

Hybrid computer modelling in plasma physics

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Abstract. Our contribution is devoted to development of hybrid modelling techniques. We investigate sheath structures in the vicinity of solids immersed in low temperature argon plasma of different pressures by means of particle and fluid computer models. We discuss the differences in results obtained by these methods and try to propose a way to improve the results of fluid models in the low pressure area. There is a possibility to employ Chapman-Enskog method to find appropriate closure relations of fluid equations in a case when particle distribution function is not Maxwellian. We try to follow this way to enhance fluid model and to use it in hybrid plasma model further.

1. Introduction

Computer modelling techniques [1] are well established tools in plasma physics research. There are two main kinds of them - particle and fluid computer models. Whereas particle models are more precise and give us more detailed information about systems of interacting particles, fluid models usually do not require so high computer performance. It was proven [2] that combination of both techniques, so called hybrid models, can bring valuable results for low temperature plasma at medium pressures where drift diffusion approximation can be used in the fluid part of the model. Our contribution wants to identify differences between particle and fluid model results and discuss possible ways to extend applicability of hybrid modelling techniques to other pressure regimes.

2. Conventional modelling techniques in plasma physics and their limits

2.1. Particle models

Particle models are based on solution of equations of motion of very large number of particles in the modelled ensemble. Thus, this modelling technique provides the most precise results, especially in non-equilibrium cases. Common particle modelling technique in plasma physics, which is implemented also in our model, is so-called PIC/MCC method (= Particle-In-Cell/Monte Carlo Collisions).

Solution process of this method consists of several steps. First of all, computational domain is initialized by charged particles of different species and with Maxwell velocity distribution. After that, iterative cycle starts. Cloud-In-Cell algorithm assigns charge density to all nodes of computational mesh and Poisson equation is solved (e.g. by finite difference method) to obtain potential distribution. Consequently, particle motion in this electrostatic field is resolved by velocity Verlet algorithm. Effects of scattering processes are solved by null-collision method;



our model uses its improved version [3]. Iterative cycle ends when convergence of solution is reached.

2.2. Fluid models

Fluid model equations are derived from Boltzmann equation as its velocity moments. Following set of fluid equations is very often used in low temperature plasma physics:

$$\frac{\partial n_{e,i}}{\partial t} + \nabla \cdot \mathbf{\Gamma}_{e,i} = 0, \quad (1)$$

$$\mathbf{\Gamma}_{e,i} = \pm \mu_{e,i} n_{e,i} \mathbf{E} - D_{e,i} \nabla n_{e,i}, \quad (2)$$

$$\Delta \phi = -\frac{e}{\epsilon_0} (n_i - n_e), \quad (3)$$

where n marks number density, $\mathbf{\Gamma}$ particle flux, μ mobility coefficient, D diffusivity coefficient and ϕ is potential of electric field \mathbf{E} .

Equation 2 is called drift-diffusion approximation and it is derived from general equation of momentum conservation:

$$mn \frac{d\mathbf{v}}{dt} = \pm en \mathbf{E} - \nabla \cdot \mathbf{P} + \sum \mathbf{F}_s, \quad (4)$$

where stress tensor \mathbf{P} and collisional frictional force \mathbf{F}_s are defined as following:

$$\mathbf{P} = \int m \mathbf{w} \mathbf{w} f(\mathbf{r}, \mathbf{v}, t) d^3 \mathbf{v}, \quad \mathbf{F}_s = \int m \mathbf{v} \left[\frac{\delta f}{\delta t} \right]_s d^3 \mathbf{v}, \quad (5)$$

where $f(\mathbf{r}, \mathbf{v}, t)$ marks particle distribution function and $\left[\frac{\delta f}{\delta t} \right]_s$ is collisional term describing collisions of one particle species with particles of species s . Velocity \mathbf{w} is defined as $\mathbf{w} = \mathbf{u} - \mathbf{v}$, where $\mathbf{u} = \int \mathbf{v} f(\mathbf{r}, \mathbf{v}, t) d^3 \mathbf{v}$.

