Fluid modelling of plasma at low pressures

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Introduction

Thanks to the increasing performance of computers in recent years computer models brought new opportunities into plasma research. Nowadays, computer models of plasma are widely used to interpret experimental measurements and to better understand plasma behaviour in cases that are too complicated for theoretical description.

The most common computer modelling techniques used in plasma physics involve particle and fluid models. Whereas particle models are able to provide us with detailed microscopic information even about a system out of thermodynamic equilibrium, fluid models are much less demanding on the computational resources. Therefore, a lot of effort has been put into development of hybrid models that benefit from advantages of both, particle and fluid models. Hybrid models have already proven their usefulness [1]; on the other hand, they also suffer from several limitations. E.g. predictions of hybrid models based on combination of PIC method and drift-diffusion fluid model fail at low pressures where the assumptions of drift-diffusion approximation are violated. Since many technological applications of plasma require low-pressure regime (e. g. semiconductor processing by CCP discharges), it would be highly desirable to extend the range of applicability of hybrid models to the area of low pressures.

Our contribution deals with the question how the drift-diffusion model can be modified so that fluid modelling could be used also for low pressure plasma with sufficient accuracy. It was proven [2] that inclusion of full electron momentum equation can improve predictions of fluid models at low pressures for CCP discharges. We would like to discuss this topic more generally and propose a way how the area of applicability of fluid models could be extended.

Effects of low pressure

We have used our 2D PIC computer model to investigate effects of low pressure on argon plasma sheath in the vicinity of a cylindrical probe with $2 \cdot 10^{-4}$ m radius. The motion of charged particles in electric field was resolved by Verlet algorithm, the electric field was obtained by finite difference method on square shaped computational mesh of 400×400 nodes. The computational domain of 4×4 cm dimensions was surrounded by sources of charged particles (Ar^{+} ions and electrons) with Maxwellian velocity distribution. Scattering processes of charged particles with neutrals were treated by modified null collision method [3].

The computations were done for two biases of cylindrical probe with respect to the plasma potential (± 5 V) and for variable pressure of neutral gas in background ($1.33 \cdot 10^{-1} - 1.33 \cdot 10^{2}$ Pa). Number density of charged particles changed between $5.03 \cdot 10^{13}\,\mathrm{m}^{-3}$ and $1.59 \cdot 10^{15}\,\mathrm{m}^{-3}$ according to square root dependance on pressure. Temperature of e^- in source of particles was set to 23 600 K, temperature of Ar^+ ions to 300 K. Cross sections of e^-, resp. Ar^+ scattering processes were considered according to [4], resp. [5].

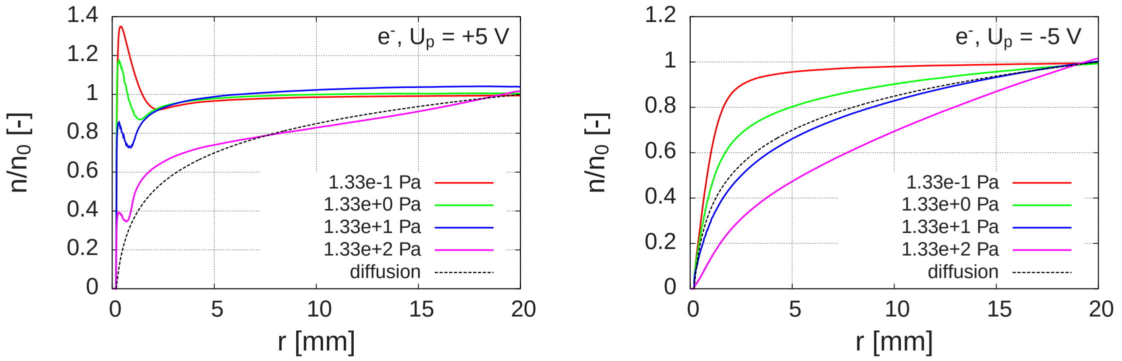

Figure 1: Normalized density of electrons in the vicinity of cylindrical probe for various values of neutral gas pressure and two probe biases.

