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A Study of Particle Collisions in Electric Propulsion Plasma Plumes

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All numerical simulations have some inherent error associated with the results but minimizing the error may also maximize the processing time of the simulation. The particle collision model used for this paper is Monte Carlo Collisions. The results of the simulations were compared to a vacuum tank experiment conducted at the Air Force Research Laboratory. The results were compared for simulations with and without collisions using different neutral densities and levels of complexity for particle collisions. The effect of particle collisions is evident in the results of the simulations. Increasing the neutral density of the simulation does not have a major impact on the results in the plume region. Outside the plume region the particle collisions can affect the results by an order of magnitude or greater.

Nomenclature

c_m	Center of Mass Velocity
c_r	Relative Velocity
\vec{c}_s	Source Particle Velocity
\vec{c}_t	Target Particle Velocity
k	Boltzmann Constant
n	Particle Number Density
n_o	Reference Number Density
m	Particle Mass
M	Number of Random Numbers
P	Probability of Particle Collision
R_i	Random Number between 0 and 1
T	Temperature
T_o	Reference Temperature
V	Volts
V_i	Particle Velocity
V_{th}	Thermal Velocity
W	Watts
χ	Random Angle between Particles
Δt	Time Step Time
ϵ	Random Angle between Particles
γ	Specific Heat Ratio
ν_s	Source Particle Initial Velocity
ν_t	Target Particle Initial Velocity
ϕ	Potential

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I. Introduction

When using a numerical method to perform a calculation, one must consider both the accuracy of the results and the processing time of the simulation. All numerical simulations have some inherent error associated with the results but minimizing the error may also maximize the processing time of the simulation. Criteria must be set as to what an acceptable level of error is for the simulation so that simulations achieve acceptable results in a reasonable time. One such criterion for plasma plume interaction simulations is whether or not to track particle collisions in the simulation.

Tracking particle collisions can add significant processing time to a simulation but may improve the results of the simulation. There are different methods of tracking particle collisions with different levels of accuracy and associated processing time. The particle collision model used for this paper is Monte Carlo Collisions (MCC).¹ MCC collides simulated particles with a defined background density of particles.

This paper performs a comparison between simulations with no collisions and MCC to determine when particle collisions are important. To perform this comparison, a simulation was created to model a vacuum tank experiment conducted at the Air Force Research Laboratory (AFRL) at Edward's Air Force Base. To determine the accuracy of the simulations, the results were compared to the experiment data and the discrepancies were analyzed.

II. Background Theory

A Monte Carlo Collision model is used in this paper for modeling particle collisions. A MCC collision model determines when particle collisions occur using simulated ion particles and a background neutral gas. There are two major steps in performing a particle collision: determine if a particle collision occurred and then perform the corresponding collision. Two types of collisions are considered for the simulations discussed in this experiment, Charge Exchange (CEX) and Variable Hard Sphere (VHS).²

A. Charge Exchange Collisions

Collision cross-section, σ , data is supplied for the simulation to calculate the probability that a collision will occur. The collision cross-section is dependant on the relative velocities between particles, c_r . The velocity of the neutral particles is assumed to be zero in this analysis. The exact collision cross-sections are not known so two CEX collision cross-sections were investigated in this paper. The first cross-section model of Pullins³ scales with the log of relative velocity, while the older model of Rapp and Francis⁴ is a function of a square of natural log. The collision cross-sections used for this paper are:

$$\sigma_{CEX,P} = 1.1872 \times 10^{-20} [-23.3 \log(c_r) + 188.81] \quad (1)$$

$$\sigma_{CEX,RF} = [-0.8821 \ln(c_r) + 15.1262]^2 \times 10^{-20} \quad (2)$$

Using the collision cross-sections, the probability of a collision is computed using Equation 3 where the particle number density, n , and time step, Δt , are known. The probability is a number between zero and one. A random number is chosen between zero and one and if the random number is greater than the probability then a particle collision is performed.

$$P = [1.0 - \exp(-n\sigma c_r \Delta t)] \quad (3)$$

After it has been determined that a particle collision occurs the simulation must perform the collisions. CEX collisions occur when an ion strikes a neutral and the ion deposits its charge on the neutral particle. The result of the collision is an ion with a velocity based on the Maxwellian distribution at the thermal velocity of the neutral gas (Equation 4) in a random direction. The final velocity is obtained by sampling the Maxwellian approximation given by Equation 5, where R_i is a random number between zero and one⁹ and M is the number of random numbers and is equal to 3.

