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QUANTIFYING STREAMER DYNAMICS FOR AZIMUTHALLY SWEPT 3D WEDGES IN PIN-TO-PLANE PIC-DSMC SIMULATIONS

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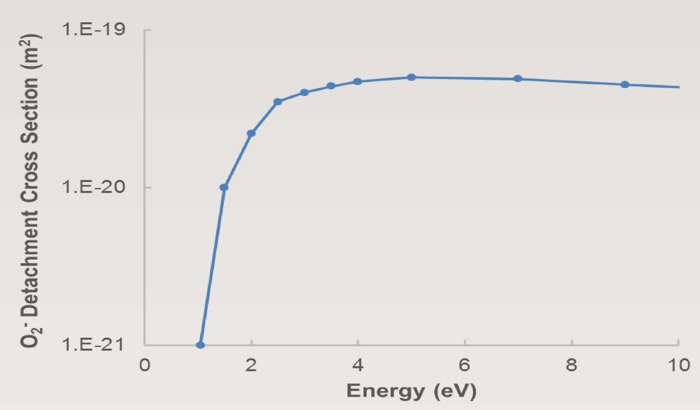
Abstract

Cathode directed streamer evolution in near atmospheric air is modeled in 3D pin-to-plane geometries using a completely resolved 3D kinetic particle-in-cell (PIC) code that simulates particle-particle collisions via the direct simulation Monte Carlo (DSMC) method. The total number of elements are confined to fractions of a full 360° geometry using 3D wedges that keep the problem space tractable. The wedge azimuthal angle is swept, resulting in 5°, 15°, 30°, and 45° angles. A DC voltage of 6kV is administered to a 100 μm hemispherical shaped anode, with a planar cathode held at ground potential, generating an overvolted state with an electric field of 4 MV/m across a 1500 μm gap. The domain is seeded with an initial ion and electron density of 10^{18} m^{-3} at 1 eV temperature confined to a 100 μm (radius) spherical region placed at the tip of the anode. The air chemistry model[1] includes standard Townsend breakdown mechanisms (electron-neutral elastic, excitation, ionization, attachment, and detachment collision chemistry and secondary electron emission) as well as streamer mechanisms (photoionization and ion-neutral collisions) via tracking excited state neutrals which can then either quench via collisions or spontaneously emit a photon based on specific Einstein-A coefficients[2,3]. In this work, positive streamer dynamics are formally quantified for each wedge angle in terms of electron velocity and density as temporal functions of coordinates r,ϕ,z. Electrons are tracked with picosecond temporal resolution out to 1.4 nsec, spatially binned, and averaged over six independent simulations each sourced with a random plasma seed. Prior 2D studies have shown that the reduced electric field, E/n, can significantly impact streamer evolution[4]. We extend the analysis to 3D wedge geometries (to limit computational cost) and examine the wedge angle's effect on streamer branching, propagation, and velocity. Results indicate that solution convergence in terms of the parameters described above are achievable.

Air and Dielectric Model[1]

- Assume N_2 and O_2 are dominant species for heavy-heavy interactions. Model dry air and neglect N–N, N – O, and O – O interactions.
  - Include elastic (VHS), charge exchange, and quenching heavy-heavy interactions
- Include e-N_2^+ and e-O_2^+ dissociative recombination
- Include O_2^- + M detachment via cross section[5]
  - Self-consistently leads to higher detachment rate in high-field regions
- e-neutral interactions included for N_2, O_2, N, O and metastable states. Use anisotropic scattering model for all electron-neutral collisions.
  - Elastic
  - Ionization: Single (ground and metastable states), double, and dissociative
  - Attachment (3-body and Dissociative)
  - Vibrational and rotational excitation
  - Electronic excitation
- Excited states have probability to radiate a photon based on transition-specific Einstein-A coefficients, quench via collision (assumed P_{quench} = ½) with background neutrals, or, in some cases, auto-dissociate or auto-ionize with state-specific rate
- Photons are modeled as discrete particles that move and stochastically collide through a simulation timestep just like all other particles
- Field solve accounts for relative permittivity



