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

PART 1:

DOUBLE LAYERS IN A TWO REGION DISCHARGE

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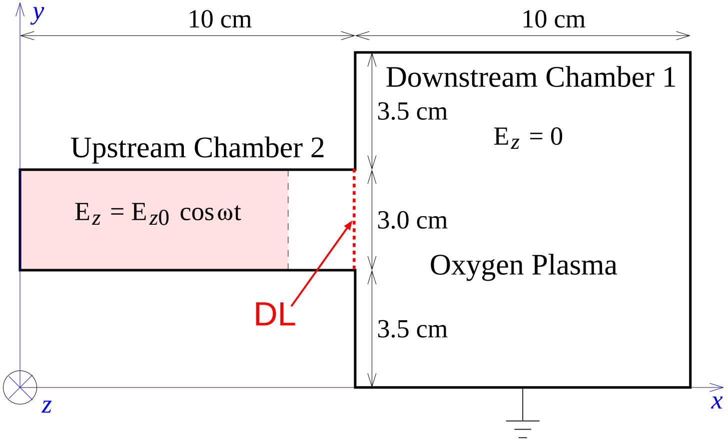
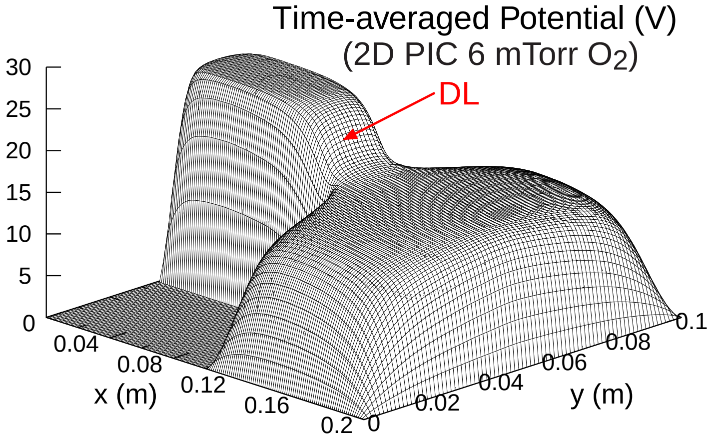
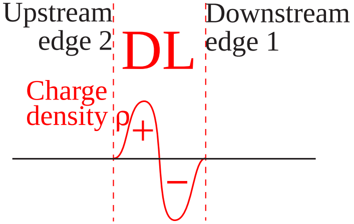
OUTLINE

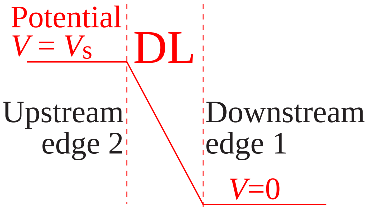
- Introduction
- “Experiments”
  — 2D particle-in-cell (PIC) simulations with rescaled oxygen cross sections
- Theory
  — 1D collisionless model of double layer (DL)
  — Global (volume-averaged) model of upstream and downstream particle and energy balances
- Comparisons
  — Reasonable agreement but also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

INTRODUCTION




Time-averaged Potential (V)
(2D PIC 6 mTorr O_2)





- 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 ⊥ 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:

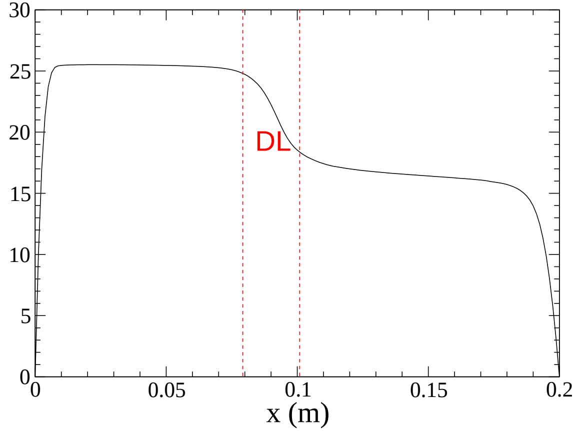
$$n_e \approx 4 \times 10^{14}\ \mathrm{m}^{-3},\ \lambda_D \approx 0.8\ \mathrm{mm}$$

