

Ultra-Long Baseline Time-of-Flight Mass Spectrometry with the AMIGAS Multi-Spacecraft Concept

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Abstract—Time-of-flight mass spectrometry allows for the study of elemental, isotopic, and molecular composition from a material sample. The mass sensitivity and resolution of time-of-flight mass spectrometers increases with the length of the instrument, where increased sensitivity indicates increased ability to distinguish between ions of similar masses. This indicates an inherent limit of traditional time-of-flight mass spectrometers designed as monolithic instruments for integration onboard a spacecraft: the length of the spectrometer, and therefore its sensitivity, is constrained by the form factor of the spacecraft. This paper motivates and presents a novel architecture for in-space mass spectrometry through the use of distinct, free-flying spacecraft that will be the subject of future research. The Advanced Mass Spectrometry in Gravity-Free Architectures (AMIGAS) concept aims to enable ultra-long baseline (10-100 m) time-of-flight mass spectrometry that could dramatically improve the sensitivity and resolution of in-space time-of-flight mass spectrometers to the point of detecting millidalton-level differences in atom or molecule mass. This paper presents the scientific motivation for why such a high sensitivity would be beneficial and explores the associated engineering constraints. A high-level overview of the AMIGAS concept is also provided along with anticipated challenges for practical implementation.

flight distances result in a greater time delay between populations of adjacent, similar-mass ions. If ions with slightly differing masses arrive closely in time to one another relative to the detector time response, the observed mass lines will overlap, and it can be difficult or impossible to break ambiguity in the resulting data. Thus, the flight distance is a primary determinant of the TOF-MS system's mass resolution, with longer flight distances producing more precise, higher mass resolution instruments.

A number of mass spectrometers have been flown on spacecraft to study the chemical composition of planetary objects. Some have been optimized to study volatiles and gases, (e.g. [1] and [2]), while others have been optimized to study dust grains ejected from planetary surfaces from orbit, such as the Cassini spacecraft's Cosmic Dust Analyzer (CDA) [3] and the upcoming Surface Dust Analyzer (SUDA) on the Europa Clipper. The CDA was highly successful at investigating the composition of various objects in the Saturn system, and in particular has been instrumental in studying the icy dust grains from Enceladus's plumes [4], [5], now known to be coming from a subsurface liquid water ocean [6]. However, because of the lower mass resolutions of the solid or ice-phase mass spectrometers, they have been unable to provide complementary measurements of, among other things, the deuterium-to-hydrogen (D/H) ratio, even as the gas-phase mass spectrometers have been able to do so.

Here we propose a tandem spacecraft mass spectrometer system, the Advanced Mass Spectrometry in Gravity-Free Architectures (AMIGAS) instrument concept. AMIGAS increases the mass resolution of typical on-orbit ice-phase mass spectrometers by spreading the flight distance between two spacecraft, which operate together, as shown in Fig. 1. One spacecraft collects icy dust grains from the target object, ionizes the material, and accelerates it towards a receiving spacecraft with detector electronics. This creates an ultra-long baseline TOF-MS system with a mass resolution that greatly exceeds that of existing ice-phase mass spectrometer instruments.

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1. INTRODUCTION

Time-of-flight mass spectrometry (TOF-MS) is one of the principal methods of studying the chemical composition of a variety of samples, both terrestrially and in space. Molecules from the sample are ionized and accelerated via an electric field towards a detector some distance away. Because the flight time of each molecule depends on its charge-to-mass ratio, the ions spread out in time according to their mass. Time delays between signals measured at the detector can then be used to determine the mass of the sample's constituent molecules, and the chemical composition of the sample can be inferred from this.

The flight distance between the ionization source and the detector is a critical parameter for TOF-MS systems. Longer

2. SCIENCE MOTIVATION

In order to demonstrate the potential value of the AMIGAS system, we contextualize the proposed concept with measurements of the D/H ratio of ice grains in the outer solar system. This ratio is deceptively difficult to measure using TOF-MS because the mass of H_2^+ molecules, 2.016 AMU, is very close to that of deuterium (D) ions, 2.014 AMU. This milli-dalton difference means these mass lines overlap in typical ice-phase mass spectrometers, and a very high mass resolution is needed to break the ambiguity between them to provide a direct measurement of the number of D^+ ions in an ice sample.

