Trapping lycopodium club moss spores with a radio frequency trap

Radio frequency traps are, theoretically, relatively simple to build and can be an asset to professional physicists, enthusiasts, and educators alike. The mathematics used to predict how the traps and the particles inside them will behave at different scales apply only to situations where air resistance need not be regarded. This report will explore these behaviours in linear radio frequency traps when air resistance is taken into consideration by simulating ions in such traps and come to a conclusion on the practicalities of building them at various scales in order to trap lycopodium club moss spores.

Introduction

The Paul trap, or radio frequency trap, is an effective tool for the containment and examination of charged particles. Attributed to German physicist Wolfgang Paul, these quadrupole ion traps were initially designed in order for use in spectroscopic examinations and are commonly used also to trap individual ions and cool them to low temperatures, or for educational purposes. This report seeks to understand the rules around the scaling of these traps when air resistance must be considered in order to determine the feasibility of building. Using them for outreach could serve to demonstrate to outreach audiences how radio frequency traps, such as those used in the GBAR experiment at CERN, work.

The traps work by using a combination of direct and alternating potentials to generate an electric field such that ions of a particular charge to mass ratio will be held in place. A simple linear Paul trap consists of four long rod electrodes and two endcap electrodes, as shown in Fig. 2. An AC voltage is applied to the rod electrodes to confine the particles radially, and a DC voltage is applied to the endcap electrodes to confine the particles axially. The AC through the top and bottom electrodes will be $180°$ out of phase with the left and right electrodes, as illustrated below:

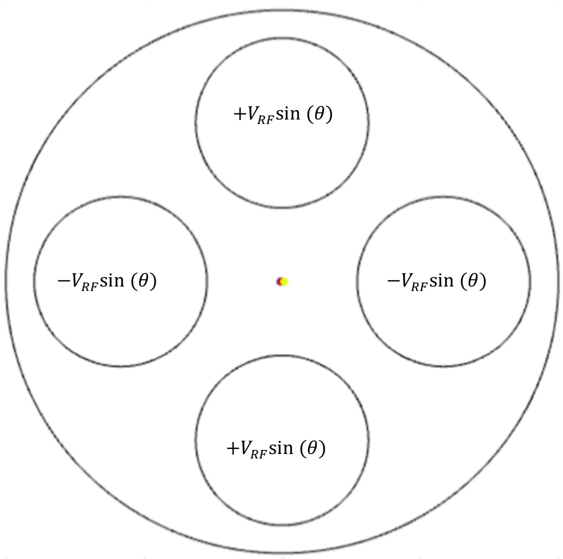

Figure 1: End view of typical Paul trap, labels to signify relative orientation of potential.

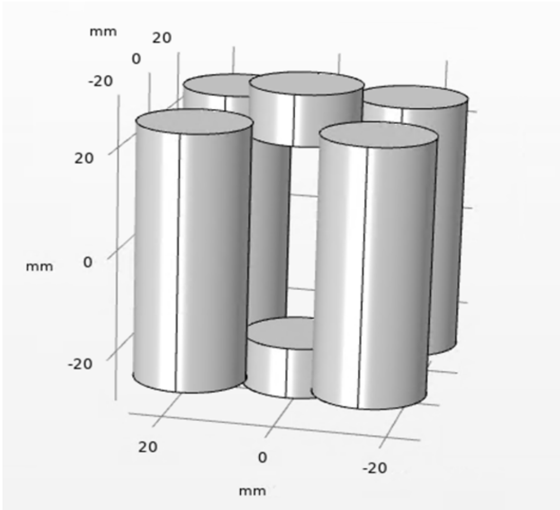

Figure 2: Vertical linear Paul trap with endcap electrodes

The ideal design parameters of a linear Paul trap can be described by a series of “magic numbers”, or “magic ratios”: $\eta = \frac{r}{(R-r)} = \frac{r}{r_0}$, the first of which being $\eta_1 = 1.14511$[1]. This then gives us $r_0 = 0.87r$, where r_0, r, and R are defined in figure 3.