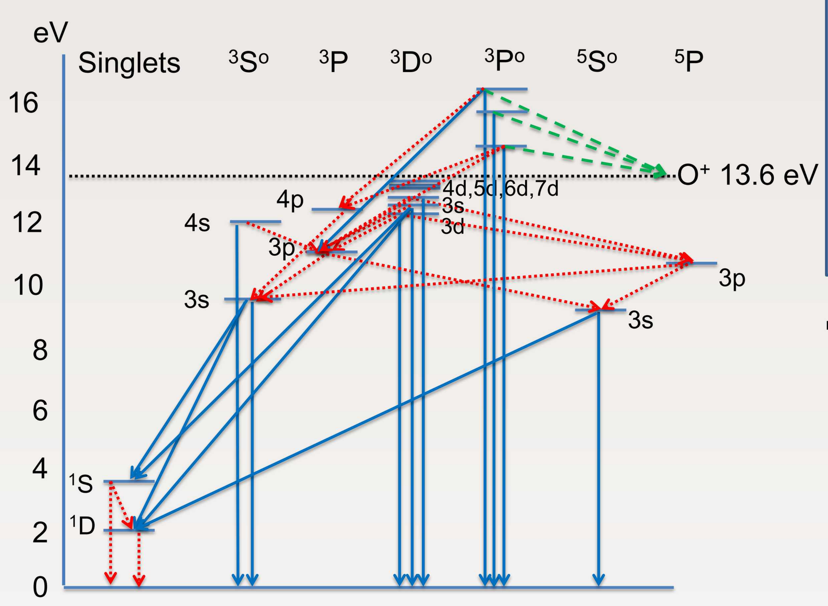
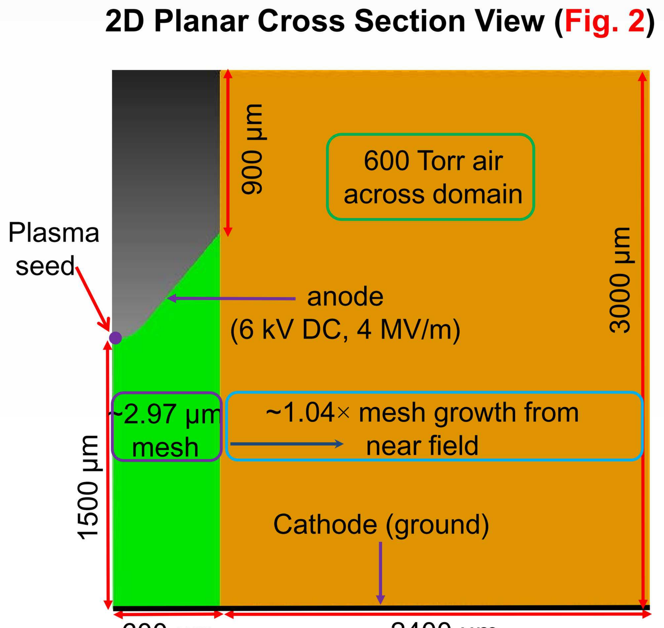


Fig. 1 Modeled energy level and transition diagram for atomic O ($^3D^o$ transitions omitted for clarity). Solid blue lines represent radiative decay in which simulation photons are generated. Red dotted lines represent decay in which a simulation photon is not generated. Green dashed lines are auto-ionizing states.

