Optimization of Cubesat-Compatible Plasma Ion Analyzer for Asteroid Composition Analysis

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Abstract

Many space probes have conducted in situ explorations of asteroids, in recent decades, intent on identifying evidence of the solar system’s earliest processes of formation within the asteroids’ interiors. Several future asteroid missions are planned, among which include ESA’s Hera mission to explore the Didymos binary asteroid pair. An ion mass analyzer is currently being designed at the Swedish Institute of Space Physics for use as part of the Hera mission.

This thesis aims to optimize the instrument such that each of its parameters meets the requirement for performance. A computer simulation is used to calculate the trajectories of low-energy ions inside the instrument, where the electrostatic potential are imposed by grids and electrodes embedded inside the instrument. From the data analysis of the simulation results, the performance for each parameter can be derived. By changing the settings of the grids and electrodes (e.g., positions and voltages), the instrument parameters are to be optimized. Two tasks are set up in this project—the first task is to optimize the focusing system of the incoming ions at the instrument’s entrance, and the second task is to investigate the reflectron system so that the mass resolution of the instrument can be optimized via reducing the spread of the ions’ time of flight spectra.

The focusing system is found to already be optimized, but instead, a relation between its position of the grid at the instrument’s entrance and the instrument’s performance is derived. The method of and parameters for optimization within the reflectron are extensively tested individually during this project. Although several performances in each trial from the reflectron analysis cannot meet at least one of the requirements, enough scenarios are examined such that every parameter tested ends with a value suitable to be applied individually to optimize the ion mass analyzer. The findings from the individual tests done in this project can be applied to further optimization, particularly to optimize multiple parameters simultaneously in the near future.
Acknowledgements

I would like to thank my supervisors, Yoshifumi Futaana and Xiao-Dong Wang for having offered me this thesis opportunity and for lending me their support through the all of the times when I was not sure on how to proceed in this project.

I also wish to thank my family for their kind wishes and understanding when work has been quite busy throughout the past few weeks.
# Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Full Form</th>
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<tbody>
<tr>
<td>NASA</td>
<td>National Aeronautics and Space Administration (US)</td>
</tr>
<tr>
<td>JAXA</td>
<td>Japan Aerospace Exploration Agency</td>
</tr>
<tr>
<td>ESA</td>
<td>European Space Agency</td>
</tr>
<tr>
<td>CNSA</td>
<td>China National Space Administration</td>
</tr>
<tr>
<td>IRF</td>
<td>Swedish Institute for Space Physics</td>
</tr>
<tr>
<td>APEX</td>
<td>Asteroid Prospection EXplorer</td>
</tr>
<tr>
<td>ACA</td>
<td>Asteroid Composition Analyzer</td>
</tr>
<tr>
<td>MS</td>
<td>Mass Spectrometry</td>
</tr>
<tr>
<td>TOF</td>
<td>Time Of Flight</td>
</tr>
<tr>
<td>AMU</td>
<td>Atomic Mass Unit</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full Width at Half Maximum</td>
</tr>
<tr>
<td>FOV</td>
<td>Field Of View</td>
</tr>
<tr>
<td>PF</td>
<td>Performance Factor</td>
</tr>
<tr>
<td>GIMP</td>
<td>GNU Image Manipulation Program</td>
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A.1 Mass Resolution and Transparency of Focal Point Test
Chapter 1

Introduction

1.1 History of Asteroid Exploration

1.1.1 Why are asteroids being explored?

Detailing the formation of the solar system is a trending topic. Processes from early on in this formation were captured in the rocks that coalesce into planets and natural satellites — though from coming together, much of their early history as individual rocks would be lost in favor of telling the story of how many together formed a handful of larger bodies. Following comets, asteroids remained the last category of bodies in the solar system to be discovered, and understanding their chemical makeup may change or improve humankind’s knowledge about how everything orbiting the sun fell into place [1, 2]. The asteroid belt was discovered in 1801, but its existence could not easily be connected with the origin of meteorites found on Earth because there was no way at the time to determine asteroid composition and compare it with meteorite samples [3]. Only once spacecraft began to visit asteroids directly in the 1990’s did it become possible to confirm that the origins of meteorites on Earth were from the main asteroid belt in the solar system [4]. Of those that reach Earth, however, the statistics show clear bias in terms of the specific location of origin within the belt and cannot accurately account for the distribution of asteroid types known to exist in the asteroid belt [2]. In turn, the discovery of the Kuiper Belt in 1992 proved there were more asteroids whose composition could not be feasibly determined by observation directly from Earth [5]. This means that any further studies on mineralogy and classification of asteroids beyond what can be seen from telescopes on (or near) Earth would need to be done in situ. Table 1.1 shows a chronological list of missions to asteroids along with their respective agencies and asteroids encountered [6].
Table 1.1: Table of successful, ongoing, and future missions to reach/pass asteroids (arranged by year (to be) launched)

<table>
<thead>
<tr>
<th>Mission</th>
<th>Agency</th>
<th>Target Asteroid(s)</th>
<th>Date</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>28/08/1993</td>
</tr>
<tr>
<td>NEAR</td>
<td>NASA</td>
<td>433 Eros</td>
<td>14/02/2000</td>
</tr>
<tr>
<td>Deep Space 1</td>
<td>NASA</td>
<td>9969 Braille</td>
<td>29/07/1999</td>
</tr>
<tr>
<td>Stardust</td>
<td>NASA</td>
<td>5535 Annefrank</td>
<td>02/11/2002</td>
</tr>
<tr>
<td>Hayabusa</td>
<td>ISAS</td>
<td>25143 Itokawa</td>
<td>12/09/2005</td>
</tr>
<tr>
<td>Rosetta</td>
<td>ESA</td>
<td>2867 Steins / 21 Lutetia</td>
<td>05/09/2008</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>10/07/2010</td>
</tr>
<tr>
<td>Dawn</td>
<td>NASA</td>
<td>4 Vesta / 1 Ceres</td>
<td>16/07/2011</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>06/03/2015</td>
</tr>
<tr>
<td>Chang’e-2</td>
<td>CNSA</td>
<td>4179 Toutatis</td>
<td>13/12/2012</td>
</tr>
<tr>
<td>Hayabusa 2</td>
<td>JAXA</td>
<td>162173 Ryugu</td>
<td>27/06/2018</td>
</tr>
<tr>
<td>OSIRIS-REx</td>
<td>NASA</td>
<td>101995 Bennu</td>
<td>12/2018</td>
</tr>
<tr>
<td>DART/Hera</td>
<td>NASA/ESA</td>
<td>65083 Didymos</td>
<td>2022</td>
</tr>
<tr>
<td>Psyche</td>
<td>NASA</td>
<td>5 Psyche</td>
<td>2022</td>
</tr>
</tbody>
</table>

1.1.2 The First In Situ Exploration

The first asteroid to ever be seen up close was asteroid 951 Gaspra when the National Aeronautics and Space Administration’s (NASA’s) Galileo spacecraft flew past it on October 29th, 1991. Its composition suggested that it was a fragment originating from the mantle of a larger object [7, 8]. Galileo went on to encounter a second asteroid, 243 Ida, in August of 1993. Ida was found to be orbited by a smaller asteroid named Dactyl, making Ida the first asteroid discovered with a companion satellite [9]. An artist’s impression of Galileo over Jupiter’s moon, Io, is shown in Figure 1.1.

![Figure 1.1: Artwork of Galileo over Io. Image credit: NASA](image)

Figure 1.1: Artwork of Galileo over Io. Image credit: NASA [10]
1.1.3 Dedicated Asteroid Missions from NASA

Asteroid 433 Eros was the next visited by the spacecraft NEAR (Near Earth Asteroid Rendezvous). This was the first time a spacecraft touched down on an asteroid’s surface [11]. Deep Space 1 was the next mission to explore an asteroid following NEAR — though it passed its target asteroid, 9969 Braille, earlier in 1999. Both Eros and Braille were identified as members of the common chondrite class: an asteroid class which constitutes many near-Earth objects [4, 12]. While the asteroids visited by Galileo and Deep Space 1 were later found to possess significant magnetic signatures from solar wind interactions, Eros did not have strong magnetic field [13]. When the Stardust spacecraft flew by 5535 Annefrank, the images of the body added more evidence suggesting many existing asteroids are former protoplanet remnants [14]. Stardust is depicted in operation in Figure 1.2.

![Figure 1.2: Artwork of Stardust analyzing the tail of target comet P/Wild 2. Image credit: NASA][15]

It took several years before the Dawn mission visited 4 Vesta and 1 Ceres. Dawn first reached Vesta in 2011 and made several crucial observations about the second largest asteroid in the asteroid belt. Out of all asteroids visited so far, Vesta had the highest albedo fluctuation. This was due to the compositional variation [16]. Among the constituents found, there are compounds associated with howardite-eucrite-diogenite (HED) type asteroids. The HED type is a small family of asteroids believed to have originated from the same protoplanetary body as Vesta [17, 18]. Vesta was also believed to hold trace amounts of water from various markings indicating hydrated material deposits [19]. In 2015, Dawn began its observations of its second asteroid when it reached Ceres. Through both visible/IR spectrometry and nuclear spectroscopy, Dawn found a significant amount of water situated on and immediately beneath asteroid’s surface [20, 21, 22]. The unusual smoothness seen over much of Ceres’ surface suggested the possibility of cryovolcanism being responsible [23]. Dawn also recorded magnetic interactions between Ceres and incoming solar wind [24]. Figure 1.3 shows an artist’s impression of Dawn near Vesta.
Lastly, NASA has the OSIRIS-REx spacecraft still in-operation. OSIRIS-REx rendezvoused with its target asteroid Bennu in late 2018 and has documented that the asteroid’s rotation rate is accelerating due to a torque applied by radiation pressure from the sun on its oblate surface — a phenomenon known as the YORP effect. In this effect, the solar radiation pressure distributes across the oblate surface, creating an offset torque (causing or increasing rotation), and the resulting thermal emission from the asteroid further accelerates its spin [26]. The spacecraft is currently preparing to land on the asteroid to obtain a sample before its journey back to the Earth [27].

1.1.4 Sample-Return Missions by JAXA

In 2003, the Japan Aerospace Exploration Agency (JAXA) launched the Hayabusa spacecraft, which reached the target asteroid Itokawa in September 2005. Besides orbiting the asteroid, the spacecraft made two touchdowns and attempted to obtain samples on its second landing on the asteroid’s surface [28]. This was also the first time that a spacecraft landed and took off from an asteroid body (NEAR still rests on Eros) [29]. While marginally successful in sampling a scant amount of particles, Hayabusa was able to return the samples to Earth for the first time. The samples were then confirmed to originate from outside Earth [30]. The success of this mission prompted Hayabusa 2 to be developed and launched. Hayabusa 2 reached asteroid 162173 Ryugu in June 2018. Ryugu was discovered to be a “spinning rubble pile” due to the frequent presence of boulders seen on its surface [31]. Itokawa’s chemical profile was found to not match typical carbonaceous chondrites, while Ryugu’s did [30, 32]. Artwork of Hayabusa 2 orbiting its target asteroid is shown in Figure 1.4.
1.1.5 Asteroid Missions by ESA

In 2004, the European Space Agency (ESA) launched their Rosetta mission to follow the comet 67P/Churyumov-Gerasimenko. Prior to reaching its destination, the spacecraft passed by two asteroids: Steins in 2008 and Lutetia in 2010. Similar to asteroid Ryugu, Steins was found to be a conic rubble pile, as opposed to a single solid asteroid [34]. Lutetia’s composition suggested it is among the carbonaceous chondrite family [35, 36].

1.1.6 China’s Asteroid Mission

As of December 2012, the China National Space Administration (CSNA) has also conducted an in situ asteroid investigation. The asteroid visited was Toutatis, and it was encountered by the CNSA’s spacecraft Chang’e-2. Prior to performing its flyby of this asteroid, Chang’e-2 had analyzed the space environment at the Sun-Earth Lagrangian point L2 [37]. Toutatis was found to resemble a ginger root, with findings suggesting that its possession of a large and small lobe are the result of a contact binary — where two asteroids connect and gradually merge at the point of contact [37, 38]. As a contact binary, Toutatis is also estimated to be comprised of a rubble pile similar to asteroid Itokawa [38].

1.1.7 Future Asteroid Missions

NASA is planning a spacecraft mission to the asteroid 5 Psyche in late 2022 [6]. Psyche stands out as an asteroid mostly comprised of metals, rather than silicates seen in most other asteroids. The mission under the same name will aim to determine whether the asteroid is the remnant of the core of a protoplanet, as opposed to a mantle or crustal fragment that some other asteroids have been assumed to be [39].

More central to the theme of this project is the planned NASA/ESA collaborative missions to 65083 Didymos, known to possess a comparatively small moon, “Didymoon”. Instead of space-borne investigations of an asteroid far from the Earth, NASA and ESA...
will this time focus on applying a proof-of-concept to redirect an asteroid’s orbit. ESA’s mission is known as Hera, while NASA’s mission is known as DART (Double Asteroid Redirection Test). The DART spacecraft will impact Didymoon at full-force, to determine the feasibility of using current spacecraft technology to redirect the orbits of asteroids [40, 41]. It will fall on Hera to then closely check the orbit of Didymoon for any discernible characteristic changes. Hera is further explained in Section 1.2.

Didymos spans approximately 780 m in diameter, while Didymoon is about 160 m wide. Didymoon orbits Didymos at a distance of 1.2 km once every 12 hours. Didymos and Didymoon are accessible, but their closest pass to Earth is estimated to be 10 million km [42].

1.2 The Hera Mission

1.2.1 Hera

Hera will arrive at the Didymos pair following DART. DART will dive toward Didymoon as a projectile, while Hera will record the aftermath of its impact from a distance and quantify the changes in Didymoon’s orbital eccentricity and inclination [41, 43]. Hera will release two clustered cubesats to view multiple perspectives of the asteroid(s) simultaneously. Hera is shown in Figure 1.5.

![Hera orbiting Didymoon with cubesats](image)

Figure 1.5: Hera (right) in orbit around Didymoon. Hera’s deployed cubesats are also visible in orbit around the small asteroid. Image credit: ESA [43]

1.2.2 Hera’s Cubesats

Two cubesats released from Hera will observe Didymos and Didymoon from their vicinities. One of the cubesats is the Asteroid Prospection EXplorer (APEX), while the second
is called Juventas. APEX will perform spectral imaging of the surfaces of each asteroid to determine surface chemical composition analysis and magnetic field measurements, and Juventas will scan Didymoon’s interior by passing radar waves through it to Hera on the moon’s opposite side. Of the two cubesats, APEX is a joint-effort project between space institutions from Sweden, Finland, Germany, and the Czech Republic. APEX will therefore possess several instruments to use in tandem to fulfill its goals — one of which is the Swedish-designed Asteroid Composition Analyzer [44].

1.3 The Asteroid Composition Analyzer

One effect from the solar wind’s interaction with asteroids is the sputtering of material from the asteroids’ surfaces due to the lack of a protective atmospheres. With asteroids having no such atmospheres present, the only major source of particles forming their environment has to come from interactions with the solar wind — most of the sputtered particles are electrically neutral, but some of the particles are charged. The sputtered ions usually have very low kinetic energy ($< 5$ eV).

