Summer student project report
Ion-Gas collision Simulations in an RFQcb using SIMION software
Name: John Onesmus Mutua
Supervisor: Maxmilian Schuett
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ABSTRACT

A methodology and procedure for ions and gas collisions in RFQcb is described and demonstrated. Simion software main menu is presented. Ion trajectories as a result of flown particles is also demonstrated. Figures showing different view planes for the simulated particles are presented and discussed.

CHAPTER ONE

1.0 INTRODUCTION

Ion simulation programs started way back in 1973 (Dahl, 2000). Since then, so many significant improvements in their functioning aspects have been done (Remes *et al.,* 2014). Features like RF capabilities were added as a result of specific needs of the day in day out simulation needs. A good example is that of improved RF capabilities which was used in the study of ion motion after collision generated disintegration in quadrupoles (Dahl, 2000). Further understanding of the problem undergone in ion motion would lead into development of first type of SIMION software by McGilvery in ordinary ionization geometry.

Many ion simulation investigation studies concerning mass-charge analysis, ion isolation, ion injection and ion activation have been done through 2D (Douglas and Konenkov, 2012) quadrupole ion trap (QIT) and 3D (Wu *et al.,* 2005). The development of QIT technology significantly transformed ion simulation through its prowess in working on several stages of mass spectrometry in single analyzer and also in full scan mass examinations (McLuckey & Wells, 2001).

SIMION software has largely been improved (Manura and Dahl, 2007) to effectively calculate electric field provided that the configurations of electrodes with voltages are defined. This has been performed in 2D and 3D arrays for an estimated billions of points. Determination of trajectories of charged particles in electric field for defined particle initial conditions such as optional RF and magnetic field have been calculated through SIMION software.

Ion propagation exercise requires intensive cooling which often is provided by use of a mixture of inert gasses. Further, the addition of buffer gas leads to transversal cooling of the ions. Additionally, increase in longitudinal potential implies that, the ions can be stored, gathered and bunched at the end of the RFQ (Babcock & Giles, 2013). Figure 1 shows Longitudinal DC potential along the RFQcb beam axis in both transmission mode and bunching mode.

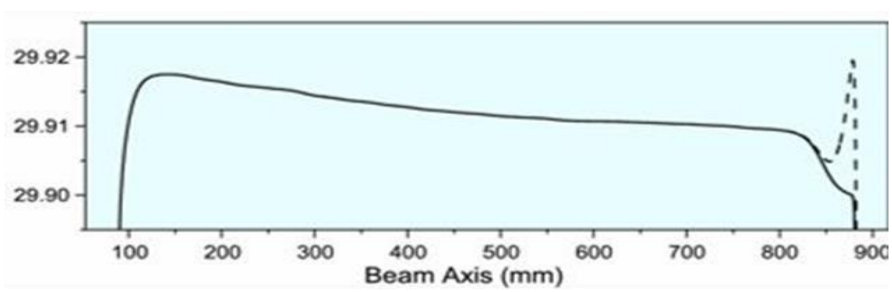

FIGURE 1; Longitudinal DC potential

Figure 2 shows a cross-section illustration of the electric fields in the transversal XY-plane depicting the alternating quadrupole electric RF fields transversally focusing the ions.

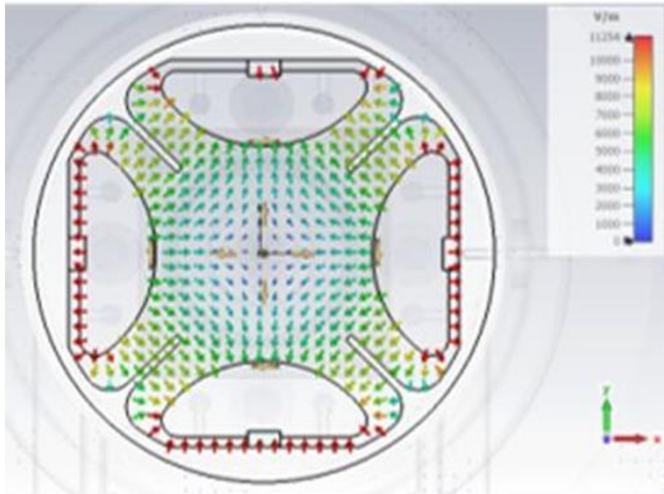

FIGURE 2; XY cross-section of focused ions.

