

ADVENTURES IN TWO-DIMENSIONAL PARTICLE-IN-CELL SIMULATIONS OF ELECTRONEGATIVE DISCHARGES

PART 1: DOUBLE LAYERS IN A TWO REGION DISCHARGE

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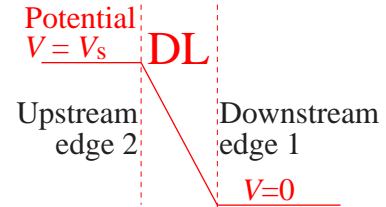
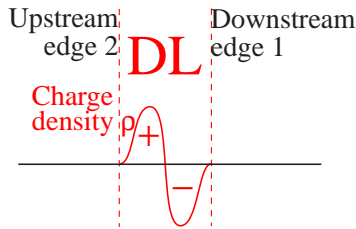
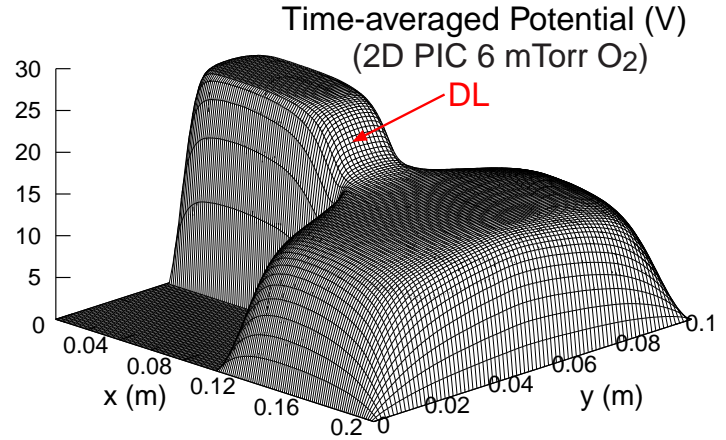
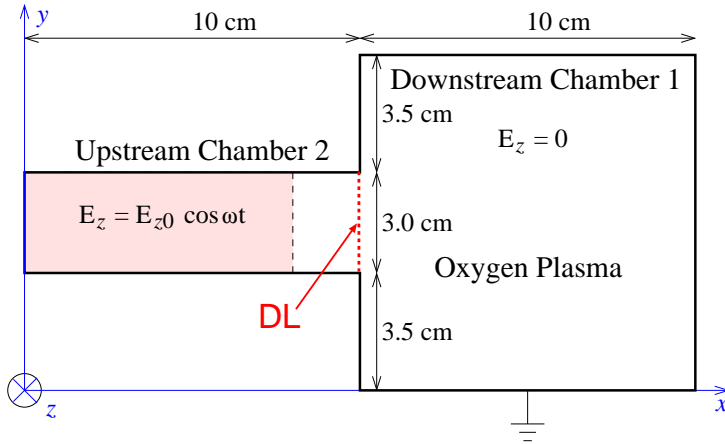
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OUTLINE

- Introduction
- “Experiments”
 - 2D particle-in-cell (PIC) simulations with rescaled oxygen cross sections
- Theory
 - 1D collisionless model of double layer (DL)
 - Global (volume-averaged) model of upstream and downstream particle and energy balances
- Comparisons
 - Reasonable agreement but also some differences
- Slow and fast waves
 - The DL has time-varying structure

INTRODUCTION



- Why does a DL form at low pressures?
 - The particle loss rate is greater upstream than downstream due to the smaller upstream radius
 - A higher ionization rate (and T_e) is needed upstream than downstream
 - A DL both “insulates” the low downstream T_e from the high upstream T_e , and it accelerates electrons upstream to increase the ionization rate there

PIC SIMULATION METHOD

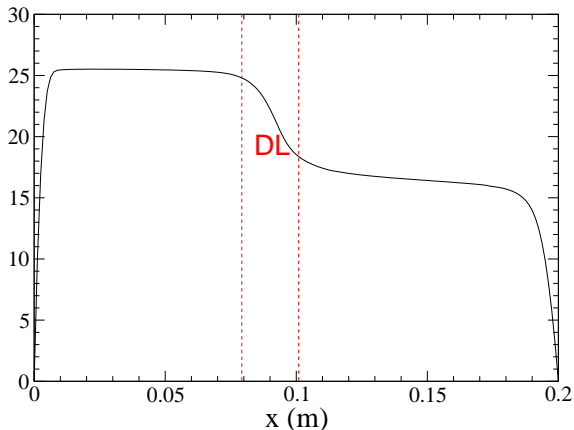
- Self-consistent results from first principles with no assumptions about electron and ion velocity distributions
- Upstream heating at 13.56 MHz \perp to the plane of the simulation
- RF field adjusted to keep number of upstream electrons constant
- Stability, speed and accuracy require small plasma reactors with low densities and large Debye lengths:

$$n_e \approx 4 \times 10^{14} \text{ m}^{-3}, \lambda_D \approx 0.8 \text{ mm}$$

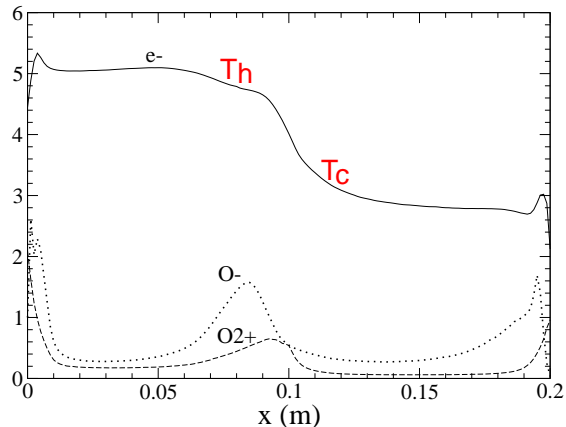
- Due to low densities, rescaled oxygen cross sections were used:
Positive-negative ion recombination $\uparrow \times 20$
Dissociative attachment $\uparrow \times 5$
- A typical simulation takes 1–2 weeks
- The pressure range explored is 0.5–24 mTorr
- A DL was observed for 1–24 mTorr

PIC RESULTS FOR 6 mTorr O₂ DISCHARGE

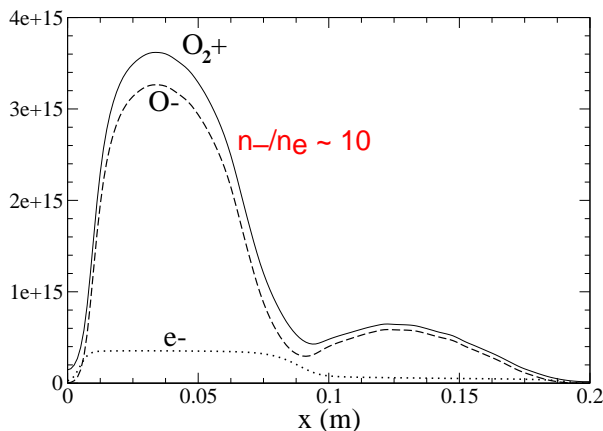
Axial Potential (V)