An ion mass spectrometer is under development by the Swedish Institute of Space Physics (IRF) to measure ions from the sputtered atoms from the day-side surface of Didymos system.

1.4 Thesis Purpose

This project aims to address parameters of ACA’s design deemed critical for meeting its individual requirements to enable scientific investigations. Optimization for a given parameter is considered complete once it had been calibrated to yield the greatest net benefit to the system’s function. Optimization for the instrument is considered complete once suitable tradeoffs between all parameters had been set.
Chapter 2

Background

2.1 Mass Spectrometry

Mass spectrometry (MS) of particles is widely used in laboratory environments, and measures the intensity of particles as a function of their masses which reveal their species. The process involves ionized atoms or molecules from a gaseous substance passing through an electric or magnetic field to discriminate against their mass-to-charge ratio (m/z ratio). Under electric or magnetic influence, the particles’ directions of travel are lined up such that they all will impact on a detector — the detector in turn produces a signal to indicate particle impact has occurred. As the ionization is usually controlled, the charge is known prior to testing meaning the detector’s signal is used to determine the particles’ masses — by how long they took to reach the detector and/or by where their impacts occur on it [45, 46]. As a general method of composition analysis, mass spectrometry has been used in several space missions.

In particular, MS has been used to measure the outer atmospheres of several planetary bodies. Data from the Apollo mission discovered sputtered material from the lunar regolith mixed with the plasma surrounding the moon through mass spectrometry [47, 46]. It helped identify elements in Europa’s ionosphere via the Galileo mission [48]. Mass spectrometry was also used aboard the Rosetta mission for analyzing the dust tail of its target comet [49].

The primary means of determining asteroid composition in the past has been through visible and near-infrared reflectance spectroscopy (VNIR), where the distribution of wavelengths of radiation reflected from an asteroid’s surface is used to predict the presence of specific elements in said surface. This process has been studied extensively in laboratory environments, documenting the reflective spectra of many elements and compounds — making those elements distinguishable among the mix of spectra typically seen on an asteroid’s surface. Albedo analysis is also used to identify elements and compounds, as each tend to absorb a specific amount of visible light, resulting in patches of varying brightness across a surface of mixed materials. As most past asteroid missions have been flybys, the observing spacecraft were primarily orbiters, hence analyses being done primarily through VNIR [2, 50].

ESA’s Rosetta carried aboard the ROSINA Double-Focusing Mass Spectrometer (DMFS) and this instrument was used throughout the course of the Lutetia flyby in an attempt to identify an exosphere over the large asteroid. While the measurements for this exploration were overwhelmed by the outgassing of the spacecraft itself, this was among the first of
cases where MS has been used from an orbiter [51]. MS has been done previously in space exploration, but only by landers, and only on planetary bodies larger than asteroids — such as Earth’s moon [47], Venus [52], and Mars [53].

2.1.1 Mass Spectrometry in ACA

Where ROSINA-DFMS was the first time MS was used in orbit around an asteroid for atmospheric analysis, ACA will be the first time MS is used in orbit to target ions sputtered off of asteroid surfaces. As it would be several years between the launch of the Hera mission and when ACA’s parent cubesat APEX is deployed to investigate the Didymos pair, outgassing of the cubesat is assumed to not have an impact on composition analysis (as well as much of the outgassed material being neutral due to it originating in a laboratory environment on Earth). ACA will provide direct elemental distribution by sampling ions — element composition via VNIR and similar methods only indirectly indicates element presence as no material is ever obtained. Because ACA will sample from an orbiter, it will provide a high spatial coverage otherwise infeasible for a lander due to its restriction of mobility and proximity to the surface.

Regardless of the technique used for composition analysis, all instruments will have selection biases with ACA being no exception. For ACA measuring ions from orbit, it will need to associate an ion sampled at a given orbital position with a corresponding area of ion origin on the asteroid surface. As many small asteroids have no magnetic fields of their own unlike larger planetary bodies, this leaves ions sputtered off of the Didymos pair to be influenced by the strength of the interplanetary magnetic field present throughout the solar system [54, 55]. The direction of the field can influence the direction of the motion of these ions, creating ambiguity on their true areas of origin. The fractions of elements in the compositional distribution may also be skewed due to ionization efficiency. Neutral particles of any element may be produced stochastically due to their lack of electric charge, but each element present will have its own ionization efficiency [47]. As such, deeper into ACA’s development, a correction factor for the interplanetary magnetic field, as well as ionization efficiency per element will need to be integrated into ACA’s electronics to balance any biases in empirical data.

2.1.2 Time of Flight Measurement

As a technique for mass spectrometry, time of flight (TOF) is simple in principle: if the time taken for a particle to fly across an known distance is recorded, its speed can be calculated. In combination with the particles’ predetermined energy, their masses can be derived. The mathematical details for this are shown in Subsection 2.2. TOF mass spectroscopy (TOF-MS) has been used in mass spectrometry for distinguishing particles from aerosol pollutants in Earth’s atmosphere [56, 57].

TOF-MS allows for the TOFs of all mass categories to be measured simultaneously for a continuous flow of inbound particles — but only for a small instance of time — this makes TOF-MS limited to pulses of information on composition over time [58].
2.2 Electric Fields within the Instrument

ACA uses an electric field to analyze ions. The force $F$ exerted on an ion in an electric field is equal to the electric field strength $E$ of the electric field multiplied by the charge of the ion $q$ (integer times electron charge of $1.6 \cdot 10^{-19}$ Coulombs) [29]:

$$F = q \cdot E \quad (2.1)$$

The equation can be expanded to emphasize that the force between the electric field and the passing particle affects the particle’s motion:

$$F = m \cdot a = m \cdot \frac{\delta v}{\delta t} = q \cdot E \quad (2.2)$$

All of ACA’s interior (excluding its reflecting devices) will be comprised of a drift tube environment. In a drift tube, electrodes line every wall, and they are all intentionally charged to the same voltage. Once particles are inside this environment they experience no electric field (save for any particles passing within very close proximity of any electrode). The drift tube region of ACA will have electrodes charged to -200 V. The purpose of this negative voltage is to accelerate the sputtered Didymos particles through its system to better discriminate among their masses by measuring TOF. Ion acceleration is needed to reduce the TOF to a reasonable range and account for the ion kinetic energy differences expected in the asteroid’s particle environment.

Based on lab data and mission data on sputtered particles, studies have found that nearly all of the sputtered particles’ energy spectrum lies under 5 eV [46, 60], hence its use as an assumed boundary. Particles with energies outside of this range may exist in the Didymos environment, but they would account for a very small fraction of the total number of sputtered particles compared to how many would have energies less than 5 eV. On its own, 5 eV is impractical for TOF measurements, as it corresponds to very slow movements of particles — but if ions with this range of energy are accelerated through a high voltage of -200 V, the energy levels of these ions effectively have 200 eV superimposed on their existing energy range, making their differences have a smaller unwanted impact on TOF measurements. The drift tube regions in ACA are shown in Figure 2.1.
Figure 2.1: (a): Current ACA layout and its ion path (signified by the orange dotted line) (b): Drift tube regions in ACA (highlighted in green). Despite being set to a high negative voltage, they yield negligible effects on particle trajectories.

The acceleration of ions in ACA is done by a curved, double-gridded structure called the entrance grid. When a new TOF cycle begins, the outer grid is set at 0 V to match the environment of space and allow particles to enter, while the potential gradient drops steeply until it reaches the inner grid set at -200 V. For the positive ions, this would metaphorically resemble a steep slide for them to gain speed. For conditions where particles are not allowed entry into ACA (due to TOF-MS requiring pulse-based ion reception rather than constant), the outer grid is set to a positive voltage to repel the same targeted ions. The time needed for one “open” and “closed” periods to pass forms one duty cycle. For this project, an ideal case of an infinitely small open time is considered as it provides the best possible performance for ACA’s TOF system. In reality, the open time will be defined by the TOF separation performance, duration of the full duty cycle, its efficiency, as well as by the performance of ACA’s electronics. At this time, no specific number has been chosen for a duty cycle length.

Many TOF instruments require a thin film of material sensitive to ion impacts to be present in order to trigger a start signal when ions pass through it, while a detector is also needed to generate the end signal to conclude the ions’ TOF. What makes ACA unique as a TOF instrument is that only a detector is needed (rather than a detector and a start film) at the end of ACA’s particle tunnel to measure the ions’ arrival time. The starting time for the ions is given by the instant the entrance grid’s outer voltage is grounded to 0 V for ions to start entering ACA. The electrostatic gating system has a heritage in the PRIMA instrument on board the Swedish PRISMA spacecraft [61].

The steps to deriving the mass of incoming particles are outlined below [62]:

---

18
The equation for an ion’s kinetic energy is:

\[ KE = q \cdot U = \frac{1}{2} \cdot m \cdot v^2 \]  \hspace{1cm} (2.3)

\( q \) is the charge of an ion, \( U \) is the potential drop of the grids in the electrostatic gate (200 V for ACA), \( m \) is the mass of the ion to derive, and \( v \) is the ion’s velocity.

The time of flight is calculated as:

\[ v = \frac{L}{t} \]  \hspace{1cm} (2.4)

Here, \( L \) is the distance traveled by the secondary ions from start to stop, and \( t \) represents the time of flight. It is a variant of the distance formula, which states that the distance an object has moved is equal to the product of its speed and the duration of its movement.

Combining the two and simplifying gives:

\[ \frac{m}{q} = \frac{2 \cdot U \cdot t^2}{L^2} \]  \hspace{1cm} (2.5)

This means TOF measurements can indicate the mass-to-charge ratio of the pre-accelerated ions. An assumption made in this project throughout its run was that the ions tested have single charge, because the probability of double ionization is negligible — a constant charge for all particles makes direct mass determination possible. A second assumption is that acceleration through the entrance grid (relating to Equation [2.2]) is not included in the TOF calculations used throughout this project. This acceleration is ignored due to it occurring over the distance between the inner and outer gates of the entrance grid being short when compared to the total distance covered by the ions’ trajectories from entrance tunnel to detector. The acceleration is considered fast enough to be instantaneous.

2.3 Reflecting Particles

Prevention of photons from reaching ACA’s detector is important, as any photon incident on the detector will cause it to register as an impact as if it were from an ion — an event known as UV contamination. Two turns in the instrument’s drift tube are needed to sufficiently reduce the UV photon count to a level that can be ignored — hence, the need for two reflection devices. The instrument’s profile has a turn in its drift tube, where an electrostatic mirror constitutes the wall forming the turn. A multi-stage reflecting component called a reflectron forms the structure at the second turn. The turns constrain the instrument’s dimensions to a 45-by-100 mm square cross-section (if the back-end electronics region is excluded), allowing the instrument to fit aboard APEX while simultaneously preventing photons (from the sun) from reaching ACA’s detector.

The turns in ACA provide the added advantage of increased tube length for increased overall TOF. Longer TOFs mean bigger differences, which are easier to detect. ACA’s objective lies specifically in differentiating between the masses of the ions it captures. ACA will in particular capture a wide range of ion masses and must be capable of resolving the
masses between the second-heaviest and heaviest possible ions it is expected to detect. These values currently sit at 70 and 71 AMU, respectively. The TOF difference between the 70 and 71 AMU categories of mass will be significantly smaller than it will for the two lightest (1 and 2 AMU), so this stresses the need for high-mass TOF differences to be large enough to be detected.

ACA’s profile starts with an entrance grid on the open end of the tube, and leads to a drift tube with a tilted mirror platform. From this mirror, the drift tube is funneled into the second turn — defined by a reflectron that is also tilted such that its cap is parallel to the mirror on the opposite side of ACA. This reflectron forms a distinctive “U” shape that then leads the particles down the final segment of the tube to the closed end, where a detector plate sits. Beyond this plate (and the outer wall of the final tube segment) lie the electronics responsible for delivering power to ACA’s entrance grid, the electrodes in the mirror and reflectron chambers, and the detector plate — these electronics components are not included in the ACA models shown.

2.3.1 Electrostatic Mirror

Recalling the layout in Figure 2.4, ACA has an S-shaped particle path to focus the incident ions in energy and to screen the photon contamination. The particle path can be divided into an entrance, a detector terminal, and two reflections to guide the particles from the entrance to the detector. The first reflection is at an electrostatic mirror: it reflects all incoming particles with an electric field. This reflecting electric field is formed by a flat panel biased to a positive voltage (e.g., 24 V) and a negatively-biased, parallel flat grid in front of the panel. In the ACA case, the grid is biased to -200 V at the same voltage as the interior of the drift tube. The uniform electric field between the panel and the grid allows incoming particles to move in parabolic trajectories. A parabolic trajectory means that the incident angle of an ion equals its exit angle, resembling an optic mirror for light. This is the reason why such a structure is called an “electrostatic mirror”.

In an ideal electrostatic mirror, the grid is 100% transparent. In practice the transparency of a real grid is less than 100 percent and results in a slightly hindered particle flux for two reasons. The first is that the grid is a solid structure, meaning there are places on it a particle can hit, ending that particle’s trajectory. The second reason is due to the distortion of the electric field at a scale comparable to the grid spacing (the interstitial gaps between the grid’s solid elements). Rather than several lost ions due to the solid portions of the grid, the hindrance of particle flux mostly results in defocusing of ions (unwanted scattering of trajectories) due to the electric field distortion affecting the particles. The transparency of a grid is on the order of 90 percent (at a best case) for a single instance of crossing per particle — and since each particle passing through the grid to the mirror will inevitably get reflected back through the grid, they will cross a second time. This reduces the overall transparency of the grid since the transparency is to the power of the total number of crossings per particle — but the efficiency can be said to remain above 80 percent always since the mirror grid should only require two crossings per particle.

The use of a reflectron can result in significantly less defocusing of ions due to it having a less critical need for a grid as well as its ability to regroup ions of the same masses initially traveling with differing velocities. It also has the ability to desegregate particles of the same mass that may have differing velocities — recombining them as a
single category for the spectrometer’s detector.

Figure 2.2: ACA mirror and its condensed electric field (shown as red contours representing lines of equal electric potential). The field is contained by a thin grid shown as a fine blue line parallel to the purple mirror plate in the design.

2.3.2 Reflectron

Where the first reflection region inside ACA is used to house a mirror, the second reflection is realized by a reflectron. As its name suggests, a reflectron is a tool that also can reflect the trajectories of incoming particles. It does so in similar fashion to a mirror at a glance — both tools rely on the use of strong electric fields to repel the particles as they enter and both tools are often tilted to change exiting particle trajectory angle. The similarities between the two devices end beyond these two facts. Where the mirror is a single electrode charged to a single uniform voltage, the reflectron possesses several electrodes specifically so that each electrode differs in voltage from its neighbors. A reflectron TOF mass spectrometer is shown in Figure 2.3.
Figure 2.3: Standard TOF reflectron set-up. Ions of one mass generated in an ion laser are accelerated through a grid with a potential difference. The red ion (with higher speed) enters the reflectron deeper than the slower blue ion (with the same mass). The red ion catches up to the blue once they are both impacting on the detector, at the same time. Image credit: K. K. Murray [63].

