An Efficient Two-Zone Model of Capacitively Driven Low-Pressure Gas Discharges

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Simulation of low pressure gas discharges is complicated by the pronounced numerical stiffness of the underlying differential equations. Recently, a novel approach has been proposed to overcome these problems by employing the technique of asymptotic scale analysis [1]. In this paper, we demonstrate the feasibility of the new method by applying it to a class of plan-parallel discharges with (at least some degree of) capacitive coupling. It is expected that the described model will serve not only academic purposes, but may also be used for quick order-of-magnitude estimates in production reactors.

Introduction

Parallel to the increasing use of plasma-based manufacturing processes in microelectronics and other industries, numerous attempts have been made to define and analyze mathematical models of the employed low pressure discharges [2,3,4]. The numerical resources required by these models have proved substantial, a consequence of the pronounced stiffness of the underlying partial differential equations. This stiffness arises from the simultaneous presence of vastly different length and time scales in the dynamics. An explicite solution of Poisson's equation in the bulk, e.g., requires resolving the Debye length $\lambda_D \approx 0.1$ mm which is a factor of 10^3 smaller than the typical discharge dimension $L \approx 10$ cm. Similarly, the ratio between the longest and the shortest time scale present often exceed values of 10^5.

To cope with these difficulties, we have recently proposed an approach to discharge modeling which takes the quoted scale separations explicitely into account [1]. The approach it is based on the well-known fact that the domain of a discharge can be divided in the bulk (which amounts to most of the volume), and relatively boundary sheaths at the electrodes or walls. The temporal stiffness is treated in a similiar way, by explicitely integating over the fast time scales of the dynamics.

It is the scope of this manuscript to demonstrate the feasibility of our concept by treating the case of electro-positive discharges with plan-parallel (i.e., one-dimensional) geometry. This restriction is not only made for academic reasons; we also expect that our model will serve as an efficient tool for fast but realistic order-of-magnitude estimates in RIE and PECVD based production reactors.

The Underlying Plasma Model

Our investigations are based on a simple but sufficiently realistic macroscopic plasma description, similiar to the models used by various other authors ([2,3,4,5]). We restrict ourselves to a plan-parallel discharge geometry and consider only one (singly charged) ion species. Under neglection of inertia effects, the electrons are modeled in terms of a standard drift-diffusion equation,

$$\frac{\partial n}{\partial t} - \frac{\partial}{\partial x}\left(\mu E n + D\frac{\partial n}{\partial x}\right) = \beta n, \tag{1}$$

where the electron density is denoted by n, the electrical field by E, the mobility by μ and the diffusion constant by D. The ionization term is linear in the density n; the rate constant $\beta \equiv k_I N_g$ is considered an arbitrary (but time-periodic) function of x and t. Its calculation lies outside of the scope of this paper.

In the description of the ions, we include inertia effects (which may dominate the dynamics because of the high ion mass m_i) but neglect any other than ambipolar diffusion (because of the low ion temperature $T_i \ll T_e$). The description thus amounts to a cold ion model, it consists of a continuity equation for the density ρ and an equation of motion for the bulk velocity v,

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = \beta n, \tag{2}$$

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = \frac{e}{m_i}E - \frac{\sqrt{c^2+v^2}}{\lambda}v. \tag{3}$$

The friction term on the right of (3) describes the effects of ion-neutral collisions including charge transfer. Note that the assumed form gives the correct expressions in the limits of high and low electrical field; the values of the parameters c and λ can easily be fitted to swarm experiments.

Finally, Poisson's equation is adopted which couples the electron and ion components to the electromagnetic field,

$$\epsilon_0\frac{\partial E}{\partial x} \equiv -\frac{\partial^2 \Phi}{\partial x^2} = e\rho - en. \tag{4}$$

The model is completed by additional conditions which state that the plasma is bounded by material electrodes at $x = \pm L/2$,

$$-\mu E n - D\frac{\partial n}{\partial x}\bigg|_{\pm L/2} = \pm\sqrt{\frac{T}{2\pi m_e}}n\bigg|_{\pm L/2}, \tag{5}$$

and that the total current through the discharge follows harmonic modulation,

$$e(\mu n E + D\frac{\partial n}{\partial x}) + e\rho v + \epsilon_0\frac{\partial E}{\partial t} = J\cos\Omega t. \tag{6}$$

The Sheath Model

In general, the partial differential equations (1-3) can only be solved numerically. To make analytical progress, we first focus on the boundary sheaths at $x = \pm L/2$. In these relatively thin zones, ionization can be safely neglected; the equations can further be simplified by assuming that i) the electron motion is fast compared to the external RF modulation, ii) the ion motion is slow compared to the external field, and iii) and the electron energy is small against the sheath potential. The sheath structure is then determined by the stationary ion equations

$$e\rho v = j_i, \tag{7}$$

$$v\frac{\partial v}{\partial x} = \frac{e}{m}\bar{E} - \frac{\sqrt{c^2+v^2}}{\lambda}v, \tag{8}$$

where the field $\bar{E}(x)$ is given as the period average of the instantaneous field $E(x,t)$. It has been shown in ref. [6] that $\bar{E}$ can be approximately represented by

$$\bar{E} = -\frac{J}{\epsilon_0\Omega}\Gamma_0 - \frac{T}{e}\frac{\partial\rho}{\partial q}\Gamma_1, \tag{9}$$

with Γ_0 and Γ_1 being two tabulated functions of $e\Omega\int_0^x \rho\, dx/J$ and $\sqrt{\epsilon_0\Omega^2\rho T}/J$. The solution characteristics of the two ordinary differential equations (8) and (9) have also been discussed in ref. [6]. Fig. 1 shows the ion density ρ and the average electron density $\bar{n}$ for the case of a 13.56 MHz argon discharge at 5 mTorr.