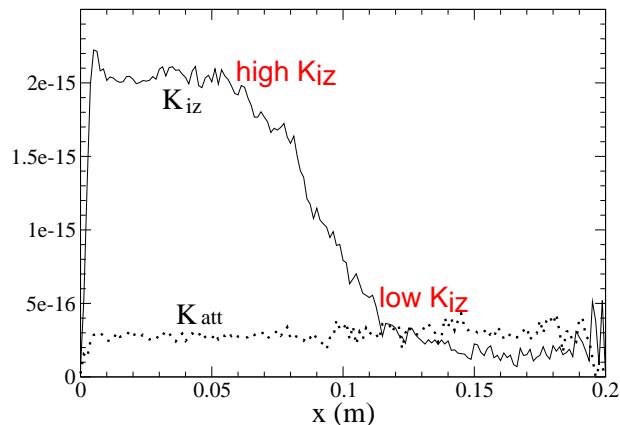
Radially averaged T (V)



Axial Density (m⁻³)

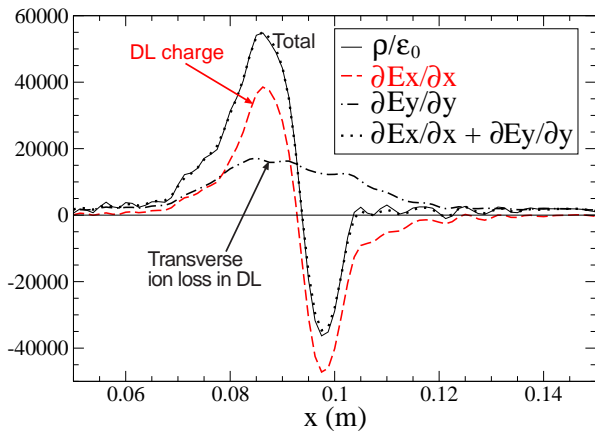


Axial Collision Rates (m³/s)

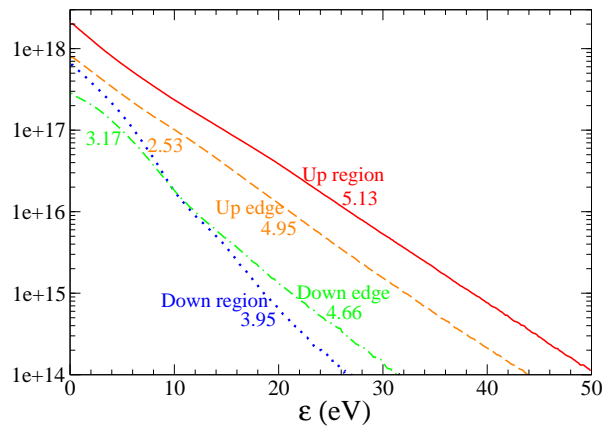


RESULTS FOR 6 mTorr O₂ DISCHARGE (CONT'D)

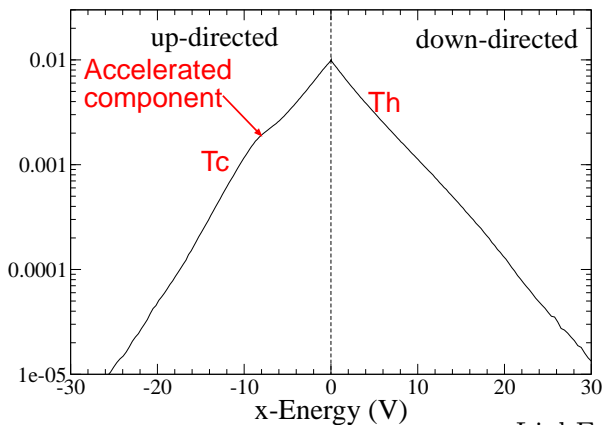
Charge Density Components in DL (V/m²)



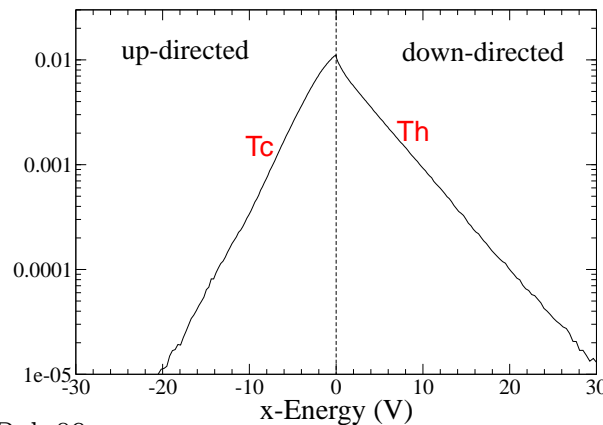
EEDF (a.u.)



Up edge x-component EEDF (a.u.)

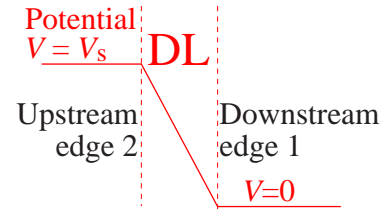


Down-edge x-component EEDF (a.u.)

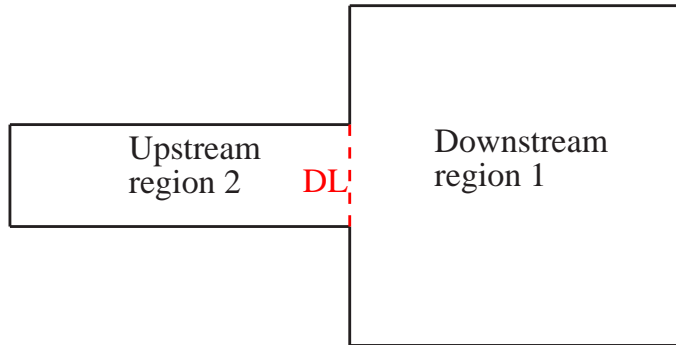


DL MODEL

- Charge density ρ and potential V within the DL are found by solving Poisson's equation
- Six types of particles contribute to ρ :
 - thermal positive ions, negative ions, and electrons
 - positive ions accelerated downstream
 - negative ions and electrons accelerated upstream
- The particle motions are 1D and collisionless
- The boundary conditions are that ρ and $d\rho/dV$ vanish at the DL edges
- An additional condition is that the sum of positive and negative charge in the double layer vanishes; equivalently, the total force acting on the double layer vanishes
- A final condition that upstream and downstream-directed electron fluxes nearly balance determines the equilibrium value of V_s/T_h .

