A Simple Monte Carlo Approach to the Diffusion of Positrons in Gaseous Media

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Abstract

In this work, we present and characterize a simple model to study the diffusion of positrons within a certain gaseous medium, which can be composed by one or more types of molecules or atoms. The positron-atom interaction is described by the partial cross sections for positron-*target* scattering, where *target* is one of the medium's components. In order to characterize the positron dynamics, we calculate quantities as the Doppler-shifted annihilation signal, penetration depths, the mean lifetime of positrons, the most probable ionization/excitation distances, and some other quantities. Simulations of this kind may be useful, for example, for astrophysicists to analyze the interstellar medium or for medical physicists to study the Positron Emission Tomography technique.

Introduction

When a high energy positron goes toward some solid, liquid or gaseous medium, it is expected to cause several ionizations, electronic excitations, molecular dissociations and other inelastic processes, transferring its kinetic energy to the medium until it reaches energies of the order of $1\ eV$ to $10^{-3}\ eV$ (thermal energies), below which the positron's destiny is certainly annihilation.

Analysis of the annihilation signal peaked around $511\ keV$ are specially useful in solid state [1], medical [2] and astrophysics [3, 4], because its Doppler shift brings information about the energy of the environment electrons which annihilate with the positrons.

Stochastic methods, like the Monte Carlo track-structure approach, are able to get the trace of the positrons along the medium and also to calculate parameters such as the positrons' average path from its source, the deposited energy in the medium, stopping powers and the energy distribution of the photons produced in the annihilation processes.

Champion and Le Loirec [2] produced simulations of this kind for positrons in aqueous medium in order to simulate *Positron Emission Tomography* (PET). On the other hand, Guessoum *et al* [4] developed a similar approach to track positrons in the interstellar medium. Positrons have a special role in many astrophysical environments, such as sunspots, supernovae and active galactic nuclei [5]. So their realization was to characterize the positron dynamics in the interstellar medium and to derive the annihilation signal expected from the Doppler broadening process, since photons are the main source of astrophysical information.

We present a computational model for diffusion of positrons in a gaseous predefined medium, which may be composed by one or more kinds of atoms or molecules. All the information about the medium itself, beyond the densities of its components, is contained in the cross sections for positron-*target* scattering, where *target* is one the medium's components, which, as a test problem, may be helium, neon or argon, or a mix of helium and argon at different ratios.

Computational Model

- Input data and interaction sorting

$$\sigma_{TOT}(E) = \sum_{i=1}^{N} \sigma_i(E) \tag{1}$$

where σ_i is the cross section for the i-th collisional channel (for instance, we can consider i $= 1$ for elastic, i $= 2$ for positronium, etc). Dividing it by σ_{TOT} we get:

$$\frac{1}{\sigma_{TOT}} \sum_{i=1}^{N} \sigma_i = \frac{\sigma_1}{\sigma_{TOT}} + \ldots + \frac{\sigma_N}{\sigma_{TOT}} = \sum_{i=1}^{N} \sigma'_i = 1 \tag{2}$$

where we defined $\sigma'_i \equiv \sigma_i/\sigma_{TOT}$ as a relative cross section.

Treating the relative cross section as the probability for the corresponding interaction, we can sort a homogeneously distributed random number in the interval $[0, 1]$ and match it with the probabilities in order to select the desired interaction.

- Positron displacement is given by the mean free path λ of any particle in a given medium:

$$\lambda = \frac{1}{n\sigma_{TOT}(E)} \tag{3}$$

where n is the number density of the scattering centers by volume unit and $\sigma_{TOT}(E)$ is the total cross section, given in the previous item, for positron scattering by the selected target. With the mean free path, we can calculate the mean time associated:

$$t = \frac{\lambda}{v}$$

where $v = \sqrt{2E/m_0}$ is the positron mean velocity while moving a distance λ. The energy E and the rest mass of the positron m_0 are parameters of the simulation, therefore:

$$t = \lambda\sqrt{\frac{m_0}{2E}}. \tag{4}$$

The direction of the scattered positron is randomly chosen by sorting a polar (θ) and an azimuthal (φ) angle, so we can decompose the mean free path to calculate the positron's new position:

$$x_{i+1} = x_i + \lambda \sin\varphi \cos\theta$$
$$y_{i+1} = y_i + \lambda \sin\varphi \sin\theta$$
$$z_{i+1} = z_i + \lambda \cos\varphi. \tag{5}$$

If the positron gets out of the sphere with radius defined by the input volume of the medium, we consider it automatically annihilated.

