

Fluid vs PIC Modeling of a Plasma Plume Expansion

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The prediction of the plasma plume properties far downstream from an electric thruster is crucial to assess its interaction with both the spacecraft and the ambient plasma. Either fluid or kinetic models can be used for this purpose. The former are generally less demanding from a computational point of view and allow exploring parametrically the physics of the expansion, but rely on strong assumptions to close the fluid equations, such as isothermal or polytropic electron thermodynamics. Kinetic simulations, on the other hand, allow reproducing the plume physics to a much deeper level of detail but require more computational power. This paper presents and compares a fluid model plume solver based on the Asymptotic Expansion Method and a full PIC simulator, benchmarking one against the other, in terms of the predicted plasma density and velocity. The suitability of fluid models to reproduce the results of a more complex full PIC simulator is investigated, identifying the limitations of a simple polytropic law and discussing the fundamental physics of the plasma plume expansion.

Nomenclature

α_0	= Initial divergence angle of the outermost streamline of the plume
δ	= Initial profile for the ions divergence angle tangent $\delta = \tilde{u}_{xi}/\tilde{u}_{zi}$
Δt	= Integration time step for the ion and electron macro-particles
η	= Initial normalized ion streamlines distance from the symmetry plane $x = 0$
ϵ_0	= Vacuum permittivity
ε	= AEM expansion parameter: $\varepsilon = 1/M_0^2$
γ	= Electron polytropic cooling coefficient
λ_{D0}	= Debye length at the plume origin ($x = 0, z = 0$)
$\phi, \tilde{\phi}$	= Electric potential and its normalized expression
ν	= Initial profile for the normalized plasma density number
v	= Initial profile for the ions axial velocity component

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ω_{pi}, ω_{pe}	= Ion and electron plasma frequency
c_s	= Ion sonic velocity
$\vec{E}$	= Electric field vector
e	= Electron charge
Err	= Error figure of merit in the PIC and AEM simulation comparison
$\vec{j}_{i0}, \vec{j}_{e0}$	= Ion and electron current density vectors at the emission plane
L_{beam}	= Plasma plume transient length
$\ln \tilde{n}^{(i)}$	= i^{th} order correction of the logarithm of the plasma number density
m_i, m_e	= Ion and electron mass
m_p	= Mass of the ion or electron macro-particles
M_0	= Plasma plume Ion Mach number at the plume origin ($x = 0, z = 0$)
n_e, n_i	= Electron and ion number densities
n_{i0}	= Ion number density at the injection plane $z = 0$ for the PIC simulations
n, n_0	= Plasma number density and its value at the plume origin ($x = 0, z = 0$)
n_{AEMij}	= Plasma number density predicted by the AEM at the node (i, j)
n_{PICij}	= Plasma number density predicted by the PIC at the node (i, j)
$\tilde{n}$	= Plasma number density, normalized with n_0
$\tilde{n}_i, \tilde{n}_e$	= Ion and electron number density in the PIC simulations, normalized with n_{i0}
q_p	= Charge of the ion or electron macro-particles
R_{beam}	= Initial size (along x) of the plasma plume
$\vec{r}_p$	= Position vector of the ion or electron macro-particles
R_0	= Normalization length (assumed equal to the Debye length at the plume origin)
T_e, T_{e0}	= Electron temperature and its value at the plume origin ($x = 0, z = 0$)
T_i, T_{i0}	= Ion temperature and its value at the plume origin ($x = 0, z = 0$)
u_{zi}, u_{i0}	= Ions axial velocity and its value at the plume origin ($x = 0, z = 0$)
u_{xi}	= Ions velocity component along x , normal to the plume symmetry plane
$\tilde{u}_{zi}, \tilde{u}_{xi}$	= Ion velocity components, normalized with u_{i0}
$\tilde{u}_{zi}^{(i)}$	= i^{th} order correction of the normalized z velocity component
$\tilde{u}_{xi}^{(i)}$	= i^{th} order correction of the normalized x velocity component
v_{beam}	= Plasma plume velocity at the plume origin, equal to u_{i0}
$\vec{v}_p$	= Velocity vector of the ion and electron macro-particles
v_{ti0}, v_{te0}	= Ion and electron thermal velocity at the emission plane $z = 0$
$v_{te,x}, v_{te,z}$	= Electron thermal velocity along x and z
$\tilde{v}_{te,x}, \tilde{v}_{te,z}$	= Electron thermal velocity along x and z , normalized with their injection values
w_{ij}	= Weight of the (i, j) node for the computation of the error figure of merit
(x, z)	= Coordinates of the plasma slab reference frame
$(\tilde{x}, \tilde{z})$	= Normalized coordinates of the plasma slab reference frame

I. Introduction

THE rapidly growing use of electric thrusters in modern satellites is demanding a deeper understanding of their interaction with the rest of the S/C and with the ambient plasma. The plasma plumes produced by such devices can induce electric charging, produce mechanical erosion/contamination and exert forces/torques on sensitive S/C components or any object they interact with. Therefore, the characterization of their expansion into vacuum has become a key element in modern S/C design (and in particular, in the novel ion beam shepherd (IBS) concept¹).

A plasma plume generally presents two distinct regions: a near region and a far region. In the near region, which extends up to a few thruster radii from the thruster exit plane,^{2,3} collisions between ions and neutrals, and electric and magnetic fields play a major role. The former, which are predominantly charge-exchange

collisions, determine the amount of total ion back-flow, a potential danger for sensitive S/C surfaces, while the latter, generated by either the thruster or locally non-neutral space-charge regions, lead to the gradual formation of a smoothed and single-peaked plasma density profile.

In the far region, on the other hand, the expansion is nearly collisionless and the only agent capable of changing the ions trajectories is the ambipolar electric field, strictly related to small plasma density gradients in the plume. This ambipolar field, in general, depends on the electron thermodynamics and, more specifically, on the evolution of the electron energy distribution function (EEDF) in the near-collisionless plume, whose prediction is not a trivial task.

While modelling near region effects necessarily requires kinetic models to treat collisions (for instance the fast neutrals that result from charge-exchange collisions), the far region can be simulated with fluid models, which have the drawback, however, of assuming a certain evolution of the EEDF to close the equations. This is typically done with an isothermal electron submodel, which gives rise to the widely used Boltzmann relation, or with a polytropic electron cooling law. In either case, the electrons are assumed to be isotropic in the velocity space and their density n_e and temperature T_e are related by the polytropic relation of Eq. 1, with $\gamma \geq 1$ and $\gamma = 1$ for the isothermal limit:

$$T_e \propto n_e^{\gamma-1} \quad (1)$$

As noted before,²⁻⁵ apart from being theoretically unjustified in a collisionless expansion, this approach also yields an unphysical behaviour in the $\gamma = 1$ case, that is, an electric potential decreasing logarithmically to $-\infty$. Indeed, in spite of the advantages of fluid models (speed and simplicity), the collisionless character of the plume warrants a fully kinetic treatment to recover the EEDF. Nevertheless, the error committed in the assumption of a simplified polytropic relation for the electrons needs to be evaluated to properly assess the limits of fluid models.

