Fully kinetic model of plasma expansion in a magnetic nozzle

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Received 23 November 2021, revised 26 January 2022
Accepted for publication 21 February 2022
Published 14 April 2022

Abstract

A self-consistent model is presented for performing steady-state fully kinetic particle-in-cell simulations of magnetised plasma plumes. An energy-based electron reflection prevents the numerical pump instability associated with a typical open-outflow boundary, and is shown to be sufficiently general that both the plume kinetics and plasma potential demonstrate domain independence (within 6%). This is upheld by non-stationary Robin-type boundary conditions on the Poisson’s equation, coupled to a capacitive circuit that allows physical evolution of the downstream potential drop in the transient. The method has been validated against experiments, providing results that fall within the uncertainty of measurements. Simulations are then carried out to study collisional xenon discharges into axisymmetric diverging magnetic nozzles (MNs). Particular discussion is given to the identification of a collision-enhanced potential well arising from chargeseparation at the plume periphery, the role of ion–neutral charge exchange, and a three-region piecewise polytropic cooling regime for electrons. The polytropic index is shown to depend on the degree of magnetisation. Specifically, in the region near the thruster outlet, the plume is weakly-magnetised due to the cross-field diffusion of electron-heavy particle collisions. Downstream, a strongly-magnetised region of near-isothermal expansion occurs. Finally, in the detached region, the polytropic index tends to that of a more adiabatic unmagnetised case. With an increasing MN field strength, an inferior limit is found to the average polytropic index of $\bar{\gamma}_e \sim 1.16$.

Keywords: particle-in-cell, fully kinetic, open boundary conditions, magnetic nozzle, magnetically-enhanced plasma thruster, collisional electron cooling

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of electric propulsion continues to receive much attention despite mature technologies such as ion and Hall effect thrusters establishing dominant flight heritage over the last two decades. However, such systems are increasingly being recognised as complex and high cost, particularly for small-satellite applications [1]. Therefore, in the last few years, particular effort has been made in the development of magnetically-enhanced plasma thrusters (MEPT). This broad category includes the helicon plasma thruster (HPT) [2–5], the electron cyclotron resonance thruster (ECRT) [6], and the applied field magnetoplasma dynamic thruster (AF-MPDT) [7]. In such systems, the plasma acceleration is driven by a magnetic nozzle (MN) [8]: a divergent magneto-static field generated by a set of solenoids or permanent magnets. The MN radially confines the hot partially-magnetised plasma beam and accelerates it supersonically via the conversion of thermal energy into directed axial kinetic energy, therefore enhancing thrust [9].
The HPT and ECRT are cathode-less devices, relying on electromagnetic waves for plasma production and heating [10, 11], while the AF-MPDT relies on annular electrodes. Since the resulting plasma beam is quasi-neutral, no additional neutraliser (e.g. a hollow cathode) is required. Thus, MEPTs are becoming an increasing option for low-thrust propulsion, being highly scalable, robust, light, low-cost and resistant to lifetime-limiting erosion [12]. MNs also have no physical walls, thus avoiding thermal loading and erosion issues. The first in-orbit demonstration of a radio-frequency MEPT took place from March 2021 by Technology for Propulsion and Innovation S.p.A. (T4i), with the 50 W ‘REGULUS’ thruster [12, 13]. At the same time, the present disadvantage of MEPTs is the relatively low thrust efficiency, generally <20% [2]. For MEPTs to be sufficiently efficient and competitive, a high ionisation ratio is mandatory (with electron temperatures of tens of eV [14–16]) or else the specific impulse achievable with the MN is limited.

The main MN physics is reasonably established and well-understood. In typical MEPTs, with magnetic fields in the 100–1000 G range, ions are weakly magnetised and are bound to the highly magnetised electrons through an ambipolar electric field, which develops to maintain quasi-neutrality [17, 18]. This results in a potential drop, both radially and axially, which confines most of the electron population while accelerating ions freely downstream. The potential drop self-consistently evolves to maintain a globally current-free plasma, ultimately determining the velocity of ions [19]. Nevertheless, there are many other aspects requiring further detailed investigation, such as the evolution of velocity distribution functions (VDF), plasma detachment, anisotropic electron cooling and doubly-trapped electron populations [20]. Specifically, the role of collisions in MN expansions is still poorly understood. At low operational power, where ionisation efficiency is <10%, neutral-collisional effects can impede ion acceleration near the thruster outlet [21]. It was conjectured that frequent collisions therefore shift the effective nozzle throat downstream, reducing thrust performance. Collisional effects were also recently studied numerically [22], where changes in the trapped electron population were observed to affect the downstream potential drop and corresponding plasma profiles. However, only electron Coulomb collisions were considered, relying on a simplified non-spatially dependant model.

Numerical efforts to understand MNs have involved both fluid and kinetic models, some of which make use of semi-analytical solutions [23, 24]. Two-dimensional (2D) fluid models have shown to be a powerful tool to understand the main phenomena [9]. However, their closure (i.e. a definition of non-local heat conduction) remains an elusive problem. One-dimensional (1D) stationary kinetic models of a MN have allowed analysis of the downstream ion and electron heat fluxes and the response to non-Maxwellian features of the ion and electron VDFs [25, 26]. However, except for 1D cases, solving the Boltzmann equation directly is often computationally intensive [27]. Both fluid and kinetic continuum approaches must further make assumptions regarding the VDF, one of the main impact parameters in magnetised plasma expansion [26]. Hence, numerical studies need to be extended to fully kinetic [28–31] or fluid-kinetic [32] approaches if the dynamics of a MN want to be treated self-consistently. The fully kinetic particle-in-cell (PIC) method represents the numerical strategy with the lowest level of assumptions. Both electron and ion populations are modelled as macro-particles, subject to the action of self-consistently computed electric and magnetic fields, as well as particle collisions [33].

PIC simulations operate by necessity on a finite domain. Due to the ambipolar potential drop along the MN, and for a typical meso-thermal plume (electron thermal velocity greatly exceeds the ion drift velocity and ion thermal velocity), most of the electron population will become trapped into the much-slower ion beam and reciprocate within the plume [34, 35]. Since the computational domain is finite, electrons may reverse their trajectories beyond the domain. If these electrons are non-physically deleted upon reaching the open boundaries, the so-called ‘numerical pump instability’ will arise [36, 37]. For this reason, simulations are usually stopped long before the ion beam reaches the open boundaries. Thus, most results in the literature deal with short time-scale transient plume expansions in small domains [38, 39].

Alternatively, to prevent the instability, an open model has been demonstrated where a virtual ion sink was implemented midway between the inlet and outer boundaries [36]. Ions are absorbed by the sink, while electrons can permeate through it, thus retaining the trapped electrons between the ion sink and the boundaries. Electrons are also reflected from the boundaries, based on global charge conservation. However, the sink must be located far from these boundaries, resulting in an unwelcome increase in the domain size. To overcome this limitation, another charge-conserving boundary condition has been proposed [40], where the number of electrons reflected at the open boundary is determined so as to maintain a globally-neutral plasma. Another approach, formulated to mimic the real physics, uses a current-free boundary condition [34]. This has been demonstrated via simulations of both a non-magnetised plume [34] and a MN [41]. The methodology proposed [34, 41] is well-founded concerning electron kinetics, but simplified conditions have been assumed for the solution of the electric field. A zero-Neumann condition was imposed at the open boundary to solve the Poisson’s equation. Such a condition is appropriate only in the limit of an infinitely large domain that encompasses nearly all the potential fall that occurs in the plasma plume. For this reason, the authors of [34] suggest ignoring the plasma dynamics in some portion of the domain near the open boundaries (e.g. ~20%). Indeed, this boundary condition does not generally provide results which are domain independent. A definition of consistent boundary conditions for treating both magnetised and unmagnetised plumes remains a challenging problem, not yet fully solved.