Description

A reflectron typically has a U-shape and comprises of arrays of electrodes on either of its internal lateral walls. These arrays of electrodes are symmetrical to one another in their electrode numbers, sizing, and voltages — this is done to ensure that similar to the case of a mirror, that particles entering with a certain velocity vector will leave with a predictable velocity vector in return. As well as having electrodes coating its lateral walls, the reflectron also must have its terminal electrodes at the deepest point along each wall extend along its bottom wall to form its cap since without this, particles are decelerated to a measurable degree before still impacting into the otherwise uncharged cap. The final part of the reflectron is the familiar grid and this is used again for similar reasons to those of the mirror — to limit external potential difference while enabling particles to pass through. Unlike with the mirror’s comparatively strong electric field and close-range potential source, the reflectron has a significantly weaker field present at its entrance due to having both more distance over which the highest potential difference can be attenuated, as well as having multiple electrode levels to dampen its effects. For this reason, the reflectron can use a grid with a higher transparency, meaning less of a reduction in particle flux — and less grid-related defocusing. Figure 2.4 shows a gradient visualization of the electrostatic potential inside the ACA reflectron.
Figure 2.4: Potential inside ACA’s reflectron (with a total depth of about 33 mm). $x$ represents the reflectron’s width while $y$ indicates depth (both in mm). The colorbar, $U$, is the potential distribution (in V) in terms of $x$ and $y$. The electrostatic voltage increases with depth and near the vertical edges where the electrodes lie. Ideally, particles enter at $x \approx 5$ mm and leave at $x \approx 20$ mm, rising from $y = 0$ mm to about $y = 17$ mm (averaging at half the reflectron depth) then dropping back to $y = 0$ mm. Both graphs use color gradients to represent voltage increasing from negative to positive (blue to yellow), but the spatial display shows the change as continuous (gradual changes in color), while the contour display discretizes the gradient into markers of specific values (i.e. $U = -200$ V, $U = -180$ V, etc.).

A visual analogy for comparing the two devices can be seen in a miniature golf course — with the ions being the golf balls. Where the electrostatic mirror is comprised of a single positively charged electrode, it shows up as a wall at the far end of the path. In reality, the wall is actually a ramp, but its gradient is so steep, it is approximated as vertical wall. The steepness of this ramp would stem from the single electrode’s high potential difference between itself and its own drift tube grid forming a steep electric field in ACA. The purpose of this wall in the course is for the incoming balls to deliberately impact onto and rebound off of it for their trajectories to continue. The reflectron in contrast has a curvature to its electric field in ACA and this carries over to a smooth ramp with a gradually increasing gradient. It is set up to redirect incoming balls by applying an amount of potential to each ball proportionate to the kinetic energy that ball had when it entered the ramp. In this way, the faster balls travel higher, but would have more potential energy to turn back into kinetic energy. This means that compared to slower-moving balls, faster ones entering the ramp will rise higher, stay on the ramp longer, and will leave traveling faster. The two examples are shown in Figure 2.5.
Figure 2.5: Mirror and reflectron concepts represented by miniature golf. (a): Mirror-wallet image created in GIMP (program described in Chapter 3). (b): Ramp image credit: Plonk Golf/ZSL London Zoo [64]

Why a reflectron is used for a second mirror

The greatest advantage in using a reflectron is its focusing property in time of flight. Ions of the same mass that enter a reflectron at the same time will exit the reflectron at the same time, regardless of each ion’s velocity, if the reflectron is correctly optimized. Additionally, by tuning a reflectron in a non-energy-focused system, the reflectron can even compensate the defocusing effects caused by other part of the TOF mass-spectrometer [65]. A mirror cannot refocus ions as such (due to its simple single-panel design) and it partly contributes to the defocusing effect instead due to its field distortion.

In a study on reflectron optimization, a reflectron with three stages of electrodes was examined [66]. The study explains how the design for this reflectron was developed with specific ratios of voltage and length between the electrodes to work optimally for their experiments. This is crucial for developing practical reflectron devices since the theoretically ideal version of a reflectron would have an infinite number of electrodes to shrink the step size to a negligible length — thus smoothening the response to a curve resembling a parabola. Modeling the geometry and underlying electronics of the reflectron to better approximate this potential curve can likely be done, but the added cost of doing so would not be worth the increases in performance, as they could be considered marginal beyond the three-electrode model. In other words, at just three electrode elements (with the correct sizing and voltages), a practical reflectron can very closely imitate a theoretically ideal one. The general position of each of the three electrodes in ACA’s reflectron, as well as their axial potential over depth in the reflectron are shown in Figure 2.6 where the three regions inside ACA’s reflectron are shown divided by dotted green lines.
Figure 2.6: (a): Ion trajectories begin in the entrance region (i) where the drift tube smoothly transitions into an increase in electric potential. j denotes the deceleration region where the particles’ velocities are the most heavily slowed, and k denotes the turnaround region, where most particles begin receding due to the outward acceleration overwhelming the particles’ diminished velocities. (b): Distribution of potential as a function of depth with \( x = 12 \text{ mm} \) (blue) marking the potential along the reflectron’s central axis. The red curve, \( x = 0.3 \text{ mm} \) shows the distribution at a close proximity to the electrodes (at 0 mm), while the green curve, \( x = 6.3 \text{ mm} \) shows the distribution half way between the central axis and the electrodes. The curvature of potential distribution across width shows that a deviation from the central axis of up to halfway to the electrode wall shows a potential line similar to that seen along the central axis itself.

In Figure 2.6a, the three electrode elements are shown labeled as i, j, and k. Their associated values were the default values for the reflectron prior to this project:

- i has a depth of 13.2 mm and has a voltage of -200 V
- j has a depth of 15.9 mm and has a voltage of -29.42 V
- k has a depth of 3.6 mm and has a voltage of 20 V

The relation between each of these values is discussed later in equations 2.10 and 2.11 in Section 3.3. Figure 2.6b shows the lateral distribution of potential inside the reflectron used — with units in cm. This stresses that the difference between an ideal reflectron and a practical three-element one is that the ideal reflectron (with an infinite number of immeasurably small electrodes) will have no field distortion at the electrode walls due to each electrode varying minimally compared to its neighbors. An ideal reflectron would also have a hyperbolic curve of increasing potential along its central axis. As far as practicality is concerned, only particles traveling dangerously close to the electrodes will experience the constraints of only three electrodes being used in a reflectron.
2.4 Allocation of Project Tasks

2.4.1 Task 1

In Figure 2.7, the results for the default version’s angular acceptance are shown. The height of the curve indicates what percentage of ions generated in the file simulation entered the instrument and reached the detector (known as the instrument’s transparency). The width of the curve at its base indicates what the maximum angular variation a stream of ions can have such that they reach the detector. The width at half the height of the curve’s peak is known as “full width half maximum” (FWHM) and is more important, as it serves as the lowest number of ions (with respect to whatever the maximum may be in a graph) that can be practically used for producing data. The FWHM is hence considered the practical angular acceptance of the instrument. The statistical formula behind this is outlined in the theory in Task 2, as FWHM will play a key role in Task 2’s objectives.

Figure 2.7: The angular acceptance at ACA’s detector with its default design. The height of the curve indicates what percentage of ions generated in the the simulation entered the instrument and reached the detector (known as the instrument’s transparency). The greatest amount of accepted particles (over 60 percent) occurs when their trajectories point straight down at -90 degrees into the entrance of ACA. Since all four mass categories with differing colors have the same acceptance angle distribution, only the highest mass is seen on the graph. This kind of graph is used to determine if over half of the particles received come from an angular range greater than a specific threshold.

At the time of this project commencing, ACA had just received a new internal design upgrade that would focus a greater portion of entering particles into the reflectron. The design affected the shape of and placement of several internal structures (wall lengths, mirror angle, reflectron angle, reflectron depth, etc.), as well as the angle of the entrance grid. Positioning of the grid, however, was left unchanged. Hence, it was decided that
the first task is to investigate the effect the entrance grid’s position on the angular acceptance. This trial for adjusting a parameter for the entrance will justify the importance of the entrance grid in ACA’s architecture: it is the first point of interaction between the instrument and the incoming particles.

Where the curvature of the grid holds significance due to it focusing the ions such that losses in intermediate portions of the tunnel are kept low, the position of the grid is imperative to defining ACA’s acceptance angle. If ACA’s acceptance angle can be changed, this is expected to have an effect on the instrument transparency, as the total number of particles reaching the detector will change. A requirement of a minimum of a 30 degree field of view (FOV) has been assigned and the adjustment of the entrance grid’s position will determine when this requirement is met.

2.4.2 Task 2

A second requirement for ACA (following that of its 30 degree FOV, which was validated through Task 1) was to have the instrument’s detector be able to differentiate between ions with masses of 70 and 71 AMU respectively. An additional requirement of having an instrument transparency of no less than 30 percent exists, as any lower does not satisfy the measurement requirement for low-energy ions sputtered from asteroid surfaces. Hence, the best case scenario is an instrument with an excellent ability to distinguish the heaviest of its target masses combined with an instrument transparency of no less than 30 percent.

The focus of this task is to adjust the elements of ACA’s reflectron since the simple design of electrostatic mirrors does not by itself improve the performance of measuring TOF by mass category near the upper limit.

Theory

Because the detector is a passive device which needs these criteria in order to differentiate between the heaviest of masses, the responsibility of meeting these criteria go to the reflectron. The reflectron therefore needs to be able to reduce the amount of deviation from the average TOF for each particle mass — thus reducing the spread of each mass profile and thereby their mutual overlap. Figure 2.8 shows two extreme examples where the difference in the widths of TOF spread is apparent. Because an ion of 71 AMU mass is the heaviest ion to be identified by ACA, accomplishing this task of maximum mass differentiation ensures that all (positive) ions of a lighter particle mass are successfully categorized by the instrument. The aim of this second task was to not only ensure that ACA meets this requirement (that is to successfully discriminate between its two heaviest target masses), but to maximize its performance. The quotients described in the figure are not used to determine if resolution between the curves is sufficient — instead, their numerators and denominators are subject to separate arithmetics before being recombined into a single fraction that determines resolution quality (Equation 2.6).
Successful differentiation between these two masses occurs when the quotient between the average FWHM value of the mass TOF distribution (the amount of TOF variance at half of the maximum number of particles per mass category) taken from both mass distributions 70 and 71 AMU and the difference between the central TOF value (the mean value of the Gaussian curve fitted over each mass distribution) results in a number less than 1. This means that the two distributions may (and often do) overlap, but can still be resolved as two peaks. If the quotient of this formula is greater than 1, then this suggests the detector is receiving a distribution that can only certainly be said to have one peak. This quotient formula output is classified as the performance factor (PF) of the system. Its equation, below is shown:

\[
PF \equiv \frac{(FWHM_{71} + FWHM_{70})}{2} \frac{TOF_{71} - TOF_{70}}{2}
\]

\[
PF < 1 \rightarrow PF \text{ is resolvable}
\]

1Gaussian curves are used throughout this project as approximations for particle histogram data and often hold few, if any counts in their long tails. When particle counts occur within the curves’ tails (often well-distanced from the curves’ centers), this usually indicates particles have either taken paths of unusual lengths, or have traveled with unusually varying velocities — both of which indicate unoptimized reflectron performance. Hence, following the completion of this project, it is recommended that a replacement type of statistical curve to be used to fit with empirical counts.

2Note that throughout the context for Task 2 any mentions about an increase in system performance equate to a decrease in performance factor.
The reason that differentiation between the highest target masses guarantees differentiation of lower masses in ACA is shown in the equations for momentum and kinetic energy, respectively shown below.

\[ p = m \cdot v \]  
\[ KE = \frac{1}{2} \cdot m \cdot v^2 \]

Particle momentum is weighted equally between mass and velocity, so if particles of all masses had the same momentum, those of mass 1 AMU would travel faster than those of mass 71 AMU — specifically 71 times faster. If all tested particles had the same kinetic energy, those of 1 AMU will be faster than those of 71 AMU by a factor of only 8.43 (the square root of 71). So, in terms of the kinetic energy equation, velocity plays a bigger part. TOF is the deciding factor for mass discrimination because it is a function of particle velocity and not mass. The particles expected to be measured by ACA will also have a close-to-constant value for kinetic energy in space (a maximum of about 5 eV prior to the -200 V acceleration, which adds 200 eV). If the instrument can differentiate between the two heaviest masses by their velocities, then the comparison of any other combination of mass categories within the 71 yield a greater TOF difference, meaning that all ionic elements/compounds up to 71 AMU can be segregated successfully.

Since the particles of each mass category have a kinetic energy variance, as well as a trajectory displacement due to differing points of origin, spread trajectories inside the reflectron are introduced — making the need for a smooth potential distribution inside the three-element reflectron all the more crucial. The parameters of the reflectron would need to be configured to maximize the amount of viable peripheral area within it — area near the electrodes that does not lose TOF resolution due to field distortion from electrode boundaries. According to the same three-electrode reflectron study, this can be achieved when the following equations were satisfied:

\[ V_j = V_k \left(1 - \frac{k}{j}\right) \]  
\[ j = i + k \]

Here, \(i\), \(j\), and \(k\) represent the lengths of each electrode (\(i\) being the outermost and \(k\) being the innermost), while \(V_j\) and \(V_k\) represent the voltages of the electrodes with the same length letters. Previously shown, Figure 2.6a attributes the regions of ACA’s reflectron to their respective letters.

These two equations (2.10 and 2.11) entail the voltages and size proportions for the electrodes in the reflectron — the variables that can be changed without the need for remodeling the reflectron’s external dimensions and positioning. From Equation 2.11 the length of electrode \(j\) must be large enough for the other two electrodes to match its length together — meaning that for a three-electrode reflectron, \(j\) must occupy half of its depth. From Equation 2.10 it can be seen that \(V_j\) must form a sizable fraction of \(V_k\). It must lie significantly closer to \(V_k\) than \(V_i\), as the expression inside the parentheses would otherwise be inverted to result in a smaller fraction. Both of these conjectures are supported by
the idea that deceleration of particles inside a reflectron is its primary priority. A smooth entry (region \(i\)) is needed only to prevent distortion of trajectory direction, while the turnaround region (\(k\)) can be smaller since its function of reversing the particles’ motion requires the least amount of space as only the fastest-entering particles reach well into this region (all slower ions have turned around, barely touching this region).

The aim of this task is to change the value of one single variable at a time within these two equations, unless other variables depended on the status of the targeted variable. The changes are mapped as a scale of points separated by constant intervals (i.e. changing a part length by 1mm every test) to see the degree of change in ACA’s performance.

Hypothesis

Prior to this thesis project commencing, the design for ACA that was used as reference for all testing had the reflectron and mirror components tilted (in place of a horizontally aligned entrance grid) to better direct particles throughout the instrument. The reflectron in particular had electrodes resized since the whole tool needed to be refitted to a smaller space due to the tilt. When the reflectron parameters were compared against the criteria of equations 2.10 and 2.11, they were found to loosely follow the formulae, but not to 100 percent satisfaction. This is explained in Subsection 3.3.1 in Chapter 3. In short, the electrodes were near proper length for optimization, but imprecise — electrode \(j\), in length came up shorter than the combined lengths of electrodes \(i\) and \(k\).

