Derivation and test of high order fluid model for streamer discharges

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Summary. A high order fluid model for streamer dynamics is developed by closing the system after the 4th moment of the Boltzmann equation in local mean energy approximation. This is done by approximating the high order pressure tensor in the heat flux equation through the previous moments. Mathematical characteristics of the system is studied. Then planar ionization fronts for negative streamers in N_2 are simulated with the classical streamer model, MC-PIC particle model, and with the present higher order model.

1 High order fluid model

Streamer discharges occur in nature and as well in many industrial applications such as the treatment of exhaust gasses, polluted water or biogas. They appear when non-ionized or lowly ionized matter is exposed to high electric fields. Here we present a high order fluid model for streamer discharges, and we use it to simulate planar ionization fronts for negative streamers in nitrogen under normal conditions; and we compare the results with those of the classical fluid model.

1.1 Model description

The high order model is derived by taking the first 4 moments of the Boltzmann equation, i.e., by multiplying the Boltzmann equation with the kth power of velocity ($k = 0,1,2,3$) and integrating over velocity space. In principle, the set of moment equations is infinite, but we consider only electron density ($k = 0$), momentum ($k = 1$), energy ($k = 2$) and energy flux ($k = 3$). The system is truncated in the energy flux equation (4) by approximating the high order pressure tensor by the product of lower order moments and by introducing factor of parametrization β. As a result the hydrodynamical formalization of the streamer dynamics in 1D is described by the nonlinear system of equations

$$\partial_t \mathbf{u} + \mathbf{A}(\mathbf{u})\partial_x \mathbf{u} = \mathbf{F}(\mathbf{u}), \tag{1}$$

where the primitive variables are

$$\mathbf{u} = (n, nv, n\varepsilon, n\xi)^{\mathbf{T}}, \tag{2}$$

the matrix $\mathbf{A}(\mathbf{u})$ is defined in following way

$$\mathbf{A}(\mathbf{u}) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{2}{3m} & 0 \\ 0 & 0 & 0 & 1 \\ -\beta\frac{2\varepsilon^2}{3m} & 0 & \beta\frac{4\varepsilon}{3m} & 0 \end{pmatrix}, \tag{3}$$

and the source term is

$$\mathbf{F}(\mathbf{u}) = \begin{pmatrix} n\nu_I \\ \frac{nqE}{m} - nv\nu_m \\ qEnv - n\{\nu_e\left[\varepsilon - \frac{3}{2}kT_0\right] + \sum_\alpha \nu_{e\alpha}\varepsilon_{e\alpha} + \nu_I\varepsilon_I\} \\ \frac{5qE}{3m}n\varepsilon - n\xi\nu_m \end{pmatrix}. \tag{4}$$

Here n, v, ε and ξ are electron number density, average electron velocity, average electron energy and electron energy flux, correspondingly. E is the electric field and T_0 is room temperature. $\nu_m(\varepsilon)$ and $\nu_e(\varepsilon)$ are the momentum and elastic energy transfer collision frequencies, $\nu_I(\varepsilon)$ is the ionization frequency and $\nu_{e\alpha}(\varepsilon)$ are the collision frequencies for inelastic processes. As charge is conserved, the continuity equation for the ion density n_{ion} is

$$\partial_t n_{ion} = n\nu_I, \tag{5}$$

when the ions are approximated as immobile. Space charge effects are taken into account through the Poisson equation

$$\partial_x E = \frac{e}{\varepsilon_0}(n_{ion} - n), \tag{6}$$

where ε_0 is the dielectric constant and e is the elementary charge.

Mathematical characteristics and numerical solution of the system

Lemma 1. *The system* (1) *is hyperbolic if and only if*

$$\beta = 0 \quad or \quad \beta \geq 1. \tag{7}$$

In the case of $\beta > 1$*, the system* (1) *is strictly hyperbolic.*

Although the eigenvalues of (1) have a simple form, the corresponding right and left eigenvectors are very complicated, which makes it impossible to work with them.