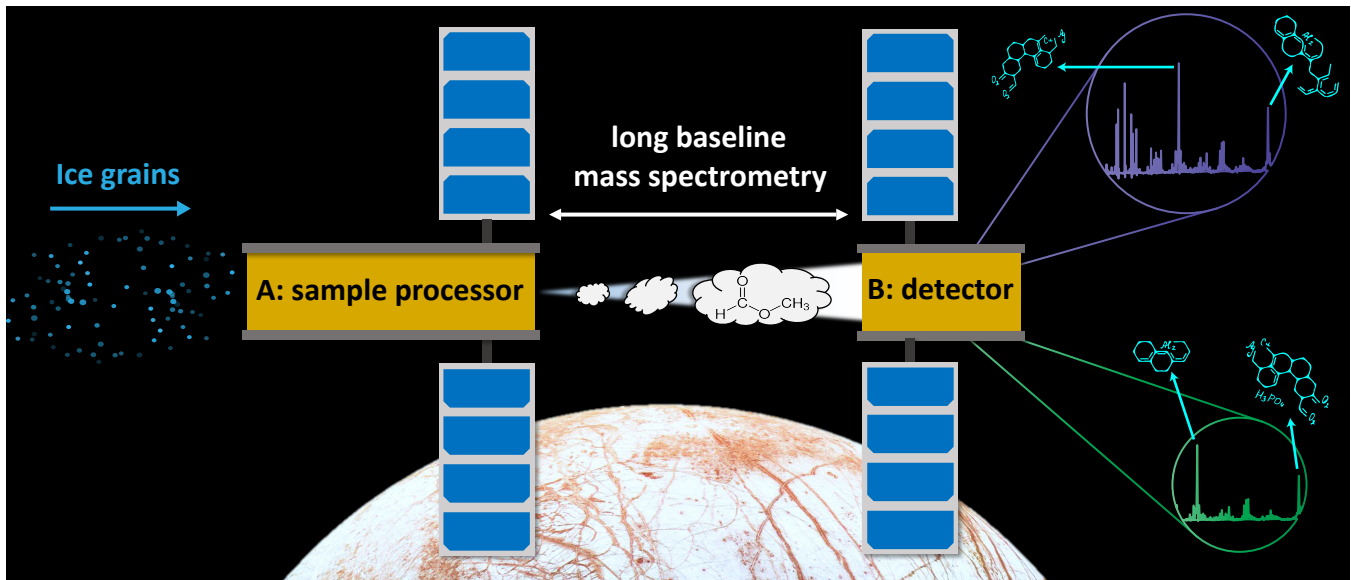


Figure 1. Illustration of the proposed long-baseline time-of-flight concept.

Stable isotope ratios are important metrics in planetary formation models and other studies of the history of the solar system [7]. The ratio between D and H is of particular importance due to rates of fractionation in planetary ices. In cold systems, typically below 50 K, there is a preferential creation and preservation of HDO ice relative to H₂O water ice. The reasons for this are complex and beyond the scope of this paper [8], [9], [10], [11], [12], but it is sufficient to say that the D/H ratio of water ice has had measurable time- and location-dependent structure throughout the history of the solar system [13], [7].

Thus, the D/H ratio of water, particularly of water ice in the outer solar system, has a rich astrophysical history, and with proper accounting for post-formation isotopic processing of H and D on planetary bodies, measurements of the D/H ratio of both bulk composition and of water ice can constrain the time and locations that planetary bodies formed in the solar system. This has made the D/H ratio an important metric for investigations into the formation and evolution of solar system bodies, including the ongoing debate about the origin of Earth's oceans [14], [15], [16], [17], [7]. Measurements of the D/H ratio can constrain these models as well as a variety of other geophysical phenomena, (e.g., [18]). As such, there is great value in providing new measurements of the D/H ratio of celestial ices, especially in the outer solar system.

Clark et al. studied the D/H ratios of the Saturnian system [7]. This study used data from the Cassini spacecraft's Visual and Infrared Mapping Spectrometer (VIMS) [19] and combined it with other published work to compare the measured D/H ratio of a wide variety of objects in the solar system. A subset of the data from Clark et al. is replotted in Fig. 2, with data color coded by the instrument family that measured it. In particular, the measurement for Phoebe's D/H ratio is 7.6 ± 1.7 times that the average of other objects in the Saturn system, strongly suggesting that it formed in a different environment than its modern neighbors and illustrating the importance of the D-H ratio for planetary science [7].

One notable feature of Fig. 2 is that the majority of observations of outer solar system D/H ratios have come from infrared spectrometers [7], shown with red triangles in Fig. 2.

Infrared spectrometers can measure only the topmost surface layers of planetary ices, where processing from radiation and other phenomena has the potential to alter the local D/H ratio through either equilibration with ambient H or through preferential ejection of the lighter H atom. On the surface of Europa, for example, the Jovian magnetosphere focuses high energy electrons on to the surface ice, dissociating water into hydrogen peroxide and hydrogen gas (which then typically escapes from the moon) via the reaction $\text{H}_2\text{O} \longrightarrow \text{H}_2\text{O}^+ + \text{e}^- \longrightarrow \text{H} + \text{OH} \longrightarrow \text{H}_2 + \text{H}_2\text{O}_2$ [20]. Subsequent reactions can then lead to H transfer, H and OH addition, and other sources of D/H disproportionation [20]. Thus, infrared spectrometers may provide D/H ratios that differ from the bulk composition, and even then, they typically involve indirect measurement through molecular spectral features [7]. Ice-phase mass spectrometers, on the other hand, may directly sample ejected ice grains [3], potentially even from the subsurface, where D/H alteration is minimized, if plume activity is present as is known to be on Enceladus and suspected on Europa [21], [22], [23], [24]. If the resolution of the ice-phase instrument is sufficient, it may provide a direct measurement of the relative abundances of D and H.