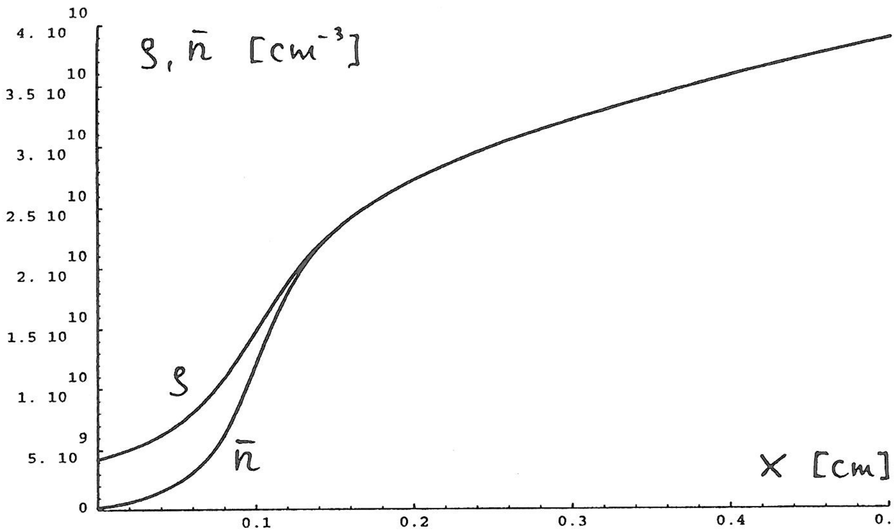

Fig. 1: Ion and average electron density in the sheath of a 5 mTorr argon plasma.

The Bulk Model

Complementary to the sheath model, we now turn to discussing the bulk physics. We can again assume that the ions are stationary and that the electron are in balance, but ionization is no longer negligible. However, quasi-neutrality holds ($n = \rho$), and the average electrial field is given by the ambipolar relation, $\bar{E} = -\frac{T_E}{e}\frac{1}{\rho}\frac{\partial \rho}{\partial x}$. The remaining non-trivial equations read ($v_B = \frac{T_E}{m_i}$)

$$\frac{\partial}{\partial x}(\rho v) = \bar{\beta}(x)\rho, \tag{10}$$

$$v\frac{\partial v}{\partial x} = -\frac{v_B^2}{\rho}\frac{\partial \rho}{\partial x} - \frac{\sqrt{c^2+v^2}}{\lambda}v. \tag{11}$$

For a general ionization function, these equations can still only be solved numerically. In the case of constant $\bar{\beta}$ (a good approximation at low pressures), however, they can be represented in terms of quadratures,

$$x = \int_0^v \frac{v_B^2 - v^2}{\bar{\beta}v_B^2 + \sqrt{c^2+v^2}\,v^2/\lambda}\,dv, \tag{12}$$

$$\rho = \hat{\rho}\exp\left(-\int_0^v \frac{\bar{\beta} + \sqrt{c^2+v^2}/\lambda}{\bar{\beta}v_B^2 + \sqrt{c^2+v^2}\,v^2/\lambda}\,v\,dv\right). \tag{13}$$

Note that this equation is a nonlinear eigenvalue problem for $\bar{\beta}$, and that $\hat{\rho}$ is an arbitrary constant. Fig. 2 displays the solution for the parameters defined above; it has been assumed additionally that the length is $L = 10$ cm.

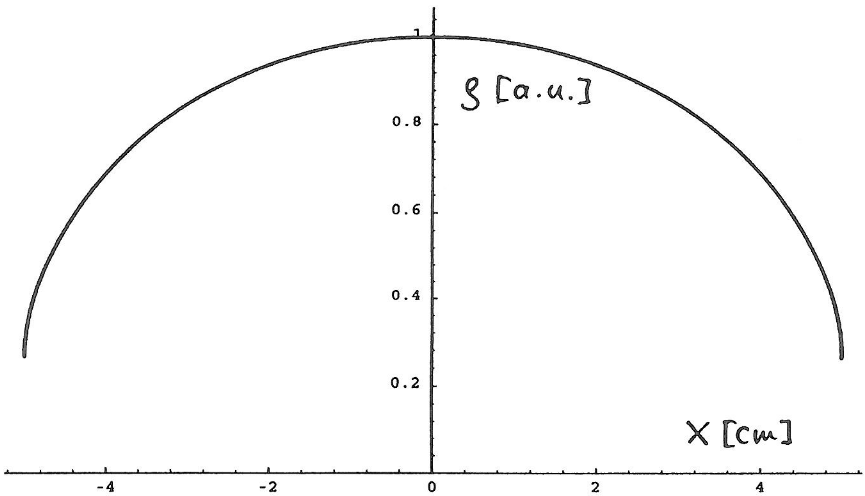

Fig. 2: Ion electron density in the bulk of a 5 mTorr argon plasma, $L = 10$ cm.

