Revisiting Paschen: Breakdown voltage calculations using PIC-DSMC

Chris H. Moore, Matthew M. Hopkins, Paul S. Crozier,
Jeremiah J. Boerner, and Lawrence C. Musson

Outline

- Motivation
- 1-D breakdown with uniform gas across gap
  - Electron source: Ionization vs. Auger neutralization vs. Field Emission
  - “Large gap” vs. “Small gap” breakdown dynamics
  - Simulated breakdown voltage vs. data & Paschen curve
  - Breakdown voltage dependence on scattering model
- 1-D breakdown with non-uniform gas density across gap
  - Comparison to uniform gas density
- Conclusions

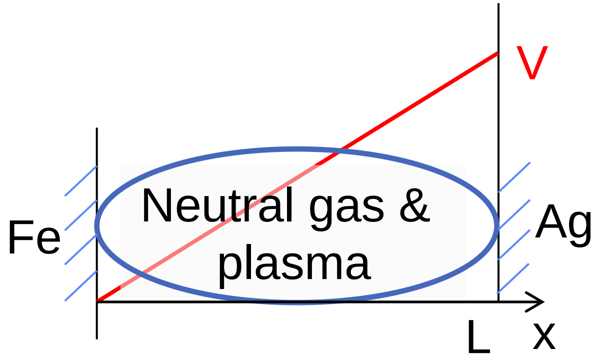
Motivation for studying breakdown

“Undesired or unintended electric arcing can have detrimental effects on electric power transmission, distribution systems and electronic equipment. Devices which may cause arcing include switches, circuit breakers, relay contacts, fuses and poor cable terminations.” Source: http://en.wikipedia.org/wiki/Electric_arc

Why PIC-DSMC to compute breakdown?

- Particle methods amenable to modeling physical mechanisms of interest (particle interactions with surfaces & particles, solving for fields, etc.)
  - PIC widely used to simulate collisionless plasmas
  - DSMC used to simulate collisional gas flows
- Yield a better understanding of breakdown phenomena.
  - Enable predictions of breakdown voltages as a function of gas composition, pressure, device geometry, and imposed E-fields.
  - Control/Delay breakdown in real devices by manipulation of sensitive parameters.
- Provide tests for models (interaction cross-sections, interaction models), which can be validated versus experimental measurements.
- Allow for analysis where Paschen equation assumptions are not valid
  - Microscale gaps where CFE matters
  - Nonuniform gas distributions

1D Breakdown in Air



- 1D3V PIC-DSMC simulations
  - Fe cathode and Ag anode
  - Gap filled with air at STP
  - Simulate various gap sizes → Find breakdown voltage
  - Uniform grid, $\Delta x < \lambda_D$ at $n_e = 10^{21}$ m^{-3} (typical “breakdown”density)
  - Timestep = 5×10^{-15} s < CFL < mean collision time < $1/\omega_{pe}$
- Define “Breakdown”: Super-exponential rise in current as voltage “collapses” and quasi-neutral plasma forms in gap
  - Simulations limited to 15 ns → Obtain upper limit $V_{breakdown}$
- “Trigger” breakdown with an initial, very low density uniform electron & ion plasma of 10^{17} m^{-3} ($\sim10^{-9} * n_{N2}$)

Gas Interactions Model

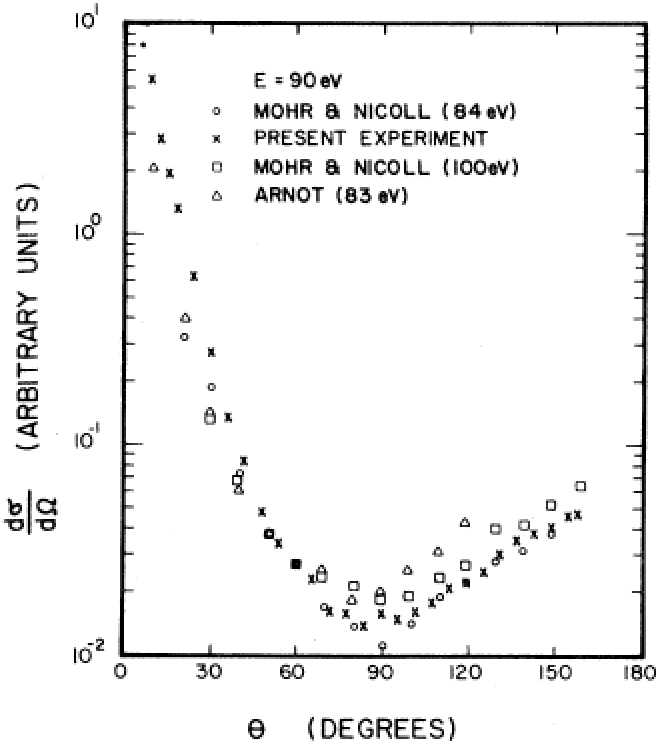
- Use lab cross sections vs. energy (linearly interpolated between lab data)
- Include $e\text{-}N_2$, $e\text{-}O_2$, $e\text{-}N_2^+$, and $e\text{-}O_2^+$ interactions
  - – Elastic, Excitation
    - Alter electron energy distribution
    - Elastic collisions can be either isotropic or preferentially forward scattering
  - – Ionization: $N_2 \rightarrow N_2^+$ and $O_2 \rightarrow O_2^+$
    - Source of ions & secondary electrons
    - Use *total* ionization cross section
    - Do not include double ionization ($N_2 \rightarrow N_2^{++}$ & $O_2 \rightarrow O_2^{++}$)
    - Do not include dissociative ionization ($N_2 \rightarrow N + N^+$ & $O_2 \rightarrow O + O^+$)
  - – Recombination ($O_2 \rightarrow O + O^-$), Attachment ($N_2^+ \rightarrow 2N$ & $O_2^+ \rightarrow 2O$)
    - Sink for electrons, ions

