A multi-stage approach for DBD modelling

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Abstract. A multi-stage numerical technique for the assessment of Dielectric Barrier Discharge (DBD) in atmospheric pressure air is presented. The model is conceived to work on the characteristic times of heavy species. The dynamics of the heavy species are computed with a 2D drift-drift diffusion model, based on a Finite Volume approach. A non-linear Poisson solver is employed for the calculation of the electric field produced by the heavy species and electrons distributions. This latter is assumed to instantly follow the Boltzmann distribution, allowing limiting the transport model to the heavy species. The main chemical reactions taking place during the discharge process between the air chemical constituents are included in the model, whereas the effects of the impact ionization are accounted by means of a simplified 1D streamer model.

1. Introduction
Over the last few decades, great attention has raised around the understanding and modelling of DBD devices and actuators, due to their many industrial and technological applications. Nevertheless, this task still represent a great challenge, mainly due to the wide differences in time and length scales of the involved physical phenomena. In this work a novel multi-stage numerical methodology is proposed, aiming to assess the regime of the main charged species (\(N_2^+, O_2^+, O_2^-, e^-\)) constituting an atmospheric pressure air plasma. The transport of the heavy species (i.e., positive and negative ions) is modelled by means of drift diffusion equations. The electrons, due to their higher electric mobility and diffusion coefficient, are assumed to instantaneously adapt to the charge density of the heavy species, following the Boltzmann distribution. Thus, the electrostatics is governed by a non-linear formulation of the Poisson’s equation. As a result of this, the time-step for the solution of the drift-diffusion equation has to follow the dynamics of the heavy species, that are nearly three orders of magnitude higher compared to the one of the electrons. This leads to great beneficial effects in terms of computational times, in comparison to existing approaches based on formulations including the drift-diffusion equation for the electrons [1, 2, 3, 4]. Streamers, whose dynamics are governed by the characteristic times of the electron drift and of the Townsend avalanche ionization, are treated by means of a simplified one-dimensional model. The purpose of this latter is not to describe in detail the evolution of a streamer, but rather to provide an estimate of the species produced by the streamer itself during his lifetime. In addition, the presence of a dielectric interface between the electrodes and the air gap has also been taken into account by adding an interface charge density accumulation process, that can occur due to fluxes of positive ions or electrons on the dielectric surface. Nevertheless, the global electric charge neutrality in the air gap is still achieved at each time step by enforcing a dedicated condition in the context of the electron density computation.
2. Physical model

2.1. Drift-diffusion

An atmospheric pressure air plasma has been considered, with 2 neutral species and 4 charged species, i.e., \( \text{N}_2, \text{O}_2 \) and \( \text{N}_2^+, \text{O}_2^+, \text{O}_2^- \), \( e^- \) respectively. Since the present work is aimed at a description of the discharge in the heavy particles time scale, the foundation of the model is constituted by the drift diffusion equations for ions:

\[
\frac{\partial N_s}{\partial t} + \nabla \cdot \Gamma_s = \Omega_s + \Omega_{\text{stream},s},
\]

in which the local quantities \( N_s \) and \( \Gamma_s \) represent the number density and the flux for the \( s \)-th ionic species, respectively. The right-hand side term in (1) is constituted by the two terms \( \Omega_s \) and \( \Omega_{\text{stream},s} \). The source term \( \Omega_s \) takes into account of the elementary processes in the plasma (i.e., thermal ionizations, recombinations, attachments), except for the Thownsend avalanche effect, that is included in \( \Omega_{\text{stream},s} \). This latter takes into account the species production due to the formation of streamers during the discharge. The flux \( \Gamma_s \) in (1) can be rewritten as the combination of a diffusion term and a convective term, as:

\[
\Gamma_s = -D_s \nabla N_s + \langle v_s \rangle N_i,
\]

where \( D_s \) is the diffusion coefficient of the \( s \)-th species. The average drift velocity \( \langle v \rangle_s = \mu_s E \) is defined via the product between the electric field and the electrical mobility of the species. The behaviour of \( E \), which on its turn depends on the distribution of the charge carriers, is described by a non-linear Poisson solver, described in detail in Sec. 2.2.