$$V_{th} = \sqrt{\frac{2kT}{m}} \quad (4)$$

$$V_n = V_t \left[\sum_{i=1}^M R_i - \frac{M}{2} \right] \left[\frac{M}{12} \right]^{-1/2} \quad (5)$$

B. Variable Hard Sphere Collisions

VHS collisions differ from CEX collisions in that two particles must be paired together to conserve momentum. First, the particles must be grouped into cells and then each particle is paired with a random target particle. The collision cross-section used for calculating the collision probability for VHS collisions is listed in Equation 6.⁵ The probability of a VHS collision is a couple of orders of magnitude lower than that of CEX collisions.

$$\sigma_{VHS} = \frac{8.2807 \times 10^{-16}}{c_r} \quad (6)$$

The probability of collision is calculated using the VHS collision cross-section and the relative velocity between the source and target particles. This process is the same as the CEX collision process. If a collision occurs for a VHS collision then the collision is performed. The random angles, χ and η , are chosen between the two particles and an elastic collision is performed along that angle. The angle χ is defined in Equation 7 and the angle ϵ is a random number between zero and 2π .

$$\chi = \cos^{-1}(2rnd - 1) \quad (7)$$

After the collision angle is determined, the center of mass velocity, c_m , can be calculated using the masses and velocities of the two particles (Equation 8). Next, the particle collision adjustment velocity, w , can be calculated using the collision angles and the relative velocity between the particles (Equation 9).

$$\vec{c}_m = \frac{m_s}{m_s + m_t} \vec{v}_s + \frac{m_t}{m_s + m_t} \vec{v}_t \quad (8)$$

$$\vec{w} = c_r \cos(\chi) \hat{i} + c_r \sin(\chi) \cos(\epsilon) \hat{j} + c_r \sin(\chi) \sin(\epsilon) \hat{k} \quad (9)$$

The final velocities of the collided particles can be determined using the particle collision adjusted velocity, particle masses and the center of mass velocity (Equations 10-11).

$$\vec{c}_s = \vec{c}_m + \frac{m_s}{m_s + m_t} \vec{w} \quad (10)$$

$$\vec{c}_t = \vec{c}_m + \frac{m_t}{m_s + m_t} \vec{w} \quad (11)$$

III. Design of Simulation

A. AFRL Experiment

The simulations used for this paper is modeled after a vacuum tank experiment performed at AFRL. The vacuum tank (Figure 1) is a cylindrical tank with a diameter of 1.8 meters and a length of 2.5 meters. The pressure of the tank during use is approximately 7×10^{-4} Pa and the vacuum is maintained by two cryogenic vacuum pumps. Graphite plates were placed in the tank to reduce sputtering of the chamber wall material.⁷

The thruster used for this experiment is a Busek BHT-HD-600 Hall Thruster with an input power of 600 W and a thrust of 36 mN. The thruster has a mass of 2.5 kg and dimensions of 100x100x66mm with the annulus diameter 56 mm. The mass flow rate of Xenon propellant of the thruster is approximately 2 mg/s and the thruster has a specific impulse of 1500 sec. The thruster has a discharge voltage of 300 V and an efficiency of approximately 46%.⁶

The thruster fired in the AFRL Chamber 6 and current data was collected during the experiment. A Faraday probe sweep at 60 cm was performed in the plume of the thruster to measure current density. The current density is plotted as a function of the angle between the probe and the thruster exit to create a baseline for the simulations conducted in this paper.

B. DRACO Simulations

The virtual vacuum tank (Figure 2), used in the simulations discussed in this paper, is modeled as cylinder containing graphite panels, vacuum pumps and thruster inside. The virtual tank has the same approximate



