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REGULAR ARTICLE

Enhancing X-ray Therapy: A Monte Carlo Study of Bismuth Sulfide Nanomaterials

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This study performs a numerical simulation of brain radiation therapy with a deep tumour at its centre using the Monte Carlo simulation program Geant4. The primary goal is to analyze the effect of nanomaterials (NMs) injected into the tumour on the dose and amount of radiation absorbed by the tumour. We built a spherical tumour measuring 1.5 cm in diameter in the middle of an adult human head while considering their chemical compositions and proportions. We are interested in studying the effects of adding bionanomaterials such as Gold nanoparticles (AuNP), hafnium oxide (HfO_2), cerium oxide (CeO_2), tantalum oxide (Ta_2O_5) and bismuth sulfur (Bi_2S_3) to the amount absorbed during an external exposure at a wavelength of energy ranging from 10 keV to 200 keV. The findings demonstrate that an absorbable dose improvement of 5.5 is obtained with a low concentration of 2% Bi_2S_3 nanoparticles inside the tumour, nearly four times with CeO_2 nanoparticles and slightly more than three times with AuNPs. According to our results, Bi_2S_3 and CeO_2 provide more enhancement in Radiotherapy than the most well-known materials in the literature, such as AuNPs.

Keywords: Radiation dose, Monte Carlo code, Nanomaterials (NMs), Tumor.

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1. INTRODUCTION

According to the American Cancer Society [1], there will be 1,958,310 new cancer cases and 609,820 deaths in the United States in 2023. From 2014 to 2019, the annual incidence of prostate cancer grew by 3, resulting in an additional 99,000 new cases. Men, on the other hand, have more positive incidence patterns. Women's lung cancer declined at half the rate of men's, whereas breast, uterine and liver cancer increased. Cervical cancer incidence has decreased by 65 as a result of the epidemic. Despite the epidemic, cancer deaths continued to fall, owing to breakthroughs in treatment. However, the increased prevalence of breast, prostate, and uterine cancers, which have the greatest racial disparities in mortality, may slow future progress. Surgery, radiation therapy, chemotherapy, and targeted therapies are just a few treatments that can be used to treat deep tumours [2, 3]. Surgery, which involves the removal of the tumour and surrounding tissue, is the most traditional and frequent kind of cancer treatment. High-energy beams are used in radiation therapy to kill cancer cells, but precise targeting is necessary to protect healthy tissue. Chemotherapy involves chemicals that can be ingested, injected into the bloodstream, or administered to the tumour to kill cancer cells. However, it may also cause side effects like vomiting, nausea, and hair loss. Drugs used in targeted therapy specifically target chemicals or processes involved in the growth and survival of cancer cells. However, they may not be effective against all cancer types [4-7]. Enhancement radiotherapy using nanoparticles is a promising new cancer treatment strategy that is promising to increase radiotherapy efficacy by providing a larger dose of radiation to tumour cells while causing less damage to healthy tissues. The special properties of nanoparticles, such as bio-compatibility, decreased toxicity, higher permeability, improved stability, precise targeting, and retention impact, make them useful in cancer treatment. Nanoparticles can improve Radiotherapy by boosting the amount of radiation energy deposited in tumour cells. This is possible with high-atomic-number (Z) nanoparticles like AuNPs or bismuth. These materials absorb X-rays and other radiation more effectively than the surrounding tissues. When nanoparticles aggregate in tumour cells, they can act as focal sites for radiation energy, resulting in a larger dose of radiation administered to the tumour while decreasing the amount provided to healthy tissues. Nanoparticles can also improve Radiotherapy by enhancing tumour cell susceptibility to radiation. This can be accomplished by delivering radiosensitizing medicines to tumour cells via nanoparticles. Radiosensitizers are medications that make tumour cells more sensi-

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tive to radiation. It is conceivable to generate a more effective tumour response while minimizing the overall dosage of radiation required by delivering radiosensitizing medicines to tumour cells using nanoparticles. Attaching tumour-specific targeting molecules to the surface of the nanoparticles can accomplish this. When these nanoparticles are introduced into the bloodstream, they collect in tumours, where they can provide a larger dosage of radiation to tumour cells while minimizing the dose to healthy organs [8]. The dose absorbed by tissues at the interface with higher Z materials is significantly increased. Indeed, due to the secondary radiation emission of kV X-rays, it has been found that AuNPs metal foils or Micro-spheres enhance the cytotoxic effect of ionizing radiation; in addition, platinum atoms have been shown to ameliorate X-ray-induced DNA breaks by enhancing the formation of hydroxyl radicals via photoelectric and Auger processes. In this paper, we are interested in novel NMs that have recently been employed in the field of Radiotherapy, such as Bismuth Sulfide (Bi_2S_3) [9-11], Cerium Oxide (CeO_2), Tantalum Oxide (Ta_2O_5), and Hafnium Oxide (HfO_2) [12-17]. We compare them to gold nanoparticles (AuNPs) [18]. We aim to investigate their dosage absorption efficiencies at a deep tumour, in this case, a brain tumour placed in the middle of a human head. As the field of nanomedicine continues to advance, this work highlights the promising role of NMs in improving cancer treatment outcomes, particularly in difficult-to-treat brain tumours.

