A Python-based Adaptive Mesh Solver for Drift-Diffusion Modelling of Streamer Discharges

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***Abstract*—Streamer discharges are fast-moving plasma fronts which can be formed in gases stressed with a sufficiently high electric field and represent a crucial stage in the evolution of an electrical breakdown. Recently, the investigation of streamer discharges has regained significant interest due to the numerous basic processes and practical applications that require their understanding. These include geophysical processes such as sprite development; gas-insulated system design for power and pulsed power equipment; and a growing number of industrial and environmental applications. Computational advances have provided deep insights into some critically important properties and characteristics of streamers, yet simulations remain highly nontrivial due to the multiscale nature of the phenomena. In the present study, the drift-diffusion approximation for the computational modelling of streamers in gases has been implemented using the open-source finite-element platform FEniCS. Equipped with a Python interface to a high-speed C++ backend, the use of FEniCS greatly improves usability by requiring less computational expertise, yet with little compromise on solver efficiency. The accuracy of the code has been verified through comparison with six other codes from a recently published benchmarking study. Thus, we conclude that the FEniCS platform may be a highly suitable alternative for furthering the study of streamer discharges.**

***Index Terms*—streamer discharges, simulation, finite element, nonthermal plasma**

I. Introduction

Streamers are a type of ionisation wave which propagate in gas, generated under sufficiently intensive electrical stress. Originally described by Meek [1], electron avalanches initiated in the gas eventually accumulate sufficient space charge to cause significant redistribution of the background electric field. The high degree of space charge induced field enhancement leads to intensive ionisation at the streamer head, which eventually evolves into a self-sustained propagation of an ionisation front, leaving behind a thin and electrically screened channel filled with non-thermal plasma. Besides being a critically important pre-breakdown process in gaseous dielectrics, streamers and streamer discharges have become of interest for a number of applications including decontamination and air cleaning [2], surface treatment [3], and chemical processing such as ozone production [4]. Therefore, deeper understanding of the processes behind streamer development is currently of high academic and industrial importance. The conditions under which streamers can form and their subsequent propagation characteristics are highly dependent on a wide range of factors, including electron transport parameters in gas, energising voltage, electrode geometry, gas density, photoionization processes, and more. The inherent complexity of streamer dynamics renders them difficult to characterise experimentally without sophisticated equipment and instrumentation. However, recent advances in computational power have led to an increased interest in the numerical modelling of the streamer discharge phenomena.

A historical lack of accessible high-performance computing has meant that plasma and streamer simulations are a relatively new innovation. While processing power remains far from able to readily simulate all possible interactions which may contribute to the development of a discharge, simulations using simplified models have been made possible on mid- to high-end desktop hardware within a reasonable timeframe. This has therefore increased the accessibility of streamer modelling, which may previously have only been available to facilities with supercomputing capabilities.

II. Mathematical Model

A. Drift-Diffusion Equations

To track the spatial and temporal evolution of a streamer discharge, the commonly used drift-diffusion approximation was employed in this study. Derived from the zero-order moment of the Boltzmann equation [5], the drift-diffusion model assumes that the plasma is weakly ionized, and that charge densities are sufficiently high to be considered a continuum. In its most general form, the drift-diffusion equation for a charged species i may be written as:

$$\frac{\partial n_i}{\partial t} + \nabla \cdot \left(\mathrm{sgn}(q_i) n_i \mu_i \vec{\mathbf{E}} \right) - \nabla \cdot (D_i \nabla n_i) = S_i \qquad (1)$$

where n is the number density in m^{-3}, q is the electric charge in coulombs, μ is the charge mobility in $m^2V^{-1}s^{-1}$, and D is the diffusion coefficient in m^2s^{-1} of the charged species i. $\vec{\mathbf{E}}$ is the electric field in Vm^{-1}, while sgn() is the sign function. S_i represents the sum of all sources and sinks from the i-th species, which may include, for example, impact ionisation, attachment, photoionization, recombination, and more. The charge densities are coupled to the electric field through the Poisson equation under the electrostatic assumption:

$$\nabla \cdot (\varepsilon \nabla \varphi) = -\rho \qquad (2)$$

$$\vec{\mathbf{E}} = -\nabla\varphi \tag{3}$$

where, ε is the permittivity of the medium in Fm^{-1}, φ is the electric potential in Volts, and ρ is the net charge density in Cm^{-3}, summed over all charged species which are under consideration. The self-consistent solution of (2) and (3) with N equations in the form of (1) yields the solution to n_i and $\vec{\mathbf{E}}$ which are the main quantities of interest, where N is the total number of charged species which are present in the model.