This article presents a new electrostatic fully kinetic PIC model for MN plasma expansions. Boundary conditions are introduced to improve on previous works in terms of both electron kinetics and the Poisson’s equation. Regarding the treatment of the electrons, a consistent approach has been
defined to selectively reflect or absorb parts of the population crossing the open boundaries. The proposed approach mimics the partial reflection of electrons that would take place further downstream (outside of the domain), by enforcing the integral current-free condition along the open boundaries and an energy-based reflection criterion. The total potential drop is self-consistently calculated to maintain the net-zero current and is included when determining a non-stationary Robin boundary condition on the plasma potential. The result is a set of mutually consistent boundary conditions, which is sufficiently general such that both the plume kinetics, and plasma potential distribution, are independent of the computational domain size and in good agreement with experiments [42].

The new model allows for significantly reduced domain sizes to be used compared to the previous state-of-the-art [34, 36], eliminating the boundary effects seen with the zero-Neumann closure in other works.

Furthermore, the model is the first to include the downstream potential drop as a self-consistent part of the solution, as well as its application in the definition of the boundary conditions. Finally, to best knowledge, this study is the first fully kinetic investigation to include a thorough analysis of collisions in a MN.

Section 2 summarises the key aspects of the PIC model and introduces the new boundary condition treatment. In section 3, the capability to produce a stable steady-state plume and a domain-independent solution is demonstrated. In section 4, the numerical approach has been benchmarked against measures of plasma density and plasma potential [42]. In section 5, the validated approach has been exploited to investigate the xenon plasma expansion in a collisional MN. The most relevant aspects analysed are: the presence of a collisionally-enhanced radial potential well that confines the plasma expansion, the role of collisions in the ion acceleration, the influence of the magnetic field intensity on the propulsive performance, and the electron cooling. The conclusions are then given in section 6.

2. Physical and numerical model

The model has been developed by adapting the fully kinetic 2D-axisymmetric PIC code Starfish, which has been used previously to model Hall thruster channels [43], ion thruster plumes [44] and the plume of a magnetically-enhanced vacuum arc thruster [45].

An overview of the simulation domain is shown in figure 1, consisting of a cylindrical 2D region (z, r). The plasma source has not been included, since the scope of this work is to simulate purely the plume expansion. Instead, ions, electrons and neutrals are injected through a boundary corresponding to the thruster outlet (I). The external boundaries (III) are treated as open to vacuum, connected to the thruster outlet (I) via a virtual free-space capacitance which ensures equal ion and electron current streams to the infinity at steady-state. Boundary (II) is the axis of symmetry.

Hereafter, the subscripts *, 0, b and ∞ shall refer to properties within the plasma source (reference), at the thruster outlet boundary (I), at the open boundaries (III) and at the virtual infinity respectively. The subscript B shall refer to the integral sum of local properties along the open boundaries. Likewise, the superscripts + and − shall refer to the forward and backward-marching components of the plasma properties.

2.1. Particle-in-cell simulation

The set of macro-particles \( p = 1, \ldots, N_p \) with positions \( \mathbf{r}_p^n = (r_p^n, \theta_p^n, \phi_p^n) \), velocities \( \mathbf{v}_p^n = (v_{r_p}^n, v_{\theta_p}^n, v_{\phi_p}^n) \), masses \( m_p \), and charges \( q_p \) describes the ion, electron and neutral g dynamics at the n-th time-step \( t^n = n \Delta t \). The particle motion is solved explicitly with the standard leap-frog Boris algorithm [46].
where $E_p^{n}$ is the electric field, and $B$ is the static background magnetic field. The movement of particles to new positions leads to a new distribution of charge density $\rho = e(n_i - n_e)$, where $n_i$ is the ion density, $n_e$ is the electron density, and $e$ is the elementary charge. It is computed by scattering particles to the mesh nodes using a second-order Ruyten shape factor $S_p$ [47],

$$\rho = \frac{1}{V} \sum_{p=1}^{N_p} q_p w_p S_p,$$

where $w_p$ is the macro-particle specific weight [46], and $V$ the mesh cell volume. The charge density is then used to solve for the self-consistent plasma potential $\phi$ according to the Poisson’s equation, using an explicit successive over-relaxation Gauss–Seidel scheme [37].

$${\varepsilon}_0 \nabla^2 \phi = -\rho,$$

where $\varepsilon_0$ is the vacuum permittivity. The electric field $E = -\nabla \phi$ is then updated for the next time-step. To comply with typical PIC stability criteria, the mesh spacing is kept below the expected Debye length $\lambda_D = \sqrt{\varepsilon_0 q_i T_k / n_e e^2}$, where $k_B$ is the Boltzmann constant.

In order to reduce the computational burden, a numerical acceleration scheme has been adopted. The vacuum permittivity is increased by a factor $\gamma^2$ and the mass of heavy species reduced by a factor $f$. This method does not require a scaled increase of the magneto-static field [41], which is particularly useful when handling a MN expansion so as not to impose intractable conditions on the time-step required to resolve the electron gyrofrequency $\omega_{ce} = |e|B/m_e$. The relationships between the simulated and physical constants, provided by $f$ and $\gamma$, are shown in equation (5). The direct consequences of these factors on $\lambda_D$ and plasma frequency $\omega_{pe}$ are provided in equation (6).

$$\tilde{m}_e = \frac{m_e}{f}, \quad \tilde{\varepsilon}_0 = \gamma^2 \varepsilon_0,$$

$$\lambda_D = \gamma \lambda_D, \quad \tilde{\omega}_{pe} = \frac{\omega_{pe}}{\gamma}.$$
at the thruster outlet $T_{0}$ since the dynamics of the backward-marching species are not known a priori (e.g., $f_{\gamma}$ might be non-Maxwellian). At the symmetry plane (II), all particles are specularly reflected.

Since ions are accelerated outward by the ambipolar electric field [19], no special treatment is required at the open boundaries (III); therefore ions reaching them are simply absorbed. Neutrals are also absorbed. For electrons, the behaviour is not as straightforward. Generating a stable steady-state plume without altering the electron kinetics requires an energy-based treatment [34]. Physically, two separate populations of electrons can be identified depending on their total energy, namely trapped and free. The former are the less energetic electrons that cannot overcome the potential drop that occurs across the plume. The trapped electrons are forced to turn back to the plasma source at a certain distance downstream. The free population are the electrons that do have energy enough to cross the potential drop and thus escape to infinity. Assuming a steady-state, and axisymmetric electric field, the total energy of each electron can be defined as

$$E_{e} = \frac{1}{2}m_{e}(v_{e}^{2} + v_{\gamma}^{2} + v_{\theta}^{2}) - e\phi(r),$$

where $E_{e}$ is a constant conserved quantity of the motion in the collisionless case. From energy conservation, trapped electrons are characterised by $E_{e} < |e\phi_{\infty}|$, while for free electrons $E_{e} \geq |e\phi_{\infty}|$. From these considerations, the following boundary condition is defined. When an electron reaches an open boundary node $b$, it’s kinetic energy is taken as $KE_{eb} = \frac{1}{2}m_{e}|v_{eb}|^2$, and then compared to the trapping potential $PE_{b} = e(\phi_{b} - \phi_{\infty})$.

- If $KE_{eb} < PE_{b}$ the electron is trapped, so it is reflected back with velocity $-v_{eb}$.
- Else, it is a free electron to be removed from the domain.

This boundary condition therefore allows the highest-energy electrons to escape, but retains the physical proportion of the trapped population, ensuring stability [34, 36]. Finally, the key assumptions in this energy-based boundary condition are, firstly, that the plasma is collisionless downstream of the open boundaries and that, beyond the domain, the magnetisation is not so strong as to induce reflection of highly energetic electrons [25].

