

Electromagnetic Propulsion Using Non-Ionized Gases

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A parallel molecular dynamics code was developed to simulate ensembles of water molecules in the presence of electric and magnetic fields to demonstrate the Abraham force. The use of the Abraham force would allow for the exploration of a new method of electric rocket propulsion without the requirement to ionize the propellant. Perfect cube ensembles ranging from 8 to 1000 molecules were investigated to find the smallest size that gave favorable behavior across 10 different initializations with random 3D orientations and velocities based on a Maxwell-Boltzmann distribution. It was sought that no matter the initialization, the average normalized z-velocity profile when the electric field was present remained higher than the profile when the electric field was absent, successfully demonstrating the Abraham force. It was found that the 512-molecule ensemble was the smallest size to produce the desired velocity profile comparisons across all initializations. A normalized Δv of 31.2 m/s/pulse and an average normalized z-acceleration of 7.8×10^8 m/s² was achievable with an 85 kV/m sinusoidal electric field applied in the x-direction at a frequency of 250 MHz and a 2.5 T static magnetic field in the y-direction. For an assumed acceleration length of 20 cm, this would provide an I_{sp} of approximately 5700 s, far surpassing that of current Hall thrusters.

Nomenclature

a	= acceleration; Virial coefficient
b	= Virial coefficient
B	= magnetic field strength
d	= separation
E	= electric field strength
F	= force
g_0	= acceleration due to Earth's gravity
I_{sp}	= specific impulse
k_b	= Boltzmann constant
L	= acceleration length
m	= mass
N	= number of molecules
q	= charge
r	= position, distance
$\bar{R}$	= universal gas constant
s	= molecular offset
t	= time
T	= temperature
v_{eq}	= equivalent velocity
V	= volume

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ϵ	=	Lennard-Jones potential well depth
ϵ_0	=	permittivity of free space
η_T	=	thruster efficiency
λ	=	third random rotation angle
μ	=	dipole moment, polarity
ν	=	specific volume
ξ	=	ionization energy
σ	=	Lennard Jones zero-energy separation distance
ϕ	=	first random rotation angle
ψ	=	second random rotation angle
ω	=	rotational frequency

I. Introduction

A. Motivation

The major loss mechanism of electrostatic and electromagnetic thrusters is the requirement to ionize the propellant. Because of recombination and radiation, the ionization energy factor is one-to-two orders of magnitude above the single ionization energy for the propellant being used, essentially wasting energy and decreasing thruster efficiency. This irrecoverable ion production energy cost is why electric thruster efficiency increases with specific impulse; the ion production energy becomes a lower fraction of the total thruster energy input as the exhaust kinetic energy increases.

The thruster efficiency is defined as the ratio of the thrust power to the sum of the thrust power and power losses. If the propellant ionization is assumed to be the only loss mechanism and a common-practice factor of 10 is implemented for the ion production energy to account for recombination, the efficiency can be expressed as

$$\eta_T = \frac{\frac{mv_{eq}^2}{2}}{\frac{mv_{eq}^2}{2} + 10\xi} \quad (\text{Eq. 1})$$

where the equivalent velocity is related to the specific impulse.

$$v_{eq} = I_{sp}g_0 \quad (\text{Eq. 2})$$

Figure 1 illustrates how thruster efficiency increases with molecular weight and, more importantly, I_{sp} for a multitude of commonly used propellants.

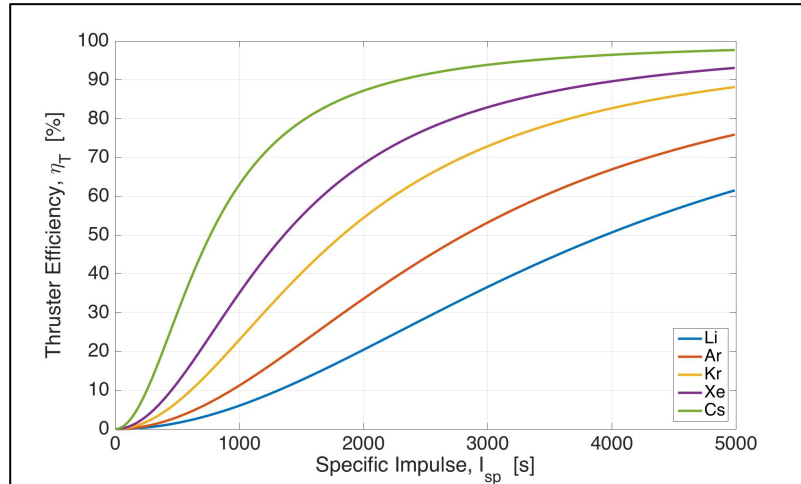


Figure 1: Electric thruster efficiency where the only loss mechanism is ionization energy.

It can be seen that the loss in efficiency due to the lost ionization energy can be substantial, even at high specific impulses. Revolutionary gains in electric thruster efficiency could be obtained if the need to ionize the propellant could be avoided.

B. Concept Derivation

The Abraham force describes how a polar molecule can experience a force in a given direction due to a time-varying polarization in a magnetic field and/or a polarization in a time-varying magnetic field¹. It is expressed as

$$\vec{F}_A = \frac{d\vec{\mu}}{dt} \times \vec{B} + \vec{\mu} \times \frac{d\vec{B}}{dt} \quad (\text{Eq. 3})$$

where the dipole moment is $\vec{\mu}$. Figure 2 shows the dynamics of a polar molecule as an electric field is applied after having an initial, hypothetical net zero polarization.

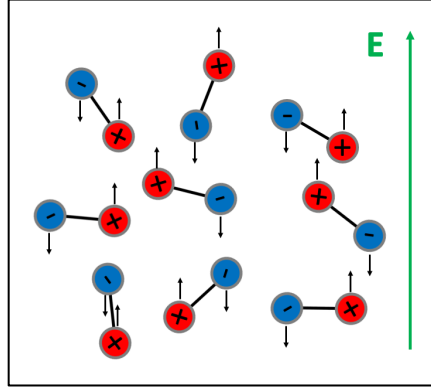


Figure 2: Inferred dynamics of a collection of randomly oriented dipoles when an electric field is present.

As the electric field is applied the dipole moments of the molecules will attempt to align themselves with the electric field, generating a force on the molecules perpendicular to both the electric and magnetic fields. Cox first proposed this acceleration scheme for Shuttle propulsion in 1980 with atmospheric gases². He derived the Lorentz body forces as follows with a supporting illustration in Figure 3³.

