Negative streamer fronts: comparison of particle and fluid models and hybrid coupling in space

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To understand ionization fronts and the growth of streamer channels, both fluid and particle models have been developed. While fluid models are computationally efficient in regions with large particle densities like the interior of a streamer finger, particle models represent the full microscopic scattering physics and are appropriate for regions with low densities and for particles with high energies like in the "pulled" ionization front ahead of the streamer finger. Furthermore, the statistics of few single particles in the front can create fluctuations of velocity and ionization rate and might trigger inherent instabilities. The goal of the project is therefore to develop a computation scheme that is hybrid in space. Here, we compare planar ionization fronts in the fluid or the particle model. The ionization density behind the particle front is higher while front velocities are similar. We analyze and explain this discrepancy. We also sketch the concept of hybrid model coupling of different spatial regions.

1. Introduction

Streamers are growing filaments of weakly ionized non-stationary plasma produced by a sharp ionization front that propagates into non-ionized matter. Streamers are used in industrial applications such as ozone generation or gas and water purification, and they occur in natural processes as well such as lightning or transient luminous events in the upper atmosphere. Therefore accurate modeling and simulation of streamers are of high interest.

Most streamer simulations are done with so called fluid models. Fluid models approximate the particles as continuous densities for different species; they should incorporate the appropriate microscopic physics included in particle models; their validity breaks down in regions with very low particle densities. It would be preferable to use a particle model such as a PIC/MCC method. However, particle models with realistic fluctuations that do not use superparticles, are computationally very expensive both in time and in memory space. Therefore, a multiscale approach is desirable combining the computational efficiency of the fluid model with the full physics of the particle model through hybrid coupling of different spatial regions.

Such hybrid computations would also contribute to the understanding two other phenomena of recent interest. 1. Streamer branching is recently understood in terms of an inherent instability of a fully deterministic fluid model [1,2,3]. However, fluctuations of the individual particles in the leading edge of the ionization front might trigger this instability earlier than it occurs in the deterministic fluid model. 2. This front region is also important for the generation of high energy electrons in streamer and leader. The recent detection [4] of x-rays emanating from lightning strokes indicates that high energy electrons can be generated during early stages of the lighting event. Both questions require a fully kinetic description of the front region.

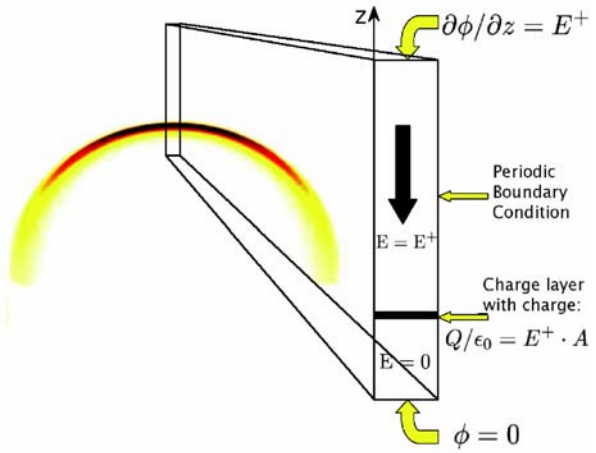

Figure 1. The relation between the full streamer problem and the planar fronts described in this paper: the left picture shows the narrow space charge layer surrounding the negative streamer head. The right picture shows a zoom into the inner structure of the space charge layer with an essentially planar ionization front as treated in this paper. In the transversal direction, periodic boundary conditions are applied.

Here we concentrate on negative streamer fronts in pure N_2 under normal conditions. We first describe the general schemes of the particle and fluid models. Then we compare the results of both models for planar fronts. Planar fronts can be simulated with reasonable particle numbers without introducing super-particles by investigating a small, essentially one-dimensional section of the ionization front as illustrated in Fig. 1. The comparison shows clear discrepancies between the results of the particle and the fluid model. We analyze and explain this discrepancy. In the end, based on observation and analysis, we explain our hybrid concept.

