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A Monte Carlo Evaluation of Gadolinium as a Neutron Capture Agent in Nanoparticle-aided Radiotherapy

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ABSTRACT

Gadolinium's large neutron capture cross section, damaging Auger cascade, and use in MRI imaging contrast agents make it an alternative to boron in neutron capture therapy. While macroscopic comparisons have been studied in the past, very little literature focuses on nano-scale properties which contribute to the emergent macro-scale effect. This study aims to compare quantities directly responsible for cell mortality between gadolinium neutron capture, boron neutron capture, as well as gold and gadolinium nanoparticle-aided photon therapies.

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INTRODUCTION

Nanoparticle-aided radiotherapy has seen a surge of interest in recent decades as a method of increasing local dose while using a lower intensity source of radiation [1]. Suitable materials will have high interaction cross sections (σ) relative to tissue and will ideally produce short-ranged, high-LET secondary radiation to contribute to cancer mortality.

Neutron Capture Therapy (NCT) [2] proposes materials with high neutron capture cross section. Boron-10 (^{10}B) is common due to it's (n,α) cross section and is the subject of worldwide clinical studies [3].

$$\begin{aligned} &(94\%)\quad {}^{10}\mathrm{B} + n \rightarrow {}^{11}B^{*} \rightarrow {}^{7}Li^{*} + \alpha + 2.31\ \mathrm{MeV} \\ &(6\%)\quad {}^{10}\mathrm{B} + n \rightarrow {}^{11}B^{*} \rightarrow {}^{7}Li + \alpha + 2.79\ \mathrm{MeV} \end{aligned} \quad (1)$$

Gadolinium (Gd) is an alternative to ^{10}B due to naturally occurring isotopes having large (n, γ) cross sections commonly resulting in internal conversion (IC) and a subsequent Auger cascade. Due to use in MRIs, Gd has theranostic potential.

$$\begin{aligned} &{}^{157}Gd + n \rightarrow {}^{158}Gd^{*} \rightarrow {}^{158}Gd + 7.9\ \mathrm{MeV} \\ &{}^{155}Gd + n \rightarrow {}^{156}Gd^{*} \rightarrow {}^{156}Gd + 7.9\ \mathrm{MeV} \end{aligned} \quad (2)$$

Table 1. Relevant neutron capture cross sections for thermal NCT.

Target	σ [barns]
Natural Gd	4.88×10^4
^{10}B	3.99×10^3
^{14}N	1.7
^{1}H	3.3×10^{-1}

METHODS AND MATERIALS

Geant4 [4] was used to simulate a single 50nm nanoparticle (NP) in four scenarios:

1. Natural Gd NP irradiated with neutrons (GdNCT)
2. ^{10}B NP irradiated with neutrons (BNCT)
3. Natural Gd NP irradiated with photons (Gdγ)
4. Natural Au NP irradiated with photons (Auγ)

The source was monoenergetic, non-diverging, 0.0253 neutrons or 100 keV photons. Energies were chosen to represent the most probable speed of a thermal neutron spectrum and to emphasize K-shell photoelectric interactions, respectively.

Geant4-DNA [5] physics was used to track particles in the surrounding water. DICEBOX [6], a Monte Carlo γ-ray cascade tool, was used for Gd secondaries.

