# Monte carlo simulation of different positron emitting radionuclides incorporated in a soft tissue volume

## Abstract

Monte Carlo calculations were carried out where compounds with positron-emitters radionuclides, like FDG ( $^{18}$ F), Acetate ( $^{11}$ C), and Ammonium ( $^{13}$ N), were incorporated into a soft tissue volume, in the aim to estimate the type of particles produced their energies, their mean free paths, and the absorbed dose at different distances with respect to the center of the volume. The volume was modeled with a radius larger than the maximum range of positrons in order to produce 0.511 keV annihilation gamma-ray photons. With the obtained results the absorbed dose, in various organs and tissues able to metabolize different radiopharmaceutical drugs, can be estimated. The code used was GEANT4.

Key words: Positrons, Absorbed dose, Monte Carlo simulation.

#### Abstract

Se llevaron a cabo cálculos por el Método Monte Carlo con diferentes compuestos de radionucleidos emisores de positrones, tales como el FDG (<sup>18</sup>F), acetato de carbono (<sup>11</sup>C), amonio (<sup>13</sup>N), etc, los cuales fueron incorporados en un volumen de tejido blando, con el propósito de estimar el tipo de partículas producidas y sus energías, los caminos libres medios y las dosis absorbida de radiación a diferentes distancias con respecto al centro del volumen. El volumen de tejido fue modelado con un radio más grande que el alcance máximo de los positrones, luego de producirse el proceso de aniquilación emitiendo fotones de 0.511 MeV. Se obtuvieron resultados de dosis absorbida y alcances máximos para varios órganos y tejidos y diferentes radiofarmacos. El código de simulación utilizado fue el GEANT4.

Palabras clave: Positrones, Dosis absorbida, simulación Monte Carlo

## 1. Introducción

The Monte Carlo method used to simulate the radiation interaction with matter allows understanding the energy delivered into the volume of interest, and to know the dynamics of the particles produced, how are their trajectories, the mean free path and the maximum range in relation to the properties of the emitting radionuclide. In nuclear medicine application the positron-emitting radionuclide is attached to a particular molecule and later is incorporated into the body through inhalation, injection, or ingestion. The radiopharmaceutical is metabolized into a tissue or organ and then the positrons emitted from the nucleus interact with electrons of the medium producing annihilation gamma photons [1]. The diagnostic image is formed by the emission of gamma photons in opposite directions that reach the PET detector array. Having an array of detectors configured ringshaped, reconstructs the volume image based on distributed positrons and therefore in vivo measurements can determine the location and size of the lesion.

Before interacting with the electrons, positrons delivered its energy to the medium through collisions and when they have reach an energy of 511 keV they annihilate with electrons to form two photons of 511 keV, that traveling in opposite directions, about 180  $\pm$ 0.5 degrees [2]. The mean free path of positrons is responsible for the resolution of the diagnostic image. The lower the path before annihilation, volume interactions occur will be smaller, improving image quality [3].

The spatial resolution is also improved by the sensitivity and size of PET detectors. Annihilation processes can be lost in the detection if they fail to reach the detectors or whether electronics of coincidence window record an event as no true. Basically, when achieve lower path before annihilation, it will have information more precise about spatial location of the lesion and the outline of the volume of interest will delimit with more accuracy, allowing discard normal metabolic processes compared with potential tumor growths [4].

#### 1.1. Theoretical basis

Positron Emission Tomography (PET) is equipment used in the field of nuclear medicine, where a patient or a living creature who has been previously administrated small quantities of radioactive material through inhalation, injection or ingestion, which is metabolized in the interest organ or tissue. Afterwards, radioactive material disintegrates producing transitions in which a proton decays into a neutron, emitting a positron (positive beta particle) and a neutrino. The interaction between a neutrino and matter has no relevance, but the positron with an energy of 1.022 MeV interacts with an electron in the medium and produces an annihilation where two 511 keV gamma photons in antiparallel direction to each other and are responsible of the formation of the diagnostic image. See Figure 1, [3], [5, 6, 7].



Figura 1. Annihilation process and gamma photons production.

The radioactive isotopes used in the PET are produced in a medical cyclotron in which usually a high energy proton beam is fired into an appropriate target. To produce <sup>18</sup>F and <sup>18</sup>O water target undergoes the nuclear reaction <sup>18</sup>O(p,n)<sup>18</sup>F, indicating that a proton (p) is absorbed and a neutron (n) lost. The most common cyclotron configuration for PET is the negative ion design, which consist of two "dee" electrodes, which are about 1m in diameter. Subsequently, radionucleide is taken to a radiochemistry laboratory, where they are combined with a chemical substance called tracer for latter administration. The mainly used radiopharmaceuticals are shown in Table1, [8].

The remarkable progress of computers and software, miniaturization and better detector efficiency lead to continuous improvement of X-ray CT, especially in reducing radiation doses in patients. The Monte Carlo method is considered to be a powerful tool to simulate a physical phenomenon of radiation interaction with the matter and obtain a precise estimation of several physical parameters of a real situation [9, 10, 11].

The purpose of this work was to determine the

Tabla 1. Main	isotopes	used in	PET [10].
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Isotope	Tracer	Physiological process	Mainapplication
<sup>11</sup> C	Methionine	Protein Synthesis	Oncology
<sup>11</sup> C	Raclopride	D2 Receptor	Movement disorder
<sup>13</sup> N	Ammonia	Blood Perfusion	Myocardial perfusion
<sup>15</sup> O	Water/Dioxise	Blood Perfusion	Brain activation
<sup>18</sup> F	Fluorine Ion	Bone Metabolism	Oncology
<sup>18</sup> F	Fluorine deoxyglucose	Glucose Metabolism	Oncology Neurology Cardiology

behavior of positrons from different emitting radionuclides with respect to its interaction with a volume of soft tissue, performing a statistical mean free path and the maximum range of the particles in order to assess what kind of radionuclide from the point physically it is more convenient according to the size of the lesion. In this work was used Geant4 Monte Carlo simulation code software.