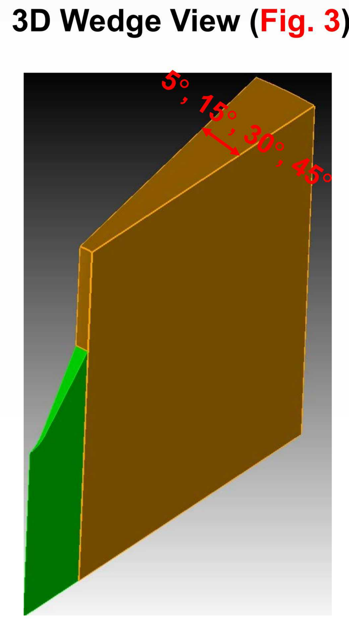
Geometry, Plasma Seed, and Mesh

- 3D wedge with azimuthal angles of 5°, 15°, 30°, and 45° used to model 1.5 mm air filled (600 Torr) pin-to-plane gap
- Unstructured tetrahedral mesh shown in Figure 4 (top) for a 45° wedge, with a factor of 4 increase in element size to improve visual clarity
- 3D volume render of a cathode directed streamer at 1.4 nsec shown in Figure 4 (bottom) for a 45° wedge
- Initial seed plasma density modeled as the following:
  - $T_e = T_i$ = 11,605 K (1 eV) and n_e =10^{18} m^{-3}
  - 100 μm (radius) sphere located at tip of pin electrode (anode)
  - Initial electron-ion particle positions generated using random numbers
  - An over-volted state (6 kV anode voltage, |E| = 4 MV/m) that allows for rapid evolution of the streamer

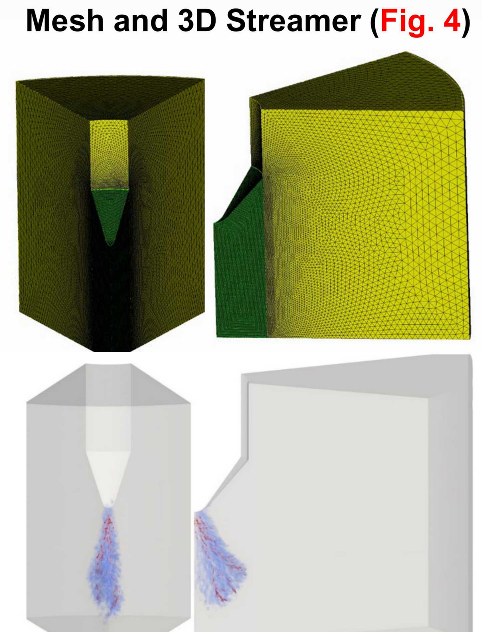
2D Planar Cross Section View (Fig. 2)



3D Wedge View (Fig. 3)



Mesh and 3D Streamer (Fig. 4)



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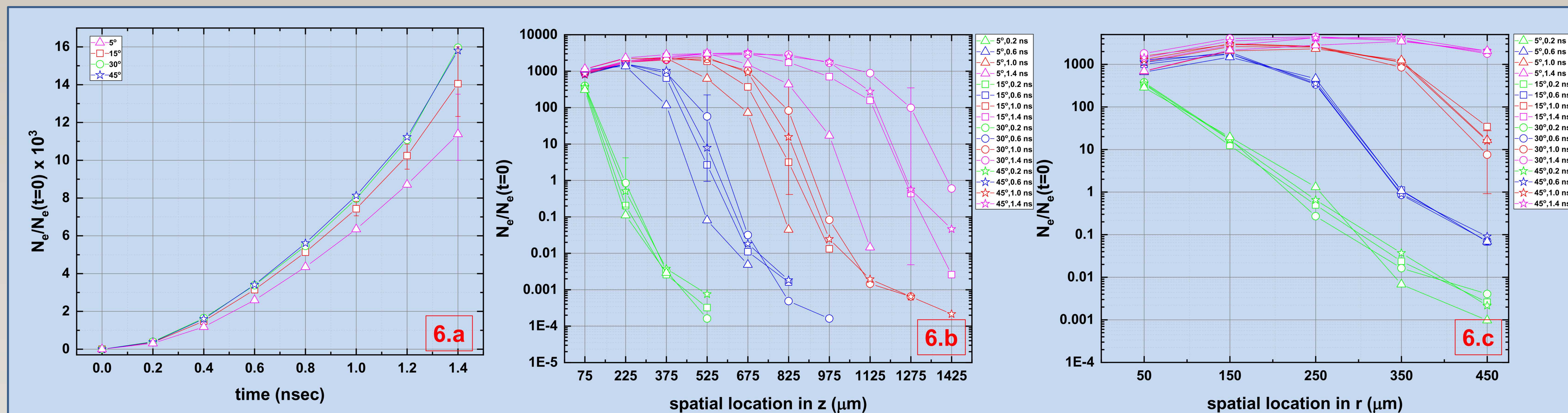
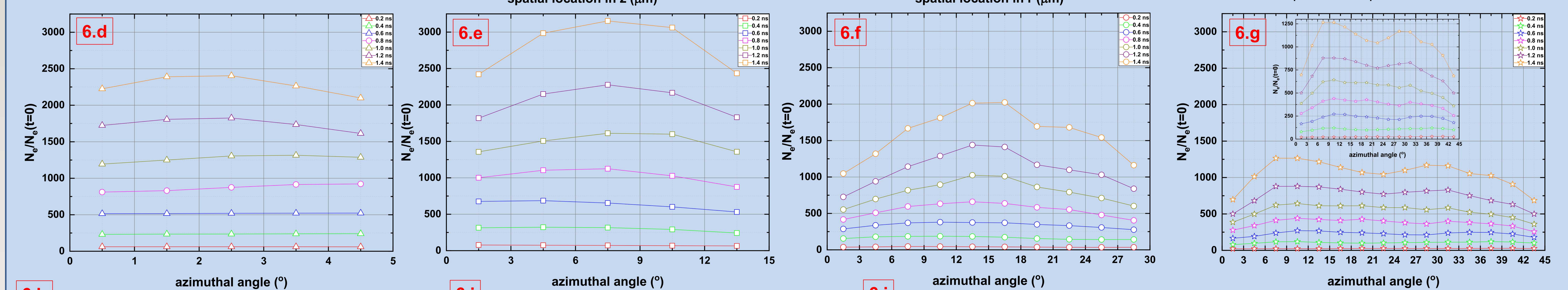
Results and Discussion