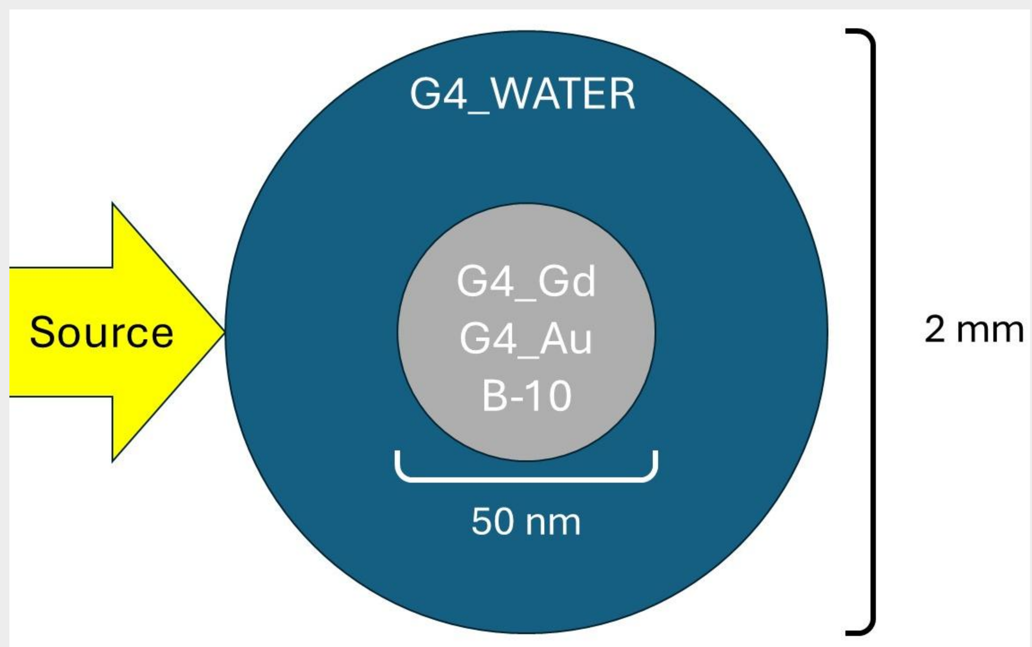

Figure 1. Simulation geometry.

RESULTS

GdNCT produces the largest flux of low energy electrons per primary history produced in the NP under the simulated conditions (Figure 2.C) with contributions from high energy IC electrons, Auger electrons, and δ-rays. GdNCT is also accompanied by a significant gamma flux from the capture reactions.

BNCT displays the highest dose deposition (Figure 3 and 4) until roughly 100nm outside of the NP where it decreases below that of GdNCT due to the short range of ^{10}B secondaries.

The ionization density outside of the NP (Figure 5) behaves similarly to the dose deposition with BNCT having a higher yield within 100nm, apart from a slight GdNCT peak within the first 5nm of the NP most likely due to the large flux of low energy Auger electrons.

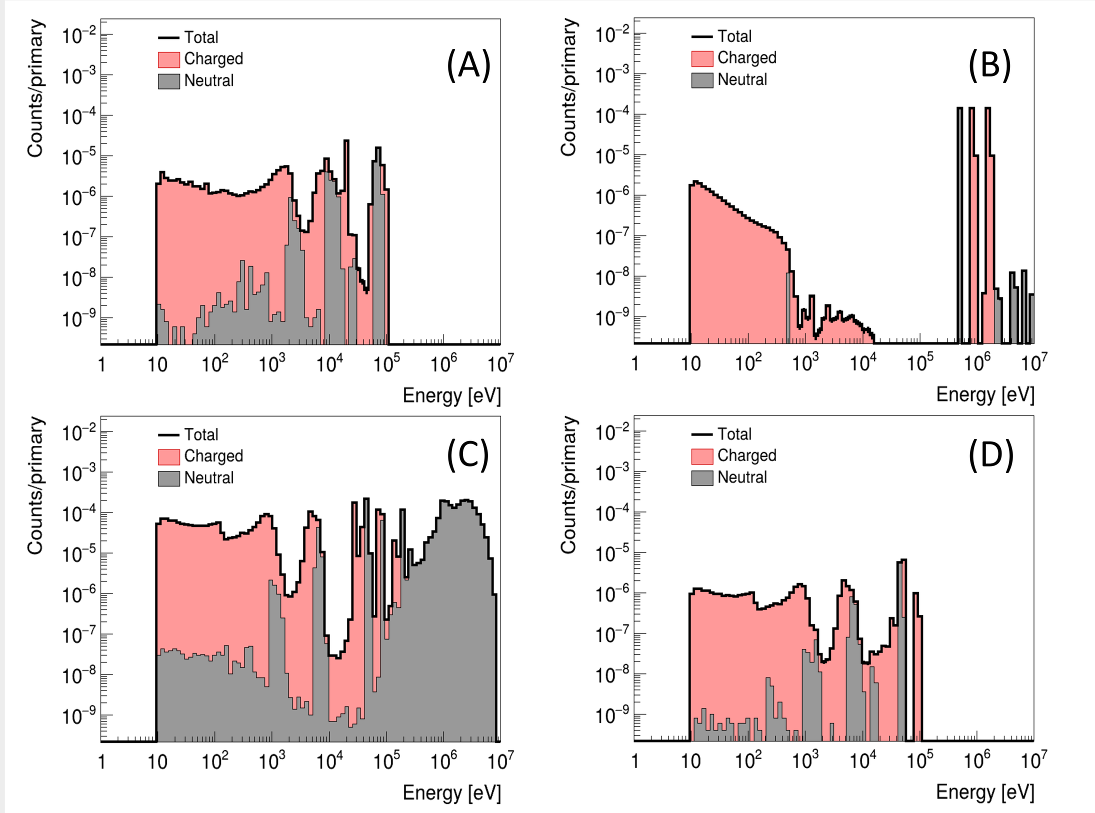

Figure 2. Secondary particle production within the nanoparticle for (A) Auγ, (B) BNCT, (C) GdNCT, and (D) Gdγ.