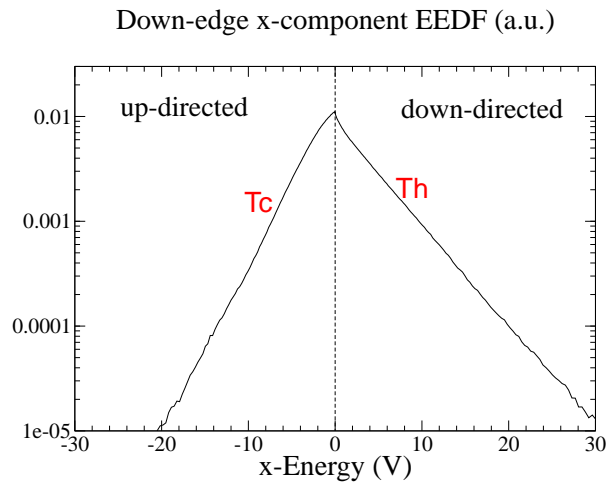
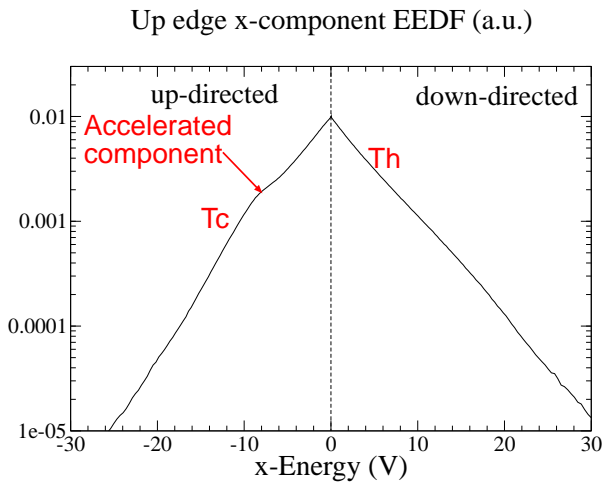
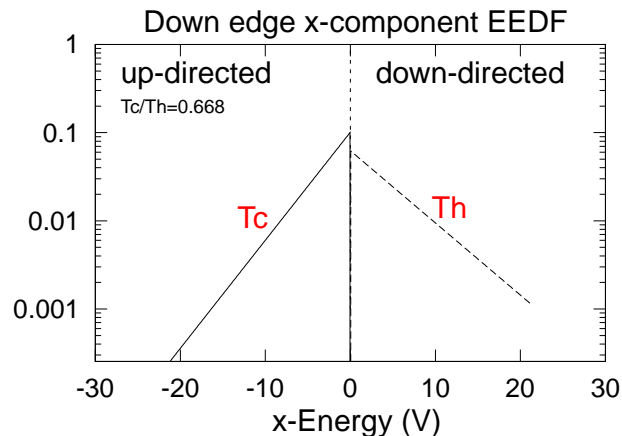
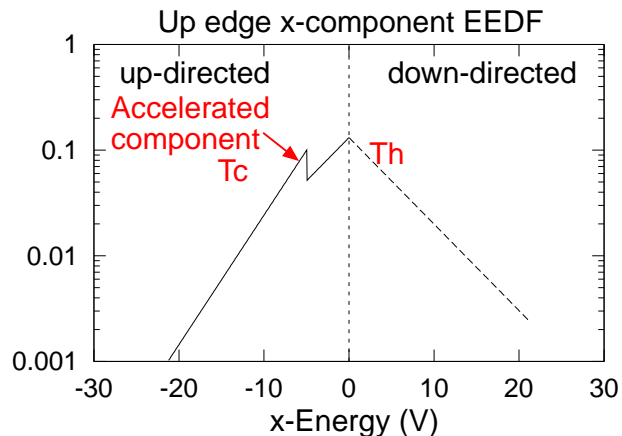


PARTICLE AND ENERGY BALANCES



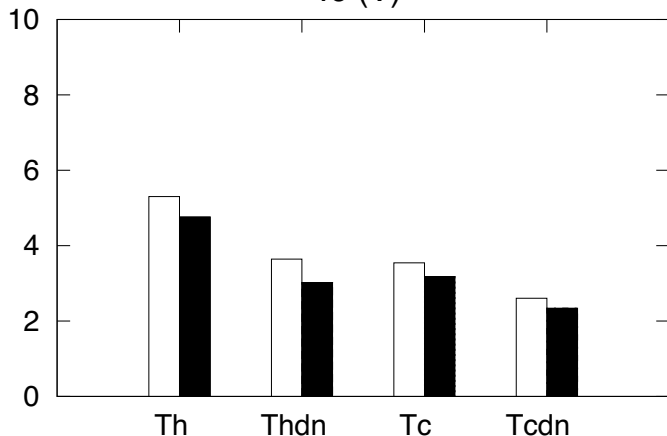
- We use a 2D rectangular geometry
- To determine the equilibrium quantities we use
 - global particle balance upstream
 - global particle balance downstream
 - global energy balance downstream
- Upstream energy balance (which determines the upstream electron density) depends on the input power; we use the PIC simulation value for the comparisons

MODEL (TOP) and PIC (BOTTOM) EEDF'S (6 mTorr O₂)

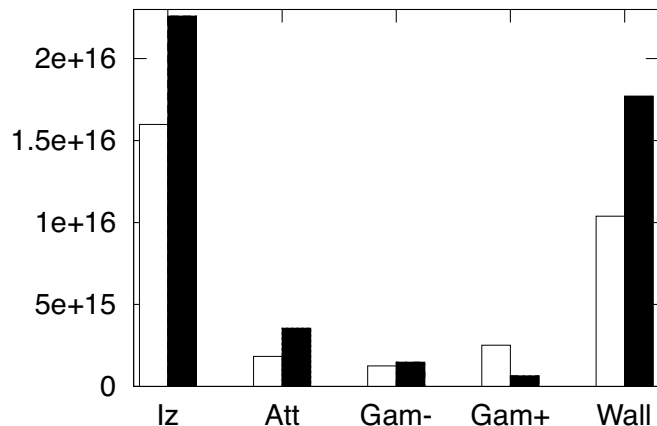


MODEL (WHITE) AND PIC (BLACK) FOR 6 mTorr O₂

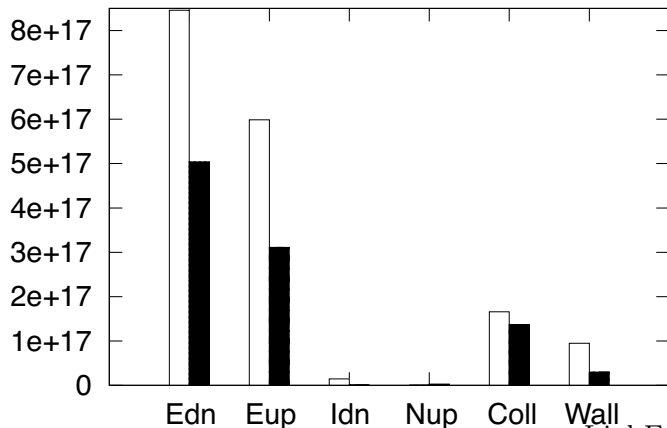
Te (V)