2.4. Capacitive circuit

The value of $\phi_{\infty}$ is a non-stationary unknown and must be calculated self-consistently as part of the solution. From the energy-based criterion discussed in section 2.3, there is a value of $\phi_{\infty}$ that reflects sufficient electrons to maintain a current-free plume. Therefore, the value of $\phi_{\infty}$ is self-consistently controlled via a virtual free-space capacitance $C$. This approach mimics other plume/spacecraft interaction codes in which an equivalent electric circuit links the spacecraft and the plasma [54, 55]. The resultant control algorithm reads

$$\phi_{\infty}^{n+1} = \phi_{\infty}^{n} \cdot \left( \frac{1}{C}I_{eb}^{n} t^{-0.5} + I_{eb}^{n} \right) \Delta t,$$

where $I_{eb}$ and $I_{eb}$ are the sum ion and electron currents leaving the open boundaries (III), with the factor $f^{-0.5}$ scaling down the ion current in accordance with the applied mass factor [48, 49]. The value of $C$ must be carefully chosen according to a compromise between fast convergence of $\phi_{\infty}$ and stability of the Poisson’s solver (see the sensitivity analysis reported in section 3.1). Alternatively, and if known, it should equal the real capacitance of the spacecraft/thruster body [54]. This method ensures that the system evolves self-consistently and inherently guarantees that, once at steady-state, the ion and electron currents are equal ($I_{eb} = -I_{eb}$) at the open boundaries (III), and therefore also at the infinity. Notably, this approach improves the method proposed in [34] to estimate $\phi_{\infty}$ based on the cut-off energy of free electrons leaving the domain. Indeed, such an assumption implies that $\phi_{b} = \phi_{\infty}$, which holds only for very large domains.

The initial value of $\phi_{\infty}$ ($\phi_{\infty}^{0}$) is set according to the theoretical value obtained by assuming a current-free condition at the thruster outlet, the absence of a magnetic field, and electron energy conservation [28]. For the Maxwellian population given by equation (8), the analytical result is

$$\frac{4\pi\Phi_{0}}{\Phi_{e}} = 1 - \exp\left(\frac{-e\Phi_{e}^{0} \Phi_{e}}{k_{B}T_{e}}\right) + \frac{4e\Phi_{e}^{0}}{\pi k_{B}T_{e}} \exp\left(\frac{e\Phi_{e}^{0}}{k_{B}T_{e}}\right),$$

where $\Phi_{e} = \sqrt{8k_{B}T_{e}/\pi m_{e}}$ is the mean reference electron velocity. For $u_{ib} = c_{s}$ with equation (11) yields $e\Phi_{e}^{0} \sim -6.4k_{B}T_{e}$.

Controlling only the value of $\phi_{\infty}$ by means of equation (10) is not itself sufficient to implement a self-consistent circuit condition. Any non-zero net current in the transient leaving the open boundaries (III) must be re-injected into the domain via the thruster outlet (I) [36]. Moreover, the injected electron current $I_{o}$ is controlled in order to enforce the quasi-neutrality condition at the thruster outlet (I), namely

$$n_{e} = n_{i0} = n_{e0}^{+} + n_{i0}^{*}.$$  

Being $n_{i0}^{+}$ unknown a priori, equation (12) can be satisfied at the steady-state by adjusting $I_{e}$ and, in turn, $n_{e0}^{+}$. From these considerations, the following conditions are imposed to the particles injected from boundary (I). Ions are injected with a constant current given by $I_{i} = n_{i0} c_{s} A_{0}$, where $A_{0}$ is the area of the thruster outlet. The injected electron current is updated each time step according to

$$I_{e}^{n+1} = (I_{i0}^{n} + I_{eb}^{n}) + n_{e0}^{+} I_{eb}^{n},$$

where the first term completes the circuit and the second enforces the quasi-neutrality. This condition guarantees that quasi-neutrality and current-free conditions are respected at the steady-state, comparable to the algorithms used previously in references [34, 36, 56]. A similar control strategy has not been imposed to ions since $I_{e} \equiv I_{i0} \equiv I_{eb}^{+}$, whereas $I_{e} \equiv I_{eb}^{+} \neq I_{i0}$. Considering that injected electrons are Maxwellian, the initial value of the current is set as
3. Verification of the numerical model

This section demonstrates the robustness of the new boundary conditions. The verification is divided into two parts. First the steady-state stability is demonstrated against the classical open-outflow boundary conditions [38, 39]. Namely, constant electron current injected at the plasma source, absorption of all electrons reaching the open boundaries (III), and the zero-Neumann condition on the Poisson’s equation. Second, a domain independence study is presented, evaluating both macroscopic plasma parameters and the propulsive performance (i.e. thrust) with respect to both axial and radial domain dimensions.

Table 1 summarises the physical and numerical parameters which are used, unless otherwise specified, throughout this article. Xenon is the propellant gas, with the reference plasma properties assumed within the source typical of the operating conditions in a low-power (50 W) HPT [12, 14]. A purely divergent MN is produced by an electromagnet of radius $R_c$, positioned concentric with the thruster outlet of radius $R_0$ [57]. Figure 2(a) illustrates the magnetic field topology B on the nominal simulation domain, normalised with its value at the magnetic throat, that is $B_0 = |B(0, 0)|$. Before commencing the PIC simulations, the DSMC method was used to pre-compute the neutral gas density field $n_g$ given in figure 2(b).

The scaling factors applied to the heavy species mass and the vacuum permittivity are $f = 250$ and $\gamma = 26.7$ respectively. The latter value is chosen such that the thruster outlet (I) is resolved with 20 cells $R_0 = 20\lambda_{De}$. The domain then spans $L_z = 25R_0$ in length and $L_r = 10R_0$ in height, with a uniform mesh spacing of $\lambda_{De}$. At steady-state $N_p \approx 1.6 \times 10^6$, which gives an average of $\bar{n}_p = 16$ macro-particles per cell (excluding neutrals, which do not contribute to the Poisson’s equation). These values of $f$, $\gamma$ and $N_p$ were selected according to the numerical sensitivity study of appendix B. The time-step adopted satisfies $\Delta t = 0.35$. In this way, the electron gyromotion is resolved in all the domain and the stability criterion on the resolution of the scaled plasma frequency [46] is also satisfied (see table 1). The Poisson’s equation is solved every $0.286\tau_{per}/\omega_{ce0}$ iterations [46]. Neutrals are sub-cycled at a larger time-step according to their Courant–Friedrichs–Lewy condition [50]. The steady-state is characterised by the number of newly injected macro-particles at the thruster outlet (I) within 0.01% for a defined number of iterations. On a machine equipped with an Intel® i7-7700 @3.6 GHz × 8, and 32 Gb...
of RAM, the computational time is approximately 9.6 h to reach steady-state. Approximately a further 8 h is required for steady-state averaging.

3.1. Steady-state stability

The stability of the new model is assessed for the unmagnetised case (i.e. \( B_0 = 0 \) G), since results can be more easily compared to theoretical values. The time-step is defined by \( \Delta t = 0.05 \). Figure 3(a) gives the evolution of the macro-particle count for both the new model and the open-outflow conditions. Although both simulations start with a similar growth in ion count during the transient, the electron count peaks around 14 \( \mu s \) with the open-outflow boundary. Despite the number of ions continuing to increase, the electron count decreases, resulting in a growing charge imbalance. This eventually results in the formation of a virtual anode [36, 37] around 32 \( \mu s \), which is followed by gradual ion loss. The vast majority of electrons are lost, thus the simulation collapses; this is the ‘numerical pump instability’ [36, 37]. No such instability is observed with the new model. The electron and ion populations closely trend each other. Steady-state is achieved near 34 \( \mu s \), and the ion and electron counts remain invariant for the reminder of the simulation. There is negligible change in the neutral count.