2. Overview of particle and fluid models

We here describe the general schemes of the particle and fluid models. Details of the methodology and numerical implementation of the models are presented elsewhere.

a. Particle model

The particle model contains all the essential microscopic physical mechanisms that are thought to be relevant for the propagation of a negative impact ionization front in pure nitrogen. The collision of electrons with neutral molecules is treated as a stochastic Monte Carlo process. While propagating freely, the electrons follow a deterministic trajectory according to Newton's law. Because the mobility of the positive ions is two orders of magnitude smaller than that of the electrons, ions are treated as immobile within the short time scales investigated in this paper. Within the ionization front, recombination can be neglected as well. The space charges in the front change the local electric field, which is accounted for by solving the Poisson equation.

The electron-neutral collisions in the particle model can be elastic, inelastic or ionizing collisions. The probability distribution of the different collision processes depends on the electron energy at the moment of impact; we use the cross section data from the Siglo Database. As the collisions are random within a probability distribution, the actual type and time of a specific collision is sampled by a Monte Carlo process. Once the collision process is chosen, the energy loss of the electron is known. Different scattering methods have been discussed in [5]. Here, the scattering method described in [6] has been used for elastic and exciting collisions. In ionizing collisions, we use Opal's empirical fit [7] to determine the energy of the ejected electron. Energy conservation and the assumption [8] that scattered and ejected electron velocities are perpendicular and coplanar with the incident electron fix all scattering angles.

b. Fluid model

The fluid model approximates the average dynamics of the local electrons as local densities depending on the local electric field. In general, it can be derived from the Boltzmann equation. But in practice, we have determined mobilities, ionization rates and diffusion coefficients from swarm experiments with the particle model.

The fluid model consists of continuum equations for electron and ion densities:

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \mathbf{j}_e = S$$

$$\frac{\partial n_p}{\partial t} = S$$

$$\mathbf{j}_e = -\mu \mathbf{E} n_e - \mathbf{D} \nabla n_e$$

where n_e and n_p are the electron and ion densities, $\mathbf{j}_e$ is the flux density, $S = |n_e \mu(E)\mathbf{E}|\alpha(E)$ is the source of electrons due to impact ionization, μ represents the mobility and **D** is the diffusion matrix; the charge densities change the electric field according to the Poisson equation

$$\nabla \cdot \mathbf{E} = \frac{e(n_p - n_e)}{\varepsilon_0}.$$

3. Comparison of planar front results in particle and fluid model

The results of particle and fluid model are compared for planar fronts. We first present results of the particle model in a field of strength E=100 kV/cm. The initial condition is a thin electron layer with enough electrons to screen the field behind the layer. Fig. 2 shows the ionization front at times t_1=450 ps (left) and t_2=900 ps (right). It shows that the front moves with approximately stationary profile to the right; its velocity is about constant.