2. EXPERIMENTAL DETAILS

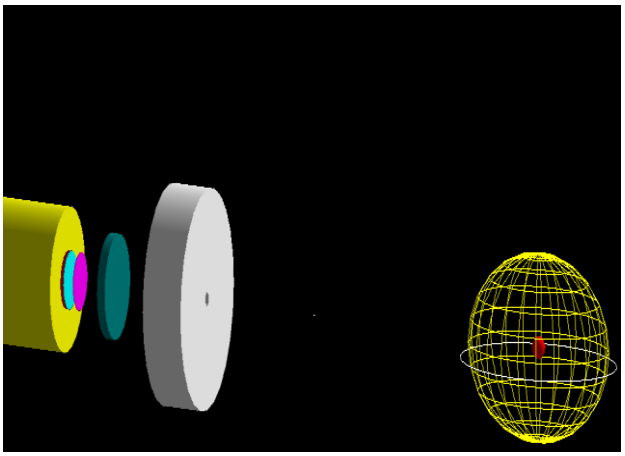
2.1 Simulation of a Tumor Inside a Human Head

The Monte Carlo approach was used in this study to examine brain tumour radiation. We are primarily interested in bio-nanoparticles' influence on the tumour and how these nanoparticles affect the absorbed dose at the tumour level. We are also particularly interested in the most competitive bio-NMs with AuNPs, such as Bismuth Sulfide (Bi_2S_3), Cerium Oxide (CeO_2), Tantalum Oxide (Ta_2O_5), and Hafnium Oxide (HfO_2).

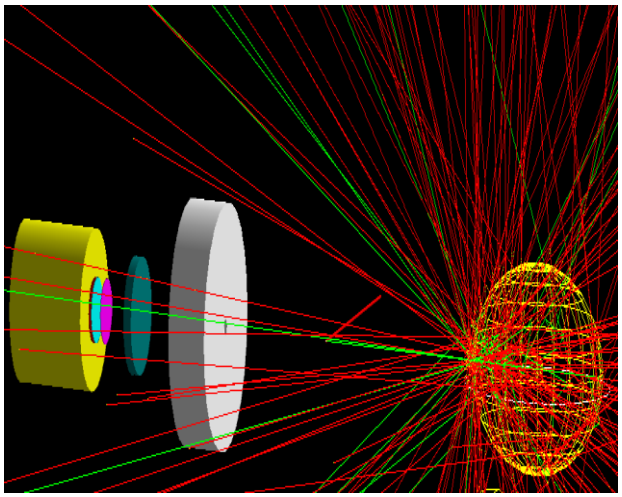
We constructed a 17 cm diameter by 8 mm wide phantom head and coated it with a 4 mm thick layer of brain tissue-containing skin (see Figure 1). Next, we constructed a 1.5 cm-diameter sphere-shaped tumour in the middle of this head. Tabl1 displays each material's atomic composition. One meter is the distance between the phantom's head and the mono-energetic X-ray beam (see Figure 1). The energy of the X-ray beam will be varied for each compilation in increments of 10 keV, from 20 keV to 200 keV. Then, 109 X-ray photons were released along the *z*-axis.

2.2 Monte Carlo Method

Geant4 code, version 11, was used for this work [19]. Based on the Monte Carlo method, the Geant4 code provides a framework for simulating the movement of particles through matter. It is utilized in several application areas, including high-energy physics, astrophysics, space sciences, and medical physics. On the project website, the Geant4 code is freely accessible and currently distributed according to the Geant4 Software License. Concerning the energy threshold for the associated physical process, its basic operational principle is to control cross-sections arbitrarily. In this simulation, we used a low electromagnetic energy package with a cutoff energy of 250 eV and a step range of 1nm [20, 21]. Geant4 provides a comprehensive set of electromagnetic methods to simulate the interaction of photons and electrons with matter [22, 23]. These processes can be divided into two broad categories: discrete processes and continuous processes. Discrete processes describe the interaction of photons and electrons with individual atoms.