The EP2 group has developed a plume solver based on a collisionless fluid model and an integration method named Asymptotic Expansion Method (AEM).^{2,3} The University of Southern California (USC), on the other hand, has developed a 3D full PIC simulator to study the plume start-up process and the electrons cooling mechanism,⁴⁻⁶ finding that the electrons do not follow a single polytropic relation, but that they are better suited by a multi-region polytropic model, with a local γ coefficient. A similar multi-region modeling for the electrons polytropic coefficient has been recently suggested in collisionless plasma expansions in magnetic nozzles,⁷ simulated with a 1D kinetic model.

The possibility to compare the results of fluid and full PIC models, has therefore motivated the work presented in this paper. The two simulators have been benchmarked one against the other in terms of the predicted ion velocity and plasma density fields, thus allowing to identify more clearly the limits of the polytropic cooling relation for the electrons.

Sec. II describes the plasma plume simulation geometry, the fluid model and the plasma plume solver used by the EP2 group. Sec. III describes the full PIC simulator employed by USC, while Sec. IV presents the set of simulations and the results obtained with both codes. In Sec. V, the results are compared and the polytropic approach limits identified, discussing also some additional plasma plume physics. Sec. VI introduces a new hybrid PIC code, being developed by EP2 for future studies of plasma plume expansions. Finally, in Sec. VII, the comparison results are summarized and new research lines are identified.

II. A Fluid Model Solver: the AEM

The full PIC simulations feature a planar plume geometry like the one depicted in Fig. 1. The plume is a plasma slab, which is symmetric with respect to the (y, z) plane, extends to infinity along y and expands in the x and z directions. This choice, instead of the more usual axisymmetric configuration, is dictated by a present limitation in the PIC code, and allows to reduce the required number of simulated macro-particles and, hence, the computational cost. To allow for a direct comparison of the results, the fluid model solver considers this plume geometry as well.

A complete description of the fluid model assumptions can be found in Refs. 2, 3 and is herein briefly summarized. Firstly, the plasma plume is considered collisionless. This is a valid assumption only in the far region of the plume, starting a few thruster radii downstream from the thruster exit, where the neutrals density has dropped so much that the ions mean free path largely exceeds the plume size.³ However, since the scope of this paper is to compare simulations of a collisionless plume, in the following, the fluid model is applied from the very exit of the thruster at $z = 0$, as shown in Fig. 1.

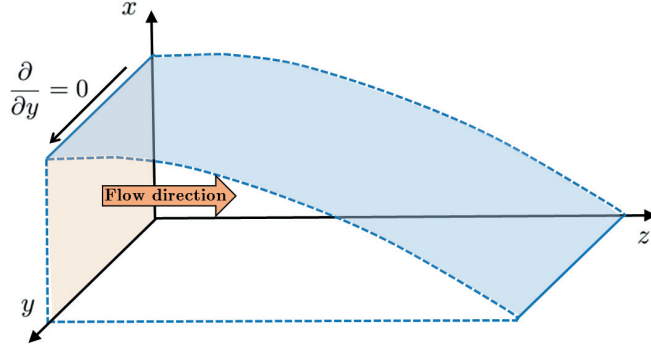


Figure 1. Simulation domain and plume geometry. The 2D plane plume is symmetric with respect to the (y, z) plane.

Secondly, the plume is considered quasi-neutral, given the relative size of the Debye length with respect to the typical radial dimension of the plume.^{2,3} This means that the ion and electron number densities are equal: $n_e = n_i \equiv n$.

Then, the electrons are assumed to be isotropic Maxwellian and polytropic, with a temperature T_e , while the ions are considered cold ($T_i = 0$). These assumptions allow us to neglect the ion pressure term, to work with a scalar electron pressure and to model the electrons cooling with the polytropic relation of Eq. 1.

Finally, the plume is considered unmagnetized and current free, meaning that the electrons drift velocity (much lower than their thermal velocity) is equal, at all points, to the ion velocity.

Although the fluid model presented in Refs. 2, 3 is applied to an axially symmetric plume case, the stationary fluid equations derived there can be easily generalized to the planar 2D geometry of Fig. 1, obtaining the following non-dimensional equations for mass conservation and momentum balance:

$$\tilde{u}_{zi} \frac{\partial \ln \tilde{n}}{\partial \tilde{z}} + \tilde{u}_{xi} \frac{\partial \ln \tilde{n}}{\partial \tilde{x}} + \frac{\partial \tilde{u}_{zi}}{\partial \tilde{z}} + \frac{\partial \tilde{u}_{xi}}{\partial \tilde{x}} = 0, \quad (2)$$

$$\tilde{u}_{zi} \frac{\partial \tilde{u}_{zi}}{\partial \tilde{z}} + \tilde{u}_{xi} \frac{\partial \tilde{u}_{zi}}{\partial \tilde{x}} = -\frac{\tilde{n}^{\gamma-1}}{M_0^2} \frac{\partial \ln \tilde{n}}{\partial \tilde{z}}, \quad (3)$$

$$\tilde{u}_{zi} \frac{\partial \tilde{u}_{xi}}{\partial \tilde{z}} + \tilde{u}_{xi} \frac{\partial \tilde{u}_{xi}}{\partial \tilde{x}} = -\frac{\tilde{n}^{\gamma-1}}{M_0^2} \frac{\partial \ln \tilde{n}}{\partial \tilde{x}}, \quad (4)$$

where $\tilde{z} = z/R_0$, $\tilde{x} = x/R_0$ are the normalized coordinates, $\tilde{n} = n/n_0$ is the normalized density, $\tilde{u}_{zi} = u_{zi}/u_{i0}$ and $\tilde{u}_{xi} = u_{xi}/u_{i0}$ are the normalized velocities components and $\tilde{T}_e = T_e/T_{e0}$ is the normalized electron temperature. R_0 represents a characteristic normalization length (assumed to be equal to the Debye length λ_{D0} at the origin) and n_0 , u_{i0} and T_{e0} are respectively the plasma density, the ion axial velocity and the electron temperature at the plume origin $z = 0$, $x = 0$. Note that the only difference with respect to the equations reported in Refs. 2 and 3 is the missing axisymmetric term.

