

Fully kinetic simulations of ion thruster plumes using PIC-DSMC

IEPC-2019-A-529

Presented at the 36th International Electric Propulsion Conference

University of Vienna, Austria

September 15-20, 2019

Revathi Jambunathan* and Deborah A. Levin†

University of Illinois, Urbana-Champaign, Illinois, 61801, USA

Ion thruster plumes, consisting of neutrals, ions, and electrons, interact with the spacecraft surface and the solar panels in the backflow region, affecting their performance. Therefore, an understanding of the plume characteristics, the charge-exchange reactions, and ion energy distribution in the backflow region plays an important role in the design of such thrusters. Generally, ion thruster plumes are modeled using an electron fluid model or a single-temperature Boltzmann relation to obtain the electric potential under the assumption of quasi-neutrality. However, these approaches assume quasi-neutrality and do not model the neutralization mechanism which affects the plume characteristics and ion backflow. In this work, we model the plasma species using a Particle-In-Cell approach to self-consistently compute the induced electric field as well as the momentum and charge-exchange collisions using Direct Simulation Monte Carlo (DSMC). The neutralization mechanism is resolved accurately as electrons are modeled as particles and its effect on the backflow ion energy distribution is studied by comparing backflow characteristics with the Boltzmann simulation.

*Department of Aerospace Engineering, University of Illinois, Urbana-Champaign, rjambunathan@lbl.gov

†Professor, Department of Aerospace Engineering, University of Illinois Urbana-Champaign, deblevin@illinois.edu.

Nomenclature

n_{io}	= thruster exit ion number density
ρ_o	= thruster exit charge density
ρ_e	= electron charge density
ρ_i	= ion charge density
ϕ	= electric potential
ω_{peo}	= electron plasma frequency
Δt	= time step

I. Introduction

Electric propulsion (EP) devices generate thrust by accelerating ionized propellant using an electric or magnetic field to generate high exhaust velocities.¹ The exhaust plasma plume consists of high-speed ions and neutrals, which undergo charge-exchange collisions to generate slow CEX ions.¹ These CEX ions are influenced by the electric field induced between the plume and the spacecraft surface, resulting in their backflow. Consequently, the backflow CEX ions impinge on solar panels and spacecraft surfaces, altering their surface properties as well as causing surface erosion and eventual failure. To prevent charge build-up within the plume, an external hollow cathode is mounted on the spacecraft to emit a beam of electrons in order to neutralize the plume. Inclusion of these electrons in modeling of plasma plumes is essential as it modifies the induced electric field and in turn affects plasma-spacecraft interactions. Furthermore, the location of the hollow cathode also plays an important role on the plume dynamics.² The focus of this work, therefore, is to study the effect of electron source location on the plume dynamics.

Numerical simulations of thruster plumes must model both the CEX collisions and the self-consistent electric field, since they are the primary driving mechanisms for the plume evolution and ion backflow. Since the thruster plume density is low ($\sim 10^{15}/\text{m}^3$), the continuum approach is not valid and particle-based methods are required. Typically, Monte-Carlo Collision (MCC)³⁻⁶ or Direct Simulation Monte Carlo (DSMC)⁷⁻⁹ methods are used to model the CEX collisions. Particle-In-Cell (PIC) is a kinetic particle-based approach that accurately computes the self-consistent electric field based on the spatial distribution of the charge species (ions and electrons) in the domain. However, to keep the computational cost of the simulations tenable, hybrid approaches have been used, where the ions are modeled as particles and the electron distribution is obtained using a model. One of the widely used assumptions to characterize the electron distribution is quasi-neutrality at a constant electron temperature, because it gives an analytical Boltzmann relation to compute the electric potential variation.⁷ However, it is well-known that due to the expansion of the plasma plume, the electron temperature is not constant. To account for this decrease in the electron temperature, a polytropic relation has been used in some works, where the isentropic exponent is chosen by using fits to experimental data.¹⁰ An electron fluid model has also been used to model thruster plumes,^{11,12} however, even in these approaches, the

conservation equations were modified to a Poisson-like form by assuming quasi-neutrality and steady-state. Recently, a non-linear hybrid approach has been demonstrated for plasma plume studies by Cichoki *et al.*,¹³ where the simulation domain was divided into neutral and non-neutral regions. However, these hybrid approaches also assumed quasi-neutrality and the effect of a shifted electron source on the plume characteristics, such as that used in a real ion thruster configuration were not studied.

