Investigation of Electric Fields for Electromagnetic Propulsion using Nonionized Dipole Gases

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A means by which water molecules may be used for electromagnetic propulsion has been investigated through the utilization of their naturally occurring permanent dipole under the effect of the Abraham force. Use of the Abraham force allows the electromagnetic acceleration of a propellant gas without the need to ionize the propellant. Two derivations of this force are presented, as well as molecular dynamics simulations of single lithium hydride and water molecules as proofs of concept. A velocity increase of approximately 0.58 mm/s was achieved under the optimal conditions of a static magnetic field of 25 T and a single cycle sinusoidal electric field of 21 kV/m at 75 GHz for one molecule. The associated acceleration is comparable to that of current forms of electromagnetic propulsion. The simulation has been scaled up to include 1000 molecules to investigate the effect of intermolecular interactions on the acceleration process.

Nomenclature

∇	Nabla operator
a	Acceleration
B	Magnetic field
d	Distance of dipole charge separation
m	Mass
E	Electric field
F	Force
L	Acceleration length
n	Principal quantum number
P	Propellant polarization
q	Charge
R	Position of negative end of the dipole
r	Distance between two molecules
r_c	Cutoff radius
t	Time
u_e	Exhaust velocity
v	Velocity
V_{cm}	Center of mass velocity
α	Damping parameter
ϵ	Ion production energy
η	Thruster efficiency
μ	Dipole moment
ω	Rotational frequency

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I. Introduction

The major loss mechanism of electrostatic and electromagnetic thrusters is the requirement to ionize the propellant. The propellant is ionized to create a net charge for acceleration but once it exits the nozzle, the energy that went into ionization is not recovered. Because of recombination and radiation, the ionization energy is one-to-two orders of magnitude above the single ionization energy for the propellant being used, essentially wasting energy. The 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. This is also the primary reason that electric thrusters are not able to operate efficiently at low specific impulses. Figure 1 shows thruster efficiencies for four propellants, lithium, argon, xenon, and cesium, as a function of specific impulse when the ion production energy at ten times the single ionization energy is the only loss mechanism for the thruster

$$\eta = \frac{\frac{mu_e^2}{2}}{\frac{mu_e^2}{2} + 10\epsilon} \tag{1}$$

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.

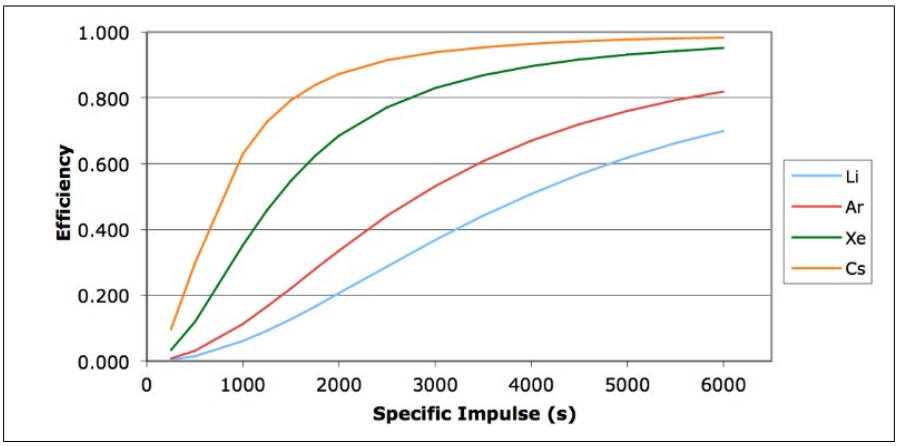


Figure 1: Electric thruster efficiency as a function of specific impulse where the only loss is ionization energy.