[a] Total number of *real* electrons, normalized to their respective values at time t=0, for 5°, 15°, 30°, and 45° wedges, as functions of time, averaged over 6 randomly seeded simulations.

[b] *Real* N_e contained in 150 μm thick dz slabs, normalized to *total* N_e at t=0, as functions of time for 5°, 15°, 30°, and 45° wedges, averaged over 6 randomly seeded simulations. Horizontal z-axis labels represent midpoint of each slab. 0 μm is tip of pin electrode and plasma seed at t=0.

[c] *Real* N_e contained in 100 μm thick dr slabs, normalized to *total* N_e at t=0, as functions of time for 5°, 15°, 30°, and 45° wedges, averaged over 6 randomly seeded simulations. Horizontal r-axis labels represent midpoint of each slab.



6.h

Wedge (°)	0.2ns	0.4ns	0.6ns	0.8ns	1.0ns	1.2ns	1.4ns
5	.213/.345	.951/1.42	2.36/2.88	3.90/4.90	5.75/7.18	7.96/10.0	10.0/13.5
15	.307/.382	1.43/1.58	3.08/3.28	4.98/5.43	7.06/7.83	9.53/10.8	12.3/16.0
30	.352/.421	1.42/1.77	3.07/3.58	5.19/5.74	7.45/8.42	10.3/12.0	14.1/18.5
45	.362/.404	1.56/1.70	3.36/3.56	5.35/5.80	7.48/8.44	10.3/11.8	13.9/18.0

6.i

Wedge (°)	0.2ns	0.4ns	0.6ns	0.8ns	1.0ns	1.2ns	1.4ns
5	70.0/17.1	64.0/19.7	42.4/23.6	37.2/18.4	30.1/17.5	29.4/18.0	39.0/33.3
15	17.9/5.8	9.1/7.6	9.1/8.5	7.4/6.8	5.9/7.8	8.1/9.3	13.0/12.5
30	2.8/4.0	9.9/4.0	9.4/0.6	3.1/1.0	0.4/0.2	0.0/1.7	1.4/2.7

6.j

Wedge Angle	$\frac{N_e}{N_{e_{t=0}}} = 10$			$\frac{N_e}{N_{e_{t=0}}} = 100$		
(°)	0.2-0.6 ns	0.6-1.0 ns	1.0-1.4 ns	0.2-0.6 ns	0.6-1.0 ns	1.0-1.4 ns
15	8.55	7.5	10.2	8.15	7.25	10.5
30	9.88	7.78	11.8	9.63	8.00	11.5
45	9.03	7.95	9.25	8.55	7.75	9.83

[d-g] *Real* N_e contained in 1° dϕ slabs for 5° wedge [6.d], and 3° dϕ slabs for 15° [6.e], 30° [6.f], and 45° [6.g] wedges, normalized to *total* N_e at t=0, as functions of time, averaged over 6 randomly seeded simulations. Horizontal ϕ -axis labels represent midpoint of each slab. 6.g inset of 45° wedge data on a magnified scale clearly shows macroscopic streamer branching.

