Drift-Diffusion Modeling of a DBD Volumetric Reactor

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Introduction

Non-thermal plasmas play a significant role in a large set of applications, ranging from the industrial and aerospace fields to agriculture and medicine [1]. One of the most common techniques to obtain a non-thermal plasma is through a Dielectric Barrier Discharge (DBD) [2]. Although being well established devices, the operation of DBD reactors is governed by a number of complex physical mechanisms, that are worth investigating. In this work we describe the implementation of a drift-diffusion model for the simulation of a volumetric DBD reactor. The aim of the model is to follow the temporal and spatial evolution of the main neutral and charged species produced in the discharge. Finally, we introduce a numerical treatment of the electron dynamics based on coupling the Poisson equation with the Boltzmann relation, and compare the obtained results against a classic full drift-diffusion approach.

Model formulation

Considering a plasma constituted by a given number n_s of species, and assuming that the validity conditions of a fluid model are met (i.e., the characteristic macroscopic length $L_c \gg$ mean free path λ_c, and the characteristic macroscopic time $t_c \gg$ mean collision time $1/\nu_c$), the foundation of the model is constituted by the drift diffusion equations for each species:

$$\frac{\partial N_s}{\partial t} + \nabla \cdot (-D_s \nabla N_s + \langle \mathbf{v}_s \rangle N_s) = \Omega_s, \tag{1}$$

in which N_s and D_s are the number density and the diffusion coefficient of the $s-$th species, respectively. The average drift velocity $\langle \mathbf{v} \rangle_s = (q_s/|q_s|)\mu_s \mathbf{E}$ is defined via the product between the electric field and the electrical mobility μ_s of the species, accounting for the sign of the species charge q_s. The right-hand side term in (1) takes into account of the elementary processes in the plasma (i.e., thermal ionisations, recombinations, attachments).

An electrostatic formulation is used to describe the electric field behaviour. That is, assuming a conservative electric field, the governing equation in the plasma region is given by the Poisson equation:

$$\nabla^2 \varphi = -\frac{\rho}{\varepsilon_0}, \tag{2}$$

where ρ is the electric charge volume density and ε_0 the vacuum dielectric constant. The charge density ρ depends on the space distribution of the ions and electrons number densities, which in turn are governed by the drift diffusion equations (1):

$$\rho = \sum_{s=1}^{n_s} q_s N_s, \tag{3}$$

Equations (1) for all the species of interest, coupled with (2), constitute a model that can be used to evaluate the evolution of a discharge over time. We will call this model Full Drift Diffusion (FDD). However, it can be observed that, among the species in the plasma, electrons exhibit markedly larger swarm parameters. As a result, numerical schemes (most notably explicit numerical schemes) that solve this problem are bound to use small time integration steps determined by the fast dynamics of the electrons. One possible way around this limitation is to consider that electrons adapt instantaneously to the local value of the electric potential, according to the Boltzmann distribution. Consequently, assuming a plasma constituted by n_H heavy species, the charge density can be expressed as:

$$\rho = \sum_{s=1}^{n_H} q_s N_s e - e N_{e,0} \exp\left(\frac{\varphi - \varphi_0}{T_{e,\mathrm{eV}}}\right), \tag{4}$$

where $T_{e,eV} = k_B T_e / e$ is the electron temperature in eV, φ_0 the electric reference potential and $N_{e,0}$ the background electron number density. The model presented in this paper is therefore constituted by the equations for heavy species, coupled with the non-linear Poisson equation in which the charge density is evaluated by means of (4). This second approach will be hereafter referred to as Boltzmann Drift Diffusion (BDD). According to this approach, the electron number density and electric potential are evaluated by means of a steady state formulation, driven by the time evolution of the heavy species. Applying (4) on a finite domain does not guarantee the global charge neutrality. Indeed, an additional condition has to be enforced:

$$Q_{tot} = Q_s + \int_V \rho\left(N_1, N_2, \ldots, N_{n_H}, \varphi, \varphi_0, N_{e,0}\right) \mathrm{d}V = 0, \tag{5}$$

where Q_s is the charge deposited on the walls. Equations (1) and (2) have been discretised by means of a cell-centred finite volume method. Convective fluxes are dealt with by means of a first order upwind scheme, and the explicit Euler method has been adopted for time integration. Assuming a 1D formulation of the problem with a space discretisation Δx, the integration time step Δt is subject to the stability condition:

$$\Delta t \leq \min\left[\frac{\Delta x}{(2D_s/\Delta x) + |\langle v_s \rangle|}\right]. \tag{6}$$

It is evident that condition (6), when applied to the BDD approach, becomes less restrictive, since only the swarm parameters of the heavy species are taken into account. On the other hand, a single time step using BDD requires a considerably higher computational effort, since the non-linear Poisson equation has to be solved. In this work, this task is carried out by means of a Newton-Raphson algorithm. The reference potential φ_0 is adjusted to satisfy the condition (5) using a bisection method.