The normalized fluid Eqs. 2 to 4 present two important non-dimensional parameters: the effective electron cooling coefficient γ and the ion Mach number reported below, with m_i representing the ion mass:

$$M_0 = \sqrt{m_i u_{i0}^2 / (\gamma T_{e0})} \quad (5)$$

The initial normalized plume profiles to be propagated downstream are then introduced: the initial normalized density $\nu(\eta) = \tilde{n}(\tilde{x}, \tilde{z} = 0)$, the axial velocity $v(\eta) = \tilde{u}_{zi}(\tilde{x}, \tilde{z} = 0)$ and the tangent of the streamlines divergence angle $\delta(\eta) = \tilde{u}_{xi}(\tilde{x}, \tilde{z} = 0) / \tilde{u}_{zi}(\tilde{x}, \tilde{z} = 0)$, with η representing the streamline distance from the symmetry plane at the initial section $\tilde{z} = 0$.

The Asymptotic Expansion method then solves for the analytical solution of the plume $\tilde{u}_{zi}^{(0)}$, $\tilde{u}_{xi}^{(0)}$ and $\ln \tilde{n}^{(0)}$, corresponding to the $M_0 \rightarrow \infty$ limit and referred to as “zeroth order solution”.^{2,3} In this limit, the ion streamlines are straight rays with constant fluid velocity and the density field is known analytically, with an expression given below, where η is related to $\tilde{z}$ and $\tilde{x}$ through the zeroth order streamline relation $\tilde{x} = \eta + \delta(\eta) \cdot \tilde{z}$:

$$\tilde{n}^{(0)}(\tilde{x}, \tilde{z}) = \frac{\nu(\eta)}{1 + \delta' \tilde{z}} \quad (6)$$

$$\tilde{u}_{zi}^{(0)}(\tilde{x}, \tilde{z}) = v(\eta) \quad (7)$$

$$\tilde{u}_{xi}^{(0)}(\tilde{x}, \tilde{z}) = v(\eta) \cdot \delta(\eta) \quad (8)$$

The zeroth order solution for the density differs from the one presented in Refs. 2 and 3 due to the absence of the axisymmetric term $(1 + \tilde{z}\delta/\eta)$ in the denominator, which models the density decrease as the streamline radius increases. In this planar 2-D geometry, the density only decreases if the streamlines diverge from one another.

After computing the zeroth order solution, the AEM solves for increasing order corrections to the fluid variables by expanding them in the small parameter $\varepsilon = 1/M_0^2$ as:

$$\begin{aligned} \tilde{u}_{zi} &= \tilde{u}_{zi}^{(0)} + \varepsilon \tilde{u}_{zi}^{(1)} + \varepsilon^2 \tilde{u}_{zi}^{(2)} + \dots, \\ \tilde{u}_{xi} &= \tilde{u}_{xi}^{(0)} + \varepsilon \tilde{u}_{xi}^{(1)} + \varepsilon^2 \tilde{u}_{xi}^{(2)} + \dots, \\ \ln \tilde{n} &= \ln \tilde{n}^{(0)} + \varepsilon \ln \tilde{n}^{(1)} + \varepsilon^2 \ln \tilde{n}^{(2)} + \dots, \end{aligned} \quad (9)$$

By equating the terms of order ε^i obtained by substituting the expansions of Eq. 9 into Eqs. 2 to 4, the evolution equations of the i^{th} order corrections along the zeroth order streamlines can be obtained. Integration of such equations^{2,3} finally yields the i^{th} order perturbations along each streamline as a function of $\tilde{z}$, and, through Eq. 9, the corrected fluid solution up to the i^{th} order. As shown in Ref. 2, the AEM method generally predicts increasing perturbations with $\tilde{z}$ and it fails when the correction terms become comparable to their previous order solutions. Such a condition arises sooner, the smaller the divergence angle of the plasma plume and the lower the Mach number M_0 .^{2,3} To avoid this limitation, the existing AEM plume solver has been upgraded by restarting it at regular intervals of $\tilde{z}$. The corrections to the fluid variables are then evaluated in subdomains of $\tilde{z}$, with the $(n+1)^{th}$ subdomain considering the perturbed ion streamlines at the end of the n^{th} subdomain as its new zeroth order streamlines. This process is illustrated in Fig. 2.

With the above described technique, the axial validity of the AEM method can be extended to infinity regardless of the M_0 value, by choosing an appropriate restarting interval $\Delta\tilde{z}$. This means that the plume does not need to be very supersonic any longer to be able to meaningfully extend the AEM simulation far downstream. Nevertheless, the method might turn out to be very inefficient for $M_0 \sim 1$, for which the restarting interval $\Delta\tilde{z}$ would need to be impractically small.

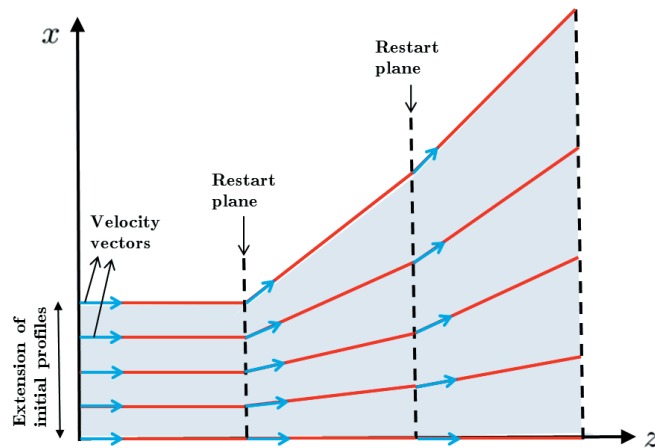


Figure 2. The restarting scheme for the AEM. Zeroth order streamlines are updated at regular intervals in the $\tilde{z}$ direction with the corrections predicted by the method. The shaded area represents the effective simulation domain.

III. A Full PIC Simulation Tool

The plasma plume expansion is also simulated using a full particle PIC simulation model developed at USC.⁴⁻⁶ In this method, both the electrons and the ions are modeled as macro-particles. The ion and electron dynamics, the space charge and the electric potential ϕ are solved self-consistently with Eqs.10 and 11, with m_p , q_p representing respectively the macro-particle mass and charge and $\vec{v}_p, \vec{r}_p$ their velocity and position vectors:

$$\epsilon_0 \cdot \nabla^2 \phi = e (n_e - n_i) \quad (10)$$

$$\frac{d}{dt} (m_p \vec{v}_p) = q_p \vec{E}, \quad \vec{v}_p = \frac{d\vec{r}_p}{dt} \quad (11)$$

The simulation setup is similar to that described in Refs.4 and 5. The simulation domain is initially a vacuum. At each step, macro-particles representing ions and electrons are emitted along the z direction into the simulation domain. The ions are sampled from a cold drifting Maxwellian distribution and have a finite temperature T_{i0} , unlike in the fluid model where they are assumed to be cold. The electrons inside the plume source, on the other hand, are thermal and stationary. Simulations are run using the real mass ratio of proton to electron, $m_i/m_e = 1836$. The temperature ratio of ion to electron at the source is taken to be $T_{i0}/T_{e0} = 0.01$, where the subscript 0 denotes the condition at the plume source plane ($0 < \tilde{x} < 10, z = 0$). This corresponds to a normalized ion thermal velocity of $v_{ti0}/v_{te0} = 0.0023$. In this paper, we present results for macroscopic drifting velocity for the plasma plume, $v_{beam}/c_s = M_0 = 5$ and 15, as shown in Tab. 1, with $c_s = \sqrt{T_{e0}/m_i}$ representing the ion sonic velocity at the plume source plane.