In this work, we perform fully-kinetic, coupled, Particle-In-Cell (PIC)/ Direct Simulation Monte Carlo (DSMC) simulations using our in-house solver called Cuda-based Hybrid Approach for Octree Simulations (CHAOS)¹⁴ to study the effect of the crucial charge-exchange collisions on the plume characteristics and backflow contamination region. The PIC and DSMC modules are invoked to compute the electric field and neutral-neutral as well as neutral-ion collisions that dominate the evolution of ion thruster plume simulations. Since the masses and velocities of the plume species, namely, neutrals, ions, and electrons, differ by orders of magnitude, we use species weighting factors and different timesteps to efficiently and accurately track the particle kinetics. A brief description of the numerical method, the charge-conserving energy-based boundary condition, and problem set-up is given in Sec. II. We perform simulations with colocated and separated electron-ion sources to study the effect of electron source location on the neutralization mechanism and plume characteristics. We also compare the flow-field properties from the fully-kinetic PIC-DSMC simulations with those obtained from the Boltzmann approach to study the assumption of quasi-neutrality and constant electron temperature on the backflow characteristics. Finally, we present the steady-state plume characteristics as well as CEX ion distribution obtained from the colocated and separated electron-ion configurations in Sec. III and IV, respectively.

II. Numerical Method and Simulation Set-Up

The flow-chart illustrating the coupled PIC-DSMC framework in CHAOS is shown in Fig. 1. The steps involved in the PIC and DSMC approaches are categorized in the code as modules, which is symbolically shown in Fig. 1 by placing the DSMC steps in one box and the PIC steps in another. Particle data is transferred to each module, where the velocity and acceleration of the particles are updated depending on the respective physical process modeled, namely, collisions in DSMC and electric field in PIC. The DSMC module alters the velocity of the xenon neutrals and ions through the momentum and charge-exchange collisions computed between the two species. The PIC module computes the self-consistent electric field based on the distribution of the charged particles and alters the acceleration and velocity of the charged particles, namely, ions and electrons. Using the updated velocity and acceleration obtained from the PIC and DSMC modules, the particles are moved to new positions using the leap-frog scheme and the species-dependent timestep. After movement, those particles that cross the computational boundary are treated with the appropriate boundary conditions. This procedure of updating particle velocities and acceleration from the PIC and DSMC modules and updating their position using the leap-frog method constitutes one cycle or one iteration.