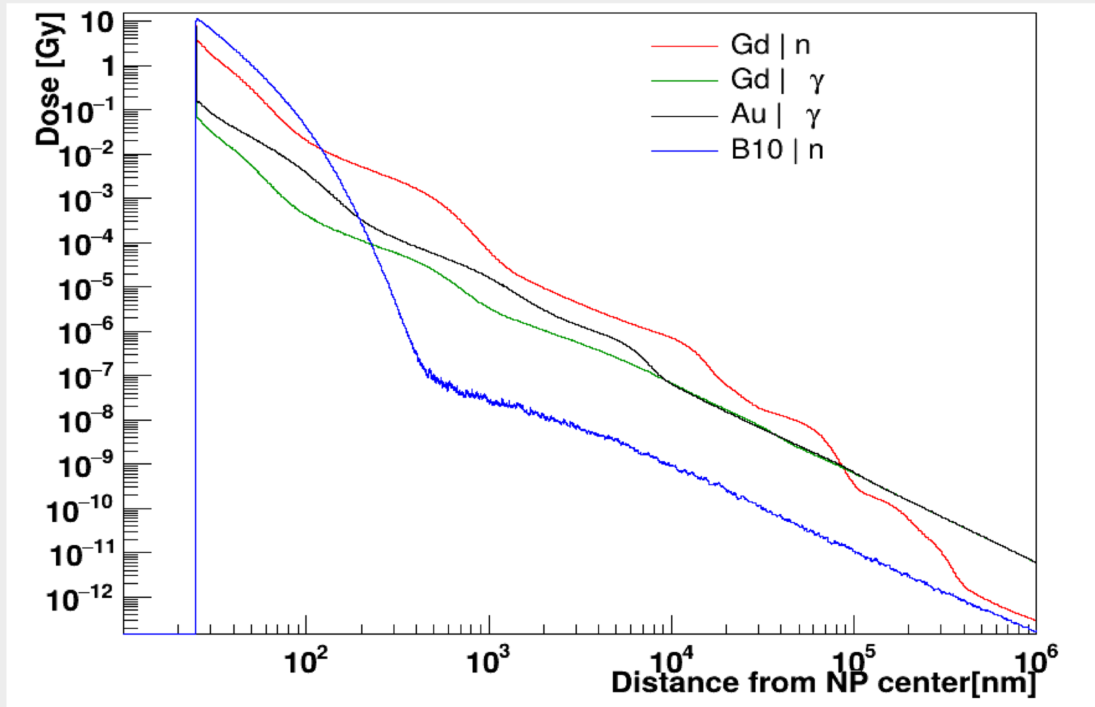

Figure 3. Dose per primary history for GdNCT [red], BNCT [blue], Gdγ [green], and Auγ [black].

