Adamantane Characterization Through Fragmentation Analysis for Plasma Propulsion Applications

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This paper characterizes adamantane's fragmentation rates, cross sections, and mass spectra using QCxMS2, a computational chemistry simulation program. The analysis of adamantane fragmentation provides an improved understanding of adamantane plasma characteristics and how this molecule interacts with other atoms. This new data, including sublimation and reaction rates, is used as input parameters into Starfish, a rarefied gas code simulating the flow of adamantane plasma in a simple thruster. These simulations calculate key propulsion parameters, including thrust, exit velocity, and specific impulse, with adamantane serving as the solid propellant. With a better characterization of adamantane's thrust and flow, its performance in plasma thrusters can be more accurately modeled and assessed. Such simulations help to gauge adamantane's viability as an alternative fuel source in plasma propulsion applications.

Nomenclature

v	=	velocity of particle
n	=	number density of target particle
$\dot{m}$	=	mass flow rate
j_{mm}	=	mass flux in particles
j_{mp}	=	mass flux in kg
F	=	thrust
V_e	=	particle exit velocity
I_{sp}	=	specific impulse
n_{adm}	=	plasma density
A_T	=	area of orifice
g	=	gravitational constant
M	=	molar mass of adamantane
N_A	=	Avogadro's constant

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I. Introduction

There is a great need for propulsion systems that are compact, small, and low-powered for nanosatellites. Current propulsion systems on CubeSats are limited mainly to chemical propulsion systems and proof-of-concept electric propulsion systems. Electrical propulsion systems utilizing cryogenic gases such as xenon or argon require bulky pressurized tanks, heavy-duty heaters, and complex feed systems, which require more space and power to be available to small-scale spacecraft. Furthermore, these propellants are rare, nonrenewable, and expensive, so less expensive propellants are necessary [1]. An alternative to gaseous propellants is solid propellants, which allow for more compact feed systems with a higher delta-V-to-volume ratio for greater thruster efficiency. However, a challenge with solid propellants is that they must first be sublimated to be used as a propellant [2]. The primary solid propellant in current consideration is iodine, but it has drawbacks, such as reacting with other components in the thruster [3]. Another category of interest in the solid propellant field is diamondoids, a type of hydrocarbon with a unique crystal lattice structure that allows it to sublimate readily.

The Advanced Spacecraft Propulsion and Energy (ASPEN) Laboratory at the University of Southern has developed a small ion thruster to explore the use of adamantane as a propellant. The adamantane-fueled thruster that ASPEN has developed operates in single-use mode to provide high specific impulse while also meeting the low power and mass requirements needed to operate. Adamantane was selected as a potential propellant due to how it readily sublimates under vacuum, is easily ionized, does not require a catalyst, and has a high mass-to-volume ratio. Adamantane can easily be loaded into a propellant chamber without need for gas lines; thus, its application eliminates the need for a complex propulsion system. Furthermore, adamantane is relatively inexpensive and originates from petroleum, meaning it is much more accessible than xenon or other commonly used propellants. These properties make adamantane favorable as a propellent for its ability to be packed into a propellant chamber without the need for heaters to achieve sublimation.

Previously, ASPEN conducted parametric studies of discharge plasma dynamics within Starfish, a two-dimensional open-source general-purpose plasma and rarefied gas code [4]. Simulations of various thruster shapes were conducted to decide upon an optimal internal geometry. Starfish requires reaction rate estimations and cross section data to accurately model the formation of material species. However, for adamantane, these values do not exist readily in literature or are limited in scope. To more accurately model the thruster efficiency, a better characterization of adamantane's fragmentation processes is necessary, which leads to the goal of acquiring mass spectrometry data.

Thus, this paper presents computational chemistry simulations using QCxMS2 to model the mass spectrometry of adamantane to determine the most likely fragmentation products, which come with associated reaction rates as a function of time and temperature. These fragmentation reactions can then be inputted into Starfish so that the program has an accurate understanding of adamantane's behavior. By running simulations in Starfish, simulated thrust data using a simple thruster geometry can be obtained, thus helping to gain a better picture of how adamantane behaves as a solid propellant. These simulations will contribute to characterizing the molecule as a whole and guide system requirements for a thruster using adamantane as its fuel source.

