

# Positron range and coincidence non-collinearity in SimSET<sup>1</sup>

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## Abstract

We have modified SimSET to model positron range and annihilation radiation non-collinearity. Positron range in water is sampled using the empirical model developed by Palmer and Brownell [1]. The positron is projected from the decay location in a random direction with adjustment for the density and effective atomic number and weight of intervening tissues. The positron range algorithm was validated by comparing simulated range distributions to the model and with data published by Derenzo [2].

Annihilation non-collinearity is simulated as a Gaussian-distributed variation from 180 degrees with a standard deviation of 0.5 degrees. Tests verify the simulated non-collinearity is Gaussian distributed and that the azimuthal angle is unbiased.

## I. INTRODUCTION

SimSET (a Simulation System for Emission Tomography) is a public domain simulation of SPECT and PET imaging. It provides photon tracking through the tomograph field-of-view (FOV), collimator and detector models for PET and SPECT, an ideal detector model, and user-configurable binned output. For PET, the currently distributed version models annihilation at the point of decay, with the coincidence photons travelling collinearly. However, positron range, the distance a positron travels from the decay that creates it, and annihilation photon non-collinearity are limiting factors in the design of high resolution scanners and studies using them [3, 4]. Thus we have created a new version of SimSET that models both these effects.

A positron travels some distance from the decay that creates it, losing momentum until it annihilates with an electron. Levin and Hoffman [5] have reported a simulation that models positron trajectories by modeling the underlying processes. The simulation shows good agreement with experimental data. However, we judge this method to be too complicated and time-consuming for SimSET: too much simulation time would be spent tracking positrons as opposed to photons.

Derenzo [2, 6] and Palmer and Brownell [1] have developed simpler parameterized models for positron range. The models are in good agreement with experimental data acquired by Derenzo. Both give empirical parameterizations of the positron range projected onto a plane, which SimSET can not use directly to simulate positron ranges. However, Palmer and Brownell's parameterization is derived from a semi-empirical expression for positron range developed by Tabata et al [7]. We use Palmer and Brownell's simplification of Tabata's expression to calculate positron range.

When positron annihilation occurs, two photons are created heading in opposite directions. There is a slight deviation from collinearity caused by the momentum of the positron-electron pair relative to the tomograph reference

frame. We model this as a Gaussian deviation from collinearity, using parameters given in Evans [8].

## II. ALGORITHMS

### A. Positron Range

Given a positron emission location, SimSET determines an annihilation location using the following three steps: (1) generate a positron emission energy, (2) sample the positron range in water from a distribution dependent on the emission energy, (3) project the positron in a random direction, adjusting the range to account for variations in the attenuating materials.

An isotope's distribution of positron emission energies depends on its endpoint energy(s) ( $E_{\max}$ ), branching ratio, and atomic number ( $Z$ ) [9]. For an isotope with only one endpoint energy, the probability of a positron with emission energy,  $E$ , is proportional to

$$N(E)dE = (E_{\max} - E)^2 W_p F(Z, W) \quad (1)$$

where  $E$  is the emission energy in keV,  $W = 1 + E/511$ , the momentum,  $p$ , is

$$p = \sqrt{W^2 - 1}, \text{ and} \quad (2)$$

$$F(Z, W) = \frac{2\pi\eta}{1 - e^{-2\pi\eta}} \quad (3)$$

$$\text{with } \eta = \frac{-ZW}{137\xi}. \quad (4)$$

For isotopes with multiple endpoint emission energies,  $N(E)$  should be computed for each endpoint energy, and summed, weighted by the branching ratios. SimSET randomly samples energies from a step-function approximation to the resulting density function.

Once the positron emission energy is chosen, the positron range in water is chosen using Palmer and Brownell's algorithm [1]. They model the annihilation density as a three-dimensional, symmetric Gaussian

$$D(\mathbf{r}) \approx \frac{1}{(\sqrt{2\pi}\sigma_{\text{water}})^3} e^{-|\mathbf{r}|^2 / 2\sigma_{\text{water}}^2} \quad (5)$$

where  $\mathbf{r}$  is a three-dimensional vector from the decay to the annihilation point, and  $\sigma_{\text{water}}$  is the energy-dependent standard deviation.

To compute  $\sigma_{\text{water}}$  we first compute the effective atomic number and weight of water. We use Tabata et al's definitions for these quantities,

$$Z_{\text{eff}} = \sum_i f_i Z_i \quad (6)$$

$$A_{\text{eff}} = Z_{\text{eff}} \left( \sum_i f_i (Z_i / A_i) \right)^{-1} \quad (7)$$

where the summation is over the constituent elements of the material and  $f_i$ ,  $Z_i$ , and  $A_i$  are the fraction by weight, atomic number, and atomic weight of the  $i$ th element.