We then consider a plasma plume emission with equal electron and ion current density vectors at the plume source plane, $\vec{j}_{e0} = \vec{j}_{i0}$. The cell size is taken to be the Debye length at this plane, λ_{D0} , with respect to which the coordinates are normalized. The simulation domain in the $\tilde{x} - \tilde{z}$ plane is $600 \lambda_{D0} \times 1000 \lambda_{D0}$. The simulation was run using a time step resolution of $\Delta t \times \omega_{pe} = 0.05$ ($\Delta t \times \omega_{pi} \simeq 1.16 \times 10^{-3}$), where ω_{pe} and ω_{pi} are the electron and ion plasma frequencies at the plume source plane. The initial plasma plume size along $\tilde{x}$ is taken to be $R_{beam} = 10 \lambda_{D0}$. For the $M_0 = 15$ case, the normalized simulation duration is $t\omega_{pe} = 856.8$ or $t\omega_{pi} \simeq 20$ (a total number of simulation steps equal to 17136). At each step, approximately 1000 simulation particles are injected. For the $M_0 = 5$ case, the simulation normalized duration is $t\omega_{pe} = 2570.4$ or $t\omega_{pi} \simeq 60$ (51408 total simulation steps). At each step, approximately 400 simulation particles are injected. Note that the simulations duration is much longer than the ion plasma period and that the beam transient length, $L_{beam} = v_{beam}t$ is much larger than the beam initial radius, R_{beam} . Therefore, a steady state for both electrons and ions is well established behind the beam front (the farthest section that the ions have reached, located at $\tilde{z} \simeq v_{beam}t$). Since the electrons oscillate back and forth many times around this front, it can be reasonably assumed that they reach a quasi-stationary condition. In the following, for the comparison with the stationary fluid simulations, we shall therefore consider a simulation region extending downstream to $\tilde{z} \sim 250$.

IV. Simulation Results

A. Simulations set

For this comparison study, a set of 4 different plume cases has been taken into account as reported in Tab. 1. The initial density profile for the plasma plume has been assumed to be uniform in the range $\tilde{x} \in [0, 10]$, while for the injection ion velocity components, the conical profile of Eq. 12 and 13 has been used:

$$\tilde{u}_{zi}(\tilde{x}, \tilde{z} = 0) = \left(1 + \left(\frac{\tilde{x}}{10} \cdot \tan \alpha_0 \right)^2 \right)^{-1} \quad (12)$$

$$\tilde{u}_{xi}(\tilde{x}, \tilde{z} = 0) = \tilde{u}_{zi}(\tilde{x}, \tilde{z} = 0) \cdot \tan \alpha_0 \cdot \frac{\tilde{x}}{10}; \quad (13)$$

The ion Mach number shown in Tab. 1 is given by Eq. 5, assuming $\gamma = 1$. This means that, if the electrons of the PIC simulation are injected with a thermal random velocity corresponding to a temperature T_{e0} , the ion injection fluid velocity at the axis is computed as: $u_{i0} = M_0 \cdot \sqrt{T_{e0}/m_i}$.

The initial density and velocity profiles are finally plotted for the Sim. 2 and Sim. 4 case in Fig. 3. The Sim. 1 and Sim. 3 cases feature an identical density profile, but with a constant initial axial velocity $\tilde{u}_{zi}$

Table 1. Simulation set parameters considered in the comparison study

Parameter	Sim. 1	Sim. 2	Sim. 3	Sim. 4
Initial Mach number, computed as $M_0 = \sqrt{m_i u_{i0}^2 / T_{e0}}$	15	15	5	5
Initial divergence angle of outermost streamline	0	10	0	10
Initial density profile	uniform	uniform	uniform	uniform

and a zero velocity component along $\tilde{x}$ ($\alpha_0 = 0$). Note that the AEM density profile has necessarily been smoothed for its correct implementation in the fluid solver, which requires a smooth transition to vacuum, while preserving the total mass flow in the $\tilde{z}$ direction. The PIC density profile, on the other hand, is provided for the ions only, since that of the electrons is slightly different and determined by the current flux condition $\vec{j}_{e0} = \vec{j}_{i0}$, as explained in Sec. III.

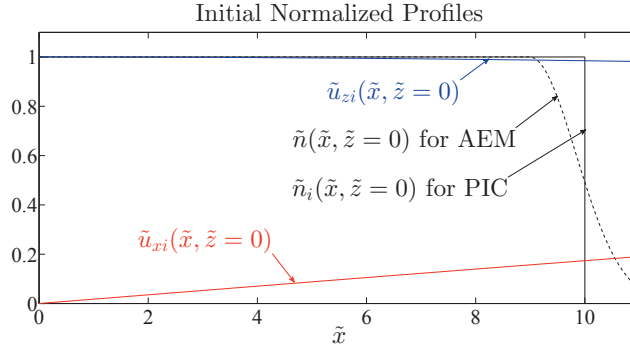


Figure 3. The initial normalized plume profiles at the beam injection: initial density profiles for the AEM (dashed black) and for the PIC (solid black), initial velocity profiles $\tilde{u}_{zi}(\tilde{x}, 0)$ (solid blue) and $\tilde{u}_{xi}(\tilde{x}, 0)$ (solid red) for both methods.

B. Full PIC Simulations Results

Full particle PIC simulations have been carried out for the simulation cases listed in Tab. 1. Their results are fully discussed in a companion paper.⁸ Fig. 4 shows the simulation result for the Sim. 2 case, featuring $M_0 = 15$ and $\alpha_0 = 10^\circ$. The ion and electron number density profiles shown in Fig. 4 (a) and (b) are normalized with respect to the ion density at the injection plane n_{i0} . Fig. 4 (c) shows the plasma charge density $\tilde{n}_i - \tilde{n}_e$. An initial region of positive charge generates because, in order to achieve an equal current density $j_{e0} = j_{i0}$, the electron density at injection must be lower than that of the ions.⁸ Fig. 4 (d) shows the normalized electric potential $\tilde{\phi} = e\phi/T_{e0}$. Finally, the magnitudes of the electron thermal velocities along the beam direction $\tilde{z}$, and perpendicular to it, along $\tilde{x}$, are shown in Fig. 4 (e) and (f). These velocities are normalized with respect to their injection values.