II. Simulation Goals

Early simulations within Starfish relied on preliminary assumptions for key cross section values, leading to thrust values that did not accurately reflect adamantane as a propellant. Previous literature lacks a deep understanding of adamantane's fragmentation behavior, necessitating an investigation into accurate reaction rates, cross section data, and resulting fragmentation species. The ASPEN lab initially measured thrust experimentally on a thrust stand but found that the values differed by three orders of magnitude when compared to the values calculated by preliminary simulations. These experimental observations demonstrated the necessity of characterizing adamantane more fully [5].

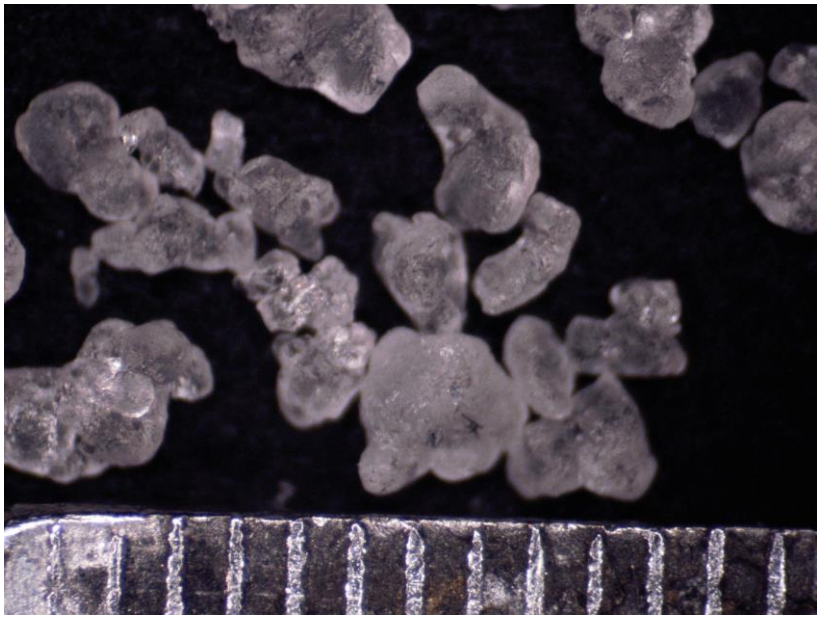


Figure 1. Adamantane grains. Ruler ticks are 1/100th inch.

Preliminary simulations were conducted in LAMMPS with ReaxFF [6]. The assumption was that this program could model the collisions that adamantane experiences under high energy. However, using two different simulation codes together, LAMMPS and ReaxFF, proved to be difficult and not easily compatible. Additionally, this method did not employ crucial chemical reactions which are necessary to model fragmentation pathways in Starfish. One of the key factors used to determine how a molecule ionizes is the fragmentation path that the particle will take. As adamantane ionizes, the electrons bombarding it fracture the structure into smaller hydrocarbon fragments that in turn will also ionize. Adamantane undergoes its first fragmentation at 9.25 eV [7]. It continues to fragment and lose carbon and hydrogen as it goes, but as the carbon chain gets smaller it becomes harder to predict experimentally.

QCxMS2, which will be discussed in detail later, was selected due to its ability to accurately simulate adamantane fragmentation and generate mass spectroscopy data. The data collected from this program fulfills the input requirements Starfish needs to complete adamantane simulations. Therefore, the goal is now to simulate fragments that adamantane ionizes. Instead of using simple electrons in previous iterations of the Starfish code, chemical reactions and fragmentation pathways will give a more accurate idea for how the molecules are breaking up and swapping electrons, which can provide more accurate Starfish results.

III. Computational Chemistry Simulation using QCxMS2

A. QCxMS2 Background and Justification for Use

QCxMS2, developed by the quantum chemistry specialized Grimme group of University of Bonn, is a program that simulates the fragmentation of molecules using automated reaction network discovery, which predicts the chemical reactions possible within a system [8, 9].

This program was chosen to simulate adamantane fragmentation since it provides information about the abundance of each adamantane ion at a specific mass-to-charge ratio. QCxMS2 gives the ability to characterize fragmentation data without the limitations of physical trials to better understand the adamantane propellant that will be used in the thruster. In physical testing, mass spectrometers typically can only operate from 60–120 eV, while ASPEN's physical thruster operates at 0.8–1.2 keV. Additionally, small carbon molecules such as methyl and ethyl groups are so small and unstable, resulting in them often going undetected in physical mass spectrometers. A benefit of the simulation is that it can accurately measure these groups since there are no detection limitations.