The same paper by Zhang and Enke also displayed the three-element reflectron with a \(j\) electrode voltage at about two thirds the difference between the \(k\) and \(i\) voltages for optimum particle turnaround — as a way to balance between off-axis homogeneity (for particles away from the reflectron’s axis to still be properly reflected back out), and axial non-linearity (for ideal TOF separation by mass of all particles in general) [66].

A reflectron with a fixed depth in ACA’s current design would mean several variables mentioned being predetermined for optimized performance. For instance, because the length of electrode \(j\) should be equal to the sum of the lengths of electrodes \(i\) and \(k\), then \(j\) must be equal to half of the depth of the reflectron. With the depth being about 32.7 mm, a \(j\) length of 16.35 mm would be ideal, meaning the current \(j\) ought to be extended by 0.45 mm. Recalling the lengths of each electrode following Figure 2.6, electrodes \(j\) and \(k\) represent the deceleration and turnaround regions for particles, respectively. In contrast, since electrode \(i\) exists mainly to smoothen the potential ramp within the reflectron (hence it being the same -200 V as the environment outside the reflectron), it could be considered the least crucial component needing to be kept the way it is. If \(j\) were lengthened from 15.9 mm to 16.35 mm (extending the deceleration region), and \(i\) shortened from 13.2 mm to 12.75 mm, it is thought that the reflectron would refocus particles more efficiently into the detector. But changing electrode \(j\) by extension requires a proportionate change in voltage:

\[
2 \times \frac{20 - (-200)}{3} = \frac{440}{3} \approx 146.67 \rightarrow 146.67 - 200 = -53.33 = V_j \ (Ideal)
\]

In turn, a change in voltage would warrant a change in electrode lengths:
Electrode \( i \) must therefore be 2/3 the length of electrode \( j \) (thereby making electrode \( k \) 1/3 of \( j \)). Since the default voltage for \( V_j \) was -29.42 V rather than -53.33 V, the 2/3 guideline could still be satisfied if \( V_j \) was fixed, and \( V_k \) instead were increased to make -29.42 V equal to two thirds of its level:

\[
-29.42 + 200 = 170.58V \rightarrow 170.58 = V_k \cdot \left(1 - \frac{k}{j}\right)
\]

\[
V_k = \frac{170.58}{\left(1 - \frac{k}{j}\right)} \rightarrow V_k = \frac{170.58}{\left(\frac{2}{3}\right)} \approx 255.87V
\]

\[
255.87 - 200 = 55.87V = V_k \ (Ideal)
\]

\( V_j \), hence could theoretically have been kept fixed, with \( V_k \) being the changed variable — either way, the idea behind the voltage changes were to satisfy the 2/3 guideline. On a related note, where length \( j \) was bound by the theory to be 16.35 mm for ACA’s design, \( i \) could be changed to avoid contradicting the 2/3 guideline for \( V_j \):

\[
\frac{2}{3} \cdot 16.35 = 10.9mm = i \ (Ideal)
\]

\[
16.35 - 10.9 = 5.45mm = k \ (Ideal)
\]

Through theory, it was hereby predicted that performance of ACA would be best when each of the following were satisfied:

1. The ratio between \( V_j \) and \( V_k \) was set to 2:3 because this was the ratio of \( i \) to \( j \)
2. The ratio between length \( i \) and \( k \) was set to 2:1 for the same previous reason
3. Length \( j \) was set equal to half of the reflectron’s depth because \( i \) plus \( k \) was equal to a second \( j \), making the reflectron depth equal to two electrode \( j \) regions
Chapter 3

Method and Apparatus

3.1 The Iterative Process

In engineering, the iterative process of optimization involves design, simulation, and analysis. Once a trial has been set up for investigation, it passes through each of these three stages before the results say whether future trials should continue in the direction the first one started.

The work to be done over this project is divided into two main tasks. Task 1 involves confirming the entrance grid could grant the instrument an acceptance angle of no less than 30 degrees as well as adjusting the grid’s position to understand its direct consequences on the entry FOV. Task 2 is focused on the effects the reflectron had on particle TOF by mass category and also involves several facets of the reflectron being changed for study.

3.2 Task 1

3.2.1 Design

Design entails the instructions for how a device is to be modeled and viewed, and eventually, how it is to be built once its testing period has consistently yielded satisfactory results. While an experiment cannot be done without a simulation to show how a device/mechanism works, utilizing a single design tells the audience only what the current version is capable of doing — its progress cannot be measured by a single instance of performance. Changes in design are imperative to understanding what brings a device closer to meeting its target requirements and what impedes it from succeeding. Every change in design will warrant its own simulation and though a large set of mandatory design changes may be necessary, the comparison between each simulation will show a better track of progress with increasing interval number.

Because the default design of ACA had a simple extruded third dimension (modeled from a planar drawing), its features could be summarized in two dimensions. They were modeled through digital sketching. The graphics-editing software GIMP was used for drawing and editing parts of the instrument due to its ability to alter details down to a pixel. The design scale was fixed to 20 pixels per mm. A change in more than two pixels in a design with a ratio of 20 pixels to 1 mm makes a significant impact on instrument performance, considering the dimensions for ACA in mm are all no more than 100 in any direction (no more than 2000 pixels in any direction). GIMP was a good
choice for its ability to assemble the overall instrument’s image from composite layers. In the context of drawing, each layer contains a specific part of the drawing, such as the structural walls or the map of electrodes lining up the inside of said walls. Drawings are often separated into layers specifically so that a change in the information in one layer does not affect the others — and this is useful for isolating change in a design. Controlling layers through GIMP made it possible for each design with respect to its immediate predecessor differ by a single altered feature constrained to just one such layer.

A view of GIMP’s interface is shown in Figure 3.1.

![GIMP interface](image)

Figure 3.1: GIMP used for drawing designs

While not directly called one, the entrance grid functions as a lens for particles entering it, as its curved outer and inner grids together focus the passing particles into a common focal point deeper within ACA. This works because the two sides of the entrance grid curve about one and the same imaginary point (as opposed to two adjacent imaginary points). Focusing of particles in turn was needed as ACA’s drift tube region constricts the particle path possibilities to a narrow range. To ensure only a single independent variable (grid position) was in effect, the curvature of the entrance grid needed to be modified proportionately to the amount of distance it would be shifted up or down per sample. Changing the curvature with the shifting was necessary to keep the focus of the ion beam in alignment with the curve of ACA’s s-tube when the ions coming from the mirror continue toward the reflectron segment. In geometric context, the two arcs forming the entrance grid were arcs from concentric circles — circles with a common center. The center needed to be identified through reversing the circle’s radius formula. A circle typically is defined at its center first, then at the radius (a set distance from the center), and finally at its perimeter — determined by having the radius pivot around 360 degrees to find all points equally distant from the center. This time, the perimeter (or
a part known as a chord) had been given, and the radius could be found through the
addition of two separate distances — the radius was found to extend past the mirror, so
that the mirror could “reflect” it, creating a second radius segment. Once the true radius
was known, then its focal point inside ACA could be located. The focal point would
need to be kept constant every time an arc in any design was moved vertically. Since the
entrance grid’s characteristics were the only part of the design that was altered for this
task, all other aspects of the design were (for now) left untouched.

The changes to the design for each test needed to be consistent. Since the entrance
grid’s curvature was getting modified for every sample, it was more feasible for a new
grid to be made for each case, rather than for the same one to be rescaled. The geometry
behind maintaining a correct focus in ACA was simple as well: the circles forming the
arcs of each entrance grid had coincident centers. Much of the procedure in this task
went into determining this center, as the changing grid position would involve the radius
being recalculated with respect to the constant center. The order for doing this came as
follows:

1. The midpoint of the entrance grid arc needed to be found. A line parallel to the
walls of the entrance passing through this point also needed to be noted. This line
is marked as $m$ in Figure 3.2.

2. The point on this line marking its intersection with the mirror platform was noted.

3. The width of the gap between the tube walls leading to the reflectron needed to be
found for that gap’s midpoint to be determined.

4. With the mirror tilted by 8 degrees, a second line (line $n$) perpendicular to the
mirror from the marked mirror point had to be drawn up to the midpoint between
the mirror and reflectron chambers. Perpendicular to the mirror, line $n$ did cross
the gap’s midpoint, meaning the particles were expected to converge there.

A concern was that particles traveling along the edges of the converging path may fail
to clear the inner entrance tunnel wall due to the path converging still further beyond this
wall — the original focal point existed at the grid of the reflectron in between the inner
entrance tunnel wall and the inner detector tunnel wall (the two walls giving ACA its
S-shaped tube). The entrance grid’s radius was shortened as a means of increasing trans-
parency by permitting more particles to enter the reflectron — through the assumption
that bringing the focal point earlier within the mirror turn would enable the particles to
converge earlier and keep the trajectory path thin enough to pass in between the two inner
walls. The focal point was decided by visual approximation and fixed for the duration
of both tasks to follow. It served as a starting point to allow the planned tasks to be
run and later be subject to its own test of position-adjustment to determine its validity
as a selected center. The results from this post-task test are described in Appendix A
and discussed in Chapter 5. Figure 3.2 shows the original focal radius compared to the
selected new one and explains their relation.

From the minimum possible depth (found to be 52.2 mm) up to the outer tip of the
entrance tunnel (about 89.0 mm), the distance was divided such that eleven instances
were created. Figure 3.3 shows three designs used in this task — each with an entrance
grid at a different depth within the entrance tunnel.
Figure 3.2: Definition of the grid arc’s radius to locate and change its center. The original radius was formed by the sum of line lengths $m$ and $n$. The new radius was formed by the sum of line lengths $m$ and $n'$. Line $n'$ was chosen in relation to line as being half the length of $n$ to shorten the distance of particle convergence.

(a) Grid at 55.9 mm distance from mirror  
(b) Grid at 59.55 mm distance from mirror  
(c) Grid at 63.25 mm distance from mirror

Figure 3.3: Three samples designed for grid position analysis
3.2.2 Simulation

Simulation gives raw data and this data sometimes may be immediately understood by whomever is conducting the simulation. Though this is possible, the data from simulations is frequently written and displayed in formats difficult for interpretation by those involved in the experiment and inadequate for reading by anyone from outside it. In general, simulations run through software may display some form of device performance in a visual manner that can be seen by all, albeit only interpreted in an abstract manner (i.e. color gradients for measuring effect intensity).

SIMION is a program developed for the tracking of ion trajectories, as well as the electric fields through which they may travel [68]. SIMION is compatible with the output PNG files produced by GIMP and can convert their pixel data into two or three-dimensional models — the models being solid structures with active electrical properties set in place by the user. For the case of ACA, the drawings are kept as two-dimensional models in SIMION, on the understanding that the third dimension has little effect on performance due to the acceleration of incoming particles occurring primarily along the plane in question. Any forces assumed to be encountered by the particles in the instrument in the third dimension would be negligible. Additionally, optimizing a planar concept is by far easier than doing so for a three-dimensional and would make three-dimensional optimization easier in future projects. SIMION can use the image color data to assign voltages specific to certain area colors. This also provides a reason for the usage of layers when in the GIMP environment, as each layer typically holds instrument parts with a certain range of colors — some have pixels of a single uniform color (again, like the external structure), while others like the reflectron layer, have 3 different colors for each electrode type in it. Through an arrangement of several panels, SIMION allows for parameters within the general environment, model, and in the simulated particles themselves to be customized to expand its focus over many potential target variables in the interest of the user.

The focus in this project is on limiting the particles’ range of velocity direction and range of kinetic energy to isolate dependent variables such as the ACA’s acceptance angle and the TOF of different mass categories of particles. The GIMP drawings got converted into models by the simulation environment SIMION, and the electrical parameters were then set up in the form of potential arrays. Potential arrays can be considered “layers” in that each correlates information about electric field strength across the model with the physical volume of the model and the permeating free space surrounding it. Similarly, each potential array is “stacked upon one another” to refine the electrical aspects so that in simulation, they approximate realistic characteristics. From the data contained within these arrays, the models could act as virtual versions of ACA — as if the instrument were already in orbit around Didymos and Didymoon. SIMION calculates electrostatic potential through the Laplace Equation:

\[
\nabla^2 V = \nabla \cdot \nabla V = 0 \tag{3.1}
\]

\[
\nabla V = \left( \frac{\delta V}{\delta x} \right) i + \left( \frac{\delta V}{\delta y} \right) j + \left( \frac{\delta V}{\delta z} \right) k = E \tag{3.2}
\]

\[
\nabla^2 V = \nabla \cdot E = \frac{\delta E_x}{\delta x} + \frac{\delta E_y}{\delta y} + \frac{\delta E_z}{\delta z} = 0 \tag{3.3}
\]
The equation states that the product between the potential at a point in three-dimensional Cartesian space and the divergence operator ($\nabla$ — the symbol used to indicate change diverging from that point) is given by the sum of the changes in potential ($\delta V$) across the three axes (x, y, and z) and is how the electric field’s strength is defined at that point. If the operator is used for differentiation and if used twice on an initial function, renders it to zero. Since electric field strength at a point is derived from the change in potential surrounding the point, differentiation of the electric field strength will be zero. Because solving such an equation can use up significant resources in a computer, SIMION approximates the Laplace solution based on the knowledge that the equation relates to the information on a point based on information on what surrounds that point.

$$V = \frac{(V_1 + V_2 + V_3 + V_4)}{4} \quad (3.4)$$

Its solution is to calculate the field strength at a point based on the values of its nearest four neighbors — done on every potential array created [69].

Figure 3.4 shows the SIMION interface with an isometric view of ACA. It is worth mentioning that for a two-dimensional model, SIMION expresses it in three dimensions, using the third to indicate levels of potential throughout the model.

Figure 3.4: SIMION used for model simulations. Display shows an isometric view of ACA to help visualize the potential as vertical topography (green mesh). Red contours indicate potential at certain values.

Each of the models for testing has the same pre-set particles flown through them to guarantee a valid comparison during the analysis phase. The particles are defined by their
mass category, charge, starting position, starting velocity, and kinetic energy. Masses are set at 1, 2, 70, and 71 AMU (to measure differences in trajectories between the minimum and maximum ion masses targeted by ACA). Charges are set to (plus) $1.6 \times 10^{-19}$ Coulomb, and absolute velocities for each particle are governed by their starting kinetic energy, ranging from 0.1 to 1 eV to simulate the Didymos particle system. The particles would be arranged to cover a 180 degree sweep over the outside of the entrance tunnel of the instrument. Imaginary test planes inside the model are programmed to capture the status of each particle parameter set at their starting position for comparison in analysis.

Each design with a new entrance grid, when finished was imported into SIMION to continue to the simulations step. No other parameters needed resizing in design, and no particle or electrical parameters were altered in this task. The electric fields were calculated by the program for each sample, before the ions were send flying through each simulation model. The same set of particles is flown through each model, and the raw results in the output file would then be collected. Figure 3.5 shows the simulated case for the model made with a grid distance of 59.55 mm from the mirror. According to the particle trajectories seen, there should be a high percentage of particles reaching the detector based on the general path’s shape and direction.