Gas Interactions: Scattering

- Post-collision velocities must be picked for each interaction type (often assume isotropic scattering)
- Above ~10 eV electrons predominately forward scatter
  - Data exists for differential scattering of elastic electron collisions
  - Reasonably approximated by (Surendra *et al.*, 1990):

$$\frac{d\sigma}{d\Omega} = \frac{\epsilon}{4\pi\left(1+\epsilon sin^2(\theta/2)\right)ln(1+\epsilon)}$$

- Will compare breakdown dynamics using isotropic and anisotropic scattering models for elastic collisions
  - Elastic collisions ~50% of total



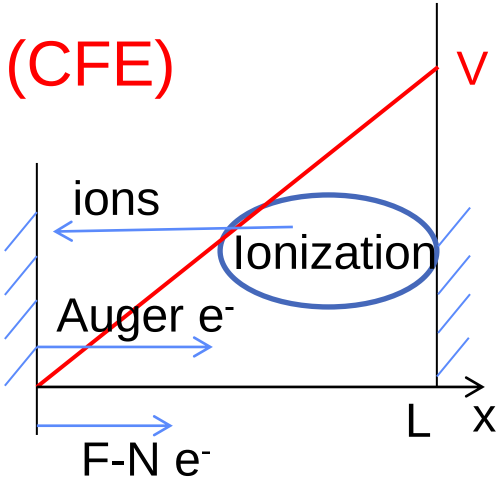
e^-–N_2 elastic differential scattering cross section vs. scattering angle at 90 eV (Shyn *et al.*, 1972)

Surface Model

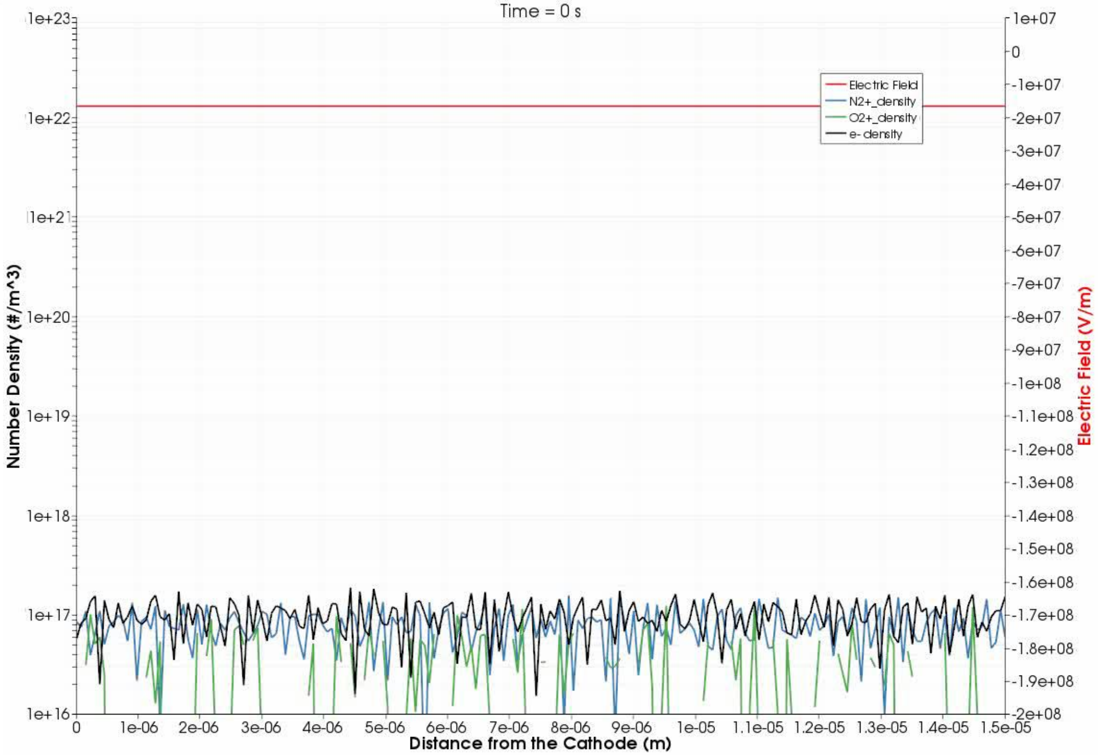
- Include Auger Neutralization
  - Upon approach to surface, ion is neutralized and liberates secondary electron with probabilty γ_e
  - γ_{e,N_2^+}=0.026, γ_{e,O_2^+}=0.018 (Lieberman & Lichtenberg, 2005)
    - Function of the ion species' ionization potential & surface work function (use ϕ=4.5 for Fe)
    - Independent of kinetic energy below ~500 eV
    - Dependent on surface contamination
- Include Fowler-Nordheim cold field emission (CFE)
  - Quantum tunneling through surface potential barrier accounting for local surface E-field, E_s

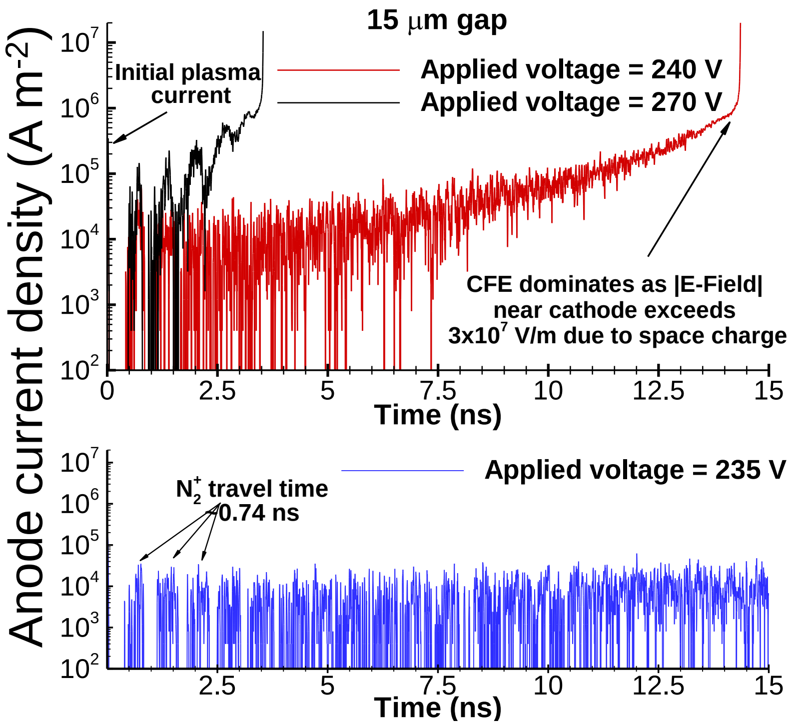
$$j = \frac{A[\beta E_s]^2}{\phi} exp\left(-\frac{B\phi^{1.5}v(y)}{[\beta E_s]}\right); \quad v(y) \approx 0.95 - \left(\frac{C[\beta E_s]^{0.5}}{\phi}\right)^2$$