II. History

A. Cox and Penfield & Haus

A viable method could be obtained by utilizing the naturally occurring dipole of molecules as Cox proposed in 1980.[1] An electric field could rotate the dipole, creating an alternating polarization. In the presence of a nonparallel, but ideally perpendicular, magnetic field, this alternating polarization would create a force perpendicular to both fields, creating the method's thrust.[2–4]Cox[1] derived the Lorentz body forces as follows and a schematic can be seen in Fig. 2. The Lorentz force is given by

$$\vec{F} = q(\vec{v} \times \vec{B}) \tag{2}$$

The velocity of each charge is the product of the rotational frequency and the radius

$$\vec{F} = q\frac{\vec{d}}{2}\omega \times \vec{B} \tag{3}$$

The dipole moment is defined to be the product of the charge and their separation

$$\vec{\mu} = q\vec{d} \tag{4}$$

Substituting Eq. (4) into Eq. (3) yields the force on one charge

$$\vec{F} = \frac{\vec{\mu}}{2}\omega \times \vec{B} \tag{5}$$

Therefore, the sum of the forces on two charges is

$$\vec{F} = \vec{\mu}\omega \times \vec{B} \tag{6}$$

The developed thrust of such a method would simply be the sum of forces acting on every dipole in the

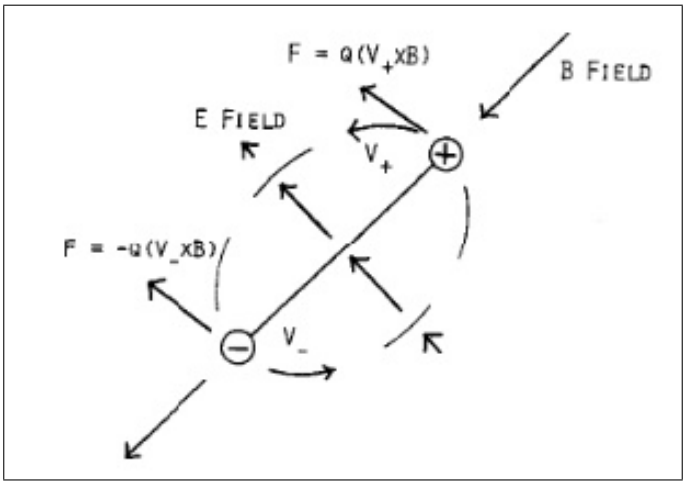


Figure 2: Schematic for Lorentz force derivation on rotating dipole molecules.[4]

interaction region.

Penfield and Haus[5] developed an earlier derivation of forces acting on dipolar gases, but their derivation differs from Coxs in that they accounted for any general motion of the dipole.[4] As seen in Fig. 3, the position of the negative end of the dipole is given by r and the dipole is acted on by both electric, E(r), and magnetic, B(r), fields which can be functions of position.

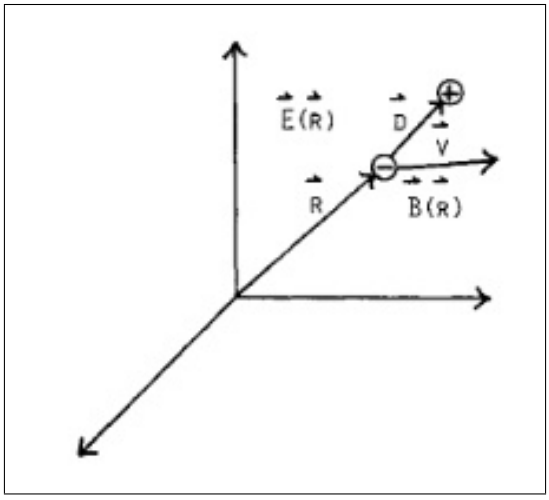


Figure 3: Dipole representation in Penfield and Haus force derivation.[4]

The force acting on the negative end is

$$\vec{F} = -q\vec{E}(\vec{r}) - q\vec{v} \times \vec{B}(\vec{r}) \tag{7}$$

and the force on the positive end, at the point r+d and traveling with the velocity $\vec{v} + d\vec{d}/dt$, is

$$\vec{F} = q\vec{E}(\vec{r}+\vec{d}) + q[\vec{v} + \frac{d\vec{d}}{dt}] \times \vec{B}(\vec{r}+\vec{d}) \tag{8}$$