Figure 3.5: Simulation of ACA with grid distance 59.55 mm. Scattering of particles (trajectories shown as black lines) results in a diffuse portion of the particle path impacting on the inner wall of the detector tunnel, while the more densely concentrated portion of the path clears the reflectron entry gap and is sent down the detector tunnel. The red pattern at the top left, as well as the horizontal red stripes crossing the instrument are markers recorded in the output data file as particle origins and test plane crossings, respectively. All other red lines seen are contours of constant potential.
3.2.3 Analysis

For cases where simulated raw data and vague visualization cannot properly convey performance in a reasonable manner, data processing comes into play. Data processing is used to take raw data and interpret (often with the assistance of a computer) it such that the same data is returned to the user, but in a more humanly comprehensible way. Examples can be taking lines of raw data and identifying the variables before arranging them to form plotted trends, or using said lines to assign the variables to colors so that the simulated visuals containing color gradients can have a scale included (if the simulation software could not return one on its own). Data processing can be done by hand by the user(s) running the simulation, but data is often entered into programs written to read and rewrite to a readable format since programs can do this at speeds several orders of magnitude higher than what humans can achieve.

The Python code organized the raw simulation data into its library of plots showing mass TOF distributions, angular acceptance, and transparency fractions. TOF information is obtained by having the times of particles’ impacts on the detector compared to their times of entering ACA’s entrance grid while angular acceptance is also found by determining the direction of the particles’ entries into the grid based on their starting position and velocity. Transparency is obtained by counting the number of detector impacts and comparing it to the number of particles entering the entrance grid. The graphs displayed particle status by mass category as they passed the aforementioned simulation test planes to elaborate on the trajectory paths seen in SIMION. Each graph explains particle behavior at different stages inside ACA. Those marking the status of angular acceptance and transparency at the detector were the ones of interest. Figure 3.6 shows the angular acceptance of ACA in regard to the same sample featured in Figure 3.5. Here, with the main objective of this task being to optimize the instrument for a 30 degree FOV, the output graph’s legend is suggesting the design was a failure, as it only yielded an acceptance of 20 degrees instead of 30. The value of 20 was the FWHM of this sample’s results, indicating that half of the particles reaching the detector came from a starting angular range of about 20 degrees. This means that particles were entering outside of this angular range, but they made up only half of the detected species. For a successful run, half of the detected particles should come from an angular range greater than 30 degrees — because these particles outside of the required FOV range will be very difficult to differentiate by mass due to TOF distribution overlap.
Figure 3.6: Angular acceptance and transparency analysis of simulated ACA sample with grid distance 59.55 mm. Despite a satisfactory level of transparency (nearly 70 percent), the angular acceptance at 20 degrees is too low to declare this sample a successful one.

3.3 Task 2

3.3.1 Trial Plan

Here, the reflectron of ACA is under the spotlight. Since it was governed by more variables (multiple electrodes with differing lengths and voltages), it definitely requires many tests, organized into several trials. Four trials were then arranged — two for adjusting the voltages of selected electrode pairs inside the reflectron, and the other two for resizing their respective lengths. For the latter two tests requiring different electrode lengths, GIMP is used for re-allocating pixels from one electrode type to another due to minute length intervals. For continued consistency, each trial consists of eleven tests, as was done with Task 1.

Similar to the changes done in Task 1, the variable adjustment started with a new design being drawn to accommodate this single variable change. From the drawing the necessary model was constructed, through which the particles to be flown. Lastly, the Python plot-generating script read the output data from the simulation and display it as a series of graphs indicating particle TOF at different checkpoints within ACA.

In task 1, only a single variable needed to be changed; there were four that would need to be investigated in Task 2, and each would warrant a trial for themselves. Table 3.1 displays the trials run and the variables changed (target variables), as well as any variables inevitably affected by the changing of others (collateral variables). Each variable in the table has been defined in the project’s background (Subsection 2.4.2).
Table 3.1: Task 2 trials and variables

<table>
<thead>
<tr>
<th>Trial</th>
<th>Target Variable</th>
<th>Collateral Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$V_j$</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>$V_k$</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>$k$</td>
<td>$i$</td>
</tr>
<tr>
<td>4</td>
<td>$j$</td>
<td>$i$</td>
</tr>
</tbody>
</table>

The order of variables to be considered are also listed below and were selected in this order due to the ease of adjustment:

1. Changing $V_j$
2. Changing $V_k$
3. Changing $k$, thus inversely changing $i$, while $j$ remains fixed
4. Changing $k$, thus inversely changing $j$, while $i$ remains fixed

While the theory called for specific parameters to be investigated, the greater focus is on identifying the behavior of the reflectron as each targeted variable was changed — over a wide range of data. This meant that the exact data points to be checked are tuned due to interval sizing, since there is always a point within about 5 V or 1 mm of the targets for comparison/approximation. Instead, the trend between the points as whole plots could be used as a means for interpolating data with little risk post-trial period.

Interpolation between known empirical data becomes especially important in Trials 3 and 4, since they involved electrode sizing. This relates to Equation 2.11, as the default design does not fully satisfy the size ratios between the electrodes. This likely occurred due to size estimation in the design stage (done by human input through GIMP). The theoretically ideal cases for electrode lengths are therefore approximated by the nearest neighboring data points in each trial.

Plan amendments from fresh data

Since the four trials were run one at a time, the end results from each one could affect the set-up for the next. Each trial’s raw results were processed up to their final plot of data points before the conditions for the next trial is set up — to better predict the results of the next trial in an attempt to improve focus on viable performance factor (PF) data points. From Trial 2 and onward, there are data points returned as undefined values stemming from no particles successfully reaching the detector of the simulated ACA. When this occurred, the TOF mass resolution criterion (equation 2.7) returned an error since it was impossible to determine the TOF distribution of a stream of particles that didn’t reach its designated terminal. In each of these trials following Trial 1, the undefined data was observed to occur on one side of their respective plots. To compensate for this, the limits that did not show invalid data were extended to include as much range as was necessary to produce graphs with the same number of visible points, if the undefined points were not counted.

\[ \text{Equations 2.6 and 2.7 define the performance factor (PF) criterion for TOF overlap resolution in Section 2.2.} \]
Table 3.2 shows the range limits set for each trial before it was run. It is worth noting that the limits shown were the final values selected. Any changes from limits initially set are explained in Subsection (3.3.2) and Chapter 4.1.

Table 3.2: Task 2 variables and their range limits

<table>
<thead>
<tr>
<th>Trial</th>
<th>Target Variable</th>
<th>Lower Limit</th>
<th>Upper Limit</th>
<th>Default Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$V_j$</td>
<td>-90 V</td>
<td>20 V</td>
<td>-29.4202 V</td>
</tr>
<tr>
<td>2</td>
<td>$V_k$</td>
<td>-35 V</td>
<td>108 V</td>
<td>20 V</td>
</tr>
<tr>
<td>3</td>
<td>$k$</td>
<td>0 mm</td>
<td>8.94 mm</td>
<td>3.58 mm</td>
</tr>
<tr>
<td>4</td>
<td>$j$</td>
<td>10.49 mm</td>
<td>22.14 mm</td>
<td>15.87 mm</td>
</tr>
</tbody>
</table>

The algorithm used for sorting data and generating the TOF distributions was the one and the same that produced the angular acceptance and transparency values for ACA simulations in Task 1 — and while they were not initially of concern, this extra data was also recorded in the event that it could be used in discussing trade-offs. As a result, ACA angular acceptance and transparency values were also used in Task 2, but were kept in the background to keep the main focus on TOF PF.

3.3.2 Simulations

Trials 1 and 2 were focused on changing electrode voltages since they could be carried out more easily due to no changes in the design drawing being necessary. This allowed for the design trial stage to be skipped for every data point obtained.

It should be stressed that changes in design were necessary for Trials 3 and 4 because they involved electrodes being resized. The changes in electrode lengths, themselves were the only ones needed and were on the order of approximately 1 mm per data interval, making electrode junctions difficult to be seen in any figures due to similar coloration of each electrode in the design drawings. Instead, their effects are shown in the simulation environment.

Trial 1

The first trial (Trial 1) to be run was on the reflectron’s middle stage voltage, $V_j$ since its range limits for measurement could easily be defined. The upper limit for the desired data range would be setting $V_j$ equal to $V_k$, the lower limit could be set as a simple intuitive fraction of $V_k$ (for instance, 50 percent that of $V_k$). The amount of data would be consistent with that obtained in Task 1 (at least ten points).

Trial 2

For Trial 2 — that of changing $V_k$, the same strategy for selecting upper and lower limits was used, but in an inverted case: The lower was set equal to the intermediate $V_j$; the higher was set to half the difference between $V_i$ and $V_k$ and summed with $V_j$. This was done because the difference between the default $V_j$ voltage (-29.42 V) and the nearest value with a confirmed PF of less than 1 (-35 V) was a comparatively small value when compared to the 220 V difference between $V_i$ (-200 V) and $V_k$ (20 V). This idea of shifting $V_j$ down to -35 V is discussed in detail in Section 4.1 (in the results). It was decided for
Trial 2 focusing on $V_k$ to instead be centered on the assumption of $V_j$ being set to the nearest value to its original that would yield proper mass resolution, since Trial 1 first revealed that the reflectron was not sufficiently separating the TOF distributions between the two heaviest masses. This approach of changing two variables within a single trial was considered too great of a risk for future trials, where the variables concerning electrode length were less understood, so all upcoming trials were set to deviate with respect to only the original unoptimized version of ACA — i.e. $V_j$ being returned to its default voltage.

For Trials 1 and 2 beginning in the simulation stage, examples of the differences between the same model under different $V_j$ and $V_k$ voltages are shown by the shifts in equipotential contours in the simulation environment — shown in Figure 3.7.

Figure 3.7: Reflectron field under different voltage settings. Where potential contours are closer together indicates steeper potential gradients and where greater particle deceleration would occur.

**Trial 3**

Trial 3 was the first of two trials to focus on how the reflectron electrode lengths affected ACA’s performance. This trial targeted electrodes $i$ and $k$, with electrode $k$’s length being the independent variable and electrode $i$’s length being changed automatically. In doing so, the length of electrode $j$ could be kept fixed, since it was understood to be more crucial to the reflectron’s performance than was $i$ (deceleration of particles requires more reflectron space than does its entrance region, as documented in Subsection 2.4.2). One
limit for electrode $k$ was having its length set to 0 mm — meaning that the portions of the lateral walls normally reserved for it now went to electrode $j$, while $k$ was reduced to just a flat plate at the bottom of the reflectron. The other specific limit of 8.94 mm was determined from increasing the interval length (about 0.89 mm) tenfold. The interval length itself was obtained by the division of the 3.58 mm by 4 since 3.58 could be rounded up to 4 mm — and that a interval resolution of less than 1 mm was considered by visual inspection to be a suitable balance between adequately mapping the effect of shrinking electrode $k$ while also seeing what would happen if it should be extended to at least double its length — and all being done without resizing electrode $j$.

**Trial 4**

Trial 4 was conducted in a similar manner to Trial 3 — the difference being that this time, it was electrode $j$ being manipulated in length and electrode $i$ whose length depended on $j$. Electrode $k$ is then kept constant. The interval length was kept the same as it was for Trial 3, and the upper and lower limits were initially set at 22.14 mm and 13.18 mm, respectively. This was done to have a ratio of data of 7:3 — seven intervals extending electrode $j$ and three reducing it. More focus was put on extending $j$ since Trial 3’s results indicate that if electrode $j$ was moved into $k$’s territory, that ACA’s performance would decrease (explained further in Chapter 4.1). In Trial 4, it turned out, extending electrode $j$ past 19.45 mm (an extension by four intervals as opposed to the seven planned) returned undefined data points, so three additional intervals focused on shrinking electrode $j$ from 13.18 mm to 10.49 mm were set up. This could be justified as electrode $j$ this time being reduced with electrode $k$ being fixed constant, as doing so would still return data different to that of Trial 3 on the matter of resizing electrodes due to the design conditions being different.

For Trials 3 and 4 requiring new designs, the subsequent models were generated in SIMION and then used for further simulations. The reflectrons of two such examples are shown with their equipotential lines in Figure 3.8.
3.3.3 Analysis

The output data files from the simulation runs in each trial were processed into plots for several response parameters using the same processing code as in Task 1. The focus was on the TOF resolution for high masses. Figure 3.9 showing the TOF histograms for masses 70 and 71 AMU at the detector was the center of attention throughout this task for every test run. The central TOFs and FWHM values were derived from the peak and width at half-peak-height values (respectively) of the Gaussian curve fitted about the histograms.

The formula for a Gaussian curve is [70]:

\[ y = a \cdot e^{-\frac{(x-b)^2}{2c^2}} \]  

(3.5)

Constant \(a\) sets the curve’s peak height, \(b\) positions the peak horizontally, while \(c\) controls the width of the curve. In practice, this made:

- \(a\) the number of particles arriving at the average TOF for a mass category
- \(b\) the value of the average TOF for the mass category (the central TOF)
- $c$ the standard deviation of the TOF spread (standard deviation multiplied by approximately 2.35 gives the FWHM)

This type of curve is frequently used for statistical estimations, and as such was applied to the histogram distribution of mass TOF data. This particular curve was chosen due to it being the least squared of statistics curves, making it the most closely-fitting curve relative to the empirical histogram distribution beneath it.

From the TOF plot's legend, the values for central TOF and FWHM for each of the two categories were taken and listed into tables for each trial run. From the four added columns, the difference between the central TOFs would form a fifth column, while the average FWHM value between the two recorded would form a sixth. The final column that would determine the PF would be created by the division between the difference between central TOFs and the average FWHM calculated. The output would indicate by its position $PF > 1$ or $PF < 1$ if the results for a given variable data point would show improvement or regression of ACA’s function, respectively.

Figure 3.9 below shows a comparison between the TOF response from the simulation of the original configuration of ACA reflectron and the TOF response from the best-performing case concerning the lengths of electrodes $k$ and $i$. The difference between the average TOF’s for 70 and 71 AMU was the same in both cases (since changing the average TOF would require resizing ACA entirely), but since the FWHM for each TOF spread was narrower in the changed-electrode-lengths case, the resulting performance was satisfactory and the case could be considered optimized. This is further discussed in Chapter 4.1.

![Figure 3.9](image.png)

Figure 3.9: Comparison of TOF responses before and after optimization between $k$ and $i$ electrode lengths. The blue distribution represents the empirical data for m70 particles while the green represents that of m71 particles. The superimposed Gaussian curve are fitted over the histogram data and are used to estimate cTOF and FWHM (displayed in the legend).
Chapter 4

Results

4.1 Task 1 Results

Once all data analyses were complete, their respective variable values were collected to be charted on one and the same plot for both variables explored in this task. The angular acceptance and instrument transparency are presented below. Figure 4.1 shows the relation between ACA’s angular acceptance over grid distancing.

