Simulation of High-Frequency Atmospheric Gas Discharges

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The generation of atmospheric gas discharges is an important concern in many industrial applications. We are investigating here a special type of high-frequency atmospheric gas discharge. The results of modelling the breakdown mechanism and of the development phase of the discharge will be presented. Furthermore we will show first numerical results.

1 Modelling

In the industrial process under investigation a plasma is used to achieve a modification of the product surface through the generated reactive particles and intense UV radiation. In order to achieve the necessary throughput the discharge is required to work under ambient pressure air. Furthermore since the product is in the path of the discharge, it has to operate with high frequency (≈ 10 MHz) electric fields. In order to gain better control of this kind of discharge an attempt is made by the authors to simulate the prevalent processes and determine fundamental plasma parameters.

In the modelling of the discharge two essentially distinct phases have to be distinguished. In the first phase, the breakdown, a fast travelling ionization wave connects both electrodes and forms a conducting channel between them. In the following phase this channel is heated and expands under the action of the high frequency electrical field.

Our main interest currently concerns the first phase in which the basis of the discharge is established. This phase usually begins with the generation of some seed electrons by various external processes like cosmic rays or UV radiation. The electrons are accelerated under the action of the electric field and produce an increasing number of free charges by impact collision. When this electron avalanche has reached a sufficiently high electron density and size it undergoes a transition to a self-propagating streamer. This streamer is able to produce its own accelerating field and through irradiation enough seed electrons in front of itself so as to cross the discharge gap at very high speeds [1].

The modelling of the electrical field $\mathbf{E}$ started with the full Maxwell equations. In the breakdown phase, however, the effective electrical current is very low and thus the magnetic field could be assumed to vanish ($\mathbf{B} \approx 0$), which was also assumed for the variation of the magnetic field ($\partial\mathbf{B}/\partial t \approx 0$). Inserting those assumptions into the Maxwell equations leads to the electrostatic approximation for the electric potential Φ and electrical field $\mathbf{E}$ given by

$$\Delta\Phi = \rho/\epsilon_0 = \sum_\alpha Z_\alpha n_\alpha/\epsilon_0 \qquad\qquad \mathbf{E} = -\nabla\Phi, \tag{1}$$

where ρ is the charge density and Z_α and n_α are the charges and number densities of the various species α.

For the particle transport model it was neccessary to limit the number of different particles to be simulated. In a discharge under atmospheric pressure air about 30 different species (i.e. atoms, positive and negative ions, molecular compounds etc.) and over 250 reactions have to be accounted for. In this first model we neglected any higher ionized particles and only incorporated electrons (e), singly positive (p) and singly negative ions (n). The different ion species were unified into one using averaged reaction and transport coefficients. The neutral density changes only marginally during the initial breakdown and was thus taken as constant. Furthermore excited and metastable states were neglected.

The transport of particles was modelled in the usual drift diffusion model with local field approximation. This means inertia effects as well as energy and momentum transport are neglected. The speed of the electrons and thus the transport coefficients are completely determined by the local electrical field. The transport for each species $\alpha \in \{\mathrm{e}, \mathrm{p}, \mathrm{n}\}$ is then given by the general transport equation

$$\frac{\partial n_\alpha}{\partial t} + \nabla \cdot (\mathbf{u}_\alpha n_\alpha - D_\alpha \nabla n_\alpha) = G_\alpha(\{n_\beta\}, \{u_\beta\}), \tag{2}$$

where D_α is the diffusivity and G_α is the production term of species α, which may depend on the densities n_β and velocities u_β of all other species β. The velocities of the charged species are proportional to the electrical field $\mathbf{u}_\alpha = \mu_\alpha \mathbf{E}$, where μ_α is the mobility of the species, which is in general a function of the reduced electrical field E/n. Mobility and diffusivity were taken from fitted experimental data [2].

The production terms G_α are composed of particle generation, transfer and loss processes. The generation processes taken into account are electron impact ionization ($e + A \to A^+ + 2e$), for the avalanche processes and photo ionization ($h\nu + A \to A^+ + e$) for the main streamer propagation mechanism. For the transfer processes electron attachment ($e + A + N \to A^- + N$)

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is considered since it plays an important role in discharges in attaching gases like O_2. Losses result from the recombination of charged particles, where we consider here electron-ion recombination ($e + A^- + N \rightarrow A + N$) and ion-ion recombination ($A^- + B^+ \rightarrow A + B$). The rate coeffi cients for the mentioned processes are given by:

$$S_{\mathrm{i}} = \alpha(E/n)u_e n_e \qquad S_{\mathrm{ph}} = \text{const.} \qquad T_{\mathrm{att}} = \eta(E/n)u_e n_e \qquad L_{\mathrm{ep}} = \beta(E/n)n_e n_p \qquad L_{\mathrm{pn}} = \beta_2(E/n)n_p n_n. \tag{3}$$

