Numerical calculations of received dose due to various geometries of radioactive material

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Abstract. The Mineral PET project aims to locate diamonds within Kimberlite by first irradiating the rock to induce beta decay in carbon atoms, then imaging the resultant positron emission signals. Due to the irradiation of large bodies of rock in an industrial context, the radiation exposure at different locations is of interest. We investigate various techniques to quantify the radiation dose received by a human-sized target from a body of radioactive material. The first technique assumes various simplified geometries, and makes use of a numerical attenuation computation to create a three dimensional dosage map. This is compared to a full Monte Carlo simulation of the physics involved using the Geant4 particle tracking toolkit developed at CERN in a high-energy particle physics context. This allows us to comment on the accuracy of the attenuation model in different configurations. This technique is also useful for identifying hotspots and ascertaining whether further shielding is required as part of the design specification of the online Mineral PET ore sorting system.

1. Introduction

Mineral PET is a project to develop a diamond imaging technique within coarsely crushed Kimberlite (±10cm rocks), without having to finely crush and expose diamonds to the surface. The technology uses Positron Emission Tomography (PET), similar in principle to medical scans. The Kimberlite is irradiated with high energy gamma rays, created by the bremsstrahlung from an electron incident on a high Z material. These gamma rays excite the giant dipole resonance, to produce the unstable ^{11}C isotope. This beta decays, and the positron emission and annihilation leads to back to back 511 keV photons. These are detected in coincidence by planes of position sensitive detectors on either side of the passing rock. The image is then constructed by constructing a 3D voxel space, populated by tubes drawn between the detector hits.

One of the concerns is quantifying the radiation exposure received by workers near different parts of the process in an industrial context. There are several areas where irradiated material is stored. One example of this is in hold hoppers. The irradiation process will create an oxygen PET isotope in addition to the desired carbon one. To let this unwanted signal die down sufficiently, the irradiated material must first be stored in a hold hopper for around 20 minutes before being sorted. Another example is the transportation of Kimberlite on conveyor belts. Most studies of radiation exposure have focussed on the long term exposure of large quantities of material in the environment, rather than a specific shape of material in a specific context.

We therefore investigate tools that can create a 3-dimensional exposure map based on known distributions of radioactive species.

In order to quantify radiation dose, we will investigate the energy delivered to a target using two different methods. The first makes use of a linear attenuation model to derive an integral that can be numerically integrated to give radiation exposure. The results from this method are compared to the second method, which involves a Monte Carlo based simulation of the physics of the radiation.

2. Attenuation model

2.1. General case

When photons are travelling through a material, the radiative energy that penetrates to a certain depth decreases as the photon interacts with the medium. The first way quantify this is with a photon attenuation model. Given a mono-energetic photon beam, the decrease in intensity can be described using a linear attenuation constant, $\mu_{\rm L}$, as follows:

$$\frac{I}{I_0} = e^{-\mu_{\rm L} x} \tag{1}$$

This does not capture the full story however, as once a photon interacts with an atom, all of its energy does not always disappear into the medium. Photons interact with the medium predominantly via pair production, the photoelectric effect and Compton scattering [1]. These can leave the primary photon with some energy, and can also release charged particles, each of is then free to interact further. One way of quantifying this is with a mass energy-absorption coefficient $\mu_{\rm en}$ (see, for example, [2]). This attempts to quantify the energy absorbed by a material through which photons are passing. If, at each step dx, the material absorbs an energy dE given by $dE = E\mu_{\rm en}dx$, then the energy that is not yet absorbed follows an exponential decay of the form of (1).

This is still not 100% accurate. The definition of $\mu_{\rm en}$ used in the commonly cited NIST database [3] takes into account only the energy given to charged particles released from the *first* photon-atom interaction site (not including the energy re-radiated by the charged particles). Any secondary interactions, plus the later interactions of secondary photons, are not included. When considering the energy that penetrates through a given length of material, we can thus expect a behaviour that is close to an exponential decay, with a decay constant that is less than $\mu_{\rm L}$, but somewhat more than $\mu_{\rm en}$. We shall refer to this effective "energy attenuation constant" as μ in what follows. This will be a function of the energy of the photon as well as the properties of the material being traversed.