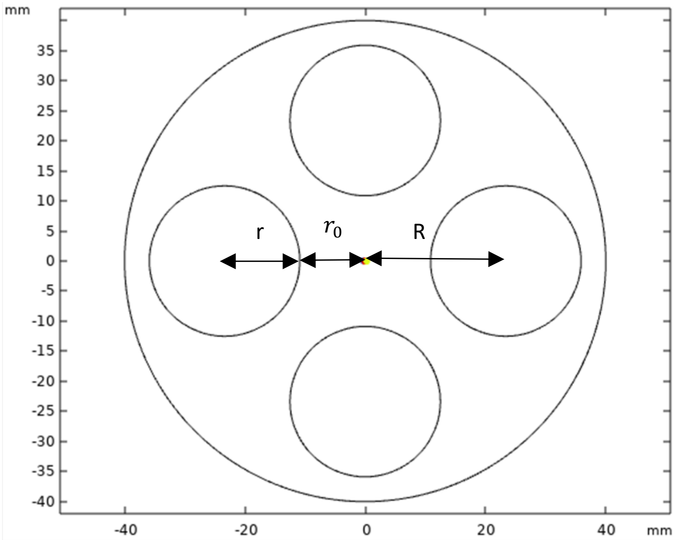

Figure 3

The stability of charged particles in a quadrupole electric field may be described by the Mathieu equations [2]:

$$\frac{d^2x}{d\tau^2} + \left(a + 2q\cos(2\tau)\right)x = 0$$

$$\frac{d^2y}{d\tau^2} - \left(a + 2q\cos(2\tau)\right)y = 0$$

When compared to the particles’ equations of motion:

$$\frac{d^2x}{dt^2} + \frac{Q}{mr_0^2}\left(V_{DC} + V_{RF}\cos(\omega t)\right)x = 0$$

$$\frac{d^2y}{dt^2} - \frac{Q}{mr_0^2}\left(V_{DC} + V_{RF}cos(\omega t)\right)y = 0$$

The solutions to q and a can be determined to be:

$$a = \frac{4QV_{DC}}{mr_0^2\omega^2}\ , \qquad q = \frac{2QV_{RF}}{mr_0^2\omega^2}$$

Where V_{DC} is the DC potential applied to opposing rod electrodes in a traditional, or horizontal, trap (which includes a contribution from the DC potential in the endcaps, the size of which depends on the trap geometry), V_{RF} is the peak of the AC potential, *a* describes the motion of the particle due to the DC field and *q* describes the motion of the particle due to the AC field, *Q* is the charge of the ion, *m* is the mass of the ion, r_0 is the length defined in figure 3 and $\omega = 2\pi f$, with *f* being the frequency of V_{RF}. The stability of the particle therefore depends only on the values of *a* and *q*.

Methods

In a horizontal trap there will be a DC potential applied to the top and bottom electrodes in order to produce a potential gradient such that the force of gravity acting on a particle of a specific charge-to-mass ratio will be counteracted.
This can also be achieved by orienting the trap vertically and using the endcap electrodes to take on the DC potential. In this case, there will be no DC potential applied to any of the main rod electrodes which, theoretically, this tells us that the value of a should be zero. In practice, however, this would not be the case. In the case of a real 3D trap of finite length, endcap electrodes would contribute an effective V_{DC} proportional to the length of the trap, and therefore, an effective value of a[3]. Imperfections in the trap geometry would also contribute to this effective V_{DC}.
By selecting the vertical Paul trap for study, it is possible to separate the balancing of gravity from the radial confinement, since there will be no contribution from gravity to the a value. For the purposes of the simulations, we may assume the trap geometry to be perfect. In the case of the 1D trap, where we are considering only the DC endcap electrode potential, the values of both a and q are irrelevant. Similarly, in the case of a 2D trap where we are considering only the AC potential V_{RF}, q is the only relevant value. Since there is no intentionally applied DC potential and the trap is long, V_{DC} will be close to zero, a can be assumed to be zero.