- Annihilation and Doppler shift calculation is treated according to Humberston and Van Reeth [10]:

$$\Delta E_1 = |p_1 - p_0|\, c = \frac{p^w_{CM}}{2}$$
$$\Delta E_2 = |p_2 - p_0|\, c = -\frac{p^w_{CM}}{2}. \tag{6}$$

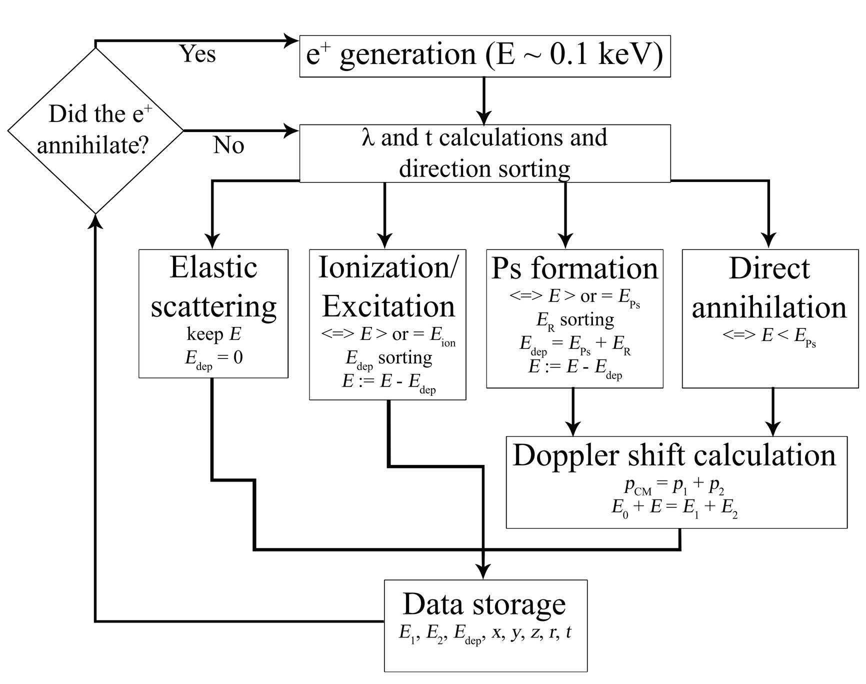

Figure 1: Algorithm flowchart. The parameters x, y and z are the positron's spatial position, r is its radial position, E_{dep} is the energy deposited in the medium and E_1 and E_2 are the Doppler shifted energy of the two photons from the annihilation process, if it had happened.

Preliminary Results

	He	Ne	Ar	He 75% + Ar 25%	He 50% + Ar 50%	He 25% + Ar 75%
Amount of positronium annihilations	99136	99601	99624	74513 24955	49189 50384	24931 74719
Amount of ion/exc events	265061	240799	241236	201265 61000	133036 121078	66736 181580
Amount of elastic collisions	87555	217507	112872	28619 66229	56958 43625	85326 21977
Total number of collisions	451752	557907	453732	114574 342007	228420 225850	341625 113644
Average number of collisions	4.5	5.6	4.5	4.6	4.5	4.6
Total deposited energy (KeV)	2881	2483	1872	2642	2377	2131
Average lifetime (ns)	80.97	52.69	9.88	63.76	45.42	27.79
Average reach (mm)	186.86	107.86	22.32	158.97	125.91	84.98
Average ion/exc distance (mm)	178.32	103.42	21.87	154.22	123.15	83.63
Gaussian FWHM for spectrum (KeV)	5.89	6.26	6.92	5.95	6.18	6.57

Table 1: Overview of the simulated media. An amount of 100000 positrons were generated for each gas mixture. Each considered media had a number density of scattering centers of 1.660539×10^{-3} mol/m^3. We have less annihilations than positrons because some annihilated going to an energy region where we did not have any data, or going outside the considered spatial volume (a sphere of 1 m^3). No positron suffered annihilation below the positronium threshold.