A simple study case: ambipolar diffusion

To validate the code a simple case of ambipolar diffusion is simulated. Ambipolar diffusion has been chosen because, under certain conditions ($\Gamma_e = \Gamma_i$, $N_e \approx N_i = N$ and no external field) the electric field can be expressed using an analytical formula [3]:

$$\mathbf{E} = \frac{D_i - D_e}{\mu_e + \mu_i} \frac{\nabla N}{N}. \tag{7}$$

For the sake of simplicity chemical reactions are not included, considering only two types of particles: electrons and ionised Argon. A one dimensional computational domain has been considered, discretised by means of 101 points, with a total length of 0.1 mm. The initial number densities of the species follow a Gaussian distribution. In the simulation constant diffusivity and mobility were assumed, using the values reported in table 1 that, according to the Einstein relation $D_e/\mu_e = T_{e,\mathrm{eV}}$ lead to an electron temperature of 0.2 eV.

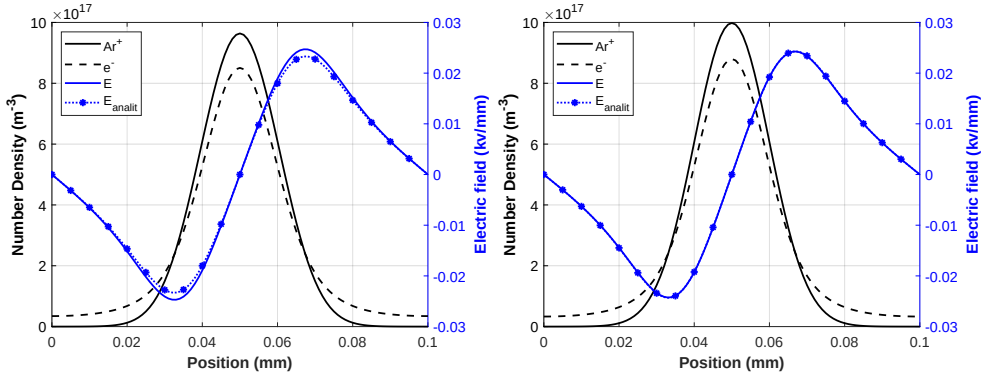
μ_e	μ_i	D_e	D_i
5.0×10^{-2}	1.5×10^{-4}	1.0×10^{-1}	5.0×10^{-6}

Table 1: Swarm parameters used in the simulations. Mobilities are in $\mathrm{m^2V^{-1}s^{-1}}$ and diffusion coefficents in $\mathrm{m^2s^{-1}}$

Results and discussion

As shown in Fig. 1 the results obtained with the two approaches considering constant parameters are in good agreement with the analytical solution. Moreover, the ion fluxes calculated using FDD and BDD method are nearly equal, as shown in Fig. 2.

It's important to notice that the BDD approach allows adopting time steps of $\sim 10^{-9}$ s compared to $\sim 10^{-13}$ s required by the FDD approach. This, depending on the simulation conditions, leads to speedup factors of 20-100.



(a) Results using BDD approach with a time step $\Delta t = 1 \times 10^{-13}\,\mathrm{s}$

(b) Results using BDD with a time step $\Delta t = 1 \times 10^{-9}\,\mathrm{s}$

Figure 1: *Comparison between analytical solution and simulation results after* $0.1\,\mu\mathrm{s}$ *with constant parameters*

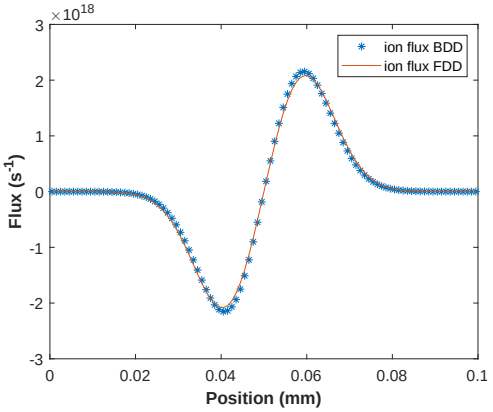


Figure 2: *Comparison between fluxes calculated using BDD e FDD approach*

Conclusion

In this paper, a novel drift-diffusion model for plasma analysis has been proposed. The model uses the Boltzmann relation to evaluate the spatial distribution of electrons. A simple case of ambipolar diffusion has been considered for validation, using the analytical solution and the results of a conventional drift diffusion model (FDD) as terms of comparison. The results have shown a good agreement. The BDD formulation is obviously not able to capture the fast dynamics of the electrons, but it allows to increase the time step by 3-4 orders of magnitude.

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