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A finite volume method for electrostatic three species negative corona discharge simulations with application to externally charged powder bells

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A three species model for steady-state negative corona discharge is studied. Ionization, attachment, and recombination reactions are modeled. A novel unstructured finite volume algorithm to solve the equations is presented, using the secondary emission of electrons from the cathode to set boundary values for the electrons.

To show the usefulness of the method for industrial applications it is used to characterize the electrostatic properties of an externally charged rotary powder bell used in the automotive industry. Experimental current density profiles are reconstructed with good accuracy, which validates the model and the method with real experimental data.

Introduction

Corona discharge has many industrial applications, e.g. spray-painting in the automotive industry, ozone-generation, and cleaning of toxic gases. Much effort has been spent on the qualitative analysis and quantitative models of the corona discharge phenomenon, see e.g. Refs. [1,2,7,8,18–21,24,27]. In this paper we focus on negative corona discharge, there is also the corresponding positive corona discharge phenomenon. In negative corona discharge a large negative potential difference is applied between two electrodes. If the potential is large enough it will ionize the gas, this primarily happens close to large curvature parts of the cathode. This, eventually, produces negative ions that flow towards the anode. The ionization region is a small region close to the cathode, outside of this ionization region mostly negative ions are present. We will restrict our attention to corona discharge in pure oxygen and air at standard temperature and pressure, but the same model works in other electronegative gases. The most interesting electronegative gas is arguably air, which is the gas used in many industrial processes.

The first choice one has to make, when modeling the corona discharge, is the number of species to use. For industrial applications, most authors use a one species model [25,29]. In Ref. [5] 70 reactions between a large number of species is considered: O, O_2, O_3, their positive and negative ions, and various excited versions. A comparison between models with different number of species is given in Ref. [20].

A one species model has several advantages, it is easier to describe mathematically and numerically, and low-resolution description of the geometry is possible. In addition, the ionization region is very small, which means that even many-species models will be one species in most of the domain. The main drawback of single species models is that they are an oversimplification of the physics. The consequence of this for a quantitative model is that the description of the boundary values close to the cathode is difficult, especially in a needle (point)-plane geometry. For wire-cylinder cases, there is Peek's law [18], which together with the Kaptzov assumption [8] allows one to assign boundary values. These

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boundary values, however, are neither numerically nor mathematically stable; on the coronating part of the needle no boundary conditions on the charge densities are set. Instead one sets Dirichlet and Neumann conditions on the potential.

In this paper we use a three species model with positive ions, represented by O_2^+, negative ions represented by O_2^-, and electrons. This captures most of the electrostatic properties of corona discharge, but ignores many of the chemical properties, and the reactions between different positive and negative ions. From the electrostatic point of view, our main simplification is that we ignore that large parts of the charge is carried by O^- and O_3^-, that have different mobilities than O_2^-. Fortunately O^- has larger mobility than O_2^- whereas O_3^- has lower mobility. Thus, on average this is an acceptable simplification.

Three species corona discharge models have previously been studied in e.g. Refs. [19,20,30]. In Refs. [19,20] only the wire-cylinder case is considered, which is essentially a one dimensional problem. We are primarily interested in the needle-plane case, which, taking rotational symmetry into account, is a two dimensional problem. This is similar to the model presented in Ref. [30], where a hybrid finite-element and method of characteristics method is presented.

Our approach is completely different. We present a stable steady-state model of negative corona discharge based on higher order convective schemes using the normalized variable diagram. In our approach both the Poisson equation and the charge density transport equations are discretized using the finite volume method. This is in contrast to many other approaches that use a combined method, e.g. the FEM-FVM approach in Refs. [12,17], FEM-MOC in Refs. [1,2,30], and FEM-FCT in Ref. [22]. In Ref. [17] an iterative second order convective scheme for the non-stationary single species case was constructed.