CHAPTER TWO

2.0 METHODOLOGY

In this section, the exact route followed in ion simulation and gas collision is explained. The main menu of SIMION software is displayed in Figure 3.

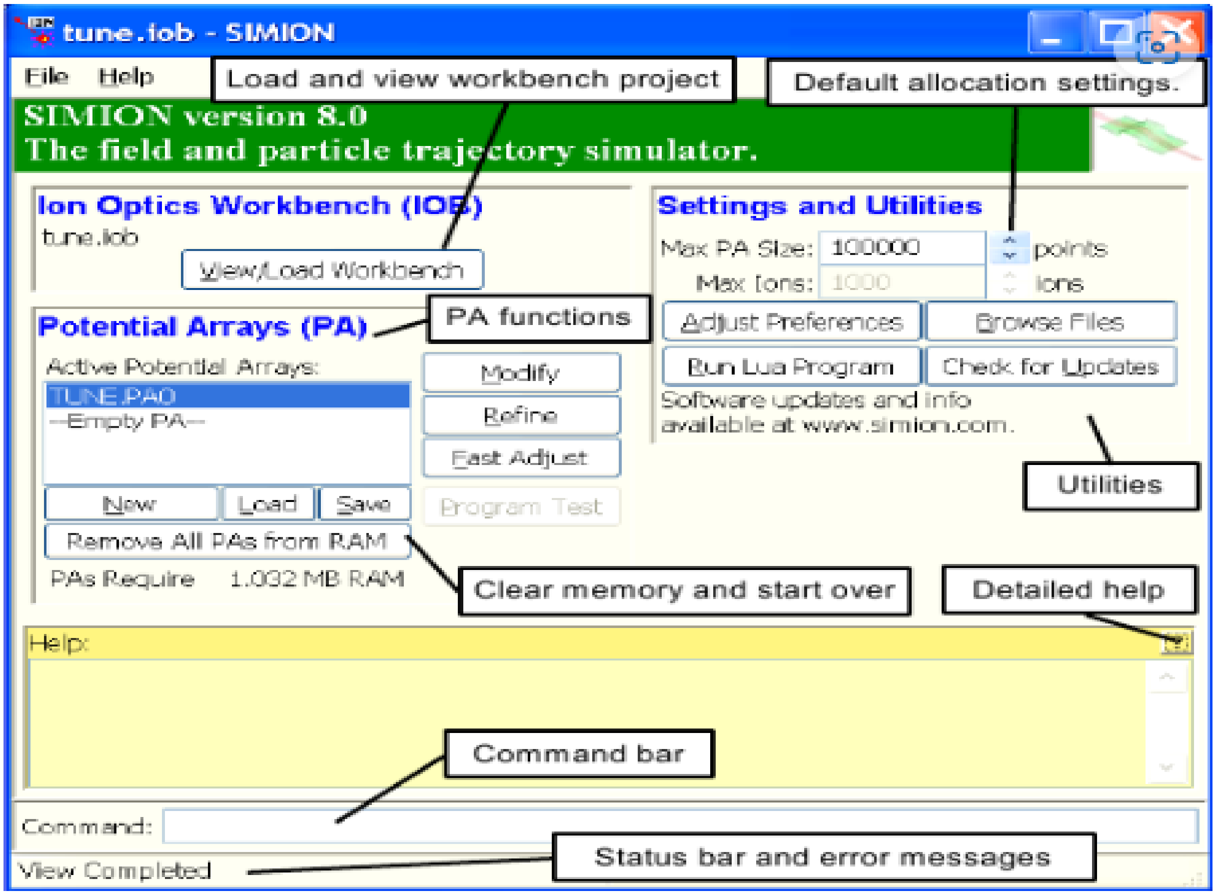

FIGURE 3; SIMION's main menu screen

The following procedure was employed in the current simulation exercise. The tabs New, Modify and Save were used in coming up with the potential array defined by electrode geometries and potentials within cylindrical volume space. The Refine tab was used in calculating the potentials in the space points of the potential array followed by potential adjustments from the Fast adjust function. Lastly, workspace was created through View/load workbench function and the already refined potential arrays, recalled and placed on the workspace and particle flown.

