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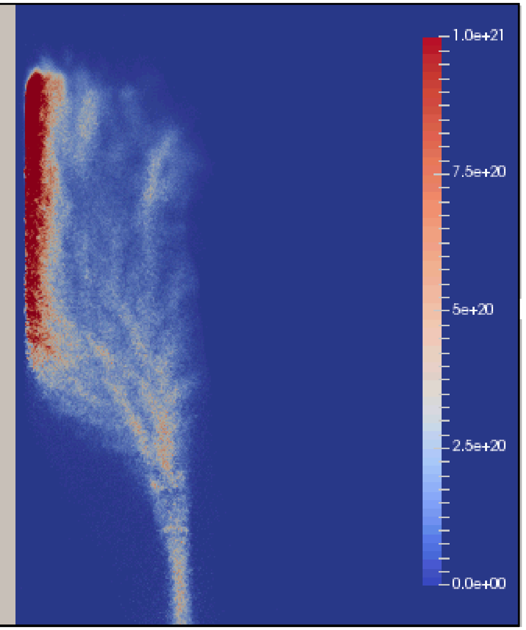

Kinetic simulation of breakdown in gaps with and without dielectric particles

Chris Moore, Andrew Fierro, Roy Jorgenson, Ashish Jindal, Paul Clem, and Matthew Hopkins

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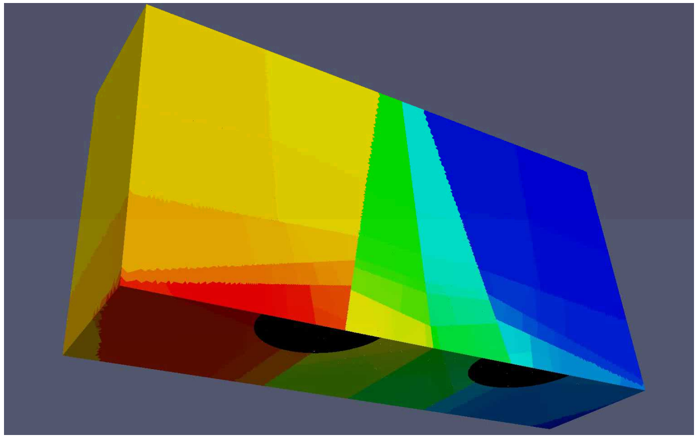
Aleph Overview

- Electrostatic Particle-In-Cell
  - Kinetic model of non-equilibrium plasma
  - 1, 2, or 3D unstructured FEM (CAD-compatible)
  - Accounts for relative permittivity of materials
- Massively parallel (scales up to ~60K procs)
  - Dynamic load balancing



Domain Decomposition

- Surface physics models:
  - Fowler-Nordheim and thermionic e^- emission, sputtering, surface charging, auger-neutralization, SEE, photoemission, sublimation
- Direct Simulation Monte Carlo Collision physics:
  - Simulate all species as simulation particles with variable particle weights
    - Can simulate evolution of neutral gas densities (important at low pressures)
  - Elastic, charge exchange, chemistry (dissociation, exchange, etc.), excited states (w/ radiative decay & self-absorption), ionization, Coulomb collisions (Nanbu model)

Air Chemistry: Model

- Lab cross sections vs. energy (linearly interpolate between data)
  - Experimental uncertainties of at ***least*** 20%

- Include elastic, charge exchange, and quenching heavy-heavy interactions. Assume N_2 and O_2 are dominant species.
  - Important for late-time thermalization of streamer channel & radiative emission intensity from excited states

$N_2 + N_2 \rightarrow N_2 + N_2$	$O_2 + O_2 \rightarrow O_2 + O_2$
$N_2 + N_2^+ \rightarrow N_2 + N_2^+$	$O_2 + O_2^+ \rightarrow O_2 + O_2^+$
$N_2 + N_2^+ \rightarrow N_2^+ + N_2$	$O_2 + O_2^+ \rightarrow O_2^+ + O_2$
$N_2 + O_2 \rightarrow N_2 + O_2$	$O_2 + N$
$N_2 + N$	$O_2 + O$
$N_2 + O$	$O_2 + A^* \rightarrow N_2 + A$
$N_2 + A^* \rightarrow N_2 + A$	

- 3-body recombination and attachment included as rate eqns.

Air Chemistry: Model

- Include e- N_2, O_2, N, O, N_2^+, and O_2^+ interactions
  - Elastic collisions: Preferentially forward scattered [1]
  - Ionization:
    - Single: $N_2 \rightarrow N_2^+$ and $O_2 \rightarrow O_2^+$
    - Double ionization: $N_2 \rightarrow N_2^{++}$ and $O_2 \rightarrow O_2^{++}$
    - Dissociative ionization: $N_2 \rightarrow N + N^+$ and $O_2 \rightarrow O + O^+$
  - Dissociation: $N_2 \rightarrow 2N$ and $O_2 \rightarrow 2O$
  - Attachment: $O_2 \rightarrow O + O^-$
  - Recombination: $N_2^+ \rightarrow 2N$ and $O_2^+ \rightarrow 2O$
  - Excitation of N_2 and O_2 vib. & rot. states (do not track them)
  - Electronic excitation:
    - 15 N_2 excited states
    - 6 O_2 excited states
    - 6 N excited states
    - 17 O excited states

[1] Okhrimovskyy et al., Phys. Rev. E. **65**, 037402

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$$e^- + N_2 \rightarrow e^- + N_2^*$$

N_2^*	E (eV)
A $^3\Sigma_u^+$, v=0-4	6.17
A $^3\Sigma_u^+$, v=5-9	7.00
B $^3\Pi_g$	7.35
W $^3\Delta_u$	7.36
A $^3\Sigma_u^+$, v=10-v_{max}	7.80
B' $^3\Sigma_u^-$	8.16
a' $^1\Sigma_u^-$	8.40
a $^1\Pi_g$	8.55
w $^1\Delta_u$	8.89
C $^3\Pi_u$	11.03
E $^3\Sigma_g^+$	11.88
a'' $^1\Sigma_g^+$	12.26
b $^1\Pi_u$	12.50
c'$_4$ $^1\Sigma_u^+$	12.85
b' $^1\Sigma_u^+$	12.94

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$$e^- + O_2 \rightarrow e^- + O_2^*$$