2.2. Electrostatics

The electrostatic formulation is used for describing the electric field behaviour. Thus, the electric field is assumed to be conservative. The governing equation in the discharge region then is given by Poisson’s equation:

\[
\nabla^2 \varphi = -\frac{\rho}{\epsilon_0},
\]

where \( \rho \) is the electric charge volume density, and \( \epsilon_0 \) the vacuum dielectric constant. The charge density \( \rho \) depends on the space distribution of the ions and electrons number densities. The heavy particles behaviour is described by the drift diffusion equations (1). Electrons, being much faster than ions, are considered to adapt instantaneously to the local value of the electric potential, according to the Boltzmann distribution. The charge density can be finally expressed as:

\[
\rho = e \left[ N_{\text{N}_2^+} + N_{\text{O}_2^+} - N_{\text{O}_2^-} - N_{e,0} \exp \left( \frac{\varphi - \varphi_0}{T_{e,eV}} \right) \right],
\]

where \( T_{e,eV} = k_B T_e/e \) is the electron temperature in eV, \( \varphi_0 \) the electric reference potential and \( N_{e,0} \) the background electron number density. Introducing (4) in (3), one finally obtains a non-linear Poisson’s equation:

\[
\nabla^2 \varphi = -\frac{e}{\epsilon_0} \left( N_{\text{N}_2^+} + N_{\text{O}_2^+} - N_{\text{O}_2^-} \right) + \frac{eN_{e,0}}{\epsilon_0} \exp \left( \frac{\varphi - \varphi_0}{T_{e,eV}} \right).
\]

Hence, electron number density and electric potential are evaluated by means of a steady state formulation, driven by the time evolution of the heavy species.
2.3. Charge accumulation at dielectric interfaces

If a solid dielectric material is interposed between an electrode and the air gap, a surface electric charge $\rho_\Sigma$ may occasionally accumulate at the interface between the solid dielectric and the air, as shown in Fig. 1. In these cases, the electric field normal component experiences a discontinuity, which can be expressed as:

$$\epsilon_d \frac{\partial \varphi}{\partial n} \bigg|_d - \frac{\partial \varphi}{\partial n} \bigg|_p = \frac{\rho_\Sigma}{\epsilon_0}, \quad (6)$$

where $\epsilon_d$ is the relative permittivity of the dielectric, and the subscripts $d$ and $p$ designate the normal derivative on the dielectric and plasma sides of the discontinuity, respectively.

In writing (6) the normal direction is assumed to be directed from the air gap towards the dielectric surface. It should be noticed that the model described so far does not guarantee that the total electric charge in the domain is equal to zero. Indeed, the (negative) electric charge obtained by integrating over the calculation domain $V$ the electron number density provided by the Boltzmann distribution depends on the two parameters $N_{e,0}$ and $\varphi_0$, and is not necessarily equal to the sum of the (positive) electric charge due to ions and the surface charge on the plasma-dielectric interface $S$. Thus an additional constrain is added, to ensure the total charge neutrality:

$$\int_V \left[ N_{N_2^+} + N_{O_2^+} - N_{O_2^-} - N_{e,0} \exp \left( \frac{\varphi - \varphi_0}{T_{e,e} V} \right) \right] dV + \int_{S_D} \rho_\Sigma dS = 0. \quad (7)$$

The interface charge density $\rho_\Sigma$ can be produced by secondary emission due to a flux of positive ions on the dielectric surface, or by a flux of electrons. In the first case, a secondary emission event is assumed to leave a hole (i.e., a positive charge) on the dielectric surface. As a result, the time variation of $\rho_\Sigma$ is described by the following equation:

$$\frac{d\rho_\Sigma}{dt} = e \gamma \left( \mu_{N_2^+} N_{N_2^+} + \mu_{O_2^+} N_{O_2^+} \right) E_n, \quad E_n > 0, \quad (8)$$

where $\gamma$ is the secondary emission coefficient. On the other hand, an electron flux toward the dielectric wall is assumed to produce an instantaneous neutralization of holes, if they are present, or a negative charge accumulation otherwise. In both cases:

$$\frac{d\rho_\Sigma}{dt} = e \mu_e N_e E_n, \quad E_n < 0. \quad (9)$$
2.4. 1D discharge model
The model described in this paper can treat phenomena evolving with the characteristic time of
the heavy species. Thus, the formation and the evolution of a streamer can not be adequately
represented. However, streamers are a fundamental feature in DBDs, as they deliver an essential
contribution in producing ionization and charge transfer. In order to take into account the
streamers’ effect on the DBD, a simplified model was developed. The streamer is represented
by the series of a non-linear time dependent resistor with two capacitors, as shown in Fig. 2.

The electric current \( I_e \) is defined as the flux of electrons through the streamer section \( S_s \), due
to the motion impressed by the electric field:

\[
I_e = \int_{S_s} e N_e \langle v_e \rangle \cdot \hat{n} dS \approx e N_e \mu_e \frac{\Delta \phi}{L_g} S_s, \tag{10}
\]

where \( L_g \) is the air gap width and \( \Delta \phi \) is the potential drop across it. A 0.2 mm\(^2\) section \( S_s \) has
been taken, based on the calculations in [5]. The electrons number density in the streamer is
governed by the equation:

\[
\frac{dN_e}{dt} = \alpha \frac{I_e}{e S_s}, \tag{11}
\]

where \( \alpha \) is the sum of the Townsend coefficients for \( N_2 \) and \( O_2 \). Defining the resistance
\( R_s (N_e, t) \) as:

\[
R_s (N_e, t) = \frac{L_g}{e \mu_e N_e S_s}, \tag{12}
\]

one may write from (10):

\[
I_e = \frac{V - (V_{C1} + V_{C2})}{R_s (N_e, t)} \tag{13}
\]

where \( V \), \( V_{C1} \), and \( V_{C2} \) are the total voltage between the electrodes, and the voltages applied to
the two capacitors \( C_1 \), and \( C_2 \), respectively. The capacitors represent the ability of the electric
charge carried by the streamer to deposit on the surface of the two dielectric interfaces, and
their capacitance values can be selected in order to match the experimental available data. The
constitutive law for each of them is:

\[
I_e = C_i \frac{dV_{Ci}}{dt}, \quad i = 1, 2 \tag{14}
\]

Introducing (13) in (11) and (14), one finally obtain a system of differential equations in the
unknowns \( N_e \), \( V_{C1} \), and \( V_{C2} \):

\[
\begin{cases}
\frac{dV_{Ci}}{dt} = \frac{1}{R_s (N_e, t)} C_i [V - (V_{C1} + V_{C2})], \quad i = 1, 2 \\
\frac{dN_e}{dt} = \frac{\alpha}{e S_s R_s (N_e, t)} [V - (V_{C1} + V_{C2})],
\end{cases} \tag{15}
\]

The solution of the system (15) gives an estimation of the total number of ions produced
by the end of the streamer (that is, when the \( I_e \) extinguishes). These number will be used to
evaluate the source terms \( \Omega_{stream,s} \) in (1).

2.5. Plasma kinetics
The source terms \( \Omega_s \) (with \( s = N_2^+, O_2^+, O_2^- \)) on the right-hand side are determined on the basis
of the reactions considered in the model. In this work, the considered elementary processes are
listed in Tab. 1, and details regarding the reaction rates can be found in [6]. It should be noted
that the impact ionization is not included in Tab. 1, since it has already taken into account by
means of the streamer model.
The problem formulated in the previous section has been numerically solved using a two dimensional Finite Volume (FV) approach. A discretization of the physical domain is performed through a subdivision in cells. For the sake of simplicity, an evenly spaced mesh will be assumed here onwards, although the method can be easily generalized to more complex mesh topologies. Referring to Fig. 3, the drift diffusion equation for the generic interface surface $\Delta S_{s,edge}$ belonging to the boundary $\partial (\Delta V)$ of the control volume is due to a diffusive and a drift contribution. The diffusive flux is discretized by means of a centred difference formula, while the drift component is expressed by means of a first order upwind scheme. Referring to the interface between the grid points $i$ and $est$, the flux can be expressed as:

$$\Gamma_{s,edge} = D_s \frac{N_{s,i} - N_{s,est}}{\Delta x} + \left[ N_{s,i} v_{s,+} + N_{s,est} v_{s,-} \right],$$