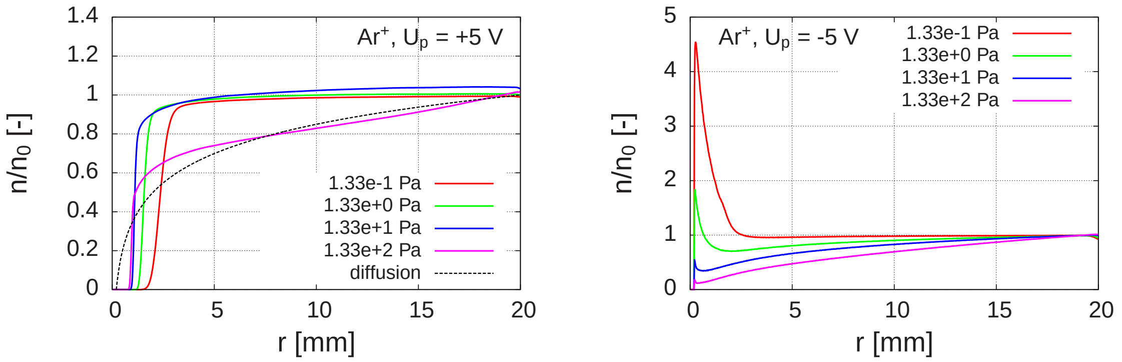

Figure 2: Normalized density of Ar^+ ions in the vicinity of cylindrical probe for various values of neutral gas pressure and two probe biases.

From Figures 1 and 2 it can be seen that with decreasing pressure of neutral gas in background charged particles that are attached by the probe bias cumulate near the probe since less collisions prevent them from getting into this area from bulk plasma. As a result, density profile of charged particles in the vicinity of the probe does not follow diffusion solution for low pressure.

Less charged particles are present in a volume unit at low pressure. For positively biased probe it has a consequence that potential is shielded out on larger distance at low pressure as

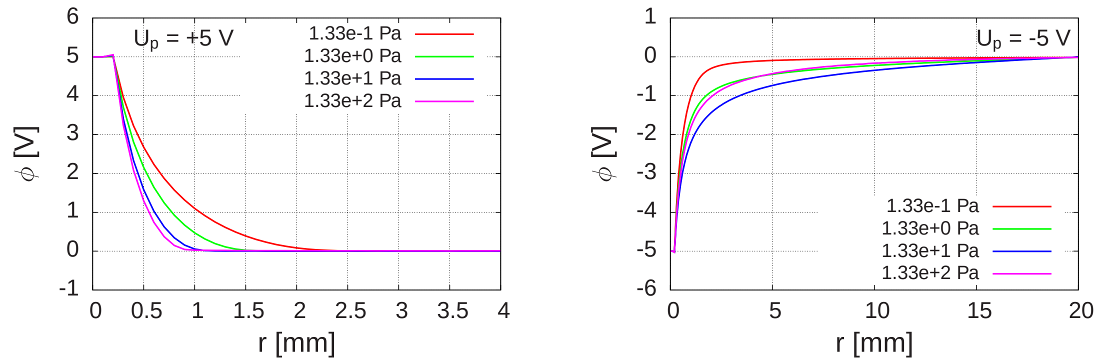

Figure 3: Electric potential in the vicinity of cylindrical probe for various values of neutral gas pressure and two probe biases.

can be seen from Figure 3. On the other hand, charged particles are cumulated near the probe at low pressure; thus, they are able to shield out the potential on shorter distance - this can be observed for negatively biased probe.

Fluid modelling at low pressure

The most frequently used fluid model of low temperature plasma is the drift-diffusion model

$$\boldsymbol{J} = \mu n \boldsymbol{E} - D \nabla n \tag{1}$$

which is derived from full-momentum equation

$$mn \left[\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} \cdot \nabla) \boldsymbol{v} \right] = qn\boldsymbol{E} - \nabla p - mn\boldsymbol{v}\nu \tag{2}$$

by neglecting terms on the left hand side (LHS) of this equation. This approximation is only justifiable if we consider steady state $\left(\frac{\partial \boldsymbol{v}}{\partial t} = 0 \right)$ and elastic collisions, whose effects are represented by the third term on right hand side (RHS) of Eq. (2), are so frequent that the second, inertial term on LHS can be neglected. Another assumptions of drift-difusion approximation: (i) Plasma can be treated as an ideal gas. (ii) The last term on RHS of Eq. (2) is only special case of velocity moment of the collisional term that emerges in Boltzmann equation. As a result, drift-diffusion model can be used to describe low temperature plasma at medium and high pressures. The usage of this approximation is discutable for positive ions because of their higher mass.