C. Fluid Model Simulations Results

The AEM fluid solution provides insight into the essential physical processes occurring in the plasma plume expansion. Fig. 5 shows the evolution of the density profiles and of the divergence profiles $\tilde{u}_{xi}/\tilde{u}_{zi}$ for the 4 simulation cases of Tab. 1 and at successive planes $\tilde{z}_i$, with the assumption of $\gamma = 2$. This γ value, allows to match well the fluid and PIC simulation results, as it will be shown in Sec. V. The reported simulations have been carried out with the re-starting scheme presented in Sec. II and a correction up to second order.

Such initial profiles are a subset of the input initial profiles, which are fed to the AEM fluid solver, at each re-start. In Fig. 5 a), the propagation of the expansion Mach line can be observed clearly. In fact, the density gradient and the related ambipolar electric field, generating at $\tilde{x} = 9, \tilde{z} = 0$ (refer to Fig. 3), propagates inwards towards $\tilde{x} = 0$ along a line with a slope given by $-\arcsin(1/M_0)$ and reaches the axis after an axial distance $\tilde{z} \sim 135$. Once the expansion wave reaches the beam symmetry plane, the wave reflection effect is that of generating a density plateau in the x-direction, which extends further downstream.

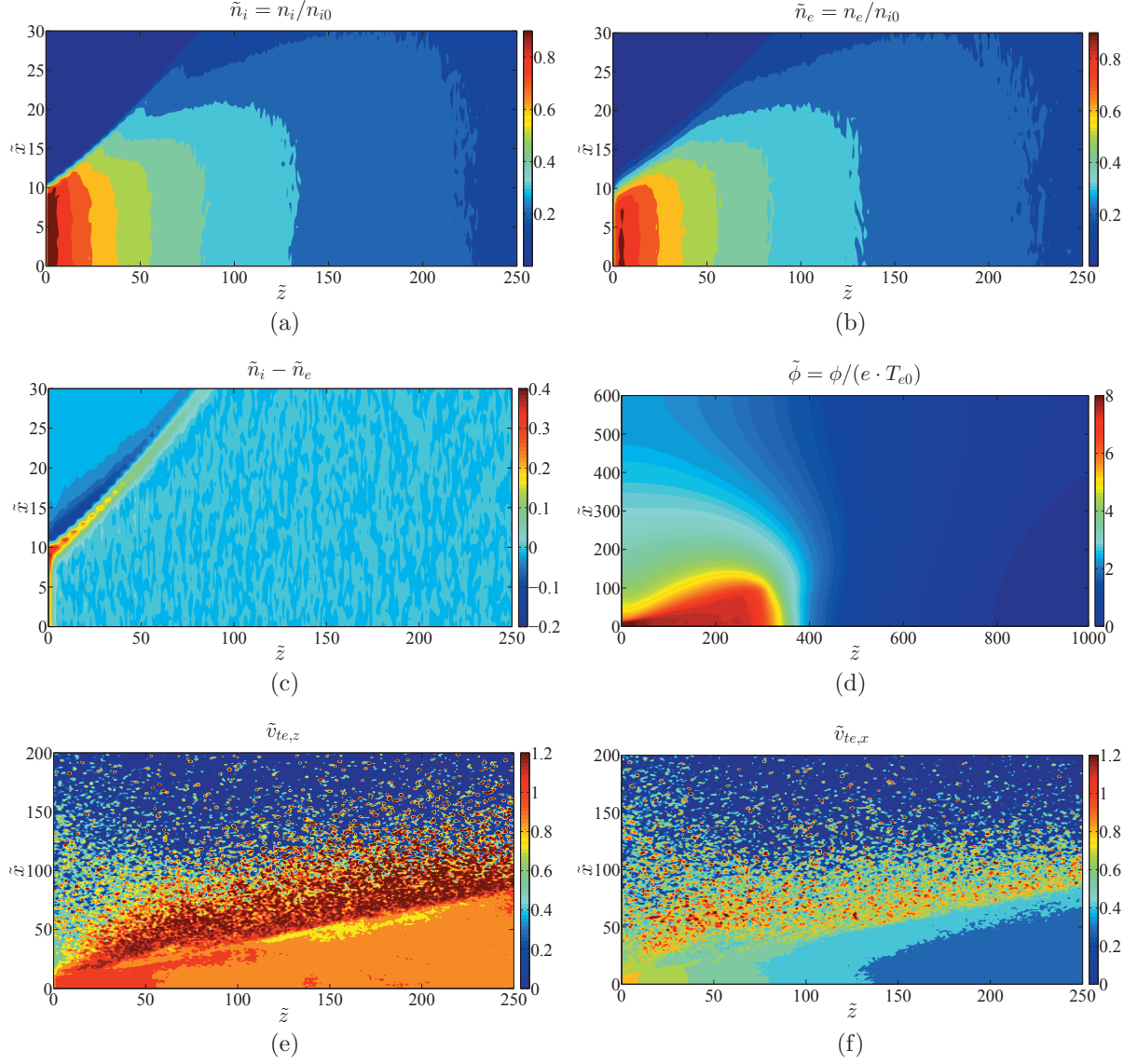


Figure 4. Full PIC simulation results for the Sim. 2 case. (a) Normalized ion number density. (b) Normalized electron number density. (c) Normalized plasma charge density. (d) Normalized electric potential. (e) Normalized electron thermal velocity along the beam direction $\tilde{z}$. (f) Normalized electron thermal velocity perpendicular to the beam direction, along $\tilde{x}$.