O_2^*	E (eV)
a $^1\Delta_g$	0.98
b $^1\Sigma_g$	1.63
c $^1\Sigma_u^+$	4.34
B $^3\Sigma_u$	6.12
"Longest band"	9.97
"Second band"	10.29

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$$e^- + N \rightarrow e^- + N^*$$

N^*	E (eV)
$2s^22p^3\ {}^2D^o$	2.38
$2s^22p^3\ {}^2P^o$	3.58
$2s^22p^2({}^3P)3s\ {}^4P$	10.33
$2s^22p^2({}^3P)3s\ {}^2P$	10.68
$2s2p^4$	10.98
$2s^22p^2({}^1D)3s\ {}^2D$	12.35

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Air Chemistry: Model

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    - 6 O_2 excited states
    - 6 N excited states
    - 17 O excited states

$e^- + O \rightarrow e^- + O^*$

O^*	E (eV)
$2s^22p^4\ ^1D$	1.97
$2s^22p^4\ ^1S$	4.19
$2s^22p^3(^4S^o)3s\ ^5S^o$	9.15
$2s^22p^3(^4S^o)3s\ ^3S^o$	9.52
$2s^22p^3(^4S^o)3p\ ^5P$	10.74
$2s^22p^3(^4S^o)3s\ ^3P$	10.99
$2s^22p^3(^4S^o)4s\ ^3S^o$	11.93
$2s^22p^3(^4S^o)3d\ ^3D^o$	12.09
$2s^22p^3(^4S^o)4p\ ^3P$	12.36
$2s^22p^3(^2D^o)3s\ ^3D^o$	12.54
$2s^22p^3(^4S^o)4d\ ^3D^o$	12.76
$2s^22p^3(^4S^o)5d\ ^3D^o$	13.07
$2s^22p^3(^4S^o)6d\ ^3D^o$	13.24
$2s^22p^3(^4S^o)7d\ ^3D^o$	13.34
$2s^22p^3(^2P^o)3s\ ^3P^o$	14.12
$2s2p^5\ ^3P^o$	15.66
$2s^22p^3(^2D^o)4d\ ^3P^o$	16.11

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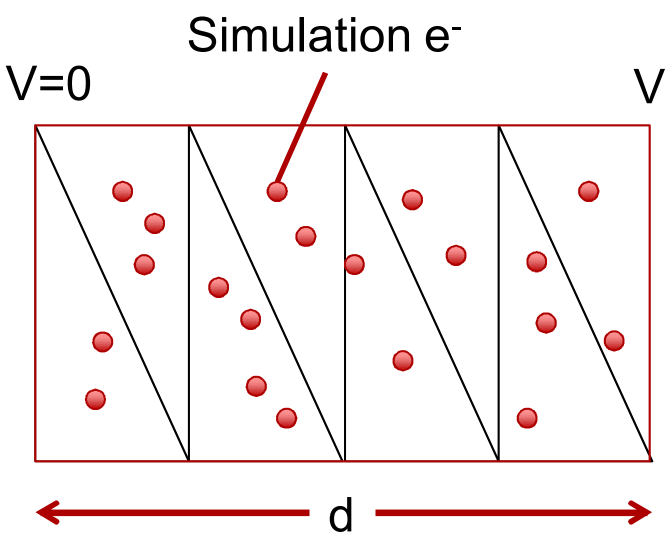
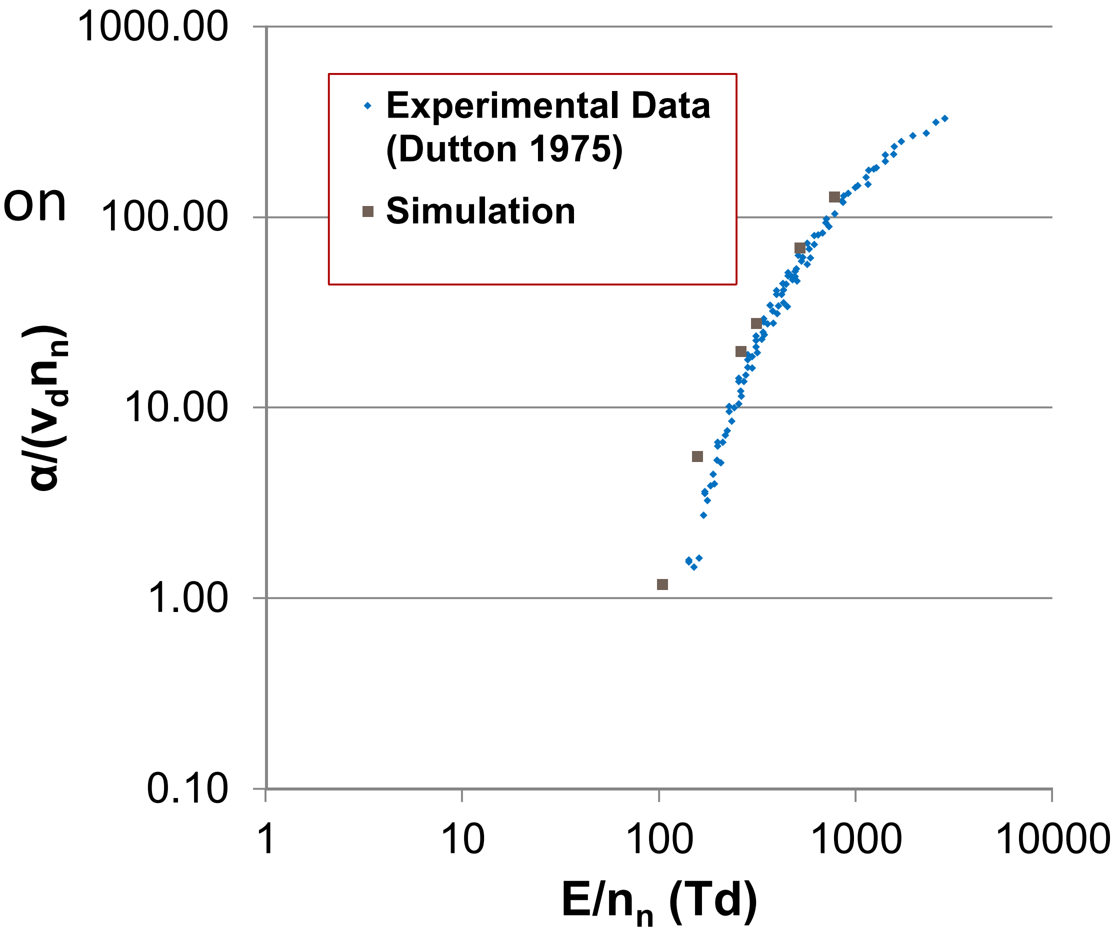
Air Chemistry: Swarm data