We have used the project FENICS [6] to implement 2D drift-diffusion model of cylindrical probe in argon plasma for different pressures. The results on Figure 4 show that drift-diffusion model is not able to capture effects of low pressure. Cumulation of charged particles near the probe with decreasing pressure can not be observed; diffusion character of density profile solution near the probe persists.

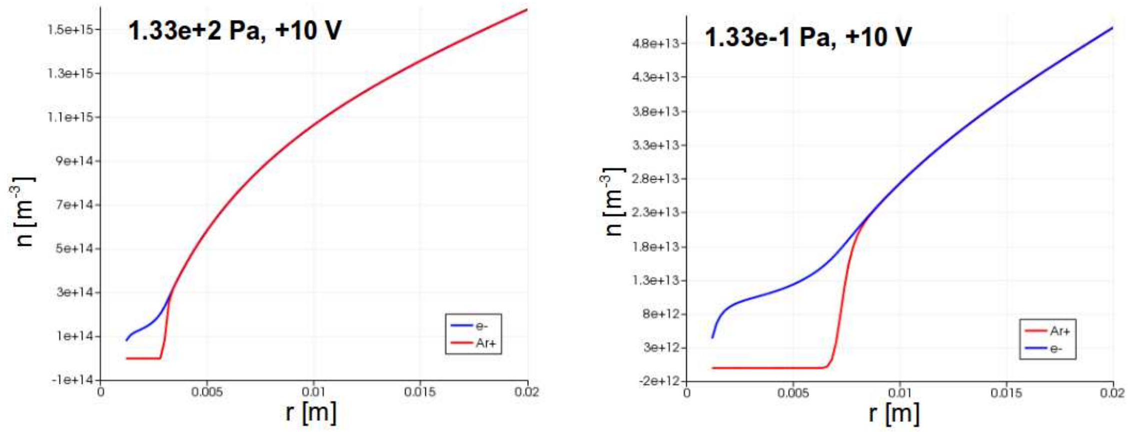

Figure 4: Number density of charged particles in the vicinity of the cylindrical probe for two different pressures. Results of 2D drift-diffusion fluid model. Probe bias: +10 V.

Conclusion

It was proven that drift-diffusion model cannot capture the effects of low pressure. To propose fluid model that would be reliable also in low pressure area we have to move to the general momentum balance equation

$$mn\frac{\mathrm{d}\boldsymbol{v}}{\mathrm{d}t} = \pm en\boldsymbol{E} - \nabla p - \nabla \cdot \boldsymbol{\pi} + \boldsymbol{F_s} \tag{3}$$

where $\boldsymbol{P} = p\boldsymbol{I} + \boldsymbol{\pi}$ is the stress tensor, $\boldsymbol{\pi}$ is viscosity stress tensor, $\boldsymbol{F_s} = \sum \boldsymbol{F_{ss'}}$ is frictional force due to collisions and $\boldsymbol{P}$ and $\boldsymbol{F_{ss'}}$ are given by

$$\boldsymbol{P} = \int m\boldsymbol{ww} f(\boldsymbol{r},\boldsymbol{v},t)\mathrm{d}^3\boldsymbol{v}, \qquad \boldsymbol{F_{ss'}} = \int m\boldsymbol{v}\left[\frac{\delta f}{\delta t}\right]_{ss'} \mathrm{d}^3\boldsymbol{v} \tag{4}$$

To find suitable closure relations for $\boldsymbol{P}$ and $\boldsymbol{F_{ss'}}$ for specific set of interactions between particles we can employ Chapman Enskog approach [7].

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