B. Photoionization

In the case of positive (cathode-directed) streamers, a source of electrons ahead of the streamer head is necessary for its sustained propagation [6]. In gases such as air, this is widely thought to be photoionization, where the de-excitation of excited nitrogen molecules emits photons of wavelength (98-102.5) nm which can ionise oxygen molecules [7]. Aside from atmospheric air, the role photoionization plays in other gases is currently not well known. However, as this study focuses mainly on air, photoionization for oxygen-nitrogen mixtures through Zheleznyak's model [8] is included. The 3-term Helmholtz approximation for the photoelectron source term S_{ph} due to the impact ionisation source $S_\alpha = \alpha\mu_e n_e|\vec{\mathbf{E}}|$ is coupled to (1) and (2), which can be written:

$$\nabla^2 S_{ph,j} - (p_{O_2}\lambda_j)^2 S_{ph,j} = -\left(A_j p_{O_2}^2 \frac{p_q}{p+p_q}\xi\frac{\nu_u}{\nu_i}\right) S_\alpha \tag{4}$$

$$S_{ph} = \sum_j S_{ph,j} \tag{5}$$

for j = 1, 2, 3. Here, p, p_q, and p_{O_2} are the total gas pressure, collisional quenching pressure of nitrogen, and partial pressure of oxygen in Torr, respectively. ν_u is the impact excitation frequency for level u, and ν_i is the ionization frequency in s^{-1}, while ξ is the photoionization efficiency [9]. Finally, λ_j and A_j are fitting parameters for the j-th equation with dimensions m^{-1}Torr^{-1} and m^{-2}Torr^{-2}, respectively.

III. Implementation

Analytical solutions to the system of equations formed by (1)-(4) are limited to a few highly simplified one-dimensional cases. Generally, these are unrepresentative of practical streamers propagating in three-dimensional space. As such, the system is typically discretized and solved on a numerical grid, using either finite-element (FEM) or finite-volume (FVM) methods. Some examples of the former include [10], [11], while codes using the latter include [12], [13]. In this work, the open-source FEM platform FEniCS [14] is chosen and evaluated for its capability to perform challenging streamer simulations. FEniCS is a collection of software packages licenced under LGPLv3 with the core aim of simplifying the definition and solution of FEM problems. The key software components are written in C++ and includes support for popular linear algebra systems. Detailed discussion of each component is beyond the scope of this study, for which the reader may refer to [15] and resources therewithin. The platform also features a high-level Python interface, which allows FEM problems to be posed using very few lines of code which are very close to the mathematical form of the problem. As a result, the platform excels in terms of user-friendliness and usability, even without computational expertise. All FEniCS components have additionally been developed with message passing interface (MPI) support for distributed memory parallelisation, allowing the same desktop-written code to be run on large HPC platforms with little to no changes.

Jovanovic *et al.* [16] had previously demonstrated that FEniCS is a capable platform for simulating streamers and dielectric barrier discharges (DBDs), using two compute nodes on a static mesh. Several comparisons between FEniCS and popular commercial software COMSOL were performed and good agreement between their results was found. However, in the present work, several major improvements to the base FEniCS code have been made which further enhances its functionality, namely:

- The aforementioned inclusion of photoionization processes is an important step for increased model fidelity.
- A custom, parallelised, and highly flexible adaptive mesh refinement (AMR) routine has been successfully developed and interfaces with FEniCS. This significantly reduces the requires computational resources and time.
- Dynamic time-stepping using an implicit Euler time integration scheme.