(17)

in which:

$$\begin{cases} v_{s,+} = \max \left[ 0, \mu_s E_{n,i} \right] \\ v_{s,-} = \min \left[ 0, \mu_s E_{n,E} \right] \end{cases},$$

where $E_n = E \cdot \hat{n}$ is the electric field normal component to the considered interface, with the normal unit vector $\hat{n}$ pointing outward the control volume $\Delta V$.

The Courant-Friedrichs-Lewy (CFL) condition requires that for the scheme (16) to be stable, the time step $\Delta t$ is subject to the following constraint:

$$\Delta t < \min \left[ \frac{1}{|\mu_s E/min(\Delta | + |D_s/(2\Delta^2)|} \right]$$

(18)

with:

$$\Delta = \min(\Delta x, \Delta y)$$
Figure 3. Finite volume approach for the nodes inside the plasma region

Figure 4. Finite volume approach at one of the dielectric interfaces

3.2. 2D non-linear Poisson solver

A similar approach is used to treat the governing equation of electrostatics (5). The discretization process yields a system of non linear algebraic equations:

\[
[K] \{\varphi\} - \{r (\{\varphi\}, \varphi_0)\} = 0. \tag{19}
\]

Referring to Fig. 4, the discrete equation in (19) for a generic internal point \(i\) can be written as:

\[
\frac{\varphi_{sth}}{\Delta_y^2} + \frac{\varphi_{wst}}{\Delta_x^2} - 2 \left( \frac{1}{\Delta_x^2} + \frac{1}{\Delta_y^2} \right) \varphi_i + \frac{\varphi_{est}}{\Delta_x^2} + \frac{\varphi_{sth}}{\Delta_y^2} + \frac{\rho_i}{\epsilon_0} = 0, \tag{20}
\]

where, according to (4), the charge density at the point \(i\) is given by:

\[
\rho_i = e \left[ \sum_s N_{s,i} - \exp \left( \frac{\varphi_i - \varphi_0}{T_e eV} \right) \right]. \tag{21}
\]

At the interface between the DBD and the dielectric, the electrostatic equation at the point \(i\) (Fig. 4) can be discretized as:

\[
\left( \frac{d \epsilon_d}{\Delta_y} + 1 \right) \frac{\varphi_{wst}}{\Delta_x^2} - 2 \left( \frac{d \epsilon_d}{\Delta_y} + 1 \right) \frac{1}{\Delta_x^2} + \frac{2}{\Delta_y^2} \right) \varphi_i + \left( \frac{d \epsilon_d}{\Delta_y} + 1 \right) \frac{\varphi_{est}}{\Delta_x^2} + \frac{\varphi_{nth}}{\Delta_y^2} + \frac{\rho_i}{\epsilon_0} + \frac{\rho_{\Sigma,i}}{\epsilon_0} + \frac{2 \epsilon_d}{d \Delta_y} \varphi_{appl} = 0. \tag{22}
\]

In (22), the effect of a dielectric with a thickness \(d\) between the electrode (with a \(\varphi_{appl}\) applied voltage) and the DBD is taken into account, as well as the surface charge \(\rho_{\Sigma,i}\) at the \(i\)-th mesh point.