QCxMS2 finds the most likely fragment and the path of lowest energy in which the starting molecule will fragment to create it. Starting with the input molecule, QCxMS2 will create possible fragments with the MSREACT mode of CREST, a quantum chemistry package [10]. Every possible fragment is initially generated at this step, but only fragments with a barrier height that does not exceed three times the fragmentation energy is used in later steps. Outside of that range, the fragments are unlikely to occur and would increase the computation time. Once the fragments are created and sorted by activation energy, MOLBAR identifies and removes duplicates to ensure proper likelihood of molecules forming to reduce redundant computation, based on matrices of atomic positions by taking into account non-central stereochemistry [11]. From physical testing, adamantane forms long carbon chains at the end of its ionization, so using a more robust molecular identifier for non-central stereochemistry provides more accurate data. Each potential reaction and fragmentation path is tested with ORCA, a quantum chemistry solver that searches and tests energy pathways. A minimum energy path search is performed by nudged-elastic band (NEB) in ORCA [12]. If NEB does not converge, then a different initial guess for the path is created by geodesic interpolation. This step works to optimize the reaction pathways to determine the minimum energy needed to reach the first transition state. Each fragment is assumed to be in a self-consistent field that assumes the electrons move in an average field with constant charge and distributes the charges equally across all fragments.

A rate constant is generated for each energy at every given temperature, and the rate constant is used to determine the reaction barriers for each temperature, which is in turn used to calculate the branching ratios. These branching ratios show the energy path of each fragment and how likely it is to break apart into smaller pieces. Each fragmentation step has its own intensity calculated and normalized to the intensity of the largest signal. The final intensity seen in the final spectrum for each fragment size will reflect the most likely fragment size, with isotope ratios considered for each new fragment that may have a slightly different mass.

B. Methodology

QCxMS2 utilizes the molecular coordinate file which contains the three-dimensional coordinates in angstroms for the 10 carbon and 16 hydrogen atoms in the adamantane molecule. The file's information is used to simulate fragmentation based on the locations of all the atoms in the mass spectrometer to predict collisions. The program operates the simulation at -29.2 Hartree, or -794.57 eV. The negative value signifies a stable molecular bond, and the magnitude of the energy is accurate to the molecular bond of adamantane. The selected gradient norm of the adamantane is set to 3.4×10^{4}. This small value indicates that the atoms are extremely close to their energy minimizing positions indicating an optimized geometry of the adamantane molecules in the simulation.

IV. Data Collection and Plasma Characterization

A. Data Processing Methodology

In the QCxMS2 simulation, every molecule is assigned a fixed charge of 1, since every species will have a fraction that is charged. Therefore, the mass per charge ratio (m/z) values can be interpreted as the mass of the molecule since *z* equals 1 for every molecule. QCxMS2 compiles each probable fragment formed with its relative intensity to create the mass spectrum graph below in Figure 2. The intensity of the peak represents the abundance of the ion relative to the base peak. Within QCxMS2, the base peak is set at 10000 for its relative intensity, rather than the typical 100 used in most other spectrums. By analyzing the largest peak, the C_9H_{12} molecule is found to be the base peak with a molecular weight of 120 g/mol. QCxMS2 outputs information on each fragment formed, with its molecular formula and relative intensity. By cross referencing the molecular formulas corresponding to individual fragments in the simulation and their relative intensities, the molecular formulas of the fragments can be found. The molecular ion peak represents the whole molecule, in this case adamantane, with one electron removed. This peak is found at 136 m/z, which corresponds to adamantane's molecular weight of 136 g/mol.