1D trap

The size of DC potential required to balance the force of gravity on an ion can be easily approximated given the mass and charge of the ion being trapped. Using the formulae for the force acting upon a charge in an electric field $F = QE$, the potential between two charged parallel plates $V = Ed$, and Newton's second law $F = ma$, we may find the formula $V = \frac{F}{Q}d = \frac{mg}{Q}d$, where V is the potential required to balance gravity, *m* and *Q* are the mass and charge of the ion, *g* is acceleration due to gravity, and *d* is the distance between two charged plates or, in this case, electrodes. In the case of lycopodium club moss spores with a mass of $4.2 * 10^{-12}\ kg$ and a charge of 10^5 electron charges [4] this potential can be found to be 25.6 V/cm.

2D trap

These parameters give us regions of stability for the x (due to the AC potential) and y (due to both AC and DC potentials) direction as detailed below:

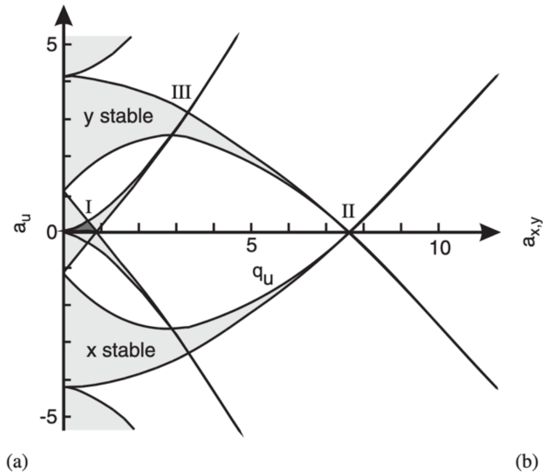

Figure 4: Plot of the regions of stability in a linear Paul trap [5]

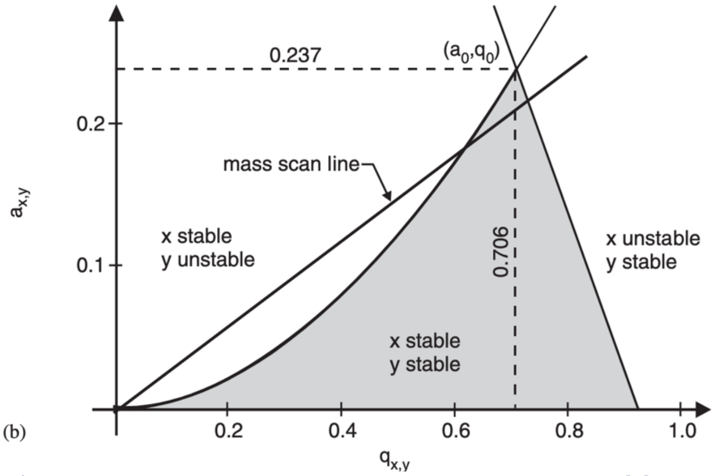

Figure 5: A closer look at region I, the closest to 0 [5]

The lowest region that provides stability for x and y simultaneously is region I (pictured in figure 5), a commonly used region owing to its practical feasibility in mass spectrometry. Since there will be no DC bias attached the RF electrodes, only the a=0 line is relevant.

Building the simulation

The simulation software COMSOL was used to design a 2D model of the trap in various sizes and test for the maximum and minimum AC voltages required to sufficiently trap the particles.