CHAPTER THREE

3.0 RESULTS AND DISCUSION

SIMION software is very useful in ion-gas collision simulations flying through non-vacuum conditions and it assumes that ions are flying within a perfect vacuum.

In SIMION software, the Ion Optics Workbench (IOB) is the main file that links all the other files. After loading a given file on the workbench, calculation of particle trajectories is done by clicking the Fly'm button. The cross sectional view can be varied across XY, ZY, XZ and 3D with each cross section generating a specific view as far as the interest of the simulator is concerned. For enlarged proper view, zoom in at the point of interest was highly effective. The PE view was useful in determining the potentials in each ring as well as the exact potentials of the electrodes. This was carried out by clicking PAs tab followed by Fast adjust voltages. Figure 4 shows the model created in this work having several rings.

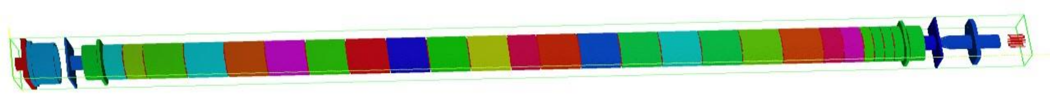

FIGURE 4; 3D view of the RFQcb modelled in SIMION.

Figure 5 and Figure 6 shows the cross sections of the injection and extraction electrodes in the YZ plane of SIMION. The injection electrodes were used as an Einzel lens to focus the beam into the RF region. The beam is stopped from the full beam energy of 30 kV to 60 kV to almost 100 eV. The ions then drift through the RF quadrupole region filled with the buffer gas. At the end of the RF channel, the ions can be completely stopped, stored and further cooled (Schuett *et al.,* 2023). Additionally, the extraction electrodes subsequently reaccelerate the ions to their previous energy.

FIGURE 5; YZ Cross section for electrodes injection. The left side shows the electrodes of the injection.

FIGURE 6; YZ Cross section for electrodes extraction. The right hand side shows the electrodes of the extraction system.

The PE view of the model is clearly shown in Figure 7 and the accompanying graphical representation illustrated in Figure 8.

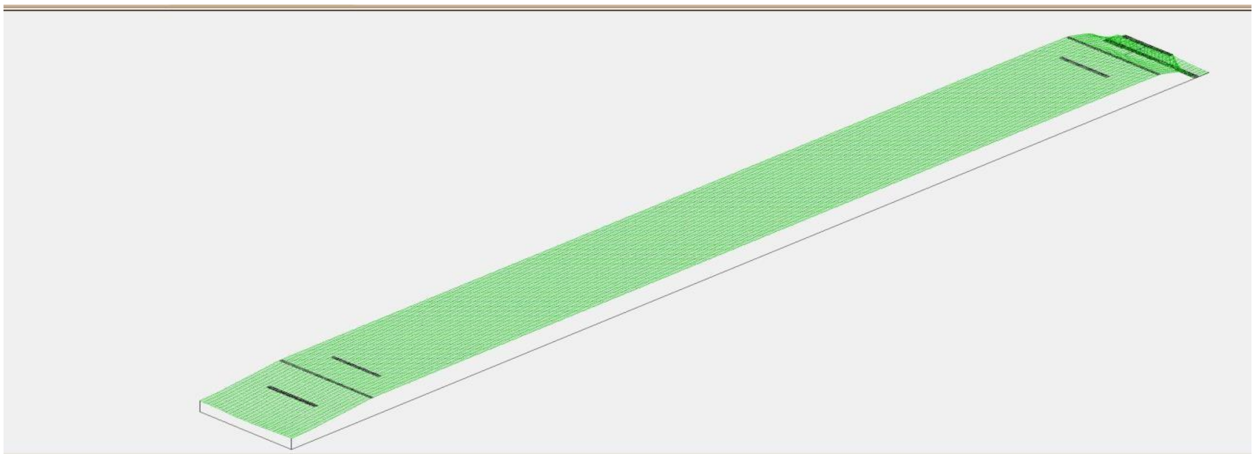

FIGURE 7; Potential energy view of potential array using the PE View function.

Figure 8 shows particles flying (PE view). The ions were flown together by selecting the Grouped check box then clicking the Fly'm button. Further, the ions were kept flying by selecting the Rerun check box. This gives a movie effect.