B. Results

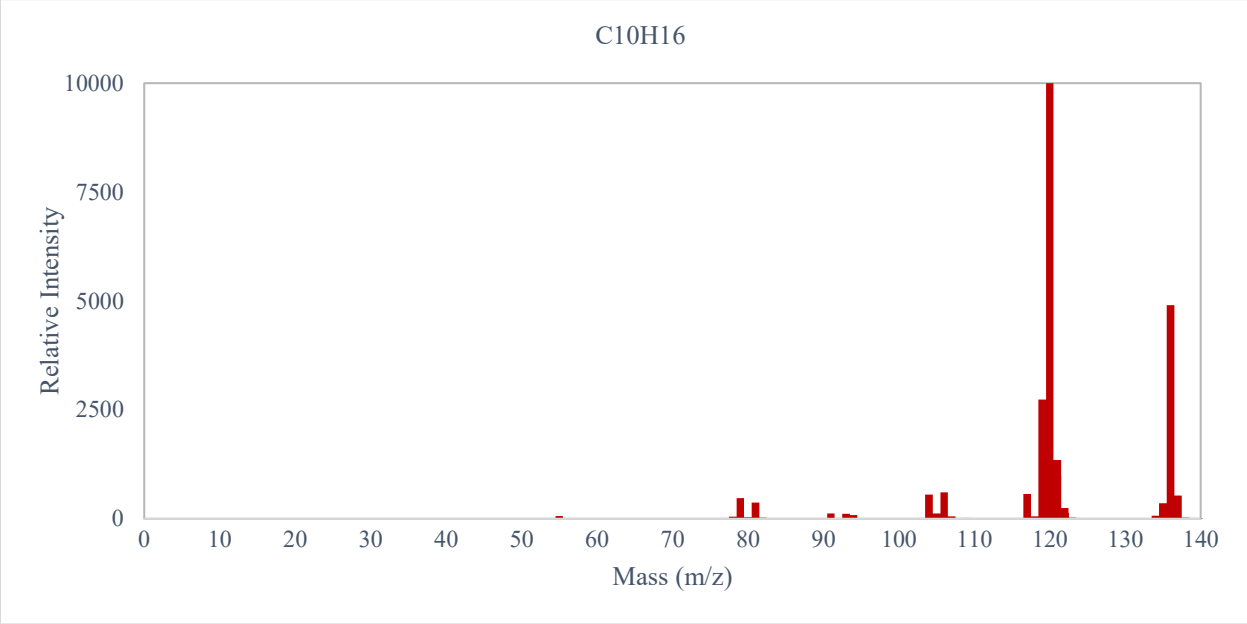


Figure 2. Mass spectrometer trial of adamantane at 790 eV.

After the base peak, by analyzing the difference in mass between the highest peaks, fragments corresponding to the loss of one carbon continue to break off the initial molecule. This is also supported by analyzing the molecular formulas QCxMS2 assigns to every fragment formed. Fragmentation is visible down to ethyl and methyl groups with one or two carbon atoms present in their structure. This is one of the benefits of using QCxMS2, as data for small fragments can accurately be obtained, which is typically not possible through physical testing.

Between 104 and 80 fragmentations there are very low intensities, which indicates the lack of a C_7 fragment. C_7 is less stable, and since adamantane has three fused cyclohexane rings, adamantane tends to break up into C_6 fragments since it has higher stability. This is why strong peaks at higher masses are common and there are small intensities in the C_7 region. In physical testing, the ASPEN laboratory observed long carbon chains formed at the end of thruster performance. Therefore, it is logical to have larger intensities for more massive hydrocarbons. At lower masses, especially past 55 m/z, low intensities of these fragments exist. Single carbons are not present due to the number of unpaired electrons which would be in the molecule which make it extremely energetically unfavorable.

Table 1. Adamantane fragmentations

m/z	136	121	105	80	55	41	30	16
Chemical Formula	$C_{10}H_{16}$	C_9H_{12}	C_8H_9	C_6H_8	C_4H_6	C_3H_5	C_2H_7	C_1H_4

V. Interpretation and Application

A. Starfish Background

Starfish, a two-dimensional open-source general-purpose plasma and rarefied gas code, was used to simulate thrust values in previous ASPEN simulations. This program generates neutral adamantane molecules in the propellant tank (shown in Figure 4) and their dispersion dynamics over multiple time steps, utilizing the Electrostatic Particle-in-Cell (ES-PIC) method and Monte Carlo Collisions (MCC) method for ionization modeling [13]. The results of these simulations are displayed in Paraview, an open-source post-processing visualization software.

Starfish does not include reaction rates for adamantane; thus, they need to be supplied via the QCxMS2 simulations. In Starfish, cross section data is used to analyze the probability of certain molecules forming. At different energy levels, certain molecules are more likely to form, so when simulating plasma, the energy in the simulation controls the molecules at the current time-step in the simulation. To determine the probabilities of adamantane fragments, QCxMS2 was used to simulate adamantane mass spectrometer trials at high energy levels. The results were used to scale the cross-sectional data from uncharged adamantane and update adamantane fragmentation information.