Despite these advantages of TOF-MS measurements, of the D/H measurements of the outer solar system, only three have come from mass spectrometers. Of these three, two have focused on the measurement of outgassing volatiles rather than direct measurement of water ice, which provides the most relevant scientific data for bulk composition [25], [7]. The third was a measurement of the Enceladus plume that used a highly indirect method to provide a measurement because it lacked the mass resolution to directly survey the isotopic fractionation [26]. All three are discussed briefly below.

High resolution gas-phase and/or ion mass spectrometers are already capable of measuring the D/H ratio of outgassing or atmospheric material, and the two measurements from this type of instrument are plotted in Fig. 2 as blue squares. The Rosetta spacecraft used its Rosetta Orbiter Spectrometer for Ion and Neutral Analysis (ROSINA) to measure the D/H ratio of outgassing vapor from 67P/Churyumov-Gerasimenko [27], [2]. This result was especially interesting, not only

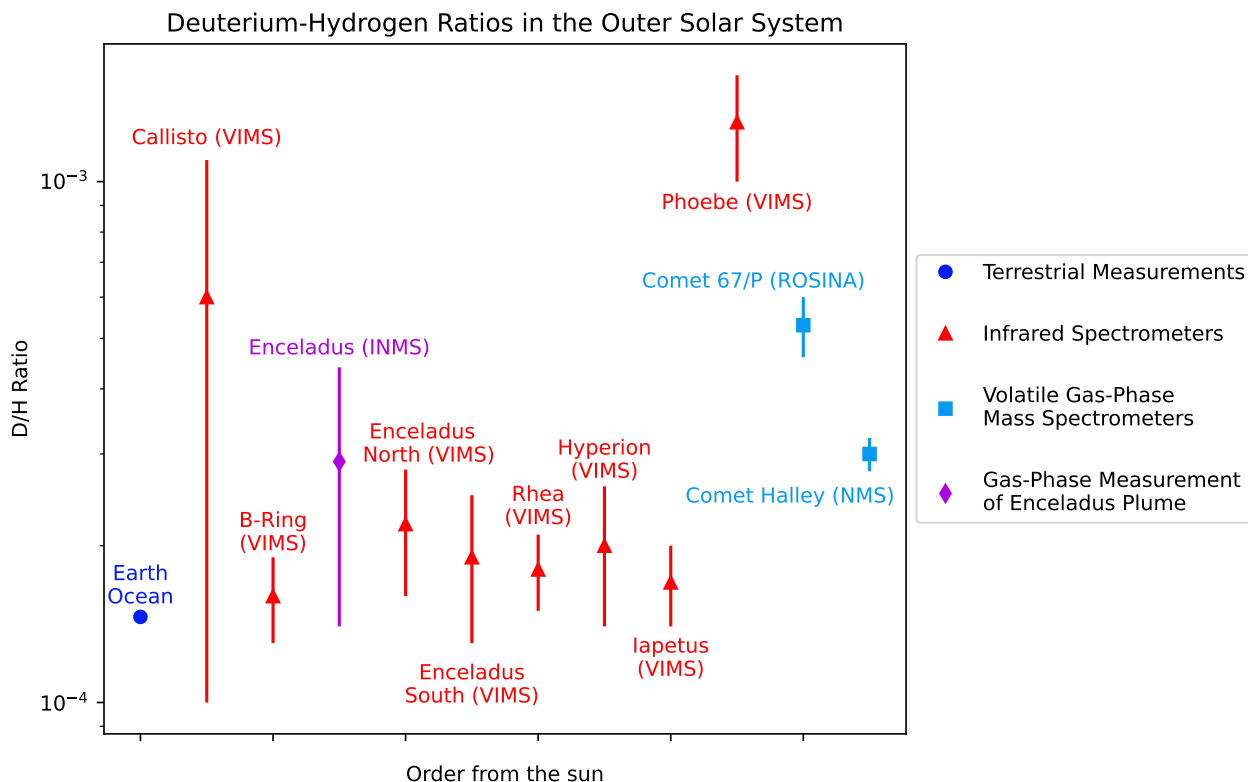


Figure 2. Comparison of the deuterium-hydrogen ratio for various objects in the outer solar system. Phoebe’s ratio is 7.6 ± 1.7 times that of its neighbors, indicating a differing formation process and location. This is a subset of the data found in Ref. [7], color-coded here by instrument type. Vertical lines represent error bars.

for being the sole use of mass spectrometry to measure the D/H of a Jupiter-family comet, but because it revealed a particularly high D/H ratio of about 530 ppm [27], over three times the terrestrial ocean’s value of 155 ppm [17], [7]. Similarly, the ESA spacecraft Giotto’s ion mass spectrometer measured the Oort Cloud Comet Halley’s D/H ratio in 1986, although the results were not published until 1995 [28], [29]. Both measurements fit lines to a family of mass peaks around mass 19 to differentiate between various water isotopologues. While these measurements of volatiles are highly valuable, there is experimental and theoretical evidence that the D/H ratio of sublimating water differs from that of the ice itself, and direct measurement of ice-phase water with a high-resolution mass spectrometer is a much more robust method of accurately determining the D/H ratio [25], [7].