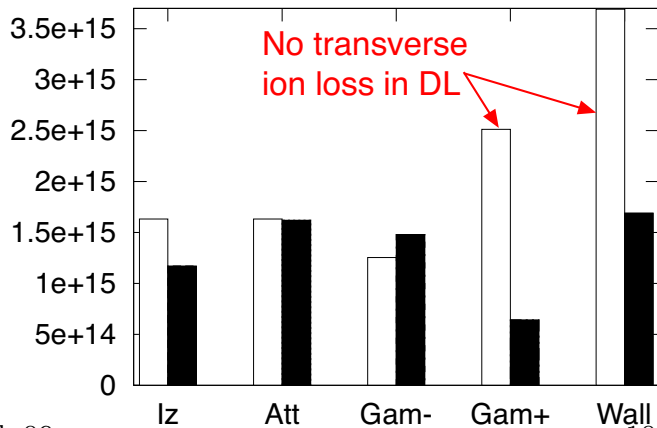
Up elec bal (#/s)



Down energy bal (eV/s)

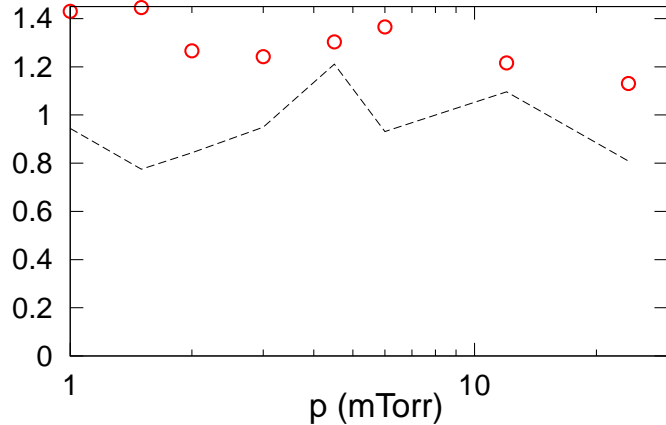


Down elec balance (#/s)

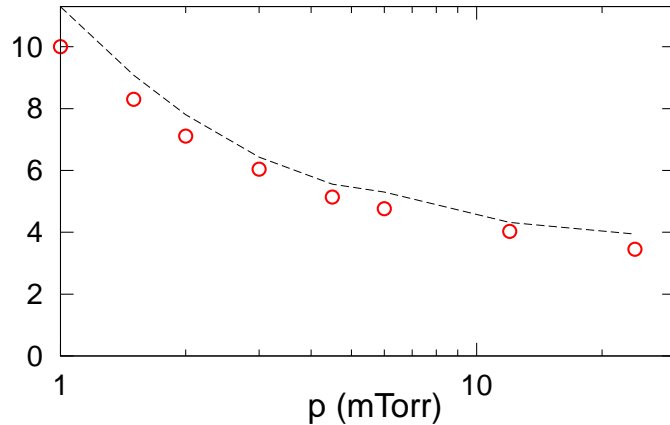


MODEL (DASH) AND PIC (CIRCLES) VS PRESSURE

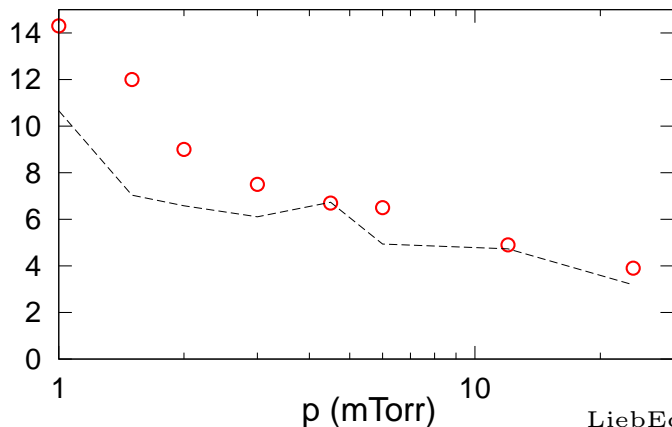
Vs/Th



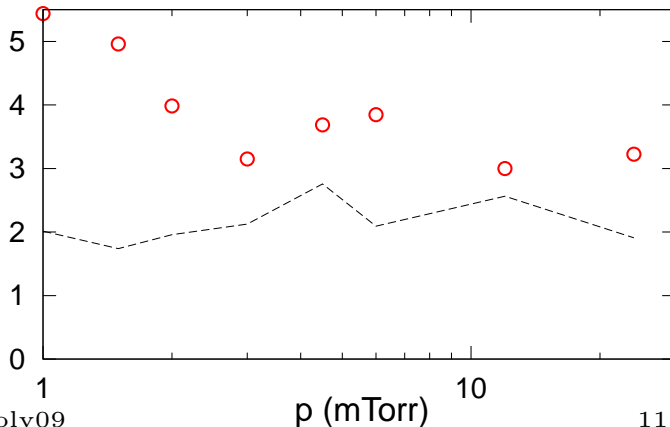
Th (V)



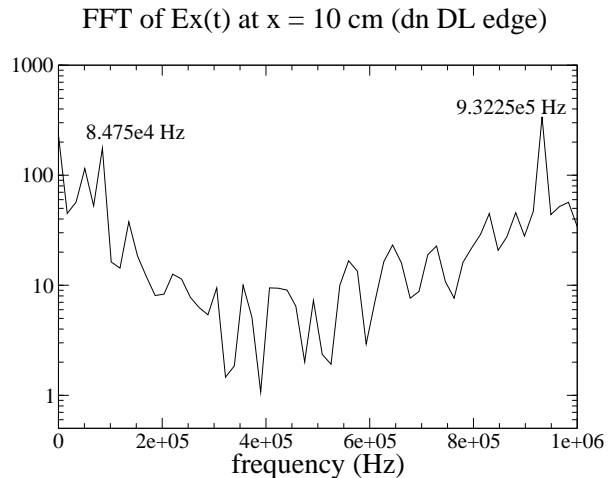
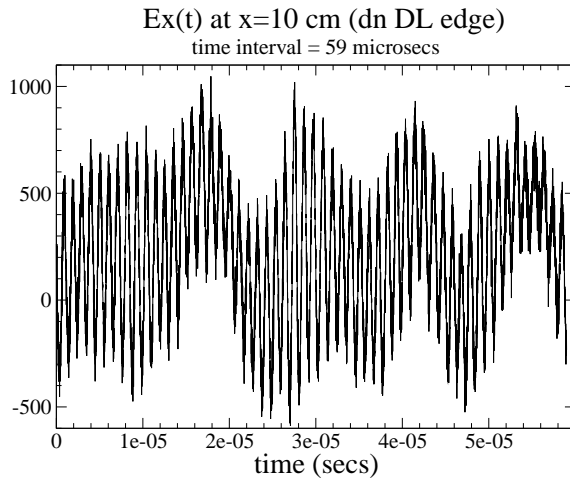
Vs (V)



ne2/ne1



SLOW AND FAST WAVES: INSTABILITIES (6 mTorr O₂)