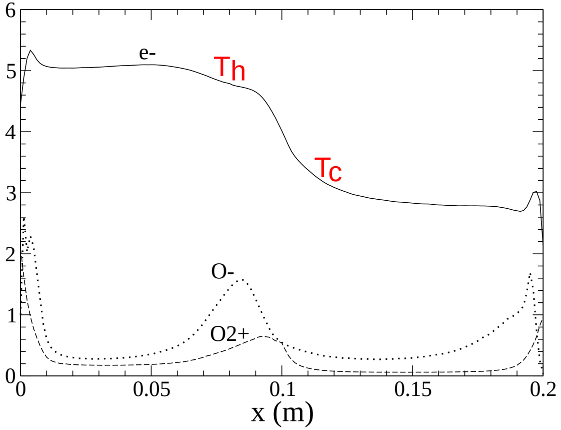
- Due to low densities, rescaled oxygen cross sections were used:

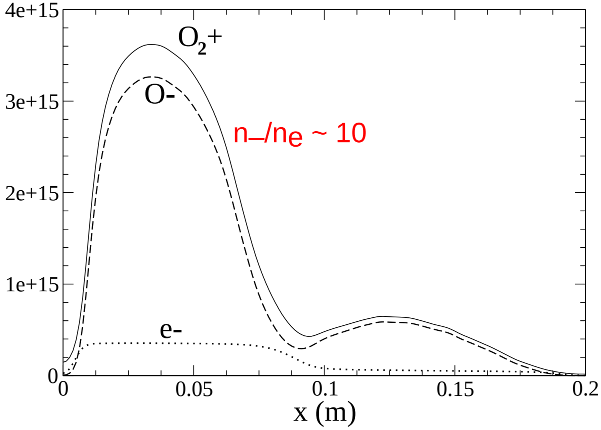
  Positive-negative ion recombination ↑ ×20
  Dissociative attachment ↑ ×5

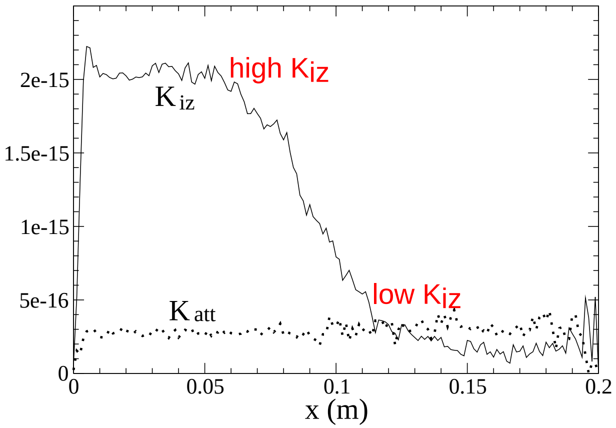
- A typical simulation takes 1–2 weeks
- The pressure range explored is 0.5–24 mTorr
- A DL was observed for 1–24 mTorr

PIC RESULTS FOR 6 mTorr O_2 DISCHARGE


Axial Potential (V)

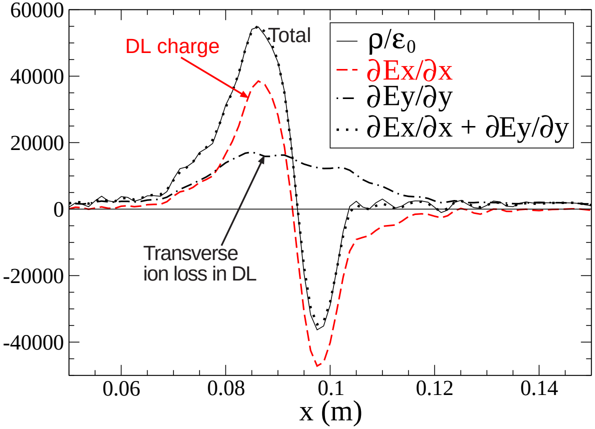

Radially averaged T (V)


Axial Density (m^{-3})