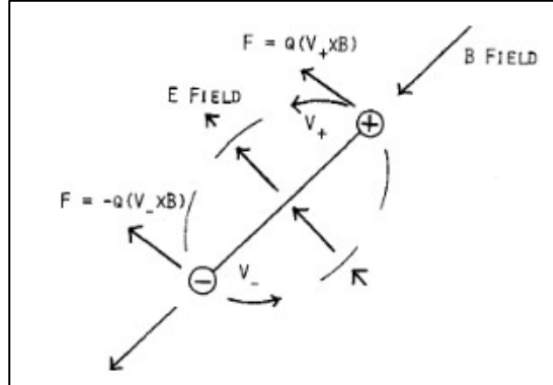


Figure 3: Illustration for Lorentz force derivation on rotating dipole molecules⁴.

The Lorentz force is given by

$$\vec{F} = q\vec{v} \times \vec{B} \quad (\text{Eq. 4})$$

where the velocity of each charge is the product of the rotational frequency and the radius. If the dipole moment is defined as the magnitude of the charge difference times the separation

$$\vec{\mu} = q\vec{d} \quad (\text{Eq. 5})$$

then the sum of the forces on the two charges is

$$\vec{F} = \omega\vec{\mu} \times \vec{B} \quad (\text{Eq. 6})$$

which can be written as

$$\vec{F} = \frac{d\vec{\mu}}{dt} \times \vec{B} \quad (\text{Eq. 7})$$

and is synonymous with part of Equation 3⁴. Penfield and Haus developed an earlier derivation of forces acting on dipolar gases, but their derivation differs from Cox's in that they accounted for any given motion of the dipole. In spatially uniform electric and magnetic fields, their derivation gives the same results as derived by Cox^{2,4,5}. Walker and Walker⁶ and Walker et al.⁷ experimentally measured this force in barium titanate crystals within 4% of the Penfield and Haus derivation. The experiment involved an alternating electric field inducing an alternating radial

polarization. The resultant force produced an alternating torque on the crystals when the steady axial magnetic field was applied. They were searching for the force described in Equation 3, but only found a force due to the first term, namely the Abraham force⁴⁻⁷.

$$\vec{F}_A = \frac{d\vec{\mu}}{dt} \times \vec{B} \quad (\text{Eq. 8})$$

Using Newton's 2nd Law of Motion in conjunction with Equation 8, the Abraham force would create an acceleration on a molecule equal to

$$a = \frac{\mu}{m} \frac{B}{\Delta t} \quad (\text{Eq. 9})$$

if the dipole's rotation is perfectly perpendicular with the magnetic field. Assuming an initial velocity of zero, the acceleration of a given exhaust velocity could be expressed as

$$a = \frac{v_e^2}{2L} \quad (\text{Eq. 10})$$

To make this acceleration scheme viable, a specific impulse of at least 1000 s is desired. With a conservative acceleration length of 20 cm, the required average acceleration is $2.4 \times 10^8 \text{ m/s}^2$.

C. Investigation of Propellants

Alkali hydride molecules – ionic, non-covalent bonds between a single hydrogen atom and an alkali metal – have significantly larger dipole moments than mixed alkali diatomics⁸. Since the molecule is diatomic and includes the lightest element, their dipole moment-to-mass ratios are highest amongst naturally occurring molecules, making them ideal for an alternating polarization acceleration scheme. Lithium hydride (LiH), sodium hydride (NaH), and potassium hydride (KH) are the three alkali hydrides with the highest dipole moment-to-mass ratios. Table 1 shows their characteristics and experimental values calculated via the QC-LAB tool on NanoHub using the TZVP basis set⁹.

Table 1: Experimental characteristics of the three lightest alkali hydrides⁹.

Molecule	Charge [C]	Bond Length [Å]	Mass [amu]	Dipole [D]	$\frac{\mu}{m} \left[\frac{\text{D}}{\text{amu}} \right]$
LiH	0.5e	1.595	4	5.967	1.492
NaH	0.5e	2.258	24	7.108	0.296
KH	0.5e	2.909	40	8.901	0.223

As one descends Group 1, the molecule becomes easier to ionize, defeating the purpose of the acceleration technique. Additionally, alkali hydrides are pyrophoric, meaning they spontaneously combust when in contact with oxygen. Fortunately, there is a molecule that is safe, abundant on Earth and in the solar system, green, and has a high dipole moment-to-mass ratio that is even comparable to that of most alkali hydrides: water.

The water molecule has an experimental dipole of 1.85 D and a moment-to-mass ratio of 0.103 D/amu. Paunescu developed a molecular dynamics simulation by simplifying the molecule to a two-particle system. The configuration, bond length, masses, and charges of the two particles were adapted to maintain the same dipole moment as that of an actual water molecule. The center-of-mass velocity reached 5 mm/s after 8 ns in the presence of a 20 kV/m saw-tooth electric field and a 25 T static magnetic field¹⁰. Figure 4 shows a detailed illustration of how the electric and magnetic fields affect the dynamics of a water molecule.

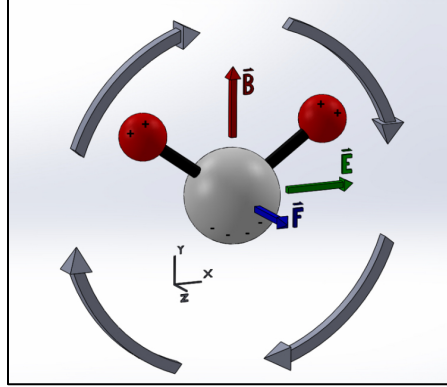


Figure 4: Illustration of how the Abraham force affects the dynamics of a water molecule.

Since water is found in various forms throughout the solar system, a spacecraft could theoretically travel to Mars, refuel, travel to an asteroid that contains ice, gather and melt it, and move on to other bodies in our solar system that harbor ice, providing for an island-hopping type of space exploration.

D. Objectives

The objectives of this study were to create a molecular dynamics simulation that modeled a large ensemble of water molecules with realistic conditions and phenomena, optimizing the operating conditions and electric field characteristics to show that the Abraham force causes a collective increase in average velocity in the z-direction. These conditions include initializing the molecules with random orientations as well as random speeds based on a Maxwell-Boltzmann distribution. Additionally, the pressure at which the molecules received their initial spacing was determined from the Paschen curve, which consequently determined the electric field strength.

The main goal was to find the smallest ensemble size of which the Abraham force is apparent, regardless of the initial conditions. This would serve to minimize the computational resources required for an extended simulation to produce an animation in which the acceleration in the z-direction is evident, another goal of the study. Successful completion of these goals would allow for the calculation of key parameters to accurately compare it to current forms of electric propulsion and provide the necessary conditions to design an experiment to physically verify the phenomenon.