Next we compute the extrapolated range,  $R_{ex}$  [10]:

$$R_{ex} = 0.1 \frac{b_1 E^2}{b_2 + E} \quad (8)$$

where  $E$  is the positron emission energy in MeV, and

$$b_1 = \frac{4.569 A_{eff}}{Z_{eff}^{1.209}} \left( \frac{g}{\text{MeVcm}^2} \right) \quad (9)$$

$$b_2 = \frac{1}{2.873 - 0.02309 Z_{eff}} (\text{MeV}) \quad (10)$$

Now we define  $\sigma$  as:

$$\sigma = \frac{R_{ex}}{2d} \quad (11)$$

where  $d$  is the density of the material the positron is traveling through in g/cc. (This is slightly different from Palmer and Brownell's formulation to allow for variations in material.)

In SimSET, the object in the tomograph FOV may be voxelized with a different material in each voxel. The experiments Tabata et al based their formula for  $R_{ex}$  on all used homogeneous absorbers. To adapt this to heterogeneous absorbers, we note that while  $R_{ex}$  assumes the absorber consists of a single material, it makes no assumptions about the density of the material; the density could even be heterogeneous. The  $A_{eff}$  and  $Z_{eff}$  of biological materials are all in a relatively small range, and therefore the  $R_{ex}$  for a given energy will also fall in a small range. Thus, to choose an annihilation location we randomly sample a positron range in water,  $r_{water}$  from the density function given in equation 5. We then project the positron from the decay in the direction given by  $r_{water}$ , adjusting the distance traveled,  $T = \sum_j t_j$ ,

until

$$\sum_j t_j \frac{\sigma_{water}}{\sigma_j} = |r_{water}| \quad (12)$$

where the summation is over the voxels that the positron is projected through,  $t_j$  is the distance through the  $j$ th voxel, and  $\sigma_j$  is computed using equations 6-11 and the same  $E$  used to compute  $\sigma_{water}$ .

### B. Non-collinearity

SimSET models the deviation from collinearity as a Gaussian random variable,  $\theta$ , with mean  $m=0$  and standard deviation  $\sigma = 0.0037059$  radians ( $= 0.5$  degrees FWHM). One of the two coincidence photons, chosen randomly, is then deflected from collinearity by angle  $\theta$ , with a random azimuthal angle of deflection.

## III. TESTING

### A. Positron Range

Three sets of tests were carried out to test our positron range algorithm and implementation. The first set of tests checked the positron emission energy spectrums produced by SimSET. The second set of tests compared the distribution of ranges generated by SimSET with those given in equations 6-11. The final set of tests compared data generated by SimSET with experimental data acquired by Derenzo.

To test SimSET positron emission energy spectrums, we first compared  $^{11}\text{C}$  and  $^{18}\text{F}$  spectrums computed directly from equations 1-4 with spectrums reported by Levin and Hoffman. Then we compared the spectrums produced by SimSET for  $^{11}\text{C}$  and  $^{82}\text{Rb}$  with spectrums computed from equations 1-4.

We tested the distribution of positron ranges in water and in lung by creating a fictional isotope with a positron emission spectrum consisting of 2 delta functions, at 200 keV (40%) and 1000 keV (60%). The expected distribution of ranges from such an isotope would be the weighted sum of two Gaussians defined by equations 6-11. We also tested positron ranges in a heterogeneous object by creating a fictional isotope with 100% of its positron emission energy at 1000 keV and looking at positron ranges from a point source at the origin in an object consisting of three layers axially: lung from  $-4$  cm to  $-0.25$  cm, water from  $-0.25$  cm to  $0.25$  cm, and lung from  $0.25$  cm to  $4$  cm. Only positrons that traveled along the  $z$ -axis ( $|z \cos \theta| > 0.995$ ) were binned. Thus the distance traveled through water will always be  $\sim 0.25$  cm. Thus the expected probability density of travel distances is proportional to

$$p(d) = \frac{\sigma_{water}}{\sigma_d} A(d)^2 \frac{1}{\sqrt{2\pi}\sigma_{water}} e^{-A(d)^2 / 2\sigma_{water}^2} \quad (13)$$

where  $d$  is the distance,  $\sigma_d$  is the standard deviation for the material at  $d$

$$\sigma_d = \begin{cases} \sigma_{water} & d < 0.25 \\ \sigma_{lung} & d \geq 0.25 \end{cases} \quad (14)$$

and  $A(d)$  is an adjusted distance

$$A(d) = \begin{cases} d & d < 0.25 \\ ((d - 0.25)\sigma_{water} / \sigma_{lung}) + 0.25 & d \geq 0.25 \end{cases} \quad (15)$$

The final tests compared distance-angle binned data from SimSET with data reported by Derenzo [2]. Point sources of  $^{11}\text{C}$  and  $^{82}\text{Rb}$  were simulated at the origin surrounded by 0.0201 g/cc foam and 0.0503 g/cc foam respectively. The simulated tomograph coordinates were taken from Derenzo, with perfect endplates and detectors. A lower energy cutoff of 350 keV was used. The simulation included coherent scatter and annihilation photon non-collinearity.

