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► **To cite this version:**

David Sarrut, Ane Etxebeste, Jean-Michel Létang. Monte Carlo photons simulation from alpha-emitter radionuclides. XXth International Conference on the use of Computers in Radiation therapy, David Sarrut; Simon Rit, Jul 2024, Lyon, France. <hal-04905635>

**HAL Id: hal-04905635**

**<https://hal.science/hal-04905635v1>**

Submitted on 22 Jan 2025

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# Monte Carlo photons simulation from alpha-emitter radionuclides

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## Abstract

We present a Monte Carlo virtual source model for generating photons emitted during the decay chain of alpha-emitter radionuclides. The model, integrated into GATE 10, utilizes Geant4 databases to extract photon emission lines from decaying daughters. Employing Bateman equations for decay chain abundances and activities within a specified time range, it generates photons' energy and temporal distribution. By avoiding the need to simulate the entire decay chain, it reduces the computation time compared to reference ion source. The source model can be applied to any alpha-emitter radionuclide in the Geant4 database. It facilitates the investigation of (SPECT) imaging photon emission from alpha-emitters.

## 1 Introduction

Targeted Alpha Therapy (TAT) is a type of Radiopharmaceutical therapy (RPT) that exploits the short range and high linear energy transfer (LET) of alpha particles ( $^4\text{He}$ ) to enhance targeted tissue dosages [1]. Examples of radionuclides for TAT include  $^{223}\text{Ra}$  (Xofigo<sup>TM</sup>) for castration-resistant prostate cancer (CRPC) with metastatic bone disease [2] and, more recently,  $^{225}\text{Ac}$  (Ac-225-PSMA-617) combined with PSMA for metastatic prostate cancer [3]. Investigation of other alpha emitters such as  $^{149}\text{Tb}$ ,  $^{211}\text{At}$ ,  $^{212}\text{Pb}$ ,  $^{213}\text{Bi}$ ,  $^{223}\text{Ra}$ , and  $^{227}\text{Th}$  is underway. The LET of alpha particles, approximately 50-200 keV/ $\mu\text{m}$ , is about three orders of magnitude larger [4] than the LET of  $\beta^-$  particles emitted by conventional radionuclides such as  $^{177}\text{Lu}$  or  $^{90}\text{Y}$ . The alpha particle's range, around 50 to 100  $\mu\text{m}$ , is close to the diameter of a few cells [5], leading to high tumor damage, but also with potential toxicity risks.

The assessment of the dose spatial biodistribution and temporal biokinetics is critical to mitigate these risks. In-vivo imaging is feasible for certain alpha emitters using emitted photons in the decay chain, detectable by SPECT systems [6]. For instance, imaging feasibility has been reported for  $^{212}\text{Pb}$  [7] (phantoms) and  $^{225}\text{Ac}$  [8] (patients).

However, each radionuclide's decay chain produces distinct photons with different energy lines. SPECT acquisition must be tailored by selecting appropriate energy windowing, scatter correction, and reconstruction methods based on the emitted photons' energy ranges and quantities. For high-energy photons (>400-450 keV), challenging for Anger camera-based SPECT systems, alternative imaging systems like Compton Camera may be considered [9]. Monte Carlo simulation is an important method for investigating SPECT image acquisition parameters and advancing new imaging systems [10, 11]. In this study, we propose an efficient source

model generating gamma and X-ray emissions from alpha emitters, encompassing associated energy spectra, intensity, and timing.

## 2 Materials and Methods

The proposed photon source model is based on two primary components. Firstly, it involves identifying and compiling all photon lines, incorporating their energies and intensities, from decay daughters and processes into a list of energy-intensity pairs. The origin of these photons is attributed to (1) isomeric transitions and (2) atomic relaxation. Bremsstrahlung radiation, depending on the media, is neglected here. Secondly, the model automatically computes and utilizes Time Activity Curves (TAC) to express the relative abundances of decaying daughters as a function of time. During simulation runtime, the Geant4 engine sequentially generates primary photon events, considering their relative intensities, energy levels, and associated timestamps.

Gamma emission data from isomeric transitions (IT) is extracted from the Geant4 database, and relative intensities are computed recursively for all decay channels and energy levels. Initial examination of a radionuclide's decay channels involves referencing the decay table of the `G4RadioactiveDecay` process object. The relevant data, including excitation energies and deexcitation channel details, are stored in files (e.g., `z89a225` for  $^{225}\text{Ac}$ ). Each deexcitation channel provides gamma transition energy, relative intensity, and the total internal conversion coefficient. Recursive computation of the final gamma emission rate considers branching ratios, gamma emission probabilities, total transition probabilities, and recursively accumulated channel probabilities. This process is performed for common radionuclides ( $^{149}\text{Tb}$ ,  $^{211}\text{At}$ ,  $^{212}\text{Pb}$ ,  $^{213}\text{Bi}$ ,  $^{223}\text{Ra}$ ,  $^{227}\text{Th}$ , etc.) and their decay daughters.

Photons from atomic relaxation (AR) are extracted from the IAEA website using the provided web API<sup>1</sup> (ENSDF Evaluated Nuclear Structure Data Files). Similar to the isomeric transition process, the obtained data are stored in a file, as lists of photon emission energies and associated probabilities. Geant4 incorporates the Bearden database, aligned with the IAEA website and activated using `/process/em/fluoBearden true`. Considering the

<sup>1</sup>API documentation: [https://nds.iaea.org/relnsd/vcharthtml/api\\_v0\\_guide.html](https://nds.iaea.org/relnsd/vcharthtml/api_v0_guide.html)

nanosecond timescale of atomic relaxation decay, characteristic X-ray emission is treated as prompt, excluding delayed fluorescence [12].

