2024 International Nuclear Atlantic Conference – INAC 2024
Escola de Guerra Naval, Rio de Janeiro, RJ, May 6 - 10, 2024

ISBN: 978-65-594-1256-3

Monte Carlo Method applied to nanobrachytherapy simulations

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1. Introduction

The term "cancer" comprises a group of diseases that arise through genetic mutations in cells, that is, alterations in their DNA that result in their malfunctioning. If the growth and uncontrolled multiplication of these cancerous cells occur, they tend to be highly aggressive and uncontrollable, leading to the formation of a tumor [1]. Among women, the most common cancer worldwide is breast cancer [1]. Brachytherapy is a cancer treatment that involves implanting a radioactive source inside or immediately next to the tumor tissue. In this type of treatment, planning is essential to damage the cancer cells with minimal harm to nearby healthy cells [2]. Another option that is under development is nanobrachytherapy, which involves using gold nanoparticles (^{198}AuNPs) as a radiation source for cancer treatment. Unlike conventional brachytherapy, which destroys cancer cells, NPs can penetrate inside them. Thus, radiation is specifically targeted at diseased cells, with the understanding that damage to healthy tissue is even lower. However, as it is a very recent treatment, further studies are still needed to establish a dosimetric protocol for future use in humans. To develop the characterization of these materials, protocol TG-143 and TG-186, used in conventional brachytherapy, recommend the use of a computational simulation tool and a practical methodology, so that the results can be compared and validated [3]. For brachytherapy, the Monte Carlo Method (MC) is recommended, a stochastic process based on probability and statistical laws to simulate the interaction of radiation with matter [4]. This work aims to discuss an initial methodology for creating a computational dosimetry code for NPs in MC, especially for breast cancer.

2. Methodology

The MCNP code has been used to solve problems in medical physics, primarily concerning the interaction of ionizing radiation with the human body and the need to ensure adequate doses in the tumor when planning treatment. The advantage of using MCNP simulation is the ability to describe reality as accurately as possible in a safe environment that allows planning and exploring treatment possibilities that cannot initially be tested experimentally. With the knowledge obtained and validated, means for application in real situations can be evaluated. MCNP allows predicting any dose distribution in a heterogeneous medium. Therefore, patients' bodies, which are composed of different tissues and bones with varying sizes, shapes, densities, and radiation attenuation coefficients, can be investigated by MCNP simulation. The Evaluated Nuclear Data File (ENDF) photonuclear data library, validated by the International Atomic Energy Agency (IAEA), is used to obtain reference simulator objects, such as breast models and other organs [5,6].

The simulation involves the following steps [5,6]:

- Geometry modeling: defining the system's geometry, source term, and surrounding materials, based on organs;
- Material assignment: specifying the properties of each material, such as density and composition, to evaluate the interaction of radiation with matter;
- Configuration of the radioactive source: initially, known radioactive sources be defined, including emission type, distribution, and energies;
- Simulation parameter configuration: defining the number of histories, termination criteria, and tallies;
- Simulation execution: the code tracks the radiation transport through the specified geometry;
- Results analysis: includes analyzing information on particle energy distribution, interaction quantities in each material, and other relevant parameters;
- Validation: Validating simulation results by comparing them with experimental data, when available. Validation is crucial to ensure that the simulation provides accurate and reliable results.

For the characterization of radioactive sources, the International Atomic Energy Agency (IAEA) Live Chart of Nuclides reference base was used to obtain the beta spectrum and gamma energies of ^{198}Au [7]. The characteristics of ^{198}Au favor permanent therapeutic application (where the source is not removed from the patient after application) due to its short half-life, penetration capability into the target, and large number of radiation-emitting gold atoms. Its properties are: half-life ($T_{1/2}$) = 2.7 days, gamma energy (Eγ) = 411.8 keV, and maximum beta energy ($E_{\beta max}$) = 961.1 keV [7].

3. Results and Discussion

Regarding radioactive NPs, there are simulation studies involving predicting dose enhancement factors in enhanced X-ray radiotherapy with NPs (Fig. 1A) [5], dose behavior in specific beams [8], proposal of synthesis, biodistribution, and in vivo testing (Fig. 1B) [6], among others.