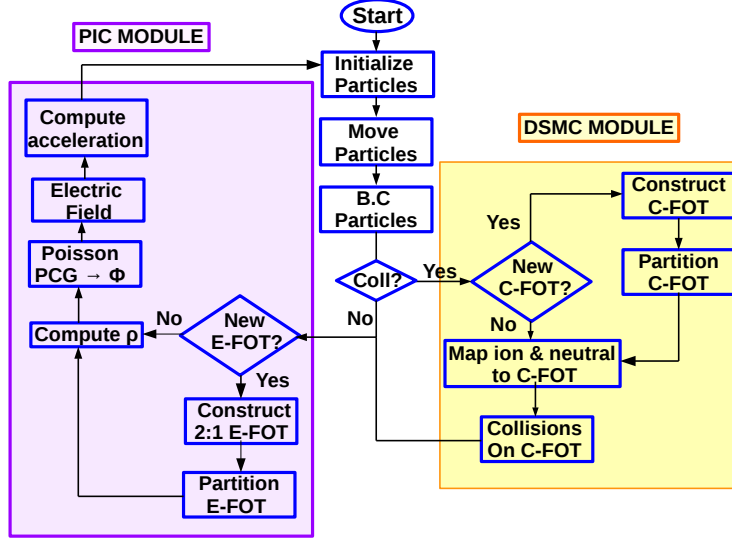


Figure 1: Flowchart for the PIC-DSMC framework in CHAOS

The details of the numerical strategies used to couple the PIC and DSMC modules in CHAOS is discussed in Ref.¹⁵ For typical ion thruster operational conditions, the local Debye length is two orders of magnitude smaller than the local mean free path which govern the PIC and DSMC modules. To reconcile these disparate length-scales, two separate linearized forest of octrees (FOTs) are used for the PIC and DSMC steps. Additionally, since the timestep required for the numerical stability of the explicit PIC approach is two orders of magnitude smaller than that required to model significant number of CEX collisions, a time-slicing methodology is used where the DSMC module is invoked after every 100 to 500 PIC timesteps. A new charge-conserving energy-based boundary condition developed in our recent work is used to overcome the ‘numerical pump-instability’ caused by the widely used outflow boundary condition for simulations with a kinetic treatment for electrons. Coupled PIC-DSMC simulations are performed for a colocated and separated electron-ion source with domain size of $(1.2 \times 1.2 \times 0.6)$ m and thruster exit ion number density on the order of $n_{io} = 10^{13}/\text{m}^3$ for this work.¹⁵

Ions are introduced at the thruster exit with a Gaussian distribution and a beam divergence angle of 12° , which is representative of ion thruster plumes.^{1,7} Electrons are initialized with a full Maxwellian in the cross-stream direction and a half-Maxwellian in the stream-wise direction at a temperature of 2 eV. The electron timestep is such that $\Delta t_e < 0.1\omega_{peo}^{-1}$, which results in a timestep of 2.8×10^{-10} for the low case presented in this paper. The ions move with the same timestep as the electrons and the PIC module is invoked at the electron timescale. However, to account for the disparate timescales, the DSMC module is invoked every 100 PIC timesteps for the low density cases. It should be noted that for the Boltzmann simulation electrons are not explicitly modeled. Therefore, a higher ion timestep of 2.8×10^{-8} s can be used for these simulations due to the assumption that the electron and ion

charge density are equal everywhere in the domain. A detailed description of the numerical strategies of coupling PIC-DSMC and the set-up of the simulations is described in Ref.15. Comparisons of the fully-kinetic and Boltzmann approaches on the flow-field characteristics is discussed next in Sec. III.