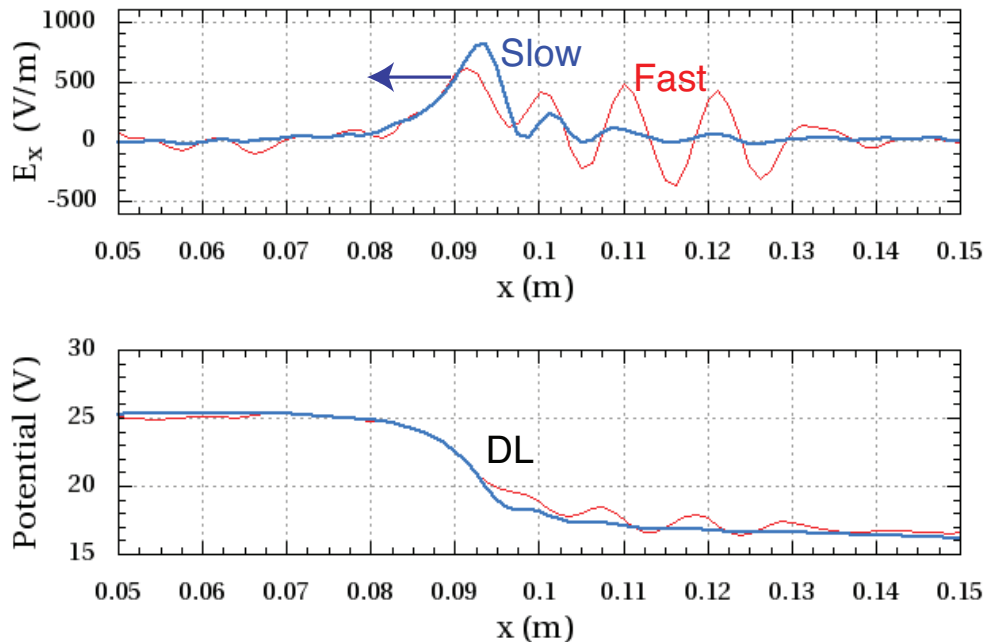


- At 2–12 mTorr, the DL coexists with an unstable slow wave that originates downstream and propagates upstream as it grows
- The wave frequency is 50–100 kHz with a wavelength of order 1 cm
- The wave produces $\sim 20\%$ oscillations in the double layer potential and ~ 0.5 cm oscillations in the DL position
- We believe the wave is driven by counter-streaming flows of positive and negative ions (Tuszewski and Gary, 2003)
- There is also a fast wave that increases spatially along with the slow wave at the higher pressures, with $f \sim 1$ MHz and $\lambda \sim 1$ cm

MOVIE SHOWING SLOW AND FAST WAVES

Red solid line: fast waves averaged over $0.1475 \mu\text{s}$ intervals
Blue solid line: slow waves averaged over $1.18 \mu\text{s}$ intervals

160. Waves in 6 mTorr DL region (23.6 microseconds)



**ADVENTURES IN TWO-DIMENSIONAL
PARTICLE-IN-CELL SIMULATIONS
OF ELECTRONEGATIVE DISCHARGES**

PART 2:

TRANSPORT IN A MAGNETIZED DISCHARGE

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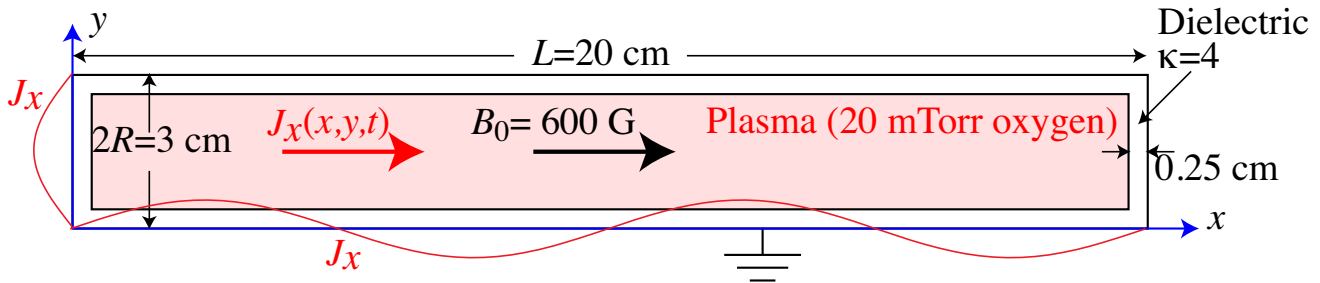
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OUTLINE

- Introduction
- “Experiments” with “uniform” electron temperature
 - 2D PIC simulations with rescaled oxygen cross sections
- Model and comparisons
 - New model (differs from Gary et al, to appear in J. Phys. D)
- “Experiments” with hot core and cold edge
 - 2D PIC simulations with “iodine-like” cross sections
- Two-region model and comparisons

INTRODUCTION

- Rectangular grounded chamber with insulating walls
- Spatially varying axial rf current density J_x



- For an unmagnetized discharge, negative ions are confined by the (positive) plasma potential
- For a magnetized discharge with uniform axial B_0 :
 - What electron temperature profiles can be obtained?
 - What is the negative ion flux to the transverse walls?
 - What are the electron fluxes to the axial and transverse walls?
 - What are the transverse diffusion coefficients for positive ions, negative ions, and electrons?