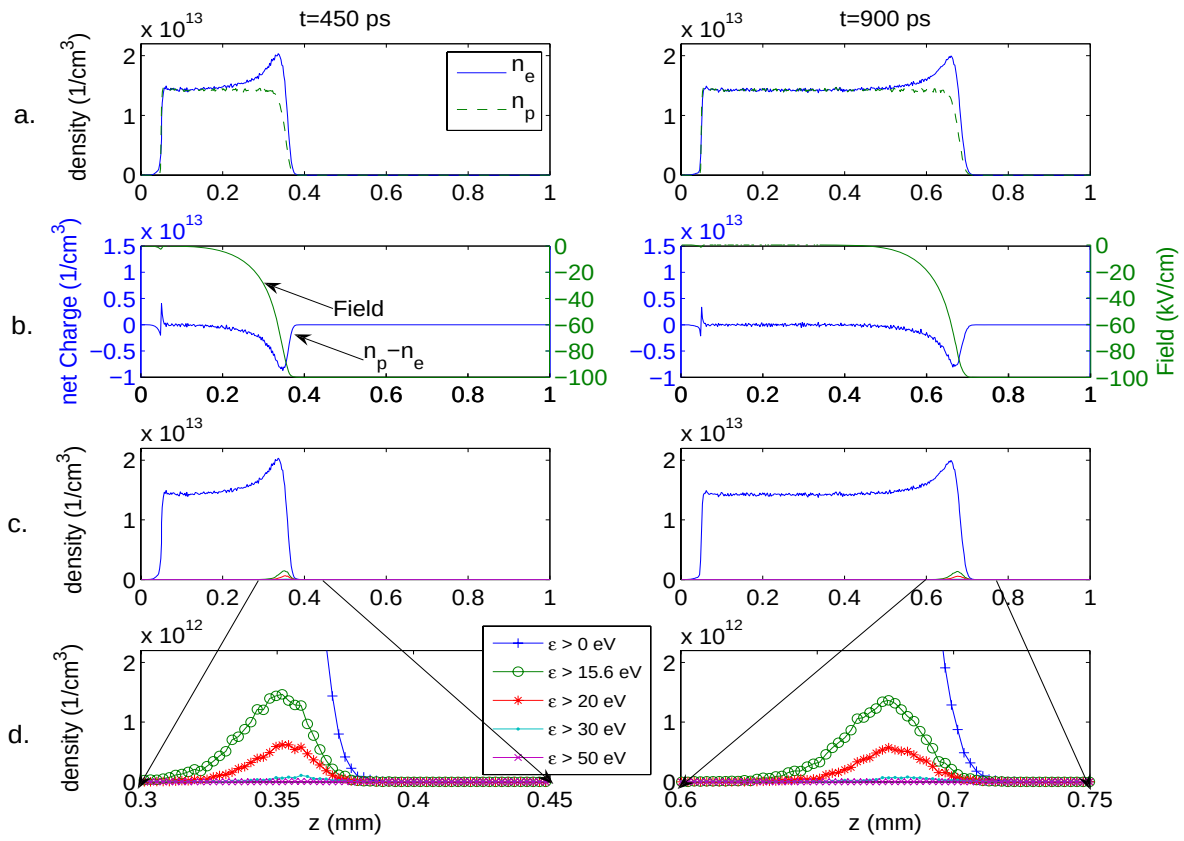

Figure 2. Spatial profile of a particle front within a field of 100 kV/cm at time t_1=450 ps (left) and t_2=900 ps (right). Panel (a) shows the density distribution of the electrons (solid) and the ions (dashed). Panel (b) shows the net negative charge distribution (solid) and the electric field (dashed). Panel (c) shows the total charge density of electrons and the charge density of electrons with an energy higher than 0, 15.6, 20, 30, and 50 eV, where 15.6 eV is the ionization energy. Panel (d) zooms into panel (c), both in space and in densities.

Both fluid and particle simulations have been carried out in the same set-up, and the parameter functions for the fluid model like mobility as a function of field strength μ(E) were derived from the particle model. In Fig. 3, we compare the spatial profile of the electron density (solid) and ion density (dotted) in a particle simulation with the electron density (dashed) and ion density (dot-dashed) in a fluid simulation in a field of 100 kV/cm. Two features are clearly visible: First, the particle and the fluid front move with approximately the same velocity. Second, the maximal electron density in the front and the saturation level of the ionization behind the front are about 20% higher in the particle than in the fluid model. The density discrepancy increases with increasing field, from 10% at 50 kV/cm to 60% at 200 kV/cm.

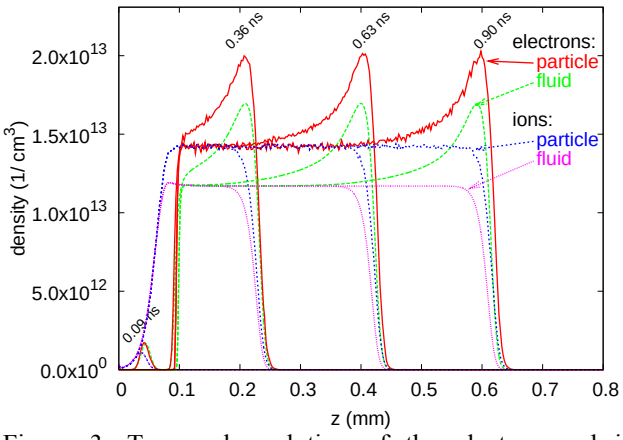

Figure 3. Temporal evolution of the electron and ion densities in a planar front in a field of 100 kV/cm. Shown are the spatial profiles of electron and ion densities derived with the particle or the fluid model at time steps t=0.09 ns, 0.36 ns, 0.63 ns, and 0.9 ns (solid lines: $n_{e,part}$, dashed: $n_{e,fluid}$, dotted: $n_{p,part}$, dot-dashed: $n_{p,fluid}$).