Figure 1. Photograph of AFRL Vacuum Tank

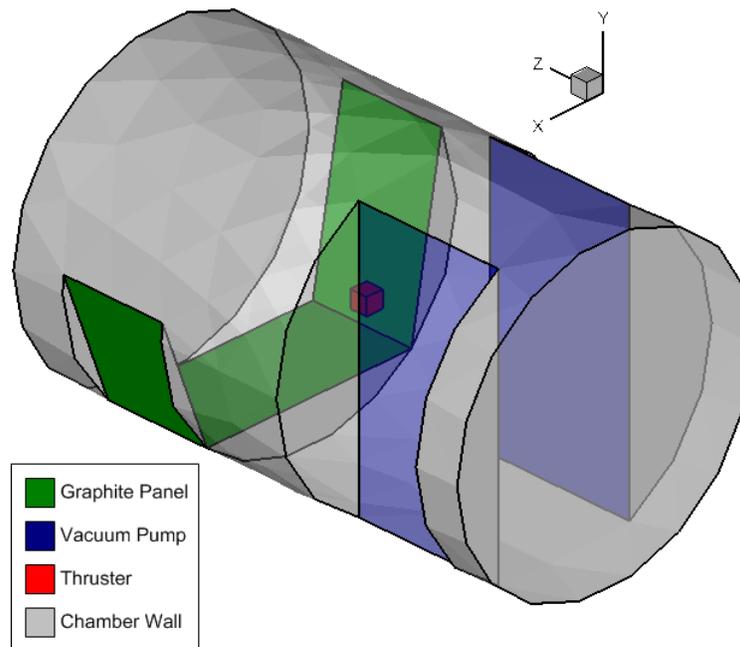


Figure 2. Geometry of "Virtual" Vacuum Tank used in Simulations

dimensions as AFRL tank. The thruster is firing in the positive z-direction and the source model for the thruster is based on LIF data taken from the Busek Hall Thruster.

For this paper, DRACO is used to perform the analysis of the plasma plume simulations.⁸ DRACO is a Particle in Cell (PIC)¹ finite element code developed at Virginia Tech as part of the AFRL Coliseum¹⁰

project. A Boltzman solver is used for this paper with a polytropic temperature model (Equation 12).

$$T = T_o \left(\frac{n}{n_o} \right)^{\gamma-1} \quad (12)$$

The PIC mesh used by DRACO is a Cartesian mesh with 38 cells in the X/Y-direction and 56 cells in the X-direction. The cells are cubes with sides of length 0.05 meters. The particle-surface collisions are handled through a newly developed DRACO algorithm based off of material types. Materials are specified for all the components of the vacuum tank so that different collision models each. When particles collide with the vacuum tank walls or the graphite plates they fly off diffusely from the point of intersection. However, the particles are removed from the simulation when they collide with the vacuum pump.

The purpose of this paper is to study the effect of particle collision modeling on simulation results. This paper will consider both collision models as well as two different collision types, Charge Exchange (CEX) and Variable Hard Sphere (VHS). This paper will consider the following test cases:

1. No Collisions

This test case tracks no particle collisions and is the simplest of all the test cases.

2. MCC with CEX Collisions only using a Projected Background Neutral Density

This test case uses MCC and only consider CEX collisions. MCC uses a background neutral density to determine the frequency of particle collisions. However, this background density must be updated with time because the neutral density of the vacuum chamber is not constant. The thruster will discharge about a tenth as many neutrals as ions and this will increase the neutral density around the thruster. For this simulation, an analytical model will be used to create the updated neutral background density. This will save significant time because the neutral particles will not require tracking during the simulation.

3. MCC with CEX and VHS Collisions using Simulated Neutral Particles

This test case uses MCC and consider both CEX collisions as well as VHS collisions. This requires the use of actual simulated neutral particles for updating the neutral density of the simulation. Tracking the neutrals for this simulation is problematic because the number of iterations required to reach a steady state solution is greatly increased. The number of tracked particles by the simulation will also be significantly increased.

The test cases described above were run until steady-state was achieved. The test cases were also run at three background neutral densities: the experimental density ($n = 2 \times 10^{17}$), perfect vacuum ($n = 0$) and a “Good” vacuum tank neutral density ($n = 2 \times 10^{16}$). The purpose of this is to determine when collisions can be ignored. The results of the simulations are discussed in the following section.

IV. Results

A. Comparison to Experimental Results

The data collected by the probe is used to validate the results of the code and compare the results of the different test cases. A virtual probe was created in DRACO to collect current density measurements during the simulation. This probe was placed 60 cm away from the thruster exit and collected current density data after the simulation reached a steady-state solution. The experimental data and the results of the simulations are plotted in Figure 3 for all of the test cases.

Figure 3 shows that the results of the current density probe for the test case with no collisions are decent in the plume region but do not match well after approximately 25 degrees. When there are no collisions in the plume, the beam remains narrow and the probe does not observe any current density beyond 40 degrees. Despite the poor agreement outside the plume region, the time for the simulation was less than 6 minutes. This test case shows that if no collisions are considered the results are a good order of magnitude approximation in the plume region.