The sum of Eq. (7) and Eq. (8) is the net force on the dipole

$$\vec{F} = q[\vec{E}(\vec{r}+\vec{d}) - \vec{E}(\vec{r})] + q[\vec{v} \times \vec{B}(\vec{r}+\vec{d}) - \vec{v} \times \vec{B}(\vec{r})] + q\frac{d\vec{d}}{dt} \times \vec{B}(\vec{r}+\vec{d}) \tag{9}$$

and when taken to the first order, the expression becomes

$$\vec{F} = q\vec{d} \cdot \nabla\vec{E} + q\vec{v} \times (\vec{d} \cdot \nabla\vec{B}) + q\frac{d\vec{d}}{dt} \times \vec{B} \tag{10}$$

The last term represents the time rate of change of the dipole moment with the magnetic field and, in spatially uniform electric and magnetic fields of Eq. (10), only the final term remains giving the same magnitude as derived by Cox.[4]

B. Further Contributors

The first physical proof for the Abraham force was given by Walker and Walker[6] and Walker et al.[7] in 1975. They measured the Abraham force on a barium titanate specimen within 4% of the Penfield and Haus[5] derivation. The experiment was performed at a frequency of 0.3 Hz and was restricted to the special case of time varying electric and fixed magnetic field in a nonmagnetic dielectric. A disc of barium titanate was suspended from a torsional pendulum and the movement of the disk was measured by optical means. Walker and Walker[6] and Walker et al.[7] were searching for a force derived by Abraham given by

$$\vec{F} = q\frac{d\vec{d}}{dt} \times \vec{B} + q\vec{d} \times \frac{d\vec{B}}{dt} \tag{11}$$

however, they only found a force due to the first term, namely the Abraham force

$$\vec{F} = \frac{d\vec{P}}{dt} \times \vec{B} \tag{12}$$

Even though they showed that Abraham‘s derivation was in error, they proved that the force exists and can be experimentally measured.

Micci[4] reexamined the concept in 1985 but concluded that the current technology was not able to produce the high strength/high freqency magnetic fields required in Cox's manifestation of the concept.

III. Challenges & Solutions

A. Static Magnetic Field

In the concept proposed by Cox, sufficient acceleration would require high strength magnetic fields (on the order of one tesla) operating at microwave frequencies. Simulations later described apply the Abraham force by using a high strength steady magnetic field. However, a problem arises when using a static magnetic field: when the dipole rotation continues past its initial alignment with the electric field, the sign of dP/dt switches, causing a force in the negative direction. A solution is to apply a single cycle sinusoidal electric field pulse to rotate the dipoles, generating the accelerating force, but then decelerated them to no rotational velocity before the sign of dP/dt can reverse. Once the dipoles relax to a random orientation, due to intermolecular collisions, the next sinusoidal pulse may be applied.

B. Propellant Selection

Selecting a propellant is contingent on the ability to achieve an acceleration and specific impulse that are competitive with current forms of electric propulsion. The force on the dipole is equal to the product of the dipole moment, magnetic field strength, and the rotational frequency. Utilizing a large dipole moment can

reduce the need for a high rotational frequency or magnetic field strength. In a conservative case where the initial velocity is zero, the acceleration associated with a given exhaust velocity is

$$a = \frac{u_e^2}{2L} \tag{13}$$

To make this a viable concept, an assumption of a specific impulse of 1000 s can be made. Assuming a conservative length of 20 cm, the required acceleration is 108 m/s. Utilizing Newtons 2^{nd} Law, the dipole acceleration can also be expressed as

$$a = \frac{\mu}{m}\omega B \tag{14}$$

Therefore, a large dipole moment-to-mass ratio would be required for a high specific impulse.[4] Rydberg atoms or molecules, lithium hydride, and water were investigated.

