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Extended dielectric relaxation scheme for fluid transport simulations of high density plasma discharges

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In order to overcome limitations on the simulation time step for fluid transport simulations of high density plasma discharges, the dielectric relaxation scheme (DRS) was developed. By imitating a realistic and physical shielding process of electric field perturbation, DRS overcomes the dielectric limitation on simulation time step. However, the electric field was obtained by assuming the drift-diffusion approximation for both the electrons and ions. Although the drift-diffusion expressions are good approximations, the inertial term cannot be neglected in the ion momentum equation for low pressure. Therefore, in this work, we developed the extended dielectric relaxation scheme (EDRS) by introducing an effective electric field. Similar to DRS, EDRS is limited to quasi-neutral plasma with zero current, i.e. EDRS is applicable when the local ambipolarity is satisfied. In order to validate EDRS, two-dimensional fluid simulations for inductively coupled plasma discharges were performed. The simulation results are then compared with experimental measurements by using a Langmuir probe.

1. Introduction

In order to simulate high density plasma discharges, various models such as particle, kinetic, fluid, and some hybrid models have been used. Among them, fluid models have been widely adopted because it provides useful global insight into the profiles of the plasma parameters [1–3]. Although fluid models are widely used in all areas of plasma physics, there are some severe restrictions on stable simulations of high density plasma discharges because the plasma frequency is too high and the sheath length is very short relative compared to the chamber scale. Therefore, various numerical methods and boundary conditions have been suggested to overcome limitations on the simulation time step and grid size [1,2,4,5].

It is well known that the upwind, exponential, and power-law schemes can efficiently overcome the limitation on the grid size for fluid transport simulations of high density plasma discharges [2,6]. In order to overcome the limitation on the simulation time step, massless electron method, semi-implicit method, and dielectric relaxation scheme (DRS) were suggested. Ventzek et al. [4] proposed a semi-implicit update technique for the electric potential. In this scheme, the Poisson's equation is solved for a future time using a prediction for the charge densities based on the present values of their time derivatives. In addition, the authors show that the semi-implicit algorithm allows the time steps to exceed the dielectric relaxation time by factors of 100–1000, or until limited by the Courant criterion. Assuming electro-neutrality in the bulk, Nam et al. [5] used the electric field in the bulk that is derived from the electron momentum balance by assuming inertialess electrons, neglecting the time dependent and inertial terms in the momentum equation. This method is called 'inertialess electron method' or 'massless electron method'. Makabe et al. [7,8] adopted the effective electric field for the electron transport in order to consider a finite time delay with respect to the local instantaneous reduced field. Kushner's group used a simple effective field approximation in order to account for the lagging relaxation response of ions subjected to high frequency electric fields [9].

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In particular, by imitating a realistic and physical shielding process of electric field perturbation, DRS overcomes the dielectric limitation on time step [1]. The authors of Ref. [1] show that DRS can provide stable values of electron density although the simulation time step is larger than the dielectric relaxation time step. Also, the results using DRS with the exponential method are in good agreement with those using semi-implicit method. Using DRS, Choe show that the drift-diffusion approximation for ion species is available at $u_B/(\nu_{i,en}L) \ll 1$, where u_B is the Bohm velocity, $\nu_{i,en}$ is the ion/electron-neutral collision frequency, and L is the dimension of the system [10]. Although, the effective electric fields were introduced to treat the inertial effect in the ion momentum equation, the electric field in DRS was not derived self-consistently but obtained assuming the drift-diffusion approximation for both the electrons and ion species.

Therefore, we derived the electric field in a self-consistent manner to treat the inertial terms in the ion momentum equation. Because the drift-diffusion representation of electrons is valid at low pressure, we also neglected the time dependent and inertial terms in the momentum equation for electrons. Using similar approach in Ref. [10], we used the modified ion momentum equation to treat the inertial term by introducing an effective electric field. By using two momentum equations and continuity equations, we derived a new electric field $\Delta\mathbf{E}$ during the time step Δt. To compare the extended dielectric relaxation scheme (EDRS) with the previous method, two dimensional fluid simulations for inductively coupled plasma discharges were performed.

This paper is organized as follows. In Sec. 2, the governing equations and numerical methods are described. Results from several specific applications are presented in Sec. 3. Finally, conclusions are given in Sec. 4.

2. Model descriptions

The basic equations for charged particles consist of the continuity, momentum, Poisson, and the electron temperature equations.

$$\frac{\partial n_e}{\partial t} + \nabla\cdot\boldsymbol{\Gamma}_e = R_e, \tag{1}$$

$$\frac{\partial n_i}{\partial t} + \nabla\cdot\boldsymbol{\Gamma}_i = R_i, \tag{2}$$

$$\frac{\partial \boldsymbol{\Gamma}_e}{\partial t} + \nabla\cdot(\boldsymbol{\Gamma}_e\mathbf{u}_e) = -\frac{en_e}{m_e}\mathbf{E} - \frac{\nabla(n_e k_B T_e)}{m_e} - \nu_{en}\boldsymbol{\Gamma}_e, \tag{3}$$

$$\frac{\partial \boldsymbol{\Gamma}_i}{\partial t} + \nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i) = \frac{en_i}{m_i}\mathbf{E} - \frac{\nabla(n_i k_B T_i)}{m_i} - \nu_{in}\boldsymbol{\Gamma}_i, \tag{4}$$

$$\nabla\cdot\mathbf{E} = 4\pi e(n_i - n_e), \tag{5}$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_e k_B T_e\right) = -\nabla\cdot\mathbf{Q}_e - e\mathbf{E}\cdot\boldsymbol{\Gamma}_e + P_{abs} - P_{coll}. \tag{6}$$