The sole measurement of D/H from a lower-resolution mass spectrometer was from the Cassini Ion Neutral Mass Spectrometer (INMS) measurement of Enceladus’s plumes [26], shown with purple diamonds in Fig. 2. It is marked differently than the ROSINA and Giotto results because, while also a gas-phase mass spectrometer studying volatiles, the confounding factors that may lead to different D/H ratios in outgassing material [25], [7] may not apply to subsurface liquid water ocean material being ejected directly into space. This result lacked the mass resolution to directly identify a number of species found within the data. Thus it relies on a complex and highly indirect measurement of fitting mixtures of multiple species to the data, including assumed rates of

reactions from adsorbed plume material on the instrument’s titanium surfaces. In that study’s own words, the analysis “requires careful deconvolution of a complex pattern of mass peaks representing both parent species and dissociative ionization products.” Because the instrument could not break the ambiguity between D^+ and H_2^+ , that study assumed effectively zero D^+ ion content in the mass 2 AMU line. It then compared mass 2, assumed to be entirely H_2^+ , with mass 3, a mixture of H_3^+ and HD^+ , using a correction factor based on instrument calibration data to subtract out the calculated H_3^+ ion content. While this result is interesting, if the instrument had had higher mass resolution, direct measurement could be made to negate the need for such complex and indirect methods.

In any case, all three of these measurements rely on gas-phase mass spectrometer systems, and there are no ice-phase measurements on Fig. 2 because none have yet been made. Thus, high-resolution mass spectrometers that can break this ambiguity may provide important new and independent measurements that constrain a number of planetary models [7], [13]. In particular, even as the Cassini VIMS was able to measure D/H ratios of Saturnian moons with infrared spectrometry, the Cassini spacecraft’s dust instrument, the CDA, was unable to provide an independent measurement of ice grains because the mass resolution required to separate D^+ and H_2^+ far exceeded the capabilities of the instrument. Thus it was unable to resolve the D/H ratios for any of the planetary bodies it studied [3]. Similarly, the Giotto Particle Impact

Analyzer and the PUMA 1 and 2 instruments aboard the Vega 1 and 2 spacecraft were unable to provide independent D/H measurements of comet Halley, even as Giotto provided volatile D/H measurements through use of gas-phase mass spectrometers [30], [31], [28], [29]. Thus, by increasing the mass resolution of on-orbit mass spectrometers, the long-baseline AMIGAS time-of-flight system proposed here may enable direct measurement of the D/H ratio of ice-phase water, potentially illuminating the formation process of objects across the solar system.

It should further be noted that the D/H ratio is but one of several important ambiguities that may be broken with a long-baseline time-of-flight mass spectrometer, and the scientific value of dramatically increased mass resolution far exceeds isotopic ratios alone. For example, identification of amino acids or other complex organics, isotopic ratios therein, and other avenues of carbon chemistry have far-reaching implications in the search for extraterrestrial life, habitability assessments of icy ocean worlds, and the study of the origin of terrestrial life [32], [33], [34].

3. LONG-BASELINE CONCEPT

In order to break the D/H ratio ambiguity, there is a clear need for in-space mass spectrometers with sufficiently-high resolution in order to differentiate atomic deuterium and molecular hydrogen and/or the family of mass peaks around water isotopologues at mass 19. Our proposed solution is to develop a new architecture for ultra-long baseline time-of-flight mass spectrometry using tandem spacecraft to provide a dramatically larger flight distance than is possible with conventional MS systems and single spacecraft form factors.

The basic principle of time-of-flight mass spectrometry is that an ion, initially at rest, of mass m and charge q , when accelerated through an electric potential of magnitude V will take a time of

$$t = L \sqrt{\frac{m}{2qV}} \quad (1)$$

to travel a flight distance of L . A detector at the far end of L measures the arriving ions, creating a series of signal peaks spread out in time. Each peak corresponds to a population of ions with an arrival time dependent upon that population's charge-to-mass ratio. From this charge-to-mass ratio, the elemental and molecular compositions of the mass peaks can be deduced.

Two of the key metrics of a time-of-flight mass spectrometer are its mass sensitivity and its mass resolution. The mass sensitivity can be quantified as the rate of change in arrival time of the ions with respect to the ion mass. An instrument with a higher mass sensitivity would have a greater time difference between the arrival of populations of adjacent, similar-mass ions, and thus would make it easier for the on-board electronics to differentiate between these populations. The sensitivity can be calculated as

$$\frac{\partial t}{\partial m} = \frac{L}{\sqrt{8mqV}} \quad (2)$$

Note that the mass sensitivity is directly proportional to the flight distance. This fact indicates an inherent limit of traditional time-of-flight mass spectrometers designed as a single, monolithic instrument for integration onboard a spacecraft; the flight distance of the spectrometer, and therefore

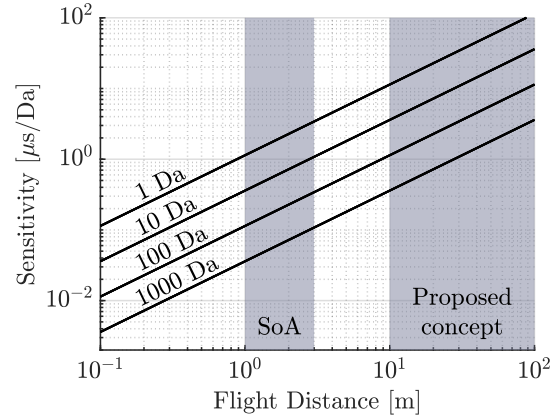


Figure 3. Comparison of time-of-flight mass sensitivity between the proposed concept and state-of-the-art (SoA).

its mass sensitivity, is constrained by the form factor of the spacecraft. Fig. 3 shows the potential increase in sensitivity from an ultra-long baseline TOF-MS system compared to current state-of-the-art ice-phase mass spectrometers (which are discussed further below).