One issue with Rydberg atoms is that the field ionization potential is proportional to n^{-4} while the force on the dipole increases with n^2. The result is that as the gas is electronically excited, the maximum acceleration which can be achieved decreases. Rydberg states are also easily destroyed by the absorption of electromagnetic radiation and resultant radiation or by collisions with other particles. In order to avoid ionizations due to collisions, operation at cryogenic temperatures would be required. Additionally, Rydberg atoms may also be photoionized by background infrared and submillimeter radiation due to their decreased ionization potential.

A molecular dynamics simulation developed by Paunescu[12] showed promising results of using lithium hydride as fuel but because of its nature of being combustible in air, especially moist air, there was a need to investigate a safer fuel.

Water has a high dipole moment-to-mass ratio of 2.07E-4 C-m/kg, is easily available, abundant in nature, and a green propellant. Paunescu[12] used the SPC/E16[16] model for the water molecule and investigated a molecule under realistic collisions. The relationship between rotational frequency (in GHz) and constant electric field strength (in kV/m), in the absence of a magnetic field, was simulated to be

$$\omega = 1.7407E^{0.5106} \tag{15}$$

The V_{cm} of the theoretical water molecule reached 5 mm/s after 8 ns.[12] In accordance with Eq. (14), water molecule acceleration in a 25 T magnetic field and a 100 GHz electric field would be 1.035E9 m/s^2, which is comparable to the acceleration experienced by propellant ions in current electric propulsion thrusters. Competing with current electric propulsion means and not requiring ionization make water an excellent propellant for an alternating polarization thruster.

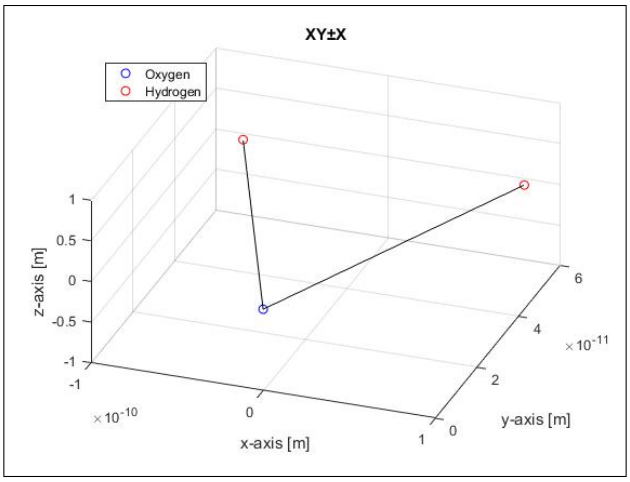
IV. Results

A. Optimization of Electric Fields

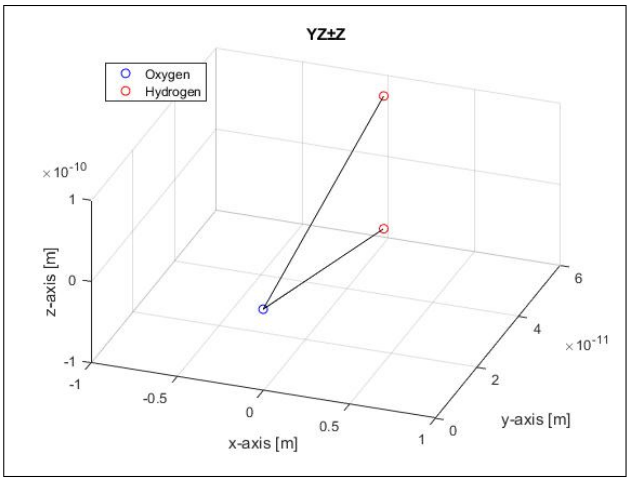
The goal is to rotate an initially stationary molecule with an electric file and bring the rotation to a halt with an electric field in the opposite direction. The moving charged particles would exhibit a perpendicular acceleration per the Lorentz force, followed by a plateaued behavior. Once the V_{cm} levels, another sinusoidal pulse of the electric field could be applied. This would give a "step-up" like behavior for the velocity increase. If the electric field were to be in the x-direction and the magnetic field in the y-direction, the polarity of the molecule would have to be along the y- or z-axes in order for the Abraham force to take effect. This would result in a net movement of the center of mass in the axial, or z-direction.