To prove the new model can self-consistently calculate the free-space potential \( \phi_\infty \), figure 3(b) plots its value against the simulation time. The trend mimics the voltage seen across the charging–discharging cycle of a capacitor [52]. Indeed, from figure 3(c), an initially large negative net current \( I_B = I_{IB} + I_{EB} \) at the open boundaries (III) is clear. Therefore \( |\phi_\infty| \) increases (the charging cycle) to slow down fast electron reflections. The rate of increase slows (see figure 3(b)) as fewer electrons can escape the growing potential barrier, and \( I_B \) becomes negligible towards 10 \( \mu s \) (see figure 3(c)). The minimum of the voltage curve, at around 10 \( \mu s \), represents the time at which ions begin to cross the open boundaries (III). \( |\phi_\infty| \) begins to decrease (the discharging cycle) as fewer electron reflections are required to balance a now net positive current that peaks at 11 \( \mu s \) (see figure 3(c)). After this initial recovery, a further, but slower, decrease in \( |\phi_\infty| \) occurs as the ion beam current—which is itself determined by the ambipolar acceleration of \( |\phi_\infty| \)—establishes an equilibrium state. After 39 \( \mu s \), \( I_B \) fluctuates about zero and a steady-state value of \( \phi_\infty = -33.5 \) V.
Figure 5. (a) Electron density $n_e$ and (b) plasma potential $\phi$ using the nominal $25R_0 \times 10R_0$ (---), three-quarter $18.75R_0 \times 7.5R_0$ (...) and half $12.5R_0 \times 5R_0$ (- - -) domains. Dotted lines (-----) indicate the boundaries of the reduced domains. (c) Electron density $n_e$ and (d) plasma potential $\phi$ sampled on the symmetry axis $r = 0$.

Figure 6. (a) Thrust $F$ for axial truncation of the domain for unmagnetised (---), 100 G (---), 300 G (...) and 600 G (-----) cases. The markers indicate the MN exit. (b) Thrust $F$ for axial and radial truncation in the 600 G case. The solid contour (---) represents the value of final thrust; the dashed line (- - - -) represents the MN exit.

is reached. This is similar to the theoretical initial value of $\phi_\infty^0 = -32.2$ V; it also falls between the values of $-28.9$ V and $-37.5$ V given by alternatives to equation (11) in references [23, 42] respectively.

At the steady-state, a zero net current $I_0 = I_\text{ion} + I_\text{ion}$ is also achieved across the thruster outlet boundary (I) as shown in figure 3(d). This arises purely as a product of the self-consistent electric field coupling electrons to the ion beam, since the current-free condition is only enforced at the open boundaries (III); only quasi-neutrality is enforced at (I). After an initially net negative current, caused by the re-injection of electrons as per the circuit condition, steady-state is achieved at around $8 \, \mu$s. Lastly, figure 3(e) provides the convergence of thrust, which achieves steady-state in the same time as $\phi_\infty$ at $39 \, \mu$s. The steady-state thrust is $F = 431 \, \mu$N.

The results obtained with different values of the virtual free-space capacitance $C$ have been compared in figure 4 in terms of $\phi_\infty$. Firstly, all three cases converge to a similar steady-state value within an accuracy of 0.4 V. Second, for smaller values of $C$, the voltage drop in the charging cycle increases: around $-69$, $-72.4$ and $-76.4$ V for $C = 0.8$, $0.4$ and $0.2$ nF respectively. This marginally increases the ambipolar acceleration of the ions during the transient. Thus, the point at which ions begin to cross the open boundaries (III) occurs $0.26 \, \mu$s and $0.22 \, \mu$s earlier for $C = 0.2$ and $C = 0.4$ compared to $C = 0.8$ nF. Analogous to a simple capacitive circuit, an increase in the value of $C$ increases the rate of voltage drop, while also decreasing the discharging time and the voltage recovery. This results in the equilibrium state being achieved at approximately the same simulation time (39 $\mu$s) for all three cases. To conclude, while the value of $C$ affects the plume during the transient phase, the solution at steady-state is independent of it. This further confirms the robustness of the proposed simulation strategy.

It is also important to note that smaller values of $C$ cause an increase in noise. This is expected for a proportional-type control law (see equation (10)), since the value of $C$ places an effective resolution on the adjustment of $\phi_\infty$. It is therefore
important to exercise care in the choice of virtual free-space capacitance. $C$ must be small enough to create the voltage drop necessary to prevent the instability, but not so small as to introduce additional noise to the solution and strain on the Poisson’s solver. For the remainder of the simulations in this work, $C = 0.8$ nF is chosen. To obtain a suitable starting point for the value of $C$, it is proposed to consider the capacitance of a conducting sphere with radius $R_0$: $C = 4\pi\varepsilon_0 R_0$ [52] which, for this work, gives $C = 0.55$ nF, in line with the found feasible range.

### 3.2. Domain independence

For the case of $B_0 = 600$ G, simulations are performed to demonstrate the domain independence using domain sizes of $18.75R_0 \times 7.5R_0$ (three-quarter) and $12.5R_0 \times 5R_0$ (half) compared to the nominal $25R_0 \times 10R_0$. Both reduced domains converged to values of $\phi_{\infty}$ within 0.8 V of the nominal $-39.1$ V. A comparison of the steady-state electron density and plasma potential distributions across the domains is shown in figures 5(a) and (b) respectively. It can be seen that the shape of the plasma obtained from both reduced domain simulations are in very good agreement with the nominal case. 

For a more quantitative analysis, the electron density and plasma potential are compared along the axis of symmetry ($r = 0$) in figures 5(c) and (d). Along the axis, results agree within 6% for the electron density, and 2% for the plasma potential. The largest disagreement occurs outside the periphery of the outermost magnetic field line connected to the source, approximated by the $10^{15} \text{ m}^{-3}$ contour in figure 5(a). The density in the reduced domain simulations is up to 68% higher in this region compared to the nominal. This difference may be attributed to the noise introduced due to the number of particles escaping and reflecting from the radial open boundary (III), which is no longer significantly removed from the thruster outlet (I). Nonetheless, the electron density within the core of the plume is in excellent agreement within 2% on average. Overall, the comparisons demonstrate that the new set of boundary conditions provides a domain-independent solution within a tolerance smaller than the typical PIC noise.

The final choice of domain size depends primarily on the phenomenon of interest. If only plume-spacecraft interactions are desired, significant computational savings can be realised by applying the new boundary conditions to a comparatively small domain. However, if the thrust is required, a domain of sufficient axial length is needed. The thrust $F$ is given by the axial flux integral

$$F = \int_{S_b} \sum_k \left( n_k m_k v_{kz} v_k + p_k \hat{z} \right) \cdot \text{d}S_B,$$  

where the two terms correspond to the species momentum flux and pressure $p_k = n_k k_B T_k$ respectively, for $k = i, e, g$. $S_B$ is the open boundary (III) surface. Figure 6(a) shows the thrust $F(z)$ calculated for different axial truncation of the domain. When the magnetic field is absent, the total axial flow momentum is conserved since no mechanism can exert force on the plasma; as a result $F(L_z) = F(0) = 431 \mu \text{N}$. In the 100 G case, $F$ increases to a converged value of $643 \mu \text{N}$ at $z \sim 12.3R_0$; for 300 G, $F = 692 \mu \text{N}$ at $z \sim 15.2R_0$; at 600 G, $F = 702 \mu \text{N}$ at $z \sim 18R_0$. This axial plane where the thrust establishes a plateau may be referred to as the exit of the MN, where plasma detachment occurs. The axial domain length must therefore include this plane so as to yield the accurate value of thrust. The domain size required is therefore proportional to the magnetic field strength.

The radial domain width must also be large enough. Figure 6(b) spatially maps the thrust $F(z, r)$ for both axial and radial truncation of the domain in the 600 G case. The size of the domain required to obtain a plateau value of $F$ is given by the area bounded by the solid contour. Accordingly, the domain must have an axial length $L_z \gtrsim 18R_0$ and radial width $L_r \gtrsim 8R_0$ to not underestimate the propulsive performance for $B_0 = 600$ G.

The results in this section show that the new model offers improvements over the current state-of-the-art fully kinetic PIC methods. Assuming the conservative criterion for the domain size related to the MN exit plane (see figure 6(b)), the new model offers $>20\%$ reduction in domain size compared to that of reference [34] where the domain must be extended to eliminate artefacts of the zero-Neumann closure. The domain is decreased by more than $50\%$ relative to reference [36], which must place an ion sink at the domain mid-point. It is also judicious to mention that the domain independence study of reference [34] yielded errors $\sim 5\%$ for the axisymmetric plasma potential, greater than the $<2\%$ observed in this study. As a result, the new methodology guarantees a reduction in the computational time by a factor $>2 - 3$, with higher accuracy in the estimation of plasma profiles.