Given the specific activity S_A (presumed measured in $Bq.m^{-3}$) of a radioactive isotope, and a photon energy E_γ, our goal is to find the overall energy incident on an object near some radioactive material per unit time. Using (1), the energy incident per unit time (dP) on a small surface area centred at point Q due to a small volume element dV centred at point P is

$$dP = \frac{d\Omega(P,Q)}{4\pi} dV S_A E_\gamma \; e^{-\mu l(P,Q)} \tag{2}$$

where $d\Omega$ is the solid angle subtended by the small area and l is the path length travelled by the radiation through the material. To find the total power incident on a target, we therefore integrate over the volume of radioactive material, and over the solid angle subtended by the object.

$$P = \frac{S_A E_\gamma}{4\pi} \int_V dV \int_S d\Omega \; e^{-\mu l(P,Q)} \tag{3}$$

If the target is small or far away, then l does not change much for different points on the target, and $l(P,Q) \approx l(P)$. The integral over $d\Omega$ collapses to the total solid angle subtended by the target, Ω. We further simplify by considering a spherical target of radius r. The solid angle subtended by a sphere can be shown to be

$$\Omega = 2\pi \left(1 - \sqrt{1 - \frac{r^2}{R^2}}\right) \tag{4}$$

The total power incident on the target due to a volume V can thus be written as

$$P = \frac{S_A E_\gamma}{2} \int_V dV \left(1 - \sqrt{1 - \frac{r^2}{R^2}}\right) e^{-\mu l} \tag{5}$$

2.2. Cuboid volume

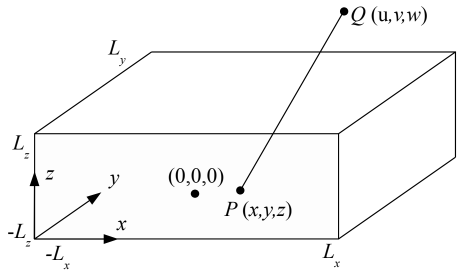

Figure 1. Rectangular Geometry

In the case of a cuboid volume, with coordinates as shown in figure 1, the path length l can be expressed in terms of R.

$$l = R\left(\frac{L_z - z}{w - z}\right) \tag{6}$$

The power will now be given by

$$P = \frac{S_A E_\gamma}{2} \int_{-L_x}^{L_x} dx \int_{-L_y}^{L_y} dy \int_{-L_z}^{L_z} dz \left(1 - \sqrt{1 - r^2/R^2}\right) e^{-\mu\left(\frac{L_z - z}{w - z}\right)R} \tag{7}$$

where $R^2 = (x-u)^2 + (y-v)^2 + (z-w)^2$. This integral does not have a readily available analytic solution and is calculated numerically.

An additional complication arises because (7) assumes that the photons passes through the upper z face. In the general case, an extra step is required at each point of the integral, that tests which face of the cuboid is intersected by the line joining P and Q. The coordinates of the term in the exponential can then be rotated appropriately.

3. Simplified simulation

In order to get results that are not limited by the assumptions that went into the analytical model described in section 2, a full simulation is desired to individually track particles from the time that they are emitted to when they hit the target. The toolkit of choice is the Geant4 framework ([4], [5]) created in a high energy particle physics context at CERN. Before introducing the full Geant4 simulation, we first introduce a simple "toy" simulation that allows us to compare the attenuation model to Geant4.

Our approach is to find the fraction of the initially released energy that makes it out to a particular distance. In order to do this, a large sphere of Kimberlite is simulated. Particles are then fired into the sphere, and each simulated energy deposition is recorded. The events are sorted and summed, and for each point the total energy that reaches that radius is calculated.

The simulated Kimberlite is composed of 14 different compounds. The constituents which make up more than 1% by mass are listed in table 1. The density is 2.8 g/cm^3.

Table 1. Simulated Kimberlite constitution

Constituent	Percentage	Constituent	Percentage
Fused Quartz	44.62	Aluminium Oxide	3.75
Magnesium Oxide	28.57	Calcium Oxide	3.73
Hydronium plus ions	8.41	Ferrous Oxide	2.77
Ferric Oxide	5.03	Other	3.12

The data from the Kimberlite ball simulation are plotted with an exponential decay in figure 2. 511 keV and 1369 keV are the energy levels from the PET isotopes and sodium respectively, which are the long-lasting isotopes created in Mineral PET. 100 keV was included as a lower energy comparison. The fit is relatively good, with small divergences at high and low energy, validating the treatment of energy loss with an attenuation model. From the slope of the exponential fits in figure 2, the effective energy attenuation constant of Geant4 for each energy level can be found. These values are shown in table 2.

