Simulations of pulses in a buffer gas positron trap

W Tattersall$^{1,2}$, R D White$^2$, R E Robson$^2$, J P Sullivan$^1$, S J Buckman$^1$

$^1$ARC Centre for Antimatter-Matter Studies, Research School of Physics and Engineering, The Australian National University, Canberra, ACT, Australia
$^2$ARC Centre for Antimatter-Matter Studies, School of Engineering and Physical Sciences, James Cook University, Townsville, QLD, Australia

E-mail: wade.tattersall@anu.edu.au

Abstract. In this study we simulate positron transport properties for various configurations of the gases and electric fields used in the Australian Positron Beamline Facility positron trap, which is based on the Surko buffer-gas trap. In an attempt to further improve the time and energy resolution of the trap and thus the associated scattering experiments, we apply a Monte-Carlo simulation procedure to a variety of possible configurations of the dumping stage of the trap.

1. Introduction

Studies of low-energy positron interactions with matter require generation of a beam with high energy-resolution, as achieved for example in the Surko trap [1, 2, 3] through thermalisation of positrons in a mixture of buffer gases. A similar trap has been developed for the Australian Positron Beamline Facility (APBF), located at the Australian National University (ANU), though the resolution of the beam has hitherto been adjusted on an empirical basis only. Moreover, the time-dependent effects of the ‘dump’ stage of the trap have yet to be investigated, something which is crucial for achieving optimal energy and time resolution of the final beam. The present paper addresses these effects using Monte Carlo simulation, which though a well-known technique in general [4, 5, 6], requires measures to treat the space- and time-dependent electric fields which exist during the dump stage of the trap. This paper will describe progress directed to that end.

2. Simulation procedure

The simulation is a typical Monte Carlo track structure code, operating in a similar manner to, but developed independently of previous simulations [7]. Electric fields derive from sharp axial changes in potential (‘potential walls’), effectively introducing a second form of elastic ‘collision’ for a positron. Temporal effects are accounted for by allowing the height of the potentials to vary with time. However motion between the potential walls is essentially free and kinetic energy is conserved, and it is not necessary to employ a null-collision method [4].
Figure 1. Comparison between experiment and simulation (a) pulse time profiles and (b) energy cut-offs. All simulation parameters are equal to those known for the experiment. Total gas pressure is 1.1 mTorr, ramping profile is logarithmic, starting at -4 V and increasing to 62 V. The final potential wall is set to 61 V. Positrons are initially thermalised to 300 K.

3. Simulation of the dumping stage

3.1. Simulation Parameters

Our simulation of the ANU beamline trap begins with positrons that have been cooled and located within the dumping electrode - the loading and cooling phases of the trap are not simulated – and the average positron energy equals that of the buffer gas, a mixture of N\textsubscript{2} and CF\textsubscript{4}, at 23°C and at experimental pressures (see details in Figure 1). Collision cross-sections are a combination of experimental and theoretical values [8]. A virtual multi-channel plate detector (MCP) was placed two metres from the dumping electrode, just as the real MCP is in the experiment. The potentials were assumed to have infinitesimal edge widths, and a fast slew rate. The energy and time at which each particle reaches the detector is recorded. In this way, the experimental pulse shape and energy cut-off curves may be simulated, with the latter determining the energies of the positrons that strike the MCP.

In the actual experiment, a retarding potential analyser (RPA) is used to resolve positron energies. As the RPA potential increases, the positron counts must monotonically decrease since the RPA is blocking an increasing proportion of the beam. This is reflected in our simulation in terms of a cumulative distribution of positron energies.

Comparisons between experiment and simulation of the pulse shape and energy cut-off curves are shown in figure 1. The agreement is better for energy cut-offs, though there is a shift of approximately 0.2 V, which may be indicative of a mis-match between the calibrations of the RPA and the final electrode of the trap, or due in part to other factors, such as contact potential differences. It should be noted that this energy cutoff is used for calibrating the experiment every time a set of data is measured, so the energy drift is known and the analysis of the results compensates for it. All in all, we would claim only a qualitative agreement with experiment, but we nevertheless feel that even these initial results help provide good physical insight and provide a useful guide for optimal tuning of experimental parameters, as outlined below.
3.2. Effect of trapping gas density

The simulation was repeated with different gas pressures, ranging from no gas to a pressure two hundred times greater than that of the experiment. Increasing pressure broadens the time and energy distribution of the resultant pulse, something which is to be expected, as collisions with gas molecules can either increase or decrease the time that the positron remains in the dumping stage of the trap.

One point of interest is that when the positrons and gas molecules are at the temperature and pressure used in the experiment, the total collision frequency is of the order of $10^5$ Hz, meaning that there are on the order of 10 gas collisions per positron during the dumping time of the trap (which is 650 $\mu$s), which has a negligible effect on any of the properties of the produced pulse.

Comparisons of the pulse time profiles and energy cut-offs are shown in figure 2. For purposes of experiment, a lower gas density is desirable, but this must be balanced against the rate at which thermalisation occurs during the cooling phase. The stepped nature of the energy cutoff is due to vibrational and rotational excitations within the area above the final wall. The positrons have a relatively high energy in this region because the dumping electrode potential is higher than that of the wall electrode, and the frequency of collisions with gas molecules becomes significant.

3.3. Effect of initial positron energy distribution

As explained earlier, our simulation begins with positrons in thermal equilibrium with the background gas, at room temperature, which corresponds to an experiment where the positrons have been allowed to cool for a sufficient time. We now look at the effect of increasing the average initial energy, from thermal energy up to a completely uncooled beam that retains an isotropic velocity spread corresponding to 1.5 eV.