(a)



(b)

Fig. 1 – Radiotherapy for a brain tumor using the Geant4 Monte Carlo model. The green lines define secondary X-rays, and the red lines define secondary electrons. (a) Geometry of tumour (red color) localized, (b) Compilation of 10 7 photons X-rays at the center of head

Table 1 – The chemical compositions of each material that constitutes the human head, expressed as a percentage of mass [24]

Materials and densities	O	C	H	N	Na	Mg	P	S	Cl	K	Ca
Scalp tissue (1.09 g.cm^{-3})	64.5	20.4	10	4.2	0.2	-	0.1	0.2	0.3	0.1	-
Skeleton (1.61 g.cm^{-3})	43.5	21.2	5	4	0.1	0.2	8.1	0.3	-	-	17.6
Brain (1.040 g.cm^{-3}) and Tumor (1.1 g.cm^{-3})	71.2	14.5	10.7	2.2	0.2	-	0.40	0.2	0.3	0.3	-

These include photoelectric absorption, Compton scattering, pair generation and arm radiation. Continuous processes describe the energy loss of photons and

electrons due to interactions with bulk matter. These include ionization and multiple Coulomb scattering. Geant4 uses these electromagnetic processes to model the interaction of X-rays with matter. Photons with energies between 100 eV and 100 MeV are called X-rays. The energy of X-rays determines the main electromagnetic processes by which X-rays interact with matter. Photoelectric absorption is the primary method for low-energy X-rays. Compton scattering is the primary method for high-energy X-rays. Geant4 simulations of X-ray interactions can be used for many different purposes, including developing new methods to treat X-ray cancers, designing and optimizing X-ray imaging systems, and studying the biological effects of X-rays. Each energy X-ray simulation requires one day on an HP Z800 workstation.

3. RESULTS AND DISCUSSION

3.1 Simulation of a Tumor Inside a Human Head

The linear energy transfer along the head for an X-ray energy of 50 keV, where a 2 % concentration of nanoparticles was added inside the tumour, is calculated and shown in Figure 2. AuNPs, Ta_2O_5, HfO_2, CeO_2, and Bi_2S_3 nanoparticles were injected into the tumour. As can be seen, the presence of nanoparticles in the tumour significantly impacts the energy deposited. Interestingly, Bi_2S_3 (red curve) and CeO_2 (black curve) have a greater impact on the amount of energy deposited at the tumour level than AuNPs (blue curve). To provide further information, we computed the absorbed dose at this tumour for every energy of the X-ray that was released. With a step of 10 keV, Figure 3 shows the tumour's absorbed dose in μGy as a function of X-ray energy from 20 keV to 200 keV. This figure shows that the radiation's energy significantly impacts the amount absorbed at the tumour level.

Furthermore, the Bi_2S_3 shows superior dose absorption, with two maximum values at approximately 50 keV and 110 keV, while the CeO_2 only shows one maximum at approximately 50 keV. Third place goes to AuNPs, which have two maximums of about 50 and 90 keV. Compared to earlier NMs, Ta_2O_5 and HfO_2 show reduced dose absorption, with two maxima at roughly 50 and 70 keV. It should be noted that, compared to NMs, AuNPs exhibit the lowest absorption at X-ray energies of about 70 keV. This finding is extremely important in Radiotherapy because Bi_2S_3 can reach relatively deep tumours, such as brain tumours.

We plotted the proportion of dose in Figure 4, and the results are impressive in the case of Bi_2S_3. The absorption dose in the tumour is nearly five times higher where the X-ray energy is around 30 keV and nearly twice as high where AuNPs are present inside the tumour. It is also worth noting that CeO_2 has a high dose absorption for an X-ray energy of around 50 keV, four times greater than in the absence of nanoparticles and two times greater than in the presence of AuNPs. The primary physical process that occurs when X-rays interact with heavy atom-based nanoparticles is known as the Auger effect, which helps to explain this [25]. This process is explained by the following: an electron ejected from the atom's inner electron shell after receiving energy from an X-ray photon leaves a hole, which is filled by an electron higher in the atom. This process results in the emission of a photon known as X-ray fluorescence.

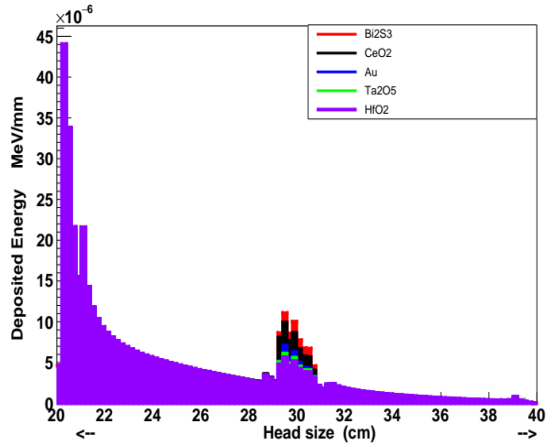


Fig. 2 – The energy deposited by a mono-energetic X-ray beam along a head. Notes: In this figure, the X-ray beam has an energy of 50 keV, and the nanoparticle concentration is 2 % relative to the tumor volume