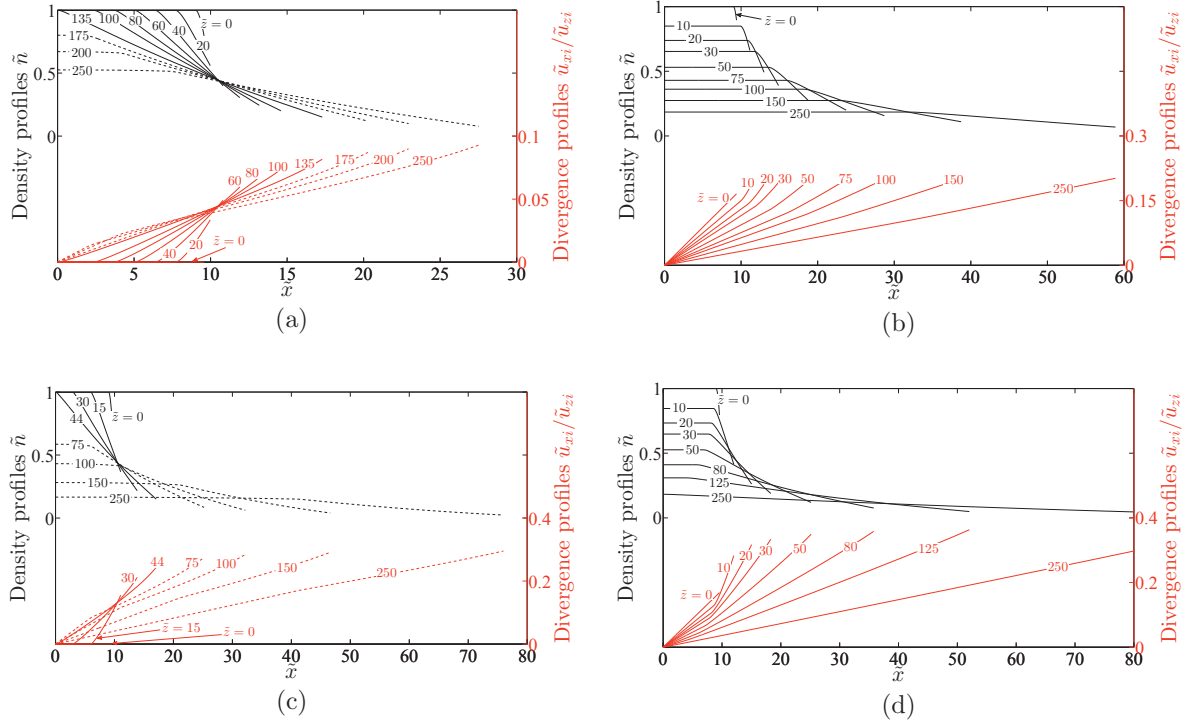


Figure 5. Density and divergence profiles at different $\tilde{z}$ sections in the AEM fluid model: (a) Sim. 1 case, (b) Sim. 2 case, (c) Sim. 3 case, (d) Sim. 4 case. The polytropic coefficient γ has been assumed equal to 2.0.

Regarding the generation of the expansion wave, this can be appreciated at the outer edge of the plasma plume, by observing the gradual onset of a non-zero divergence angle region (red curves), which propagates inwards. An interesting conclusion is that the plume develops a conical velocity field, or a divergence profile linear with $\tilde{x}$ at the expansion wave reflection, but not elsewhere. This conical divergence profile is the only admitted profile of the fluid models based on the self-similarity assumption.^{2,3,9–11} After the expansion wave reflection, the divergence profile is no more completely self-similar (or linear in $\tilde{x}$), since it displays two regions of different divergence slope.

Fig. 5 b) shows the evolution of the plume profiles for the Sim. 2 case. Now, the expansion Mach line generating at the plume periphery has a slope relative to the outermost streamline lower than $\alpha_0 = 10$ degrees. Therefore, it gradually gets farther away from the symmetry plane, producing an increasingly wider region with $\tilde{z}$, which is completely unaffected by the expansion and simply expands conically, according to Eq. 6. Eventually, the expansion wave will reach the symmetry plane, as it crosses plume regions with a decreasing ion divergence angle, and this crossing is farther downstream the higher the γ coefficient. In fact, this parameter controls the temperature and consequently the slope of the Mach lines with respect to the streamlines velocity vector.

Fig. 5 c) shows the evolution of the plume profiles for the Sim. 3 case. At a much lower Mach number, the reflection wave reaches the symmetry plane much quicker and at an axial distance $\tilde{z} \sim 44$. The same considerations made for Fig. 5 a) apply here, with the difference that the expansion is now stronger, being the Mach number lower. Therefore, the divergence angle of the ion streamlines grows to much higher values.

Finally, Fig. 5 d) shows the evolution of the plume profiles for the Sim. 4 case. Unlike for the Sim. 2 case, the ion Mach line slowly approaches the symmetry plane, crossing it at $\tilde{z} > 100$. The difference is due to the lower Mach number $M_0 = 5$ and hence the higher Mach cone half-angle, now larger than $\alpha_0 = 10$ degrees.

V. Discussion and Comparison of the Results

In order to match the PIC simulation results with those of the fluid model, an error figure of merit has to be introduced. This is defined as the root mean square of the relative density error over a common AEM-PIC

simulation domain, with a weight, for each common node i, j , given by $w_{ij} = n_{AEMij} / \sum_{i,j} n_{AEMij}$:

$$err = \sqrt{\sum_{i,j} w_{ij} \cdot \left(\frac{n_{AEMij} - n_{PICij}}{n_{AEMij}} \right)^2} \quad (14)$$

Regarding the domain considered, this extends from $\tilde{z} = 0$ to $\tilde{z} = 250$, the upper boundary being due to the PIC “stationary” region extension. In the $\tilde{x}$ direction, on the other hand, such domain is limited by the radius of the outermost AEM streamline solution.

The fluid model parameters have then been tuned to minimize this figure of merit. This has been done by evaluating the fluid solution for a set of γ and M_0 values contained in a 2-D solution space. The results for the Sim. 1 case are shown in Fig. 6.

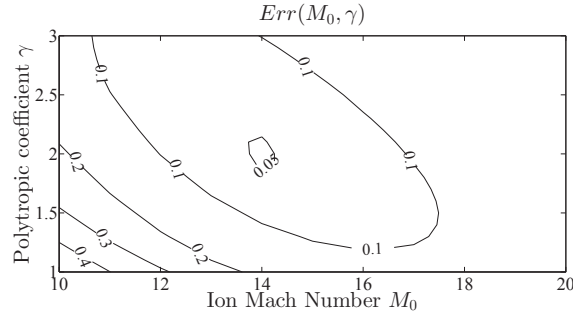


Figure 6. Error figure of merit as a function of the M_0 and γ parameters of the fluid model for the Sim. 1 case.

The R.M.S. relative density error ranges between a minimum of 3.4% for the $M_0 = 15$, $\alpha_0 = 10$ deg. case and a maximum of 7.5% for the $M_0 = 5$, $\alpha_0 = 0$ deg. case. The pairs of γ and M_0 that minimize the errors and the corresponding R.M.S. error are finally reported in Tab. 2, for all the simulation cases:

Table 2. Optimal γ and M_0 values

Parameter	Sim. .1	Sim. .2	Sim. .3	Sim. .4
Ion Mach number M_0	14	15	4.5	4.0
Electron polytropic cooling coefficient	2.0	1.7	1.6	1.9
R.M.S. relative density error	5.0%	3.4%	7.5%	5.3%

Apparently, the optimal M_0 is not very different from the PIC simulation one, computed with Eq. 5 and taking $\gamma = 1$. However, the most effective γ coefficient appears to be somewhere between 1.6 and 2, depending on the simulation case, with 2 representing the adiabatic γ value for the considered geometry. In fact, although the ions and the electrons have always three degrees of freedom (along x, y, z), it is clear that the degree of freedom in the infinite direction (y) does not participate at all in the expansion, thus remaining frozen. Therefore, in the computation of the adiabatic specific heat ratio, only two degrees of freedom should be taken into account, leading to an adiabatic value equal to $\gamma = 1 + 2/N_{DOF} = 2$.