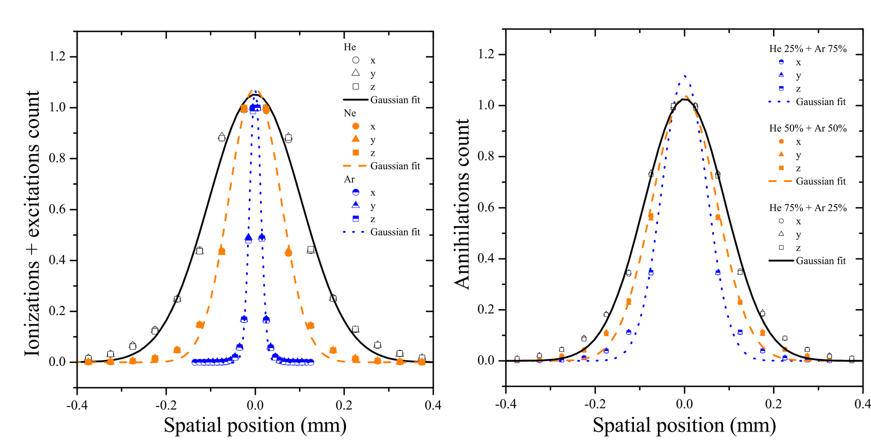

Figure 2: Comparison of the spatial distributions of the inelastic processes for all the considered media, fitted by Gaussian curves.

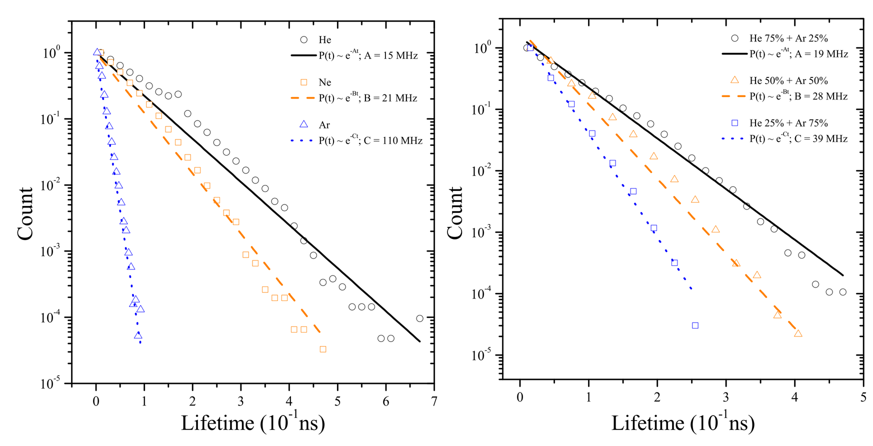

Figure 3: Comparison of the lifetime distributions for positrons' dynamics within all the considered media. The data were fitted by exponential distributions.

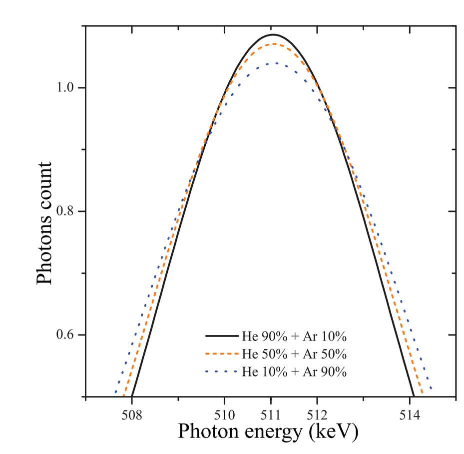

Figure 4: Comparison of the annihilation photons spectra for single-component media and mixture media. Notice that even though the data were not in a satisfactory Gaussian shape (although they can be fitted by 3-peak Gaussians), the fitted single-peak Gaussians are such that we can distinguish between the different media. The same happens for the mixture situation: the higher the concentration of Ar, the similar it becomes to the single-component Ar simulation.

Conclusions and Expectations

Through this work, we developed a simple Monte Carlo diffusion model for positrons in gaseous medium. We were able to characterize the atomic species by their annihilation spectra, even though they had to be fitted by a Gaussian function, due to the considerably amount of annihilations in relatively big energies (greater than the positronium threshold for each medium) and to discard the triplet annihilation channel even for positronium. Just for the record, these could be implemented, with a better description of the media with DCS's and orbital energies in order to enhance the accuracy of the simulations. The results obtained are promising and show that understanding the positrons' dynamics in different media can be useful to identify the medium components. To this extent was the work of Guessoum *et al* [4] in order to get a better comprehension of the interstellar medium.

Besides, with media like H_2O and radioactive positron sources, as did Champion and Le Loirec [2], the spatial, radial and lifetime distributions are of interest for the PET industry, since they have to optimize the detection of the annihilation photons and to minimize the damage to the patients' health.

Finally, this model resembles a diffusion model, since we have Gaussian spatial distributions for the positrons after some time period of evolution of the system, as evidenced by the annihilation and ionization/excitation spatial position distributions.

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