PIC SIMULATION METHOD

- 13.56 MHz **axial** RF current density J_x
- Adjust amplitude and spatial variation to obtain $T_e \approx \text{const}$

$$J_x = 1 \cdot \sin \frac{4\pi x}{L} \sin \frac{\pi y}{2R} \quad [\text{A/m}^2]$$

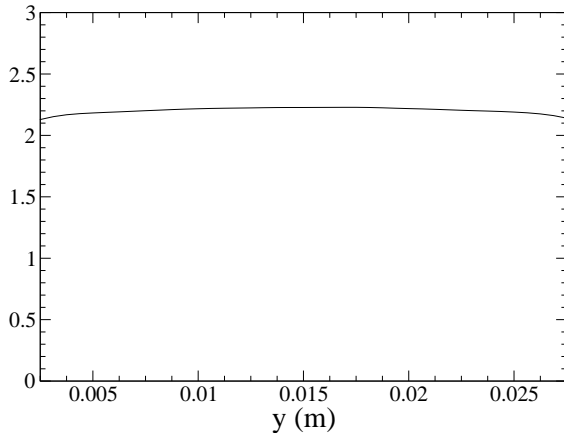
- Transverse heating (E_y 's or E_z 's) did not work
- Larger amplitudes or uniform J_x 's \Rightarrow large T_e 's at the transverse and/or axial edges
- $B_0 = 600$ G (sometimes 300 or 1200 G)
- Stability, speed, accuracy, and $T_e \approx \text{const}$ require low densities and large Debye lengths:

$$n_e \approx 2 \times 10^{13} \text{ m}^{-3}, \lambda_D \approx 0.8 \text{ cm (!)}$$

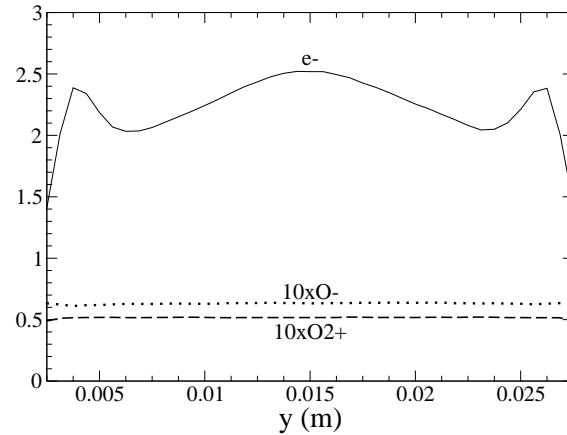
- Due to low density, rescaled oxygen cross sections were used:
Positive-negative ion recombination $\uparrow \times 20, \times 100, \text{ etc}$
- A typical simulation takes 1–2 weeks

PIC RESULTS FOR $100 \times K_{\text{rec}}$ O₂ DISCHARGE

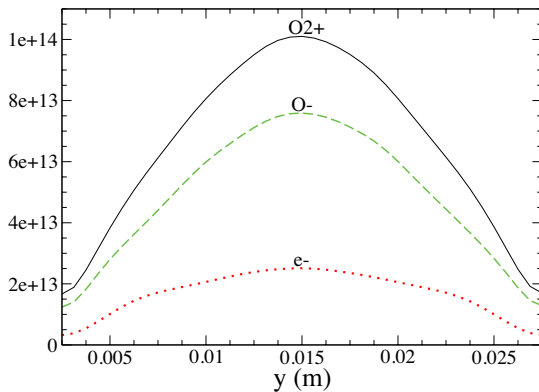
Radial Potential (V)



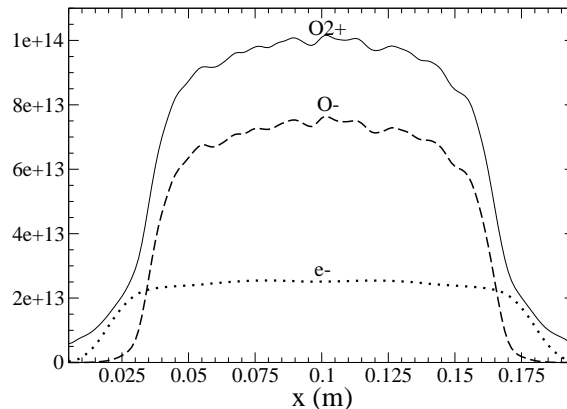
Radial T (eV)



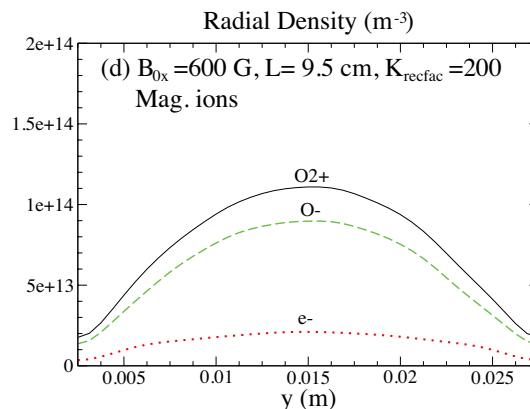
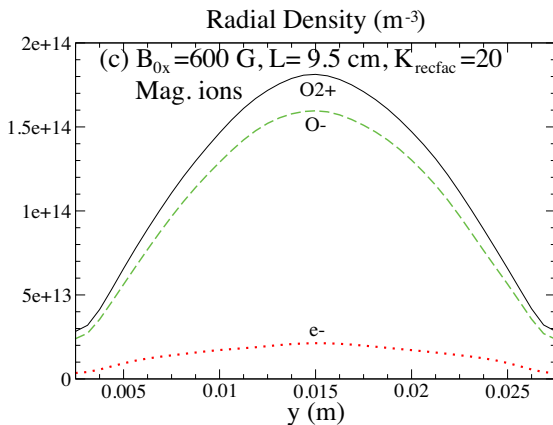
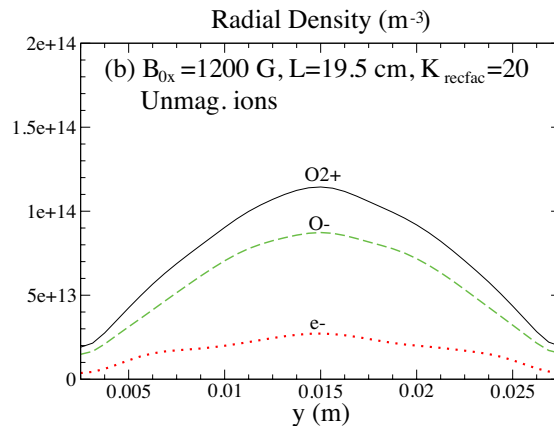
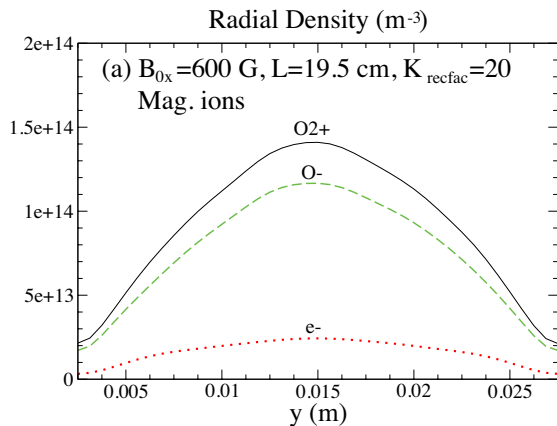
Radial Density (m⁻³)