Assuming the molecule starts from rest, there are four configurations which allow for a maximized Abraham force. The configurations can be seen in Fig. 4. The nomenclature for the "ab±c" designation is as follows: a & b are the axes of the plane in which the molecule lies and c is the axis in which the hydrogen molecules span. An investigation of which initial configuration of a single water molecule resulting in the best V_{cm} increase for one sinusoidal pulse of the electric field with a static magnetic field was launched. Once an optimal configuration was determined, the magnitude of the electric field was varied to determine the optimal conditions.

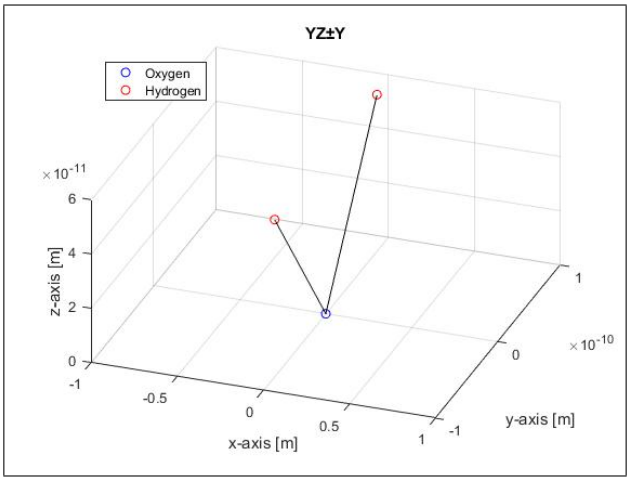
As with Paunescu's[12] research, a molecular dynamics (MD) simulation using the velocity Verlet algorithm[13] and the RATTLE constraint dynamics algorithm[14] were utilized. The SPC/E[16] model for the water molecule also allowed for the assumption that the magnitude of the partial negative charge on the oxygen atom is evenly countered and distributed to the partial positive charges of the hydrogen atoms.



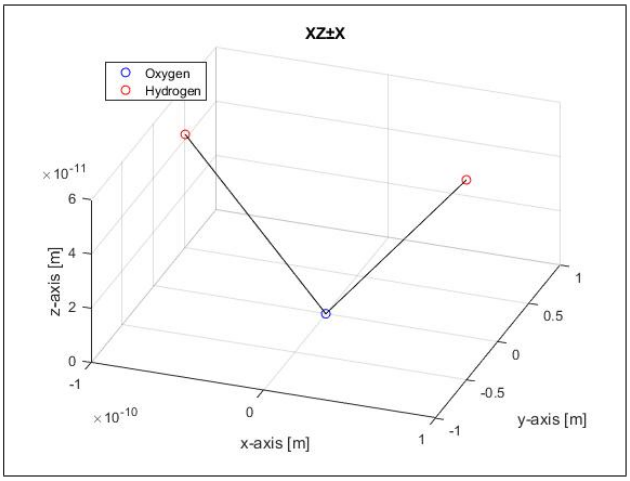
(a) XY±X configuration



(b) YZ±Z configuration



(c) YZ±Y configuration



(d) XZ±X configuration

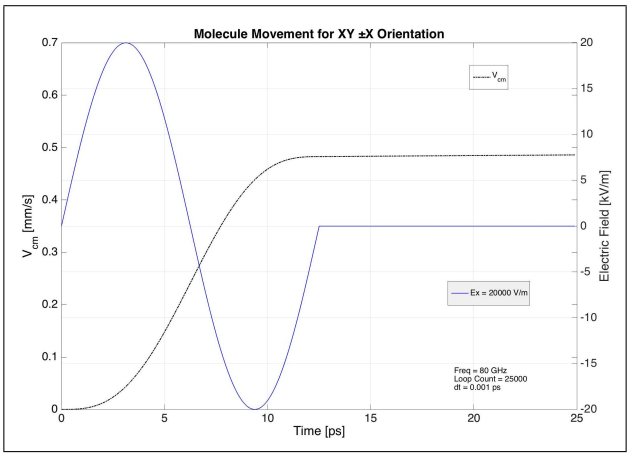
Figure 4: Possible initial configurations of water molecule for optimal V_{cm} results.