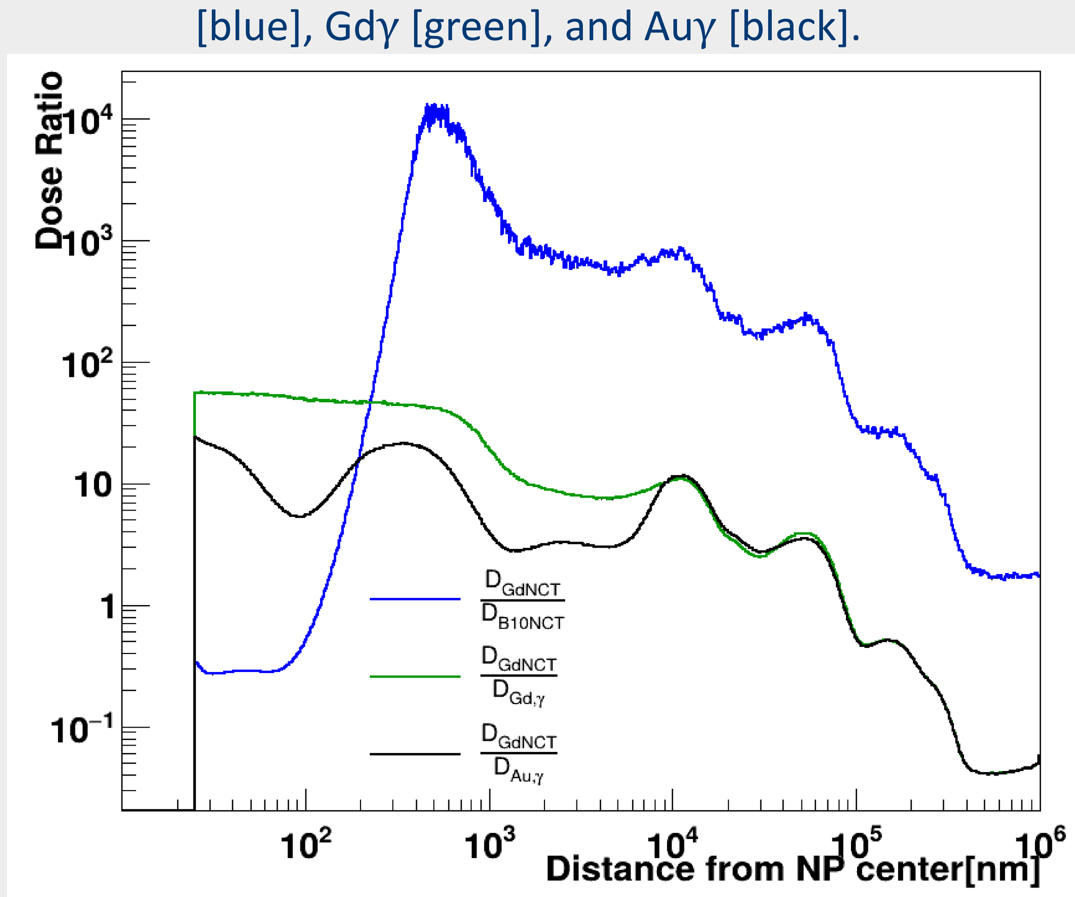

Figure 4. Ratio of GdNCT dose to that of BNCT [blue], Gdγ [green], and Auγ [black].

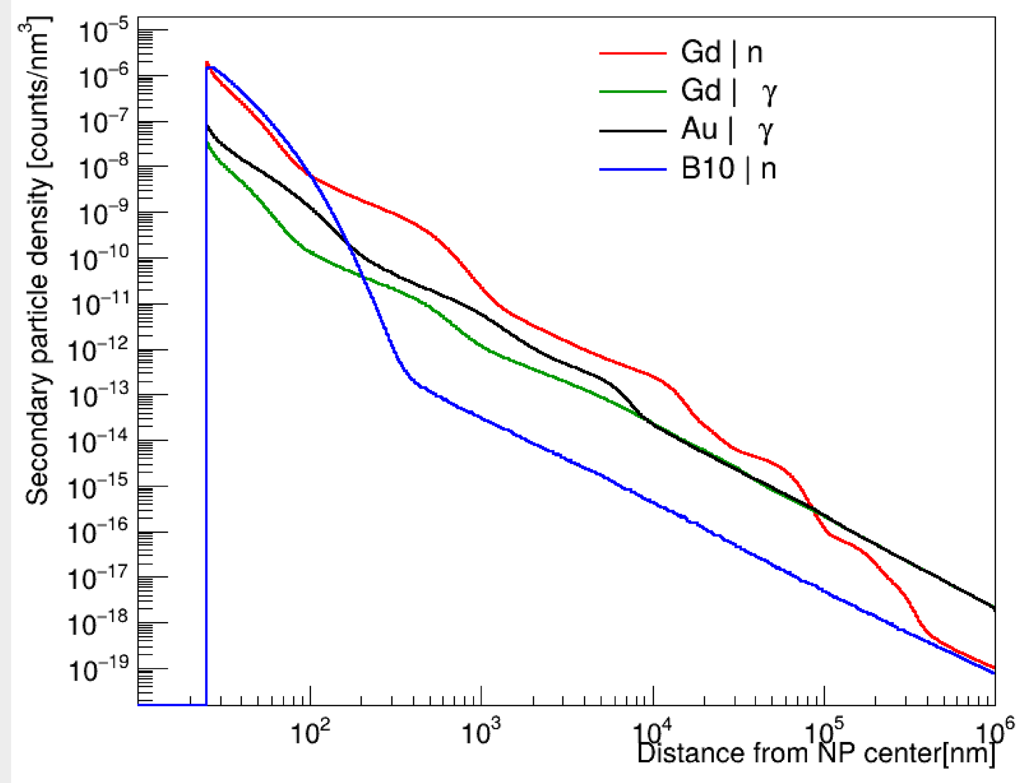

Figure 5. Ionization density of GdNCT [red], BNCT [blue], Gdγ [green], and Auγ [black].

DISCUSSION

GdNCT outperforms both photon simulations, with higher dose deposition, and ionization density around the NP but is less than that of BNCT at short distance. The further range of GdNCT IC electrons could allow extranuclear nanoparticles to contribute to cell mortality and better tumor coverage with a potential for increase to peripheral healthy cells.

The resultant gamma flux from GdNCT does not significantly contribute to the presented results due to their long mean free path (O(10cm)). The effects of these gammas need to be further study on patient dosimetry.

CONCLUSIONS

GdNCT has potential for a viable alternative to BNCT as a neutron capture agent. Future evaluation of gamma dose is necessary to definitively rule on GdNCT's viability as a therapeutic method.

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