III. Comparison of Fully-kinetic and Boltzmann simulation - Colocated electron-ion sources

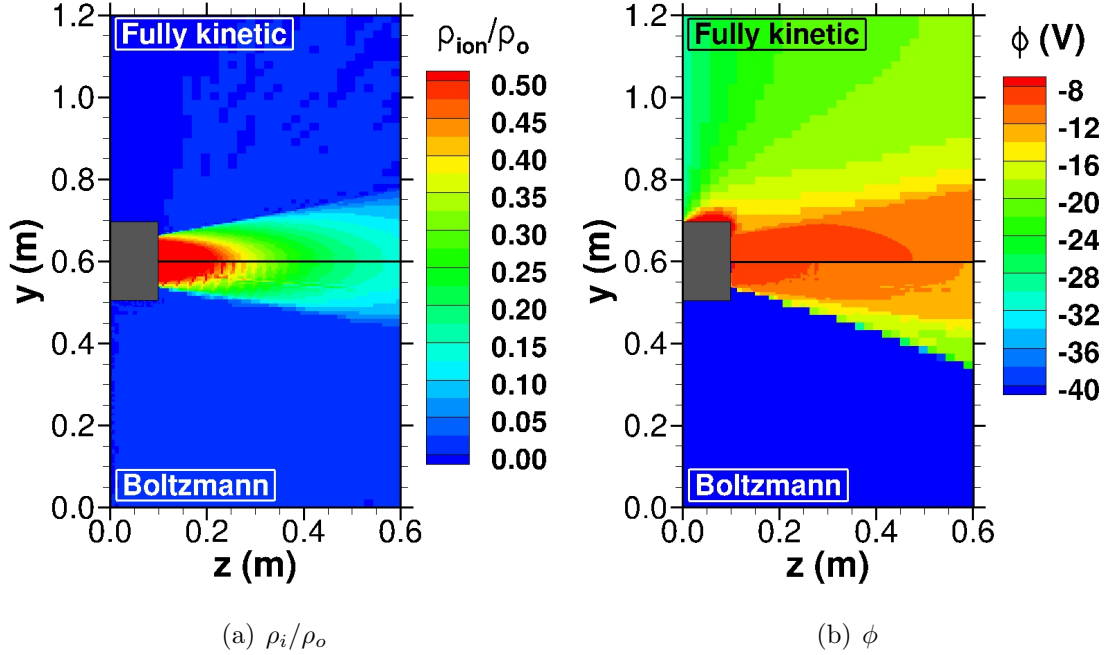


Figure 2: Comparison of ion charge density normalized by $\rho_o = e \cdot n_{io}$ and electric potential obtained from fully kinetic case (top) and Boltzmann simulation case (bottom).

The effect of assuming a Boltzmann relation for the electric potential is assessed by comparing the flow-field properties from the Boltzmann simulation with those obtained from the fully-kinetic PIC-DSMC simulation. Neutral-neutral and ion-neutral collisions are performed in both the simulations, however, the differences between the two simulations occur due to the different approaches used for computing the electric field. For the fully kinetic case, the self-consistent electric potential is obtained by solving the electrostatic Poisson's equation, while for Boltzmann case, the electric potential is obtained from the Boltzmann relation.⁷ Note that, the value of the reference potential, (ϕ_o) and reference number density (n_o) used for the Boltzmann equation are set equal to the thruster exit potential and initial ion number density obtained from the fully PIC simulation. The electric field for the fully-kinetic simulation reached steady-state after $t = 42 \text{ } \mu\text{s}$, i.e., $t\omega_{peo} = 7500$, and the CEX ion number density in the domain reached steady-state after $t = 280 \text{ } \mu\text{s}$. The difference in the time-scale

required for the electric field and CEX number density to reach steady-state, respectively, allowed us to turn off the Poisson solver after the steady-state electric field was sampled for 50,000 timesteps beyond $t=42 \mu\text{s}$. The sampled electric field was then used to perform DSMC collisions and move the charged ions species, until the CEX ions in the domain and the backflow region reached steady-state.

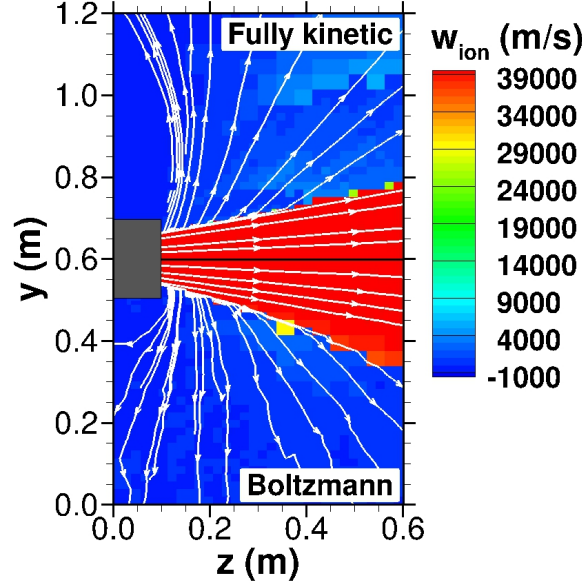


Figure 3: Comparison of Xe^+ streamwise velocity variation obtained from the fully kinetic simulation and Boltzmann simulation (bottom), along with their respective three-dimensional ion velocity streamlines.

A comparison of the steady-state ion charge density distribution normalized by the initial thruster exit ion charge density, $\rho_o = e \cdot n_{io}$, across the $y-z$ plane passing through the center of the domain, obtained from the fully-kinetic and Boltzmann simulation is shown in Fig. 2(a). The variation of ion charge density in the plume core region predicted from the two methods are in agreement, suggesting that the use of the Boltzmann relation for the electric potential does not significantly affect the ion density in the plume core-region. A comparison of the corresponding steady-state electric potential is shown in Fig. 2(b). Even though the electric potential in the plume core region are in agreement within 2-4 V, the potential predicted by the Boltzmann case in the region surrounding the plume is significantly lower compared to the fully kinetic case. In some regions outside the plume, the ion number density is zero, and therefore, to prevent the logarithm term in the Boltzmann relation from blowing up in the Boltzmann simulation, a floor value of $n_e = 1 \times 10^5 / \text{m}^3$ is used. The sudden drop in the ion density and the use of a floor value to model $n_e = n_i$ everywhere in the domain, causes the potential to abruptly decrease at the radial edge of the plume for Boltzmann relation case, as shown in Fig. 2(b). In contrast, the electric potential obtained from the fully kinetic simulation decreases gradually in the radial direction as observed from Fig. 2(b).