- Compare experimental and simulated electron drift velocity and ionization coefficient vs. E/n



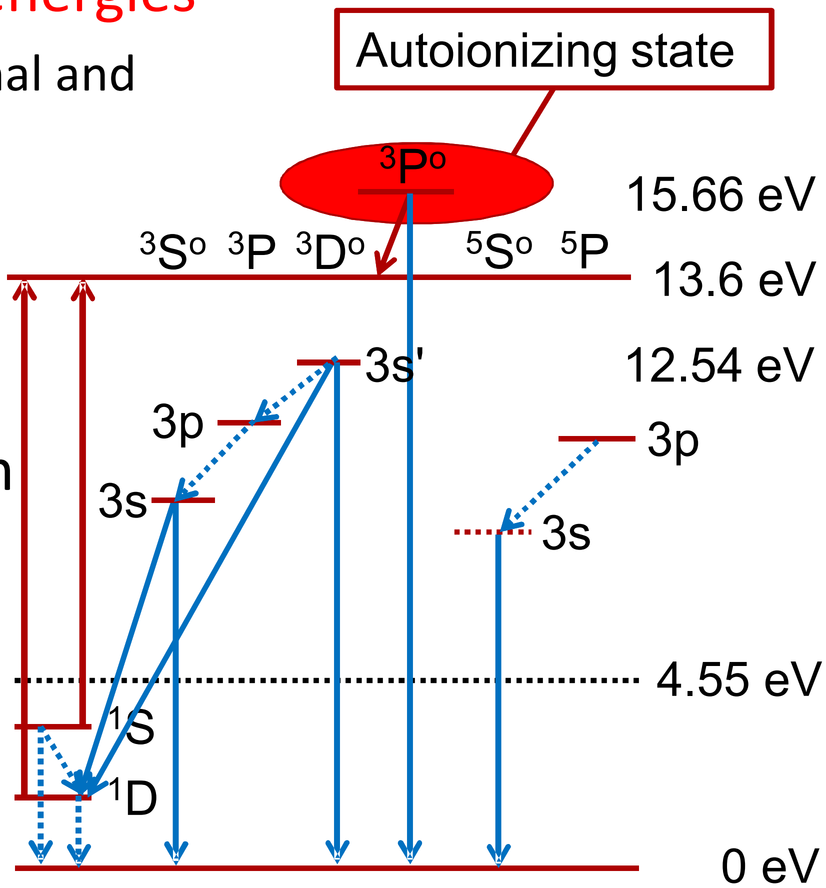


- Electrons undergo collisions with background air and gain energy in const. E-field

Convergence required
$\Delta t < 5\times10^{-14}$ s $<< \nu_{col}^{-1} < \omega_{pe}^{-1}$
$\Delta x^{*}E < 1$ V $<< \lambda_{MFP}$

Photons: Spontaneous Emission

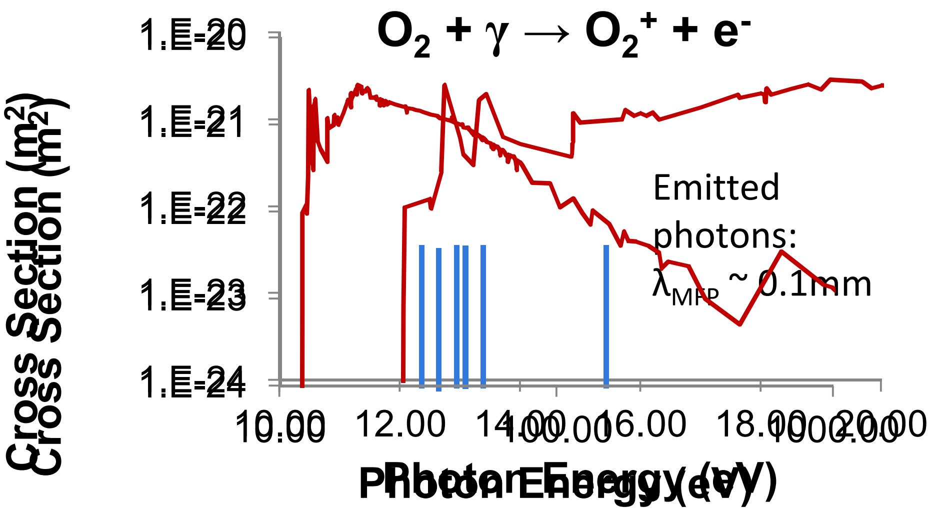
- Model excited states of N_2, O_2, N, and O due to electron impact
- Assume photon interaction cross sections vary little over rotational and vibrational energies
  - Group all excited molecules into rotational and vibrational ground state (v=0, j=0).
- Allow spontaneous emission to multiple lower states based on Einstein-A coefficients
- Emit multiple sim. photons in random directions per emitting particle
  - Reduces numerical streamer branching due to sim. noise in particle count
- Include electron de-excitation (quenching) and ionization from metastable excited states