The design of our algorithm is based on methods in computational fluid dynamics for solving continuity and convection equations on unstructured grids. We present a detailed study of the convergence properties of our algorithm. In addition, the algorithm is validated with analytic solutions to a one dimensional one-species case, and a separately implemented one dimensional FEM three-species solver. Another novelty with our approach is that it avoids the double iterative loop, used in e.g. Refs. [1,28,30], where the boundary condition is updated separately from the PDE solver iterations.

The motivation for this work is the electrostatic modeling of externally charged spray-painting, see e.g. Refs. [14,25,28,29]. The three species solver is introduced to enable a detailed description of the electrostatic properties both inside the ionization region close to the bell, and between the bell and the target.

Experiments on the current density profiles of negative corona discharge is difficult and time-consuming, see e.g. Refs. [7,16,23,27]. To use our model to characterize a corona discharge system, either a single needle system or one of the multi-needle systems often used for spray-painting applications, one can either measure the current density profiles, or the curvature of the needle together with the total current. To illustrate the applicability of this approach to externally charged spray-painting in the automotive industry, we have performed current density measurements of an externally charged rotary powder bell, and estimated the radius of curvature of the needle and the second Townsend ionization coefficient. We stress, however, that to measure the total current it is not necessary to measure the current density profiles, instead one can measure how much current that is emitted from the needle. Once the curvature and the total current is known, γ — the second Townsend ionization coefficient, can be varied until the simulations yield the same total current as the corona discharge system.

The structure of this paper is as follows: in Section 2 we present the details of the model, reactions, and equations studied in this paper, in Sections 3 and 4 we present the algorithm and its validation. We present results for needle-plane geometries in Section 5, including parameter studies in the needle radius of curvature, the second Townsend ionization coefficient, and the cathode potential. In Section 6 the experiments and their analysis is presented. Finally, in Section 7 we make some concluding remarks and comments.

Three species corona discharge model

To describe a three species model of the negative corona discharge we need four variables: the electric potential and the charge densities of electrons, negative ions, and positive ions. The equations governing the negative corona discharge consists of two parts, the Poisson equation for the potential, and convection-reaction equations for the charge densities.

We will restrict ourselves to the steady state case. Thus, in the absence of sources the current density is conserved. Since the diffusion of electrons and ions has a negligible effect on the corona process, the current density is given by $j = \mu\rho E$, where μ is the mobility, ρ is the charge density, and E is the electric field. For a single species model of the negative corona discharge, only the negative ions are considered. In this case one solves the Poisson equation and the conservation of current density, $\nabla \cdot j = 0$. The reactions between the three species will appear as source terms in the equations.

Equations

We will consider the five reactions described in Refs. [30], many more occur between different forms of oxygen [5,21], in Ref. [20] models with up to seven species are compared. The reason for restricting to three species is that this is the simplest model which still captures the physics of the ionization process. We are not primarily interested in the exact concentrations of different atoms and molecules among positive and negative ions. This means that we will use O_2^+ to model all positive ions, and O_2^- to model all negative ions. The five reactions can be split into two groups: two are linear in the unknown charge densities and three are quadratic. The quadratic reactions only have a minor effect on the solutions. The values of the reaction parameters are taken from Ref. [5] for pure oxygen gas and [21] for air, they are described in detail in Section 2.2.

Linear reactions:

$$e + O_2 \rightarrow 2e + O_2^+ \quad (\textit{ionization}),$$

and

$$e + O_2 + M \rightarrow O_2^- + M \quad (\textit{attachment}),$$

with M an uncharged species (primarily O_2 or N_2), the role of M is, e.g., to preserve energy, momentum, and electron excitations. We denote the reaction rate coefficients with k_i, and k_a for ionization and attachment, respectively.

Quadratic reactions:

(*electron-positive ion recombination*)

$$e + O_2^+ + O_2 \rightarrow 2O_2$$

(*two body negative-positive ion recombination*)