### 4. Experimental validation

The results of the PIC simulations are compared against the measurements performed in the Piglet Helicon plasma reactor, filled with argon gas at 0.04 Pa as described in reference [42]. The magnetic configuration considered is generated by an electromagnet, referred to as the source coil in reference [42], which provides a throat intensity of $B_0 = 4$ G. The validation input parameters are given in table 2. The domain is a truncation ($L_e = 0.25$ m, $L_f = 0.13$ m) of the physical vacuum chamber used in the experiment (length 0.288 m radius 0.16 m), such to allow the use of the open boundaries. The plasma reference properties were taken directly from the experimentally measured values within the source tube, where $\mu_0 = 0.8c_s$.

In the experiment, electron density was evaluated with a Langmuir probe, with the local plasma potential obtained from a retarding field energy analyser (RFEA). The results along the axis of the discharge, have been reported in figures 7(a) and (b). The experimental plasma potential has been normalised so as that $\phi_{\min} = 0$ at $z = 0$. Due to the possible overestimation of the Langmuir probe sheath area by about 15% [42], the errorbars associated to the number density are asymmetrical between $-5\%$ and $27\%$. RFEA measurements have a given uncertainty of $\pm 5\%$.

Focusing on the axial density profile in figure 7(a), the experimental trend is reproduced by the PIC model. The maximum local error is $10\%$ at $z = 0.05$ m, well within the uncertainty bands reported. Concerning the plasma potential profile
Table 2. Validation parameters.

| Parameter                      | Unscaled      | Scaleda |
|-------------------------------|---------------|---------|
| Reference plasma density      | $n_e \ (\text{m}^{-3})$ | $5 \times 10^{16}$ | — |
| Ion mass ($Ar$)               | $m_i \ (\text{kg})$ | $6.63 \times 10^{-26}$ | $1.66 \times 10^{-27}$ |
| Reference ion temperature     | $T_{i*} \ (\text{K})$ | 298 | — |
| Reference electron temperature| $T_{e*} \ (\text{eV})$ | 9 | — |
| Ion speed                     | $u_i \ (\text{m s}^{-1})$ | 3724 | 23520 |
| Axial domain length           | $L_z \ (\text{m})$ | 0.25 | — |
| Radial domain length          | $L_r \ (\text{m})$ | 0.13 | — |

$^a f = 40, \gamma = 33.1.$

Figure 7. Experimentally measured data (○) with relative uncertainty bands and PIC output (——) on the axis of the Piglet Helicon reactor: (a) electron number density $n_e$, and (b) plasma potential $\phi$.

Figure 8 shows the 2D spatial fields for the $B_0 = 600 \text{ G}$ case, including (a) the electron number density, (b) plasma potential, (c) electron temperature and (d) ion axial velocity. The plasma expansion follows the magnetic field lines which determine the divergence of the plume. Specifically, the plasma properties propagate monotonically downstream under the dominance of a self-consistently developed ambipolar electric field [2]. Electron density drops outside the periphery of the plume, with an electron void occurring near the thruster outlet in figure 8(a).

A notable feature is observed in the potential field of figure 8(b): a radially non-monotonic dependence. This is characterised by an effective potential well along the vacuum interface line (the outermost magnetic field line starting at edge of thruster outlet boundary). This has been noted in a number of magnetically confined plasmas [21, 41] and can be interpreted as the consequence of charge separation that results from ions with sufficient radial energy surpassing the attached electron fluid, causing secondary ion expansion beyond the vacuum interface line. A potential barrier forms to counter this radial ion inertia and return the ion streamlines back toward the MN-aligned electron trajectories. This is clearly seen in figure 8(d) by the radial discontinuity in ion axial velocity along the vacuum interface line. Indeed, the charge separation across the plume periphery is evident in figure 9: there is a highly negative space charge along the outermost magnetic field line connected to the thruster outlet. Beyond this layer, near the thruster outlet, there is then a strong positive charge density as the result of secondary expanding ions. Within the plume, plasma is substantially quasi-neutral.

Cooling of electrons downstream in figure 8(c) occurs as electron thermal energy is evidently converted to ion kinetic energy, facilitated by the ambipolar potential drop, with the magnetic field acting as a mediating factor. The region of high $T_e > 6 \text{ eV}$ at the radial peripheries of the thruster outlet (beyond the vacuum interface line) occurs since only the most highly-energetic electrons can detach early from the MN and overcome the radial potential well. A deeper analysis of this region, including the high currents that are known to form [41], is possible with the methodology presented in this work since fully kinetic PIC simulations can handle non-neutrality [54]. Nonetheless, interactions with spacecraft surfaces must

is then given on the nature of electron thermodynamics in the MN and the equivalent polytropic indices.

5. Physical analysis

In this section, the plasma profiles are first examined, where the role of collisions has been discussed in detail. Second, the effect of varying $B_0$ on the global parameters, including the propulsive performance indicators, is presented. A discussion
be properly modelled to investigate in detail the radial peripheries of the plume [54]. Provided that this is beyond the scope of the article, such analysis will be the subject of future work.

In order to provide a more quantitative comparison, 1D plasma profiles have been sampled along the $z$-axis in figure 10 for $B_0 = 0, 100, 300$, and 600 G. From figure 10(a), the application of the MN yields higher plasma density because of the increased radial confinement of the plume, but there is no significant change between 100 and 600 G. The MN effect tends to increase electron current due to the $\mathbf{v}_e \times \mathbf{B}$ force exerted on electrons. As a consequence, the potential drop increases with $B_0$ (figure 10(b)), so as to maintain the current-free plume. Consistently, the ion axial speed increases (figure 10(c)). It is interesting to note that the potential drop/acceleration occurs in a larger axial span in the magnetised cases. This might be explained with mass conservation, since the ion beam divergence for the unmagnetised case is much higher, so a faster geometric expansion is expected.

The electron cooling is reduced with the increase in $B_0$ (figure 10(d)). It is reasonable to associate the slower cooling of the electrons to the increased plume confinement and so a reduced loss of energy through the periphery of the MN; this enables more electron energy to be available downstream. Strong temperature anisotropy is developed as shown in figures 10(e) and (f). Electron temperature along the $z$-axis ($T_e$) decays to a non-zero value ($\sim 3.6$ eV regardless the MN strength), while $T_i$ decays to zero. Interestingly, no magnetic field means a higher divergence of the plume, and this decreases greatly $T_e$ in the region close to the thruster outlet, resulting in the smaller mean temperature seen in figure 10(d).

On the other hand, the anisotropy on $T_e$ increases downstream for both MN strengths which confirms the conversion of electron internal energy into ion axial kinetic energy [25].

5.1.1. The role of collisions. Particular emphasis should be given to the role played by collisions in the dynamics of a MN. Specific features associated to collisional processes are discussed in the following.

The on-axis collision frequency $\nu$ is presented in figure 11, for the 600 G case, to identify the the most relevant processes included in the simulations. Most apparent is that in-plume ionisation is negligible, which was expected since $T_e$ is relatively low ($< 5$ eV). The most significant collisions are the $e$–$e$ and $e$–$i$ Coulomb interactions, which remain non-negligible even downstream. The processes responsible for the electron cross-field diffusion [49] are the $e$–$i$ collisions, along with the $e$–$n$ scattering. The latter is most critical at the thruster inlet but decreases by nearly three orders of magnitude due to the drop-off in neutral density. Charge exchange collisions occur at approximately half the frequency of $i$–$n$ scattering, with both two orders of magnitude less significant than the Coulomb and neutral scattering. The $i$–$i$ Coulomb collisions are half the magnitude of other Coulomb processes near the thruster, but tend toward equal value downstream, most likely due to the difference in electron and ion cooling.