### B. Non-collinearity

1,000,000 events were simulated with the coincidence photons traveling from  $(0,0,0)$  in opposite directions along the  $x$ -axis before the adjustment for non-collinearity. After adjustment, the photons were tracked through air to a 100 cm radius target cylinder. All unscattered coincidences were

binned (1) according to which photon had been deflected, (2) by the (y,z) coordinates of the deflected photons, and (3) by the angle of deflection,  $\alpha$ :

$$\alpha = \arcsin\left(\frac{\sqrt{y^2 + z^2}}{100}\right) \quad (16)$$

We used binning method (1) to look for bias in the choice of the deflected photon. Row and column sums of method (2) were examined for any evidence of bias in the azimuthal angle of scatter. The distribution of angles in method (3) was compared to the Gaussian distribution we use to model non-collinearity.

#### IV. RESULTS

##### A. Positron Range

Spectrums generated for  $^{11}\text{C}$  and  $^{18}\text{F}$  using equations 1-4 agree with the data presented in Levin and Hoffman. The spectrums generated for  $^{11}\text{C}$  and  $^{82}\text{Rb}$  using SimSET show the staircase pattern expected from a step-function approximation as well as some statistical noise, but are in general agreement with spectrums generated using equations 1-4. Figure 1 compares the SimSET spectrum with the spectrum generated by Equation 4 for  $^{11}\text{C}$ .

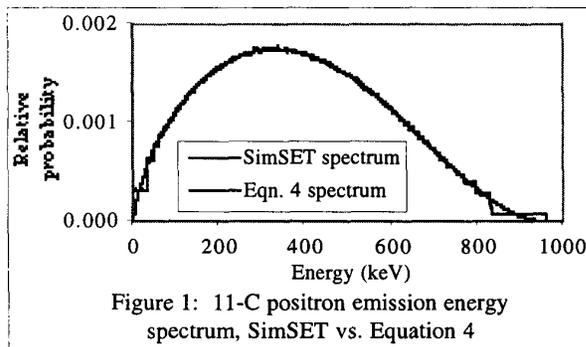


Figure 1:  $^{11}\text{C}$  positron emission energy spectrum, SimSET vs. Equation 4

The SimSET distributions of positron annihilations in lung and water from the fictional two-delta function spectrum isotope match the theoretical distributions well. The curves are indistinguishable, as is shown for water in Figure 2.

Similarly, in the test of the heterogeneous water-lung object, the SimSET range distribution matches the theoretical distribution given in Equation 13 well. However, the curves are distinguishable in near the boundary between water and lung (Figure 3). We believe this is caused by the fact that the positrons are not forced to travel exactly in the axial direction, and hence the positrons in SimSET will travel slightly further than 0.25 cm in water.

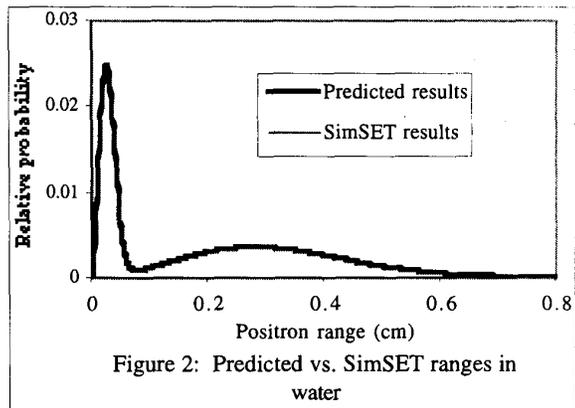


Figure 2: Predicted vs. SimSET ranges in water

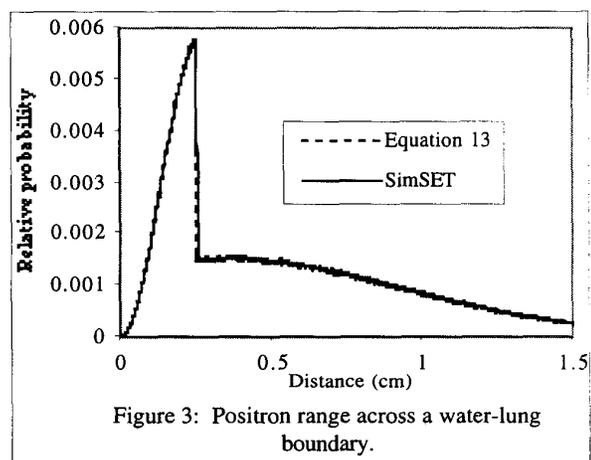


Figure 3: Positron range across a water-lung boundary.