  - Assume β=50 (typical for polished metals)



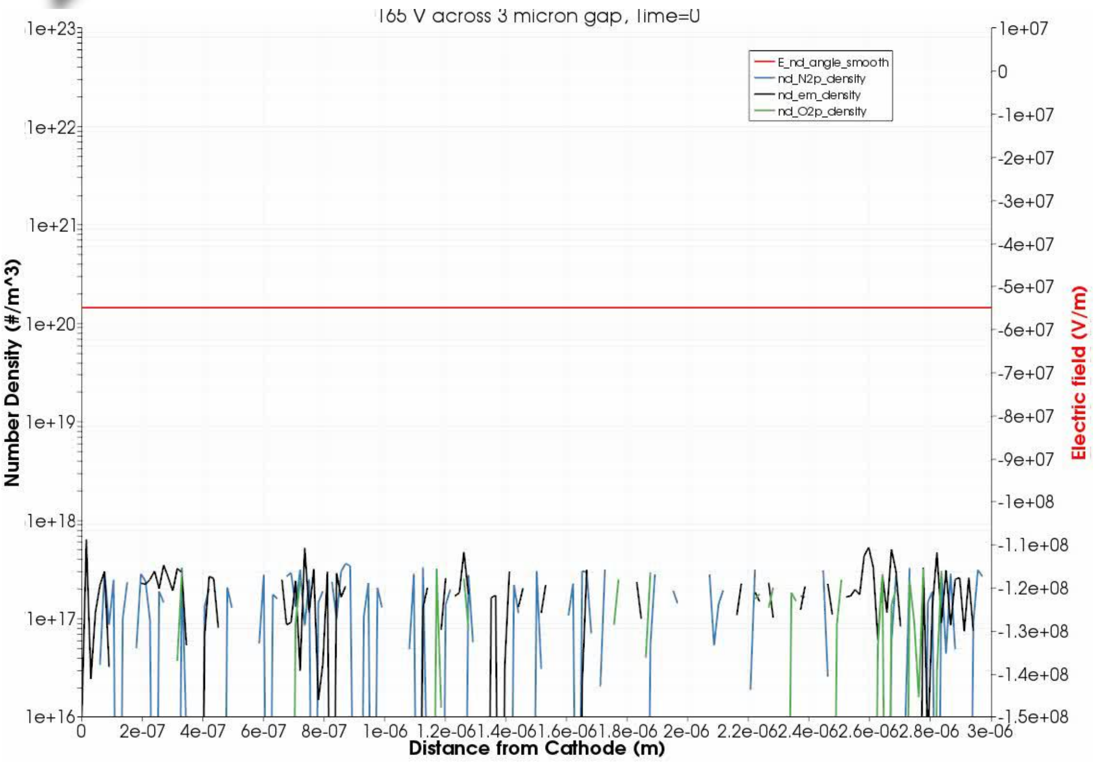
“Large” Gap Breakdown

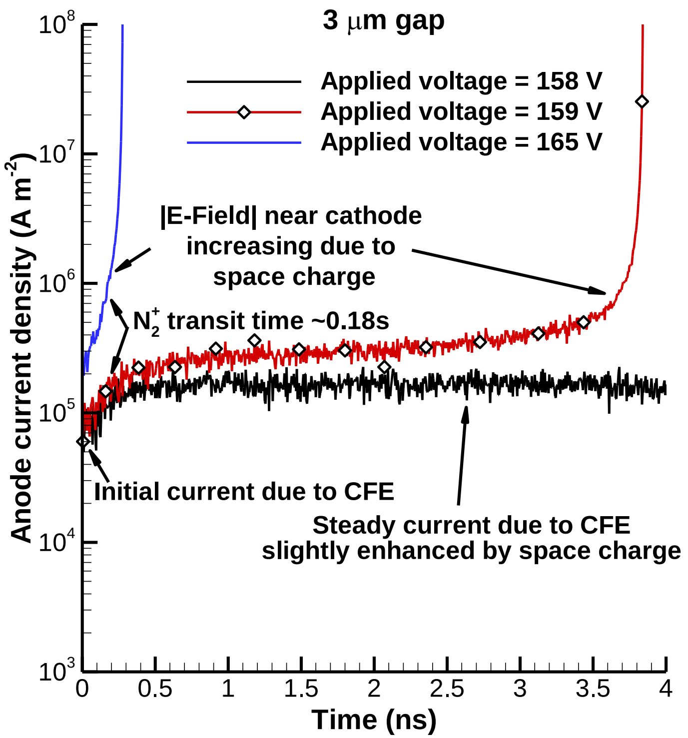




- Initial pulsing of current as ions transit gap and release electrons from cathode which then generate more ions
- Eventually quasi-neutral plasma established
  - Gap voltage drop only across sheath → Fowler-Nordheim emission accelerates breakdown
  - Most ionization events occur at edge of sheath