Partial energy level diagram for O

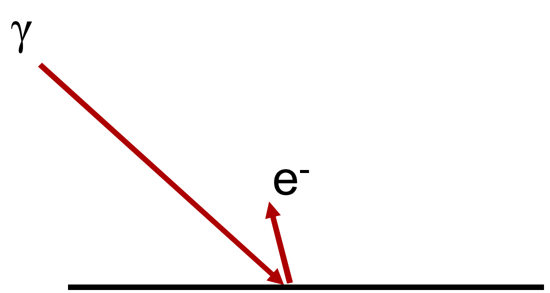
Photons: Neutral Interactions

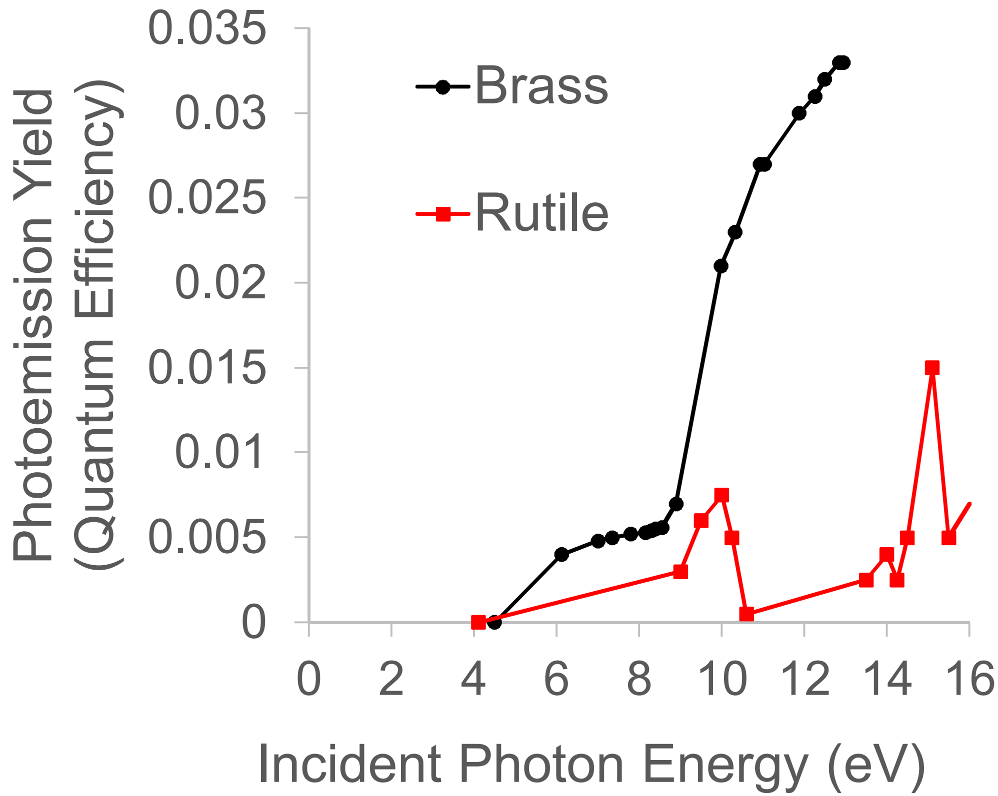
- Photons are simulation particles
  - During push: Velocity is constant, but spatial position updated
  - During collide: Photon can interact with any other simulation particle in the same element (DSMC) provided the input deck specifies a cross section for the interaction
- λ-dependent photon interactions
  - Photon absorption based on Einstein-B coefficients
  - Photo-ionization of O_2 and N_2
  - Photo-dissociation of N_2 & O_2
  - Photo-emission from surfaces
- Current results do not include self-absorption!
  - Need to track vib. & rot. states



Photons: Photoemission

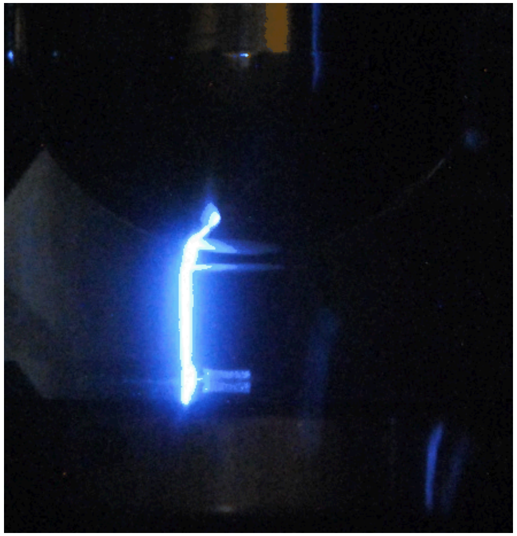
- Photons incident on the electrodes and dielectric have material specific electron emission yields
  - Use experimental yields
  - Dependent on the photon energy
  - $E_{e-} = E_{\gamma} - \varphi_w$





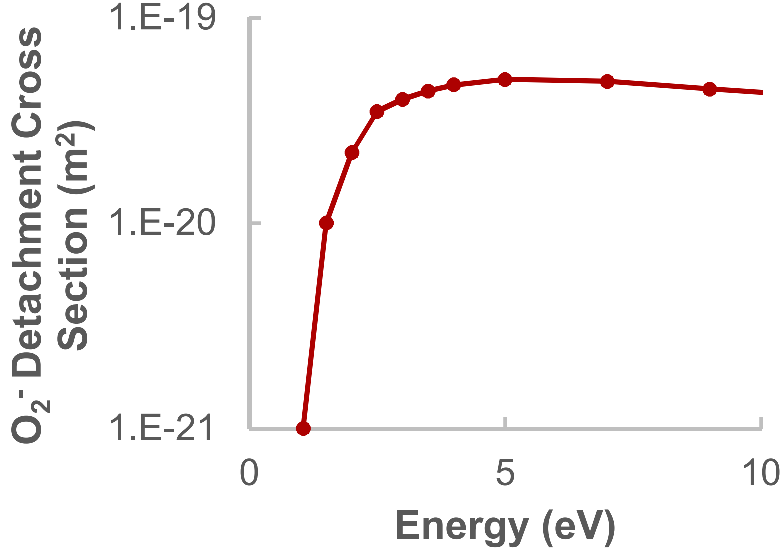
(Some) Open Questions

- How much does dielectric photoemission yield matter to streamer dynamics (velocity, attachment to dielectric, etc.)?
- 2D vs. 3D: sustainment/branching/etc. ?
- At ~ion timescales (~100ns) does the small gap fill with plasma allowing a streamer to propagate/start outside of the gap and travel down the dielectric surface?
- How important (to streamer dynamics) is accounting for vibrational and rotational states when spontaneously emitting photons?
- How important is self-absorption?