2 Implementation and results

For the numerical solution of the coupled system equations (1) and (2) have two be solved in each time step. For the spatial discretization a fi nite elements approach was chosen. The discretization of the Poisson equation is fairly standard within this framework, whereas for the transport equation some form of stabilization had to be employed. With the well-known SUPG method the test functions are modifi ed in the direction of advection leading to

$$\mathrm{M}^\alpha_{ij} = (\phi_j, \phi_i + \frac{\delta h}{\|\mathbf{u}\|}\mathbf{u}\nabla\phi_i) \quad \mathrm{K}^\alpha_{ij} = (\mathrm{D}^\alpha\nabla\phi_j, \nabla\phi_i) + (\mathbf{u}^\alpha \cdot \nabla\phi_j, \phi_i + \frac{\delta h}{\|\mathbf{u}\|}\mathbf{u}\nabla\phi_i) \quad \mathrm{g}^\alpha_i = (G_\alpha, \phi_i + \frac{\delta h}{\|\mathbf{u}\|}\mathbf{u}\nabla\phi_i),$$

where M denotes the mass matrix, K the stiffness matrix and g the right hand side. The drift velocity is calculated from $\mathbf{u} = \mu \sum_k \Phi\nabla\phi_k$ after fi rst having solved the Poisson equation (1).

The resulting system of ordinary differential equations for the vector of nodal unknowns $\mathbf{u}^\alpha$ is given by $\mathrm{M}^\alpha(t)\dot{\mathbf{u}}^\alpha + \mathrm{K}^\alpha(t)\mathbf{u}^\alpha = \mathbf{g}^\alpha(t)$. This system of ODEs is solved by a θ-method with $\theta = 1/2$ whereby the implicit part was only applied to the $\mathbf{u}$ terms while the matrices and right hand side were kept fi xed from the beginning of the time step:

$$(\mathrm{M}^\alpha_n + \Delta t\theta\mathrm{K}^\alpha_n)\mathbf{u}^\alpha_{n+1} = (\mathrm{M}^\alpha_n - \Delta t(1-\theta)\mathrm{K}^\alpha_n)\mathbf{u}^\alpha_n + \Delta t\mathbf{g}^\alpha_n \tag{4}$$

The scheme was implemented using the Deal.II library [3] with bilinear quadrilateral elements and adaptive local refi nement. As refi nement indicator a local error estimator based on work by Kelly et al. provided by the library was employed. The resulting linear systems were solved using a CG method with SSOR preconditioner for the Poisson problem and with a BiCGStab and SOR preconditioner for the transport problem.

The geometry was only that section of the full discharge gap where the electron avalanche is started. Due to the initial cylindrical symmetry a cylinder of radius 2 mm and height 15 mm was chosen. On the top and bottom Dirichlet boundary conditions were chosen to account for the applied external fi eld. At r=0 symmetry boundary conditions had to be applied and on the outer boundary homogeneous Neumann boundary conditions fi t best the free fi eld conditions. The initial state was chosen to be an equally normal distributed density of electrons and positive ions, such that charge neutrality was satisfi ed. Time steps where chosen in accordance with typical streamer velocities and the given mesh spacing to be $1\mathrm{ns}$.

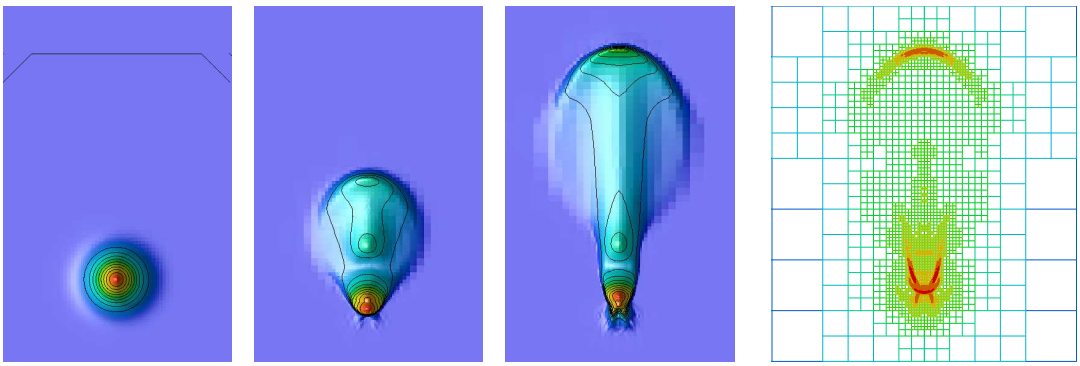

Fig. 1 Evolution of the electron density n_e after $t = 10\mathrm{ns}$, $20\mathrm{ns}$ and $30\mathrm{ns}$ (left). The refined grid after $t = 30\mathrm{ns}$ (right).

Results for the evolution of the electron density are shown in fi g. 1. It can be seen how the initial normal distributed electron distribution is accelerated in y direction creating more electrons on its path. Further the steepening of ionization front can be observed. The current scheme unfortunately the becomes unstable after about $t \approx 60\mathrm{ns}$, so that the transition to the streamer mechanism cannot be clearly observed.

To avoid the instabilities the use of conservative and positivity conserving schemes is considered. Especially discontinuous Galerkin (DG) or flux corrected transport (FCT) methods seem to be well suited [4]. Further it will be seen, whether the time stepping scheme has to be adjusted.

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