FAST TRACK COMMUNICATION

Spatial coupling of particle and fluid models for streamers: where nonlocality matters

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Abstract

Particle models for streamer ionization fronts contain correct electron energy distributions, runaway effects and single electron statistics. Conventional fluid models are computationally much more efficient for large particle numbers, but create too low ionization densities in high fields. To combine their respective advantages, we here show how to couple both models in space. We confirm that the discrepancies between particle and fluid fronts arise from the steep electron density gradients in the leading edge of the fronts. We find the optimal position for the interface between models that minimizes the computational effort and reproduces the results of a pure particle model.

(Some figures in this article are in colour only in the electronic version)

Streamers generically occur in the initial electric breakdown of long gaps. They are growing filaments of weakly ionized nonstationary plasma; they are produced by a sharp ionization front that propagates into nonionized matter within a self-enhanced electric field. Streamers are used in industrial applications such as lighting, gas and water purification or combustion control, and they occur in natural processes as well, such as lightning or transient luminous events in the upper atmosphere. Recent important questions concern (i) propagation and branching of streamers and the role of avalanches created by single electrons, (ii) the electron energy distribution in the streamer head and the subsequent gas chemistry that is used in the above applications as well as (iii) runaway electrons and x-ray generation, possibly in the streamer zone of lightning leaders. This paper deals with efficient simulation of these problems.

Monte Carlo particle simulations model these effects as they contain the full microscopic physics; the deterministic electron motion between collisions is calculated and collisions of electrons with neutrals are treated through a Monte Carlo process with appropriate statistical weights. The particle model includes the complete electron velocity and energy distribution as well as the discrete nature of particles. However, a drawback of such models is that the required computation resources grow with the number of particles and eventually exceed the CPU space of any computer. This difficulty is counteracted by using superparticles carrying the charge and the mass of many physical particles, but superparticles in turn create unphysical fluctuations and stochastic heating.

Streamers are therefore mostly modelled as fluids (see, e.g. [14–18]) since a fluid model is computationally much more efficient. In the case of a negative discharge in a pure nonattaching gas such as nitrogen, it consists of continuity equations for the densities of electrons $n_e$ and positive ions $n_p$ coupled to the Poisson equation for the electric field $E$. The electron mobility $\mu$ and diffusion matrix $D$ and the impact ionization rate $\alpha$ are calculated from microscopic scattering and transport models such as the Boltzmann equation or directly from Monte Carlo simulations as, e.g. in [20]. In streamer calculations, it is generally assumed that these transport and reaction coefficients are functions of the local electric field.

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We have recently compared the properties of streamer ionization fronts of particle models and conventional fluid models [20] for negative planar fronts in nitrogen; the transport coefficients for the fluid model were generated from swarm experiments in the particle model. We found that the models agree reasonably for fields up to 50 kV cm$^{-1}$ at standard temperature and pressure, but that differences increase with increasing electric field. For example, in a field of 200 kV cm$^{-1}$, the ionization level behind the front is 60% higher in the particle model than in the fluid model. We have related this to the fact that the electron energies and, consequently, the ionization rates in the leading edge of the front are considerably higher in the particle than in the fluid model; they are actually at the edge of the runaway. We found that this effect is due to the strong density gradients in the front, and not due to field gradients. So for high fields and consequently strong density gradients at the streamer tip, there is a clear need for particle simulations, and particles, rather than superparticles, should be used to get physically realistic density fluctuations when modelling, for example, the branching process of a streamer.

The basic idea of this paper is demonstrated in figure 1, namely, to follow the single electron dynamics in the high field region of the streamer where the electron density gradient is steep and to present the interior region with large numbers of slower electrons through a fluid model with appropriate transport coefficients. As in [20], we study negative streamers in nitrogen, and we simplify the notation by referring to the standard temperature and pressure, but that differences scales with the gas density. The particle and the fluid models by themselves are taken as described in detail in [20]. But how should the particle and fluid models be coupled in space? And where should the interface between the models be located to get fast but reliable results? The answers to these questions will be given below. They required us to correctly identify the spatial region where the particle and fluid models deviate, and this allowed us to then compute the full electron physics efficiently in the relevant region.

**Figure 1.** The streamer ionization front, that is here indicated by the electron density $n_e(z)$, and its presentation by the particle or the fluid model in different spatial regions.

When coupling the models, the model interface should move with the ionization front; this keeps the total number of electrons limited and superparticles need not be introduced. The position of the interface can be chosen according to either the electron densities or the electric field. As the electron densities fluctuate stronger than the electric field, we relate the position of the model interface to the electric field. More precisely, the interface is placed where the local field $E$ is a given fraction $x$ of the maximal field $E^*$: $E_{\text{interface}} = x E^*$. By varying $x$, the region modelled by particles can be varied.