Initial Seed Plasma

- Desire a more physical initial seed plasma in order to explain variability in breakdown voltage/time
- In un-stressed state Cosmic Rays result in free electrons which then rapidly attach to O_2
- O_2^- long-lived at room temperature and no E-field
- Applied fields accelerate O_2^- resulting in sufficient energy for $O_2^- + M \rightarrow O_2 + e^- + M$
  - Source of initial e^- in regions of high fields (e.g., dielectric corners)



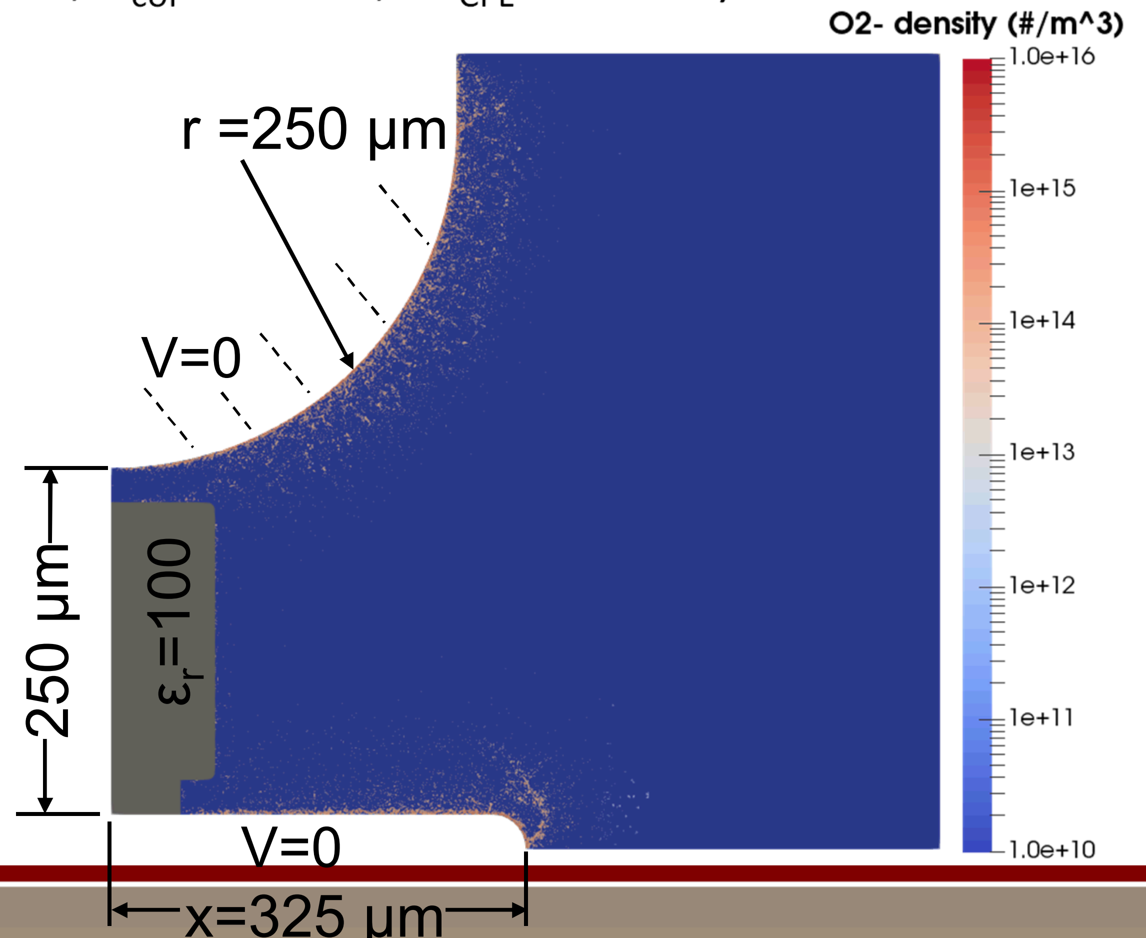
Simulation Domain

- 2D simulation of a 600 Torr, air-filled hemisphere-to-plane 250 μm gap with 200 μm TiO_2 ($\varepsilon_r = 100$) cylinder on top of a 25 μm dielectric ($\varepsilon_r = 3$) spacer between brass electrodes.

- $\Delta t = 5 \times 10^{-14}$ s ($\omega_{pe}^{-1} \sim 10^{-12}$ s; $\nu_{col} \sim 10^{-12}$ s; $\Delta t_{CFL} \sim 10^{-13}$ s)

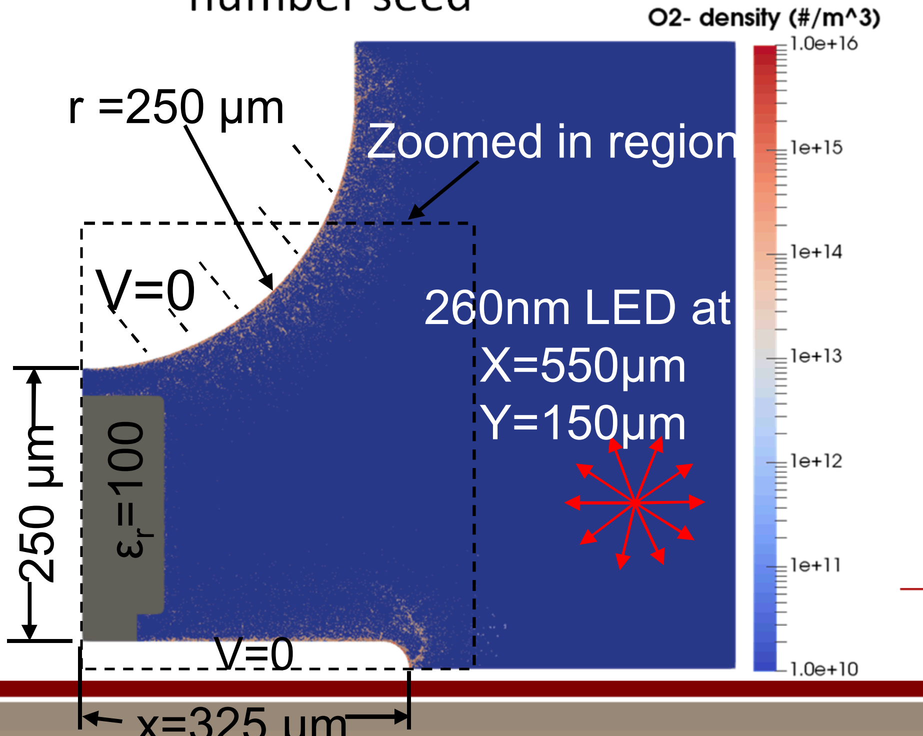
- "Δx" = 0.2 μm ($\lambda_D \sim 0.2$ μm in streamer channel)
  - ~30 million elements

