3D Models for nanosecond pulsed discharges: with new codes to quantitative understanding

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Computer simulations are an important method to study and understand nanosecond pulsed discharges. We give a brief introduction to the numerical modelling of discharges and our open source codes. Then, two studies with a 3D particle model are presented: the inception of discharges near a needle electrode and the guiding of streamers by pre-ionization. A 3D particle model is computationally expensive, even with adaptive mesh refinement and adaptive particle control. As an alternative, we have developed a framework for plasma fluid simulations in 2D and 3D on adaptively refined grids. Electrodes and dielectric surfaces can be included. We can now perform quick tests in 2D, and study problems that could not be tackled before in 3D.

1. Introduction

Computer simulations can help to understand discharges for which we do not have a suitable theoretical description. Compared to ‘real’ experiments, numerical simulations have some advantages, e.g.: one can decide what physics (not) to include, one has complete information about the system and one can perform simulations under conditions that are experimentally hard to realize. On the other hand performing simulations can be challenging, because computers are much less powerful than nature itself. It is often necessary to use simpler, approximate models, which have to be validated by experiments. Simulation and experiment should therefore go hand-in-hand.

Here, we will focus on the modelling of nanosecond pulsed discharges. In such discharges the electron energy can be controlled quite well, which can be interesting for applications such as the production of radicals [1,2]. Space charge effects often control the development of these discharges, so that they behave non-linearly. This complicates the development of both theory and simulations.

Below, we first give a brief introduction to the modelling of nanosecond pulsed discharges. Then we present two studies performed with a 3D particle model: the inception of discharges near a positive needle electrode in nitrogen/oxygen mixtures and the simulation of laser guiding. Particle simulations are computationally expensive, especially in 3D. The last part of this paper describes a framework that we have developed for plasma fluid simulations in 2D and 3D.

2. Modelling of nanosecond pulsed discharges

Even though modern computers are quite powerful, one quickly runs into their limitations with computational models. This is especially true when performing time-dependent discharge simulations in 3D. Therefore, making the right approximations is

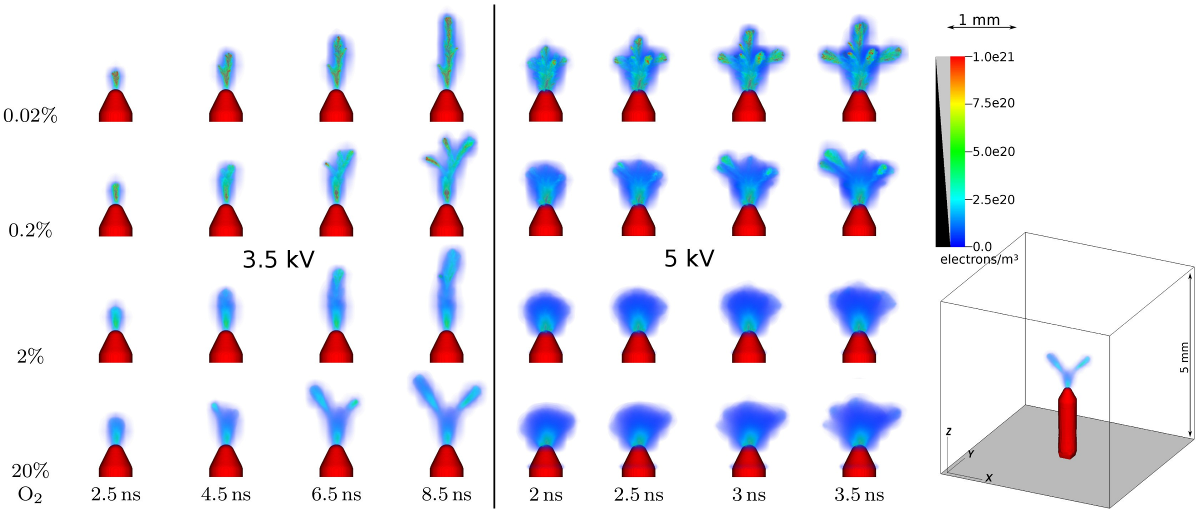

Figure 1: 3D Particle simulations of the inception of discharges near a positive needle electrode. Left: electrode voltage 3.5 kV, right: 5 kV. The background gas is nitrogen with oxygen (percentage indicates on the left), at 1 bar. The simulation domain is shown on the right.

essential. These are some of the approximations that we typically use for gas discharge simulations:

1. The gas can be treated as a constant background (no turbulence or heating) and is weakly ionized.
2. On nanosecond time scales, ion motion and most chemical reactions can be ignored.
3. The electric field is calculated in the electrostatic approximation.