A Newton-Raphson solver has been used for the non-linear system (19). At the given \(n\)-th iteration, the variation \(\{\Delta \varphi\}^{(n)}\) that the solution \(\{\varphi\}^{(n)}\) must undergo to evolve on to the next step is obtained by solving the linear system:

\[
[J] \{\Delta \varphi\}^{(n)} = - [K] \{\varphi\}^{(n)} + \{r (\{\varphi\}^{(n)}, \varphi_0)\}. \tag{23}
\]

Here, the jacobian matrix \(J\) of the system (19) is given by:

\[
[J] = [K] + [D], \tag{24}
\]
where \([D]\) is a diagonal matrix, whose non-zero entries at the \(i\)-th row is:
\[
d_{i,i} = \frac{1}{\epsilon_0} \frac{\partial \rho_i}{\partial \varphi_i} = -\frac{e}{\epsilon_0 T_e eV} \exp \left( \frac{\varphi_i - \varphi_0}{T_e eV} \right).
\]

The solution of the system (19) yields the distribution of the electric potential as a function of the reference potential \(\varphi_0\). This quantity is adjusted to meet the neutrality of the total electric charge constraint (7) by means of an iterative solver running externally to the Newton-Raphson solver. In carrying out this task, the bisector method showed good reliability and robustness.

3.3. Source terms
At the \(k\)-th time step, a semi implicit approach was adopted to compute the array \(\{\Delta N_i\}_{\Omega_i}^{(k)}\), whose generic entry \(\Delta N_{i,j}^{(k)}\) has been defined above in (16). Let’s define \(\Omega_s^{(k)}\) as the local jacobian matrix of the source terms at point \(i\). The generic term \(\Omega_s^{(k)}\) in \(\Omega_s^{(k)}\) is defined as the derivative of the source term \(\Omega_s^{(k)}\) of the species \(s\) at the point \(i\), with respect to the number density \(N_{w,i}^{(k)}\), referred to the species \(w\) at the point \(i\). The source term array can be now linearized in the form \(\Omega_s^{(k)} = \Omega_s^{(k)} + [O^{(k)}(i,j)]\Delta t/2\). The increment array \(\{\Delta N_i\}_{\Omega_i}^{(k)}\) in the \(\Delta t\) time interval due the the chemical reactions is found by solving the system:
\[
[M] \{\Delta N_i\}_{\Omega_i}^{(k)} = \{\Omega_s\}^{(k)} \Delta t,
\]
where:
\[
[M] = [I] - \frac{1}{2}[O^{(k)}] \Delta t.
\]

4. Results and Discussion
4.1. Test-case description
In order to verify the correct behaviour of the presented numerical model, the physical conditions taking place during a DBD in air were simulated on a rectangular domain of size \(0.8 \times 4.0\ mm^2\), which has been discretized with a uniform bi-dimensional grid consisting of \(111 \times 61\) nodes. The assumption of a 2D approximation is justified by the geometric uniformity of the configuration in the axial direction. Parallel plates electrodes are positioned at the two ends of the short edges of the rectangle, separated from the air gap by a \(0.5\ mm\) thick layer of teflon \((\epsilon_d = 2.1, \gamma = 0.1)\). A sinusoidal voltage of amplitude \(1\ kV\) and frequency \(50\ kHz\) has been enforced between the two electrodes, in order to represent the voltage source employed for the plasma generation. The test has been conducted in atmospheric pressure, hence assuming a constant number density of \(1.88 \cdot 10^{25}\ m^{-3}\) and \(0.63 \cdot 10^{25}\ m^{-3}\) for the \(N_2\) and \(O_2\) distributions respectively. For this test, the simplified streamer model has been deactivated. The temperatures of the electrons and the heavy species have been set to 20000 \(K\) and 400 \(K\) respectively, whereas the initial number densities of the heavy species were \(0.75 \cdot 10^{15}\ m^{-3}\), \(0.25 \cdot 10^{15}\ m^{-3}\) and \(0.9 \cdot 10^{15}\ m^{-3}\) for \(N_2^+\), \(O_2^-\) and \(O_2^+\) respectively. Ion mobilities are taken from [6], while the diffusion coefficients are evaluated using the Einstein relation, i.e., \(D_s = \mu_s T_e v\), where \(T_e v = k_B T/e\) is the heavy species temperature in \(eV\). The high \(O_2^-\) initial density that has been assumed serves the purpose of starting the simulation with physical conditions close to global charge neutrality. Figure 5 shows the electric potential at one side of the air gap and the computed time-step for each iteration of the simulation. The electric potential does not correspond to the applied electrode potential, due to the voltage drop across the teflon layer and the surface electric charge accumulation mechanism. As one can see, the obtained time-step decreases for raising applied voltages. This is due to the higher values of drift velocities of charged species and of the diffusion coefficients dependency from the local electric field strength. Here the details of the obtained charged species