The electrostatic particle-in-cell method simulates computational particles using the Lorentz force instead of directly calculating Coulomb's force [14]. This model is designed so that plasma can be modeled as macroparticles, representing random samples of the velocity distribution function. To reduce calculation time and simplify the formulas, it is assumed that due to the low-density plasma, the particles generate a very low current, and the generated magnetic field can be neglected. ES-PIC also assumes that the macroparticles follow the Boltzmann relationship. The main purpose of this simulation is to generate data for thruster plumes.

Particle collisions are modeled with Monte Carlo Collisions [15]. This simulation is primarily designed for thruster plumes where the target density is significantly larger than the source particle density. Under this condition, it becomes possible to model the target as a cloud. In a very similar manner to ES-PIC, the MCC requires the assumption that no interior magnetic field is produced. To run the actual simulation each source particle is tested for probability collision and the action continues from there if a collision is likely. The model runs and generates a fixed electric field that provides charge exchange collisions.

To run a Starfish simulation, commands entered directly into the terminal to generate neutral, positively charged, and negatively charged adamantane particles over a maximum of 10,000 time-steps. To perform calculations within Starfish, the adamantane tank and ionization chamber were composed of a mesh which was split into cells with areas of 10^{-4} x10^{-4} m^2 (see Figure 3). In each mesh cell, calculations were performed from Starfish particle data to find the average particle density and mean velocity in each mesh cell. The particle density was used for thrust and specific impulse calculations. Then, a calculator in Paraview was used to calculate mass flux across the exit orifice. A symbolic equation for mass flux was created by multiplying the particle density of charged molecules by their exit velocity at the orifice. To calculate the mass flux at the exit of the thruster, a vertical slice was created at the orifice, extending from bottom of the model to the top and with its vertical coordinate aligned with the thruster opening. Next, a clip was added onto the slice, which was positioned at the top of the orifice to only gather data at the opening of the orifice. For the mass flux calculator data, its variables were integrated to find the total mass flux at the whole orifice area rather than as a set of points for each mesh area. The calculator function in Starfish is particularly useful in finding other key values such as mass flow rate, thrust, and specific impulse. By creating multiple calculators at the orifice slice, inputting the respective equations, and either integrating variables to find singular values for the orifice area or opening a spreadsheet view of the clip, values for each mesh segment of the orifice can be pinpointed. This maintains the consistency of the data between models and ensures that results are driven by the base values provided by Starfish of plasma density and horizontal velocity.

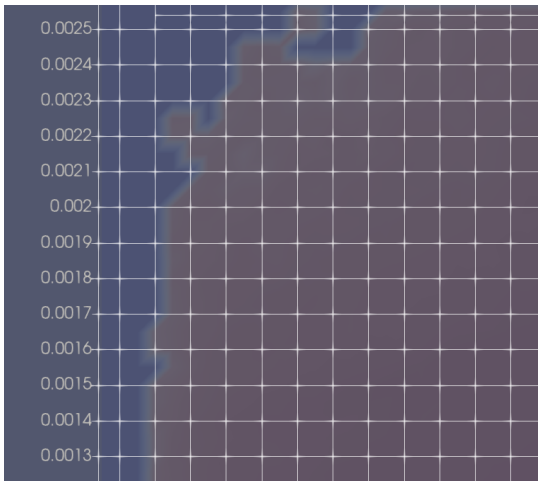


Figure 3. 10^{-4} x 10^{-4} m^2 mesh grid used in Starfish.

B. Starfish Usage

To improve Starfish's accuracy when handling adamantane, the mass spectrum data was inputted by adding in chemical reactions to model the fragmentation of the hydrocarbon. The first five chemical equations below were modeled in Starfish. Since the percentage of charged species in the mass spectra is not known, the assumption is made that an equal probability of both charged and uncharged products form in all chemical equations used. In reality, the probabilities of the charged and uncharged molecules forming are not the same, but determining the exact probabilities would require further data processing. The probability is based on the cross-sectional area of different molecules in the simulation based on the energy level in eV. At different energy levels, molecules will have different average cross-sectional areas, which determine the likelihood of molecules colliding and fragmenting further. Larger cross sections indicate a higher area for collisions to occur which leads to more interactions. The cross-sectional data for adamantane at various energy levels is averaged in the Starfish code to calculate a single value [15]. This average value is then scaled using the normalized intensities from the mass spectrum. Since C_9H_{12} has a larger relative intensity relative to adamantane, its cross-sectional area is multiplied by the ratio of C_9H_{12} relative to adamantane to determine the predicted cross-sectional area of C_9H_{12}.

