $\leftarrow$ Cy) (Gy / Bq.s)
^{44}Sc	4.64×10^{-5}	6.01×10^{-5}
^{64}Cu	5.76×10^{-5}	1.45×10^{-4}
^{68}Ga	4.21×10^{-5}	6.76×10^{-5}
^{124}I	5.68×10^{-5}	1.82×10^{-4}

4. Conclusion

The DPKs and cellular S-values of four PET radionuclides (^{44}Sc , ^{64}Cu , ^{68}Ga , and ^{124}I) were evaluated using Monte Carlo simulations to compare their radionuclide-specific dosimetric characteristics. The DPKs showed decreasing energy deposition with increasing distance from the source, with ^{124}I exhibiting a distinct spatial distribution compared with the other radionuclides. These differences may be associated with radionuclide-specific decay characteristics, including the ranges of emitted positrons and the numbers and energies of Auger and internal conversion electrons.

At the cellular scale, the S-values were higher for the cytoplasm than for the nucleus when the radionuclides were distributed within the cytoplasm. In particular, larger differences between (Cy $\leftarrow$ Cy) and (N $\leftarrow$ Cy) were observed for ^{64}Cu and ^{124}I , indicating that radionuclide-specific emission characteristics can lead to different absorbed-dose distributions within cellular compartments.

Overall, the DPK and cellular S-value results demonstrate radionuclide-dependent differences in energy deposition at both the medium and cellular scales. The combined evaluation of these quantities provides complementary information for comparing the microscopic dosimetric characteristics of PET radionuclides and highlights the importance of accounting for their individual decay characteristics.

REFERENCES

- [1] J. Perl, et al., TOPAS: an innovative proton Monte Carlo platform for research and clinical applications, Medical Physics, Vol. 39, No. 11, pp. 6818–6837, 2012.
- [2] B. Faddegon, et al., The TOPAS tool for particle simulation, a Monte Carlo simulation tool for physics, biology and clinical research, Physica Medica, Vol. 72, pp. 114–121, 2020.
- [3] S. Incerti, et al., The Geant4-DNA project, International Journal of Modeling, Simulation, and Scientific Computing, Vol. 01, No. 02, pp. 157–178, 2010.
- [4] S. Incerti, et al., Comparison of Geant4 very low energy cross section models with experimental data in water, Medical Physics, Vol. 37, No. 9, pp. 4692–4708, 2010.
- [5] M. A. Bernal, et al., Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit, Physica Medica, Vol. 31, No. 8, pp. 861–874, 2015.
- [6] S. Incerti, et al., Geant4-DNA example applications for track structure simulations in liquid water: A report from the Geant4-DNA Project, Medical Physics, Vol. 45, No. 8, pp. e722–e739, 2018.
- [7] H. N. Tran, et al., Review of chemical models and applications in Geant4-DNA: Report from the ESA BioRad III Project, Medical Physics, Vol. 51, No. 9, pp. 5873–5889, 2024.