Monte Carlo modelling of positron transport in real world applications

S Marjanović, A Banković, M Šuvakov and Z Lj Petrović

Institute of Physics, University of Belgrade, 118 Pregrevica, 11080 Belgrade, Serbia

E-mail: msrdjan@ipb.ac.rs

Abstract. Due to the unstable nature of positrons and their short lifetime, it is difficult to obtain high positron particle densities. This is why the Monte Carlo simulation technique, as a swarm method, is very suitable for modelling most of the current positron applications involving gaseous and liquid media. The ongoing work on the measurements of cross-sections for positron interactions with atoms and molecules and swarm calculations for positrons in gasses led to the establishment of good cross-section sets for positron interaction with gases commonly used in real-world applications. Using the standard Monte Carlo technique and codes that can follow both low- (down to thermal energy) and high- (up to keV) energy particles, we are able to model different systems directly applicable to existing experimental setups and techniques. This paper reviews the results on modelling Surko-type positron buffer gas traps, application of the rotating wall technique and simulation of positron tracks in water vapor as a substitute for human tissue, and pinpoints the challenges in and advantages of applying Monte Carlo simulations to these systems.

1. Introduction

Owing to the antimatter nature of positrons, it has always been a struggle to obtain large numbers of positrons and store them for long periods of time [1]. The development of buffer gas positron traps (or Surko traps) [2,3,4,5,6] over the last two decades allowed for a constant increase in positron yields and storage times. This advancement in the experimental facilities for handling positrons led to an increased accuracy in the measurements of cross-sections for positron-matter interaction for various atoms and molecules, especially at lower energies [7,8]. In turn, the assembled cross-section data sets, if sufficiently complete (in terms of number, momentum and energy balances) [9], can be used as an input for different theories and computer simulations.

With the exception of few cases where obtaining positron plasma is the primary experimental goal [3], most positron experiments do not reach, or even aim at, such high particle densities where positron-positron interactions control the properties of the ensemble [4,5,6]. Other positron applications, like positron emission tomography (PET) scans, due to their nature, also do not produce a high enough positron density to observe positron-positron interactions. This is why most real-world applications of positrons can be analyzed using swarm calculations. The Monte Carlo technique [10], in particular, lends itself perfectly to modelling experimental conditions and geometries, as opposed to the Boltzmann codes [11], where the boundary conditions implementation can be very complicated.

1 To whom any correspondence should be addressed.
Additionally, the Monte Carlo technique accuracy is limited only by the quality of the statistics (i.e., calculation time) and the accuracy of the cross-sections.

As many modelled applications require treatment of positrons at nearly thermal energies, it is important to include thermal effects into the calculations. Concerning the Monte Carlo technique, the problem of thermalization has only recently been adequately solved [12] providing a proper finite value of the mean energy. This technique is included in the present simulation.

2. Modelling buffer gas positron traps

The buffer gas positron trap (Surko trap) is a cylindrical device filled mostly with nitrogen gas that is used to capture, accumulate and cool a large number of positrons. Typically, the number of captured positrons ranges from $10^5$ – $10^7$ e+/s with trapping efficiencies of 10 – 25% [2,3,4,5,6].

The main operating principle of the Surko trap is the utilization of a $^1\Sigma_1$ electron excitation of the $\text{N}_2$ molecule [2]. The incoming positron energy is adjusted by a bias potential to target the cross-section for this molecule excitation just above its threshold where the process cross-section is comparable with the cross-section for positronium (Ps) formation. Through this excitation, the positrons transfer energy to buffer $\text{N}_2$ molecules and remain trapped. The threshold energy for this process is $\sim 8.5$ eV, which is (roughly) the energy that a positron loses in the collision. Unfortunately, the threshold for Ps formation lies very close to the threshold for a $^1\Sigma_1$ electron excitation, so that the efficient trapping window is less than 1 eV wide [2].

We model this interaction of positrons with the $\text{N}_2$ background in our Monte Carlo code [13] by using the cross-section set from [9]. The fact that conditions change along the axis of the trap is taken into account by separating the simulation in three segments with different chamber diameters, gas pressures and electric potentials, which represent actual segments of the apparatus. The conditions in each segment are considered uniform.

The potential gradient existing between the segments of the trap is neglected in the model without reducing the accuracy of the simulation as this transient region is very short, much shorter than the mean-free-path of positrons under the conditions in question. Instead, as a positron reaches the end of a segment, it is immediately transferred to the next one if it has enough axial energy to overcome the potential difference. Its axial energy is increased or decreased depending on the potential difference between the segments and the direction of the positron motion. In the case when a positron’s axial energy is insufficient to overcome the potential barrier, it is reflected back.

To investigate the operation of the trap, we can sample the properties of the swarm of positrons at each stage separately or, sample the entire swarm inside the trap. Through such sampling, we can observe the evolution of the positrons’ energy distribution, and see how inelastic collisions with high thresholds and transitions over different potential levels first split one particle beam into several beams with well-defined discreet energies [13]. This structure is analogous to the Frank-Hertz experiment. In time, and due to collisions with smaller energy losses, these separate beams all relax to a single cloud of positronium at thermal temperature. This can be seen in figure 1, which presents the temporal development of the energy distribution function (EDF) where the magnitude is color coded while the vertical axis represents the energy. The beam enters the trap with 10-eV of energy. It bifurcates for a very brief period of time to two beams when the next stage is entered and

![Figure 1. Evolution of the positrons’ kinetic energy distribution [13].](image-url)
no collisions have occurred. On the other hand, the three-pronged EDF is due to different inelastic collisions and each group represents positrons that have undergone one inelastic collision. Due to elastic and further inelastic collisions (with smaller losses), these three-beam-like distributions merge into one broad distribution that is then thermalized to the trap temperature. The thermalization time may be determined from such a simulation and compared to experiments to verify the model and the cross-sections.