Axial Density (m⁻³)

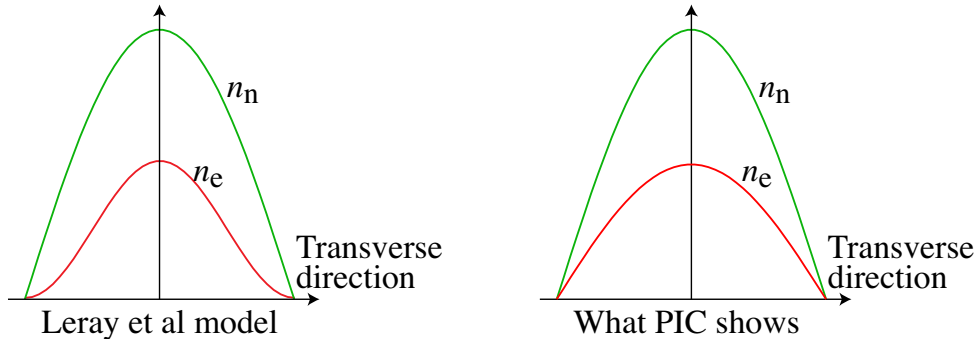


PIC RESULTS FOR OTHER O₂ DISCHARGES



CONCLUSIONS FROM PIC SIMULATIONS

- Cosine transverse electron and negative ion density profiles
 \Rightarrow constant electronegativity $\alpha_0 = n_n/n_e$



- Transverse electron/negative ion flux $\Gamma_{\perp e}/\Gamma_{\perp n} \approx D_{\perp e}/\alpha_0 D_{\perp n}$
- Leray et al model confirmed for axial loss frequency

$$\nu_L \approx \frac{2D_i}{RL} \left(1 + \frac{T_e}{T_i} \right)^{1/2}$$

- Transverse diffusion coefficients $D_{\perp e}$, $D_{\perp i}$, and $D_{\perp n}$ are classical

1D MODEL

- Electron balance

$$-D_{\perp e}^* \frac{d^2 n_e}{dy^2} = (\nu_{iz} - \nu_{att})n_e - \nu_L(n_e + n_n)$$

- Negative ion balance

$$-D_{\perp n}^* \frac{d^2 n_n}{dy^2} = \nu_{att}n_e - K_{rec}n_n(n_e + n_n)$$

- $D_{\perp e}^*$ and $D_{\perp n}^*$ are the transverse ambipolar diffusion coefficients, obtained from

$$\Gamma_{\perp i} = \Gamma_{\perp e} + \Gamma_{\perp n}$$

in terms of the species mobilities and diffusion coefficients

- Cosine density profiles with $n_n = \alpha_0 n_e$ (from PIC)
- Boundary conditions $n_e = n_n = 0$ at transverse wall

⇒ good agreement with PIC results

SCALINGS FOR 1D MODEL

- Transverse wall negative ion current = $2\pi \frac{L}{R} D_{\perp n}^* \alpha_0 \cdot n_e$
- Transverse wall electron current = $2\pi \frac{L}{R} D_{\perp e}^* \cdot n_e$
- End wall particle current = $2D_i(1 + \alpha_0)(1 + \frac{T_e}{T_i})^{1/2} \cdot n_e$

- Negative ion balance:

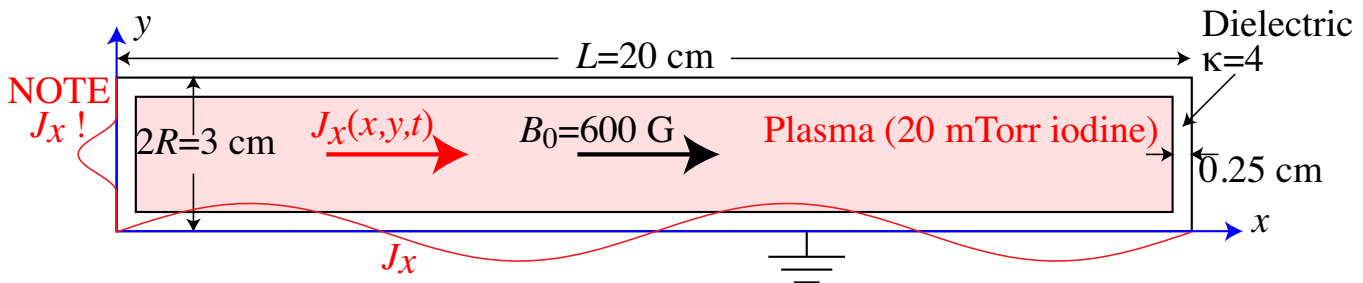
$$\frac{4R}{\pi} \nu_{\text{att}} = \frac{\pi}{R} D_{\perp n}^* \alpha_0 + K_{\text{rec}} n_{e0} \alpha_0 (1 + \alpha_0)$$

- Range of solutions:

$$0 < \alpha_0 < \frac{4}{\pi^2} \frac{R^2}{D_{\perp n}^*}$$

TWO-REGION IODINE SIMULATIONS

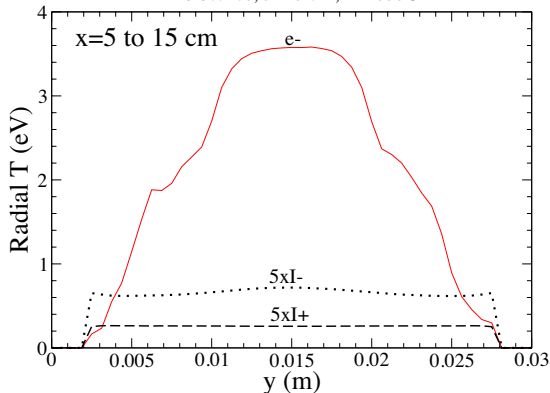
- Goal was to obtain a high T_e core with a cold T_e periphery
- Rectangular grounded chamber with insulating walls
- 13.56 MHz J_x peaked at transverse midplane



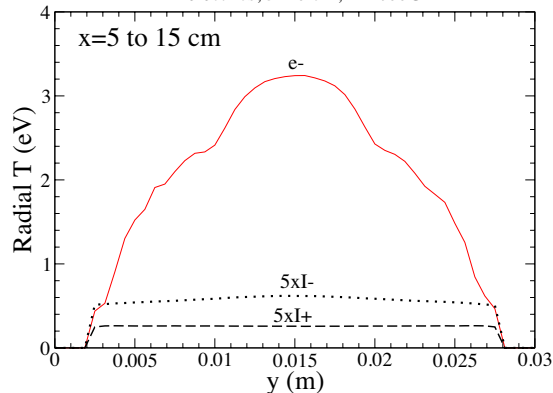
- Rescaled oxygen cross sections were used:
 - Positive-negative ion recombination $\uparrow \times 20$
 - Attachment $\uparrow \times 5$ (w/wo 4.2 V threshold energy)
- Iodine masses were used