Table 2. Adamantane fragmentation products and probabilities

Equation	Fragmentation Reactions	Cross Section (m^2)
I	$C_{10}H_{16} + e^- \rightarrow C_{10}H_{16}^+ + 2e^-$	2.7E-19
II	$C_{10}H_{16} + e^- \rightarrow C_9H_{12}^+ + CH_4 + 2e^-$	4.6E-19
III	$C_{10}H_{16} + e^- \rightarrow C_9H_{12} + CH_4^+ + 2e^-$	4.6E-19
IV	$C_9H_{12} + e^- \rightarrow C_8H_9^+ + CH_3 + 2e^-$	7.8E-20
V	$C_9H_{12} + e^- \rightarrow C_8H_9 + CH_3^+ + 2e^-$	7.8E-20
VI	$C_8H_9 + e^- \rightarrow C_6H_8 + C_2H^+ + 2e^-$	8.6E-20
VII	$C_8H_9 + e^- \rightarrow C_6H_8^+ + C_2H + 2e^-$	8.6E-20

New molecules for the chemical reactions were defined with their molecular weight and charge. A scaling factor was used to define how many particles would be present in each simulation particle, to decrease the number of particles for more efficient simulation processing by diving the total particle amount by 2000. Updated boundary files were used to gather measurements for the simulated thruster geometries, which is the same as the physical thruster being studied (Figure 4). The reaction rate used in the simulation is k[n.reactant1][n.reactant2], so the updated number densities of the two reactants based on the fragmentation probability scaling has allowed for more accurate reaction rates.

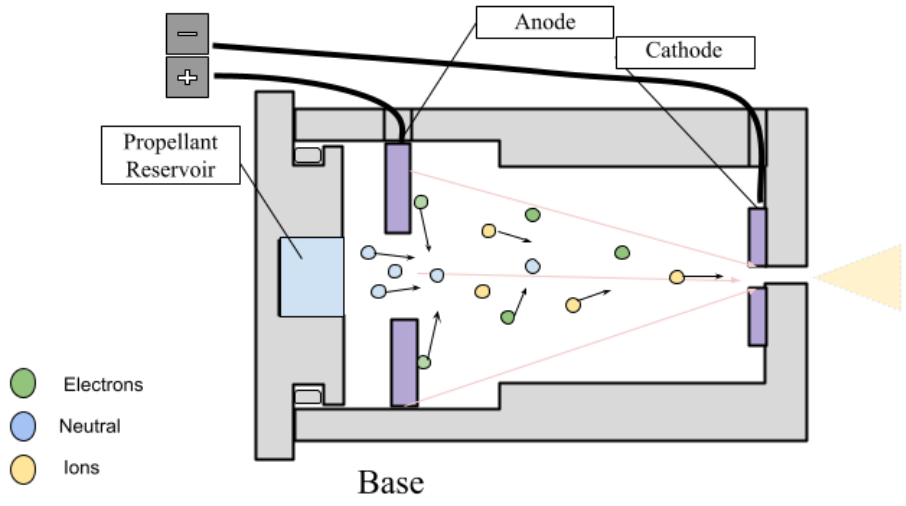


Figure 4. Representation of physical base thruster geometry used in experimental data collection and in simulations.

Higher intensities for molecules with larger masses in the simulation correspond to results from physical testing in which large carbon chains are formed at the end of the ionization process. When analyzing the mass spectrum results, the intensities can be used to scale average cross section values. The uncharged adamantane average cross section is known, so the normalized data from the QCxMS2 simulation is used to get the ratios between the adamantane intensity relative to other peaks in the mass spectrum. By using these ratios, the cross-section data for the fragments formed can be scaled with the cross section of adamantane, to determine the collision probability of each molecule.