“Small” Gap Breakdown

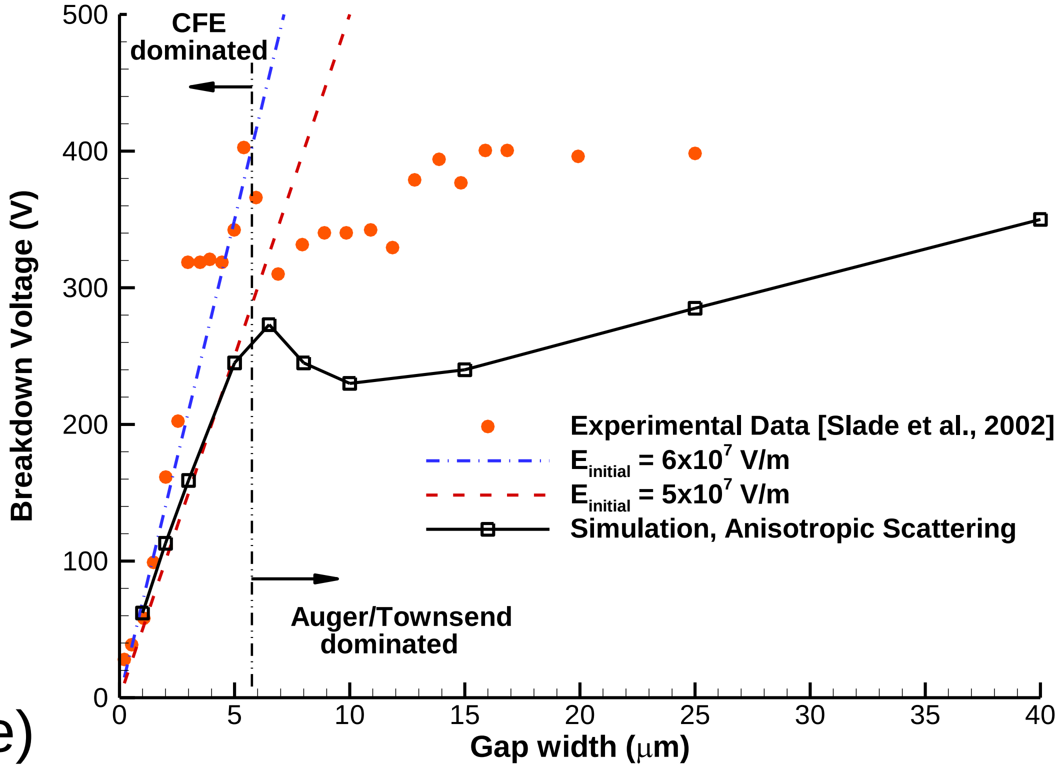




- For small enough gaps, Fowler-Nordheim field emission dominate source of electrons
- Ionization of gap gas → Net charge buildup near cathode leads to increased field emission and breakdown

Breakdown vs. Gap size: Experiment

- Small gaps: Fowler-Nordheim emission
  - Sensitive to β (Field Enhancement Factor) due to microscopic roughness & ϕ (cathode work function)
  - Data requires initial E-field of ~6×10^7 V/m to breakdown
  - Simulation requires smaller initial E-field as gap size increases (still Fowler-Nordheim regime)



- Large Gaps: Auger neutralization electron emission
  - Sensitive to secondary emission coefficient and e^- - neutral interactions

Paschen Breakdown Curve

- Obtain analytic breakdown criteria → compare to simulations
- Paschen breakdown criteria:

$$d\Gamma_e = \alpha(z)\Gamma_e dz, \qquad \alpha(z) \equiv \frac{1}{\lambda_{iz}(z)}$$

Change in e$^-$ flux due to ionization

$$\Gamma_i(0) - \Gamma_i(d_{gap}) = \Gamma_e(d_{gap}) - \Gamma_e(0)$$

Ionization charge neutral

Assume γ_{se} constant

$$\Gamma_e(0) = \gamma_{se}\Gamma_i(0)$$

Self-sustaining breakdown

$$\Gamma_i(d_{gap}) = 0$$

Assumption

Put it all together to get breakdown criterion (when field emission negligible):

$$1 + \frac{1}{\gamma_{se}} = exp\left(\int_0^{d_{gap}} \alpha(z)dz\right)$$

Paschen Breakdown Curve

- Further assume form for α(z): $\alpha(z) = const = A_p p\, exp\left(-\frac{B_p p}{E}\right)$
  - A_p & B_p fit to breakdown data and ≈constant over range of E/p
  - A_p & B_p based on e^--gas interactions (net ionization rate)

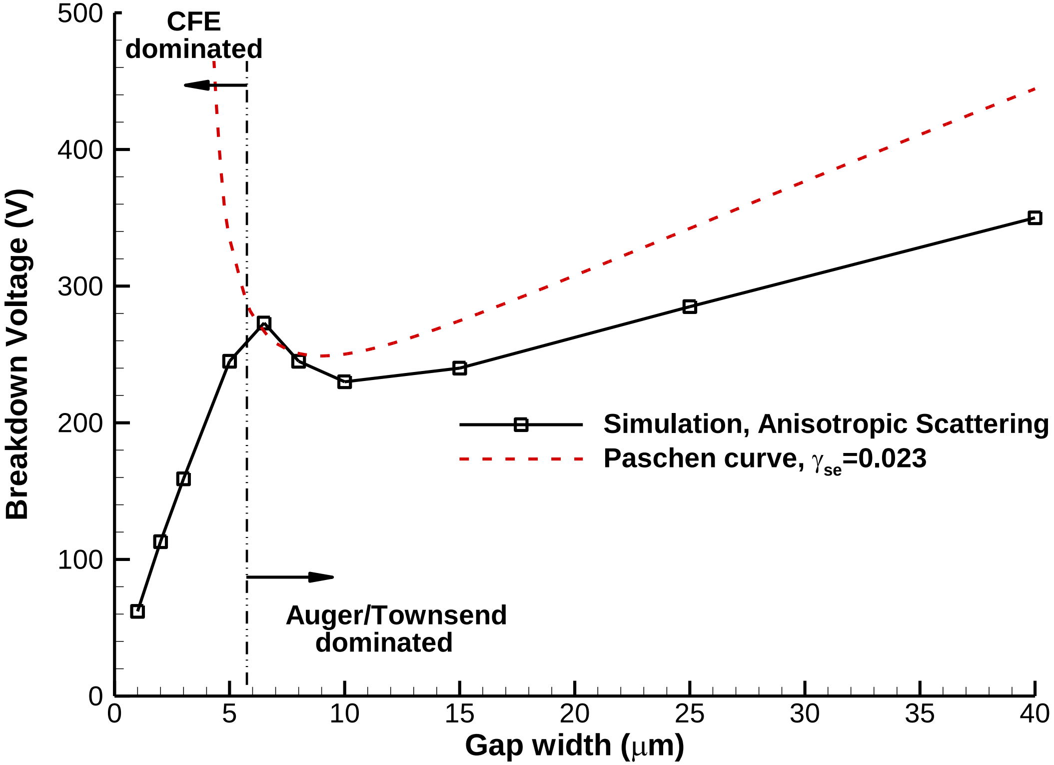
- Assume space charge negligible: $E = \frac{V_b}{d_{gap}}$