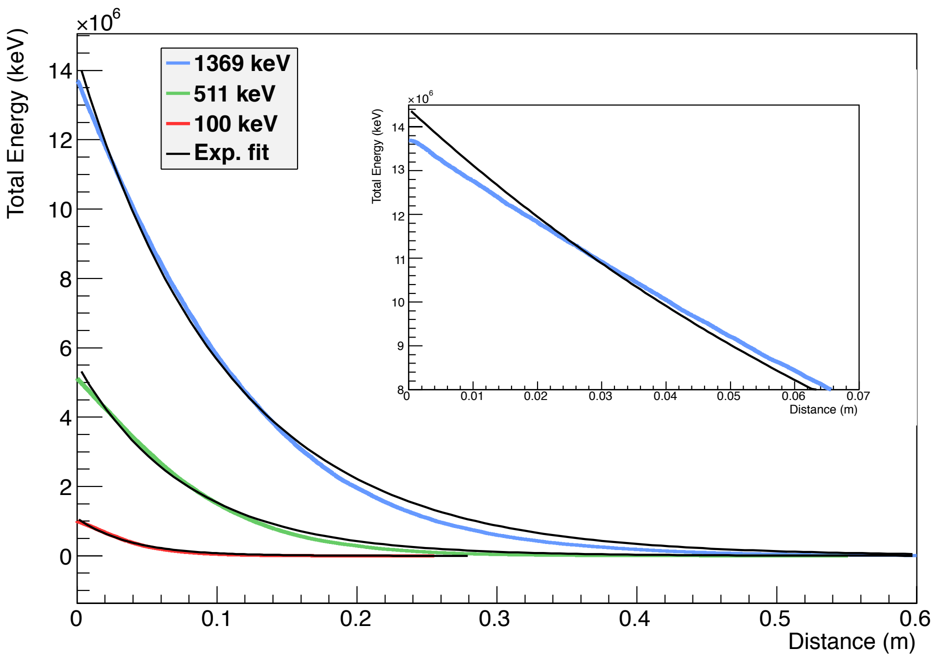

Figure 2. Comparison between Geant4 and attenuation model. Coloured lines show simulated data from Geant4. The inset shows a magnified view of the lower radius region for 1369 keV.

Table 2. Effective energy attenuation constants, from slopes in figure 2

Energy (keV)	Eff. atten. const. (m^{-1})
1369	9.352 ± 0.002
511	12.804 ± 0.004
100	26.37 ± 0.02

The linear attenuation constant μ_L is additive; if the medium is made up of several materials labelled by i, and the proportion of material i is p_i, then the effective attenuation constant is $\mu_L = \sum_i p_i \mu_i$. Using the elemental values from the NIST database [3] for the compounds listed in table 1 and using a density of $2.8 g/\text{cm}^3$, μ_L for 500 keV is 24.70 m^{-1} and for 600 keV it is 22.81 m^{-1}. We can thus extrapolate to roughly 24.5 m^{-1} for 511 keV. μ_{en} is not additive, but we can get a ballpark figure by taking the value for concrete with a density of $2.8 g/\text{cm}^3$, which is 8.49 m^{-1}. We can see now that the fitted value for our effective energy attenuation constant μ of 12.8 is slightly higher than μ_{en}, but lower than μ_L. This matches the expectations from the discussion in section 2.

4. Example model and simulation results

The full Geant4 simulation consists of Kimberlite volume and a target. A water sphere approximates a human, with a radius of 0.5m that roughly corresponds to the frontal cross-section area of a standing person. If more accuracy is desired, a more realistic shape can easily be created, but the advantage of a sphere is that the results are directly comparable to those from the attenuation model. 511 keV photons are then created and fired in random directions, and the total energy deposited in the target is recorded. At first only the photons initially directed towards the target were considered. This approach was discarded however, as it was found that a significant portion of the energy deposited resulted from photons that had an initial velocity pointing away from the target, due to scattering, creation of secondary particles, etc.

An example geometry was created with a Kimberlite cuboid 2m high, 4m wide and 6m long. A 0.5m radius spherical target was then moved along a horizontal plane at a height of 0.6m above the cuboid, and the energy deposited was calculated using both the attenuation model and the Geant4 simulation. The attenuation model was integrated numerically using the Vegas algorithm from within ROOT [6]. The Geant4 simulation fired 1 000 000 particles for each data point and recorded the energy that hit the target. The results are shown in figure 3. The agreement is quite good. The major qualitative difference is that the Geant4 simulation is not as smooth, based as it is on a stochastic Monte Carlo simulation.