Simulations began at the lower frequencies (10 to 60 GHz) but the V_{cm} would not plateau before the electric field was finished. A frequency of 80 GHz and a static magnetic field of 25 T were chosen to compare the four configurations. The electric field was varied from 1 to 25 kV/m to determine the "best plateaued" behavior of the V_{cm} for each configuration. As the electric field was varied, the V_{cm} plot was visually inspected to determine the electric field strength which resulted in the smoothest, most level, plateau, as remaining rotation would eventually reverse and start to act to decelerate the molecule. The optimal plots for each configuration can be seen in Fig 5 with the tabulated results in Table 1. The largest velocity increase through one pulse of the electric field was approximately 0.51 mm/s for the XZ±X configuration at a strength of 21 kV/m.

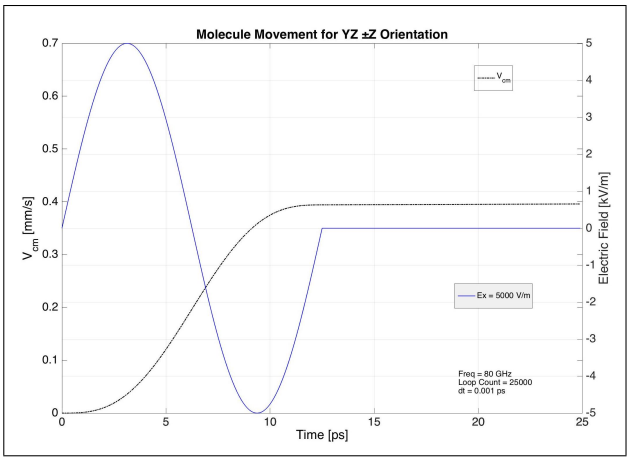
Table 1: V_{cm} plot comparison of all four initial configurations.

Parameter	**XY±X**	**YZ±Z**	**YZ±Y**	**XZ±X**
Electric Field [kV/m]	20	5	4	21
Plateaued V_{cm} [mm/s]	0.48	0.39	0.32	0.51

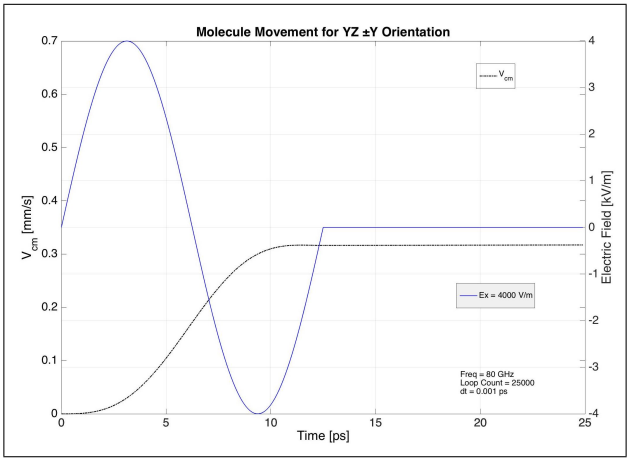
Once it was determined that the XZ±X produced the highest increase in V_{cm}, the electric field fre-