The near-field potential surrounding the electron-ion sources at the thruster exit is equal to the imposed Dirichlet value of 0 V for the fully-kinetic simulation, while for the Boltzmann simulation, it decreases to -40 V, as shown in Fig. 2(b) since the Boltzmann relation does not directly account for the electric potential or electric field boundary conditions.

The spatial variation of the streamwise ion velocity in the $y - z$ plane extracted at the center of the domain and the three-dimensional ion velocity streamlines, obtained from the fully-kinetic and Boltzmann simulations are compared in Fig. 3. From the spatial variation of streamwise ion velocity, it can be seen that the plume predicted by the Boltzmann case is wider than that for the fully kinetic case due to the higher radial electric field obtained for the Boltzmann plume as seen from the gradient in the electric potential shown in Fig. 2(b). For both cases, the xenon ions flow radially outwards with some ions flowing towards the solar panel due to the lower potential in the backflow region. However, because the Boltzmann case predicts a rapid decrease in the potential both radially as well as in the z -direction as shown previously in Fig. 2(b), the slow CEX ions impinge on the solar panel in the backflow region at a higher angle of incidence, compared to the shallower angles observed for the streamlines from the fully-kinetic case.

IV. Effect of electron source location on plume characteristics

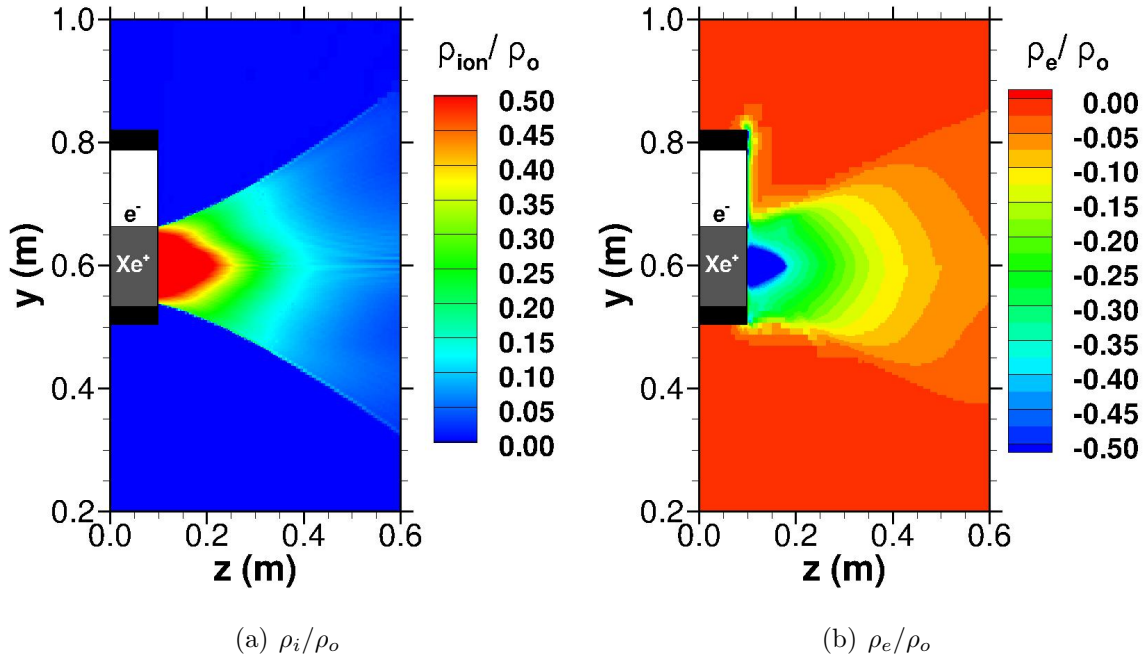


Figure 4: Spatial variation of the ion and electron charge density normalized by $\rho_o = e \cdot n_{io}$ in the $y - z$ plane obtained for the fully kinetic simulation with a shifted electron source.