- Put it all together to obtain traditional Paschen Curve:

$$V_B = \frac{B_p pd}{ln\left(A_p pd\right) - ln[ln(1 + 1/\gamma_e)]}$$

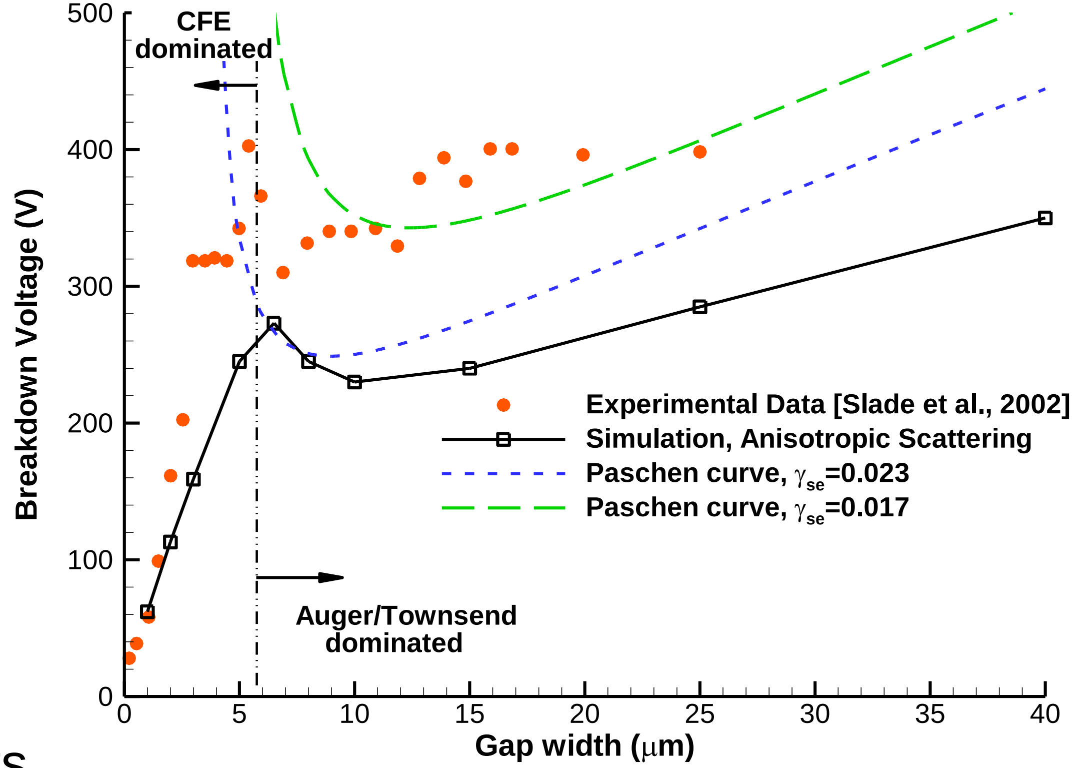
Breakdown vs. Gap size: Paschen

- Compare to Paschen curve: $V_B = \dfrac{B_p p d}{ln\left(A_p p d\right) - ln[ln(1 + 1/\gamma_e)]}$
- Decent agreement where CFE is negligible
- Discrepancy vs. Paschen (with γ_e=0.023) grows for large gaps → likely due to interaction physics model
  - Missing/inaccurate large energy loss mechanisms such as double ionization & dissociative ionization at higher energies?
  - Charge loss interactions inaccurate?