Since higher energies result in a higher collision frequency, gas molecule interactions have a larger impact on the results of the simulation in precisely the same manner as in the earlier gas density variations. To avoid conflating these interaction effects with the effects of faster positrons colliding with the walls in the time-dependent potential, the gas density was set to zero.

Figure 3 shows a comparison of pulse time profiles and energy cut-offs. A lower initial positron temperature results in less variability in the energies and times at which the positrons are detected. However, the slower velocities of the positrons mean that they travel across the dumping potential relatively slowly, and hence have less frequent opportunities to escape the trap, which can lead to a larger energy spread. This is discussed further below.
Figure 3. Comparison between different initial positron energies for (a) pulse time profiles and (b) energy cut-offs. Temperatures refer to equivalent isotropic velocity distribution for positrons with three degrees of freedom. No gas was included. All other parameters are as in Figure 1.

3.4. Effect of dump ramp profile

At room temperature, the average energy of a positron is given by $\epsilon = \frac{3}{2}kT \approx 0.0388$ eV, with a corresponding average speed of $v = \sqrt{\frac{2\epsilon}{m_e}} \approx 1.168 \times 10^5$ m/s$^{-1}$. The average velocity component in the direction of the electrodes is then $v_z = v/\sqrt{3} \approx 6.743 \times 10^4$ m/s$^{-1}$. The width of the dumping electrode is 6cm, so the positron on average bounces from wall to wall at a frequency of 1.1 MHz, meaning that during a typical dumping time of 650 µs, the positron has approximately 325 opportunities to leave the trap. If the dumping potential exceeds the potential required to eject a positron from the trap in between two of these opportunities, then the positron will pick up excess energy, leading to a broadened energy distribution and slightly higher average energy. The details depend on the rate at which the dumping function changes in this period. Ideally, the dumping potential should stop precisely when it has reached the same level as the wall potential, but this is not practical due to fluctuations in the potentials set by the amplifiers.

In the ANU experiment, three different types of functions have been used to control the dumping electrode to varying effect. The instant dump consists of switching the electrode from low to high as quickly as the equipment allows (the slew rate is approximately 30 V/µs). The result would be a pulse of positrons that would have an energy distribution of the same width, but shifted up by an amount corresponding to the potential of the final electrode, were it not for the transport time effect mentioned above. This effect results in 90% of the positrons remaining in the dumping electrode until the end of the ramp, rendering the potential of the final electrode inconsequential, and setting the beam energy to that of the top of the dumping ramp. In addition, every positron will gain sufficient potential to leave the trap within a few microseconds, leading to a high time resolution.

The bilinear ramp style consists of two linear ramps that share a common centre point. The logarithmic ramp initially increases quickly, but only gradually approaches the final value, thereby reducing the energy variation between positrons located in different parts of the dumping electrode when the dump potential passes the wall potential. The pulse shapes and energy cutoffs for each of these dumping functions are provided in figure 4.

3.5. Other Variables

Several other possible variables were investigated, and found to have little effect on the resultant pulse. Thus, for example, a spatial gradient in the electric potentials has little effect, other than to increase the collision rates with gas molecules, resulting in a longer time within the trap and additional signal loss due to positronium formation and annihilation. On the other hand, modifying the ratio of gases has a similar effect to modifying the gas density.
Figure 4. Comparison between different ramping functions for (a) pulse time profiles and (b) energy cut-offs. Ramping functions are as described in section 3.4, no gas was included, all other parameters are as in Figure 1.

4. Concluding Remarks
We have addressed key questions relating to optimising the operation of the traps used in the ANU beamlines. In future work we will improve the accuracy of the simulation to achieve better agreement with experiment, and consider the effect of altering a wider range of experimental variables. This will allow experimentalists to achieve better time and energy resolution in experiment and ultimately more precise data.

Acknowledgments
The authors are grateful to the Australian Research Council for support under the Centres of Excellence Program, and to experimentalists J. Machacek and A. Jones for data and discussions on the topics related to this work.

[1] J P Sullivan, A Jones, P Caradonna, C Makochekana, and S J Buckman. A positron trap and beam apparatus for atomic and molecular scattering experiments. Review of Scientific Instruments, 79(11):113105, 2008.
[2] A Jones, P Caradonna, C Makochekana, D Slaughter, D Mueller, J P Sullivan, and S J Buckman. High resolution positron interactions. Journal of Physics: Conference Series, 194(1):012033, 2009.
[3] C M Surko, G F Gribalakin, and S J Buckman. Low-energy positron interactions with atoms and molecules. Journal of Physics B: Atomic and Molecular Physics, 38(6):R57–R126, March 2005.
[4] H R Skullerud. The stochastic computer simulation of ion motion in a gas subjected to a constant electric field. Journal of Physics D: Applied Physics, 1(11):1567, 1968.
[5] C Champion and C Leloirec. Positron follow-up in liquid water: I. a new monte carlo track-structure code. Physics in Medicine and Biology, 51:1707–1723, April 2006.
[6] S Duško, R D White, K F Ness, Z Lj Petrović, and R E Robson. Non-conservative electron transport in CF₄ in electric and magnetic fields crossed at arbitrary angles. Journal of Physics D: Applied Physics, 39(22):4788, 2006.
[7] M Šuvakov, Z Lj Petrović, J P Marler, S J Buckman, R E Robson, and G Malović. Monte carlo simulation of non-conservative positron transport in pure argon. New Journal of Physics, 10(5):053034, 2008.
[8] A Banković, J P Marler, M Šuvakov, G Malović, and Z L Petrović. Transport coefficients for positron swarms in nitrogen. Nuclear Instruments and Methods in Physics Research B, 266:462–465, February 2008.