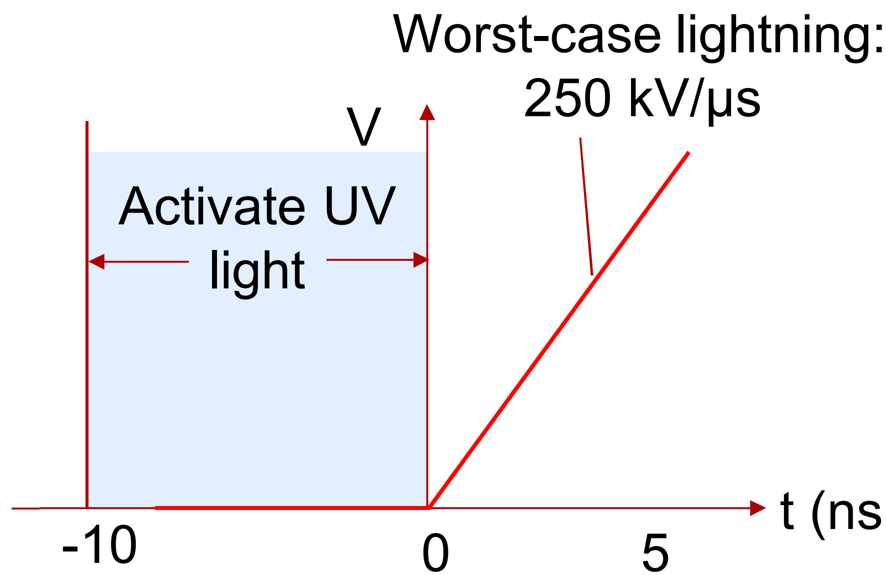
- Particle merger kept ~128 charged particles per element



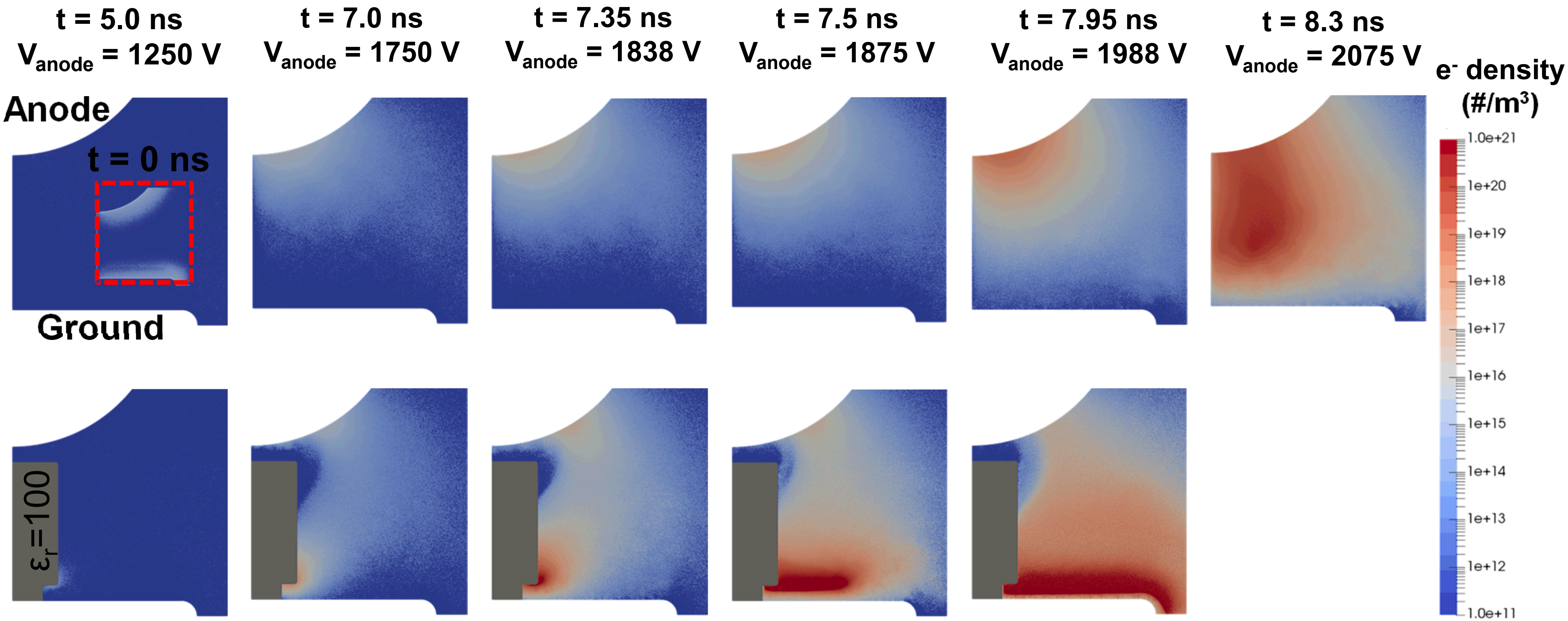
Generation of Initial O_2^-

- Activate isotropic, 260 nm UV LED light source (1.6 mW/cm^2 on axis) for 10 ns with no applied potential and then ramp anode voltage at 250 kV/µs
- Electrons diffuse through the background neutral gas and attach to O_2 through 3-body collisions
  - Gives initial density distribution for e^- & O_2^- which varies with random number seed





Results: e- densities



- Initial photoemitted e^- swept out of the gap in the first several ns while the field is still too low to result in breakdown