A related metric is the mass resolution, defined as

$$\frac{m}{\Delta m} = \frac{t}{2\Delta t}, \quad (3)$$

where Δm is the difference in mass for two adjacent ion populations and Δt is a measure of the ion spread of a population as measured by the detector (and thus Δt is complex and contains information about the methods of ionization and acceleration, detector electronics response, initial kinetic energy spread in the ion population, etc.), often taken as the full-width-at-half-maximum of a given mass line. Substituting Eqn. 1, it can be seen that the mass resolution is simply the mass sensitivity multiplied by $\frac{m}{\Delta t}$, and thus it is also linearly dependent upon the flight distance.

Thus we propose to separate the mass spectrometer into two spacecraft: a source spacecraft and a disconnected, free-flying detector spacecraft. A diagram of the proposed concept is shown in Figure 1. A source spacecraft, which houses the sample to be analyzed and an ion source, emits a pulsed ion beam at a free-flying detector spacecraft. Based on the travel time of the ions from the source spacecraft to the detector spacecraft, the mass spectrum can be determined. Since the source and detector spacecraft are no longer physically attached, the flight distance—or baseline—can be made significantly longer than traditional time-of-flight architectures. Initial predictions estimate an increase in sensitivity by an order of magnitude or more as shown in Figure 3. Compared to current state-of-the-art ice-phase spectrometers such as SUDA, the mass resolution may be improved by over an order of magnitude shown for most masses.

There are a number of representative examples for the state-of-the-art for TOF-MS systems, both for terrestrial applications and for spacecraft applications. A comparison of several of them illustrates the great lengths that instrumentation goes to to solve mass resolution problems and demonstrates the potential benefits of an ultra-long baseline TOF-MS system. Fig. 4 shows the mass resolutions of the Europa Clipper's SUDA instrument [35], the Rosetta ROSINA's two methods of TOF-MS [2], and a terrestrial MS system that utilizes a

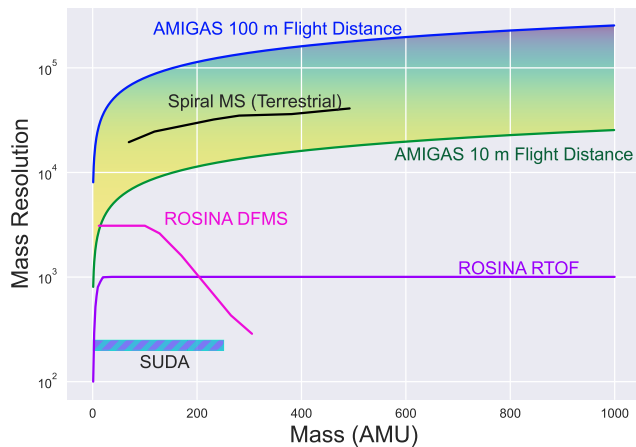


Figure 4. A comparison of the mass resolutions of various TOF-MS systems and the potential resolutions offered by AMIGAS. While the upper bound, provided with a flight distance of 100 m, may not be feasible in actual operation, even the lower bound with a 10 m flight distance provides a significant boost in mass resolution compared to the current state-of-the-art ice-phase mass spectrometers, such as SUDA. It also provides significant gains over gas-phase spectrometers, such as ROSINA in both its modes of operation. These ranges assume a $\Delta t = 10$ ns and an accelerating potential of 2 kV.

unique, spiral ion trajectory to create a long flight distance [36]. We also briefly consider the highly advanced MASPEX instrument, although its complicated design and multiple mass range operations [1] precludes simple plotting of its mass resolution on Fig. 4. The figure also shows a range of potential AMIGAS mass resolutions, ranging from a flight distance of 10 to 100 meters, although it should be noted that the potential challenges to the AMIGAS concept, discussed in Section 4, will likely restrict operation far below this upper bound. The estimates shown here assume a $\Delta t = 10$ ns and an accelerating potential of 2 kV.

The SUDA instrument is a reflectron time-of-flight mass spectrometer (RTOF-MS) on the upcoming Europa Clipper mission [35]. While SUDA can trace its lineage to the CDA instrument that studied the Saturn system [3], it is a highly advanced TOF-MS with vastly superior capabilities, such as its ability to map dust populations to surface features [37] despite its small form factor, measuring just 26.8x25x17.1 cm. However, because it utilizes an RTOF configuration, where the beam is reflected on a parabolic arc inside the instrument volume, the flight distance can significantly exceed the largest dimension. This enables SUDA to achieve a mass resolution of $\frac{m}{\Delta m} = 200-250$ over the mass range 1 – 250 AMU [35], making it among the most capable ice-phase mass spectrometers available. Its mass resolution is shown with a striped box in Fig. 4.