PIC RESULTS FOR IODINE DISCHARGE

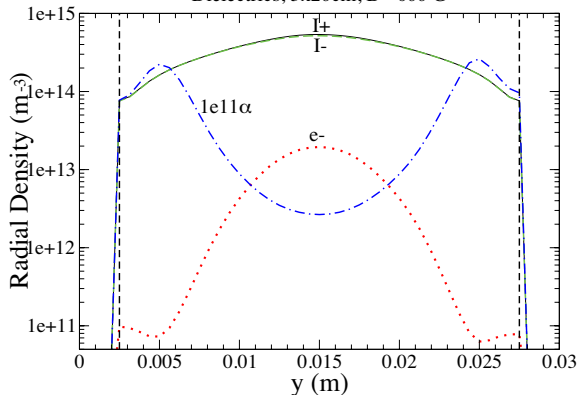
20 mT 20xKrec, 5xKatt(No Thr.)
Dielectrics, 3x20 cm, B= 600G



20 mT Iodine 20xKrec, 5xKatt(4.2V Thr.)
Dielectrics, 3x20 cm, B= 600G

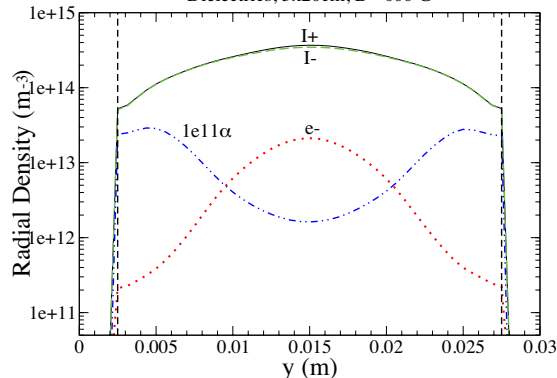


20 mT Iodine 20xKrec, 5xKatt(No Thr.) Discharge
Dielectrics, 3x20cm, B= 600 G



No attachment threshold

20 mT Iodine 20xKrec, 5xKatt(4.2V Thr.) Discharge
Dielectrics, 3x20cm, B= 600 G



4.2 V attachment threshold

TWO-REGION 1D MODEL

- Electron balance

$$-D_{\perp e}^* \frac{d^2 n_e}{dy^2} = (\nu_{iz} - \nu_{att})n_e - \nu_L(n_e + n_n)$$

(ν_{iz} in the core, $\nu_{iz} = 0$ in the periphery)

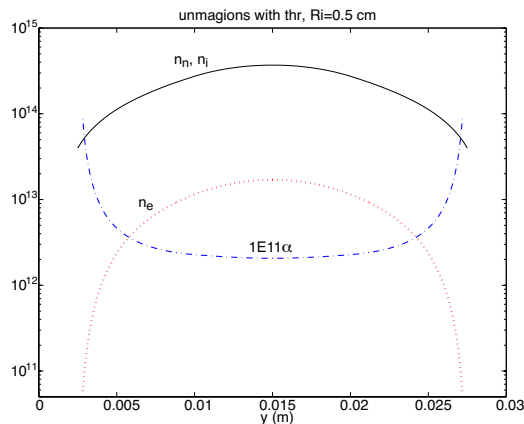
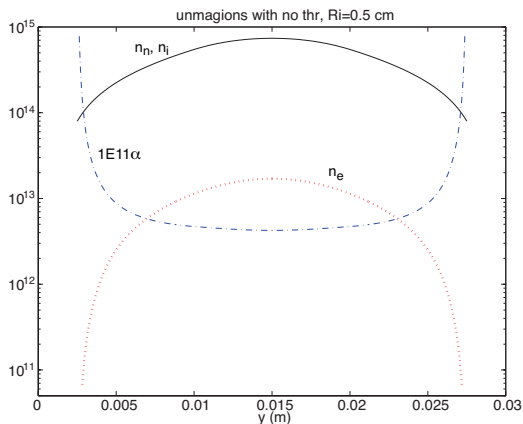
- Negative ion balance

$$-D_{\perp n}^* \frac{d^2 n_n}{dy^2} = \nu_{att}n_e$$

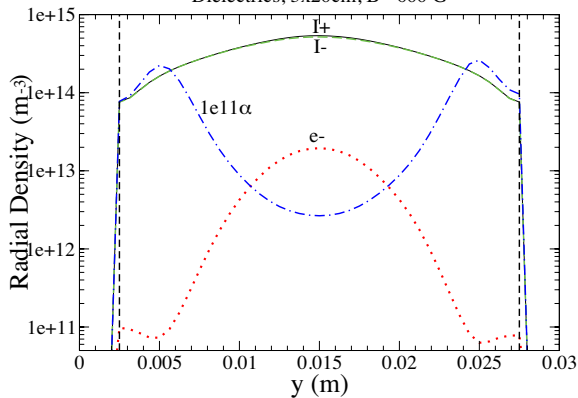
(Neglect recombination compared to negative ion transverse loss)

- Match densities and fluxes at the core-periphery transition
- Boundary conditions $n_e = n_n = 0$ at transverse wall
- This linear system can be solved exactly

COMPARISON OF MODEL WITH PIC

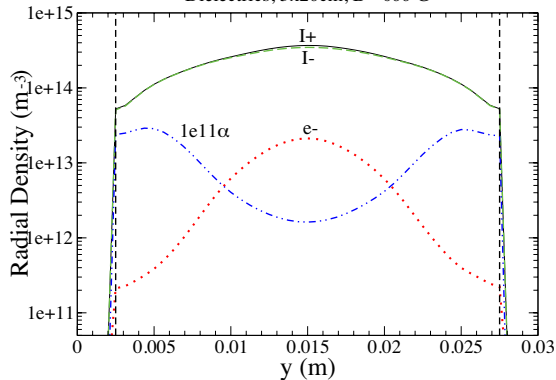


20 mT Iodine 20xKrec, 5xKatt(No Thr.) Discharge
Dielectrics, 3x20cm, B= 600 G



No attachment threshold

20 mT Iodine 20xKrec, 5xKatt(4.2V Thr.) Discharge
Dielectrics, 3x20cm, B= 600 G



4.2 V attachment threshold

CONCLUSIONS

- 2D PIC simulations can be powerful tools to study the physics of electronegative discharges
- Experimental parameters can be easily varied; various physics can be turned “on” and “off”
- These simulations can provide diagnostics that would be very difficult to do in laboratory experiments
- The models, verified by PIC, can give important scalings that can be used to design new PIC and experimental configurations

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