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An axisymmetric unstructured finite volume method applied to the numerical modeling of an atmospheric pressure gas discharge

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ABSTRACT

We develop a finite volume method based on unstructured triangular and/or quadrangular meshes for the numerical modeling of gas discharges at atmospheric pressure. The discretization of the computational domain is performed with median-dual control-volumes. Gradient calculations at the faces of the control-volumes are based on finite-element interpolation using shape functions. An FCT method was chosen for the species transport integration. The accuracy of the numerical scheme is verified for different types of mesh-elements in a plane-to-plane DBD geometry. We present comparisons with literature results based on the immersed boundary method in a point-to-plane geometry and investigate the need of a high-order scheme for an accurate model of a filamentary discharge. Finally, we apply our scheme in a study of a discharge between two hemispherical electrodes covered with dielectrics, while focusing on sufficient spatial resolution in the vicinity of the dielectric surface.

1. Introduction

A large number of works have been devoted to the numerical modeling of non-equilibrium cold plasma at atmospheric pressure (AP). Most of these works were motivated not only by the need to improve our understanding of the basic mechanisms of gas discharges, but also by their potentially important industrial applications [1]. However, in spite of the complex design of many industrial reactors, most of the numerical codes described in the literature are based on a structured mesh approach. This allows to handle quite easily simple geometries, such as plane-to-plane; when more complex geometries are of interest though, special techniques should be used. As an example, Célestin et al. [2] used the Immersed Boundary Method (IBM) in a point-to-plane geometry. However, such techniques require significant modifications when a new geometry is considered and, in the case of IBM, the choice of the immersed structures which can be used is rather limited.

Unstructured meshes offer means to achieve good flexibility in handling complex reactor geometries. Surprisingly, only a few unstructured-mesh codes have been developed in the field of non-equilibrium cold plasmas. To our knowledge, the first code of this type was developed by Georghiou et al. in 1999 [3] and applied to the numerical modeling of a filamentary discharge in air. Several other studies by the same team have followed this pioneering work [4–7]. The Georghiou and Morrow

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code employs the finite element method (FEM). These codes are 2D axisymmetric. In order to resolve steep gradients in the solution and to avoid the occurrence of negative values in the charged species density, their method uses the concept of flux-corrected transport (FCT). FCT was initially developed by Boris and Book [8] and Zalesak [9], and later extended to unstructured meshes by Löhner et al. [10] and Kuzmin [11].

Recently, three-dimensional codes were introduced [7,12,13]. Photoelectric effect was taken into account together with photoionization based on the works of Bourdon et al. [14] and Luque et al. [15]. Furthermore, the local field approximation was used and only three different charged species (i.e. electrons, one positive and one negative ionic species) were taken into account to describe the air discharge. An adaptive mesh was used to allow for an accurate treatment of steep gradients with a small number of mesh nodes.

The FEM was only employed by Georghiou's team. Most of the other unstructured mesh codes available in the literature are based on the finite volume method (FVM), such as the work of Kushner's team [16]. Unlike Georghiou, Kushner includes the equation for electron energy rather than using the local field approximation. Photoionization, together with various modules for hydrodynamic effects induced by the discharge, are included in the code. However, compared to Georghiou's FEM, Kushner uses a simpler numerical method based on the exponential Gummel scheme [17], whose discretization leads to a system of equations which is linearized and solved with a quasi-Newton method [18].

Another FVM was developed by Min et al. [19] for the modeling of plasma display panels. In this work a hybrid FVM and FEM was used together with an FCT algorithm and the Gummel scheme.

One of the most recent works on unstructured meshes was presented by Deconinck et al. [20,21] and Breden et al. [22]. A cell-centered FVM was developed for the study of plasma bullets and micro-hollow cathode discharges on hybrid meshes (combination of triangles and quadrangles). A vertex-centered FVM based on triangular meshes was recently developed by Benkhaldoun et al. [23]. They used an adaptive mesh to simulate the propagation of planar ionizing waves in plane-to-plane geometries.

This work describes a 2D axisymmetric code, based on the integration of fluid equations, which aims to model non-equilibrium high-pressure discharges. The code uses vertex-centered control volumes and allows for the simultaneous use of triangular and quadrangular elements.

The layout of the paper is as follows. In Section 2 we describe the fluid equations and the corresponding boundary conditions (BCs) used. Then, in Section 3, we present the numerical techniques with an emphasis on the use of a specific FCT method. In Section 4 we analyze the accuracy of our numerical scheme and compare it with other codes for plane-to-plane (Section 4.1) and point-to-plane (Section 4.2) geometries. Finally, in Section 4.3 we give results for a reactor described by Kozlov et al. [24], designed to study the transition between a filamentary and homogeneous discharge in nitrogen and air.

2. Model description

2.1. Plasma–fluid equations

Our model is based on a fluid (hydrodynamic) description of the motion of charged and neutral species. The transport of species is governed by the continuity equations

$$\frac{\partial n_k(\boldsymbol{r},t)}{\partial t} + \nabla \cdot \boldsymbol{\Gamma}_k(\boldsymbol{r},t) = R_k(\boldsymbol{r},t), \quad \text{for } k = 1(e), 2, \ldots, N_t, \tag{1}$$

where $n_k(\boldsymbol{r},t)$ is the density of species k at position $\boldsymbol{r}$ and time t, k is equal to 1 (or e) for electrons and lies between 2 and N_c for ions, where N_c is the number of charged species. The species subscripts between N_c+1 and N_t correspond to neutral species. R_k is the signed production rate of species k resulting from the relevant chemical reactions and photoionization. Because we assume that photoionization leads only to the photoelectron-coupled ionic species with $k=2$, the photoionization source term S_{ph} (see Section 2.2) is included in R_k only for $k=1,2$. The flux of species k, $\boldsymbol{\Gamma}_k$, follows from the drift–diffusion approximation, with the total flux composed of a convective flux $\mathcal{C}_k$ and a diffusive flux $\mathcal{D}_k$,

$$\boldsymbol{\Gamma}_k = n_k \boldsymbol{w}_k - D_k \nabla n_k(\boldsymbol{r},t) = \mathcal{C}_k + \mathcal{D}_k, \tag{2}$$

where $\boldsymbol{w}_k$ is the drift velocity of the charged species,

$$\boldsymbol{w}_k = -\operatorname{sgn}(Z_k)\mu_k(\boldsymbol{r},t)\nabla V(\boldsymbol{r},t), \tag{3}$$

and μ_k and Z_k are, respectively, the absolute value of the mobility and the charge number of species k. The diffusion is assumed to be isotropic with a scalar diffusion coefficient D_k. $V(\boldsymbol{r},t)$ is the electrical potential at position $\boldsymbol{r}$ and time t.

We work within the framework of the local field approximation (LFA): the transport parameters and the electron-dependent reaction rates at position $\boldsymbol{r}$ are functions of the magnitude of the local reduced electric field $E(\boldsymbol{r},t)/N$, where N is the background neutral gas density.

The motion of the space charges influences the electrical potential $V(\boldsymbol{r},t)$ governed by the Poisson equation:

$$\nabla \cdot \big(\varepsilon(\boldsymbol{r})\nabla V(\boldsymbol{r},t)\big) = -|q_e| \sum_{k=1}^{N_c} Z_k n_k(\boldsymbol{r},t), \tag{4}$$