II. Simulation Setup

A. Water Molecule

The SPC/E model of the water molecule was utilized because of its simplicity^{11,12}. The atoms were modeled as point charges and point masses, while the bonds were modeled as rigid rotors. Table 2 displays the characteristics of the chosen model.

Table 2: SPC/E water molecule model characteristics¹¹.

Hydrogen (H) atoms	Mass: 1.6739×10^{-27} kg Charge: 0.4238e
Oxygen (O) atoms	Mass: 2.6568×10^{-26} kg Charge: $-0.847e$
O-H bond length	1 Å
H-O-H bond angle	109.47°

These characteristics gave a dipole moment of 2.35 D, which is higher than the experimental value due to the model's approximations.

B. State Parameters

Van der Waals' equation of state, sometimes referred to as the Virial Theorem, was utilized to more accurately set the initial volume of the system and the corresponding molecular separation.

$$Pv^3 - (Pb + \bar{R}T)v^2 + av - ab = 0 \quad (\text{Eq. 11})$$

The specific volume is denoted by v and $\bar{R}$ is the universal gas constant. This third order relation contains two gas-specific constants, a and b , which are $580 \text{ J}\cdot\text{m}^3/\text{kmol}^2$ and $0.0319 \text{ m}^3/\text{kmol}$ for water, respectively¹³. Once the pressure and temperature were chosen, the specific volume could be obtained, which allowed for the calculation of the domain volume and initial molecular separation.

The Paschen curve relates the RMS electric field strength at which a gas will break down and ionize (ie., the breakdown electric field) to the gas pressure. Figure 5 shows the Paschen curve for dry air, H_2O , and a mixture of both at 293 K¹⁴.

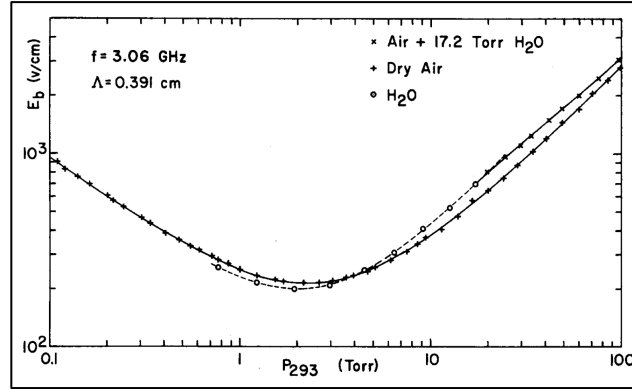


Figure 5: Breakdown electric field strength vs. total pressure¹⁴.

At conditions below the curve, the gas will not ionize, therefore, it is important to choose a pressure and electric field strength in this region for this method of propulsion. At first, 4,000 Pa was chosen because it correlated to a high electric field strength, around 100 kV/m. Simulations provided minimal-to-no evidence of the Abraham force on the system because it was found that the Coulomb force between particles greatly dwarfed that of the Lorentz force. The pressure was then decreased and the electric field strength was altered accordingly. As the pressure decreased, so did the number density, reducing the Coulomb interaction greatly, and allowing the Lorentz force to become more prominent. The lowest pressure of 13.33 Pa (0.1 Torr) was finally chosen to minimize the number density and maximize the electric field strength.

The application of a polar propulsion method requires the propellant to be in the gaseous state. At 293 K and 13.33 Pa, water is gaseous. A temperature of 300 K was chosen to err on the side of caution and to maintain the phase requirement. As the pressure was decreased to the left side of the Paschen curve, the choice of temperature remained the same so that as few variables were being changed at a time.

C. Electric and Magnetic Fields

A higher electric field will result in a higher Lorentz force, and thus an enhanced Abraham force. Given the experimental data in Figure 5, the maximum electric field associated with a pressure of 13.33 Pa is approximately 85 kV/m. A sinusoidal electric field with this maximum value was applied in the x-direction. It was found that the optimal frequency was 75 GHz for simulating a single molecule. It was given four different initial orientations with the dipole along either the y- or z-axis. The spread of the hydrogen atoms was then oriented in-plane so as to maximize the Abraham force. As the electric field was applied, the center-of-mass accelerated in the z-direction with the positive half of the electric field, and decelerated with the negative half. The goal was to create a plateaued velocity profile. The frequency was varied from 60 to 100 GHz to find the best balance between a velocity-increase and a plateau, and 75 GHz provided just that.

Both Penfield & Haus¹⁵ and Walker and Walker's⁶ derivations only found a force when the magnetic field was constant. Therefore, a static magnetic field was applied in the y-direction. Equation 9 shows that the acceleration will be greatest with a high magnetic field. A relatively inexpensive (~\$1000) high permanent magnet has been developed with a high field strength of 2.5 T. It is also much lighter than conventional equivalent electromagnetic systems by more than an order of magnitude and for these reasons, a 2.5 T magnetic field was chosen for the simulations¹⁵.

D. Assumptions

Various assumptions attributed to making the code less computationally expensive, as well as simplifying the relevant physics, which also reduced computation time. As the ensemble of molecules was generated to more accurately represent how a real-world scenario would behave, the molecules were initially configured into a cube, equally spaced from one another. They were offset by half the molecular separation,

$$s = \frac{1}{2} \left(\frac{V}{N} \right)^{1/3} \quad (\text{Eq. 12})$$

to center them in the domain. Figure 6 shows the initial layout of an ensemble of 1000 molecules.

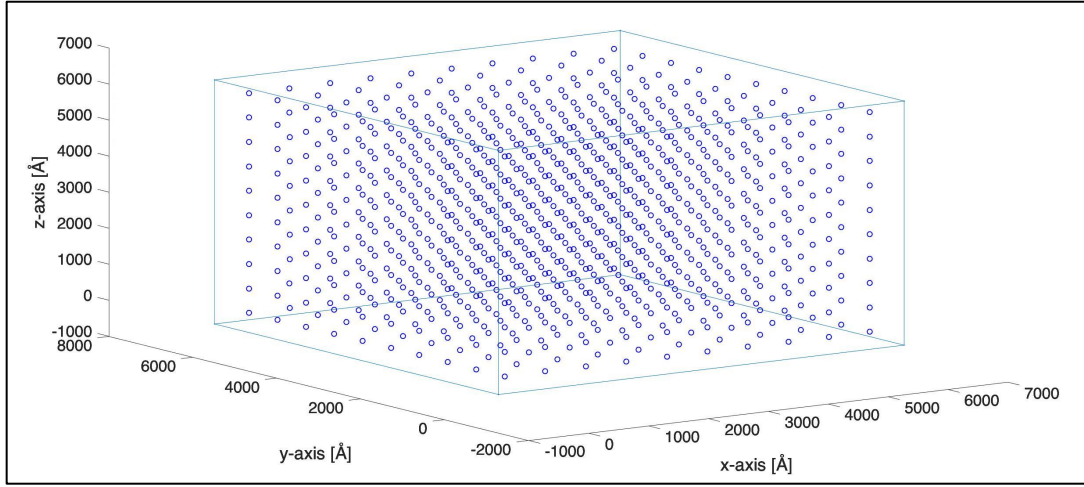


Figure 6: Initial arrangement of a 1000-molecule ensemble.