The model was built according to the ideal geometry for a trap of this kind, as detailed below:

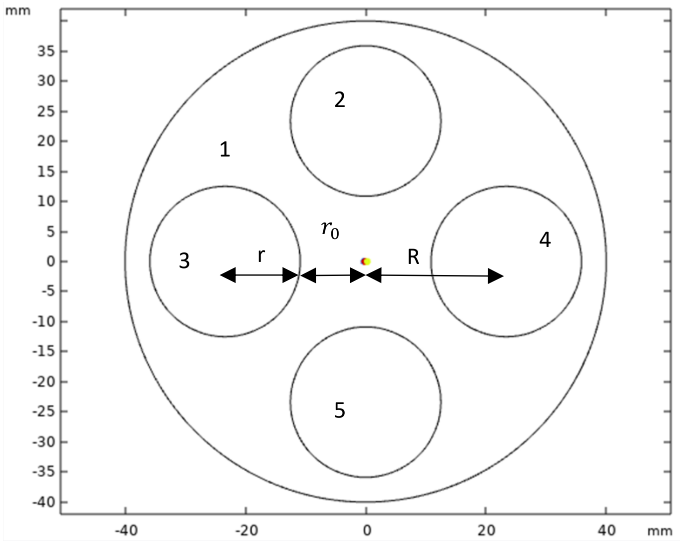

Figure 6: 2D model built in COMSOL labelled with lengths and domains

Electric current (ec) component terminals were attached to electrodes (COMSOL domains) 2 and 5, 3 and 4, with voltages $V_{RF} * \sin(\omega t)$ and -$V_{RF} * \sin(\omega t)$ respectively, such that V_{RF} could be defined by the global parameters. These domains were set as copper while domain 1, the surrounding area, was set to be air. The charged particle tracing (cpt) component was added to domain 1, through which the electric force, governed by the ec component, was able to act on the particles.

The charged particles chosen were the commonly found lycopodium club moss spores, and so the particles were given a mass $4.2 * 10^{-12}$ kg, and charge $10^5 e$ in accordance with recorded values [4].

A friction component was added to cpt to represent air resistance in order to produce a more accurate simulation, but also to study how the ideal q value changes. The background number density was set to the number density of air, $2.5 * 10^{25}\ \mathrm{m}^{-3}$ [6,7]. The collision cross section to $4.90874 * 10^{-24}\ \mathrm{m}^2$, calculated from a given diameter of the spores $d = 25\ \mu\mathrm{m}$ with an adjustment of 10^{-14} which was necessary due to COMSOL assuming the frictional force to be proportional to the mass of the spore particles ($4.2 * 10^{-12}$ kg), rather than the mass of the air particles ($4 * 10^{-26}$ kg).

Two studies were added, the first to simulate the electric fields from ec, the second to simulate the motion of the particles due to those electric fields. The time-step for each study was 0.005s, with a total time of 10s.

Running the simulation

The sizes of trap chosen to study were r = 5 mm, 10 mm, 15 mm, 20 mm, 25 mm. A new particle was released at position (r/5, r/5) every 0.01 s over the course of the first 0.5 s of the simulation. For each size of trap, a theoretically ideal V_{RF} was calculated from Mathieu equation using q = 0.706 and $f = 50$ Hz. Particles were given the maximum initial speed possible for this initial V_{RF}, with $v_{0x} = -v_{0y}$, that wouldn't result in a signification portion of them quickly escaping the trap. This was in order to more easily visually determine which runs of the simulation were less or more stable.

It was found that there was a minimum V_{RF} that the trap needed in order to prevent the particles from escaping and a maximum V_{RF} that the trap could handle before the particles became unstable. These are referred to as the “maximum” and “minimum” V_{RF}’s. First V_{RF} was slowly increased, until the maximum potential that still resulted in the particles being held stably at the centre of the trap was determined. V_{RF} was then decreased until the minimum potential that could still trap the majority of the particles was determined. The particles were deemed suitably stable if they were fixed in the centre of the trap rather than performing a small orbit around the centre, as detailed in figure 7:

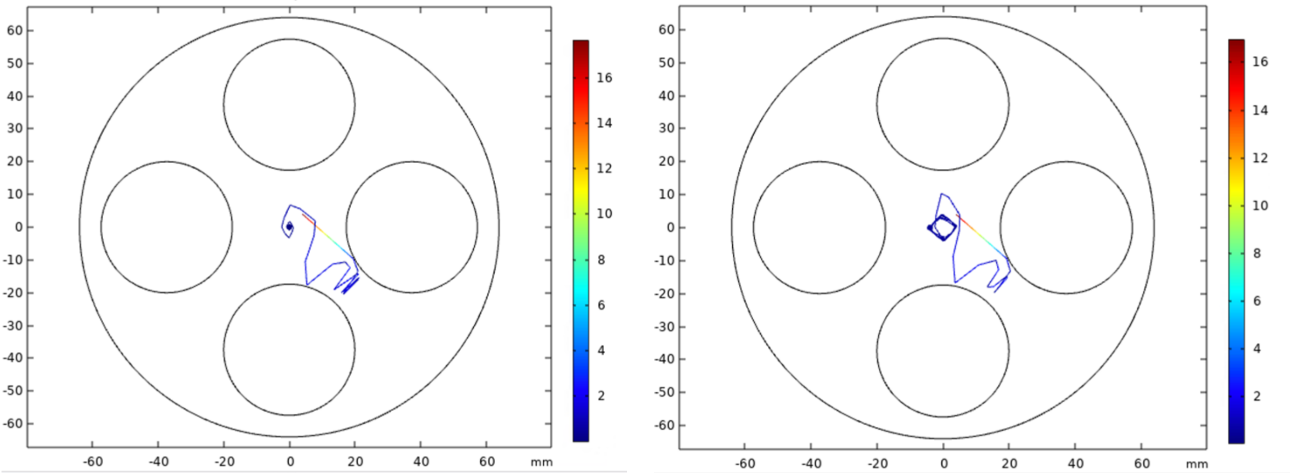

Figure 7: Two versions of the r=20 mm trap operating with a single particle. The line shows the path of the particle colour of the line indicates the speed in m/s of the particle at that point.

V_{RF} = 1400 V (left) quickly stabilises and then remains approximately stationary in the centre of the trap, while V_{RF} = 2000 V the particle never stabilises; instead it oscillates around the centre.

An additional increase in the particles initial velocity was sometimes required in order to more clearly distinguish between the stabilities of the most stable simulations.
After the maximum and minimum V_{RF}’s were determined for this initial sample of r’s, r=2.5 mm, 7.5 mm, and 12.5 mm were studied to provide more detail to the results.