The Rosetta spacecraft’s ROSINA is a gas-phase MS instrument that measured the D/H ratio of volatiles from comet 67/P [27]. The ROSINA features an RTOF-MS instrument with an overall volume of 0.104 m³ with the largest dimension, by far, being its length at 114 cm [2]. With such scale, RTOF configurations can, in principle, create flight distances of perhaps a few meters. The system also features a double focusing mass spectrometer (DFMS), where the intrinsic spread in initial ion velocity is reduced by focusing

fields in flight. This has the result of decreasing the Δt term in Eqn. 3, and thus it increases the mass resolution by ensuring that ions with a single m/z value arrive closer together and are thus easier to distinguish from adjacent mass lines. However, this DFMS is only designed to operate over a small mass range (specifically 12-150 AMU) because of the difficulty of manipulating the full spectrum of ion populations with significantly different m/z values. The ROSINA RTOF-MS mass resolution is shown in Fig. 4 with a purple line, while the DFMS mass resolution is shown with a pink line.

Sato et al. describe a TOF-MS system that forces ions to ride a spiral or corkscrew path towards its detector [36]. This flight path was used to eliminate low mass ion ‘lapping’ of high mass ions. If ions are made to fly in a circular or otherwise looping trap, the faster, lower mass ions will eventually overtake the higher mass ions from behind. Thus, when the ions are released into the detector, they will likely not arrive in the order of m/z values and may overlap with one another. The spiral flight path eliminates this lapping problem to create a flight distance of approximately 20 meters, wherein a mass resolution of 20,000 or better was achieved over the mass range of $75 < m/z < 500$. This spiral mass spectrometer is shown in Fig. 4 with a black line.

Finally, the MASPEX instrument is a highly advanced, multi-bounce spectrometer. This system takes a plume of ions and bounces them back and forth between two opposing electrostatic reflectrons numerous times to create a TOF-MS system with an ultimate flight distance many times greater than its largest dimension [1]. By artificially increasing the flight distance in this manner, a tremendous leap in mass sensitivity and resolution for space-borne instruments can be achieved, reaching nearly 25,000 for some masses. However, such an instrument is necessarily highly complex, and the observable mass range decreases as the number of bounces increases (that is, the extremely high mass resolution enabled by the multi-bounce method applies only to a small mass range). Because of the ‘lapping’ problem, sample analysis must be broken down into numerous small mass ranges (called ‘regions of interest’) with different instrument operation parameters (called ‘Science Operation Methods’) and vastly different mass resolutions. Because of the complexity of the design, the instrument suffered numerous cost and schedule overruns. These problems were so significant that the instrument was considered for cancellation, but eventually allowed to proceed with a change to the instrument’s risk classification (From Class “B” to Class “D”, indicating acceptance of higher risk to the instrument’s goals) and a modification of the Level 1 science objectives of the entire Europa Clipper mission to facilitate this change. Given the complexity of the instrument and its revolutionary leap in mass resolution for spacecraft instrumentation, these complications are not surprising, but they nonetheless indicate that alternative, less complicated methods of increasing the mass resolution may be ideal.

4. CHALLENGES

This long-baseline time-of-flight concept has the potential to dramatically improve the capabilities of in-space mass spectrometry and could provide the required sensitivity for the scientific studies of Section 2. However, there are many challenges that need to be addressed in order to assess the feasibility of the long-baseline concept. First, the impact of the relative position control and estimation precision and accuracy on the ability to determine a mass spectrum must be analyzed; since the source and detector spacecraft are

no longer physically attached, the resolution of the resulting mass spectrum is dependent on the performance of the relative position control and estimation architecture. Second, methods for sufficiently focusing the ion beam over the proposed long baselines in order to generate a time-of-flight signal need to be explored. Finally, the impact of the ambient environment on the ion beam and resulting mass spectrum needs to be quantified.

Due to the statistical spread of ions in a given population from the initial temperature of the ion packet, ions will spread out in time as they travel towards the detector. For an ultra-long baseline TOF-MS such as AMIGAS, this problem becomes more acute because the longer flight time allows for greater spread. This has the effect of increasing the Δt term in Eqn. 3, thus negating some of the advantage of the ultra-long baseline. This spreading out effect also produces a mass peak that is lower in amplitude but more spread out in time. Thus, even as the mass line preserves its integral, it becomes more difficult to measure against background noise. While this is a problem in TOF-MS systems that artificially increase flight distance (e.g., by multi-bounce or spiral TOF-MS), those systems are able to have a set of ion optics that can refocus ion packets during flight. It may be possible to mitigate this spread by adding a focusing element to the detector spacecraft (or perhaps on both spacecraft), but this will increase the system complexity and the cost of the spacecraft. While there are potential solutions that need to be explored, the spread is a significant hurdle that needs to be studied. The merits of various ionization strategies will be explored in future work.

