Development of Ion Optics for a Spaceflight Ion Mass Spectrograph

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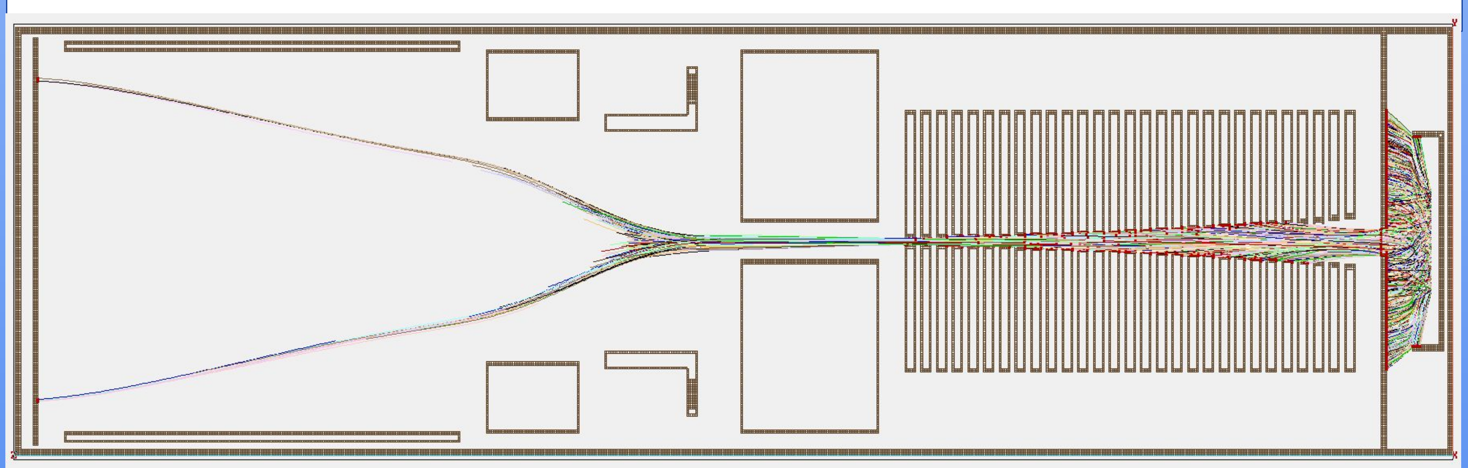
Statement of the Problem

The goal is to modify the design of an existing mass spectrometer, REFIMS in order to accommodate a larger detection plate and to improve performance generally so that it is sensitive to mass differences of one amu from one to 81 amu. In particularly, how the geometry and voltages of the ion optics analyzer at the heart of the instrument can be optimized to do so. REFIMS is for use in space flight missions, so there are constraints on its size as well as other considerations.

Methods of Simulation

In order to develop the ion optics system, the electrodes were modeled in Solidworks and exported into the ion optics simulation software, Simion. Simion is able to convert the STL file into a 3D array of points, each with an associated electric potential. Simion allows the user to set the voltages of each electrode, and then it populates the rest of the points in the 'potential array', by the relaxation method, essentially repeated averaging, as well as some other clever tricks. Simion will then calculate the trajectories of ions through the instrument. A vertical cross section of ion trajectories for mass 16 amu ions is depicted below. The rotating electric field is modeled using supplemental user programming written in lua. The floating electric potential outside of the rocket is modeling using with a box shaped electrode, with a permeable screen (ions pass through, electric potential stays in).



Changes to Design

Most of the work on the ion optics system has involved optimizing the voltages of the electrodes with the geometry of electrodes fixed. However I also tried dozens of variations of electrode configurations. The first major change to the geometry of the system is to the collimator.

The previous design of the collimator had a fixed inner radius for every electrode. (the electrodes are washer shaped.) Instead I gradually decreased the radii so that the first electrode was wider than the original, and the last was narrower. The effect of this is that an ion coming in at a slightly eccentric angle has more time to get back on track before it collides with one of the electrode plates rather than pass through to be analyzed by the instrument. The intention is to get more ions to pass through a smaller aperture. Despite the similar appearance, this is not an ion funnel. Unlike an ion funnel, the voltages on the electrodes are static, and it operates under vacuum.

Several changes we made to the inner radii of the other electrodes as well. The first electrode after the collimator was made narrower, which I found limited how much the beam spread out, and the electrodes after the eight electrodes which generate the rotating electric field were widened, which helps to accommodate the larger detection plate, and stops them from causing interference with the ions which can happen if they get too close.