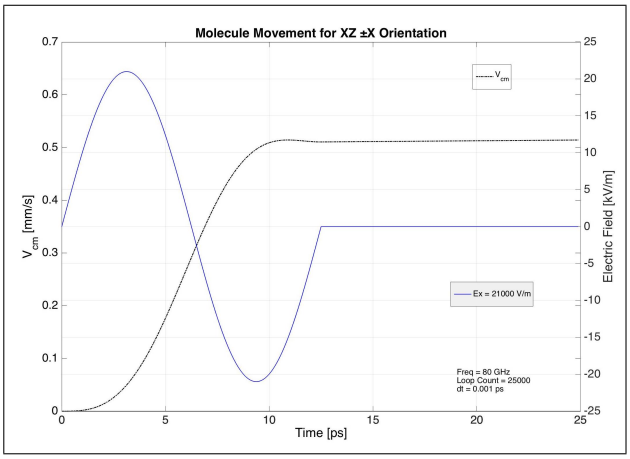
(a) XY±X configuration



(b) YZ±Z configuration



(c) YZ±Y configuration



(d) XZ±X configuration

Figure 5: Optimized V_{cm} results for respective configurations.

quency was varied from 60 to 100 GHz to determine the highest increase, without deviating too much from a plateaued state.

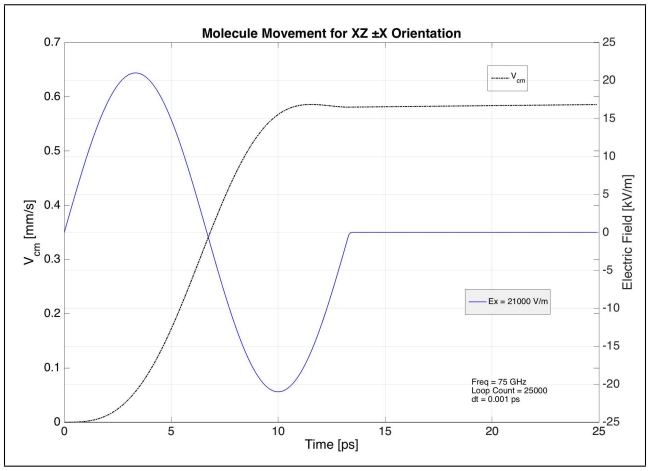


Figure 6: Optimal electric field strength and frequency for water.

Fig. 6 shows that at an electric field strength of 21 kV/m and a frequency of 75 GHz, with a perpendicular static magnetic field of 25 T, the water molecule achieves a V_{cm} increase of approximately 0.58 mm/s. These are the optimal conditions for which further studies were conducted under. It should be noted that at frequencies below 60 GHz, the V_{cm} would peak above 2 mm/s, but the behavior would oscillate.

B. N-Body Simulation

The optimal electric field frequency and strength was then applied to an MD simulation containing 1000 water molecules. The molecules were initially placed 132 $\AA$ apart from each other in each direction, based on the Ideal Gas Law with a pressure of 3000 Pa and a temperature of 500 K. The molecules were also given an initial randomized thermal velocity based on a Maxwellian distribution at 500 K. Coulomb and Lennard-Jones force were added to the Lorentz force applied to each atom. The initialized system is shown in Fig 6.