The first phenomenon analysed is the potential peak of $\sim 3.5$ V near the thruster outlet (see figure 8(b)), which is not a
Figure 10. Plasma on-axis profiles for $B_0 = 0$ (——), $B_0 = 100$ G (——), $B_0 = 300$ G (———) and $B_0 = 600$ G (-----): (a) electron number density $n_e$, (b) plasma potential $\phi$, (c) ion axial velocity $u_i$, (d) electron temperature $T_e$, (e) axial electron temperature $T_{ez}$, (f) radial electron temperature $T_{er}$.

Second, a deeper analysis is conducted to explain why, independent of the MN strength, the plasma potential and axial ion speed are almost equal for $z \lesssim 3R_0$ (see figures 10(b) and (c)). The relatively high neutral density near the thruster outlet leads to CEX ion collisions, which act as a drag term on the ions. To assess this, the CEX mean free path $\lambda_{\text{CEX}}$ can be compared to the characteristic length scale of axial ambipolar acceleration $\lambda_\nabla \phi = |(\phi - \phi_\infty)/E_z|$ [52]. $\lambda_{\text{CEX}}$ can be estimated from the PIC simulation as $\lambda_{\text{CEX}} \sim |v_i|/\nu_{\text{CEX}}$, where $\nu_{\text{CEX}}$ is the CEX collision frequency taken from the MCC module. If the CEX mean free path is shorter than the acceleration length scale, the ions are experiencing a drag force through frequent CEX collisions. Otherwise, the ion acceleration is not significantly impeded by these collisions.

The on-axis length scales are given in figure 13. The axial location at which the CEX mean free path becomes equal to the acceleration length scale occurs at $z \sim 1.2R_0$ independent of the MN field strength. The action of this CEX drag may explain why the potential drop, and subsequent ion velocity, in the near thruster outlet region is identical in each case presented in figure 10. Drag from CEX collisions may explain also why the plasma choke point ($v_{iz} = c_*$) is located downstream from the MN throat at $z \sim 1.5R_0$, a consequence also observed in reference [21]. Figure 12(b) compares the collisionless and collisional axial ion velocity. As expected, in the absence of collisions, the injected velocity is the same as that imposed. Notably, the final velocity is $\sim 5\%$ less than in the collisional case; this is associated to a lower magnitude of the potential drop $|\phi_\infty|$ of $\sim 5$ V. Critically, figure 12 proves that the collisional plasma undergoes CEX drag in the near-thruster outlet region. Finally, it is worth noting that to better estimate plasma profiles in the near thruster outlet region, the plasma source should be included in the model. In fact the MN field strength would alter the ionisation efficiency, and therefore the ratio of plasma to neutral density. As a result, the CEX drag is expected to produce milder effects for higher values of $B_0$. 

usual feature observed in collisionless PIC simulations [41]. Its presence can be justified in the role played by collisions. Radially accelerating CEX ions, combined with increased electron collisional cross-field mobility, enhance the secondary ion expansion, increasing the positive space charge and hence the strength of the potential barrier. Moreover, the large ion mass (the propellant gas is xenon) is expected to enhance the amplitude of the potential peak, since heavier ions should require a larger electric field to return their trajectories into the MN. A collisionless case was simulated for comparison. Figure 12(a) illustrates the collisionless plasma potential for $B_0 = 600$ G; there is no distinct radial peak, since it’s magnitude is approximately that of the thruster outlet potential. Finally, it is worth noting that the results reported in appendix B guarantee that the radial potential peak registered in figure 8(b) is not generated by numerical artefacts.

Figure 11. On-axis collision frequencies, for $B_0 = 600$ G, from the MCC/DSMC module for e–e (——), i–i (———), e–i (——), e–n (-----), i–n charge exchange (———), i–n scattering (-----) and ionisation (-----).
Figure 12. The collisionless MN: (a) plasma potential field $\phi$ for 600 G; (b) comparison of the ion axial velocity $v_i$ in the collisionless (---) and collisional (- - -) cases for 600 G.

Figure 13. Comparison of the on-axis CEX mean free path (solid lines) to the ion ambipolar acceleration length (dashed lines) for $B_0 = 0$ (——), 100 G (---), 300 G (——) and 600 G (——).

The two phenomena analysed highlight the significance of collisional processes within the MN plasma expansion. Previous models in the literature [34, 36, 41, 58], that have neglected both neutrals and collisions, ignore phenomena such as the electron cross-field transport, the enhanced potential peak and CEX ion drag. Neglecting such features will directly affect the plasma profiles, consequently affecting the magnitude of global values such as $\phi_\infty$ and performance parameters by more than 10%.

5.2. Global parameters

The propulsive performance of the MNs is illustrated in figure 14. As the magnetic field strength increases, thrust also increases at a diminishing rate. The magnetic thrust in the 100 G case accounts for approximately 50% of the total. At 1200 G the magnetic thrust is around 65%, showing there is limit to the performance enhancement the MN can provide. The gain in thrust between the unmagnetised and magnetised cases is namely due to the increased radial confinement of ions and the corresponding increase in downstream density. Indeed there is a clear trend in the thrust of figure 14(a) and the plume divergence $\dot{\theta}_i = \langle \cos^{-1}(v_i \cdot \hat{z} / |v_i|) \rangle_i$ of figure 14(c). As $B_0$ is further increased, the additional thrust is due to the higher ion axial velocity achieved in association with the greater potential drop, seen in figure 14(b). The potential drop must increase to balance a growing electron current induced by the MN effect. Note, that in practice, the influence of the MN on performance is far more complex because it also affects the source region. The magnetic field strength affects the source confinement [14], deposition of power into the plasma [2], and the electron distribution function [19] of the discharge into the MN throat.

5.3. Electron thermodynamics

The electron cooling in MN expansions may be described by a polytropic relation $T_e/T_{e0} = (n_e/n_{e0})^{\gamma_e - 1}$ where $\gamma_e$ is the polytropic index [9]. It can be calculated considering that

$$\gamma_e = 1 + \frac{n_e d T_e}{T_e d n_e} \quad (15)$$

with $\gamma_e$ derived by the linear regression of the $\log_{10} T_e$ versus $\log_{10} n_e$ relation, an example of which is given in figure 15 for the 600 G case. The average value is shown to be $\bar{\gamma}_e \sim 1.16$, but it is clear that a single polytropic index cannot represent the electron cooling in the MN. Three separate regions are therefore identified for a piecewise polytropic relationship. Nearest the thruster outlet there is a region with a mildly-adiabatic value. Further downstream, and for most of the expansion, there is a region with a near-isothermal $\gamma_e \sim 1.13$. Finally, farther downstream, there exists a region with a markedly greater value of $\gamma_e \sim 1.30$. Piecewise polytropic behaviour has also been observed in reference [58], where the measurements of an ECR thruster plume agree with the first and second regions identified here.

The break between the second and third polytropic regions agrees with the locations of the MN detachment planes identified in figure 6. It can therefore be inferred that the second region is where the electrons are well-magnetised and frozen to the magnetic field lines. The third region represents that where the plasma has detached from the MN and so the electron cooling tends to the same as that for an unmagnetised expansion. The first region possesses an average value that lies between the indices found in the other two regions, therefore it may be assumed that here electrons are not fully attached to the MN.

Figure 16 shows the effect of the MN strength on the indices describing the different polytropic regions. Notably, the value of $\gamma_{ed}$ is approximately constant, and roughly equal to the unmagnetised average $\bar{\gamma}_e = 1.29$, for all cases. This confirms
Figure 14. Effect of MN field strength on (a) thrust $F$; (b) potential drop $|\phi_\infty|$ and (c) ion divergence angle $\bar{\theta}_i$.

Figure 15. Polytropic index fitting of the 600 G case.