Another aspect investigated by us is the loss processes that take place inside the trap and limit the number efficiency of the trap. What we see in our simulations is that at every occasion where positrons are trapped through a \( ^1\Sigma \) electron excitation of \( \text{N}_2 \), approximately 50% of them are lost to positronium formation. This is due to the fact that the intrinsic energy width of the modern solid neon moderators is \( \sim 1.5 \text{eV} \), which is relatively broad compared to the width of the trapping window between the \( ^1\Sigma \) electron excitation and the \( \text{Ps} \) formation channel of \( \text{N}_2 \). Since most Surko trap applications use a three-[2,3], or two-stage design [4,5,6], the maximum number efficiency that such devices can achieve is 12.5 – 25%. Additional losses may arise due to losses to the walls, direct annihilation, and particles escaping the trap, but these losses can be reduced through experimentation and by changing the geometry and pressures inside the trap.

3. Modelling the rotating wall compression technique

Once all the positrons have been accumulated inside the Surko trap, and in order to use them efficiently in an experiment, the positron cloud needs to be compressed to be as narrow as possible. The rotating wall compression technique has long been applied to compression of single component plasmas [14]. Recently, it has been demonstrated to work even in the single particle regime, but apparently the proposed compression mechanisms differ [15,16]. As the effect occurs under the swarm conditions, our Monte Carlo code is the appropriate tool to analyze this system.

In modelling the rotating wall compression, we follow an approach similar to that of Isaac et al. [17], with the exception of the treatment of positron collisions with the background gas. Instead of adopting an effective viscous term in the equations of motion, we use our Monte Carlo procedure with the full set of interaction cross-sections. As the compression is reported to work for buffer gases that have a strong vibrational channel [16], we run the simulations for \( \text{CF}_4 \) [9]. We can thus observe the compression for different conditions of the applied magnetic and rotating electric fields. The difficulty of employing the MC approach in modelling this particular application lies in the fact that the effect is observable at a ms timescale, while the highest characteristic motion frequency is of the order of GHz. This limits the time step of simulation to the order of several picoseconds and significantly lengthens the computation. Any practical computer code would have to be parallelized in order to achieve results at reasonable execution times. Fortunately, the Monte Carlo approach lends itself perfectly to parallelization as long as this problem is linear in nature. This is why a number of particles can be assigned to each computing unit for calculation while at predefined intervals they each report their state and entire swarm is sampled for its properties.

Figure 2 shows the profile of the positron beam at different moments [18]. The conditions simulated are: 1.5 V of applied rotating voltage at 9.63 MHz; axial magnetic field of 250 Gauss; while the axial bounce frequency of the positrons is 9.49 MHz. The pressure inside the chamber is 40 \( \mu \text{Torr} \) of \( \text{CF}_4 \). The radius of the positron ensemble is half the dimension of the box presented in the figure and is provided above each frame. As the rotating field is applied, the positrons are heated but lose energy preferentially near the center and remain trapped in a narrower distribution. The development is shown in frames. At the same time, the ensemble thermalizes back to a very low mean energy. Both a low energy and a small radius are required in order to optimize the production of anti-hydrogen.

4. Modelling positron interaction with tissues

The last example of positron application modelling that we address in this paper is modelling the positron interaction with a living tissue. This line of research is important for positron emission in view
Figure 2. Profile of the positron beam sampled at different moments of compression. The white arrow shows the direction of the applied field at the moment of sampling [18].

Figure 3. Example of a positron track in a water vapor background at atmospheric pressure. Inset: the same positron track with points of electron-H₂O collisions included [20].
of investigating the damage inflicted by positrons on the surrounding tissue. It also provides an insight into a possible positron radiation therapy.

As a first-order approximation for the living tissue model, we use cross-sections for water vapor at atmospheric pressure [9]. The positrons are initialized at one point and released isotropically into the medium with an energy of 1 keV. Using our MC code, we are able to follow the trajectory of positrons up until the formation of positronium, and then the newly formed positronium until annihilation. We are also able to follow any secondary electrons produced in ionization events, either by original positrons, or by other secondary electrons. The velocity of the electrons produced in an ionization event is determined by the Opal-Peterson-Beaty [19] formula, while obeying the conservation laws. As a single positron can produce several electrons, and there is no efficient loss channel for electrons, the number of electrons can become very high very fast. This has a detrimental effect on the speed of simulation. For this reason, when an electron thermalizes (in effect reaches energy less than 100 meV) it is considered harmless and is removed from the simulation.

Figure 3 shows an example of a visualized track that a positron makes. Included in the inset of the figure 3 as blue dots laid over the positron’s track are the points of collisions of the secondary electrons. This shows that the range of electrons can be much larger than that of positrons, collisions are much more frequent and that electrons could actually play a more direct role in tissue damage. This can be seen more accurately in the energy deposition to the medium by both electrons and positrons reported in [20].

5. Conclusions
A large part of positron applications lies in the domain of swarm physics, where Coulomb interactions do not play a significant role. Monte Carlo simulation, as a well-developed swarm tool, allows us to investigate these systems in detail, and proceed from such fundamental properties as cross-section data, through sampling of averaged observables, to estimating the macroscopic qualities of large-scale, applicable, devices. The flexibility of this numerical method allows us to adapt it quickly to many different, collision dominated, gas-filled systems.

In this paper we show how the simple Monte Carlo technique may be used in combination with accurate available data for cross-sections in much the same way as it is applied to electron kinetics in ionized gases and plasmas to describe the transition from beams to swarms of charged particles, to manipulate those ensembles and to describe their major applications. This paper gives an overview of our technique, while a more detailed description of particular applications will be given in focused technical papers.

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