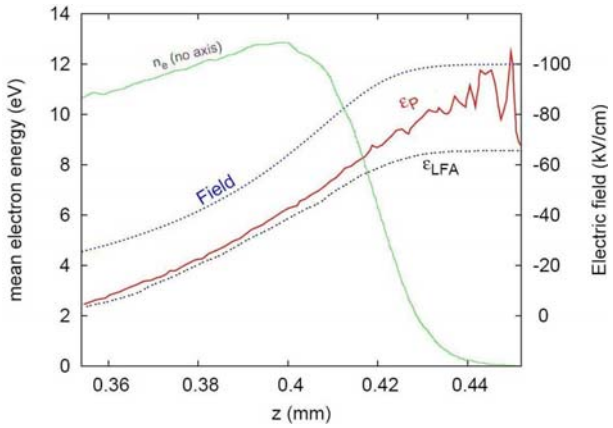

Figure 4. Zoom into the particle ionization front of Fig. 3 in a field of 100 kV/cm at time 0.63 ns: shown are electron density distribution n_e (solid line), local average electron energy ε_p(dotted line), local average electron energy ε_{LFA} according to the local field approximation (dashed line), and electric field strength E (dot-dashed line).

Having excluded numerical discretization errors or inconsistent parameter functions, deviations must be due to the approximations in the fluid model. Fig. 4 zooms into the ionization front shown in Fig. 3 at time t=0.63 ns. Here we show the electron density (solid line) and electric field (dot-dashed line) in the particle model. Furthermore the local mean energy of the electrons in the particle model is indicated with a dotted line. Finally, the mean electron energy according to the local field approximation is derived from the local field E; it is indicated with a dashed line. It can be seen that the average electron energy nicely follows the local field approximation in the interior of the ionized region while it is considerably higher in the region where the electric field is large and constant and the electron density decreases rapidly.

The electron energies in the leading edge substantially exceed the local field approximation and indicate that a larger fraction of electrons has energies in the tail of the distribution above the ionization threshold. This leads also to higher ionization rates than estimated by the local field approximation and results in a higher electron density behind the front.

A detailed discussion will be given elsewhere. Basically, high fields generate strong density gradients, and the density decay length can approach the electron energy relaxation length; in this case the fast and energetic electrons get ahead of the slow ones.

4. Hybrid model coupling in space

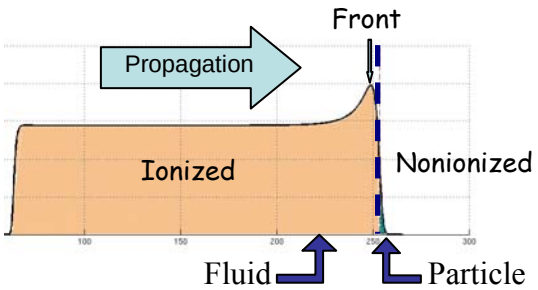

Figure 5. In our concept of hybrid coupling in space, the fluid model is used in the streamer body and the particle model is used in the ionization front.

The comparison shows that the electron energy overshoot in the leading edge of the ionization front cannot be reproduced in the fluid model. But in lower fields, the fluid model is a rather good approximation. This sets the stage for our hybrid model coupling in space as shown in Fig. 5: We use the fluid model in the streamer body where (i) electrons and ions can be approximated as densities and (ii) the fluid model is a good approximation. The particle model is applied in the region where (a) the electron density is low and their discreteness has to be taken into account, and (b) the fluid model fails. As the ionization front propagates, the model interface moves with the front so that the number of electrons followed by the particle model is limited.

Acknowledgments

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