[h] Minimum / maximum values for ratios of *Real* N_e normalized to *total* N_e at t=0, as functions of time, for 5°, 15°, 30°, and 45° wedges, taken from 6 randomly seeded simulations. All values to be multiplied by 10^3. [i] Absolute values of percent differences for all minimum / maximum data in 6.h with respect to a 45° wedge. [j] Z-directed streamer velocities for 15°,30°, and 45° wedges over various Δt = 0.4 nsec windows, evaluated using *Real* N_e to *total* N_e at t=0 ratios of 10 and 100. All values to be multiplied by 10^7 cm/s.

Temporal/Spatial n_e – ϕ=0 Planar Slice (#/m^3)

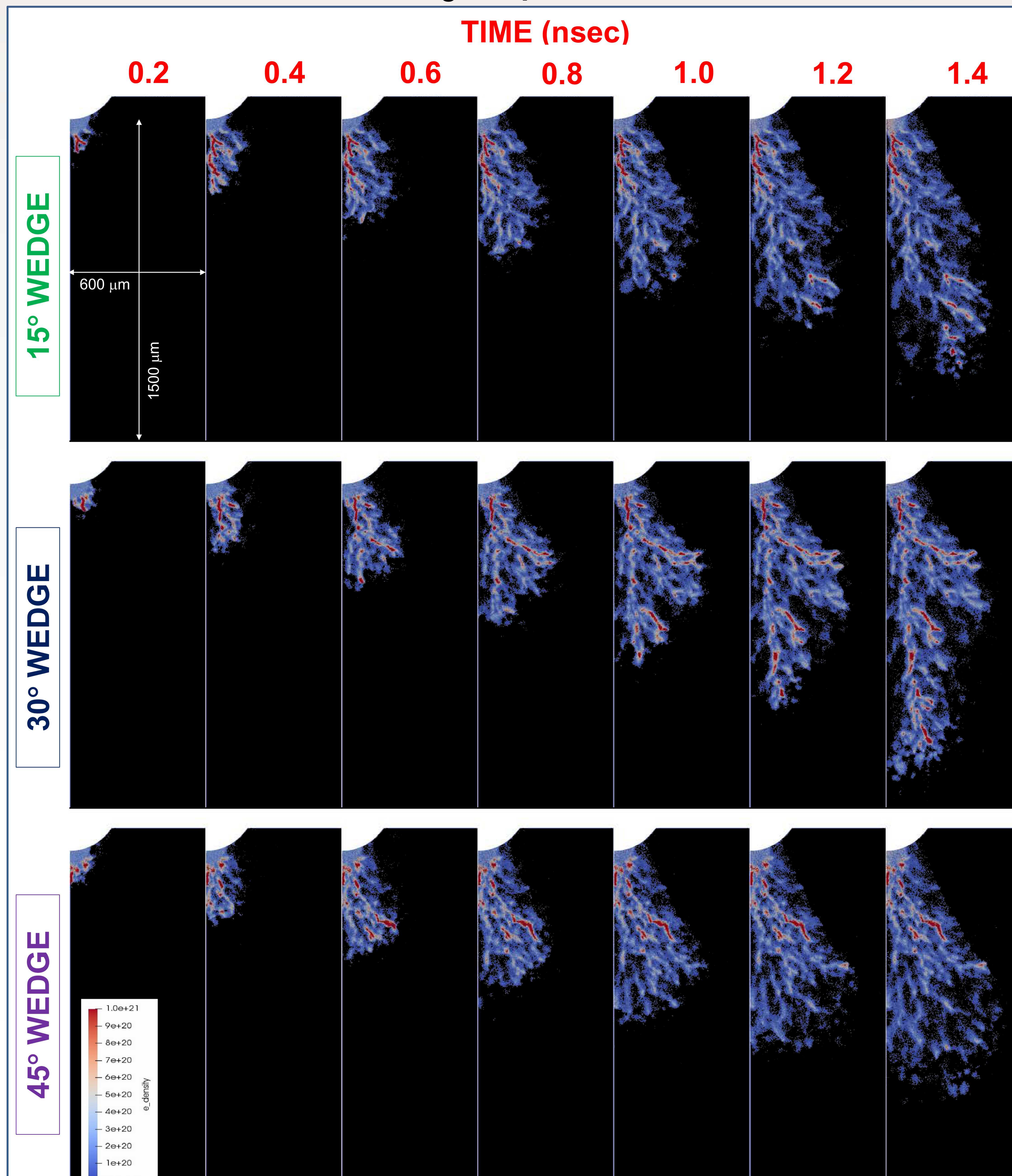


Fig. 5

- Figure 5 depicts the temporal and spatial evolution of cathode directed streamers for 15°, 30°, and 45° wedges along a slice in the ϕ=0 plane, using a spherical (r = 100 μm) plasma seed density of 1x10^{18} m^{-3} located as shown in Figure 2. Figure 6 above represents the analysis of this data (along with a 5° wedge), averaged over 6 randomly seeded simulations.
- In Figure 6.a, the total number of real electrons normalized to their respective values at time t=0, averaged over 6 randomly seeded simulations, depict approximate independence from the wedge angle for 15°, 30°, and 45° wedges, as the data points are tightly distributed. The larger spread for the 5° case is more clearly observed when the minimum and maximum values from 6 simulations are presented (temporally) for each wedge, along with the percent differences in these values when compared to the 45° case, in tables 6.h and 6.i, respectively. Table 6.i shows up to a 70% difference in minimum recorded values between the 5° and 45° cases at early time and as high as 33% in maximum values at late time. In stark comparison, there is less than a 10% difference for all values at early and late times between 30° and 45° cases.
- In Figure 6.b, the temporal and spatial distribution of the total number of real electrons contained in 150 μm thick dz slabs normalized to their respective values at time t=0, averaged over 6 randomly seeded simulations, for 15°, 30°, and 45° wedges, show that they are essentially independent of wedge angle. Again, greater deviation for the 5° case is observed even as early as 0.6 nsec.