Figure 16. The values of the polytropic index, taken using the linear regression, as a function of $B_0$. This region is post plasma detachment. The value of $\gamma_{eM}$ is almost constant, consistent with the mild effect that the intensity of the MN has on $n_e$ and $T_e$ profiles upstream of the detachment plane for $B_0 \geq 100$ G (see section 5.1). Increasing the magnetic field strength reduces the average electron cooling rate, tending to $\bar{\gamma}_e \sim 1.16$ for 600–1200 G. This is due to the larger axial length in which electrons are magnetised, since the detachment plane moves downstream with increasing $B_0$ (see section 3.2). The values found for $\bar{\gamma}_e$ are in good agreement with experiments on xenon MNs, which have reported magnitudes between 1.1 and 1.23 [21, 58]. Measurements of $\bar{\gamma}_e = 1.15 \pm 0.02$ have been reported also in reference [59] and a theoretical limit of $\bar{\gamma}_e = 1.16$ was predicted in reference [60].

In order to interpret the behaviour of $\gamma_e$ in the region near the thruster outlet, consider the electron Hall parameter

$$\Omega_e = \frac{e|B|}{m_e \nu},$$

where $\nu = \nu_{en} + \nu_{ei}$ is the total of the electron–neutral and electron–ion collision frequencies calculated from the MCC module. $\Omega_e$ is equal to the ratio between the cyclotron frequency and the collision frequency, so it is an indicator of the level of electron magnetisation/attachment. In figure 17 the electron Hall parameter is shown for 100, 300 and 600 G. Sufficiently upstream near the thruster outlet, collisions act to de-magnetise the electrons. The plasma remains dominated by collisions in the near-field plume. This collisionality reduces the plasma conduction and thermalises the electron distribution, increasing the near-throat polytropic index towards the

Figure 17. Electron Hall parameter $\Omega_e$ along the axis for the 100 G (---), 300 G (-----) and 600 G (----) case.
adiabatic. This precludes the accelerating action of the magnetic field until the neutral gas becomes sufficiently sparse that the electrons become strongly magnetised again.

6. Conclusions

In this article, a new set of self-consistent, open boundary conditions for electron kinetics and the Poisson’s equation have been introduced. They were developed to perform steady-state fully kinetic PIC simulations of plasma expansion in the MN. The newly developed boundary conditions correct the non-physical loss of electrons by reflecting them at the open boundaries according to an energy-based criterion. A virtual free-space capacitor allows equal ion and electron currents to infinity at steady-state. The electric field at the external boundaries is also self-consistent with the potential drop according to a new Robin-type condition on the Poisson’s equation. This approach generates a stable, steady-state plume with axisymmetric 2D fully kinetic simulations for typical operative conditions of a low-power (50 W) MEPT.

The robustness of the new model was established by changing the value of the virtual capacitance and thus the transient evolution of the plasma potential and plume. It was demonstrated that identical steady-state solutions are obtained, and thus the boundary conditions yield results independent of the choice of capacitance. Domain-independence studies were performed to study the sensitivity of the computed number density and plasma potential to changes in the location of the domain boundaries. The results of the new set of boundary conditions were benchmarked against experiments providing electron density and plasma potential profiles that fall within the uncertainty band of the measures.

The validated model was exploited to investigate the collisional xenon plasma expansion in a MN. A potential well forms at the periphery of the plume to counterbalance the cross-field diffusion of the weakly-magnetized ions. The performance indicators increase with the strength of the MN because of the enhanced radial confinement and ion acceleration. Nonetheless, the increase in the performance a MN can provide is limited at about 70% [25].

The major effects of collisions on the MN have been revealed. Namely, the CEX collisions act as a drag term on the ions in the near-exit region, such that ion acceleration is reduced over the collisionless case. Collisions are also responsible for a radial potential peak at the plume periphery, near the thruster outlet, caused by the scattering of CEX and highly energetic ions. Finally, the electron cooling correlates with the electron-heavy particle collisions.

- There exists a three-region polytropic cooling regime, defined by a partially-detached near-exit region, a strongly attached near-isothermal region, and a more adiabatic detached region.
- The third region occurs downstream of the detachment plane, here the polytropic index is equal to the one of an unmagnetised plume.
- The average polytropic index decreases with the strength of the MN since the detachment plane moves downstream and so the electrons are strongly attached to the MN in a larger portion of space. An inferior limit of $\gamma_e = 1.16$ was found.
- The electron cooling in the near-exit region is determined by collisions that tend to partially-detach electrons from the MN.

The new boundary conditions offer a valuable tool in the performance evaluation and optimisation of MEPTs (and indeed unmagnetised thrusters also), reducing the computational time compared to the large domains required by other models [34, 36], and including the behaviour of collisions, previously omitted in the literature [41, 58]. Future work will involve iterative coupling of the PIC to the fluid model 3D-VIRTUS, developed to simulate the source region of such devices [15, 29, 61, 62], allowing for multi-scale modelling of MEPTs. The boundary conditions will also be applied within the framework of a 3D PIC code [28], to assess the limitations of the 2D axisymmetric assumptions, and analyse the plume interactions with non-axisymmetric spacecraft bodies.

Acknowledgments

This work was partially funded by Technology for Propulsion and Innovation S.p.A. (T4i). S Andrews was also supported by a scholarship from the European Union Horizon 2020 MSCA-RISE project PATH, under Grant Agreement 734629.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Appendix A. Robin boundary condition

Generally, the plasma potential generated by $N_p$ charged particles with positions $\mathbf{r}_p$ is obtained by the sum of the individual point charges. However, consider the potential very far from the localised charge distribution of the plume; it resembles one total point-like charge. Reference [52] developed a multipole expansion for the approximate potential at large distances $\mathbf{r}$ from such a localised charge distribution, which is modified here to the discrete form and referenced to the potential at infinity,

$$
\phi(\mathbf{r}) = \phi_\infty + \frac{1}{4\pi\varepsilon_0} \sum_{s=0}^{\infty} \sum_{s=0}^{\infty} \sum_{p=1}^{N_p} |\mathbf{r}_p|^s P_s (\cos \theta_p) q_p,
$$

(A.1)

where $P_s$ is the Legendre polynomial operator, and $\theta_p$ is the angle between $\mathbf{r}$ and $\mathbf{r}_p$. This is the multipole expansion of $\phi$ in powers of $1/|\mathbf{r}|$. The first term ($s = 0$) is the monopole contribution $1/|\mathbf{r}|$; the second ($s = 1$) is the dipole contribution $1/|\mathbf{r}|^2$; and so on. Equation (A.1) is exact, but it is useful primarily as an approximation scheme. The lowest non-zero term in the expansion provides the approximate potential at
large \( \mathbf{r} \), and the successive terms improve the approximation if greater precision is required. In the following, it is proven that the monopole term is sufficient to define suitable boundary conditions for studying the plasma expansion in the MN. Therefore equation (A.1) has been truncated at the second term, the dipole contribution, to prove that it is negligible with respect to the monopole. The multipole expansion truncated at the second term reads

\[
\phi(\mathbf{r}) \approx \phi_\infty + \frac{1}{4\pi\varepsilon_0} \left( \frac{1}{|\mathbf{r}|} \sum_{p=1}^{N_p} q_p + \frac{1}{|\mathbf{r}|^2} \sum_{p=1}^{N_p} |\mathbf{r}_p| \cos \theta_p \mathbf{q}_p \right), \tag{A.2}
\]

where \( Q = \sum_{p=1}^{N_p} q_p \) is the total net charge in the plume, which, for a partially confined plasma, is not null \([46]\). Since \( |\mathbf{r}_p| \cos \theta_p = \hat{\mathbf{r}} \cdot \mathbf{r}_p \) and given the dipole moment of a collection of point charges \( \mathbf{p} = \sum_{p=1}^{N_p} q_p \mathbf{r}_p \), the potential can be more succinctly written,

\[
\phi(\mathbf{r}) \approx \phi_\infty + \frac{1}{4\pi\varepsilon_0} \left( \frac{Q}{|\mathbf{r}|} + \frac{\hat{\mathbf{r}} \cdot \mathbf{p}}{|\mathbf{r}|^2} \right), \tag{A.3}
\]

where \( \hat{\mathbf{r}} \) is the unit vector parallel to \( \mathbf{r} \). Equation (A.3) is the standard monopole–dipole decay into vacuum. Taking the gradient of the potential in equation (A.3) gives

\[
\nabla \phi(\mathbf{r}) = -\frac{1}{4\pi\varepsilon_0} \left( \frac{Q}{|\mathbf{r}|^2} + \frac{3(\hat{\mathbf{r}} \cdot \mathbf{p}) \hat{\mathbf{r}} - \mathbf{p}}{|\mathbf{r}|^3} \right)
\]

\[
= -\frac{1}{4\pi\varepsilon_0} \left[ \left( \frac{Q}{|\mathbf{r}|^2} \right) \hat{\mathbf{r}} + \frac{\hat{\mathbf{r}} \cdot \mathbf{p}}{|\mathbf{r}|^2} \hat{\mathbf{r}} + \frac{2(\hat{\mathbf{r}} \cdot \mathbf{p}) \hat{\mathbf{r}} - \mathbf{p}}{|\mathbf{r}|^3} \right]. \tag{A.4}
\]