![ACA Angular Acceptance per Sample](image)

Figure 4.1: ACA’s angular acceptance as a function of grid distance

Figure 4.2 outlines how ACA’s instrument transparency is affected by grid distancing.
As seen in each plot, there were linear correlations between the grid positioning and the derived performances of ACA. This trend was distinct enough to be approximated by a line of best fit — the degree chosen being for a linear correlation. For the case of angular acceptance, the correlation was found to increase by approximately 1.13 degrees for every millimeter fewer between the entrance of ACA’s ion tube and the start of the grid itself. With transparency, the trend was found to increase by about 1.48 percent for the same amount (and direction) of change.

There remains a question of why the sample with grid distance 74.25 mm yields a comparably lower transparency at ACA’s detector when compared to either of its neighboring samples. Figure 4.3 shows the simulations for this sample centered between its preceding and succeeding test samples. The spread of the ion path in Figure 4.3a is less than that of the path in the sample in question (Figure 4.3b), but the path itself is denser as a result. In the sample with grid distance 77.95 mm shown in Figure 4.3c, the path of the ions is also denser than that of the outlier, but its spread is approximately equal to that of the latter. This means that between 70.6 mm and 74.25 mm grid distance, more and more ions (with respect to those that reached the entrance grid) are reaching the detector region, but those that arrive have smaller original angles of entry. This way, the trends for the graphs of both ACA’s angular acceptance and for its ion efficiencies are validated. In turn, the source particle trajectories responsible for this phenomenon are visible in the figures described: Comparing Figure 4.3a with Figure 4.3b, the densities of the particle paths that terminate just prior to the detector region increase visibly, while the densities of those passing the detector boundary have hardly changed visually. Then between Figures 4.3b and 4.3c, the densities of all the paths succeeding in reaching the detector region have caught up and rebalance the path spread mentioned.
This is likely the consequence of increasing the angular acceptance, as the increased FOV would allow particles with more lateral pre-acceleration velocities to enter the instrument. This is continued in Chapter 5.

4.2 Summary

The task of revising ACA’s design to create samples, each with entrance grids at positions varying by a constant interval was completed. The compiled results following analysis proved not only to verify the existence of the trend between the entrance grid’s position and ACA’s angular acceptance, but to also calculate its gradient. The same was achieved for the tests on ACA’s instrument efficiency as a second function of the entrance grid’s positioning. While the original version of ACA is already calibrated to meet the requirement of having a detector FOV of 30 degrees, it nevertheless helps in having these linear functions documented, as they may be assumed to apply to future revisions in ACA’s design, if with some changes to the given coefficients.

4.3 Task 2 Prologue

4.3.1 Particle Rejection and the Analysis of Transparency in Task 2

Starting in Trial 1 and remaining apparent throughout all following trials, a phenomenon coined “particle rejection” was observed. Being a more extreme version of particle scattering due to increasing convexity of the reflectron’s potential, this phenomenon often aided
in delivering particles to the detector with less TOF variance, thereby increasing mass
discrimination and decreasing PF values below 1. Unfortunately, the same phenomenon
made tracking transparency per test seem unreliable — until direct sightings were con-
firmed down to the tests where they first began in Trial 1. Figure 4.4 corresponds to
the tests on either side of the default value of $V_j$, where the total number of particles
confirmed to successfully enter ACA began to rise beyond the mode value of 785 particles
per mass category (as of Task 2 it was assumed to always be constant). In the screenshots,
particles can be seen exiting the instrument out the entrance grid — either as stark
lines overlaid upon the otherwise red-marked region of particle genesis (Figure 4.4a), or
as paths exiting to the right of those entering on the left side of the grid (Figure 4.4c).
Figure 4.4b which displays trajectories for $V_j$ at -35 V shows no rejection due to the
voltage being much closer to the default value of -29.42 V.

Figure 4.4: Trial 1 particle rejection starting at high deviations of $V_j$

The screenshots provided evidence of the direct cause of particle count increases and
the surplus amount could be attributed to duplicate counts for all particles exiting ACA,
which would need to cross the test planes marking their inward progress a second time. It
could now once again be assumed that all particles reaching the detector were valid, since
the detector possessed no repulsive charge, meaning any particle making contact with its
surface would remain there indefinitely (i.e. only one termination marker per successful
particle). With all valid total particle counts essentially returned to 785, transparency
measurements could once again be considered reliable, and this criterion, along with
angular acceptance could be used now in Task 2 to further discriminate among the data
for PF values less than 1.
4.4 Task 2 Results

4.4.1 Reflectron Voltage Trials

Trial 1

The values for PF (performance factor defined by equation 2.6) across the two trials involving voltage analysis are presented below. Table 4.1 and Figure 4.5 mark the listed and plotted results for Trial 1 and show the relation between ACA’s mass resolution performance over the change in $V_j$. As is seen in the plot, there was a positive correlation (across the range recorded) between an increase in the electrode’s voltage and ACA’s performance factor. This meant that the first value that could guarantee sufficient high-mass resolution was -35 V. Since the condition for a working instrument was for this PF to be kept below 1 and/or further decreased as much as was possible, the reflectron discriminated among higher masses more efficiently as $V_j$ decreased and approached $V_i$. The theoretically best-suited $V_j$ value according to the Task 2 hypothesis was found to be -53.33V. The nearest point to -53.33 V tested was -57 V. When compared to the total 220 V difference between $V_i$ and $V_k$, this difference could be considered small enough for an approximation of the PF for -53.33 to be made by linear interpolation between -46 V and -57 V:

$$PF_{(-53.33V)} = 0.62875 + \left(\frac{0.6635 - 0.62875}{11}\right) \cdot 3.67 = 0.64033$$

Table 4.1: Trial 1 result. Columns from left to right: The target variable unique to its trial. The mean or central TOF (cTOF) of the ion category of mass 70 AMU (m70) in microseconds ($\mu$s). The FWHM of the ion category of mass 70 AMU. The central TOF of the ion category of mass 71 AMU. The FWHM of the ion category of mass 71 AMU. The difference between the 70 and 71 AMU cTOFs ($\Delta$TOF). The average FWHM ($\bar{x}$FWHM) between 70 and 71 AMU. The performance factor (PF) as a quotient between the ($\Delta$TOF) and ($\bar{x}$FWHM) values. The angular acceptance ($\alpha$) in degrees ($^\circ$). The instrument transparency ($\tau$) as a percentage.

<table>
<thead>
<tr>
<th>$V_j$ (V)</th>
<th>m70 cTOF ($\mu$s)</th>
<th>m70 FWHM ($\mu$s)</th>
<th>m71 cTOF ($\mu$s)</th>
<th>m71 FWHM ($\mu$s)</th>
<th>$\Delta$TOF ($\mu$s)</th>
<th>$\bar{x}$FWHM ($\mu$s)</th>
<th>PF</th>
<th>$\alpha$ ($^\circ$)</th>
<th>$\tau$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-90</td>
<td>10.75</td>
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Figure 4.5: ACA’s Mass Resolution PF as a function of $V_j$ voltage

Simulated particle trajectories for three of the data points from Trial 1 are displayed in Figure 4.6. Figure 4.6a shows the marginally acceptable outcome of $V_j$ at -35 V, Figure 4.6b shows the marginally unacceptable outcome of $V_j$ at -24 V, and Figure 4.6c shows the outcome of the highest limit ($V_j$ at 20 V). Increasing $V_j$ showed the trajectory path inside the reflectron getting laterally “pinched” — particles were now being more heavily repelled towards the center of the reflectron before leaving.
Figure 4.6: Trial 1 trajectory comparison for different $V_j$

The data points for $V_j$ at -57 V and -46 V, respectively, are shown below in Figure 4.7. The two points surround the theoretically significant position for $V_j$ at -53.33 V (hypothesized to be the best point for deceleration potential), and its respective particle trajectory figure can be considered as a cross between the visual appearance between the two existing images (with more bias toward -57 V due to voltage proximity). Though, -53.33 V had a more favorable PF compared to the marginal value of -35 V, all data points less than it had better PF values in turn. The theoretically ideal value, however did not yield a high transparency, and all values less than -57 V yielded unacceptable transparency values less than 30 percent.
It is estimated that a “saturation” occurs in the PF trend at a point between -35 V and -46 V having to do with the voltage being reduced from its default value. This is speculated further in Chapter 3. Transparency and angular acceptance together made PF data points from -90 V to -46 V impractical for ACA, as they would each suggest not enough particles would reach its detector, even if the results were high TOF resolution (low PF). With all voltages higher than -35 V yielding insufficient TOF discrimination, only -35 V as a voltage for $V_j$ could be considered approved for use in reflectron optimization.

**Trial 2**

Table 4.2 and Figure 4.8 outline how ACA’s mass resolution performance was affected when the voltage $V_k$ was adjusted. The $V_k$ trial data shows the same profile shape across the visible data as seen in the results from Trial 1, though the correlation is negative. If traced from right to left, the curve formed by the data points halted between -2 V and -13 V. This halt can be predicted to the accuracy of a single data interval as Trial 2 included three tested data points that are not visible on the graph because their TOF readings were indeterminate. This occurred because for $V_k$ values -13 V, -24 V, and -35 V, all flown particles impacted prior to reaching the detector, meaning no TOF could be measured.

**Table 4.2: Trial 2 result conversion**

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<th>$V_k$ (V)</th>
<th>m70 cTOF (µs)</th>
<th>m70 FWHM (µs)</th>
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<th>m71 FWHM (µs)</th>
<th>$\Delta$ TOF (µs)</th>
<th>$\bar{x}$ FWHM (µs)</th>
<th>PF</th>
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<tr>
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<td>0.133</td>
<td>0.09</td>
<td>0.132</td>
<td>1.47</td>
<td>25</td>
<td>46.6</td>
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</table>
Figure 4.8: ACA’s mass resolution PF as a function of $V_k$ voltage. The space on the left devoid of points indicates three invalid intervals due to no particles leaving the reflectron.

The particle trajectories for three of the data points from Trial 2 are displayed in Figure 4.6. At a $V_k$ voltage of -2 V, the impacts of a significant amount of the particles were seen at the site of the $k$ electrode bottom plate — a consequence of excessively weakening the turnaround region of the reflectron. As is supported by this graphic evidence, reducing $V_k$ by any further interval resulted in no particles escaping the reflectron as the potential gradient became too weak in the turnaround region due to being governed by negative voltages (while trying to repel ions of positive charge). Figures 4.9b and 4.9c express the outcome of increasing $V_k$, thereby increasing the turnaround region’s effectiveness. The potential gradient was steepened, making an increasingly larger amount of the particles entering the reflectron leave it as well. Compared to the path “pinch” seen in Trial 1, the convex potential seen in Trial 2 occurred due to the potential gradient between
the turnaround region and the deceleration becoming too steep; its steepness was most pronounced about the axis and the effect less severe further away into the periphery. Particles not bound for reflection before crossing the central axis were reflected away from the detector in the and risked being “rejected” by the instrument. An example outlining this phenomenon of “particle rejection” is described in the following subsection for Trial 3. With increasing $V_k$ though, came an increase in the detector area receiving impacts from particles.

![Figure 4.9: Trial 2 trajectory comparison for different $V_k$](image)

Since all data within Table 4.2 and Figure 4.8 relied on the condition that $V_j$ was reduced from -29.42 V to -35 V, the trial’s results were initially considered inaccurate. By visual inspection, the points in the plot for Trial 1 (Figure 4.5) formed a nonlinear trend — this included the range -24 V to -35 V that surrounded the default $V_j$ of -29.42 V. It was because of this trend the Trial 2 data (Figure 4.8 and Table 4.2) couldn’t be considered valid at first glance since Trial 2 depended on a voltage value in Trial 1’s results that differed from its default value. A second, closer glance at the Trial 1 plot, as well as a re-examination through its axial/peripheral potential gradient plots suggested otherwise. The plots of the latter category most relevant to suggesting nearly-linear differences are arranged in Figure 4.10.
(a) Reflectron potential for $V_j = -24V$

(b) Reflectron potential for $V_j = -29.4202V$

(c) Reflectron potential for $V_j = -35V$

(d) Reflectron potential for $V_j = -46V$

Figure 4.10: Difference between axial and peripheral potential curves for $V_j = -29.4202V$ and $V_j = -35V$. Red represents the reflectron potential just 0.03 cm away from the electrode wall, making its “step-like” values nearly equal to the electrode voltages themselves. Since Trial 1 had the middle red “step” change over constant intervals, the change was linear. The linear effects carry over to the two deeper axes of reference for the reflectron, represented by the space between the green line (half-way to the central axis) and the blue line (central axis) closing with decreasing $V_j$. From -24 V to -29.42 V and from -29.42 V to -35 V, the two changes to the space are roughly equal to one another due to -29.42 V being nearly equally distant from both voltage points. From -35 V to -46 V, the space reduction is doubled because the electrodes’ voltage drop is now doubled as well. The effects of the electrode voltage interval changes on the central axis’ potential would be assumed to be small linear increments.

The nearly linear variations between the $V_j$ central axis potential between each of the graphs showed that it was possible to assume a linear translation of the existing data for Trial 2 with negligible consequence. All points in the trial were from then on assumed to be increased by 5.58 V voltage in any further calculations. The reasoning behind this decision is continued in the Discussion chapter under Trial 2.
For a valid comparison between theory and empirical data to take place, the theoretically ideal $V_k$ position of 55.87 would also need to be translated by 5.58 V, along with its nearest point of 53 V. This would set the two points to 61.45 V and 58.58 V, respectively, with the difference between them (translation or not) being 2.87 V. The entire voltage range between $V_i$ and $V_k$ would depend on the current Trial 2 data point — in this case, 58.58 V:

$$V_k = 20 + 5.58 + 53 - (-200) = 258.58V$$

A difference of 2.87 V therefore, could also be considered small enough for linear interpolation between 53 V and 64 V for the theoretical PF (irrespective of the 5.58 V translation):

$$PF_{(55.87V)} = 0.6327142857 + \left(\frac{0.50225 - 0.6327142857}{11} \cdot 2.87\right) = 0.6208538961$$

Table 4.2 showed that the PF data points from 31 V and up were rendered obsolete despite their less-than-1 PF due to having angular acceptances of less than 30 degrees. Past 75 V, the transparency had also dropped below 30 percent due to the excessive particle scattering preventing sufficient detector-focused trajectories in the reflectron. This left only the point at 20 V (meaning approximately 25.58 V due to the 5.58 V translation) as a useful point for the reflectron’s turnaround region.

### 4.4.2 Electrode Sizing Trials

#### Trial 3

Table 4.3 and Figure 4.11 show the relation between ACA’s mass resolution performance over the trade in length between electrodes $i$ and $k$. While the correlation in the data from this trial was not as clear as they were for the $V_j$ and $V_k$ trials, it can still be seen that lengthening electrode $k$ in question decreased the performance of the system by raising the PF. Even though the peak in the plot for this trial showed lower values on either of its sides, it could be seen that invalid data points eventually occurred. The final test in Trial 3 failed to direct any particles to the detector, occurring when the $k$ electrode was made 8.94 mm long. Trial 3 was, hence kept with 10 visible data points due to the fact that an extra valid point could not be placed beyond either side of the range limits — on one side, the length already measured 0 mm, while on the other side, the final test already showed no particles reaching the detector (Figure 4.12c). Adding an extra point for consistency would have meant resizing the interval length, increasing the plot range resolution, but insignificantly.