Each atom was given an initial thermal velocity based on a Maxwell-Boltzmann distribution around the given temperature, but all atoms on a given molecule were given the same velocity. Ergo, there was only translational movement and no rotational movement initially. Once they experienced the interactions from other molecules and the electric field was applied they would be free to rotate.

The vibrational, and thus rovibrational, modes of the molecules were not accounted for. While this would provide for a more accurate model, the length scale of the simulation domain was far greater than the deviation in an atom's position due to vibrations.

Plasma may be generated through four main processes: electron impact ionization (EII), secondary electron emission (SEE), field emission (FE), and cosmic radiation (CR). By staying below the Paschen curve, Townsend Avalanches were avoided and EII could be neglected. Field emission only applies to microgaps of distances smaller than 7 μm and since any practical application of this acceleration scheme would involve a gap larger than that, FE was ignored^{16,17}. Finally, SEE & CR were disregarded to focus on a simpler simulation. For these reasons, the molecules were assumed to never be ionized and no randomly generated electrons were added to the simulation.

Because of the lack of experimental data for water's Paschen curve and the complexity of deriving one, the Paschen curve for water was assumed to follow that for dry air in Figure 5. Dissociation was neglected due to the lower temperature.

E. Initializations

Each molecule was given an initial random orientation and velocity using the ran2 random number generator¹⁸. A direction cosine matrix (DCM) was applied to the orientation of each molecule where the three rotation angles were randomly chosen. The velocity was determined using the gasDev function, which gives a speed by integrating a Maxwell-Boltzmann distribution of thermal speeds via kinetic theory¹⁸.

Each molecule was initialized with its oxygen atom at a local origin; its dipole aligned with the x-axis, and its hydrogen atoms in the xy-plane. Three rotations were then performed to give each molecule its own random initial orientation. The first rotation was about the z-axis, denoted by ϕ and ranged from 0 to 2π radians of rotation in the xy-plane. The second rotation, denoted by ψ , was about the y-axis and ranged from $-\pi/2$ to $\pi/2$ radians, bringing the molecule above or below the xy-plane. The final rotation, denoted by λ , was about the x-axis and rotated the molecule around its dipole between 0 and π radians. The full DCM in Equation 13 was applied to the position of both hydrogen atoms where the trigonometric expressions are abbreviated (ie. ' $\cos(\phi)$ ' is ' $c\phi$ ') for simplicity's sake.

$$\underline{DCM} = \begin{bmatrix} c\phi c\psi & s\phi c\psi & -s\psi \\ -s\phi c\lambda + c\phi s\psi s\lambda & c\phi c\lambda + c\phi s\psi s\lambda & c\psi s\lambda \\ s\phi s\lambda + c\phi s\psi c\lambda & -c\phi s\lambda + s\phi s\psi c\lambda & c\psi c\lambda \end{bmatrix} \quad (\text{Eq. 13})$$

Once each molecule had a unique random orientation, the ran2 generator was again used to assign each molecule a random speed via the 'gasDev' function¹⁸. Each atom on a given molecule was given a unique, random speed in

each direction determined from an integrated Maxwell-Boltzmann distribution centered on the initial temperature of 300 K¹⁹.

$$f(v) = 4\pi v^2 \left(\frac{m}{2\pi k_b T} \right)^{3/2} \exp \left(-\frac{mv^2}{2k_b T} \right) \quad (\text{Eq. 14})$$

This was so that the molecule had no initial rotation. Table 3 shows the computed average, RMS, and most probable speeds with respective errors against their theoretical values, which are stated in the second row.

Table 3: Computational speeds and respective errors across all ensemble sizes.

Number of Molecules	$v_{ave} \left[\frac{m}{s} \right]$	$v_{rms} \left[\frac{m}{s} \right]$	$v_{mp} \left[\frac{m}{s} \right]$	$Error_{ave} [\%]$	$Error_{RMS} [\%]$	$Error_{mp} [\%]$
	594.00	644.72	526.41	-	-	-
8 (2 ³)	538.50	581.28	400.00	9.342	9.840	24.014
27 (3 ³)	559.19	599.41	475.00	5.859	7.027	9.766
64 (4 ³)	627.80	670.20	475.00	5.692	3.952	9.766
125 (5 ³)	606.97	657.14	490.00	2.184	1.926	6.917
216 (6 ³)	578.54	630.15	525.00	2.601	2.260	0.268
343 (7 ³)	607.12	655.71	490.00	2.211	1.704	6.917
512 (8 ³)	599.79	647.10	520.00	0.975	0.370	1.218
729 (9 ³)	617.14	669.76	490.00	3.897	3.884	6.917
1000 (10 ³)	589.64	636.00	585.00	0.732	1.352	11.130

The relatively low errors – around or below 5% - give great credibility to the ran2 random number generator.

III. Molecular Dynamics

A. Forces

The SPC/E model of the water molecule assumes the atoms are point charges, with the net charge evenly distributed along its dipole¹². Because of this, the Abraham force can be simplified to the Lorentz force, which describes the behavior of the charge of particle i moving in an electric and magnetic field.

$$\vec{F}_{L,i} = q_i (\vec{E} + \vec{v}_i \times \vec{B}) \quad (\text{Eq. 15})$$

Additionally, the Coulomb force results from the electrostatic potential between two point charges. The point charge assumption allows the total force on atom i to be expressed as

$$\vec{F}_{C,i} = \sum_{j=1, j \neq i}^{3N-2} \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}^3} \vec{r}_{ij} \quad (\text{Eq. 16})$$

where the summation does not exceed $3N-2$ because the Coulomb interaction between two atoms on the same molecule is neglected due to the rigid rotor assumption.