A formal relation between \( \phi \) and \( \nabla \phi \) is then obtained by substituting equation (A.3) into (A.4),

\[
\nabla \phi(\mathbf{r}) = -\frac{\hat{\mathbf{r}}}{|\mathbf{r}|} (\phi(\mathbf{r}) - \phi_\infty) - \frac{1}{4\pi\varepsilon_0} \frac{2(\hat{\mathbf{r}} \cdot \mathbf{p}) \hat{\mathbf{r}} - \mathbf{p}}{|\mathbf{r}|^3}. \tag{A.5}
\]

The projection of equation (A.5) along a unit vector \( \hat{\mathbf{n}} \) subsequently reads,

\[
\frac{\partial \phi}{\partial \hat{\mathbf{n}}} + \frac{\hat{\mathbf{n}} \cdot \mathbf{r}}{\mathbf{r} \cdot \mathbf{r}} (\phi(\mathbf{r}) - \phi_\infty) + \frac{1}{4\pi\varepsilon_0} \frac{2(\hat{\mathbf{r}} \cdot \mathbf{p}) \hat{\mathbf{r}} - \mathbf{p}}{|\mathbf{r}|^3} \cdot \hat{\mathbf{n}} = 0 \tag{A.6}
\]

which, when \( \hat{\mathbf{n}} \) is the normal to the domain boundary, provides an open boundary condition on the Poisson’s equation for plasma expansion into vacuum. The second term of equation (A.6) (hereinafter referred to as \( E_\text{dip}^{\text{mon}} \)) is associated to the monopole field and the third term (\( E_\text{dip}^{\text{dip}} \)) to the dipole contribution.

To prove that the dipole term is negligible in the study of the MN, simulations were performed with the open boundary conditions defined by equation (A.6); all the other parameters are listed in table 1. Figure A1(a) shows the contribution of the dipole term \( E_\text{dip}^{\text{dip}} \) to the total axial electric field along the central axis \( E_\text{ax}^{\text{tot}} = E_\text{mon}^{\text{mon}} + E_\text{dip}^{\text{dip}} \). At the open boundary \( z = 25R_0 \) the greatest contribution from the dipole is \( -0.56\% \) for \( B_0 = 600 \text{ G} \). So, it is clear that the dipole term is negligible and the open boundary condition can be reduced to purely the monopole term

\[
\frac{\partial \phi}{\partial \hat{\mathbf{n}}} + \frac{\hat{\mathbf{n}} \cdot \mathbf{r}}{\mathbf{r} \cdot \mathbf{r}} (\phi(\mathbf{r}) - \phi_\infty) = 0. \tag{A.7}
\]

Indeed, the on-axis plasma potential given in figure A1(b) shows negligible difference in the solution with purely the monopole term (i.e. the reference case adopted in section 3) compared to that inclusive of the dipole. The error between the two (<1%) is indistinguishable from the natural order of statistical variance.

The fact that the dipole term becomes more significant at smaller \( \mathbf{r} \) may limit the application of the monopole condition for certain reduced domain size. However, note that figure A1(a) was generated with a dipole moment \( \mathbf{p} \) calculated using the full domain. It is important to consider that with reduced domain sizes, there may be error in the value of \( \mathbf{p} \) due to the reduced sample of the charge distribution. Thus, a domain size limit likely exists, even with the addition of the dipole term. So, as a general principle, considering only the monopole term is reasonable for domains where \( z > 10R_0 \). In general, it must be noted that neglecting the dipole term, while valid here, may not be valid in the general application of the boundary condition; especially in cases of highly quasi-neutral plasma with greater degrees of charge separation. Therefore, a contribution analysis of multipole terms should precede any investigation. Finally, it is worth noting that neglecting the dipole term improves the numerical efficiency of the overall simulation since the condition expressed in equation (A.7) does not depend on the parameters \( Q \) and \( \mathbf{p} \), which must be computed each time step by cycling over all the macroparticles.

### Appendix B. Numerical sensitivity analysis

A convergence study has been conducted to select acceptable values of the average macroparticle number per cell \( N_p \) at steady-state, the heavy species mass factor \( f \), and the artificial permittivity factor \( \gamma \). The main scope of this analysis is to verify that the numerical acceleration strategies do not introduce false artefacts. If not otherwise specified, the simulation parameters are given in table 1 and the magnitude of the magnetic field is \( B_0 = 600 \text{ G} \). Table B1 summarises the values of global parameters (i.e. \( \phi_\infty \) and \( F \)) and the computational time to steady-state \( \tau_{ss} \) for each simulation.

#### B.1. Macro-particles per cell

Figure B1(a) shows the macro-particle convergence study in terms of the on-axis number density. Increasing \( N_p \) from 4 to 40 shows good agreement near the thruster outlet where the average number of macro-particles per cell always remains above 20. For \( N_p = 4 \) and 8 the number density is underestimated further downstream, where errors arise due to reduced particle samples in the cells along the axisymmetric boundary. The increase in noise is also clear, since these fluctuations relate to \( 1/\sqrt{N_p} \). Despite the differences apparent in
the plasma profile, table B1 shows insignificant variance in the global parameters, including $\phi_\infty$ and $F$. The computational cost of $\hat{N}_p = 40$ is three-times that of 16. Given the near-perfect agreement in figure B1(a), the latter is considered a very acceptable number of particles to use for this study.

**B.2. Heavy species mass factor**

Figure B1(b) presents the sensitivity study on the value of the heavy species mass factor $f$ applied to ion and neutral macro-particles. While $f = 250$ agrees well with the reference case where no factor is applied, for $f = 2500$ the solution no longer holds. When $f = 2500$, the magnitude of the potential peak in figure B1(b) is underestimated by 1 V and the non-monotonic trend is less pronounced compared to $f = 1$. This is because the electron cross-field transport is no longer conserved for high values of $f$ [49]. Electrons therefore non-physically radially diffuse and damp out the potential peak due to the reduced charge separation. Excellent agreement between $f = 250$ and the reference case is seen in table B1, within 0.3 V for $\phi_\infty$ and negligible difference in $F$; $f = 2500$ however underestimates both. The time to steady-state can be seen to follow approximately the predicted $\sqrt{f}$ scaling [49]. Critically, $f = 250$ is a suitable value to apply in the study.

**B.3. Artificial permittivity**

Figure B1(c) presents the sensitivity study of the artificial permittivity scaling factor for $\gamma = 13.4$, 26.7, 53.4, and 106.8, which corresponds to a Debye length scaling allowing 5, 10, 20 and 40 cells per $R_0$ respectively. There appears to be a transition point between acceptable and too-large choice of $\gamma$: figure B1(c) shows that $\gamma = 26.7$ replicates well the less-scaled case at 13.4, but at greater values the behaviour is lost. Notably, high values of $\gamma$ fail to capture the radial potential peak; it is damped out due to the enlargement of charge separation provided by increased permittivity. As a result, the plume confinement in the MN is also reduced, apparent in the noticeable underestimation of thrust in table B1. The same effect induces a decrease of $\phi_\infty$ with increasing $\gamma$. A computational
saving of 4.6 is achieved with \( \gamma = 26.7 \), and it reproduces the physical behaviour well, thus it is acceptable for this study.

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