The finite volume method is used to spatially discretize the system (1),(5),(6) on uniform control volumes or cells V_j as follows:

$$V_j := [j\Delta x, (j+1)\Delta x), \quad x_j := \left(j+\frac{1}{2}\right)\Delta x, \quad (8)$$

where $j = 0, 1, ..., M-1$, $\Delta x = L/M$ is the spatial grid size and L is the length of the simulation domain. To approximate the spatial derivative in (1) we use the second-order central difference discretization [1]. In our numerical experiments we saw that this spatial discretization approximates quite well the analytically predicted front velocity for the minimal model [2].
The time derivatives are approximated with the Runge-Kutta 4 method [1]. This is an explicit method, which always has a bounded stability domain. In our case the stability condition or CFL restriction is

$$\beta\sqrt{\frac{2}{3m}}\sqrt{\max\varepsilon}\frac{\Delta t}{2\Delta x} \leq C, \quad (9)$$

where C depends on the particular method and space discretization. In our simulations we use the value $C = 0.1$.

1.2 Particle model and classical fluid model

In essentially all numerical fluid models for streamers in the past 30 years, except for [3,4], the electron density is approximated by a reaction drift diffusion approximation

$$\partial_t n - \partial_x(\mu E n + D\partial_x n) = n\nu_I\,, \quad (10)$$

This model is called the minimal model; it implies a local field approximation of reaction and transport coefficients.
As a second reference model we use the MC-PIC particle model from [5].

2 Results and discussion

Fig. 1 compares the results of the high order model, the particle model and of the minimal model for the same initial and boundary conditions and for the same electric field ahead of the ionization front. A multi term theory for solving the Boltzmann equation [6] is used to calculate flux transport coefficients and mean-energy dependent collisional rates required as an input in fluid equations.

The following main conclusions can be drawn:

1) The overall front structure is the same, but the particle model is much better approximated by the high order model than by the minimal model.

2) That the mean electron energy ahead of the front increases while the electric field is constant, was also seen in Monte Carlo simulations before [2], but not yet included in fluid models. The mean electron energy behind the front where the electric field vanishes, is close to 1 eV, because energy relaxation is slow in this region. This feature was not included in fluid models before.

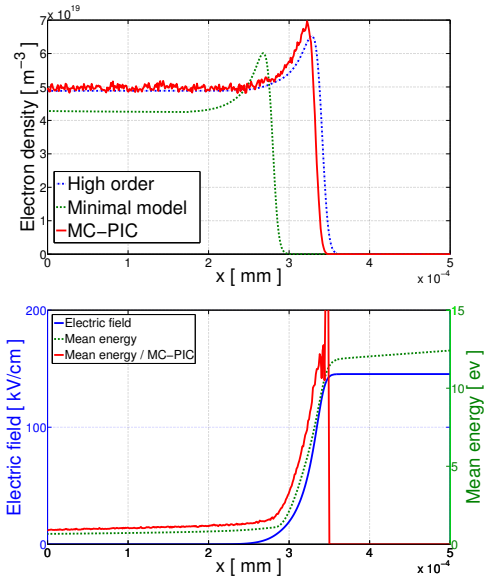

Fig. 1. Top: Electron density profile for the high order model (dashed dotted line, blue), the particle model (solid line, red) and for the minimal model (dashed line, green), bottom: mean electron energy (dashed line, green) and electric field (solid line, blue) profiles in the high order model, mean electron energy in the particle method (solid line, red). The plots show the simulation for instant 0.7 ns for identical initial conditions. The electric field ahead of the ionization front is 145 kV/cm at standard temperature and pressure, which corresponds to 590 Td.

In summary, the new high order fluid model captures effects in streamer simulations that up to now were only inherent in the more microscopic Monte Carlo simulations. This is a step forward for long time calculations.

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