Modelling for RF-CCPs at Intermediate Pressure: Doubts on Drift-Diffusion Models

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Radio-frequency capacitively coupled plasmas (RF-CCP) at gas pressures above ~1 Torr are often simulated by fluid models since Particle-in-Cell (PIC) models are too computationally intensive. The drift-diffusion approximation, is widely employed in fluid models [1]. Drift-Diffusion models require the electron transport coefficients (mobility, μ, diffusion, D, energy mobility μ_ε and energy diffusion D_ε), as well as the rate constants (for ionisation, energy loss, etc.), which are calculated from the electron energy distribution function (EEDF). Fluid models do not copntains information on the EEDF, which must be estimated in other ways. In this pressure range, the local energy approximation is commonly used (with an approximation on the energy transport coefficients and using the Einstein relation) [1], but a detailed comparison to PIC results is needed in order to quantify the impact of the abovementioned approximations. In this study we compare simulations of Argon plasmas using three different approches for the EEDF: the local energy assumption, Maxwellian assuming constant collision frequency, and Maxwellian with full calculation of the transport parameters. The fluid model results using these theree assupmtions are then compared to a benchmark PIC simulation.

In the local mean energy model, the EEDF is calculated, as a function of the electron mean energy <E>, using the Loki Boltzmann solver [2]. This assumption is well justified for homogeneous DC glow discharges, but its applicability to time-varying fields (e.g. RF-CCP) with strong spatial gradients is more debatable. When all four coefficients (μ, D, μ_ε and D_ε) are directly calculated from the local-field EEDF, the RF-CCP simulation gave unphysical negative values in the sheath for the electron density and energy, causing failure of the simulation. A widely-used solution for RF-CCP simulation [1] is to use the local energy mobility, and calculate the other coefficients from the mean electron energy using the Einstein relations (which are only strictly valid for a Maxwellian distribution) assuming a constant momentum-transfer collision frequency. This solution gives improved numerical stability and convergence speed.

For the Maxwellian assumption, the transport coefficients and rates can be calculated from the EEDF, most simply by assuming constant collision frequency assumption, or by a full calculation using the energy-dependent cross-section. The electron temperature is determined by the power balance in the simulation. However, at intermediate pressures (1-10 Torr) the EEDF is expected to deviate significantly from Maxwellian due to inelastic collisions.

The results of the different models (fluid and PIC) are compared in Fig. 1. Compaed to the PIC model, the local energy assumption overestimates the mean electron energy, (Fig. 1 (a)), while both Maxwellian assumptions (with and without a constant collision frequency assumption) underestimate

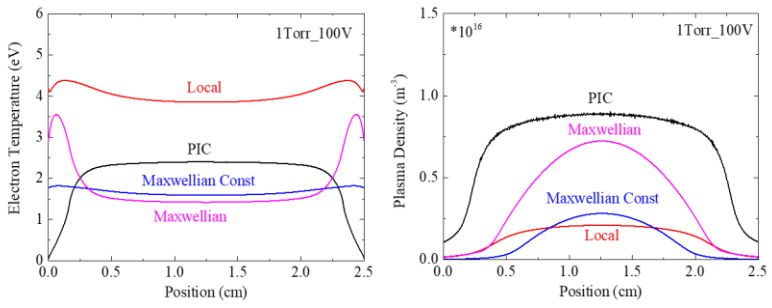

Fig. 1: (a) Mean electron energy, (b) Ion density profile at 1 Torr 100 V, with different models

it. This can be attributed to differences in the density of high-energy electrons: the EEDFs provided by the local energy assumption contain few high energy electrons, so that a high mean electron energy is necessary to provide enough ionization. Considering the central plasma density (Fig. 1 (b)), the full Maxwellian model is closest to the PIC, although there is poor agreement in the profile. While the density is very underestimated as compare to PIC.

The PIC model provides the true EEDF at different pressures and positions, shown in Fig. 2 (b). The problems in the fluid models can be explained by the spatial variation of EEDF. At low pressure (0.1 Torr), the EEDF at both the center and the ionization peak region is quite Maxwellian. At higher pressure, the high energy tail is depleted compared to a Maxwellian distribution due to the inelastic collisions, but this effect is more marked at the center compared to the regions of peak ionization (at the sheath edges).

At 1 Torr, the center EEDF, (Fig. 2 (f)) is already close to that predicted by the local energy assumption. As a result, the density profile is quite well predicted by this model. However, in the peak ionization regions neaer the sheath, the EEDF is much more Maxwellian, explaining why this model is betyter at predicting the peak density. Most of the electron heating and ionization happens in the peak ionization region, so the EEDF in this region decides the density.

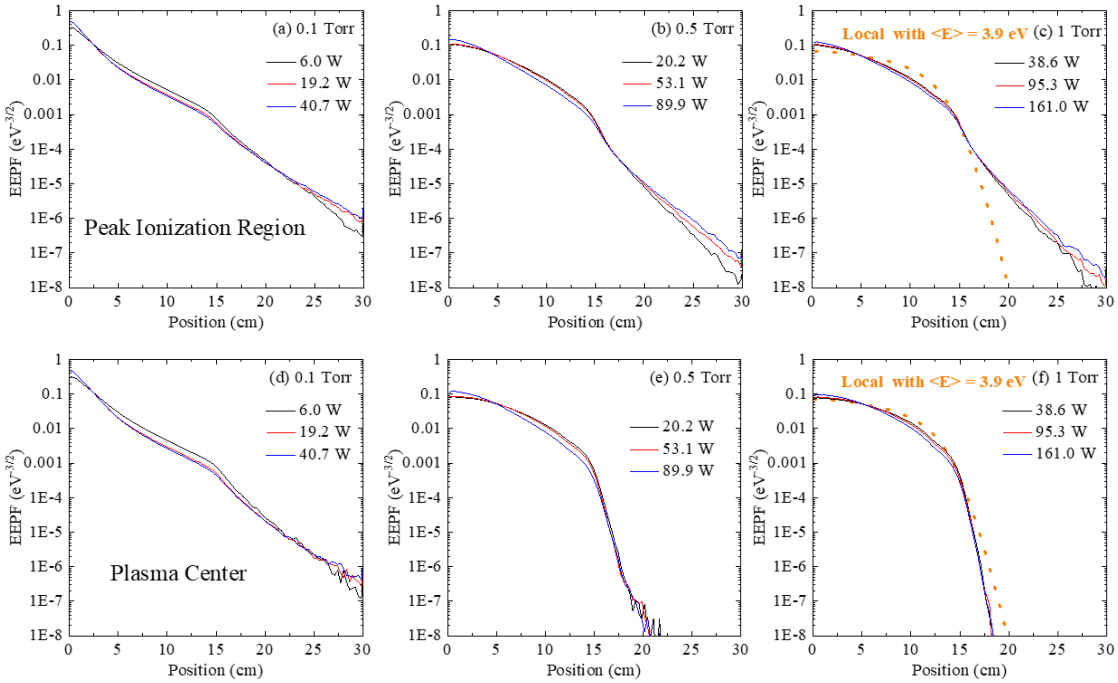

Fig. 2: (a) Ion density profile, (b) Mean electron energy at 1 Torr 100 V, with different models

In conclusion, we present a comparasion of Drift-Diffusion fluid simulations using different EEDF assumptions with a PIC benchmark. The source of the errors inthe Drift-Diffusion models are discussed. Drift-Diffusion fluid models should be used with caution in this pressure range due poor estimation of the EEDF.

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Reference

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