- In Figure 6.c, the temporal and spatial distribution of the total number of real electrons contained in 100 μm thick dr slabs normalized to their respective values at time t=0, averaged over 6 randomly seeded simulations, for 15°, 30°, and 45° wedges, show that they are essentially independent of wedge angle. In contrast to the results from 6.a and 6.b, the 5° case appears to align reasonably well with larger wedge angles.
- Figures 6.d – 6.g depict the total number of real electrons contained in 1° dϕ slabs for the 5° wedge and 3° dϕ slabs for all others, normalized to their respective values at time t=0, and averaged over 6 randomly seeded simulations. Emergence of macroscopic branching is slightly observed for the 30° case and clearly visible in the inset for the 45° case.
- Z-directed streamer velocities in table 6.j for 15°, 30°, and 45° wedges, averaged over 6 randomly seeded simulations, indicate that they are approximately independent of wedge angle.
- Collectively, Figure 6 results suggest that solution convergence may be achievable at an angle as small as 15°, but requires modeling 3D streamers at angles in excess of 45° for verification.

References

[1] C. Moore *et al.*, "Development of Kinetic PIC-DSMC Model for Breakdown in the Presence of a Dielectric", ICOPS, Banff, 2016
[2] C. Moore *et al.*, "Development and Validation of PIC/DSMC Air Breakdown Model in the Presence of Dielectric Particles," Pulsed Power Conference, Austin, TX, 2015.
[3] A. Fierro *et al.*, "Discrete Photon Implementation for Plasma Simulations," Physics of Plasma, 23, 013506, 2016.
[4] Jindal A. et al., *Streamer Formation Near a Dielectric Surface with Variable Quantum Efficiency*, ICOPS, 2017.
[5] A. Ponomarev and N. Aleksandrov, "Monte Carlo simulation of electron detachment properties for O_2^- ions in oxygen and oxygen:nitrogen mixtures," PSST 24, 035001, 2015.

Future Work

- **Investigate any possible effects on streamer propagation for wedges exceeding 45°, constrained to the same mesh resolution**
- **Two papers are in the works and expected to be submitted in the near future**