Abstract

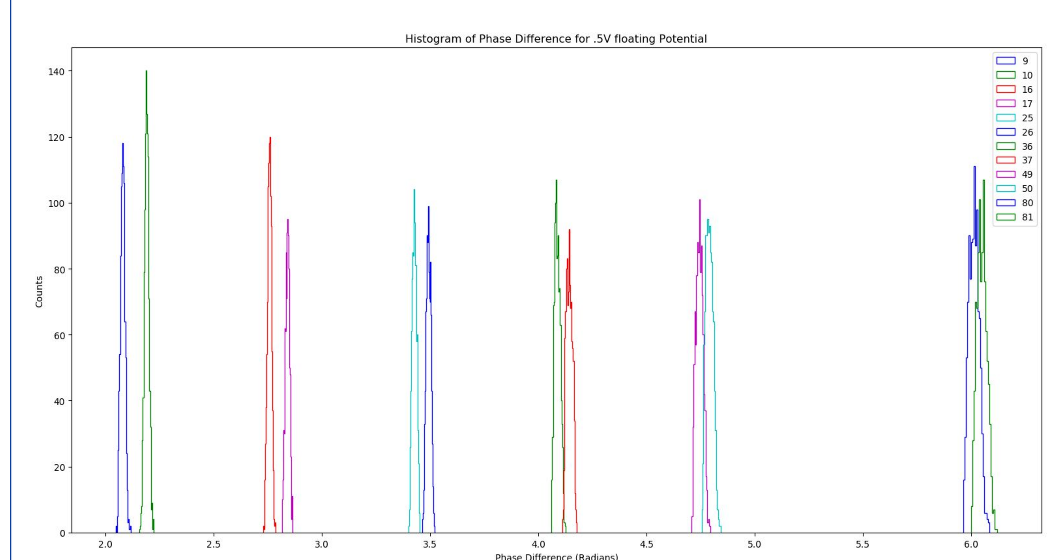
The work is the development of the ion optics analyzer of an ion mass spectrograph, REFIMS, for use in near-space and space, on various upcoming missions. The goal is to improve the resolution and precision of the mass spectrum reading, by adjusting the shape, spacing, and voltages of the electrodes. The electrodes, which make up the ion optics analyzer, generate electrostatic lenses, which guide the trajectories of the ions through the instrument. A complete discussion of the operating principles of REFIMS, and the theory of ion optics, in general, is provided. This presentation also explains how Solidworks and the ion optics simulation software, Simion, were used to design the ion optics analyzer. Data from these simulations will show how far development has progressed towards the goal of focusing the instrument such that it is precise to a single atomic mass unit, up to 80 atomic mass units.