<table>
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<th>$k$ (m)</th>
<th>$\ell$ (m)</th>
<th>$m_{70}$ cTOF ($\mu$ s)</th>
<th>$m_{70}$ FWHM ($\mu$ s)</th>
<th>$m_{71}$ cTOF ($\mu$ s)</th>
<th>$m_{71}$ FWHM ($\mu$ s)</th>
<th>$\Delta$ TOF ($\mu$ s)</th>
<th>$\bar{x}$ FWHM ($\mu$ s)</th>
<th>PF</th>
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The ideal length for electrode \( k \) for a reflectron of ACA’s size was thought to be 5.45 mm, making the nearest two points of data those marking 5.36 mm and 6.26 mm. 5.36 mm was so close to 5.45 mm that their difference was less than a tenth of a millimeter apart (0.09 mm). The interval difference between empirical points was higher for length than for voltage, where one interval spanned 0.89 mm compared to the entire depth, which was 32.7 mm. This still however, could be considered small (around 2.7 percent) along with the PF difference between 5.36 mm and 6.26 mm visually being small compared to the difference between 0 mm and 6.26 mm (maximum PF difference). Linear interpolation could once again be used:

\[
P_{F_{5.36mm}} = 1.3975 + \left( \frac{1.44875 - 1.3975}{0.89} \cdot 0.09 \right) = 1.4027325843
\]

The PF for Trial 3’s theoretical optimum lay above the acceptable threshold, meaning particles were reaching the detector, but with insufficient TOF discrimination. In this
case, the first confirmed point with an applicable PF was at 2.68 mm for electrode $k$ — a difference of 2.77 mm from the theoretical best point and about 0.90 mm less than the default length of 3.58 mm. The effect of this first viable point (2.68 mm) is shown in the trajectory display in Figure 4.12a. The trajectories through the reflectron in Figure 4.12a show a shape closer to achieving symmetry than do the trajectory shapes in Figures 4.12b and 4.12c. Figures 4.12b and 4.12c show the tests for 8.05 mm and 8.94 mm $k$ electrode length, respectively. From 2.68 mm to 8.05 mm, it could be seen that extending the length of the target electrode decreased the depth of the turnaround region, while reducing its potential gradient — making the curves of the trajectories smoother. Unfortunately, this also had the added effect of reducing the off-axis homogeneity, so nearly all particles impacted prematurely on the inner wall of the detector tunnel. Enough were still able to reach the detector to produce TOF spreads, however. In contrast, once the electrode was lengthened to its final data point of 8.94 mm, the entire path of all trajectories leaving the reflectron pointed away from the detector, resulting in an invalid output.

![Figure 4.12: Trial 3 trajectory comparison for different electrode $k$ length](image)

When electrode $k$ was reduced all the way to 0 mm (leaving just a flat bottom plate), the PF dropped not only to its lowest value seen in Trial 3, but to the lowest seen throughout all of Task 2 — 0.312. The transparency values for this test revealed an anomaly: where typically 785 (or occasionally 784) particles successfully enter ACA’s entrance grid, this time a greater number of particles was recorded at entry — 798. Rerunning the simulation, the culprits were isolated as particles whose trajectories were completely reversed once inside the reflectron (another issue stemming from improper potential gradients and poor off-axis homogeneity). These particles not only never reached the detector, they instead (loosely) retraced their entry paths and left the instrument, returning to space. The outcome of this was a seemingly unreliable transparency grade for this test and others that showed similar trajectories and/or “total particles entered” values.
Figure 4.13: Trial 3 best PF test showing particle rejection mid-simulation

Despite a 0 mm turnaround region dropping the reflectron’s PF to the lowest it was recorded, the PF point for this length, as well as for 0.90 mm and 1.79 mm were rejected due to insufficient angular acceptances (short by about 5 degrees of particle trajectories that ended before reaching the detector). The default turnaround region length of 3.58 mm and all intervals adding length to it led to PFs greater than 1, so the resolution of particle masses became too scrambled to be resolved by the detector on the high end of the masses. A turnaround region of 2.68 mm depth within the reflectron could be used in future optimization endeavors.

Trial 4

Table 4.4 and Figure 4.14 show how ACA’s mass resolution performance depends on the length assigned to electrodes \( j \) and \( k \). In the case of Trial 4, the data points for electrode \( j \) lengths 20.35 (Figure 4.15a), 21.25, and 22.14 mm were also returned as invalid for diverting all particle trajectories away from the detector. This set the longest viable length for electrode \( j \) at 19.45 mm. These two trial plot behaviors may suggest that in each case, there may (possibly) be a second point where the plots could cross the \( PF = 1 \) line for practical performance. Finding these points may however prove to be time-consuming and possibly fruitless if the reflectron conditions cut off particle detection before they can once again sufficiently segregate among the highest ion masses. Towards the end of the data range for higher \( j \) lengths, PF started to decrease and approach 1 - meaning differentiation between the heaviest ions was increasing. Simultaneously, the reflectron and tunnels’ transparency rapidly dropped, signaling that more particles were impacting portions of the reflectron and tunnel walls rather than the detector. If only a few dozen particles out of normally about 785 reached the detector, then the TOF differences between those of 70 and 71 AMU would be easier to distinguish, but the data sample size would be deplorable — well below the 30 percent transparency guideline.
Table 4.4: Trial 4 result conversion

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<td>0.0510</td>
<td>0.728</td>
<td>25</td>
<td>46.4</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>10.49</td>
<td>10.78</td>
<td>0.0514</td>
<td>10.85</td>
<td>0.0518</td>
<td>0.07</td>
<td>0.0516</td>
<td>0.737</td>
<td>25</td>
<td>39.4</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 4.14: ACA’s mass resolution PF as a function of j electrode length

For this final trial, the theoretical optimum was calculated to be a length of 16.35 mm for electrode j. Among the empirical data gathered for Trial 4, the points surrounding this value were the j lengths 15.87 mm (the original starting value) and 16.76 mm. The
point 16.76 mm was closer, lying at a distance of 0.51 mm from the theoretical point. Here, the difference between the two data points was larger than it had been for any of the previous trials. It formed a visible fraction of the difference between the points with the highest and lowest PF values, however linear interpolation could still be used. The two points, while near an inflection point (between 14.97 mm and 15.87 mm) and a vertex (between 17.66 mm and 18.56 mm) did not cross either, making the use of an imaginary straight line between them less inaccurate:

\[
PF_{(16.35\text{mm})} = 1.360625 + \left( \frac{1.571875 - 1.360625}{0.89} \cdot 0.51 \right) = 1.4816783707
\]

Inaccuracy or not, a PF of 1.482 would not do as far as TOF discrimination of high masses was concerned. Figure 4.15 shows three subfigures that illustrate the outcome of electrode \(_j\) being lengthened and shortened. The effects of trajectory path pinching and tilting can be seen straightaway in Figures 4.15b and 4.15c as they were seen with Trial 3 with similar results. As electrode \(_j\) was increased in length from 15.87, these problems became apparent. As the path became more tilted and compressed, it was once again diverted from the detector plate to instead impact mostly (and eventually entirely) on the inner wall of the tunnel. The PF mainly increased for this period until the reflectron began to choke the path reaching the detector. With fewer particles arriving, the ability for the detector to discriminate among their masses increased, dropping the PF again. Then, with no further impacts on the detector the PF became invalid. Similar to the effect of reducing electrode \(_k\) in Trial 3, reducing electrode \(_j\) to 10.49 mm reduced the PF to 0.737 and yielded a symmetrical particle path throughout the reflectron (though again with spread scattering of particles).

(a) Electrode \(_j\) = 10.49 mm  (b) Electrode \(_j\) = 14.07 mm  (c) Electrode \(_j\) = 20.35 mm

Figure 4.15: Trial 4 trajectory comparison for different electrode \(_j\) length

Trials 1, 2 and 3 resulted in several PF-viable values for their respective variables being discarded for having too low an angular acceptance response or an insufficient
transparency. Each trial mentioned so far had ended up with one working point of data for use in the future. Trial 4 presented a different case, as this time, several candidates would withstand the test of Task 1’s parameters being used for additional validation of data. The range of PF data from electrode \( j \) length 12.28 mm up to 14.07 mm would result in three possible deceleration region lengths that could be used for future experimentation. Lengths greater than 14.07 mm left PFs higher than 1 and less than 12.28 mm resulted in inadequate angular ranges.

Recapitulating from Task 1, the data would be considered applicable for every point that yielded transparency values higher than 30 percent and showed an angular acceptance of 30 degrees. Each trial presented a range of variable values with PFs less than 1, but the inclusion of Task 1 parameters (angular acceptance and transparency) as further criteria for assessing the ranges of viable values per Task 2 variable disqualified many previously acceptable data points. Trials 1 through 3 were left with only a single viable point and Trial 4 had only three. The ranges before and after filtering by this method are displayed below in Table 4.5.

<table>
<thead>
<tr>
<th>Trial</th>
<th>Viability by PF</th>
<th>Viability by PF, ( \alpha ), and ( \tau )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-90 V — -35 V</td>
<td>-35 V</td>
</tr>
<tr>
<td>2</td>
<td>20 V — 108 V</td>
<td>20 V</td>
</tr>
<tr>
<td>3</td>
<td>0 mm — 2.68 mm</td>
<td>2.68 mm</td>
</tr>
<tr>
<td>4</td>
<td>10.49 mm — 14.07 mm</td>
<td>12.28 mm — 14.07 mm</td>
</tr>
</tbody>
</table>

### 4.5 Summary

The task of revising ACA’s design to manipulate its reflectron’s parameters for performance increases was completed. The results from the four trials could be condensed into two reflectron properties individually (or both) requiring adjustment. These properties were increasing the electric field gradient from the entrance to the cap of the reflectron and/or decreasing the length of the electrodes — both of these properties specifically pertaining to changes to the intermediate and cap electrodes (though the entrance electrode is affected as well, by proxy). This suggests that the reflectron should be modified to possess dimensions closer to those of a mirror, though theory contradicts this by emphasizing the required balance between mirror diameter and depth. Replacing the reflectron with a second mirror is second option.
Chapter 5

Discussion

5.1 Task 1

5.1.1 Further Analysis

Regarding the linear trendlines, specific numbers themselves were relevant only in the context of ACA’s current entrance grid curvature(s) combined with its current internal part parameters. What was relevant is the fact that reducing the depth of the entrance grid increased the angular acceptance and the transparency, meaning that if any internal parameters in the later task were changed and negatively impacted Task 1’s variables, the entrance grid could be raised as a possible solution. If ACA’s entrance tunnel were elongated to an arbitrary, large number, setting the entrance grid at the bottom would never yield zero degree angular acceptance. This would make the theoretical trend between grid position and angular acceptance an exponential growth profile that peaks and ends at 180 degrees (when the entrance grid is placed at the outer rim of the entrance tunnel). This post-result evaluation for instrument transparency would likewise, yield an exponential relationship, rather than a linear one. The reason for each trend seen being linear had to do with the range of angular variance being small enough to be approximated by a straight line in both cases.

5.1.2 Speculations

When the values for transparency of ACA were tallied per tested grid distance, one point stood out: a design with a grid at 74.25 mm underperformed in terms of the transparency expected it. The lower-than-average transparency was traced to the behavior of the particle trajectories forming the path from the reflectron to the detector, where it was seen that the particles were beginning to diverge more to the edges of the detector (meaning many of the newer particles were simply impacting onto the tunnel walls just a few mm above the detector itself). Despite letting in a greater number of particles, this grid position let a smaller fraction of them hit the detector. The transparency of this plot point at 66 percent was lower than the deepest grid position offering the least amount of particles entry (still at 67 percent transparency). Because of that, it would mean the 74.25 mm grid position didn’t just have the smallest ratio of particles detected to particles entered, it had the lowest number of particles out of all trials hit the detector in the first place. While this anomaly is not fully understood, the likelihood is that it was caused by
a greater number of particles with a specific lateral velocity being allowed into ACA that otherwise would never reach the entrance grid. The grid would accelerate them, but only in forward velocity, so the particles would still travel sideways at speeds proportional to their angles of entry. Presumably, the transition of the entrance grid to this height from the level beneath it may have raised the amount of particles within this lateral velocity range by enough such that they add a large number to the particle population, but crash into the drift tube walls or reflectron due to their higher lateral speeds compared to the particles that always can enter and rarely impact into walls.

5.2 Task 2

5.2.1 Further Analysis

Trial 1

As $V_j$ was increased, the clustering of particle trajectories within the reflectron became more tightly condensed and shifted off-center, pointing toward off-axis homogeneity being compromised, and less area within the reflectron being used. Less area was used due to a greater potential gradient within the reflectron occurring increasingly closer to the entrance due to the contrast between the deceleration region and the turnaround region being reduced (as $V_j$ approached $V_k$). Increased potential gradient occurring earlier within the reflectron meant less opportunity for slower particles to catch up to faster particles, and all factors resulted in PF increasing with increasing $V_j$. The particle path “pinch” mentioned in the results of Trial 1 occurred because particles straying too close to the $j$ electrodes and because the deceleration region was being made more powerful and left less work for the actual turnaround region controlled by $V_k$. The result of the pinch was similar to the case of the Task 1 test outlier — the amount of detector area hit by particles was increased by the reflectron’s pinching, but this action confined both the faster and slower-moving particles to a smaller amount of depth, reducing the displacement for the fast particles significantly. This could explain the high PF values recorded, as the TOF distributions for tests exhibiting this pinch could expect to have no high-mass resolution whatsoever due to particles of any single mass arriving with a large amount of TOF variation — making discrimination between masses nigh-impossible.

Where initially it was thought that having $V_j$ equal to or less than -35 V would be enough for continued design optimization, a single data point at -35 V remained valid after this trial’s data was put through the criteria for determining sufficient transparency and angular acceptance of ACA. Even though all points from -46 V to -90 V had better PF values, only this point could certainly be used for future optimization runs. The deceleration voltage of -35 V was the only case that supported an angular acceptance of 30 degrees along with allowing more than 30 percent of all entering particles to reach ACA’s detector.

It was also found that decreasing the PF point past -35 V brought the PF values to a form of saturation — where they began decreasing far more slowly than they did before, as if behaving asymptotically. This was estimated to be caused by the deceleration region being used to its full volume by -46 V, so that all particle trajectories entering when the deceleration voltage is lower than this would penetrate far into the turn-around region, maximizing the used depth within the reflectron. This also resulted in more of the
detector’s area being used for particle impacts, but this time with proper TOF separation due to the faster ions covering much greater distances inside the reflectron than the slower ions would. In this way, there would be less TOF variation per mass, but the increased scattering from a weaker deceleration region would result in limited transparency and angular acceptance due to the particles with high lateral velocity impacting more easily through scattering.