To model the development of streamer discharges at atmospheric pressure, a grid spacing of a few micrometer is typically required within the ionization front. To make 3D simulations feasible, we use adaptive mesh refinement: different parts of the domain have a different grid spacing. A major challenge has been to efficiently solve Poisson's equation on such an adaptive mesh:

$$\nabla\cdot(\epsilon\nabla\varphi)=\rho.$$

3. 3D Particle model

In recent years, we have developed a particle-in-cell, Monte Carlo collision model, in which electrons are tracked as particles. Besides the adaptive mesh refinement mentioned above, we also investigated methods for changing the weights of the simulation particles [3]. A 3D particle model is computationally expensive, but allows one to study effects of electron density fluctuations, such as the breaking up of an inception cloud or the branching of a streamer.

3.1 Inception near a positive needle electrode

When a high voltage is suddenly applied to a sharp electrode, a so-called *inception cloud* can form [4]. We have investigated the formation of such inception clouds with 3D particle simulations, in different nitrogen/oxygen mixtures. In figure 1, results are shown for 3.5 and 5 kV. At 5 kV, the formation of a ionized cloud is visible with 2% or 20% oxygen, but not with 0.02% oxygen. The discharges with more oxygen are smoother because there is more photoionization around them.

3.2 Guiding streamers with laser pre-ionization

Streamers usually propagate along electric field lines. However, it was demonstrated in [5] that streamers can be guided in a different direction by weak pre-ionization from a laser. With the 3D particle model, we have performed simulations to investigate this guiding, see figure 2.

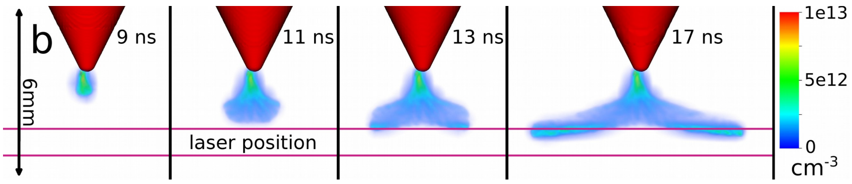

Figure 2: 3D Particle simulations of laser guiding. Between the purple line, weak laser pre-ionization was initially present. Nitrogen with 10 ppm oxygen, 133 mbar. This is part of a figure from [5].

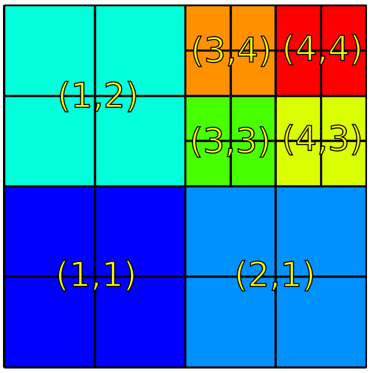

Figure 3: A quadtree grid

4. AFiVO: plasma fluid models

In plasma fluid models, the electrons are described as a density. This approximation makes them computationally cheaper than particle models. We have created AFiVO, a framework that can be used for plasma fluid simulations on adaptively refined meshes in 2D and 3D. So-called quadtree/octree grids are used, see figure 3. The included multigrid solver (for Poisson's equation) supports the inclusion of electrodes and dielectric surfaces. Furthermore, we have also implemented a Monte Carlo algorithm for photoionization.

Since AFiVO was designed with performance in mind, 2D simulations (Cartesian or cylindrical symmetry) can often be performed in a couple of minutes, allowing for interactive exploration. We are also pushing the borders of what is possible in 3D simulations.

We would like to emphasize that AFiVO and the plasma models that we have implemented are fully open source (see *http://cwimd.nl*), and that we are interested in collaborations.

5. References

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