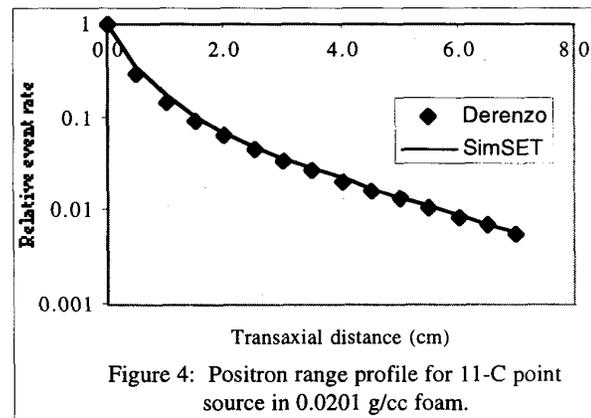


Figure 4: Positron range profile for  $^{11}\text{C}$  point source in 0.0201 g/cc foam.

In Figure 4 we compare profiles from a simulated  $^{11}\text{C}$  point source in 0.0201 g/cc foam with data reported by Derenzo. Figure 5 shows the same comparison for a  $^{82}\text{Rb}$  point source in 0.0503 g/cc foam. In both cases the simulated data is in close agreement with the Derenzo data.

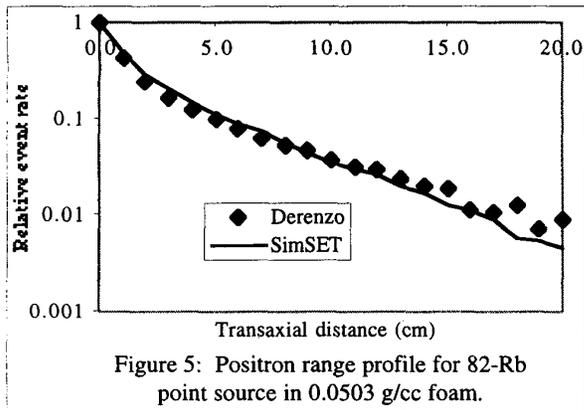


Figure 5: Positron range profile for 82-Rb point source in 0.0503 g/cc foam.

### B. Non-collinearity

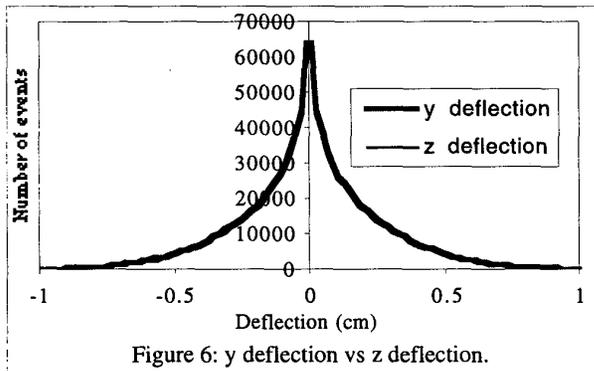


Figure 6: y deflection vs z deflection.

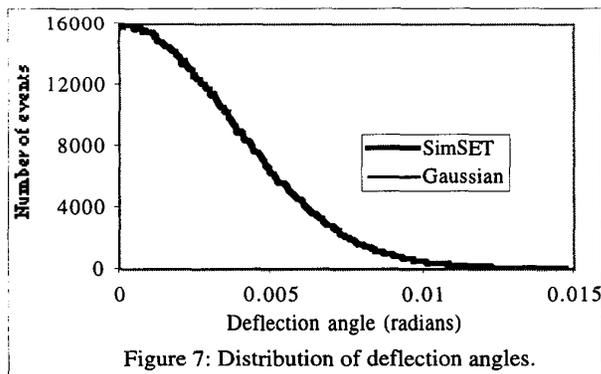


Figure 7: Distribution of deflection angles.

Out of 1000000 decays, the photon moving in the positive x direction was deflected 500093 times, the photon moving in the negative x direction was deflected 499686 times, and 221 decays were discarded when one or both of the photons scattered before reaching the cylinder.

Figure 6 compares the sum over all y and the sum over all z of the data binned by y and z position on a 100 cm radius cylinder. The two curves overlay each other so closely it is impossible to tell them apart. Similarly, plotting the deflection angle against a Gaussian with a standard deviation of 0037059 radians yields two indistinguishable curves (Figure 7).

## V. CONCLUSION

The positron range and non-collinearity algorithms appear to be properly implemented.

We made several approximations in the positron range algorithm. However, the excellent fits to Derenzo's data shown in Figures 6 and 7 indicate that the approximations did not cause significant bias.

## VI. REFERENCES

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