IV. Code Benchmarking

Following a benchmarking study performed by Bagheri *et al.* [17], which compared streamer modelling codes from six different international groups, we further compared our FEniCS code with AMR to their provided data. Full details regarding the computational domain, boundary conditions, and transport parameters can be found in [17] but are briefly described below for completeness. The study involved three cases of an axisymmetric positive streamer initiating and propagating through air: Case 1: with background ionization; Case 2: with reduced background ionization levels; and Case 3: inclusion of photoionization. Only the results from the Case 3 comparison are presented here, which best showcases the capability for FEniCS to successfully perform the simulation with the additional complexity of photoionization.

A. Computational Domain and Boundary Conditions

Following Figure 1, the 2D domain consists of a square with dimensions r, z = [1.25, 1.25] cm, which is rotationally symmetrical around r = 0 cm. The anode and cathode are located at z = 1.25 cm and z = 0 cm and are held at constant voltages of 18.5 kV and 0 kV, respectively. Neumann-zero conditions are prescribed for the potential on the left and right boundaries only but are prescribed on all four boundaries for the charge densities and photoionization source terms. To initially enhance the uniform background field, a seed of positive ions following a Gaussian distribution with peak value N_0 = 5×10^{18} m^{-3} is placed at z = 1 cm on the axis of symmetry.

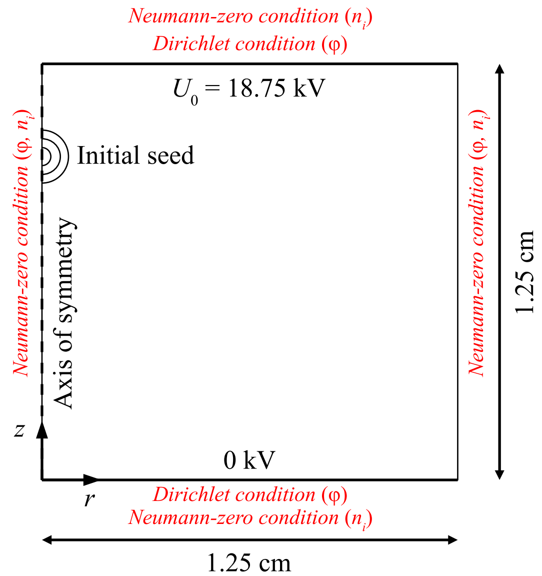

Fig. 1. Diagram of computational domain, boundary conditions, and initial seed for benchmarking study. Diagram adapted from [17].

B. Transport Parameters

As used in the original study, empirical expressions for the electron mobility, diffusion coefficient, and effective ionisation coefficient are used. We remark that the present code can also accept tabulated coefficients. The local-field approximation is used such that the parameters are dependent only on the local electric field magnitude (with the exception of the attachment coefficient which is constant). The expressions are given as equations (6)-(9).

$$\mu_e = 2.398 E^{-0.26} \tag{6}$$

$$D_e = \left(4.3628 \times 10^{-3} E^{0.22}\right) \tag{7}$$

$$\alpha = \left(1.1944 \times 10^{6} + \frac{4.3666 \times 10^{26}}{E^3}\right) e^{-2.73\times10^{7}/E} \tag{8}$$

$$\eta = 340.75 \tag{9}$$

where α and η are the ionisation and attachment coefficients in m^{-1}, respectively. Only electrons are assumed to be diffusive, and ions are taken as immobile over the nanosecond timescales of the simulation.

All results presented below were generated on a 16-core desktop computer at 3.4 GHz base frequency with 64 GB of memory. Hyperthreading was disabled (though no noticeable performance gain was found with it enabled) and AMR was set to refine every 30 iterations based on the magnitude of electron production and electric field strength. Linear Lagrange elements were used alongside dynamic time-stepping with a maximum step of 2 ps. FEniCS was running through Anaconda on Ubuntu 20.04. The generalized minimum residual method (GMRES) was used as a linear solver inside of a non-linear Newton iteration, preconditioned with an algebraic multigrid method from the PETSc [18] solver library, on default settings.