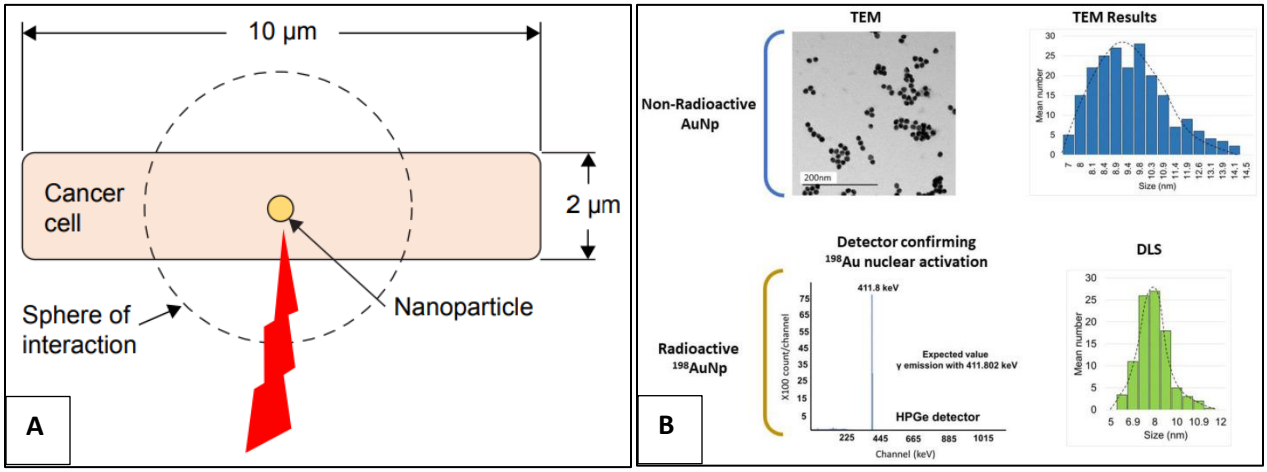

Figure 1: Reference studies on the simulation of NPs in Monte Carlo found in the literature. A) Analytical simulation scheme, where a single nanoparticle is at the center of a cell modeled as a slab of tissue. B) Results for the non-radioactive product and radioactive AuNPs. Source: T. Gray, *et al.* 2021 and C.D. Souza, *et al.* 2022.

Although several studies address the increase in dose of ^{198}AuNP in radiotherapy, a knowledge gap persists between Monte Carlo simulation and in *vitro/in vivo* investigations, a point highlighted in most of the literature's conclusions. In this initial proposal, a simulation of a breast with a diameter of 11.5 cm and a tumor of 2.0 cm (early stage without reaching lymph nodes) was performed, where the ^{198}AuNps were distributed homogeneously throughout the tumor (Fig. 2). For the simulation, the following parameters were adopted:

- Water was chosen as the material for both tumor and healthy tissue, as its radiation absorption and scattering properties resemble those of muscles and soft tissues, besides being a readily available material for reproducibility.
- The source term was defined by the SDEF card. The distribution of beta spectrum and gamma radiation from ^{198}Au were obtained from the Live Chart of Nuclides table [7], made available by the IAEA.
- The absorbed dose in the tumor and healthy breast tissue was calculated using Tally *F6 of MCNP 6.2 with 10^7 histories. The result generated by MCNP is given in GJ/g. To convert to J/kg or Gy per decay, the calculated values were multiplied by 10^{12} and are presented in Tab. I.
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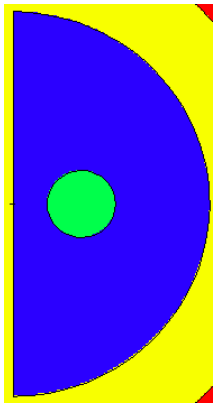

Figure 2: Simulation of 2 cm tumor in a breast with MCNP 6.2 – Visualization by VISED.

Table I – Calculation of dose rate in the treatment of cancer by ^{198}AuNps.

	Dose Rate (Gy/Bq/s)	
Region	**Beta**	**Gamma**
Healthy human tissue	4.54E-15	1.05E-14
Tumor	7.77E-12	2.22E-13

According to the treatment prescribed by the physician, the specific activity of the source used is determined. Based on this activity, it is possible to calculate the absorbed dose per second in the tumor through the *Specific activity of the source (Bq) x Dose rate (Gy/Bq/s)*. For example, in a cancer treatment where ^{198}AuNPs of 15 MBq [6] are implanted (tested *in vitro*), the calculation of the absorbed dose is presented in Tab. II.

Table II – Calculation of absorbed dose in the treatment of cancer by ^{198}AuNps with 15MBq.

	Absorbed dose (Gy/s)		Absorbed dose (Gy/h)	
Region	**Beta**	**Gamma**	**Beta**	**Gamma**
Healthy human tissue	6.81E-8	1.57E-7	2.45E-4	5.65E-4
Tumor	1.17E-4	3.33E-6	4.21E-1	1.20E-2

4. Conclusions

The absorbed dose was obtained by the relationship between *Specific activity* and *dose rate*, considering the insertion of ^{198}AuNPs with 15 MBq showed greater energy deposition in the tumor, which is suitable for brachytherapy treatment, aiming to preserve healthy tissue. However, it is still necessary to study in detail the parameters for representing the ^{198}Au more accurately, considering, for example, its cellular absorption property. Additionally, it is necessary to strike a balance to achieve a high level of statistical convergence and the processing time of MCNP.

Acknowledgements

Acknowledgment to the agencies FINEP 0941/22, CNPq INCT-INTERAS 406761/2022-1, IPEN/CNEN 2020.06.IPEN.37, FAPESP 2017/50332-0 and 2020/07065-4, CAPES, CNEN and IAEA BRA6026 for Project funding and scholarship support.

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