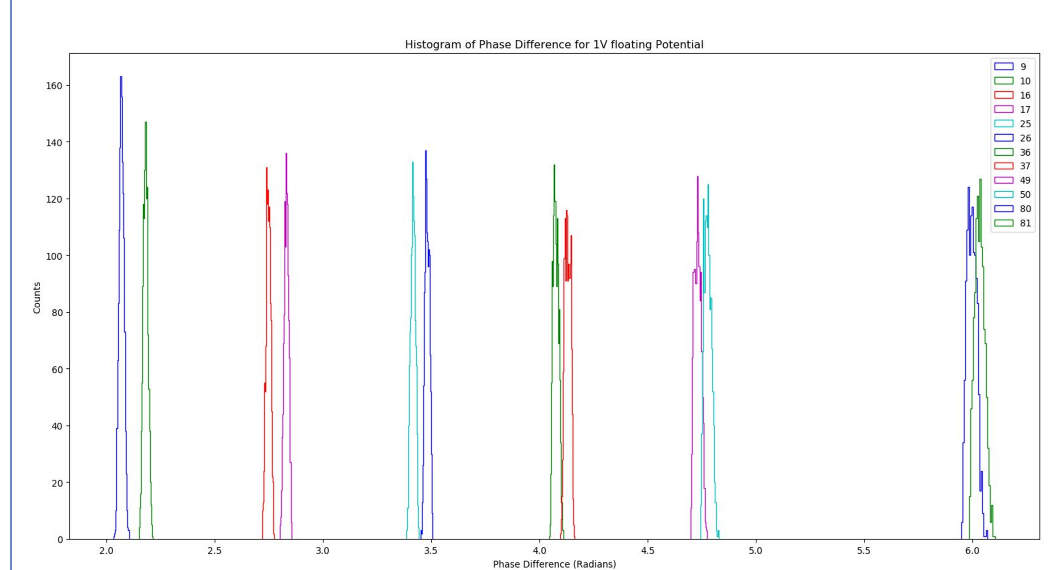
Progress towards goal

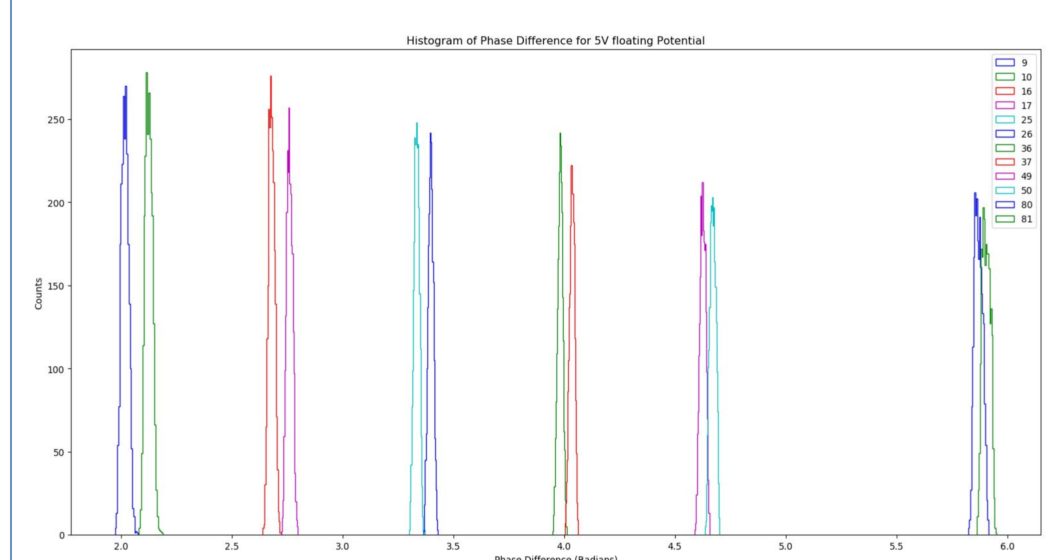
To the left are three plots summarizing some of the data from my last set of comprehensive trials, testing what seemed to be the most optimal configuration from previous trials. Each plot shows the simulated data processed and presented similarly to the way data collected by the real instrument would be. The plots are histograms of the rotation of the electric field during the flight of each ion, which is proportional the square root of mass. (See methods of operation for more detail). The masses included in the trials are 9, 10, 16, 17, 25, 26, 36, 37, 49, 50, 80, and 81, which I felt to be representative of the mass spectrum.

Each of the three plots represents data taken from simulations representing different conditions outside of the instrument. There is an effect caused by the rocket traveling through the plasma that causes a floating electric potential outside of the rocket. We expect the floating potential will be around .5V, but we want the design to work for up to 5V. From top to bottom, the plots correspond to .5 to 5V of floating potential.

The masses are color coded in this distribution, but if it were actual data, we would have to infer the mass from the data, so when two adjacent mass distributions are in contact we have no way of knowing what mass is responsible for the count. Ideally, every mass distribution would be neatly separated from adjacent mass distributions. In practice, this is difficult to achieve. Fortunately, so long as the distributions have distinct peaks we can still get some sense of the size of the distribution from measurements like the full width at half maximum. We would like to be able to distinguish between ions by 1 amu all the way up to 81 amu (as you can see if becomes more and more difficult to do so, as the mass increases), however we do not seem to be at that level yet. Fortunately most of the masses we are really interested in are much smaller mass, where we have fairly decent separation.







Acknowledgement and Citations

I would like to thank Professor Clemmons for taking me on to work on this project, which continues his original research, and for his extensive guidance on the project. His article on REFIMS is cited below