Matching of Bulk and Sheath Model

In the final step, the bulk and the sheath models (which were so far discussed separately) must now be merged into a description of the gas discharge as a whole. The matching can be carried out systematically by considering a third "pre-sheath" model, derived by imposing the assumptions of the bulk and the sheath together. This solution can easily be formulated in terms of quadratures:

$$x = \int \frac{v_B^2 - v^2}{\sqrt{c^2 + v^2}\, v^2/\lambda}\, dv = x_c - \lambda \left(\frac{\sqrt{c^2 + v^2}\, v_B^2}{c^2 v} - \ln\left(\sqrt{c^2 + v^2} + v\right) \right), \quad (14)$$

$$\rho = \exp\left(- \int \frac{1}{v}\, dv \right) = j_i / ev. \quad (15)$$

The pre-sheath solution exhibits the same singularity as the bulk model at $v = -v_B$, and behaves like the sheath model for $v \longrightarrow 0$. We can thus define a bulk and a sheath model as matched, when they are both asymptotics – in the respective regimes – to the same pre-sheath model (14)-(15). Our experience shows, that this matching prescription leads to convincing results already for rather moderate ratios of the scale parameters. (It is strict, of course, only in the limit of infinite scale separations.) Fig. 3 shows the outcome the matching procedure applied to the solutions of figs. 1 and 2, i.e., the combination of the sheath and the bulk model in one common scale. It can be seen that the obtained result is is quite satiscactory, in spite of the fact that the scale separation amounts to not more than a factor of 10.

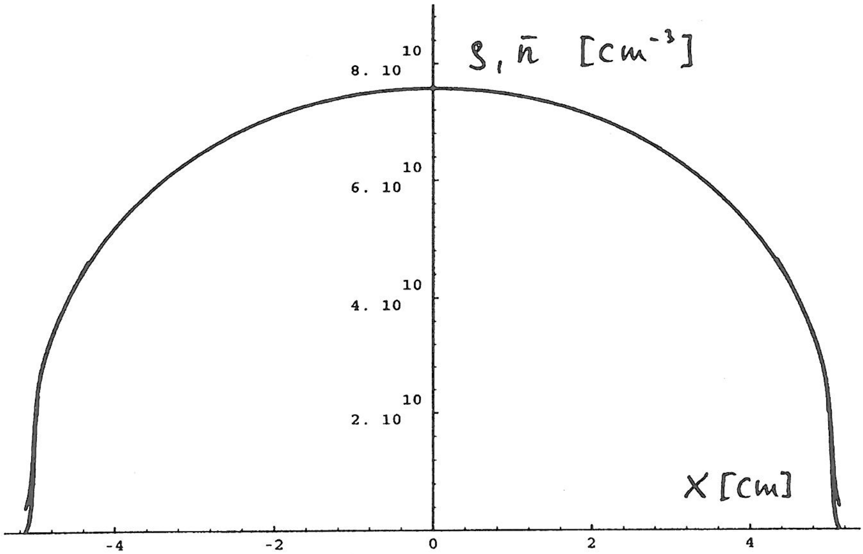

Fig. 3: Electron and ion density in a 5 mTorr argon plasma, matched solution.

Conclusions

In this work, we have demonstrated that the analysis of capacitively coupled gas discharges can be considerable simplified by means of asymptotic scale analysis. Our approach combines the benefits of first-principles models (physical motivation, spatial resolution) with those of engineering oriented approaches (quick response). Compared to an implementation of the original fluid-dynamics description (1-3), our model cuts the numerical effort of discharge simulation by a factor of more than hundred: The total CPU-time for solving the tow-zone model is less than 10 s on a 486 PC, comparable fluid-dynamical calculations require at least 1h on a work station. The main difference, of course, is that the original formulation amounts to a system of partial differential equations, whereas the two-zone model is represented ny ordinary differential equations.

As already stated, we expect our model already to be useful for a first (fast but still realiable) analysis of production reactors. It is clear, however, that a one-to-one simulation of such reactors can only be endavoured if a better than one-dimensional representation can be obtained. A closer investigation of our two-zone approach shows that the bulk model lents itself easily to generalization to two or three dimensions. The sheath model, however, is inherently one-dimensional. Fortunately, because the overall extension of a discharge is typically large against the thickness of the boundary sheaths, errors introduced by a one-dimensional representation will be small.

For these reasons, we are convinced that the presented two-zone approach represents a further step toward the goal of incorporating the simulation of plasma manufacturing processes into a commercially utilized TCAD environment.

References

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