Inputting the first three fragments with the largest relative intensity peaks into Starfish and modeling their chemical reactions, Starfish can more accurately model the size and charge of the molecules colliding within the boundary. The probability of charged molecules formed from each fragmentation is assumed to be the same, so the same cross section is used for both the charged and uncharged products in Starfish. New material properties for each molecule are created by inputting the molecular weight and charge.

The mass flux calculation in particles divided by 1 m^2 s can be done in Paraview by making a *y-z* planar slice at the thruster orifice and clipping this slice to only measure values at the orifice. Then, values of plasma density and particle velocity in the *x* direction (generated by Starfish) can be inputted into the calculator function in Paraview to output mass flux. The following equation details the Paraview input for mass flux. Where there are square brackets, the 'species name' as defined in Starfish should be written in place for the species whose value is being calculated. For example, the calculator input for ionized adamantane would be: "nd.adm+" x "u.adm+_v.adm+".

$$j_{mp} = \frac{particles}{time}(area) = nd.[species] * u.[species]\_v.[species] \quad (1)$$

To calculate the mass flow rate, mass flux must be converted to kilograms over area per second. To do this, the original mass flux is multiplied by the molar mass of the species and divided by Avogadro's number [4].

$$j_{mm} = j_{mp} \cdot \frac{M}{N_A} \quad (2)$$

Mass flow rate can now be calculated by multiplying the converted mass flux by the circular orifice area. The radius of the orifice is 0.32 mm.

$$\dot{m} = j_{mm} \cdot A_T = j_{mm} \cdot \pi r^2 \quad (3)$$

To calculate the total thrust, mass flow rate is multiplied by the exit velocity at the orifice.

$$F = \dot{m} \cdot V_e \quad (4)$$

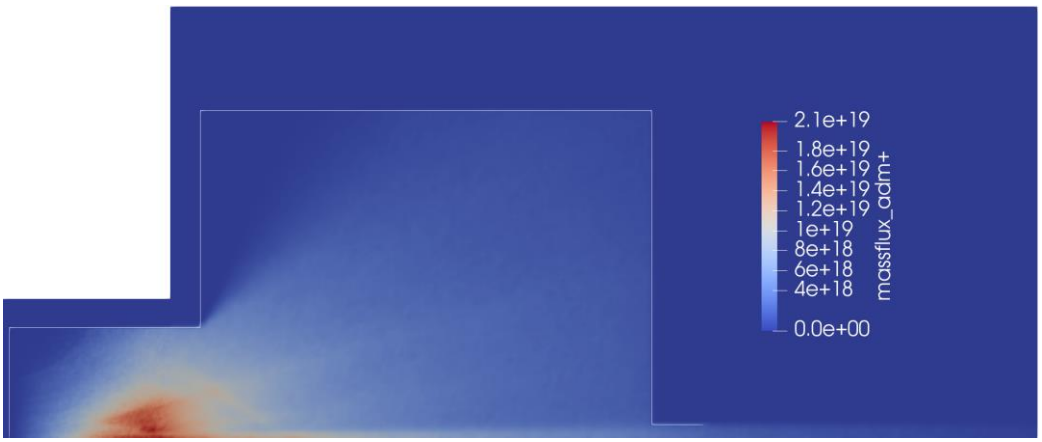
To calculate the specific impulse, thrust is divided by mass flow multiplied by gravity.

$$I_{sp} = \frac{F}{\dot{m}g} \quad (5)$$

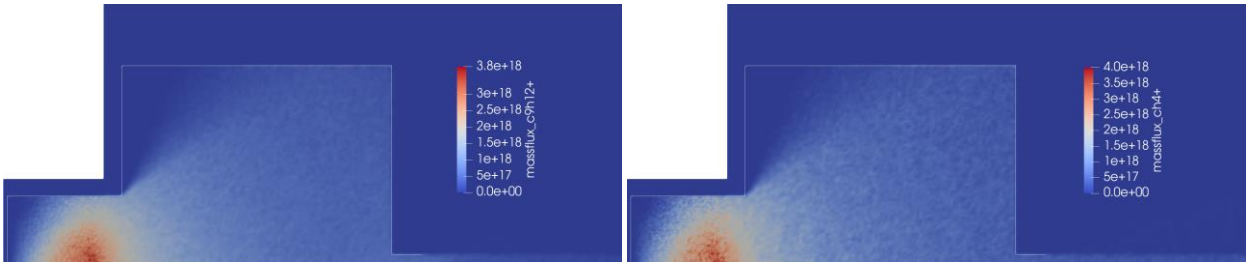
To gather thrust generation from all the molecules, plasma density and velocity had to be included within the input files so Starfish would output the plasma density and velocity of the now three ionized molecules in the thruster. Independent thrust calculations were performed for each species with the same methodologies, then added to calculate the thrust for the whole thruster.