This problem is exacerbated by another challenge for the AMIGAS spacecraft, which is the effect of ambient plasma on the noise levels. While the intrinsic spread due to temperature means ion packets will spread out in time as they travel towards the detector spacecraft, they will also spread out perpendicularly. Thus, the detector must have a larger surface area than is typical for TOF-MS systems to collect the spread out ion packet. Unlike traditional MS systems, where the detector is encased, the detector on the receiver spacecraft must be exposed to space. This will increase the amount of stray ions from ambient plasma that may reach the detector, thus increasing the noise floor for the electronics. While a shroud or some other simple spacecraft geometry may be used to reduce this effect (or again, perhaps with a focusing element on the receiver spacecraft), it remains a significant challenge to overcome.

This paper has also deliberately avoided mentioning the specific mode of ionization and acceleration for the sample molecules. This is because, in its present form, the AMIGAS concept is somewhat agnostic to the ionization source given that current studies focus on the spacecraft dynamics. However, the choice of an ionization source directly affects the Δt ion spread, and thus has important implications for the overall mass resolution of the instrument.

While these challenges are not trivial, they are challenges that certainly align with those that have been solved in many terrestrial TOF-MS systems (and indeed, solutions such as these are part of the reason why there is a great variety of mass spectrometer architectures). Future work will thus determine how these challenges can be best mitigated, both through adaptation of terrestrial techniques and development of new techniques that may exploit the unique features of the ultra-long baseline tandem spacecraft mass spectrometer system.

5. PRELIMINARY ANALYSIS

Initial analyses were focused on the propulsive cost and stability of maintaining a desired baseline distance between a source and detector spacecraft. As an example scenario, control of the detector spacecraft relative to the source spacecraft was conducted in the Clohessy-Wiltshire frame where the source spacecraft was assumed to be in a 400 km altitude circular orbit around Earth. The detector spacecraft is assumed to have an onboard propulsion system with a minimum thrust of 10 mN, representative of a cold-gas propulsion system, capable of producing thrust in all three axes of the Clohessy-Wiltshire frame independently. Changes to the thrust value were assumed to occur every 0.5 seconds, effectively giving the propulsion system a minimum impulse bit of 5 mNs. This scenario is intended to assess the initial feasibility of the long-baseline mass spectrometer concept while being extendable to intended scientific missions.

The position controller for the detector spacecraft was designed assuming perfect state (position and velocity) knowledge and using an infinite-horizon, discrete-time linear-quadratic regulator. No feed forward control was considered, and the position of the detector spacecraft is controlled purely using proportional-derivative feedback control. The weighting matrices for the linear-quadratic regulator will impact the controller performance, but were chosen arbitrarily here for preliminary analysis. Given the feedback control gain, K , from the linear-quadratic regulator, the desired control input at any time step is calculated according to

$$\vec{u}_d = -K(\vec{s} - \vec{s}_{\text{ref}}) \quad (4)$$

where \vec{s} is the current state vector of the detector spacecraft containing its relative position and velocity with respect to the source spacecraft in the Clohessy-Wiltshire frame and \vec{s}_{ref} is the desired reference state. In all cases the reference state has zero velocity and represents a desired position offset of the detector spacecraft. To account for the minimum thrust output of the propulsion system, the control vector is saturated on a component-by-component basis

$$u_i = \begin{cases} 0 & u_{d,i} < F_{\text{min}} \\ u_{d,i} & u_{d,i} \geq F_{\text{min}} \end{cases} \quad (5)$$

where u_i and $u_{d,i}$ represent the i^{th} component of the actual and desired control vector respectively. Note that a maximum control output is not discussed here as the controller spends almost all of the simulation time near the minimum thrust criterion—a maximum thrust value would have negligible impact on the regulator's performance.

Due to the minimum thrust of the propulsion system, the detector spacecraft will not be able to maintain a fixed reference point and will instead oscillate about or near the desired reference point in a deadband-like behavior. This behavior means that there will always be a propulsive cost of maintaining a desired relative position of the detector spacecraft with respect to the source spacecraft, even if there is no relative acceleration acting on the detector spacecraft. In addition, there will exist some error in the actual baseline between the source and detector spacecraft relative to the desired baseline. As part of this preliminary analysis there were two metrics of interest. The first is the propulsive, Δv , cost of maintaining a desired position offset between the source and detector spacecraft. The second is the error in the baseline between the source and detector spacecraft relative to the desired baseline.

Both metrics were assessed in a simulation environment for different directions of the position offset between the source and detector spacecraft. For a desired baseline distance of L , the reference position is defined as

$$\vec{r}_{\text{ref}} = L \begin{bmatrix} \sin \phi \cos \theta \\ \sin \phi \sin \theta \\ \cos \phi \end{bmatrix} \quad (6)$$

where ϕ is a polar angle referenced to the cross-track direction and θ represents angular displacement in the radial-along-track plane referenced to the radial direction. If $\phi = 0$ then the detector spacecraft is displaced from the source spacecraft by a distance of L in the cross-track direction. If $\phi = \pi/2$ and $\theta = \pi/2$ then the detector spacecraft is displaced from the source spacecraft by a distance of L in the along-track direction. In the analysis presented here, $L = 100$ m unless otherwise specified.