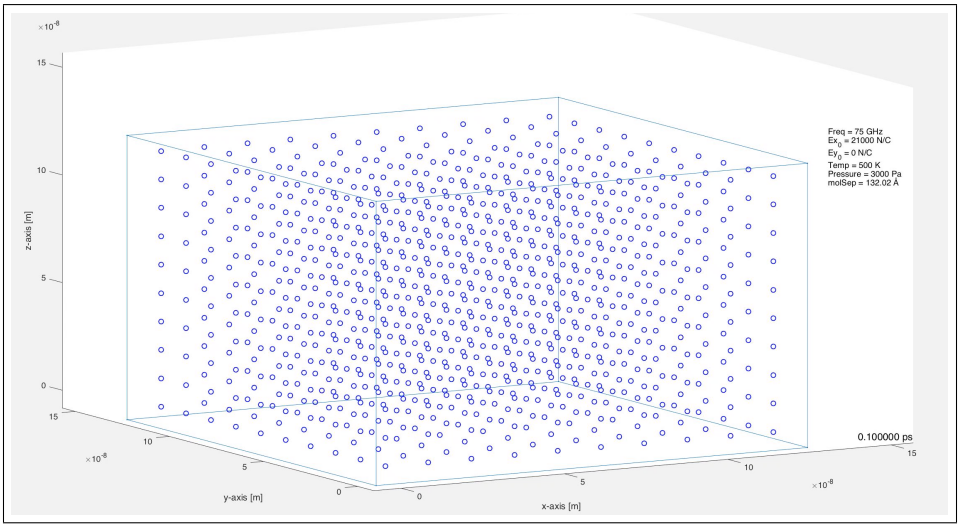


Figure 7: Initial screenshot of 1000 molecule simulation.

C. Kinetic Energy

Calculating the kinetic energy involves taking into account the three forces used in the simulation: Lorentz, Coulomb and Lennard-Jones. The Lorentz force is given by

$$\vec{F_L} = q(\vec{E} + \vec{v} \times \vec{B}) \tag{16}$$

The Coulomb Force is considered a long range interaction and the most popular computational method is the Ewald method.[17] However, in 1999, Wolf presented an alternative method which reduces the computational time of the Ewald method by 2-3 times.[17] Wolf's method for calculating the Coulomb force is

$$\vec{F_C} = q_1 q_2 \left(\frac{erfc(\alpha r)}{r^3} - \frac{erfc(\alpha r_c)}{r_c^3}\right)\vec{r} + \frac{2\alpha}{\sqrt{\pi}}\left(\frac{exp(-\alpha^2 r^2)}{r^3} - \frac{exp(-\alpha^2 r_c^2)}{r_c^3}\right)\vec{r} \tag{17}$$

where

$$erfc(\alpha r) = 1 - \frac{\alpha r}{r_c} \tag{18}$$

for radii less than the cut-off radius and zero everywhere else. The best suited value of the parameters α and r_c for water were selected from Reference (18).

The Simple Truncation method was used for calculating the Lennard-Jones potential.[19] The Lennard-Jones force from one molecule is only calculated on surrounding molecules which are within a specific radius called cut-off radius. This method gives fairly accurate results because the Lennard-Jones force is short

range interaction and becomes negligible as the distance between particles increases more than the cut-off radius. The force here is given by

$$\vec{F}_{LJ} = 24\epsilon(\frac{2\sigma^{12}}{r^{14}} - \frac{\sigma^6}{r^8})\vec{r} \tag{19}$$

for distances smaller than r_c - usually 2.5σ - and zero everywhere else. The Lennard-Jones parameters for water can be seen in Table 2.[19]

Table 2: L-J parameters for all L-J interactions between two water molecules.

Atomic Interaction	σ [$\AA$]	ϵ [J]
H-H	2.81	$8.6k_\mathrm{b}$
O-O	2.95	$61.6k_\mathrm{b}$
H-O	2.88	$23.0165k_\mathrm{b}$

The tolerance used in the velocity verlet should be chosen such that the kinetic energies before the constraint and after the constraint remain constant. The energy is re-scaled up to 500,000 time steps by using a re-scaling factor f as

$$f = \sqrt{\frac{KE_{ave,i}}{KE_{ave}}} \tag{20}$$

where $KE_{ave,i}$ is the initial average kinetic energy and KE_{ave} is the average kinetic energy at every 1000^{th} time step. This re-scaling helps to bring back the energy to the initial value and after finding the correct tolerance, the kinetic energy remains constant when the re-scaling is removed after 500,000 time steps.

V. Conclusion

Simulations are proving promising for the use of the naturally occurring dipole of water and other molecules as the propellant for an alternating polarization thruster. Bulk behavior is now being examined to further validate the concept and provide optimal operating conditions for a proof of concept experiment. The ability to obtain electromagnetic acceleration of a propellant as ubiquitous throughout the solar system as water without the need to ionize it would open up a range of missions not currently achievable.

Acknowledgments

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