The photon lines with their respective energy and probabilities extracted from IT and AR are not sufficient, we also need the relative abundance of each daughter radionuclide. This is done by solving Bateman equations that compute the time-dependent decay of radioactive nuclides and their daughter products, accounting for changes in population over time due to parent nuclide decay and subsequent daughter decay. These equations yield to TAC for all daughters based on specified time points.

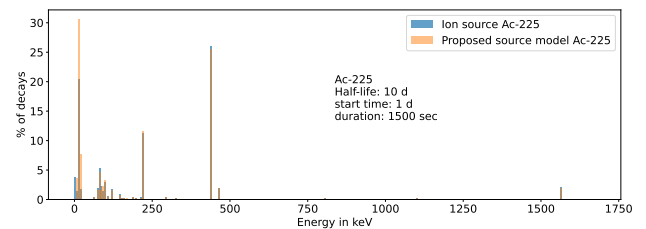
In summary, the proposed source model automatically retrieves comprehensive information (daughters, half-life, TAC, etc.) for a given radionuclide. It incorporates relative activity from computed TAC, coupled with emitted photons from isomeric transitions and atomic relaxation, to selectively generate primary photons with accurate energy, intensity, and timing within the specified timeframe.

### 3 Experiments and results

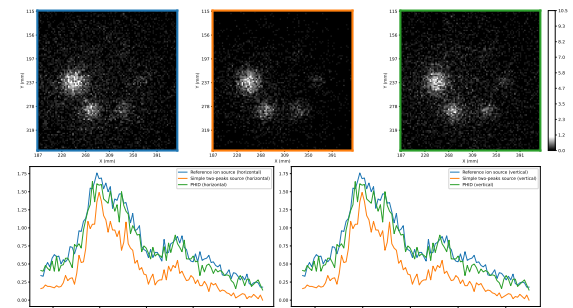
We compared the photons emitted from a reference Geant4 simulation and the proposed model. The simulation used a  $^{225}\text{Ac}$  point-like source of 1000 Bq, in a water box, during an acquisition time frame of 1000 seconds starting 14 hours after injection of the radionuclide. Photons from the reference simulation were extracted from a phase space that contains all particles that have been created and tracked together with the kinetic energy, their Geant4 creator process, and their associated timestamps. At the end of the simulation, the phase space was processed to extract the photons whose creator process is IR or AR and whose timestamps are between 14 hours and 14 hours plus 1000 seconds. The resulting reference photon energy spectrum was compared to the one obtained from a second simulation in the same condition but using the proposed source model. Figure 1 shows very good concordance between most of the photon lines except for the very low energy (<20 keV).

We also simulate a projection from Siemens Intevo Bold SPECT/CT device equipped with High Energy collimator (8000 holes of 4 mm, 2 mm septal thickness) coupled to 9.5 mm thickness NaI crystal. We simulated the NEMA IEC body phantom with six spheres filled with 100 kBq/mL  $^{225}\text{Ac}$  (around 0.5 MBq total) and no background activity. The acquisition was one single-angle orientation with a time frame of 210 seconds starting at  $t=24\text{h}$  like in [8]. We compared three types of sources: (1) the reference  $^{225}\text{Ac}$  ion source, (2) a simplified dual gamma source of 218.12 keV (11.4%) and 440.45 keV (25.9%), like the one in [13], and (3) the proposed source model. Figure 2 shows the obtained projections and associated profiles. The proposed source model is in good agreement with the reference profile, while the simplified model depicts larger discrepancies.

Using the reference ion source involved the tracking of a lot of different particles and required to start from  $t=0$ , and filter the desired photons. If we consider an acquisition of 200 seconds with a  $^{225}\text{Ac}$  source of 3 kBq, about  $15.8 \times 10^6$  particles will be tracked for only  $2.7 \times 10^5$  photons that should be simulated (32 seconds vs 1.4 seconds). In the previous experiment, computation time was 28 hours for the reference source, 1.6 hours for the simplified two peaks source and 3.7 hours for the proposed one.



**Figure 1:** Comparison of emitted photons from the reference ion source and the proposed source model for  $^{225}\text{Ac}$ .



**Figure 2:** Top:  $^{225}\text{Ac}$  SPECT projections of the IEC phantom for an energy window around 218 keV (energy window equal to 196-240 keV), with the reference ion source (left), the simplified two-peaks model (middle), and the proposed source model (right).

### 4 Conclusion

We presented and evaluated a specialized Monte Carlo source model for alpha emitters, specifically designed for the generation of photons within a specified timeframe. This approach provides computational efficiency benefits compared to conventional ion sources that require the generation and tracking of all decay products. Obtained photons are in good agreement with the reference ones except for the low energy range below 20 keV. The proposed source model is versatile and has been applied to various other alpha emitters. It can be useful for optimizing acquisition protocols, refining scatter correction parameters, and exploring advanced reconstruction methods. The source model is open source and available in GATE 10.

## Acknowledgments

This work was performed within the framework of the MO-CAMED project (ANR-20-CE45-0025), the SIRIC LYri-CAN+ Grant INCa-DGOS-INSERM-ITMO cancer18003. We gratefully acknowledge the support of NVIDIA Corporation with the donation of the Titan Xp GPU used for this research. This work was granted access to the HPC resources of IDRIS under the allocation 2019-101203 made by GENCI (Jean Zay computing center).

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