The electric field for the low density simulation with separated electron-ion sources

reached steady-state after 80,000 PIC timesteps, i.e., $t\omega_{peo} = 4000$, or $t = 22.4$ s. Similar to the colocated cases, the Poisson solver module was by-passed after the electric field was sampled for 50,000 timesteps after reaching steady-state. This sampled electric field was used to continue the DSMC collisions which required an additional 20,000 DSMC collision timesteps to reach steady-state. The steady-state spatial variation of ion and electron charge densities, normalized by $\rho_o = e \cdot n_{io}$, in the $y - z$ plane extracted at the center of the domain are shown in Figs. 4(a) and 4(b), respectively. In both figures, the ion and electron sources are indicated by the grey and white blocks, and the black region surrounding them represents the thruster geometry. Comparison of the spatial variation of the ion and electron charge densities shows that, even though the electrons are emitted from a separate source, at steady-state, they become trapped within the positively charged ion plume, thus neutralizing the net-charge within the plume. The ion charge density is maximum near the thruster exit, at $z=0.1$ m, and decreases rapidly as the plume expands. Consistent with the variation in the ion charge density, the electron charge density is maximum at the thruster exit, where the ion charge density is maximum, and decreases downstream due to the expansion of the ion beam. The self-consistent electric field that attracts the electrons towards the plume, also causes the ions within the plume to repel each other, resulting in a stronger ion beam expansion for the shifted electron source simulation, shown in Fig. 4(a), compared to that obtained from the colocated case, shown previously in Fig. 2(a).

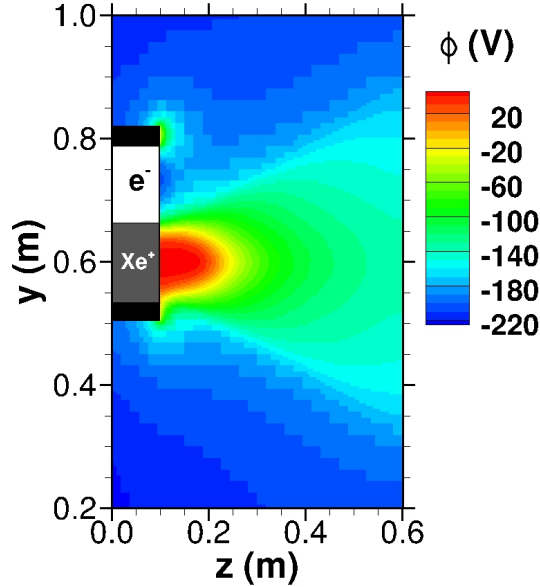


Figure 5: Spatial variation of the steady-state electric potential along the $y - z$ plane from the fully kinetic case with a shifted electron source.

The steady-state electric potential variation along the $y - z$ plane, obtained for the fully kinetic simulation with separated electron-ion source is shown in Fig. 5. The electric potential is a maximum at the thruster exit with a value of 40 V and decreases gradually to

a negative value in the streamwise direction. Near the electron source, at $y=0.725$ m, the potential drops to -190 V due to the concentration of electron charge density after emission. The potential in the vicinity of the sources at $z=0.1$ m is 0 V due to the Dirichlet boundary condition implemented on the leading edge of the thruster body, which is represented by the black block shown in Fig. 5. In addition to the difference in the plume characteristics, the fully kinetic simulation of the separated ion-electron simulation also results in a more negative potential in the region surrounding the plume compared to the colocated case, shown in the top half of Fig. 2(b). Since electrons are emitted with a high thermal velocity component and the electron source is shifted from the ion source, a substantially higher number of electrons escape the attraction of the positively charged plume compared to the colocated case, where electrons are trapped more efficiently within the plume core-region. As a result, the potential within the plume core-region is more positive for the shifted case compared to the colocated case, and since the electrons are lost to the region surrounding the plume, the potential outside the plume is more negative than that obtained for the colocated case, shown previously in Fig. 2(b). The separation of electron-ion sources thus increases the radial electric field compared to the colocated plume, causing a stronger (or broader) ion plume expansion for the shifted electron source case, as shown in Fig. 4(a) compared to the colocated case shown previously in the top half of Fig. 2(b). The differences in the electric