Results and Analysis

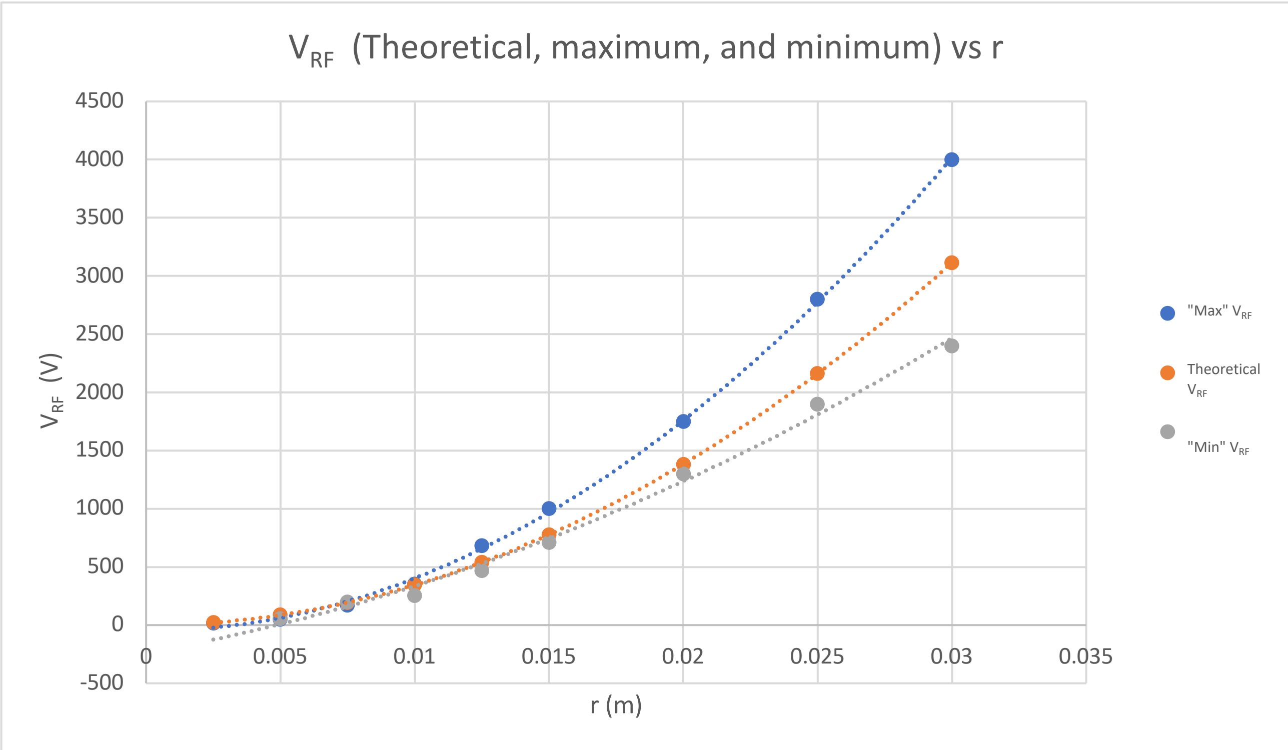

Figure 8: Graph of the three V_{RF} values against r

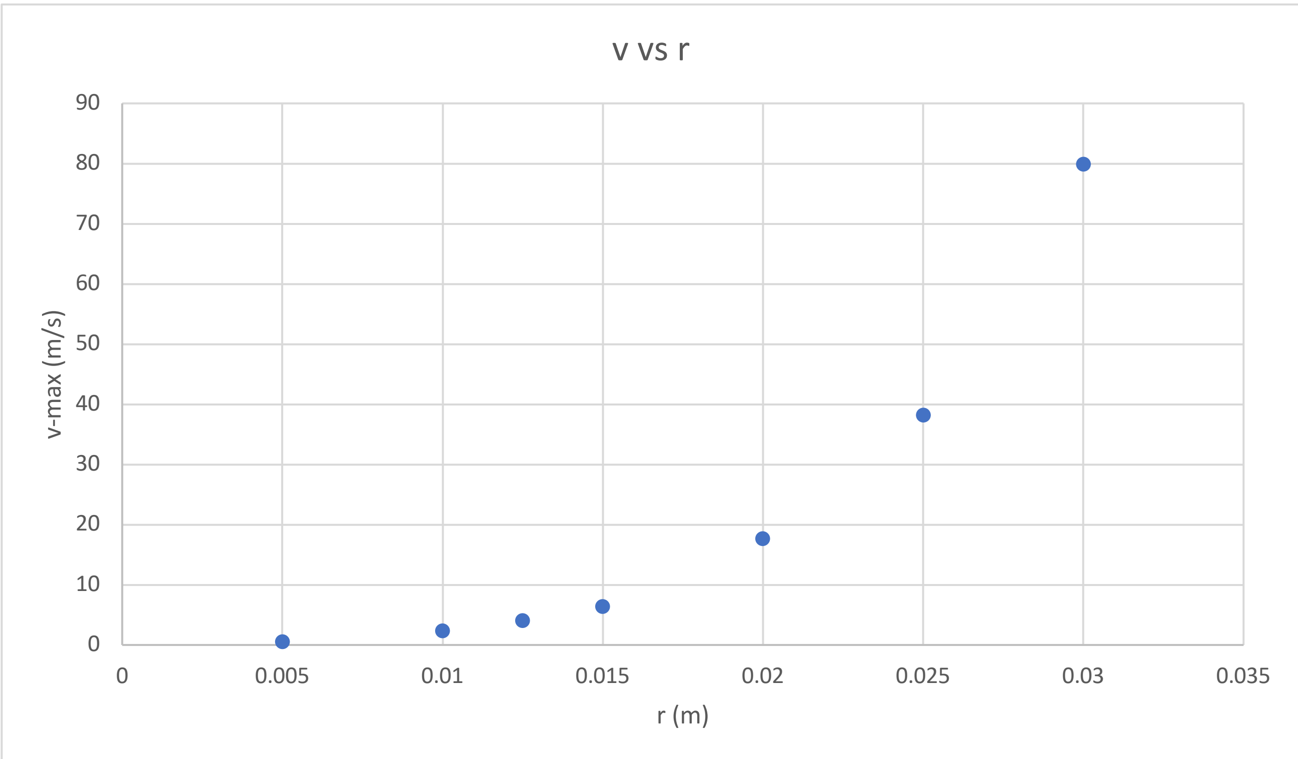

Figure 9: Plot of the maximum velocity v the particles could initially be given in the bottom right direction without flying out of the trap against r (for "max" V_{RF}).

r(m)	"Min" V_{RF} (V)	Theoretical V_{RF} (V)	"Max" V_{RF} (V)	v-max (m/s)
0.005	55	86.4	52.5	0.57
0.01	255	346	355	2.31
0.0125	470	540	680	4.03
0.015	710	778	1000	6.36
0.02	1300	1380	1750	17.7
0.025	1900	2160	2800	38.2
0.03	2400	3110	4000	80

Similar to what the Mathieu equations predict with $V_{RF} = \frac{qmr_0{}^2\omega^2}{2Q}$, the "maximum" V_{RF} increased approximately proportionally to r^2. The "minimum" V_{RF} increased slightly differently, appearing to be approximately proportional to $10r^2 + r$.

For the smaller trap sizes ($r \leq 7.5\ \mathrm{mm}$), no stable value could be determined as any value of V_{DC} high enough to trap the particles led to too unstable a hold. This could be due to the timestep of the simulations. Since these traps are so small, it is possible that too high a timestep led to the particles escaping the trap in just one step, where with smaller timesteps the particles could potentially be trapped with a lower V_{DC}, allowing the required stability. In future, a smaller timestep would be a better candidate.