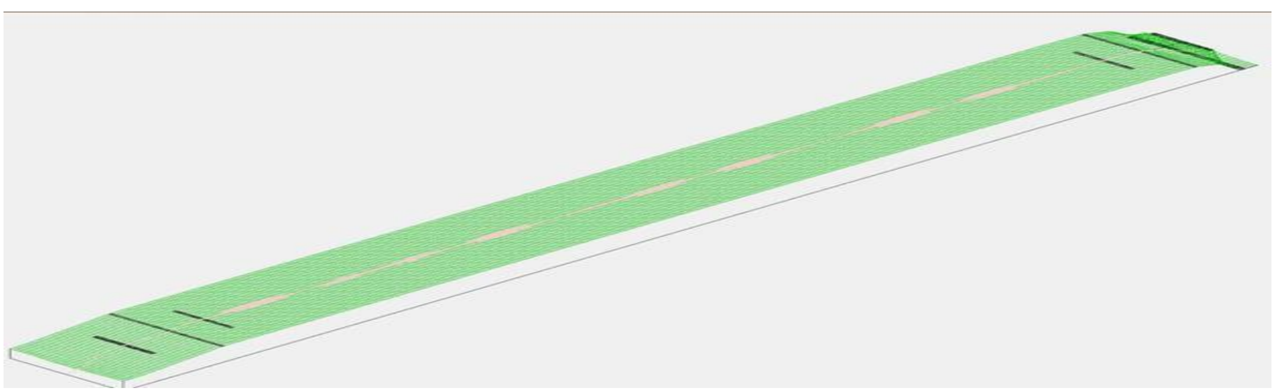

FIGURE 8; Particle trajectories flown while displaying potential energy view.

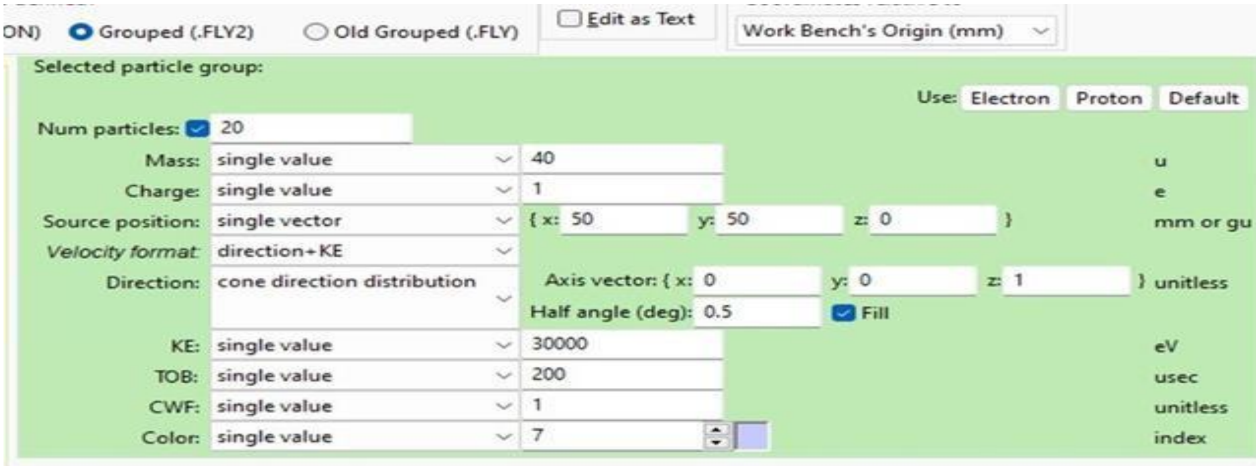

FIGURE 9; Defining initial conditions of ions to fly.

The existing gas collision model (Collision Model HS1) in SIMION software and modification of the necessary parameters were useful in ion beam simulation in non-vacuum conditions. Figures 10 and 11 shows the ion beam collisions with the background argon gas.