With the optimal values for M_0 and γ of Tab. 2, the AEM solutions have been finally compared with those of the PIC, in terms of density contours and ion streamlines, as shown in Fig. 7.

In all cases, the agreement is quite satisfactory, both in terms of the density contours and of the ion streamlines. Regarding the former, the iso-density lines only depart significantly at the outer periphery of the plume, where the difference between the initial profiles for AEM and PIC simulations is important (refer to Fig. 3). Regarding the latter, it can be noticed that the AEM slightly overestimates the divergence growth of the core streamlines (e.g. the 25 % ion current streamlines), while underestimating the divergence growth of the outermost streamlines. This is clearly due to the assumption of a single polytropic coefficient for the fluid model, while the PIC simulations show that the effective γ value changes from streamline to streamline.^{5,8} In particular, the outermost streamlines present a lower γ value, thus retaining their thermal energy farther downstream and expanding more than the core streamlines. The AEM optimal solution thus assumes an average effective polytropic coefficient, that minimizes the overall error.

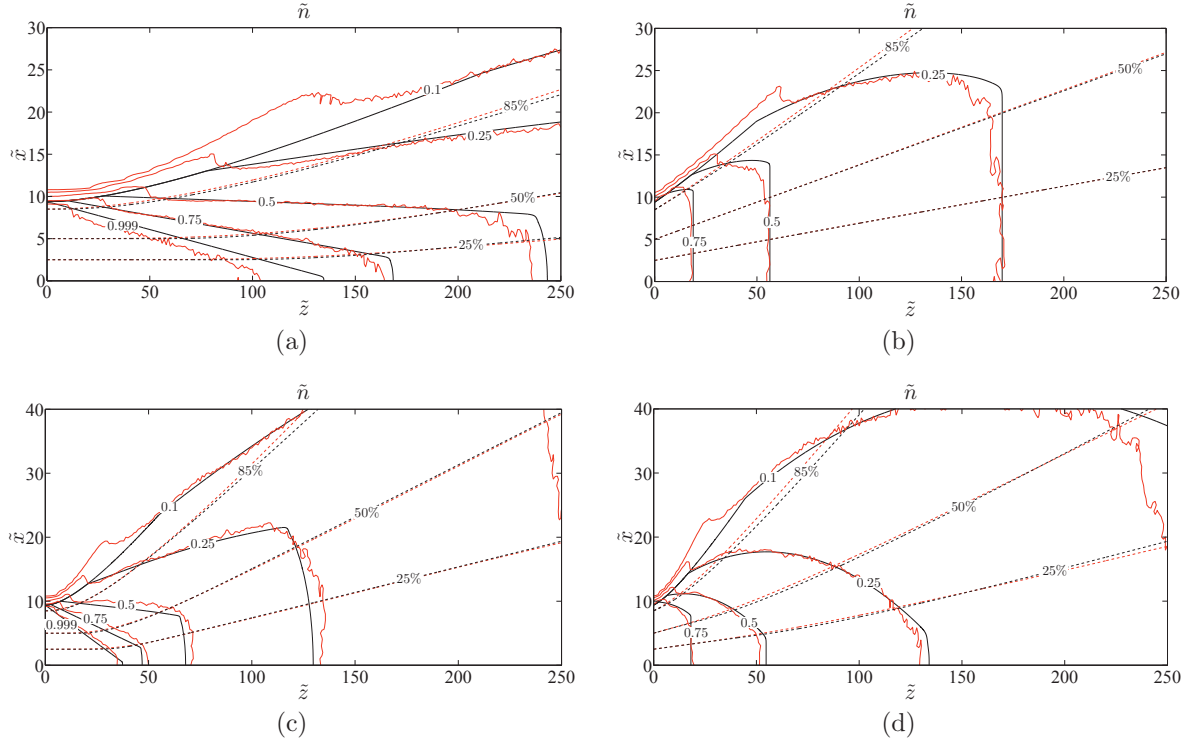


Figure 7. Density contour (solid lines) and streamlines (dashed lines) comparison (25, 50 and 85% ion current). Red lines refer to the PIC, while black lines to the AEM. (a) Sim. 1 case, (b) Sim. 2 case, (c) Sim. 3 case and (d) Sim. 4 case.

Regarding the optimal Mach numbers of Tab. 2, they do not coincide exactly with those of Tab. 1 for two reasons. Firstly, the optimal Mach number should approach the value of the effective Mach number, which controls the real speed of density perturbations within the supersonic plume. Such effective Mach number is lower than the Mach number of Tab. 1 because it depends on an effective coefficient $\gamma > 1$, through Eq. 5. Secondly, the optimal Mach number minimizes the error figure of merit and, therefore, it does not necessarily coincide with the effective Mach number. Referring to Fig. 7 (a), the density perturbation, represented by the iso-density line with value 0.999, moves towards the plume symmetry plane more quickly in the PIC simulation than in the fluid one. This suggests that the effective initial Mach number is lower than the optimal initial Mach number, used for the fluid simulation.

The major conclusions that can be extracted from this comparative study are finally summarized below:

- The fluid model reproduces correctly the results of the PIC simulations in terms of plasma density and velocity at least down to a distance of 25 initial plume radii.
- A single value for the polytropic exponent ($\gamma \simeq 1.6 - 2$) appears to be reasonably good for all the 2D plane plume simulations considered. Although a detailed analysis⁸ suggests the existence of different γ regions, this is not particularly relevant for the global behavior of the plume. In particular, a near adiabatic γ coefficient seems to correctly model the ion streamlines divergence growth and hence the density field.

The above-mentioned conclusions, however, do not reduce the importance of kinetic simulations in the study of the plasma plume expansion. Firstly, they remain the only way to study the evolution of the electron and ion energy distribution functions and to study the effect of heavy particles collisions (charge and momentum-exchange). Secondly, they allow to properly study the electron cooling mechanism, which affects the electric potential drop, far downstream. In fact, this is strongly related to the local γ coefficient in the far region of the plume, whose value may be different from the optimal one obtained here.