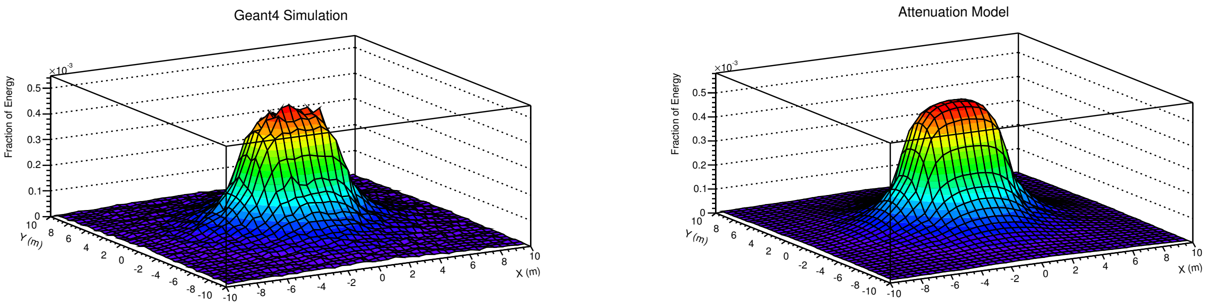

Figure 3. Fraction of activity reaching target in Geant4 simulation and attenuation models.

The difference between the models is shown in figure 4 together with a one-dimensional slice through the middle showing the relative difference. We can see that far from the Kimberlite, the difference consists mostly of noise, though the attenuation model slightly under counts. Closer to the Kimberlite, the attenuation model over counts. This can explained by two factors. Firstly, from the inset in figure 2, we can see that the exponential decay is larger than the data at small distances. When the target is near the material, the solid angle from nearby points in the Kimberlite is the greatest, and so photons that have travelled through less Kimberlite have a proportionately larger contribution. Secondly, the attenuation model assumed that the target was small, thus neglecting the path length difference to different points on the target. This is a good assumption at large distances. When the target is close however, this plays more of a role.

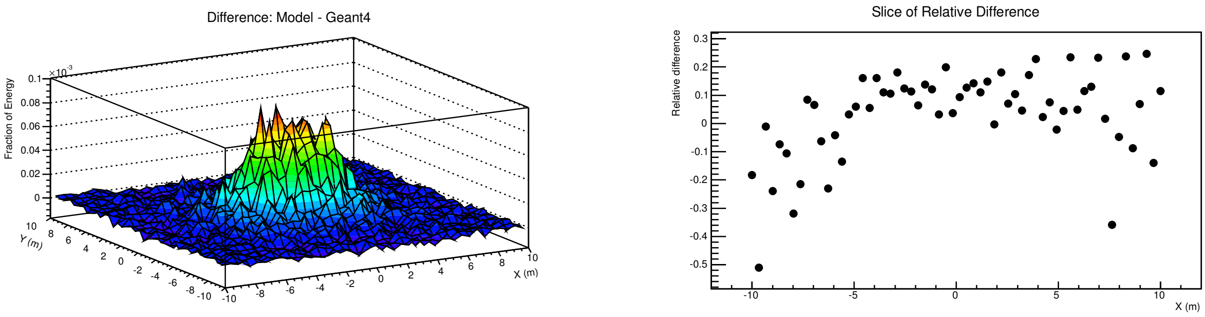

Figure 4. Difference between models, and relative difference between models for constant y.

5. Conclusions

We have developed two techniques for finding position specific radiation exposures due to specific geometries of radioactive material. The results for each are in close correspondence, increasing our confidence in both techniques. The attenuation model is quick to calculate, and is useful for simple geometries such as cuboids. Calculating the data for figure 3 took seconds on a personal computer. The Geant4 simulation is far more powerful, as it can simulate any geometry, and can easily be extended to include layers of shielding etc. The downside is that it is far more computationally intensive. A single (x, y) point from figure 3, with one million events, took 5 minutes to compute on a personal computer. The University of Johannesburg's cluster computer [7] was therefore used. It took about four and a half hours to compute the data shown (3 600 points). Fewer events can be used per point, but this increases the stochastic roughness.

The final step now remains to create an actual body of irradiated material and measure energy deposited at different points to compare to the models described above.

References

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[6] Brun R and Rademakers F 1997 *Proceedings AIHENP'96 Workshop, Lausanne, Sep. 1996, Nucl. Inst. & Meth. in Phys. Res.* A **389** 81–86 see also http://root.cern.ch/.

[7] See webpage for details: URL `http://physics.uj.ac.za/cluster`