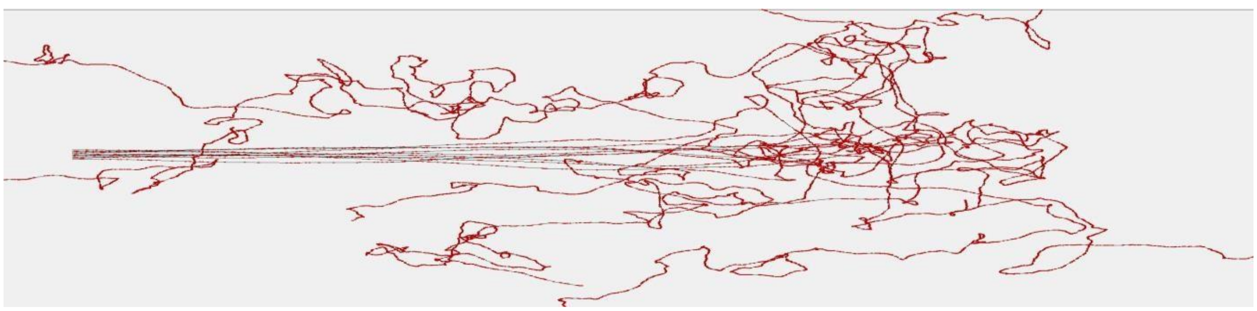

FIGURE 10; XY cross-sectional view of the proton beam colliding with the background argon gas

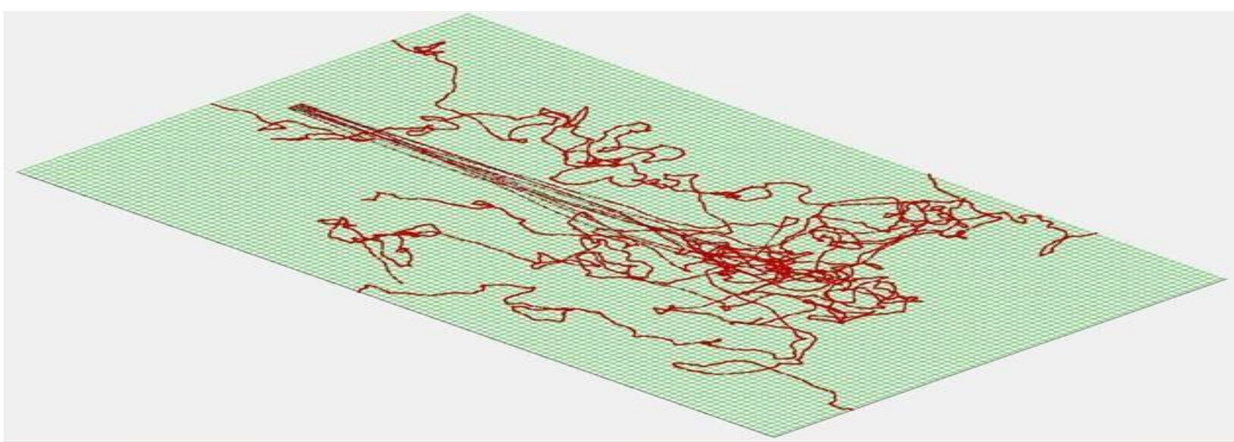

FIGURE 11; XY cross-sectional PE view. The ions collide against background argon gas and undergo random deflection.

Collision models assumes that ion collisions are elastic and the background gas is neutral in charge, its velocity follows the Maxwell-Boltzmann distribution, mean velocity may be non-zero and kinetic energy of cooling and heating is negligible over many collisions.

To exactly determine the behavior of ions behind the front surface, pealing-off of a selected surface was done, clearly exposing the particles to the viewer. Furthermore, contour maps of electrostatic fields were also drawn giving much insights to the potentials along the contours.

CHAPTER FOUR

4.0 CONCLUSION

The simulation of individual collisions between ion and gas particles was done. Kinetic theory of gases is used to tell the expected frequency of collisions due to variation in pressure, temperature, and collisional cross sections of colliding particles. Collisions between ion and gas particles is responsible for energy transfers, particle scattering and absorptions. Fast moving ion and slow moving ion have their kinetic energy coming from the energy transfers. The colliding particles are often taken as hard-spheres and are assumed to undergo elastic collisions.

Lastly, adjustment of Potential Array was very significant in this project. This is because often we needed to change the electrode potentials of an already refined array to adjust a magnet's field. This was supported by SIMION software through Modify the Potential(s) and Re-Refine tabs. The Modify function was used to change the potentials of the points of one or more electrodes in the basic potential array (PA) while the Refine function re-refined the basic potential array (PA) to obtain the resulting potentials of the non-electrode points.

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