Table 3. Properties for plasma and propellant flow from simulation of adamantane

Species	Plasma Density (n, particles / m^3)	Exit Velocity (V_e, m/s)	Thrust (F, N)	Specific Impulse (I_{sp}, s)
$C_{10}H_{16}^+$	1.08E+14	3.13E+04	7.66E-06	3.19E+03
$C_9H_{12}^+$	1.58E+13	3.35E+04	1.15E-06	3.41E+03
CH_4^+	4.44E+12	1.03E+05	3.96E-07	1.05E+04
Total			9.20E-06	3.32E+03



(a)



(b) **(c)**

Figure 5. Mass flux of ionized a) charged adamantane, b) $C_9H_{12}^+$, c) CH_4^+ at 6401 time steps.

After updating the Starfish simulations, the total thrust was found to be 9.2 μN which is the same order of magnitude as experimental results verified in a companion paper [16]. Previous Starfish simulations were outputting thrust values averaging 1.5 x 10^{-9} N because adamantane's fragmentation reactions were not modeled. By adding chemical reactions to create and simulate the first molecules adamantane fragments into, the increased chemical interactions exhibited larger thrust values [17]. Physical thrust stand data has been measured as 20 μN, so the increase from results on the order of 10 x 10^{-9} to 10 x 10^{-6} proves to be a significant improvement. A total specific impulse of 3320 seconds was calculated, which is comparable to the 2500–4000 seconds specific impulse range that is typical of ion thrusters [18]. This improvement in data accuracy allowed for more accurate plasma density and velocity values which thrust and specific impulse calculations are derived upon. The addition of charged species in the simulation allowed for more interactions, thus increasing accuracy during data processing.

It is important to note the assumptions made and possible sources of error in the calculations. Starfish is an ongoing and evolving code, meaning many properties of adamantane are assumed or simplified. In the code, the volume of adamantane is modeled as a fixed number of particles, and the shape of each particle is assumed to be perfectly cubic. However, the adamantane particles that the ASPEN lab uses are not one size and are not perfectly packed into the propellant chamber like how they are modeled in the simulation. With more computing power and time, further research could be done to address this incongruency within the code.

VI. Conclusion

The purpose of the ASPEN simulation team is to enhance and supplement experimental testing of an adamantane thruster. Initial starfish simulations with inaccurate assumptions of adamantane's behavior calculated thrust values that were off by a factor of a thousand. To make the simulation more accurate, adamantane's fragmentation pathway had to be updated to represent the real molecular interactions occurring. Accurate physical data for adamantane is

sparse and incomplete due to the high sublimation rate that makes it hard to characterize without interfering with physical instrumentation. To produce a more accurate fragmentation model, QCxMS2 was used to perform an accurate simulated mass spectrometer trial that demonstrated the most probable fragments adamantane creates. Adamantane's fragmentation reactions have made it possible to update the Starfish plasma simulations with more accurate chemical interactions to generate data closer to physical results. The thrust data from Starfish increased in accuracy by 1000x and is now within a factor of two from physical testing results. More accurate simulations have allowed for better understanding of the thruster operation and support of experimental data collection.

By updating adamantane's chemical interaction parameters in Starfish, it will be possible to quickly model iterations of the base thruster model. Future work in determining an optimal thruster design for maximum thrust and specific impulse will be supported by accurate simulations. The goal is to utilize the data from Starfish described in this work to determine the best internal thruster geometry and support its implementation on a CubeSat design.

The properties of adamantane require continued investigation for use as a propellant. Vapor pressure and additional fragmentation information would help determine its efficiency. Further study would have to be conducted to determine its viability as an alternative fuel source for electric propulsion applications. The addition of functional groups could alter its properties and open different applications; however, this transition may be beyond the scope of our laboratory at the undergraduate level.

Acknowledgments

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