\[
\text{evaluated using the Einstein relation, i.e., } D_s = \mu_s T_e v,\text{ where } T_e v = k_B T/e = \text{the heavy species temperature in eV}.\text{ The high } O_2^-\text{ initial density that has been assumed serves the purpose of starting the simulation with physical conditions close to global charge neutrality. Figure 5 shows the electric potential at one side of the air gap and the computed time-step for each iteration of the simulation. The electric potential does not correspond to the applied electrode potential, due to the voltage drop across the teflon layer and the surface electric charge accumulation mechanism. As one can see, the obtained time-step decreases for raising applied voltages. This is due to the higher values of drift velocities of charged species and of the diffusion coefficients dependency from the local electric field strength. Here the details of the obtained charged species}
\]
4.2. Low applied voltage - 725th iteration (4.89 µs)

After 4.89 µs, upon reaching the 725th iteration, the voltage applied to the left-hand side of the air gap shown in Fig. 6 has dropped to almost −10 V, having started from 1 kV. The right-hand side of the gap has now a slightly higher potential and hence is repulsing the positive ions. However, as shown in Fig. 7 and 8 respectively, the heavy species distributions still correspond to an opposite polarity. This lag in the adaptation of the heavy species distribution to the external electric field is explained by the fact that at the 725th iteration the polarity inversion has just took place, and by recalling that the drift speed is given by the product of the (at this point low) electric field and the electrical mobility. The distribution of the electron number density is shown in Fig. 9. As discussed in Sec. 2.2, these have been considered to instantaneously adapt to the electric field distribution. This assumption yields a consistent behaviour of this species, which is expected to react much more quickly to the external electric field due to the higher electric mobility with respect to the heavy species. It is worth pointing out that the low external electric field allows noticing the effects of the space charge on the electric potential distribution (Fig. 6), which is deformed in the central part of the gap.

4.3. High applied voltage - 1200th iteration (8.21 µs)

This other relevant moment of the performed simulation takes place after 8.21 µs, at the 1200th iteration, when the maximum of the sinusoidal applied voltage is almost reached. As shown in Fig. 10, the right-hand side of the gap is the positive electrode, and so has been for almost a quarter of cycle. Hence, a higher density of electrons can be found close to the anode (see Fig. 13). Regarding the positive ions, Fig. 11 shows two steps, due to a combination of the drift towards the negative pole and the effects of the ionization, which depends on the local electric field value. In contrast to the situation shown at the 725th iteration, now the combination of higher electric field values and a longer evolution time allows the effects of the drift to be relevant.
Figure 6. Electric potential distribution after 4.89µs (725th iteration).

Figure 7. $N_2^+$ number density after 4.89µs (725th iteration).

Figure 8. $O_2^-$ number density after 4.89µs (725th iteration).

Figure 9. Electron number density after 4.89µs (725th iteration).

also for the $O_2^-$ distribution, shown in Fig. 12. As one can see on the left-hand side, the negative ions are drifting towards the positive pole, where a considerable generation is taking place due to electron-oxygen attachment reactions.

5. Conclusions
A multi-step approach has been presented for the numerical modelling of air pressure DBDs and their fluid dynamic effects on the charged species, aiming to use the drift-diffusion approximation only for the heavy species. As expected, the CFL stability condition is satisfied by notably larger time steps with respect to other explicit DBD models where the electrons are included in the drift-diffusion equation. The provided simulation results are consistent with the expected physical behaviour of both the heavy species and the electrons. In particular, the results proof that the externally enforced electric potential is able to generate a drift of the heavy species
and electrons, leading to a charge density distribution which is in turn creates distortions of the electric potential distribution in the bulk of the plasma. The provided results have been obtained with a few hours long computation on a single physical core, therefore leaving room for further optimization and parallelization.

6. References
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