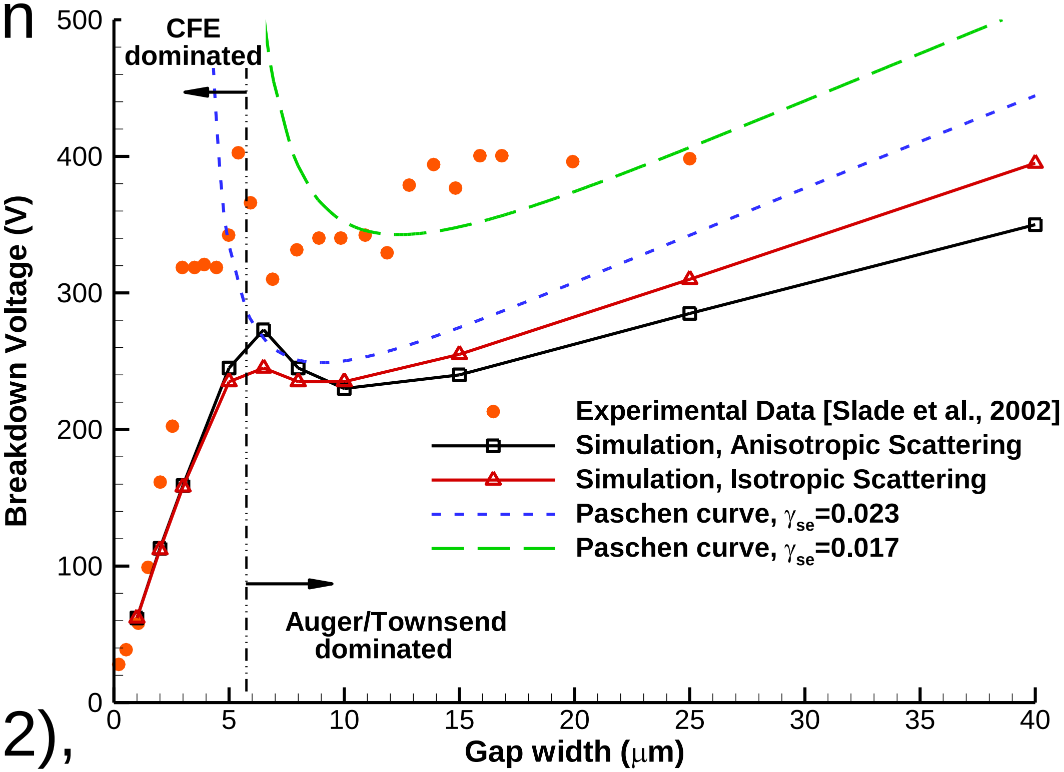
Breakdown vs. Gap size: Paschen

- Experimental breakdown voltages in large gaps (where Paschen should be valid) better fit by $\gamma_e \cong 0.017$
  - Small change in γ_e gives very different Paschen curves
  - Low γ_e for experiment (compared to data on clean surfaces) likely due to surface contamination/geometry
    - Implies higher surface work function
    - But CFE agreement gets (slightly) worse for higher work funtion!



Breakdown vs. Gap size: Scattering

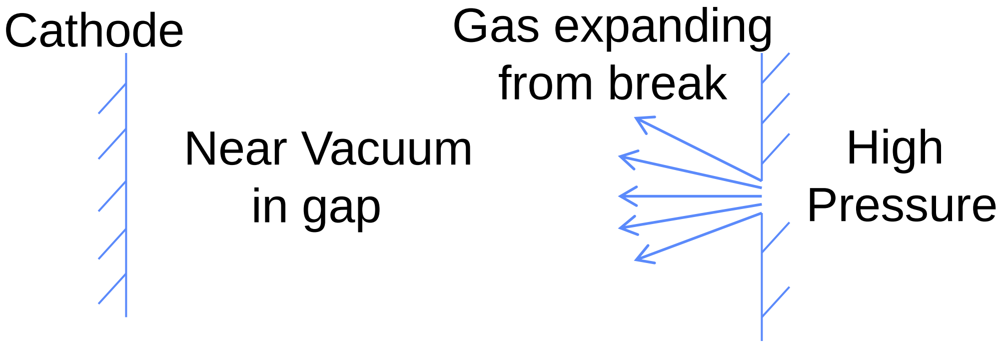
- Isotropic scattering for all collisions doesn’t change the breakdown voltage for very small gaps dominated by Fowler-Nordhiem emission
- For small gaps not CFE-dominated, V_b decreases with isotropic scattering
  - $Kn_{gap} \sim 0.2$
  - Isotropic scattering has more backscatter which yields a longer effective gap width and lower V_b



- For large gaps ($Kn_{gap} < 0.2$), V_b increases with isotropic scattering
  - Increased backscatter not as important as effect on eedf

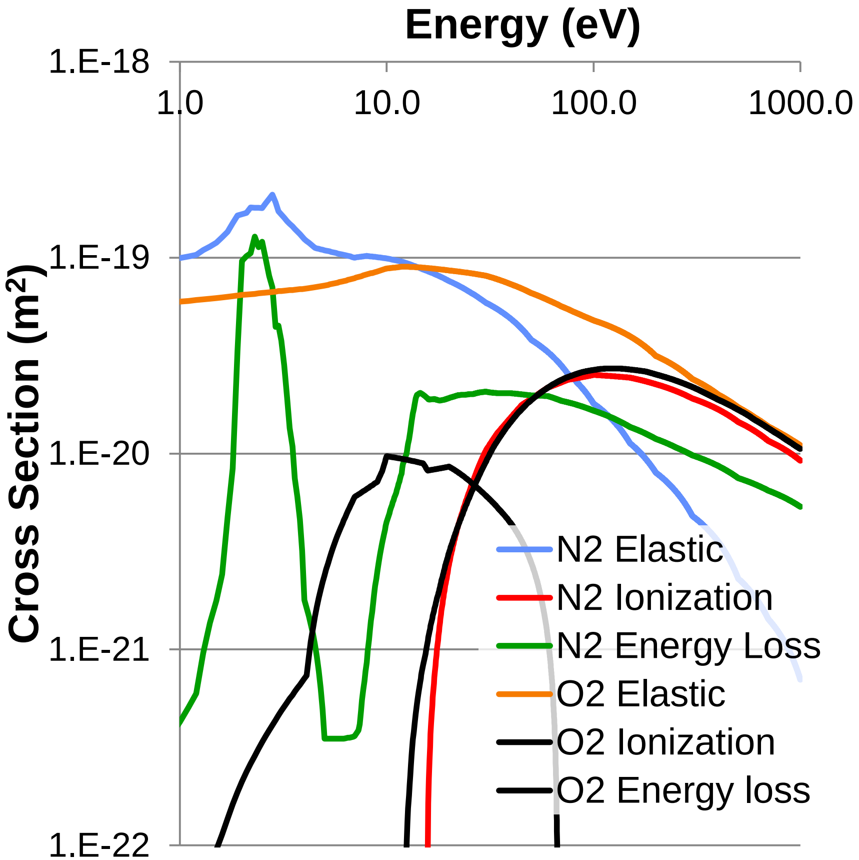
Non-uniform neutral gas breakdown

- Previously assumed the neutral gas in the gap was spatially uniform… what if it wasn't (assuming equal gas columns)?
- While Paschen's curve depends on the neutral gas column density (pd), implicit in the derivation is an ionization rate, $\alpha(z)$, *which depends on the electron energy distribution*
  - If gas density distribution allows for different eedf, change in ionization rate might change the breakdown voltage