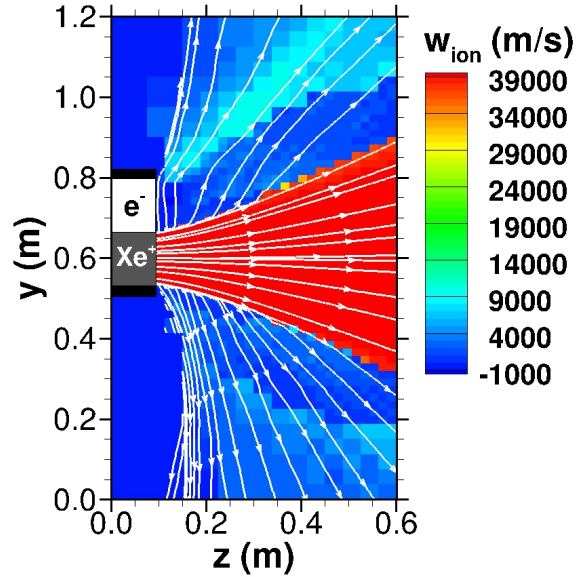


Figure 6: Streamwise ion velocity variation along the $y - z$ plane with velocity streamlines obtained from the fully kinetic shifted electron cases with CEX collisions.

field due to the shift in the electron source affects the acceleration and the distribution of the slow CEX ions in comparison to that obtained for the colocated plume. The three-dimensional ion velocity streamlines for the fully kinetic simulation with separated electron-ion sources is shown in Fig. 6. Similar to the colocated case shown in the top half of Fig. 3,

the slow CEX ions generated in the core-region of the plume with a shifted electron source are attracted by the radial electric field and flow radially outwards to the region surrounding the plume. However, in contrast to the colocated case, the three-dimensional ion velocity streamlines in the separated electron-ion case do not backflow to the region upstream of $z < 0.1$ m. This difference in the trajectory of the CEX ions is due to the difference in the electric field obtained for the colocated and separated electron-ion configurations.

For the shifted electron source, the maximum radial electric field is 2200 V/m, which is an order of magnitude stronger than the -100 V/m axial electric field.¹⁶ Since the radial electric field is stronger, it drives the ions primarily in the radial direction and thus the backflow is negligible compared to that observed for the colocated case. Due to the potential gradient from 40 V at the ion source to -190 V at the electron source, shown in Fig. 5, some slow CEX ions are attracted towards the electron source as indicated by the trajectory of the ion streamlines at $z=0.1$, for $y > 0.68$ m, in Fig. 6. However, this flow of ions towards the electron source is mainly due to the wide radius of the electron source generating a large area with negative potential, which is not typically observed in real ion thrusters with smaller hollow cathode radius. The simulations with higher number density and smaller electron source with realistic radius is performed in Ref. 16.

V. Conclusions

Coupled PIC-DSMC simulations of ion thruster plumes are performed to study the ion characteristics in the backflow region. A new charge-conserving energy-based open boundary condition is used to enable steady-state plume simulations without numerical instabilities. Comparison of fully-kinetic simulation with the Boltzmann approach demonstrate that resolving the electric field accurately is crucial for accurate predictions of the backflow ion characteristics. The electron source location affects the neutralization mechanism which in turn affects the electric field variation and as a result, the ion backflow characteristics. The effect of electron source location and thruster exit number density on the ion energy distribution in the backflow region and electron kinetics is studied in detail in our recent work.^{15,16}

Acknowledgments

We are grateful for the funding support provided by AFOSR through the Grant AF FA9550-16-1-0193. This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications. We also acknowledge Xsede for the computational resource on XStream.