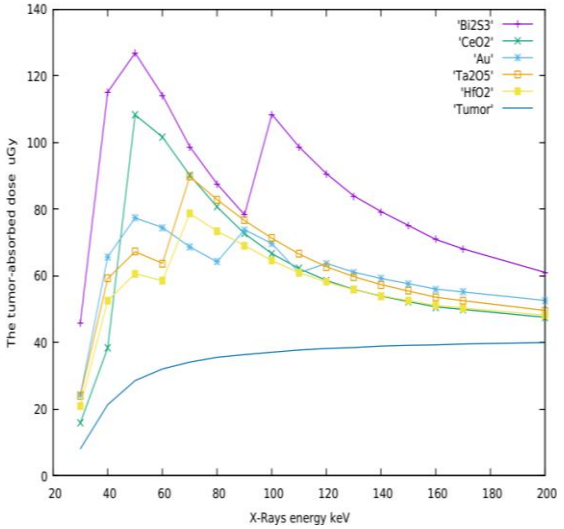


Fig. 3 – Calculate the absorbed dose at the tumour in the presence of nanoparticles within the tumour. The X-ray energy changes from 20 to 200 keV in 10 keV steps at each compilation. The nanoparticle concentration is set at 2 % of the tumour volume

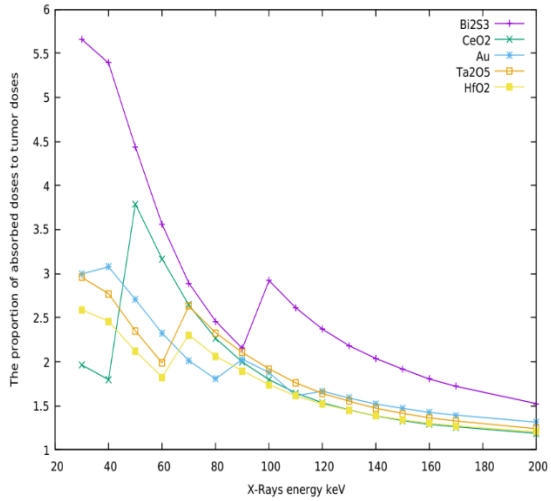


Fig. 4 – The proportion of the dose that the tumor absorbs when nanoparticles are present compared to the dose that the tumor absorbs when they are not

4. CONCLUSIONS

This paper investigates brain tumour radiation using a Monte Carlo method. The main areas of interest are bio-nanoparticles' impact on the tumour and their effect on absorbed dosage at the tumour level. The most competitive bio-NMs with AuNPs, such as hafnium oxide, cerium oxide, tantalum oxide, and bismuth sulfide (Bi_2S_3), are of special interest. Bi_2S_3 has promising benefits in radiation therapy, particularly in deep brain-type tumours, with twice as high dose absorption as AuNPs.

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Покращення рентгенотерапії: дослідження наноматеріалів на основі сульфіду вісмуту методом Монте-Карло

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Це дослідження проводить числове моделювання променевої терапії мозку з глибоко розташованою пухлиною в її центрі за допомогою програми моделювання Монте-Карло Geant4. Основною метою є аналіз впливу наноматеріалів (НМ), що вводяться в пухлину, на дозу та кількість випромінювання, що поглинається пухлиною. Ми створили сферичну пухлину діаметром 1,5 см посередині голови дорослої

людини, враховуючи її хімічний склад та пропорції. Нас цікавить вивчення впливу додавання біонаноматеріалів, таких як наночастинки золота (AuNP), оксид гафнію (HfO_2), оксид церію (CeO_2), оксид танталу (Ta_2O_5) та сірка вісмуту (Bi_2S_3), до кількості, що поглинається під час зовнішнього опромінення на довжині хвилі енергії від 10 кеВ до 200 кеВ. Результати дослідження показують, що покращення поглинальної дози на 5,5 раза досягається при низькій концентрації 2 % наночастинок Bi_2S_3 всередині пухлини, майже в чотири рази при використанні наночастинок CeO_2 та трохи більше ніж у три рази при використанні AuNPs. Згідно з нашими результатами, Bi_2S_3 та CeO_2 забезпечують більше покращення в радіотерапії, ніж найвідоміші матеріали в літературі, такі як AuNPs.

Ключові слова: Доза опромінення, Код Монте-Карло, Наноматеріали (НМ), Пухлина.