A force unique to molecular dynamics simulations is the Lennard-Jones (LJ) force, which accounts for the interatomic interactions between atoms i and j . The strong repulsion at short distances, due to the Pauli Exclusion principle, is characterized by the r^{-12} term, whereas the r^{-6} term characterizes the weak, long-range attractive van der Waals force^{20,21}. The total LJ force on particle i can be expressed as

$$\vec{F}_{LJ,i} = \sum_{j=1, j \neq i}^{3N-2} \frac{24\epsilon_{ij}}{r_{ij}^2} \left[2 \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \vec{r}_{ij} \quad (\text{Eq. 17})$$

where the upper limit on the summation is the same as with the Coulomb force, for the same reason. The Lennard-Jones potential has two parameters specific to the elements the potential is between. The zero-energy separation distance is σ and the depth of the potential well is ϵ . The interaction between two unlike atoms requires the use of the Lorentz-Berthelot mixing rules²².

$$\sigma_{ij} = \frac{1}{2} (\sigma_{ii} + \sigma_{jj}) \quad (\text{Eq. 18})$$

$$\epsilon_{ij} = (\epsilon_{ii} \epsilon_{jj})^{1/2} \quad (\text{Eq. 19})$$

Table 4 shows appropriate LJ parameters for interactions between the atoms of water molecules.

Table 4: Lennard-Jones parameters for O and H interactions.

Atomic Interaction	σ [Å]	ϵ [J]
H-H	2.81	$8.6k_b$
O-O	2.95	$61.6k_b$
O-H	2.88	$23.0165k_b$

Because the atomic separation is raised to such a high order, the potential and force rapidly approaches zero. This allows for truncation, greatly reducing the number of computations for each time step. Common practice sets the cutoff distance, r_{cut} , equal to 2.5σ where the LJ potential is only 1.6% of its minimum energy. The following equations show the conditions on how the Lennard-Jones force is implemented in the code where r_{min} is the distance at which the potential is equal to $-\epsilon$.

$$\vec{F}_{LJ,ij} = \vec{F}_{LJ,ij}(\vec{r}_{ij}) \quad r_{ij} < r_{min} \quad (\text{Eq. 20a})$$

$$\vec{F}_{LJ,ij} = \vec{0} \quad r_{ij} = r_{min} \quad (\text{Eq. 20b})$$

$$\vec{F}_{LJ,ij} = \vec{F}_{LJ,ij}(\vec{r}_{ij}) \quad r_{min} < r_{ij} < r_{cut} \quad (\text{Eq. 20c})$$

$$\vec{F}_{LJ,ij} = \vec{0} \quad r_{ij} > r_{min} \quad (\text{Eq. 20d})$$

The total force on particle i , therefore, can be expressed as the sum of the three forces.

$$\vec{F}_{tot,i} = \vec{F}_{L,i} + \vec{F}_{C,i} + \vec{F}_{LJ,i} \quad (\text{Eq. 21})$$

This is essential for computing the acceleration felt by the particle to advance its position and velocity.

B. Equations of Motion

The ‘velocity Verlet’ algorithm was used to integrate the equations of motion of the water molecules²³⁻²⁵. It is a two-part algorithm that calculates the acceleration felt by each particle directly for each part,

$$\vec{a}_i(t) = \frac{\vec{F}_{tot,i}(t)}{m_i} \quad (\text{Eq. 22})$$

The first part advances the position by a full time step and the velocity by a half time step.

$$\vec{r}_i(t + \Delta t) = \vec{r}_i(t) + \Delta t \vec{v}_i(t) + \frac{\Delta t^2}{2} \vec{a}_i(t) \quad (\text{Eq. 23})$$

$$\vec{v}_i\left(t + \frac{\Delta t}{2}\right) = \vec{v}_i(t) + \frac{\Delta t}{2} \vec{a}_i(t) \quad (\text{Eq. 24})$$

The second velocity calculation occurs after the second set of forces has been calculated and advances the velocity of the particles by another half time step.

$$\vec{v}_i(t + \Delta t) = \vec{v}_i\left(t + \frac{\Delta t}{2}\right) + \frac{\Delta t}{2} \vec{a}_i(t + \Delta t) \quad (\text{Eq. 25})$$

This algorithm determines the position and velocities at the current time step to $\mathcal{O}(\Delta t^2)$ with a minimized round-off error²⁴.

C. Constraint Dynamics

As the positions of the atoms are advanced, the bond lengths between the hydrogen atoms and oxygen atom may shorten or lengthen slightly. The RATTLE algorithm is utilized to apply constraint dynamics to retain the proper bond length within a certain tolerance²⁴. A time step of 1 fs was chosen to advance the equations of motion as a conservative measure and for simplicity.

D. Boundary Conditions

Periodic boundary conditions were used to contain the molecules within a cubic domain. These conditions allowed for the assumption that the cube was infinitely replicated through space; once all the atoms on a molecule left the cube, it entered from the opposite side with the same velocity, conserving the total number of molecules²⁰.

E. Parallelization

The Message Passing Interface (MPI)²⁶ allowed the parallelization of the code and communicated the position and velocity arrays between all the processors. The arrays were first created on the master node and then sent to all the remaining processors via the Broadcast²⁷ routine. Having had access to the entirety of the position and velocity

arrays, a given processor was then designated to only calculate the forces, positions, and velocities of a certain set of molecules. Once completed, that data was then communicated between the processors via the Allgather²⁸ routine – a combination of the MPI Gather and Scatter routines. Table 5 summarizes the simulation conditions for the results in Section IV.

Table 5: Summary of simulation parameters.

Time Step	1×10^{-15} s
Electric Field Strength (x-direction)	85 kV/m
Electric Field Frequency (x-direction)	75 GHz
Magnetic Field Strength (y-direction)	2.5 T
Pressure	13.33 Pa
Temperature	300 K

IV. Results

A. Introduction

The number of molecules simulated was varied through all the perfect cubes from 8 to 1000. Depending on the number of molecules they contained, different ensembles were assigned to different classes. Namely, $2^3 - 4^3$ were considered small ensembles, $5^3 - 7^3$ were considered intermediate ensembles, and $8^3 - 10^3$ were considered large ensembles.

The objective was to find the minimum ensemble size, for which results were “favorable” and fairly consistent across multiple seed values for different initializations. For a simulation to be considered favorable, the velocity profile when the electric field was present needed to be greater than when the electric field was absent, so as to exemplify the Abraham force. Furthermore, for a simulation size to be considered the smallest necessary for further research, all the different seed values needed to provide favorable results. The average velocity was normalized by taking the initial average velocity of the center-of-masses and subtracting it from every atom in each respective direction.

$$v_{i,new} = v_{i,old} - \bar{v}_{0,cm} \quad (\text{Eq. 26})$$

This was conducted so that the initial average z-velocity read zero and an easier comparison of the magnitude of the velocity profiles could be made across simulations regardless of their size and initializations.

Initial simulations ran for 50 ps for the sake of computation time and found that the velocity profiles were nearly identical no matter the ensemble size or initialization. Since there needed to be a distinction between different ensemble sizes and seeds, the timespan was lengthened to 250 ps.