Breakdown of non-uniform neutral gas

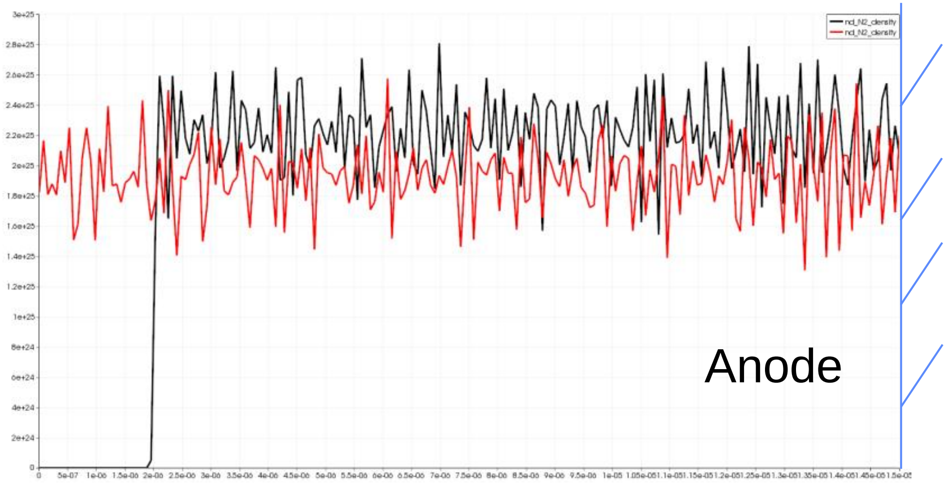
- V_B might decrease if gas is distributed such that e^- freely accelerate & avoid inelastic collisions
  - Hit gas near peak ionization cross section
  - Competition between losing path length for ionizations vs. more energy for ionizations
  - Effect probably dependent on gap size vs. mean free path (Kn_{gap})
- V_B might decrease if (more) ions can accelerate to E>1 keV such that their auger neutralization yield increases (large gaps or high pressures)



Breakdown of non-uniform neutral gas

- Assume step function gas density scaled so that gas column in gap is equal to the uniform gas density case

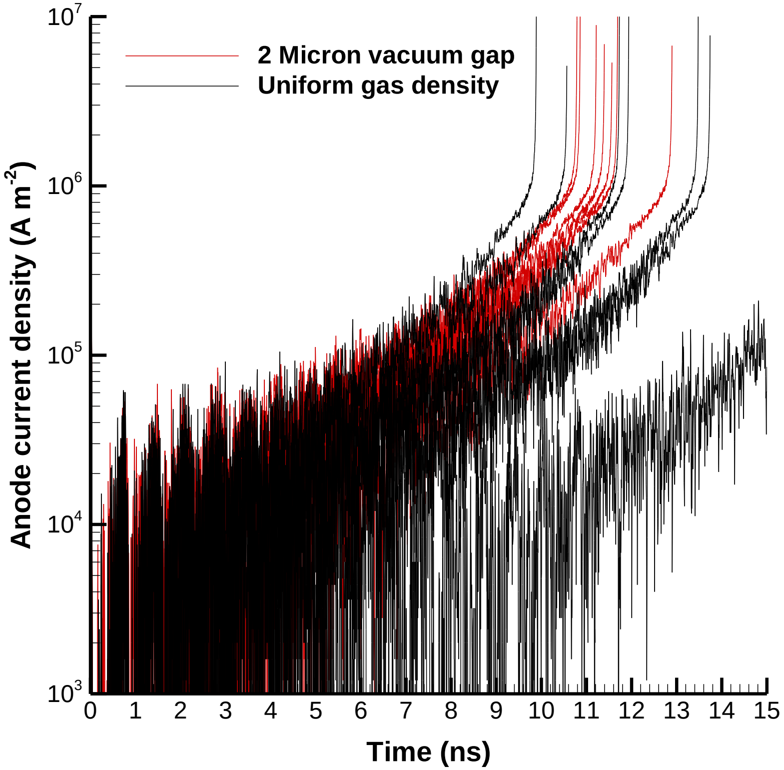
- Simulate 15 μm gap with vacuum out to 2 μm



  - 2 μm chosen because $V_{B,uniform}$ = 240 V → electrons will have an energy of 32 eV upon reaching neutral gas avoiding most inelastic excitation interactions

- Could just simulate this initial condition with the code
  - This would be slow: require a reservoir that would fill the gap with atmospheric pressure air for comparison to prior results