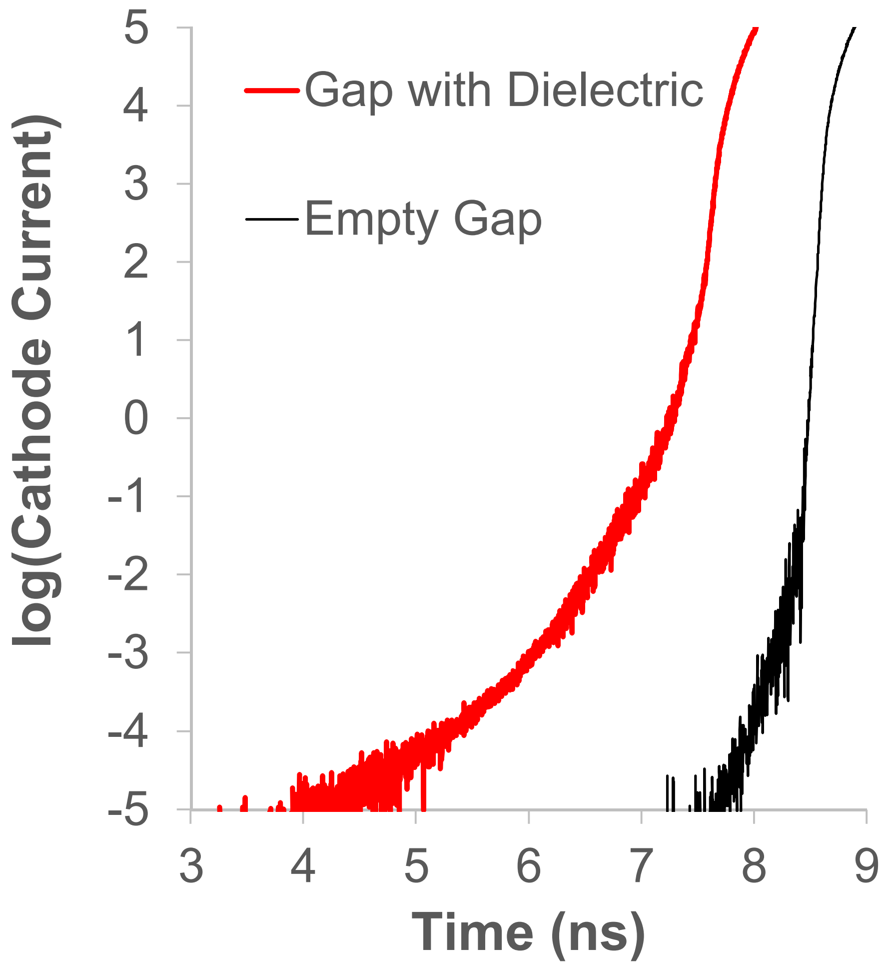
- After ~5ns the field near the dielectric corner causes significant O_2^- detachment supplying e^- in the high-field (and thus high α) region
- In contrast, there is much less O_2^- detachment in the empty gap (with lower E)

- After 7ns significant e^- avalanche starts near cathode in the high-field region near the dielectric corner and leads to 2nd positive excitation of N_2.
- In the empty gap e^- densities are highest near the anode as would be expected from seed e^- avalanching back to the anode

Cathode Currents

- The empty gap breaks down in ~8.5ns via a positive streamer
  - Breakdown voltage ~2125 V
  - Significant variation in breakdown voltage for different random seeds

- Presence of dielectric particle causes gap to breakdown in under 8ns
  - Breakdown voltage ~2000 V
  - Less variation in breakdown voltage when changing random seed



(Some) Open Questions

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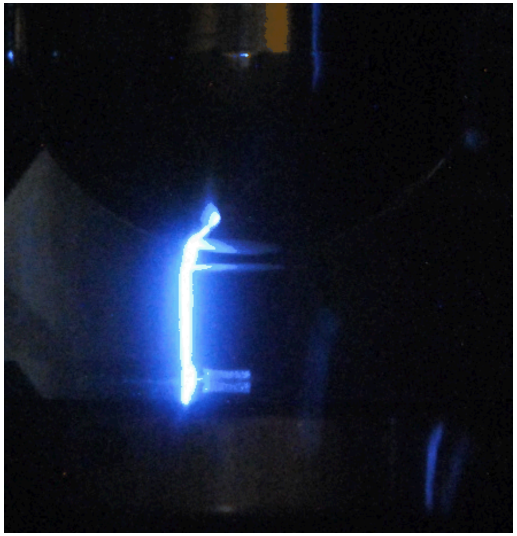
- How do initial seed plasma/electrons form and influence breakdown delay time?
- 2D vs. 3D: sustainment/branching/etc. ?
- At ~ion timescales (~100ns) does the small gap fill with plasma allowing a streamer to propagate/start outside of the gap and travel down the dielectric surface?
- How important (to streamer dynamics) is accounting for vibrational and rotational states when spontaneously emitting photons?
- How important is self-absorption?

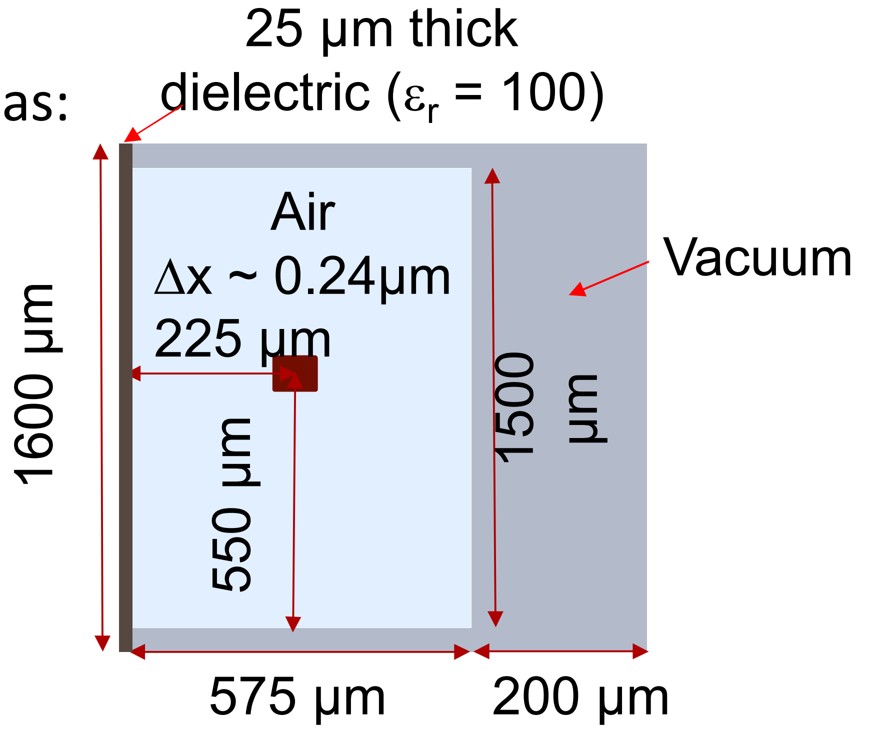


Domain: Photoemission Sensitivity

- 2D simulation of a 760 Torr 1.5 mm air filled gap with a 25 µm thick TiO_2 (ε_r = 100) cylinder between electrodes