B. Results for Smaller Ensembles

Smaller ensemble sizes were first simulated and provided inconsistent results where the velocity profile when the electric field was present was not always greater than when the electric field was absent for the entirety of the simulation for various initializations. Figures 7 and 8 show results of the average normalized z-velocity and z-acceleration for a simulation of 125 molecules with and without the electric field present, along with the amplified average dipole components.

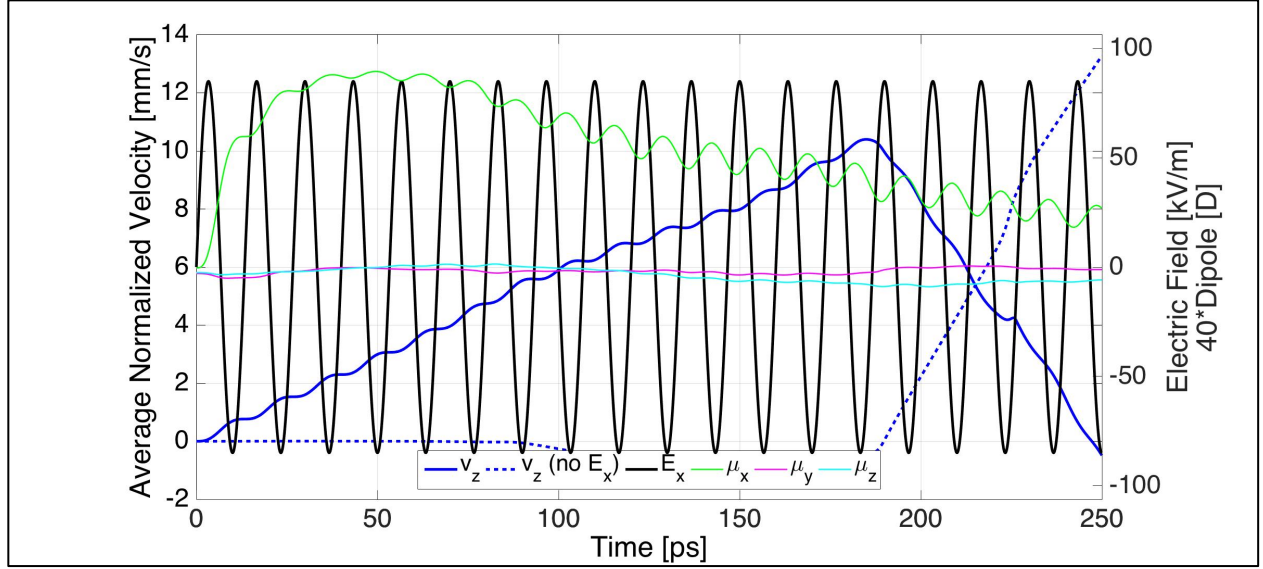


Figure 7: Average normalized z-velocity of 125 molecules with and without an electric field (Conditions: $E_x = 85$ kV/m @ 75 GHz; $B_y = 2.5$ T; $T = 300$ K; $P = 13.33$ Pa; Seed = -2).

As with the velocity profile, the respective acceleration profile was unfavorable, indicating ineffectiveness of the electric field.

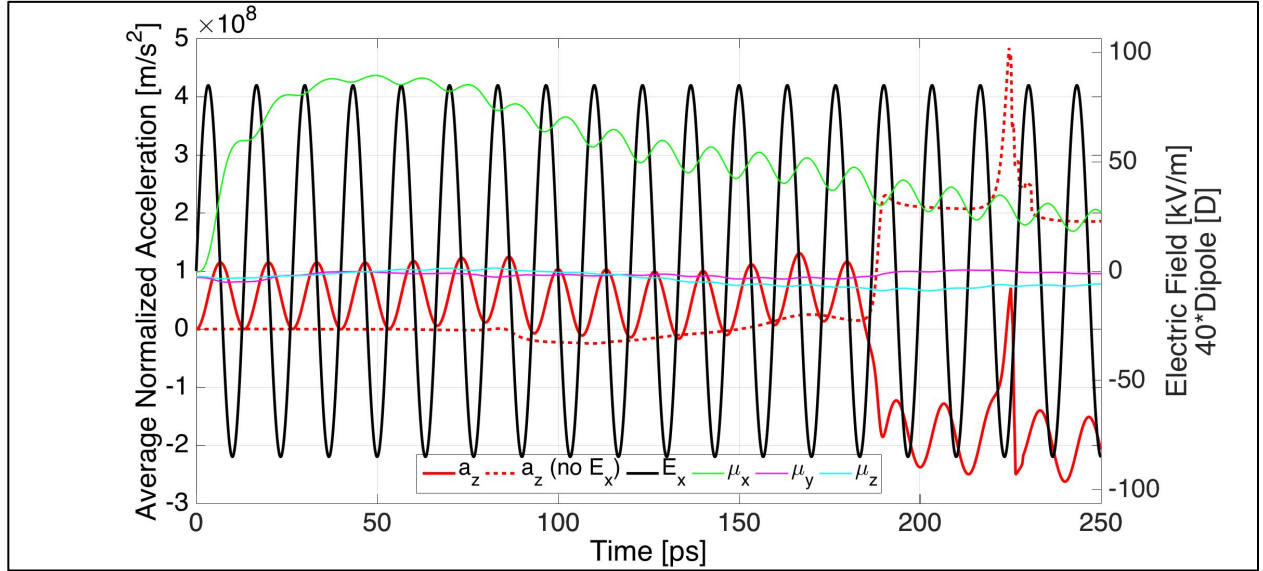


Figure 8: Average normalized z-acceleration of 125 molecules with and without an electric field (Conditions: $E_x = 85$ kV/m @ 75 GHz; $B_y = 2.5$ T; $T = 300$ K; $P = 13.33$ Pa; Seed = -2).

Even for the intermediate ensemble sizes, unfavorable simulations occurred for at least one out of the 10 different initializations. Consistent, favorable results were not found until the larger ensemble sizes were investigated.

C. Results for Larger Ensembles

An ensemble of 512 molecules proved to be the smallest ensemble size at which consistent velocity and acceleration profiles were found across all 10 initializations. Figure 9 shows that, when the electric field was present, the average normalized z-velocity was always higher than when the electric field was absent, and was ever-increasing in a “step-up” like manner. After 250 ps, the velocity reached about 30 mm/s over almost 19 electric field pulses. This translates to an average acceleration of 1.2×10^8 m/s² and a Δv of 1.6 mm/s/pulse.