VI. A New Hybrid PIC code for Future Work

In order to extend the simulation capabilities of the fluid model, the EP2 group is developing its own hybrid PIC 3-D code named EP2-Plus: Extensible Parallel Plasma PLUme Simulator. Such a tool considers the heavy species as particles (neutrals and ions). The electrons, on the other hand, are treated as a fluid, whose momentum equations have to be solved in order to determine the electric and magnetic fields, once the heavy species density distribution is known. The most relevant tool capabilities are listed below:

- 3D simulation of the near region plume physics
- 3D simulation of the plume interaction with either a target debris or sensitive S/C surfaces (solar panels, sensors, thruster, etc...)
- Simulation of an oblique magnetic field effects on the plume expansion (e.g. the geomagnetic field)
- Asymmetric initial plume profiles and equi-potential surfaces for the electrons fluid equations (e.g. neutralizers)

Simulation of the near region plume physics will be achieved with a detailed modeling of the charge-exchange collisions between neutrals and ions, thus enabling a correct quantification of the ion backflow towards S/C sensitive surfaces. Regarding the magnetic field effects, an oblique magnetic field shall be included in both the propagation of the charged particles trajectories and in the fluid solution of the electron momentum balance equations.

A preliminary plume simulation is shown in Fig.8, featuring a view of the trajectory of 100 tracked particle ions and the corresponding weighted ion density at a given plume cross section.

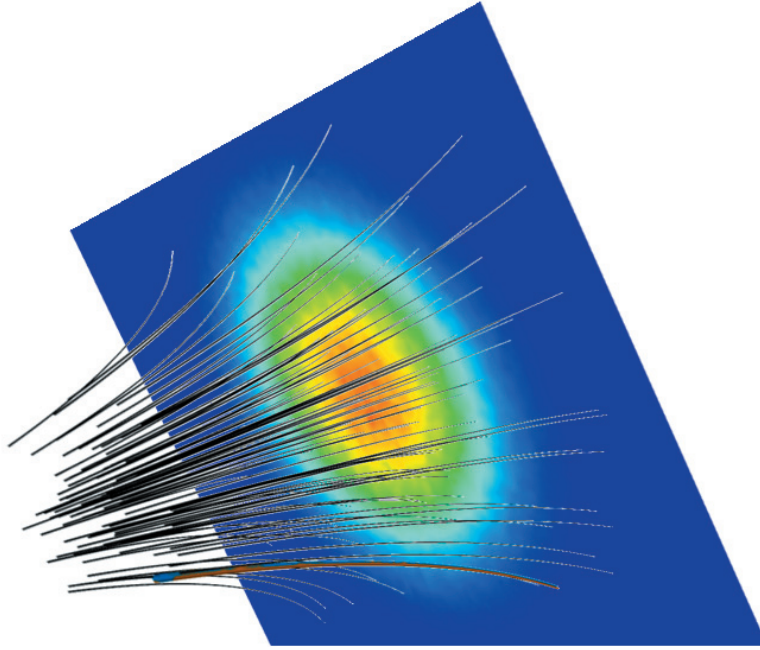


Figure 8. EP2-Plus preliminary simulation results showing 100 tracked ion particles trajectories and the corresponding weighted ion density at a given plume cross section.

VII. Conclusions

In this paper, a comparative study between full PIC and fluid simulations of a collisionless plasma plume expansion into vacuum has been carried out.

A PIC simulator treating electrons as particles has been presented, featuring a 2-D plasma slab geometry, with periodic boundary conditions along y . In this way, the overall computational load is reduced. A fluid

model solver based on the AEM method, firstly introduced in Refs. 2, 3, has then been described and used to match the results of the PIC simulations. The re-starting technique, presented here, allows to extend the validity of the AEM fluid solution far downstream and to study plumes that are not necessarily hypersonic.

A comparison between the fluid and the PIC simulations has then been carried out by finding the optimal values for the 2 free parameters of the fluid model, namely the Ion Mach number M_0 and the electron polytropic cooling coefficient γ . It has been found that the optimal Mach number is very close to that used in the PIC simulations. The optimal polytropic cooling coefficient, on the other hand, assumes values close to 2, the adiabatic limit for the 2-D geometry of the plasma plume slab considered here.

The expected relative density errors over a large domain, extending up to 25 initial plume radii downstream, has been estimated to be between 3 and 8%, depending on the simulation case. Results show that a good accuracy can be reached even with a fluid model based on polytropic electrons. Such assumption is not justified and, in fact, it is not strictly valid, as shown by the kinetic PIC simulations.⁸ In fact, the polytropic coefficient depends on the plasma density number and on the ion streamlines and features three characteristic regions: a rapidly cooling region during the plume start up, an almost isothermal region and a gradually cooling region with $\gamma > 1$ extending indefinitely downstream. A related but different behavior is also seen in the 1D kinetic simulation of the plasma expansion in a magnetic nozzle.⁷

Finally, the capabilities and some preliminary results of a new hybrid PIC code, being developed by the EP2 group, have been presented.

Regarding future work, an extension of this comparison study to a more realistic 3-D axisymmetric plume geometry shall be carried out and the existence of an optimal gamma value in that case will be investigated.

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References

- ¹C. Bombardelli and J. Peláez. Ion beam shepherd for contactless space debris removal. *Journal of Guidance, Control, and Dynamics*, 34(3):916–920, May 2011.
- ²F. Cichocki, M. Merino, and E. Ahedo. Modeling and simulation of ep plasma plume expansion into vacuum. In *50th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Cleveland, OH*, AIAA 2014-3828, 2014.
- ³M. Merino, F. Cichocki, and E. Ahedo. Collisionless plasma thruster plume expansion model. *Plasma Sources Science and Technology*, 24(3):035006, 2015.
- ⁴Y. Hu and J. Wang. Fully kinetic simulations of mesothermal plasma expansion. In *13th Spacecraft Charging Technology Conference*, number 197, 2014.
- ⁵Y. Hu and J. Wang. Electron properties in collisionless, mesothermal plasma expansion: Fully kinetic simulations. *IEEE Trans. Plasma Science*, 2015.
- ⁶J. Wang, O. Chang, and Y. Cao. Electron-ion coupling in mesothermal plasma beam emission: Full particle pic simulations. *IEEE Trans. Plasma Science*, 40(2):230–236, 2012.
- ⁷J. Navarro-Cavallé, S. Correyero, and E. Ahedo. Collisionless electron cooling on magnetized plasma expansions: advances on modelling. In *34th International Electric Propulsion Conference, IEPC-117*, 2015.
- ⁸Y. Hu and J. Wang. On the validity of the boltzmann assumption for electrons in plasma plume modeling. In *34th International Electric Propulsion Conference*, number 90872, 2015.
- ⁹DE Parks and I. Katz. A preliminary model of ion beam neutralization. In *14th International Electric Propulsion Conference*, Fairview Park, OH, 1979. Electric Rocket Propulsion Society.
- ¹⁰J. Ashkenazy, A. Fruchtman, Y. Raites, and N.J. Fisch. Modelling the behaviour of a Hall current plasma accelerator. *Plasma physics and controlled fusion*, 41:357, 1999.
- ¹¹AG Korsun, EM Tverdokhlebova, and FF Gabdullin. Mathematical model of hypersonic plasma flows expanding in vacuum. *Computer physics communications*, 164(1-3):434–441, 2004.