## 2. Materials and Methods

The work was carried out using the Geant4 code; in the simulation model was constructed several 10 mm-radius spheres, considering that sphere radius must be greater than maximum range of positrons used in nuclear medicine for water. The materials of elemental spheres were chosen: water, muscle, adipose tissue and compact bone tissue, the components by weight they are taken from [12].

The radioactive source is located in the center of the sphere with 10.000 initial radioactive nuclei. Positrons interact with the matter creating ionizations and delivering energy until to produce the annihilation gamma photons. Subsequently, the simulation data are sent in ROOT software for processing and analysis of multiple interactions.

In the Figure 2a it shows the simulation with 10 decays, in the Figure 2b it shows the simulation with 3 decays of <sup>18</sup>F in water. We can be observed positrons trajectories before happens the annihilation process and ionization produced.

List physical reference Geant4 LBE 5.3 was used because allows information about the decay processes at the same time that positrons are emitted. With this application we can know the history of events interaction positrons until annihilation with electrons of the medium [13].

Results for various positron emitting radionuclides and various tissues were compared in relation



Figura 2. Simulation decays in <sup>18</sup>F.

to energy deposited into sphere mass to determine the dose absorbed by the tissue [14]. We can see in both figures the path streams of positrons, as soon path ends appears straight lines that joining the annihilation photons. Radial distance between origin and annihilation point is the maximum length of one positron.

## 3. Results

In the Figure 3 it show the average range of positrons emitted from by <sup>18</sup>F, <sup>11</sup>C and <sup>15</sup>O, we might show at the center of each sphere the intensity and the length lines that represent the region where positrons delivered its energy based on initial energy of positrons. Below are shown the maximum length and average distance calculated through Gaussian fitting.

Where Full Width Half Maximum (FWHM) =  $2\sqrt{2\ln 2 \sigma} = 2,355 \sigma$ , corresponds to average range of positrons. Full Width Tenth Maximum (FWTM)  $= 2\sqrt{2\ln 10 \sigma} = 4,292 \sigma$  corresponds to maximum length reached by positrons.



*Figura 3.* Maximum length for: a)  ${}^{18}$ F=2.4 mm b)  ${}^{11}$ C=5.0 mm c)  ${}^{15}$ O=8.2 mm.

Simulation data are stored in ROOT software and are shown the results in following histograms, see Figure 4. In Figure 4 shows the largest frequencies are given for shorter maximum lengths. It's clear to see that as much energy delivered by positrons in a small range and the greatest contribution is obtained by <sup>18</sup>F.

The relation between maximum length in water sphere and compact bone for <sup>18</sup>F is 1.880, <sup>11</sup>C is 1.673 and <sup>15</sup>O is 1.920, this meaning that there is a relationship between tissue density and maximum length. A higher density of tissue decreases the maximum length. In Table2 shown the maximum lengths in different tissues.

In Figure 5 the functional relationship between the energy of positrons corresponding to the three radionuclides simulated <sup>18</sup>F, <sup>11</sup>C and 150 and the maximum length of the positrons have a linear behavior. Allowing predict the range of positrons for any medium in terms of energy. Taking account decay time for each radionuclide and the relationship between the number of positrons simulated and the activity was evaluated the absorbed dose into the volume. The results are shown at the Table3.



*Figura 4.* Figure 4. The maximum length in water sphere (a) and compact bone (b).



*Figura 5.* Relation between positron energy and maximum length for blood, adipose and muscle tissue).

This work can be extended to situations where knowing the volume and density of a tumor the radiopharmaceutical covers fully the region of interest not exceeding the amount of radioactive material in order to obtain an accurate diagnosis reducing the absorbed dose to the patient and the workers that delivered it.

## 4. Conclusions

Using different positron emitters is established that type of radionuclide it is needed for each kind of lesion and its volumetric configuration. The Monte Carlo method can accurately assess the maximum and averages ranges for any tissue and generally

Isotope	Water	Adipose Tissue	Muscle Tissue	Compact Bone
		[mm]		
<sup>18</sup> F	$2.319\pm0.003$	$2.457\pm0.003$	$1.854\pm0.003$	$1.233\pm0.002$
<sup>11</sup> C	$3.438\pm0.003$	$3.785\pm0.003$	$2.723\pm0.003$	$2.055\pm0.002$
<sup>15</sup> O	$6.970\pm0.003$	$7.365\pm0.003$	$5.508 \pm 0.003$	$3.630\pm0.002$

Tabla 2. Maximum lengths in different tissues.

Tabla 3. Absorbed dose in a distance from center of sphere.

Isotope	Distance	Dose rate	Dose integrated
		Dose Tale	in 10 minutes
	[mm]	$[mSv \cdot h^{-1}]$	[mSv]
<sup>18</sup> F	2	$0.356\pm0.01$	$0.119\pm0.01$
<sup>11</sup> C	3	$0.427\pm0.01$	$0.142\pm0.01$
<sup>15</sup> O	6	$0.608\pm0.01$	$0.203 {\pm}~0.01$

a lot of materials that are defined in the database Geant4 simulation code.

The maximum length of the positrons before annihilation is directly related to the spatial resolution of diagnostic images. The smallest maximum range gives the largest spatial resolution. This is one of the reasons why most studies with positron emission tomography are carried out with the compound FDG based on  $^{18}$ F.

The absorbed dose into the volume depends of initial energy of positrons. The 18F due to have lowest energy compared with <sup>11</sup>C and <sup>15</sup>O allows reduce the absorbed dose in a tissue.

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