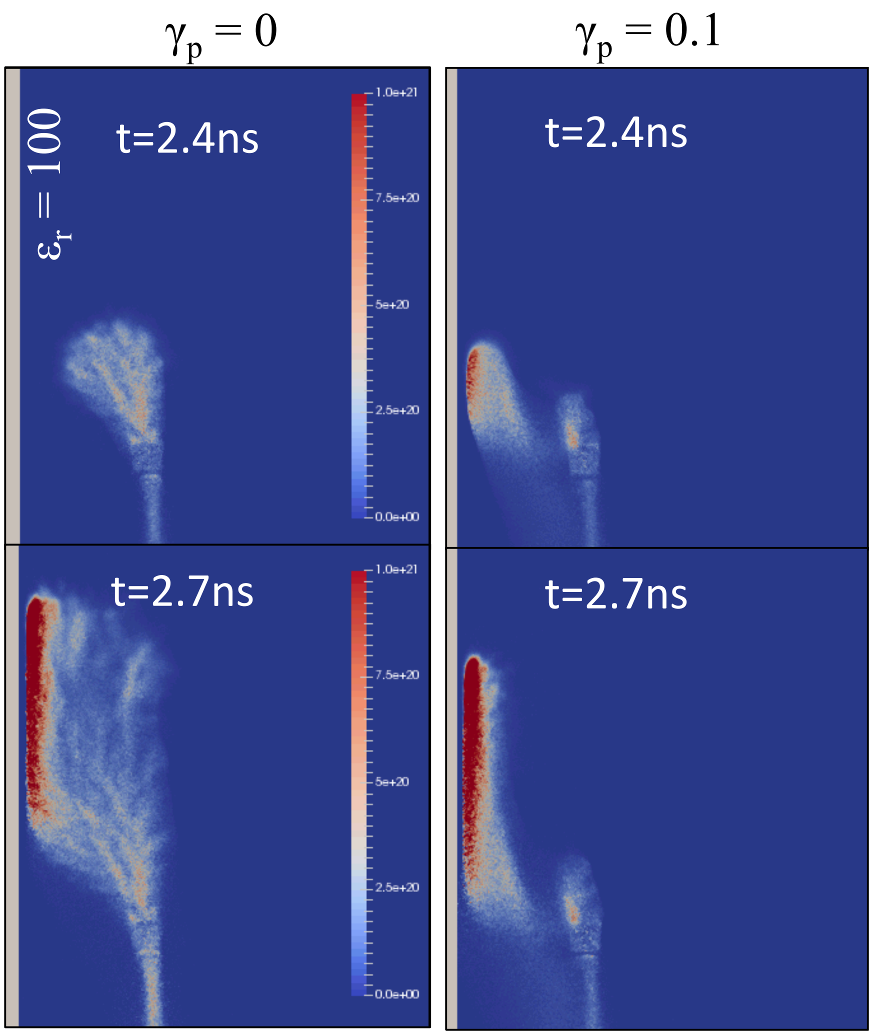
- Over-volted state (8 kV anode voltage) allows for rapid evolution of the streamer

- Initial seed plasma density modeled as:
  - $T_e = T_i = 1$ eV and $n_e = 10^{20}$ m^{-3}
  - 50 µm^2 square centered at 225 µm radially from dielectric surface and 550 µm axially from bottom vacuum interface



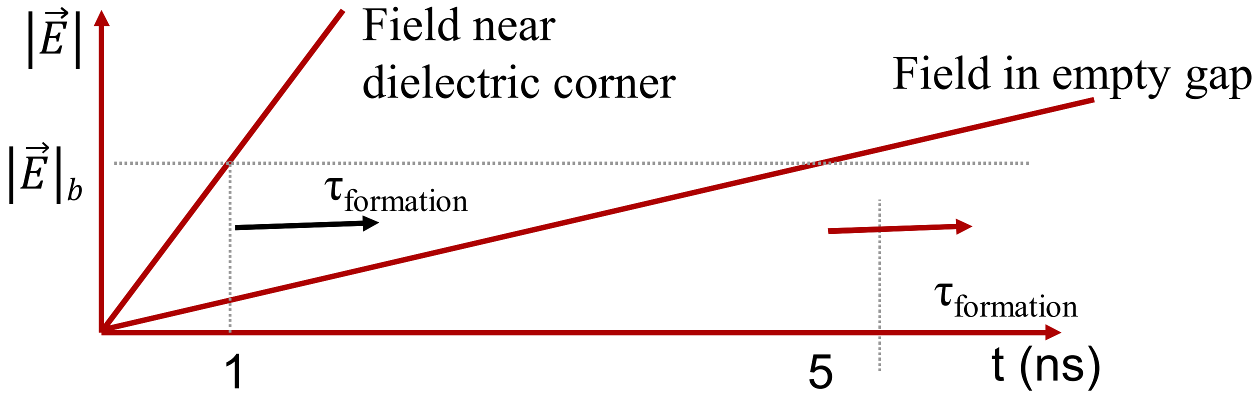
Results: Photoemission Sensitivity

- At 2.4 ns:
  - Elevated E/n near the dielectric surface results in an increase in α (net ionization). This “attracts” the streamer to the dielectric as e^- created in this region avalanche more strongly
  - With a photoemissive dielectric surface two distinct cathode directed streamers form
- At 2.7 ns:
  - The streamer travels along the dielectric surface in both cases; however, it is much more diffuse for the case without photoemission



Conclusions

- Kinetic model for breakdown in the presence of dielectric particles:
  - Townsend mechanisms (e^- - neutral collisions, ion induced SEE)
  - Ion and neutral transport (O_2^- detachment)
  - Photon transport (photoionization and photoemission)
- Dielectric particles create regions of high fields that detach O_2^- at earlier times supplying initial electrons which then initiate breakdown sooner (and more reliably) during lightning pulse



- Increased E/n near dielectric results in amplification of net ionization rate, α, preferentially directing streamer growth towards the surface even under conditions of zero quantum yield