Trial 2

The short lateral branches of the bottom \( k \) electrode emphasized the purpose of the turnaround region to be mainly focused on repelling incoming particles with a deceleration vector perpendicular to the bottom plate itself — and at high \( V_k \) values, this effect pronounced itself as a convex contour formation in the potential distribution. Convex potential would reflect particles in a similar manner that a convex mirror would scatter light. While the entire detector would receive particle impacts (with comparatively fewer premature impacts on the detector tunnel’s walls in turn) the same curvature of potential would lead to increased particle rejection from ACA.

The effect of Trial 2 being based on the nearest viable \( V_j \) value (-35 V) manifested itself upon the generation of the plotted results. The default \( V_k \) voltage was 20 V for the original design, and Figure 4.5 suggests that this voltage was high enough for the PF to be below 1. This, however could not work if the the default \( V_j \) voltage of -29.42 V was used in tandem, meaning that the PF should have been just over 1 at \( V_k = 20V \). In reality, \( V_k \) would need to be higher. It could be assumed that with most of the particle turnaround taking place over the boundary between the \( j \) and \( k \) electrodes, that a \( V_j \) shift by 5.58 V in the negative direction could be countered by displacing the entire Trial 2 plot by the same amount in the positive direction (adding 5.58 V to all data points). This assumption was based on the knowledge that a relatively small change over a curve could be considered linear — the “curve”, in this case being the term given to describe the change in the reflectron’s potential gradient when its \( V_j \) voltage was changed from -29.4202 V to -35 V. The difference between -29.42 V and -35 V on the \( V_j \) plot — could be approximated as a straight line, as shown by the changes in (middle) step height in each of the graphs in Figure 4.10. Going by this assumption, this made the new minimum viable \( V_k \) value about 25.58 V. Because a change of less than 6 V over a much larger \( V_j \) to \( V_k \) range of 220 V (if \( V_k \) was kept at its default 20 V) was considered small enough to count as negative linear displacement of Trial 2’s results (before being plotted), it was proposed that the results be interpreted as if shifted positively by the same amount of displacement for the trial’s true values (with no \( V_j \) meddling) to be documented.

In spite of the offset of 5.58 V, the Trial 2 relation (Figure 4.8) makes it clear that increasing the \( V_k \) voltage would improve ACA’s performance.

Trial 3

Trial 3 was the first trial that disputed the theoretically ideal position of a parameter within the reflectron by revealing its effect on instrument performance to be contrary to what was desired.
It was discussed earlier that electrode \( k \) in the reflectron possessed short lateral branches (occupying little depth along the reflectron’s walls) as its purpose was mainly to exert a repulsion vector parallel to the reflectron’s central axis with its bottom plate. It was shown that reducing the length of the \( k \) branches improved the reflectron’s performance in TOF discrimination — and that completely eliminating the lateral electrodes resulted in the best PF for Task 2, regarding ACA’s differentiation of the highest of ion masses. With only a bottom plate establishing the turnaround region, the particle path showed nearly perfect symmetry about the reflectron’s central axis, though as with Trial 2, the shape of the potential contours indicated a convexity was forming at this point — with plenty of scattering also being responsible for the symmetrical appearance. Increasing the length of the same electrode eliminated the issues of scattering and the steepness of axial potential gradient that came with it, however the off-axis homogeneity was made worse with an excessive lateral repulsion force coming from the extended turnaround region; particles entering the reflectron were laterally pushed to the side of the reflectron above the detector tunnel, but the equal opposite lateral force from the latter side of the reflectron responded by overcorrecting the trajectories of these particles such that by the time electrode \( k \) was extended to 8.94 mm, all particle were sent into the inner tunnel wall instead. In a way, a pinching effect similar to that in Trial 1 was seen here, but this effect also was accompanied by an off-axis tilt due to the distorted proportions of electrode \( k \) with respect to the reflectron’s width.

Similar to both voltage trials, Trial 3 returned only a single viable value for its electrode \( k \) length after lengths shorter than 2.68 mm did not allow for a 30 degree angular acceptance. This aside, the working value of 2.68 mm could be kept for future runs.

**Trial 4**

As with Trial 3, this trial too disproved the validity of its theoretically best value for its target variable. The theory pointed to a \( j \) electrode length of 16.35 mm being best suited for optimization, yet it resulted in a PF over 1.4. Instead, reducing the length of the electrode in question boosted the performance of the reflectron.

 Though one difference was apparent when compared to its counterpart result in Trial 3 — the curvature of the path was nearly flattened, but still retained visible concavity. Particle scattering still did occur, as seen in Subfigure 4.15a where the region near the detector, across the inner wall was normally sparsely filled with particles (if with any at all). The scattering however was less apparent, due to the potential still being concave deep within the reflectron. Scattering aside, this effect reduced the PF all the way to 0.737; a good sign for TOF high-mass differentiation. The gradient between the deceleration and turnaround regions was steepened, but this effect was more concentrated in the axial periphery and less so the closer to the central axis a particle reached — the opposite effect of what caused the convex potential shape. This helped more particles get reflected in directions suitable for exiting the reflectron from the correct side in order to reach the detector and less scattering was seen.

In PF context, Trial 4 was the least successful not due to failure to produce any points with PF below 1, but due to it not returning any PF values below 0.5 (contrary to the previous trials). Despite this minor setback, Trial 4 ironically did best running against the filtering criteria assigned to Task 1 originally — it returned the range of electrode \( j \) lengths from 12.28 mm to 14.07 mm as usable in future runs.
5.2.2 Grand Results

The graphical statistics of the accepted Task 2 values are displayed below, arranged by their designated trial number. For comparison, the starting version of ACA had:
An angular acceptance of 30 degrees and an instrument transparency of 76 percent. Based on its TOF distribution parameters, it also had a PF of 1.36.

Trial 1

![Graph showing angular acceptance and transparency for Trial 1](image)

(a) Angular acceptance and transparency

![Graph showing m70 to m71 TOF Resolution for Trial 1](image)

(b) m70 to m71 TOF Resolution

Figure 5.1: Accepted result from Trial 1: $V_j = -35$ V. This point had an angular acceptance of 30 degrees, an instrument transparency of 68 percent, and a PF of 0.979.

Trial 2

![Graph showing angular acceptance and transparency for Trial 2](image)

(a) Angular acceptance and transparency

![Graph showing m70 to m71 TOF Resolution for Trial 2](image)

(b) m70 to m71 TOF Resolution

Figure 5.2: Accepted result from Trial 2: $V_k = 20$ V (25.6 V with translation). This point had an angular acceptance of 30 degrees, an instrument transparency of 68 percent, and a PF of 0.990.
Trial 3

(a) Angular acceptance and transparency

(b) m70 to m71 TOF Resolution

Figure 5.3: Accepted result from Trial 3: $k = 2.68$ mm. This point had an angular acceptance of 30 degrees, an instrument transparency of 68 percent, and a PF of 0.965.
Trial 4

(a) 12.28 mm Angular acceptance and transparency

(b) 12.28 mm m70 to m71 TOF Resolution

(c) 14.07 mm Angular acceptance and transparency

(d) 14.07 mm m70 to m71 TOF Resolution

Figure 5.4: Accepted results from Trial 4: \( j = 12.28—14.07 \) mm. Point 12.28 mm had an angular acceptance of 30 degrees, an instrument transparency of 57 percent, and a PF of 0.805. Point 14.07 mm had an angular acceptance of 30 degrees, an instrument transparency of 71 percent, and a PF of 0.955.

It could safely be assumed that the greater the difference between \( V_k \) and \( V_j \), the greater the clarity becomes between identifying particles of or near the highest mass targeted. The changes needed for the original version of ACA to meet this PF requirement were for either:

- The \( V_j \) voltage to be reduced from -29.42 V by a minimum of 5.58 V. The viable voltage range begins at -35 V and lower.

— OR —
• The $V_k$ voltage to be raised from 20 V by the same minimum of 5.58 V. The viable voltage range begins at approximately 26 V and higher.

Like with Trial 1, Trial 2’s TOF-viable data was reduced to only a single point at 20 V (25.6 V), when it came to the Task 1 criteria, so it would appear that changing either $V_j$ or $V_k$ would have close to the same effect. In this case, it is recommended for $V_j$ to be put at higher priority due to it holding a lower PF value than 25.6 V for $V_k$. A second benefit would have to do with the power budget cost being slightly reduced due to electrode $j$ being reduced by 5.6 V instead of $V_k$ being increased by that amount.

Similarly, the reflectron’s depth divisions could be improved. Either:

• The $k$ electrode length could be reduced from 3.58 mm down to 2.68 mm, with the subtracted length going to electrode $i$.

— OR —

• The $j$ electrode length could be reduced from 15.87 mm to anywhere from 14.07 mm down to 12.28 mm, with the subtracted length also going to electrode $i$.

5.2.3 Speculation

The combined findings from these trials suggest two directions to be taken for improving the reflectron’s performance:

1. Increasing the voltage gap between electrodes $j$ and $k$ will reduce the TOF distributions’ spread by reducing the volume of the particles’ turnaround region (thereby limiting the velocity variation).

2. Decreasing the lengths of either electrodes $j$ or $k$ (and possibly both) will similarly confine the turnaround region to a smaller space with a steeper electric potential gradient.

Both of these qualities are akin to the properties of the electrostatic mirror and this suggests that the best reflectron for ACA would be overall shallower than the one currently in use. This may yet again contradict the ideal reflectron architecture, which was stated in the three-element-reflectron study that it must have a depth of about 25 percent the focal length [66]. Most likely, there are still places to optimize the three-element-reflectron, but the optimized parameter ranges could be small. Exploring in wider parameter space is a possible future study. Disrupting the reflectron’s current aspect ratio may also distort its efficiency with its transfer of particles being reflected off-axis. A mirror trades the complex electric potential curvature over a wide space in favor of a simple strong electric field condensed into a small space for increased simplicity — taking care of the issue of off-axis homogeneity by reflecting all incoming particles equally (but defocusing them as a consequence).

Despite the Task 1 filtering criteria eliminating data territory previously thought ideal for use in instrument optimization, it is now known that for each trial in Task 2 run, there exists a small island of possible points centered around the values documented in the trials (variance about said points may exist, but has not as of yet been documented). Overall, optimization trials testing multiple variables have the possibility of continuing due to these data islands existing.

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5.3 Sources of Error

On the subject of focal length, a source of error warranting investigation would be the decision for the focal point of the entrance grid to have been changed based on a visual assumption that particles may risk hitting the edge of the inner entrance tunnel wall. While not stated directly, nearly every trajectory screenshot shown has indicated that the particles now hit the broad side of the inner wall of the detector tunnel as a consequence. While this did not seem to impede the process of optimizing the other goal parameters of this project, the focal point selection did deserve a test of its own. The test was set up such that the data range would start at the focal distance used for the two tasks and extend to the maximum depth of the reflectron — a range of just over 6 cm distance for interval testing. The minimum distance was kept at the used focal point position on the assumption that moving it further away from the reflectron would only worsen the amount of particles hitting the inner wall of the detector tunnel. The plots for the test’s PF (Figure A.1a) and transparency values (Figure A.1b) along with an angular acceptance (Table A.1) table are shown in Appendix A, but they can be summarized into one definite finding: For all other parameters at their defaults, the currently used focal point had the lowest PF with a viable angular acceptance and transparency — though at all default parameters, the PF was above 1, at about 1.36. As it turned out, the original focal depth prior to being changed (close to 47.25 mm in the test) would have yielded an angular acceptance of only 25 degrees as opposed to 30 for a given entrance grid depth. The original entrance grid would have therefore been less efficient in capturing ions with lateral velocities than would the selected focal point. This would mean that though based on a poor assumption initially, the decision to decrease the focal distance from the mirror by a factor of 2 yielded more benefits than errors over the course of this project.

A second source of error was the decision to change $V_j$ in Trial 2, which was focused on the reflectron’s behavior about changes in $V_k$. All four trials were mapped initially to cover broad ranges of voltage or length to obtain as much information on the changes between individual variables as could be gathered — all part of a safeguard, in case there would be insufficient time for any further trials exploring the crossovers between two or more of the target variables changing simultaneously to be covered. Trial 2 was modified, such that its data could be directly “fitted” over the data of Trial 1 to follow sequential iterative optimization — where each variable in a trial would be changed depending on how the variable in the previous trial was changed. Doing this could improve the reflectron performance, while underscoring the dependent behaviors of each Trial’s target variables. Following Trial 2, this idea was scrapped in favor of the project returning to branching optimization, where each change to a variable in a trial originated from the default design of ACA to simplify and ground the conclusions gathered from the data.

A third source would come from ACA’s design using a 20:1 pixel to mm ratio. Given the instrument’s 45 by 100 mm dimensions, that would set it at 900 by 2000 pixels. The area is not a small number of pixels by any means, but it is limited such that the quantization of elements by the pixels was seen in the circular entrance grid. The grid’s curvature was constrained by the number of pixels forming its arc, meaning that adjustments in focal distance and direction would also be limited in combinations.
Chapter 6

Conclusion

6.1 Optimization Findings

The entrance grid of IRF’s TOF-MS instrument, as well as the internal parameters of its reflectron were investigated in their own respective trials over two tasks. Regarding the entrance grid’s positioning, the trends between its placement and ACA’s functional FOV and transparency became understood. Respectively, their relations were found to be: $y = 1.13 \cdot x + 42.5$ degrees per mm and $y = 0.148 \cdot x + 59$ percent per mm. ACA’s reflectron in terms of individual elements is also understood now to by default operate at near-optimized levels, and was optimized with respect to each studied element individually. The hypothesis gathered for predicting the reflectron’s best calibrations was disproven — narrowly in terms of element voltages, and severely in terms of electrode lengths. Deceleration and turnaround voltages were found to ideally sit at -35 V for the deceleration region and 25.6 V for the turnaround region if tested individually. Similarly, for individual testing, the best lengths for the same governing electrodes were found to be anywhere from 12.3 mm to 14 mm for the deceleration electrodes and 2.7 mm for the turnaround electrode. Despite an invalidated hypothesis, each trial run found individual conditions now known to optimize ACA’s performance.

6.2 Future Research

As individual variables affecting ACA’s performance have now been subject to in-depth experimentation, any runs done to further optimize ACA should be done in tests crossing multiple variables per trial for more comprehensive data to be obtained. Multiple element voltage and length changes should be attempted per trial once a comfortable understanding of their effects on each other has been reached. This should eventually expand to include variables outside of ACA’s reflectron until the whole instrument’s design is fully optimized without compromising its cubesat compatibility.
References


Appendix A

Test on shifting focal distance

Table A.1: Focal depth against PF, angular acceptance, and transparency

<table>
<thead>
<tr>
<th>Focal Depth from Mirror</th>
<th>$\alpha$ (°)</th>
<th>PF</th>
<th>$\tau$ (%)</th>
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Figure A.1: (a): ACA’s mass resolution PF as a function of focal distance from ACA’s mirror. Weak positive correlation is seen between increasing distance and increasing PF. Individual variance of PF per point heavily skews the correlation. (b): Transparency as a function of focal distance from ACA’s mirror. The profile appears to be skewed similarly to how that of the PF is for this test. With increasing focal distance comes increasing transparency.