The results of the test case with CEX collisions using a projected background neutral density are also listed in Figure 3. The results in the plume region match the experimental results more closely than the

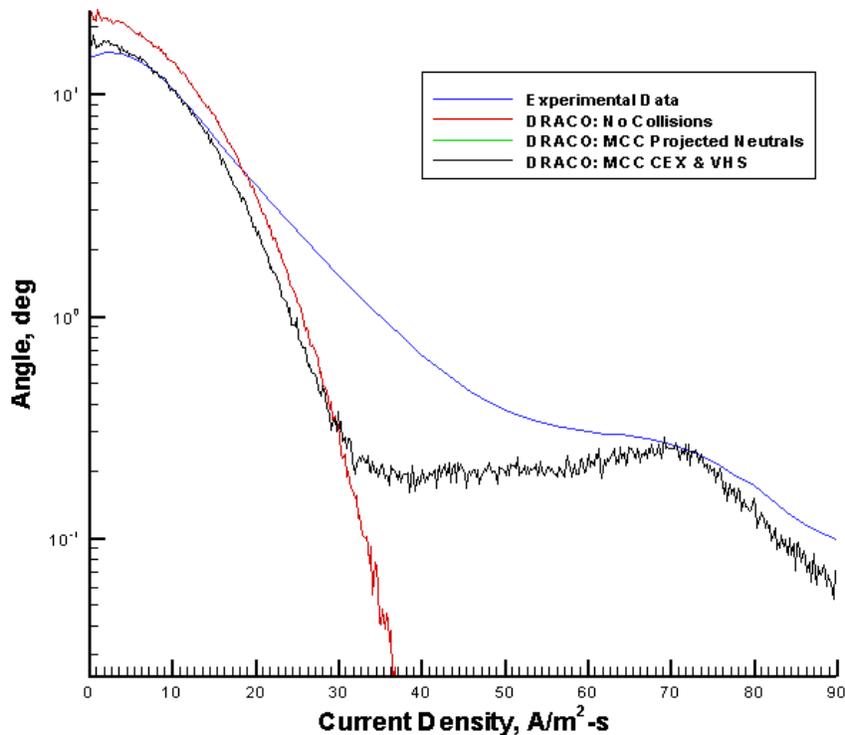


Figure 3. Plot of Simulation Results and Experimental Data

previous test case with no collisions. Additionally, the results outside the plume region match considerably better for this test case. The curve diverges from the experimental results at approximately the same location as the test case with no collisions and then matches the experimental results again from approximately 70 to 90 degrees. This is the charge exchange region. The effect of collisions on the results of the simulation is obvious in these results. The collisions cause the plume to expand. The results of this test case are an improvement over the simulation with no collisions but are still not perfect. The processing time for this simulation was under 6 hours.

The results of the final test case using MCC for CEX and VHS collisions models neutral particles with a uniform background density instead of a projected background density. The results of this test case are also plotted in Figure 3. The plot shows that for this test case the results in the plume region also match the experimental data very well as well as the charge exchange region. The area between the plume and charge exchange region has improved for this test case. This is mainly due to the addition of scatter collisions to the simulation. The results of this simulation are by far the best of the test cases but the processing time for the simulation was over 24 hours.

B. Effect of Neutral Density

The background neutral density used in the simulations has a major impact on the number of particle collisions. The previous section shows that at relatively high neutral densities the results are very dependant on particle collisions. Although it is obvious that at high neutral densities it is important to track particle collisions but it is still not known at what neutral density particle collisions are important. To determine when particle collisions are important the simulations above are run again at different neutral densities. The two other densities investigated in this paper are perfect vacuum and an improved vacuum tank with a background neutral density an order of magnitude lower then the AFRL tank (2×10^{16} particles/ m^3). In both cases the neutral particles discharged from the thruster due to inefficiencies are tracked in the simulation.

The results of the simulation without particle collisions are not affected by the neutral particle density. The results of the simulation using a projected background neutral density with CEX collisions only are