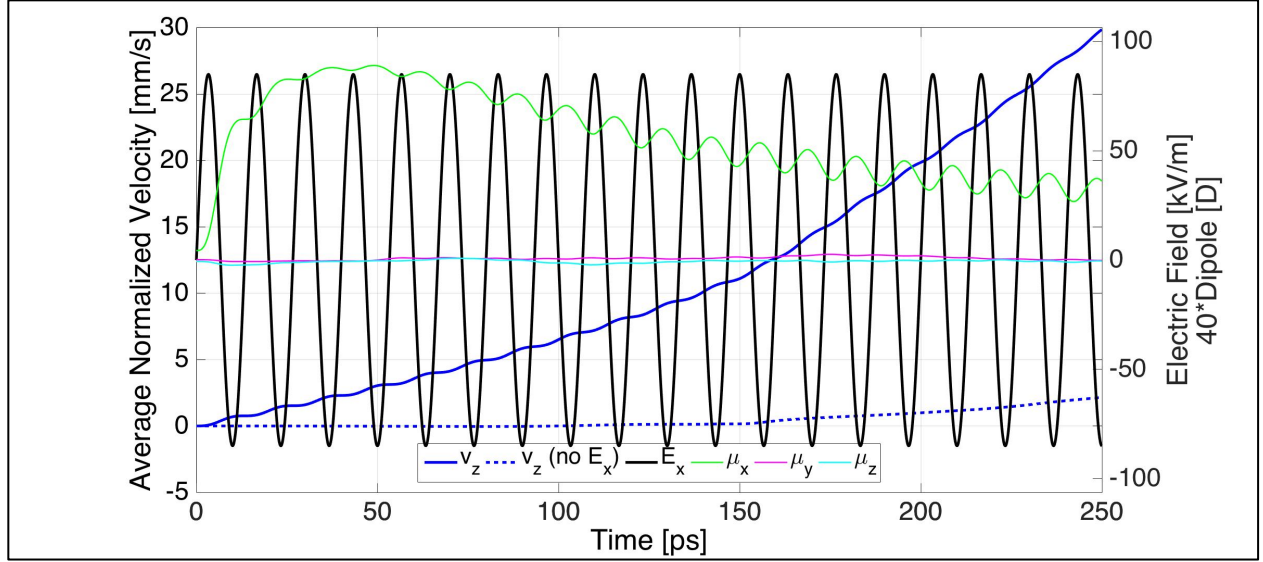


Figure 9: Average normalized z-velocity of 512 molecules with and without an electric field (Conditions: $E_x = 85$ kV/m @ 75 GHz; $B_y = 2.5$ T; $T = 300$ K; $P = 13.33$ Pa; Seed = -4).

Figure 10 shows that the respective acceleration profile when the electric field was present was also greater than when it was absent. Additionally, the average acceleration calculated from Figure 10 is on par with the behavior in Figure 9: the acceleration varies from zero to approximately 2.6×10^8 m/s².

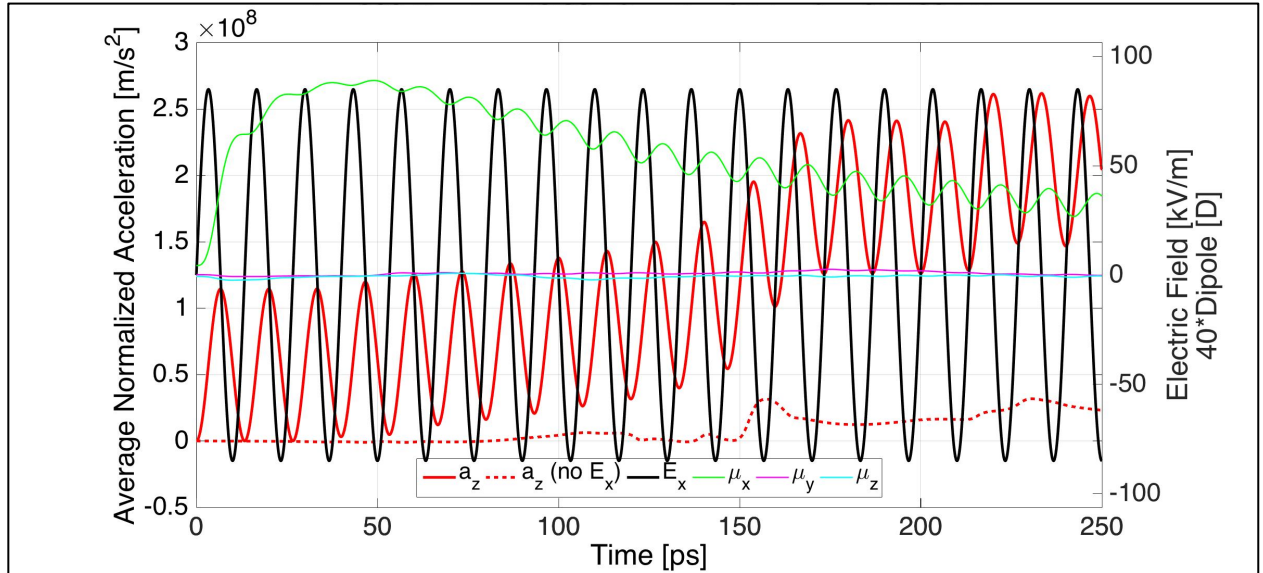


Figure 10: Average normalized z-velocity of 512 molecules with and without an electric field (Conditions: $E_x = 85$ kV/m @ 75 GHz; $B_y = 2.5$ T; $T = 300$ K; $P = 13.33$ Pa; Seed = -4).

As predicted, the 729- and 1000-molecule ensembles also provided consistent, favorable profile comparisons across all initializations.

D. Exploration of the Electric Field Frequency

The initial frequency simulated was 75 GHz per the explanation in Section II. C. After the optimal ensemble size was determined, the electric field frequency was further varied to determine if a higher exit velocity could be achieved.

The frequency was first varied in 15 GHz increments to cover a wider range with fewer simulations needed. After determining that increasing the frequency provided a smaller Δv per pulse, lower frequencies were

investigated where it was found that the Δv per pulse increased as the frequency decreased. Figure 11 shows the average normalized z-velocity profiles for frequencies ranging from 15 GHz to 90 GHz.