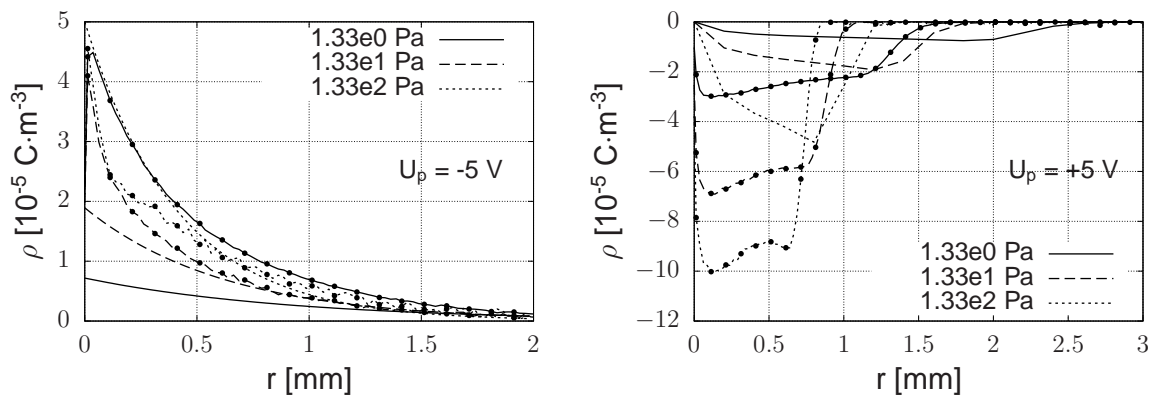
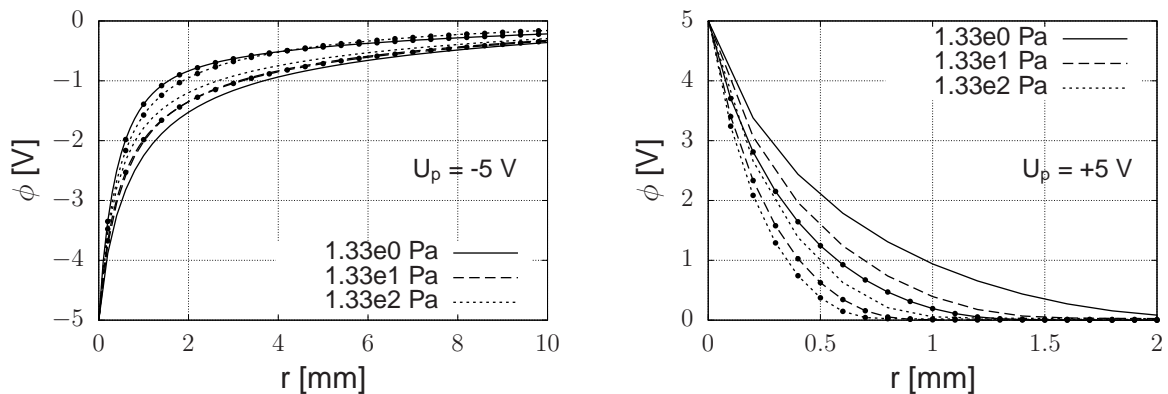
Derivation of drift-diffusion approximation from general momentum equation takes into account several approximations: 1. Inertial term in full momentum equation is neglected, 2. steady-state is considered only, 3. plasma is treated as ideal gas (particles interact only during collisions), 4. special case of velocity moment of the collisional term in Boltzmann equation: $\mathbf{F}_s = -mn\nu\mathbf{v}$, where ν is frequency of elastic collisions. These considerations limit application of drift-diffusion model in plasma physics.