References

- ¹Goebel, D. M. and Katz, I., *Fundamentals of electric propulsion: Ion and Hall thrusters*, Vol. 1, John Wiley & Sons, 2008.
- ²Xu, K. G. and Walker, M. L., “Effect of External Cathode Azimuthal Position on Hall-Effect Thruster Plume and Diagnostics,” *Journal of Propulsion and Power*, Vol. 30, No. 2, 2014, pp. 506–513.
- ³Taccogna, F., “Monte Carlo Collision method for low temperature plasma simulation,” *Journal of Plasma Physics*, Vol. 81, No. 1, 2015.
- ⁴Bondar, Y. A., Schweigert, V., and Ivanov, M., “Modeling of the Hall-Effect Thruster Plume by Combined PIC-MCC/DSMC Method,” *AIP Conference Proceedings*, IOP Institute Of Physics Publishing Ltd., 2003, pp. 549–556.
- ⁵Birdsall, C. K., “Particle-in-cell charged-particle simulations, plus Monte Carlo collisions with neutral atoms, PIC-MCC,” *IEEE Transactions on Plasma Science*, Vol. 19, No. 2, 1991, pp. 65–85.
- ⁶Wang, J. and Brophy, J., “3-D Monte-Carlo particle-in-cell simulations of ion thruster plasma interactions,” *31st Joint Propulsion Conference and Exhibit*, 1995, p. 2826.
- ⁷Korkut, B., Li, Z., Levin, D., et al., “3-D Simulation of Ion Thruster Plumes Using Octree Adaptive Mesh Refinement,” *IEEE Transactions on Plasma Science*, Vol. 43, No. 5, 2015, pp. 1706–1721.
- ⁸VanGilder, D. B., Font, G. I., and Boyd, I. D., “Hybrid Monte Carlo-particle-in-cell simulation of an ion thruster plume,” *Journal of Propulsion and Power*, Vol. 15, No. 4, 1999, pp. 530–538.
- ⁹Hyakutake, T., Nishida, M., Kuninaka, H., and Toki, K., “DSMC-PIC analysis of a plume from MUSES-C ion engines,” *Transactions of the Japan Society for Aeronautical and Space Sciences*, Vol. 46, No. 151, 2003, pp. 24–30.
- ¹⁰Taccogna, F., Pagano, D., Scortecchi, F., and Garulli, A., “Three-dimensional plume simulation of multi-channel thruster configuration,” *Plasma Sources Science and Technology*, Vol. 23, No. 6, 2014, pp. 065034.
- ¹¹Boyd, I. D. and Crofton, M. W., “Modeling the plasma plume of a hollow cathode,” *Journal of Applied Physics*, Vol. 95, No. 7, 2004, pp. 3285–3296.
- ¹²Boyd, I. D. and Yim, J. T., “Modeling of the near field plume of a Hall thruster,” *Journal of Applied Physics*, Vol. 95, No. 9, 2004, pp. 4575–4584.
- ¹³Cichocki, F., Domínguez-Vázquez, A., Merino, M., and Ahedo, E., “Hybrid 3D model for the interaction of plasma thruster plumes with nearby objects,” *Plasma Sources Science and Technology*, Vol. 26, No. 12, 2017, pp. 125008.
- ¹⁴Jambunathan, R. and Levin, D. A., “CHAOS: An octree-based PIC-DSMC code for modeling of electron kinetic properties in a plasma plume using MPI-CUDA parallelization,” *Journal of Computational Physics*, Vol. 373, 2018, pp. 571–604.
- ¹⁵Jambunathan, R. and Levin, D., “Kinetic, three-dimensional, PIC-DSMC simulations of ion thruster plumes, Part 1: A colocated ion-electron source,” *submitted to IEEE Transactions on Plasma Science*, 2019.
- ¹⁶Jambunathan, R. and Levin, D., “Fully kinetic, three-dimensional, PIC-DSMC simulations of ion thruster plumes, Part 2: Separated ion-electron sources,” *submitted to Plasma Sources Science and Technology*, 2019.