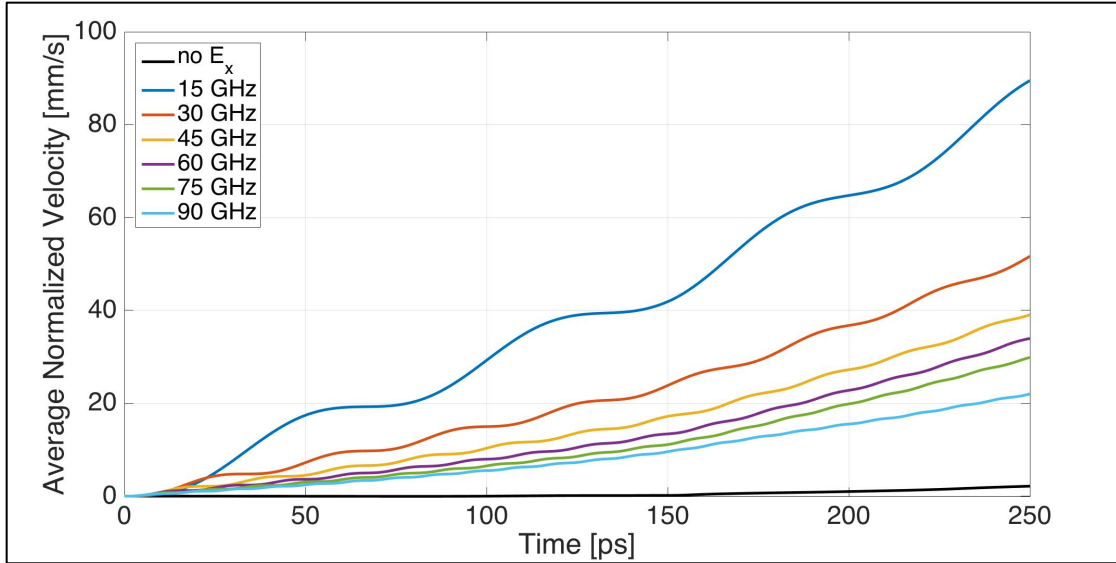


Figure 11: Comparison of average normalized z-velocity profiles across lower GHz-ranged frequencies (Conditions: $E_x = 85$ kV/m; $B_y = 2.5$ T; $N = 512$; $T = 300$ K; $P = 13.33$ Pa; Seed -4).

Because the velocity profile kept steepening with a decreasing electric field frequency, the frequency was reduced in greater intervals. Lower frequencies had longer periods, requiring the simulations to be extended by an order of magnitude to observe the behavior over multiple pulses. Figure 12 shows the velocity profiles for frequencies between 250 MHz and 1000 MHz in 250 MHz intervals. The discontinuities in the profiles are the results of collisions between particles.

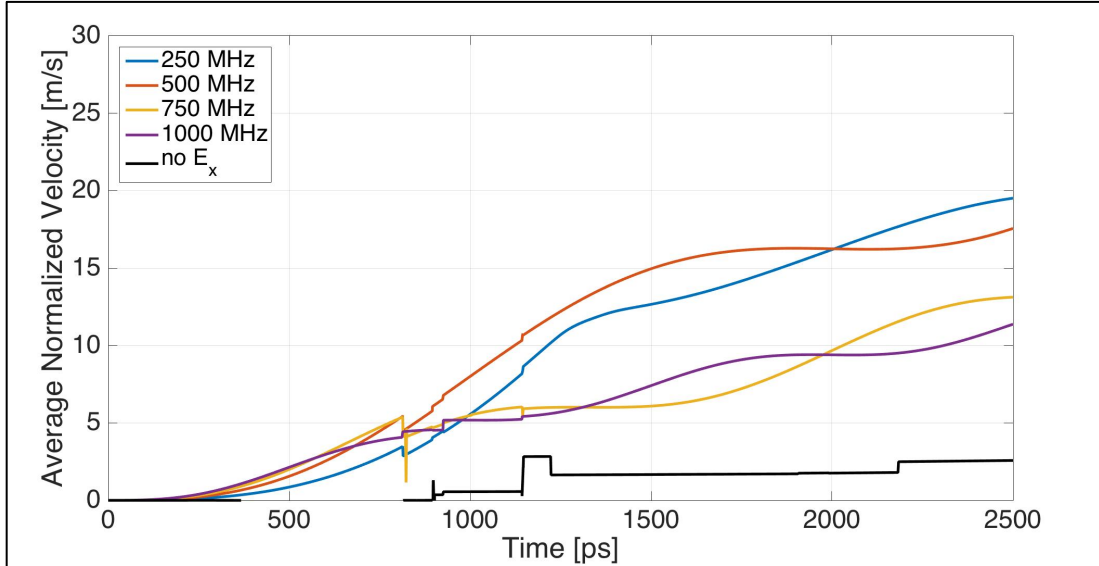


Figure 12: Comparison of average normalized z-velocity profiles across upper MHz-ranged frequencies (Conditions: $E_x = 85$ kV/m; $B_y = 2.5$ T; $N = 512$; $T = 300$ K; $P = 13.33$ Pa; Seed -4).

The highest final z-velocity coincided to the lowest electric field frequency. At 250 MHz, the final average normalized z-velocity was 19.5 m/s, occurring over 2500 ps, for an average acceleration of 7.8×10^9 m/s² and Δv of 31.2 m/s/pulse. Assuming an acceleration length of 20 cm, Equation 10 gives an I_{sp} of 5700 s, vastly outperforming current methods of electric propulsion.

V. Conclusions

A. Summary

Current methods of electric propulsion expend considerable power when ionizing the propellant. Avoiding this requirement would lead to an increase in thruster efficiency and could be done by taking advantage of the Abraham force on a dipole molecule in perpendicular electric and magnetic fields. Simulating an ensemble of water molecules to observe the collective effect of the Abraham force provided insight into the validity of this method of propulsion.

One of the goals of this research was to determine the smallest ensemble size that gave average normalized z-velocity and z-acceleration profiles that were higher with an electric field present for the entirety of the simulation. The primary goal was to accomplish this with realistic conditions by implementing random initial orientations and random speeds based on a Maxwell-Boltzmann distribution. Additionally, restrictive conditions on pressure, temperature, and electric field strength from water's assumed Paschen curve and phase diagram were implemented. Consistency was first confirmed across 10 different initializations for an ensemble of 512 (8^3) molecules and also for larger ensembles.

The highest velocity achieved was approximately 19.5 m/s, with an average acceleration of 7.8×10^9 m/s² and an average Δv of 31.2 m/s/pulse. Assuming an acceleration length of 20 cm, and utilizing Equations 2 and 10, an I_{sp} of 5700 s could be reached, dwarfing that of current Hall thrusters.

B. Future Work

While the results presented herein are promising, there are still areas for advancement. Running much longer simulations – which would showcase the effect of collisions on a longer scale – would provide a more direct look at an achievable exit velocity. Additionally, an experiment could be conducted with the optimized operating parameters to verify the phenomenon. The use of water as the propellant would allow for an “island-hopping” type of space exploration due to water's availability in the solar system, revolutionizing the electric propulsion industry.

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