V. Results

In the Case 3 study, photoionization was enabled, with uniform background ionization levels of $N_b = 10^9$ m^{-3} for both electrons and positive ions. Fitting parameters from Bourdon *et al.* [9] are used for the Helmholtz coefficients. The simulation was run up to $t \sim 16$ ns, where the streamer had effectively bridged the electrode gap. Figure 2 and 3 shows the spatial variation of the electric field and electron density at t = 3, 9, and 15 ns, respectively. Comparisons of the streamer length over time and the maximum electric field strength as a function of the streamer length to other groups from [17] are shown in Figures 4 and 5. Note that only five additional groups are present, as one group from [17] did not participate in the case 3 study.

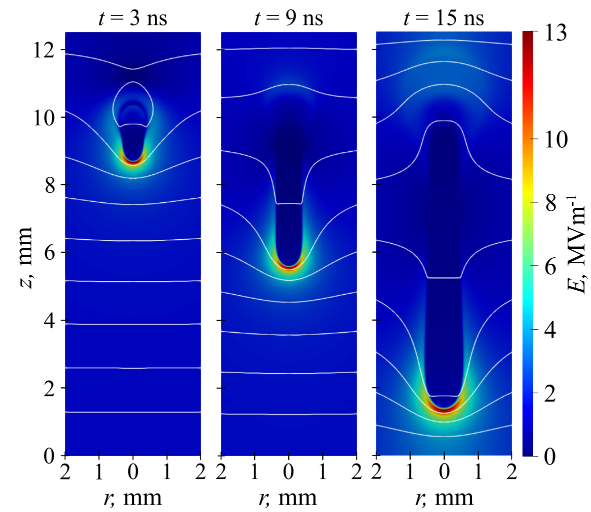

Fig. 2. Electric field distribution of the Case 3 positive streamer at t = 3, 9 and 15 ns. Equipotential lines are spaced by 2 kV. The simulation domain extends beyond the boundary of the figure.

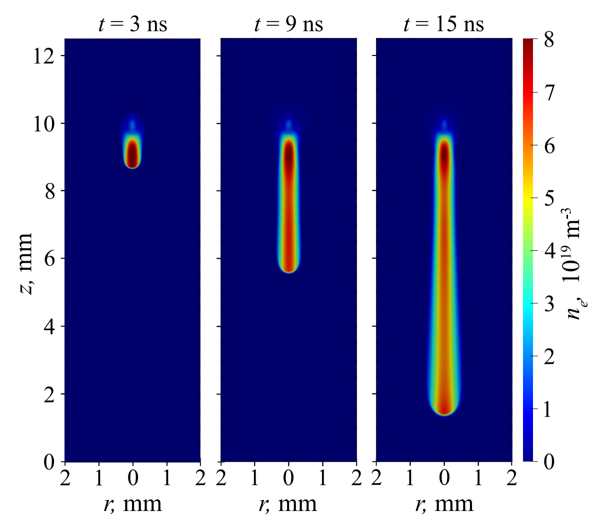

Fig. 3. Electron density distribution of the Case 3 positive streamer at t = 3, 9 and 15 ns. Equipotential lines are spaced by 2 kV. The simulation domain extends beyond the boundary of the figure.

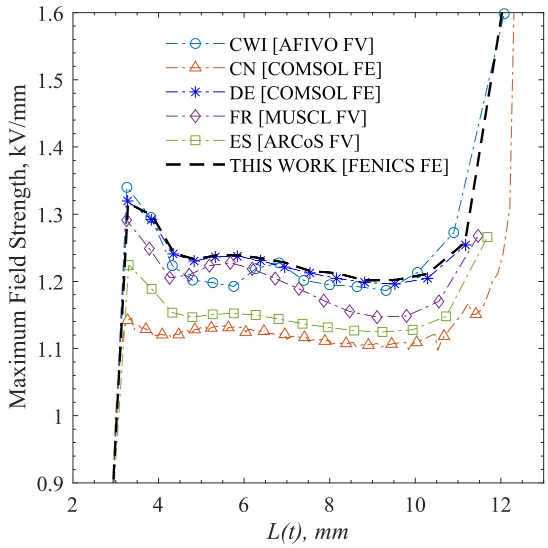

Fig. 4. Comparison of the Case 3 maximum field strength over the length of the streamer. Data for other groups from [17].