3. Comparison between particle and fluid models

2D particle and fluid models were used to investigate sheath structure and IV characteristics of a cylindrical probe with $2 \cdot 10^{-3}$ m radius to compare their results. We have considered electropositive argon plasma where temperature of electrons was 23 600 K and that of Ar^+ ions was 300 K. Computational domain had dimensions of $(4.0 \times 4.0) \cdot 10^{-2}$ m. Regular rectangular mesh with 400×400 cells was used to solve Poisson equation by finite difference method in particle model. Scattering processes that were considered in particle model; $\text{Ar} + e^-$ collisions: elastic scatter, excitation and ionization [4]; $\text{Ar} + \text{Ar}^+$ collisions: elastic scatter and charge transfer [5]. Equations of fluid model were solved by finite element method on triangular mesh with approximate number $4 \cdot 10^5$ of triangles. Open source project FENICS [6] was used to build the fluid model. Our study was done for different values of neutral gas pressure and table 1 presents corresponding plasma densities. Exact pressure dependence of plasma density was neglected, square root dependence was considered.

Table 1. Plasma density for different values of neutral gas pressure

| Neutral gas pressure [Pa] | 1.33e-1 | 1.33e0 | 1.33e1 | 1.33e2 |
|------------------------------------|---------|---------|---------|---------|
| Plasma density [m^{-3}] | 5.03e13 | 1.59e14 | 5.03e14 | 1.59e15 |

**Figure 1.** Net charge density in the vicinity of biased cylindrical probe for different pressures of neutral gas on the background computed by 2D particle (lines with markers) and fluid model (without markers). Two probe biases were considered, $U_p = \pm 5$ V.**Figure 2.** Potential profile in the vicinity of biased cylindrical probe for different pressures of neutral gas on the background computed by 2D particle (lines with markers) and fluid model (without markers). Two probe biases were considered, $U_p = \pm 5$ V.

3.1. Plasma sheath around cylindrical Langmuir probe

Figures 1 and 2 show sheath structure around cylindrical probe in terms of net charge density and potential profile for different pressures. It can be seen that fluid model is able to capture formation of sheath in some level of accuracy. Still fluid model results differ from that obtained by particle model.

For almost all investigated cases net charge density in the near surroundings of a probe obtained by fluid model is lower than that obtained by particle model. Fluid solution tend to

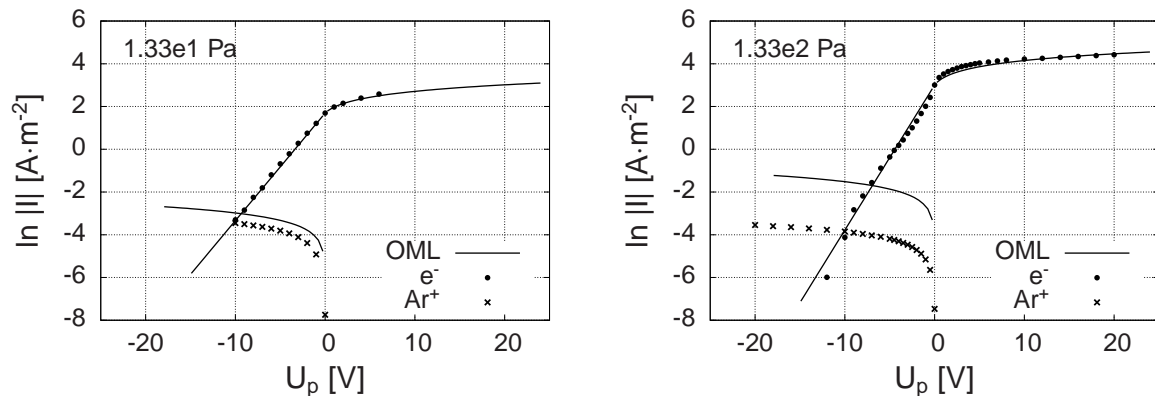


Figure 3. Comparison of IV characteristics of cylindrical Langmuir probe computed by 2D particle model with OML theory for two different pressures of neutral gas.