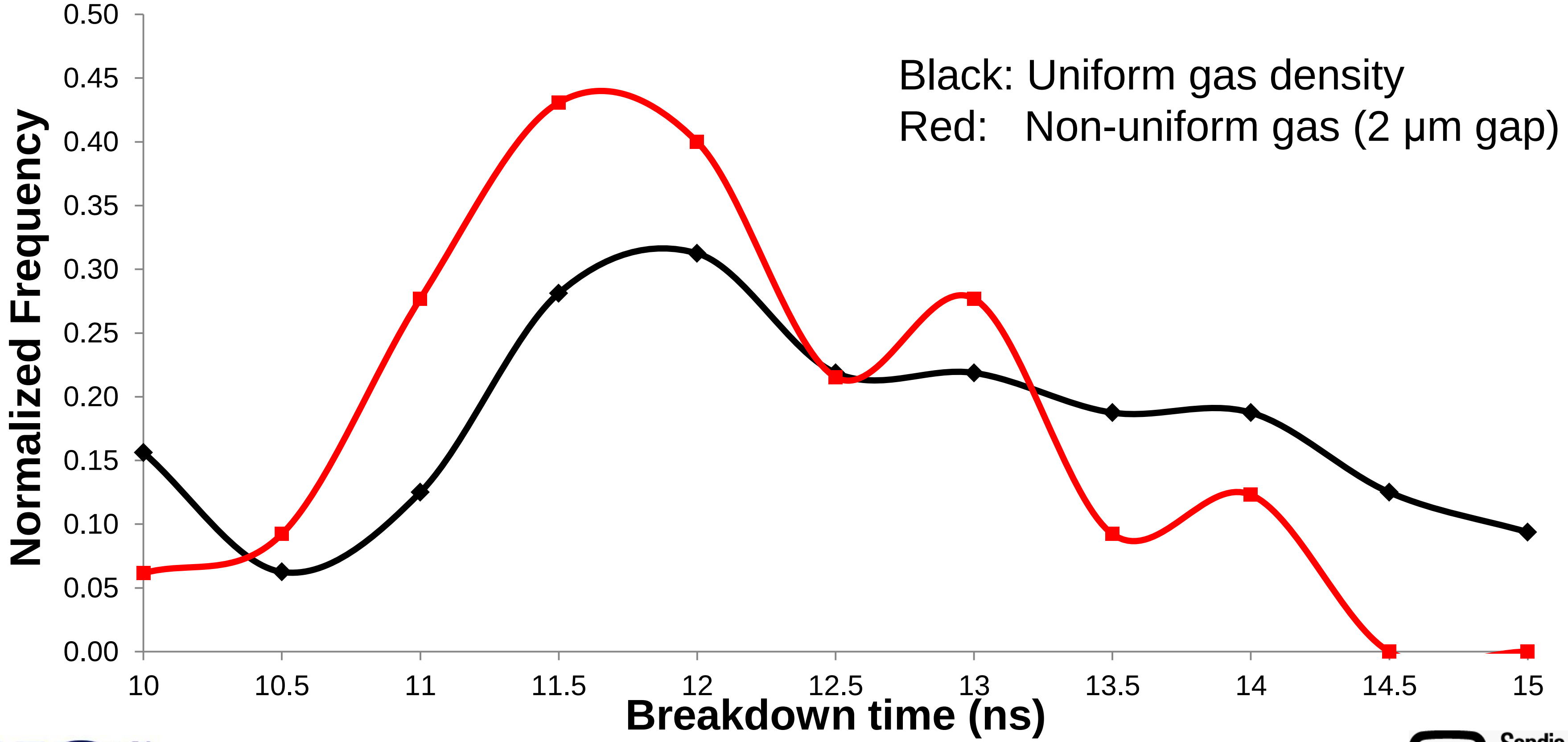
15 μm Gap: Current vs. time



- Breakdown time at a fixed voltage indicative of how close system is to V_b
- Difference between in breakdown times for uniform and non-uniform gas distributions just noise?

“Breakdown Time” Distribution

- 65×2 simulations with unique RNG seeds
- Breakdown Time ≡ when anode current density > 5×10^6 A/m^2
- Difference between distribution of breakdown times negligible



Why so little effect?

- Analytic (Paschen) breakdown criteria: $1 + \frac{1}{\gamma_{se}} = exp\left(\int_{0}^{d_{gap}=d_{eff}} \alpha(z)dz\right)$
- So whether non-uniform gas distributions change the breakdown voltage is a competition between
  - Reduced distance over which ionizations can occur:
    - $d_{eff} = d_{gap} - 2\mu m$
  - Increasing initial $\alpha(z)$ so that more ionization/unit length
- As defined, $\alpha(z)$ is the inverse of the ionization m.f.p.

$$\alpha(z) \equiv \frac{v_{iz}}{v_d} = \frac{n_g \int_{\varepsilon_{iz}}^{\infty} \left[n(\varepsilon,z)\sigma(\varepsilon)\sqrt{2\varepsilon/m_e} \right] d\varepsilon}{v_d}$$

EEDF contains the effect of all other collision types and accelerating field (as does v_d)

Why so little effect?

$$1+\frac{1}{\gamma_{se}} = exp\left(\int_{0}^{d_{eff}} \alpha(z)dz\right)$$

$$\alpha(z) \equiv \frac{v_{iz}}{v_d} = \frac{n_g \int_{\varepsilon_{iz}}^{\infty}\left[n(\varepsilon,z)\sigma(\varepsilon)\sqrt{2\varepsilon/m_e}\right]d\varepsilon}{v_d}$$

- $n(\varepsilon)$ can be made more favorable (larger α) by a vacuum gap out to some distance past the cathode (d-d_{eff})
  - But this increase is not sustained over the entire gap as the EEDF goes to steady state (not Maxwellian due to inelastic collisions) after ~few mean free paths
  - Steady state distribution is slightly *less* favorable for ionizations
    - Due to increased number density (to keep the column density the same) and hence less acceleration by the field between collisions
  - Also: $\alpha(z<d\text{-}d_{eff})=0$ since there is no neutral gas!

Conclusions 1

- Large Gaps:
  - – Auger neutralization is primary source of initial e^-
  - – Current “waves” as breakdown develops plasma in the gap
  - – Anisotropic (preferential forward) scattering is important:
    - For very large gaps ($Kn_{gap} << 1$) it *decreases* V_b
    - For moderate gap sizes ($Kn_{gap} > 0.1$) it *increases* V_b
  - – Discrepancy between simulation and experiment/theory indicates gas interaction model needs improvement

- Small Gaps:
  - – Fowler-Nordheim field emission e^- flux source – no “trigger” plasma needed
  - – Collisional processes with neutral gas not as important

Conclusions 2

- For all gap sizes, final breakdown occurs when quasi-neutral plasma forms a sheath and Fowler-Nordheim field emission results in super-exponential current growth
- Non-uniform gas distributions in the gap (for air)
  - For $Kn_{gap} < 0.25$ (right side of Paschen curve) the breakdown voltage does not change appreciably
    - Cancellation between increased initial ionization rate, reduced ionization rate several mean free paths into the gas, and the reduction in length over which ionization can occur
  - It is possible that for $Kn_{gap} > 0.25$ (left side of the Paschen curve) that the breakdown voltage will be reduced due to higher initial ionization rate in the first few mean free paths
    - Need to simulate low Kn_{gap} at lower gas pressures!