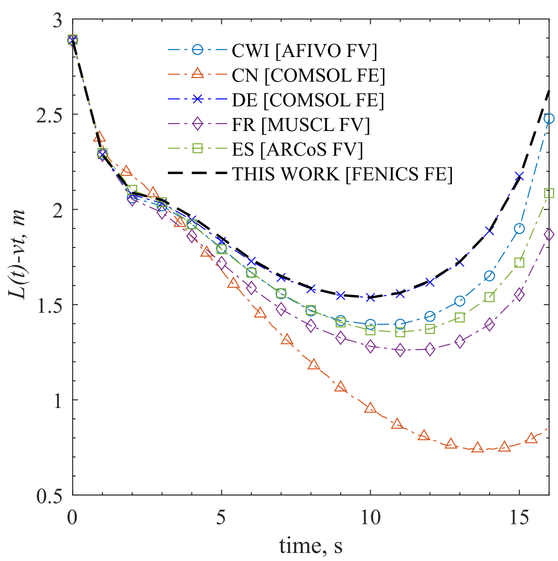

Fig. 5. Comparison of the Case 3 streamer length over time (with vt subtracted to emphasise the differences, v = 0.005 cm ns^{-1}. Data for other groups from [17].

The results obtained using the developed FEniCS code show good agreement when compared with other groups, of whom employed a mixture of fully custom and commercial codes. The FEniCS implementation appears to match the CWI and DE groups most closely. With the use of AMR, the necessary computational time was also reduced. Though the number of CPU cores which were used in this study exceeds that of all other participants, after the consideration of imperfect parallel scaling, the FEniCS code would still appear to complete the simulation faster than groups using COMSOL with AMR. Table 1 provides a detailed comparison of the various platforms used by each group, including the present work. The grid sizing and maximum number of grid cells which were necessary are of a similar order to that of other published codes.

TABLE I
COMPARISON OF FENICS PLATFORM TO OTHER GROUPS

	CWI	ES	FR	CN	DE	THIS WORK
FV/FE	FV	FV	FV	FE*	FE*	FE
Unstructured grid				✓	✓	✓
Spatial order	2	2	2	1	1	1
Temporal order	2	2	2	1-2	1-5	1
Mesh refinement	✓	✓	✓	✓	✓	✓
AMR	✓	✓		✓		✓
Parallel	✓		✓	✓	✓	✓
Tabulated Data	✓	✓				✓
Case 3 Simulation Settings						
Min. grid, μm	3.0	3.9	6.0	2.0	4.1	2.2
Max. grid, μm				8.0	5.0	
Max N_{cells}, 10^5	0.76	20	2.9	7.2	7.6	7.8
Time step	dyn.	1.0 ps	dyn.	dyn.	dyn.	dyn.
CPU Cores	4	1	1	4	6	16
Run time	<5 m	72 h	34 m	26 h	42 h	6 h

*These groups used COMSOL Multiphysics.

VI. CONCLUSION

In summary, the present work proposes that the open-source FEM platform FEniCS is a highly suitable alternative for the simulation of streamer discharges. Through its simple Python interface coupled with a high-speed C++ backend, the platform requires less computational expertise, yet demonstrates excellent computational efficiency and flexibility. We have briefly presented our custom FEniCS streamer modelling code, complete with photoionization processes, adaptive mesh refinement, and dynamic time-stepping. By comparing our simulated results to the data from a recent benchmarking study, we found excellent agreement between our results and six other groups who participated. The flexibility of FEniCS has allowed further studies involving complex gas-solid topologies and curved electrode geometries to be conducted. We aim to further apply the developed code in exploring streamer dynamics in contexts relevant to pulsed power applications.

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