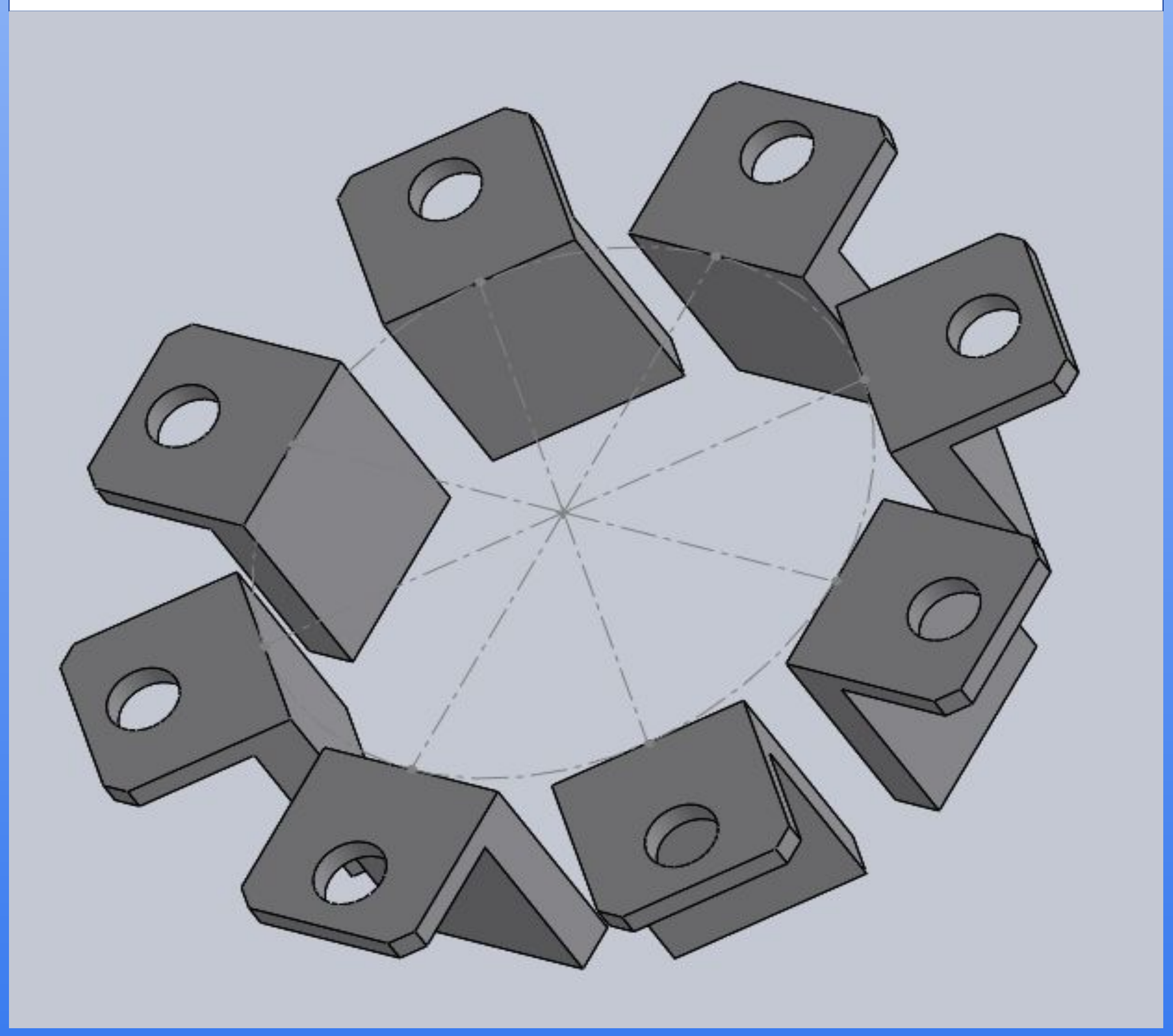
Clemmons, J. H., and F. A. Herrero. "Mass Spectroscopy Using a Rotating Electric Field." *Review of Scientific Instruments*, vol. 69, no. 6, June 1998, pp. 2285–2291., doi:10.1063/1.1148933

Mode of Operation

First, ions diffuse into the instrument. Then they are dropped through an electric potential difference so that they all have approximately the same energy (we give them enough energy such that their random thermal energies are negligible), and focus them into a beam by the collimator. This has the effect that the heavier elements will be travelling slower than the lighter ones, a fact we will use to distinguish them. The other electrodes also help to focus the ions, but I believe the ones before the rotating electric field have more of an effect.

The beam of ions is then passed through a rotating electric field perpendicular to the path of the ions. The direction the ion is deflected depends on the time the ion passed through the electric field. In this way, the time that the ion passes through the electric field is encoded into its angular position. The electric field is generated by eight electrodes (below), set to oscillating voltage, each one eight out of phase with each other.

The ions are allowed to drift to larger radii before landing on the detection plate. The detection plate has many radial channels, so it is able to detect at what angle the ion lands. This is assumed to be the angle at which it was deflected. The difference of that angle and the current phase of the electric field are compared. This value, which is the rotation of the electric field while the ion was in flight, is ultimately proportional to the square root of the mass of the ion.



Theory of Ion Optics

The ions that pass through REFIMS are guided by electrostatic lenses, generated by the electrodes. The electric potential difference between adjacent electrodes creates a curved electric field. Ions that are traveling further from the central axis of the device are accelerated towards the central axis. You can imagine it a bit like an electromagnetic shoot.

Working out the trajectories of ions through a system like this analytically would be extremely difficult, if not impossible. For this reason we use simulations. See methods of simulation for more details.