To properly handle the interaction of the two models, we introduced a so-called ‘buffer region’ where a particle model coexists with a fluid model. The separation of the full computational region into fluid, particle and buffer regions is indicated in figure 1. Buffer regions have been introduced in [21–23] for rarefied gases coupling a direct simulation Monte Carlo (DSMC) scheme to the Navier–Stokes equations and in other applications [24, 25]. Physical observables are evaluated from the fluid model in its whole definition region up to the model interface. Beyond that point, the particle model is used. The particle model extends back beyond the model interface into the buffer region where particle and fluid models coexist; it supplies particle fluxes to the fluid model on the model interface. However, correct particle fluxes require correct particle statistics within the buffer region whose length should be as small as possible to reduce computation costs, but larger than the electron energy relaxation length [20]. In many cases, new particles need to be introduced into the buffer region, which have to be drawn from appropriate distributions in the configuration space. This would pose a particular problem since a Boltzmann or even a Druyvesteyn distribution can be inaccurate. But for negative streamers, where electrons on average move somewhat slower than the ionization front, the electron loss at the end of a sufficiently long buffer region does not affect the calculation of particle fluxes at the model interface. Therefore, the particle loss at the end of the buffer region can be ignored and new electrons do not need be created artificially.

In more detail, the calculation is performed as follows. One hybrid computation step from $t_n$ to $t_{n+1}$ is described in the flow chart in figure 2. The electric field $E$, the electron

![Flow chart for one time step from $t_n$ to $t_{n+1}$ in the complete hybrid calculation.](image)
and ion densities $n_e$ and $n_p$ in the fluid region and the kinetic information of particles in the particle and buffer regions are given at time step $t_n$. First, the positions and velocities of all old and newly generated particles are updated to time step $t_{n+1}$ in the particle and buffer regions. Their collisions during this time step are treated stochastically and their new velocities and positions are calculated by solving the equation of motion. The number of electrons crossing the model interface during this time step is recorded. This particle flux across the interface provides the required boundary condition for calculating the time step is recorded. This particle flux across the interface needs several time steps to move over one unit length, $\Delta x$. By choosing $\Delta t$ and the grid size are chosen so that the ionization front need several time steps to move over one $\Delta x$, e.g. $10\Delta t$ at 100 kV cm$^{-1}$ and $3\Delta t$ at 200 kV cm$^{-1}$.

The length of the buffer region is another crucial factor in the hybrid computation. A buffer region with a length of 32$\Delta x$ has been used in the current simulations, which ensure a reliable flux across the model interface and stable results of hybrid simulations. The length of the buffer region is much larger than the energy relaxation length found in [20]. The long buffer region does not bring a heavy burden to the simulation of the planar front system but will considerably reduce the computational efficiency in a more complex geometry. Therefore, the minimal length of the buffer region as well as other features of fluid and particle models shall be investigated in more detail in a future paper.

We first show the simulation results of this coupled model for a front propagating into a field of $E^*=100$ kV cm$^{-1}$ and with the model interface located at $x=0.6, 0.9$ and $0.98$; the positions of these interfaces are indicated in figure 3. The field ahead of the front is fixed, and the system is always taken long enough such that effects at the outer boundaries are not felt. The coupled model generates different electron and ion densities behind the ionization front as shown in figure 4; for $x=0.6$, the density is as in the particle model, for $x=0.98$, it is as in the fluid model, and for $x=0.9$, it takes some intermediate value. We conclude that the solution of the pure

![Figure 3](image-url)  
**Figure 3.** Electron density $n_e$ and ion density $n_p$ (solid and dotted lines) and electric field strength $|E|$ (dashed–dotted line) in a streamer ionization front in nitrogen in a field of $E^*=100$ kV cm$^{-1}$ at standard temperature and pressure within a pure particle model. Our units are related to other commonly used units such as 1 kV cm$^{-1}$ bar$^{-1} = 1.316$ V cm$^{-1}$ Torr$^{-1} = 0.424$ Td at $T=300$ K. Below we will model the leading edge of the front by a particle model and the streamer interior by a fluid model where the model interfaces are located at $E_{interface} = x E^*$ with $x=0.6, 0.7, 0.8, 0.9$ and $0.98$. These interface positions for figures 2 and 3 are marked by vertical lines, with ‘o’ for the fields and with ‘+’ for the densities.

![Figure 4](image-url)  
**Figure 4.** Electron and ion densities in the coupled model (thick lines) in a field of $E^*=100$ kV cm$^{-1}$ with model interfaces at $E_{interface} = x E^*$ with (a) $x=0.6$, (b) $x=0.9$ and (c) $x=0.98$; these interface positions are indicated by vertical dashed lines. The densities in the particle model (electrons: solid, ions: dotted–dashed) and in the fluid model (electrons: dashed, ions: dotted) are shown as well; they are discussed in [20].
Coupling particle and fluid models in space with varying interface positions confirms our prediction [20] that the density discrepancies between particle and fluid model are due to strong density gradients in the leading edge of the front. This investigation also lays the basis for constructing a fully 3D coupled particle–fluid model where the fields ahead of the ionization front are changing in space and time.

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References