Here, n_e (n_i), $\boldsymbol{\Gamma}_e$ ($\boldsymbol{\Gamma}_i$), $\mathbf{u}_e$ ($\mathbf{u}_i$), m_e (m_i), and T_e (T_i) are the density, flux, velocity, mass, and temperature of the electrons (ions). k_B is the Boltzmann constant, ν_{en} and ν_{in} are the electron and ion collision frequency with neutrals, respectively. $\mathbf{Q}_e$ is the energy flux of the electron given by $\mathbf{Q}_e = 5/2 n_e \mathbf{u}_e k_B T_e + \mathbf{q}_e$, where

$$\mathbf{q}_e = -\frac{5}{2}\frac{n_e k_B T_e}{m_e \nu_{en}}\nabla(k_B T_e). \tag{7}$$

R_e and R_i represent the generation rates for the electrons and ions, P_{abs} and P_{coll} represent the power absorption from external power and collisional power loss per unit volume.

As shown in Ref. [1], when Eq. (5) is solved along with Eq. (1) in an explicit time integration scheme, severe time step limitation occurs. In order to overcome this limitation on the time step, Choe et al. [1] derived the electric field $\Delta\mathbf{E}$ during the time step Δt shown as

$$\Delta\mathbf{E}(\Delta t) = -4\pi e\tau_d(\boldsymbol{\Gamma}_i - \boldsymbol{\Gamma}_e)\left[1 - \exp\left(-\frac{\Delta t}{\tau_d}\right)\right], \tag{8}$$

with assuming the drift-diffusion approximations shown as

$$\boldsymbol{\Gamma}_e = -\frac{en_e}{\nu_{en}m_e}\mathbf{E} - \frac{\nabla(n_e k_B T_e)}{\nu_{en}m_e}, \tag{9}$$

$$\boldsymbol{\Gamma}_i = \frac{en_i}{\nu_{in}m_i}\mathbf{E} - \frac{\nabla(n_i k_B T_i)}{\nu_{in}m_i}, \tag{10}$$

where $\tau_e = \nu_{en}/\omega_e^2$, $\tau_i = \nu_{in}/\omega_i^2$, and $1/\tau_d = 1/\tau_e + 1/\tau_i$ [1,11]. Here, ω_e and ω_i are electron and ion plasma frequencies, respectively. After introducing the effective electric field $\mathbf{E}_{eff}$ [10], Eq. (10) can be written as

$$\boldsymbol{\Gamma}_i = \frac{en_i}{\nu_{in}m_i}\mathbf{E}_{eff} - \frac{\nabla(n_i k_B T_i)}{\nu_{in}m_i}. \tag{11}$$

Assuming $\partial[\nabla(n_i k_B T_i)]/\partial t \approx 0$, Eqs. (4) and (11) yield

$$\frac{1}{\nu_{in}}\frac{\partial\mathbf{E}_{eff}}{\partial t} = \mathbf{E} - \mathbf{E}_{eff} - \frac{m_i}{en_i}\nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i). \tag{12}$$

Using similar approach in Ref. [1], we can obtain the continuity equation shown as

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\mathbf{J}_i - \mathbf{J}_e) = 0, \tag{13}$$

or

$$\nabla\cdot\left[\frac{1}{4\pi}\frac{\partial\mathbf{E}}{\partial t} + \mathbf{J}_i - \mathbf{J}_e\right] = \nabla\cdot(4\pi\mathbf{J}_t) = 0, \tag{14}$$

where $\rho = e(n_i - n_e)$, $\mathbf{J}_i = e\boldsymbol{\Gamma}_i$, $\mathbf{J}_e = e\boldsymbol{\Gamma}_e$, and $\mathbf{J}_t$ is the total current density. Assuming locally ambipolar diffusion, $\mathbf{J}_t$=0, Eq. (14) can be written as

$$\frac{\partial\mathbf{E}}{\partial t} = 4\pi(\mathbf{J}_e - \mathbf{J}_i). \tag{15}$$

Substituting Eq. (9) into Eq. (15) gives

$$\frac{\partial\mathbf{E}}{\partial t} + \frac{1}{\tau_e}\mathbf{E} = -\frac{4\pi e}{m_e\nu_{en}}\nabla(n_e k_B T_e) - 4\pi\mathbf{J}_i, \tag{16}$$

where $\tau_e = m_e\nu_{en}/4\pi e^2 n_e$. In order to apply finite difference method in time evolution, we integrate Eq. (16) during finite time step Δt. This leads to

$$\Delta\mathbf{E}(\Delta t) = -4\pi e\tau_e(\boldsymbol{\Gamma}_i - \boldsymbol{\Gamma}_e)\left[1 - \exp\left(-\frac{\Delta t}{\tau_e}\right)\right]. \tag{17}$$

Notice that Eq. (17) is similar with Eq. (8) except for τ_e. However, the extended model of Eq. (17) can be applied for low pressure region because $\boldsymbol{\Gamma}_i$ in Eq. (17) includes the effective electric field as shown in Eq. (11).

To compare EDRS with the previous method, two dimensional fluid simulations for inductively coupled plasma discharges are