As shown in figure 9, the maximum velocity the particles could be given grew dramatically with r after $r = 15\ \mathrm{mm}$. This is presumably because in a larger trap the air resistance has more time act on the particle and slow it down before it reaches the boundary at the edge of the trap where it can escape.

Conclusion

For any person looking to make one of these traps an ideal trap size, an appropriate V_{RF} could be selected anywhere between the "min" and the "max" V_{RF} based on the size of trap available and the anticipated initial velocity of the particles. Alternatively, if only a set supply voltage is available, then it is possible to determine the size of the trap required by ensuring the voltage falls somewhere between the "max" and "min" for that size.

Based on these results and ideal trap would be somewhere between $r = 12.5\ \mathrm{mm}$ and $r = 15\ \mathrm{mm}$. These sizes do not require an impractically high voltage to operate as required but can still withstand a reasonably sized initial velocity from the particles. $r = 10\ \mathrm{mm}$ could be a reasonable alternative if a smaller sized trap was required, given that particles entered the trap at an angle such that they would bounce off one of the electrodes in order to slow them down, preventing them from flying straight through the trap. For example, anyone working with a mains voltage supply of $V_{RF} = 325\ V$, a trap with size $r \sim 10\ \mathrm{mm}$ would be ideal but would require a small initial velocity.

Sources

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