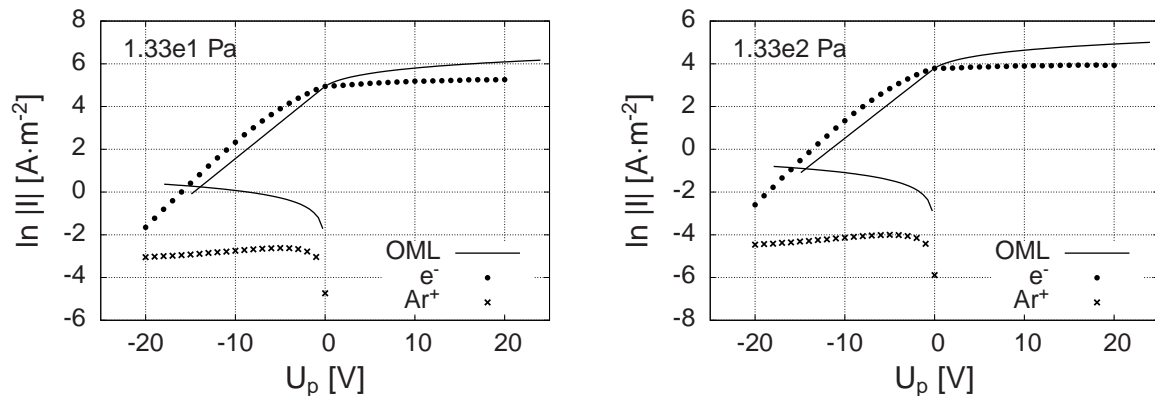


Figure 4. Comparison of IV characteristics of cylindrical Langmuir probe computed by 2D fluid model with OML theory for two different pressures of neutral gas.

preserve diffusion profile which is logarithmic in 2D case. As a result we can see that potential is shielded out on larger distance in fluid case.

It can be stated that differences between particle and fluid model results are greater for lower pressures. We also expect greater differences between fluid and particle model results in a case the average kinetic energy per particle increases. If a particle has higher kinetic energy it is more probable that it will undergo one of the inelastic scattering processes (excitation, ionization etc.) and it will affect particle's velocity distribution function in a way that it will become much more distinct from Maxwellian distribution (which is an assumption of fluid plasma models).

3.2. IV characteristic of cylindrical probe

Differences between particle and fluid models were also investigated for the case of IV characteristics of cylindrical Langmuir probe, results are presented on figures 3 and 4.

Particle model results are in very good agreement with OML theory for 13.3 Pa pressure. For higher pressure we can see disagreement caused mainly by scattering processes that are not considered by OML theory. Disagreement is observed especially for ion current.

Fluid model provides electron current that is qualitatively in agreement with OML theory. The agreement is better for lower pressure. At low pressure fluid model is able to capture

increasing electron current for positive probe bias. However, fluid model is not reliable in computation of ion current at all.

4. Concept of hybrid models

Main idea which is behind hybrid models is to combine advantages of both particle and fluid models so that the resultant model would be sufficiently precise and fast enough to solve large 3D problems. Results obtained by hybrid modelling approach have already been published, e. g. [7]. There are many ways how the particle and fluid models can be combined. It was proven [2] that so-called iterative hybrid model can provide reliable results in medium pressure area. Since this model uses drift diffusion approximation it can not be used for low pressure problems.

To extend usability of hybrid models to the low pressure regime Chapman Enskog method [8] can be used. It is a method of solution of Boltzmann kinetic equation with prescribed collisional term and force law between interacting particles. Particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ is expanded around equilibrium Maxwell distribution according to small parameter ϵ which can be e. g. mean free path or Larmor radius:

$$f(\mathbf{r}, \mathbf{v}, t) = f_0 + \epsilon f_1 + \epsilon^2 f_2 + \dots \quad (6)$$

Usually, only first two terms are considered and inserted into Boltzmann kinetic equation. Consequently, this integral equation is solved for f_1 using e. g. Sonine polynomials. Obtained distribution function is used in equations 5 to derive expressions for stress tensor \mathbf{P} and collisional frictional force \mathbf{F}_s .

5. Conclusions

In our contribution we compared results of two well established computer modelling techniques used in plasma physics - particle and fluid models. The differences between these techniques were discussed on sheath structure around cylindrical Langmuir probe and its IV characteristic. We identified that differences are greater for low pressure where drift diffusion approximation fails. We also discussed hybrid modelling techniques and possibilities of their usage in low pressure area.

Acknowledgments

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