Figure 5 shows the resulting Δv cost for different ϕ and θ in polar coordinates. For the polar plot, ϕ is the radial coordinate and θ is the angular coordinate such that the cross-track direction is the axis directed out of the page. The positive radial and along-track directions are indicated on each plot. Due to symmetry only $\phi \in [0, \pi/2]$ are shown here and symmetric results to Figure 5 exist for $\phi \in [\pi/2, \pi]$. As can be seen, the propulsive Δv cost is quite low with typical costs of approximately 1 m/s per hour that the detector spacecraft is displaced from the source spacecraft. As expected, the Δv cost is minimized in the along-track direction—where the relative acceleration between the source and detector spacecraft are minimized—with a cost of approximately 0.03 m/s per hour. Such Δv costs are well within the realm of feasibility for a simple cold-gas propulsion system onboard a small CubeSat-like spacecraft. While these costs would change with different controller designs and mission scenarios, it is expected that the feasibility of maintaining the relative position displacement between the source and detector spacecraft would not be nullified.

Also shown in Figure 5 is the root mean square error in the baseline between the source and detector spacecraft. Typical baseline errors are around 0.5 m, but would depend significantly on the controller design and propulsion system minimum thrust value. Unlike the propulsive cost, the baseline error is not minimized in the along-track direction, and instead has a minimum value of approximately 0.01 m for $\phi = \pi/4$ and $\theta = 0, \pi$. While error in the baseline does not strictly impact the performance of the long-baseline time-of-flight mass spectrometry concept, it may become relevant when defining requirements for the minimum resolution that the mass spectrometer needs to achieve; if the error in the baseline is of a similar order of magnitude to the desired baseline, then notable deviations in the resolution of the mass spectrometer from what is desired may exist. However, the more relevant metric for influencing the resolution of the mass spectrometer will be uncertainty in the knowledge of the baseline. Uncertainty in the baseline knowledge will be driven by the onboard estimation of the relative position of the detector spacecraft with respect to the source spacecraft, and will be explored in future analyses. What this preliminary analysis shows is that there may exist a tradeoff between propulsive cost and error in the source-detector baseline.

6. CONCLUSION

While there are significant technical hurdles to be overcome to bring the AMIGAS instrument concept to life, the potential

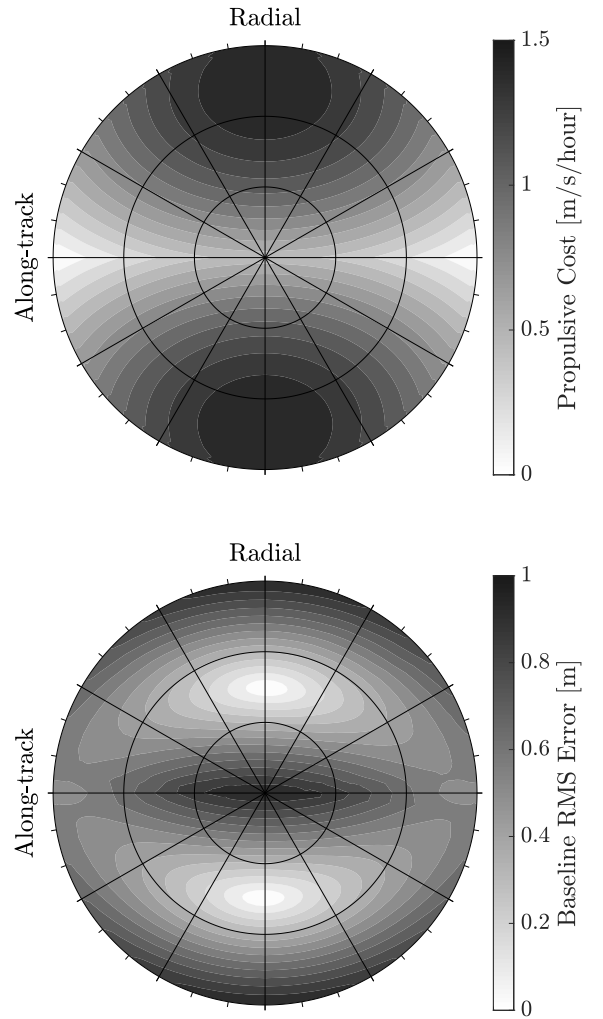


Figure 5. Propulsive Δv cost over time in order to maintain the relative separation between the source and detector spacecraft (top) and root mean squared error in the baseline (bottom) for different displacement directions of the detector spacecraft relative to the source spacecraft.

leap in mass resolution that such a platform offers warrants further study. By splitting the ionization and detection elements of a TOF-MS system across two spacecraft, an ultra-long baseline time-of-flight mass spectrometer can be created, boosting mass resolution beyond what is capable with a single spacecraft form factor. This simple method of increasing mass resolution may allow for new measurements of isotopic ratios or other difficult-to-resolve ambiguities in present time-of-flight mass spectrometer datasets, whether for ice-phase water dust grains or a number of other potential targets. Future work will determine how ion packet spread can be mitigated across the long flight distance and how increased noise floors resulting from the open nature and large size of the detector can be reduced or eliminated. Potential solutions will consider both analogy to how similar problems have been solved in terrestrial, laboratory mass spectrometers as well as through the development of new techniques that may be possible only in space and only with the unique AMIGAS tandem spacecraft architecture.

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