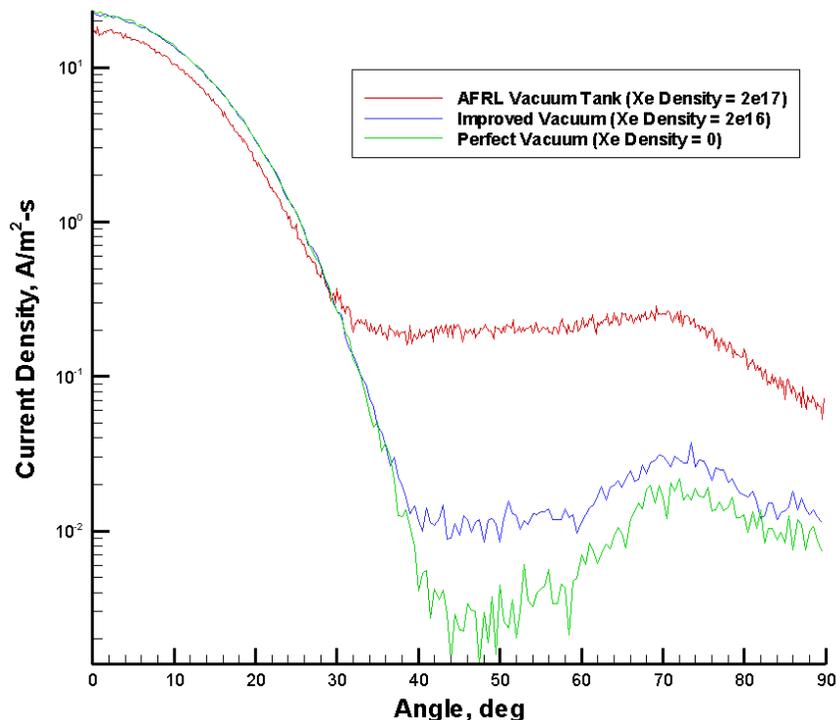


Figure 4. Plot of Simulation Results at Different Neutral Densities for Projected Background Neutral Density with CEX Collisions only

plotted in Figure 4.

The current density results shown in Figure 4 show that the plume region is not significantly affected by the neutral density. The results of all three densities are almost exactly the same up to an angle of thirty degrees but from thirty to ninety degrees the current density drops by approximately an order of magnitude for the two lower densities. The results for the two lower densities are approximately the same because of the projected background density produced by neutral particles drifting out of the thruster. The projected background density produced by the thruster contains areas with densities on the order of magnitude of 10^{16} particles/ m^2 .

The current density results for the test case using simulated particles with CEX and VHS collisions are shown in Figure 5. Again, the effect of the neutral density on the plume region is minimal. Outside the plume region the neutral density has a major impact on the current density.

V. Conclusion

Although particle collisions increase the processing time of simulations they are often necessary for acceptable results. Simple order of magnitude results in the plume region can be obtained without the use of collisions but outside the plume region the results are not good. Using a projected background neutral density, instead of simulating neutral particles, can be used to decrease processing time while maintaining good results.

VI. Acknowledgements

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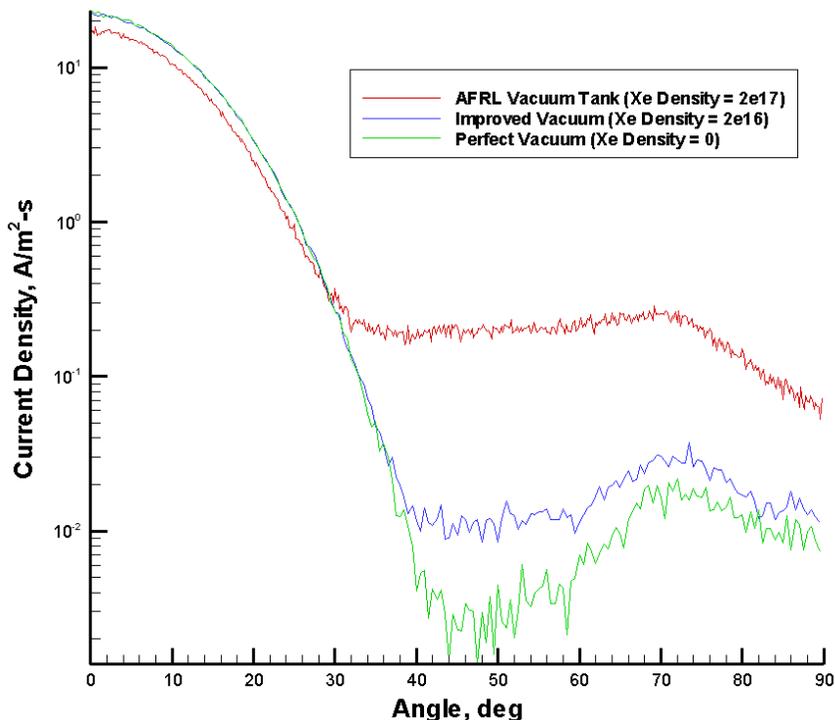


Figure 5. Plot of Simulation Results at Different Neutral Densities with Simulated Particles with CEX and VHS Collisions

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