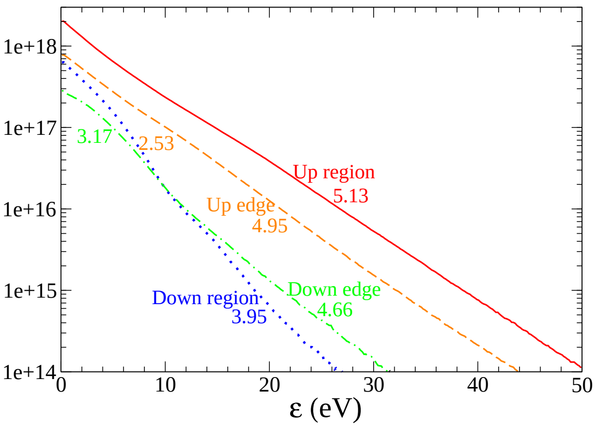

Axial Collision Rates (m^3/s)

RESULTS FOR 6 mTorr O_2 DISCHARGE (CONT'D)

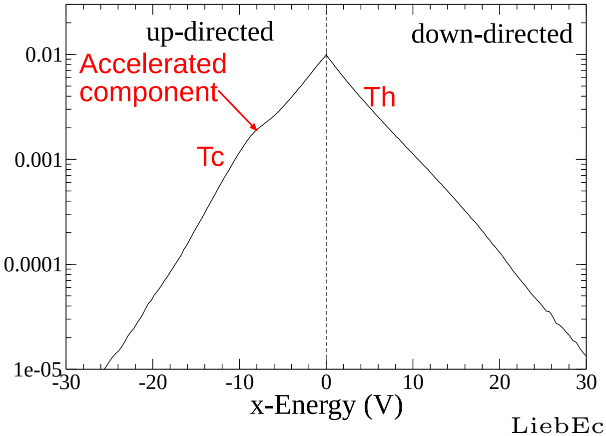
Charge Density Components in DL (V/m^2)



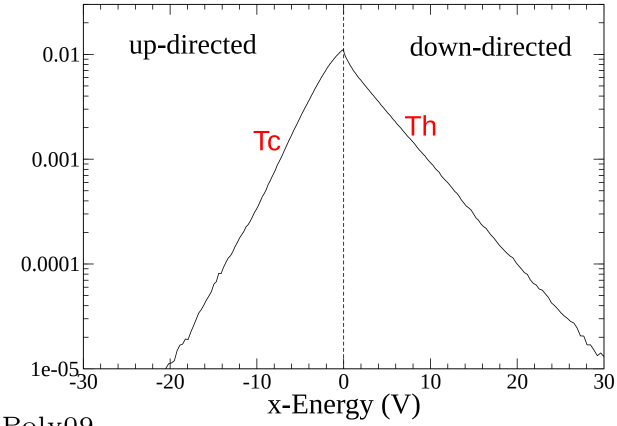
EEPF (a.u.)



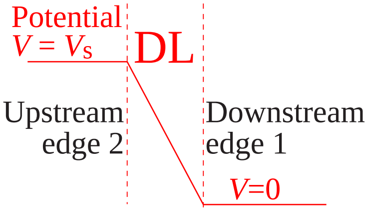
Up edge x-component EEDF (a.u.)



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

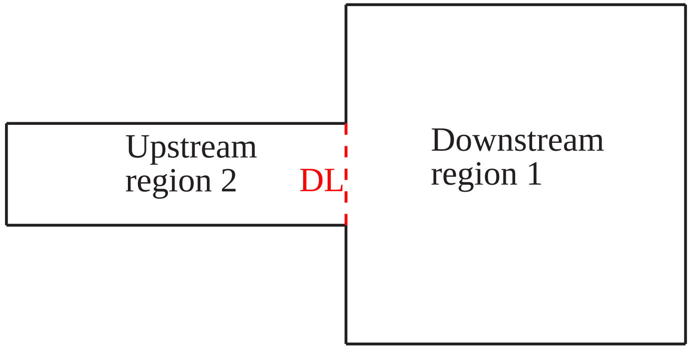


DL MODEL



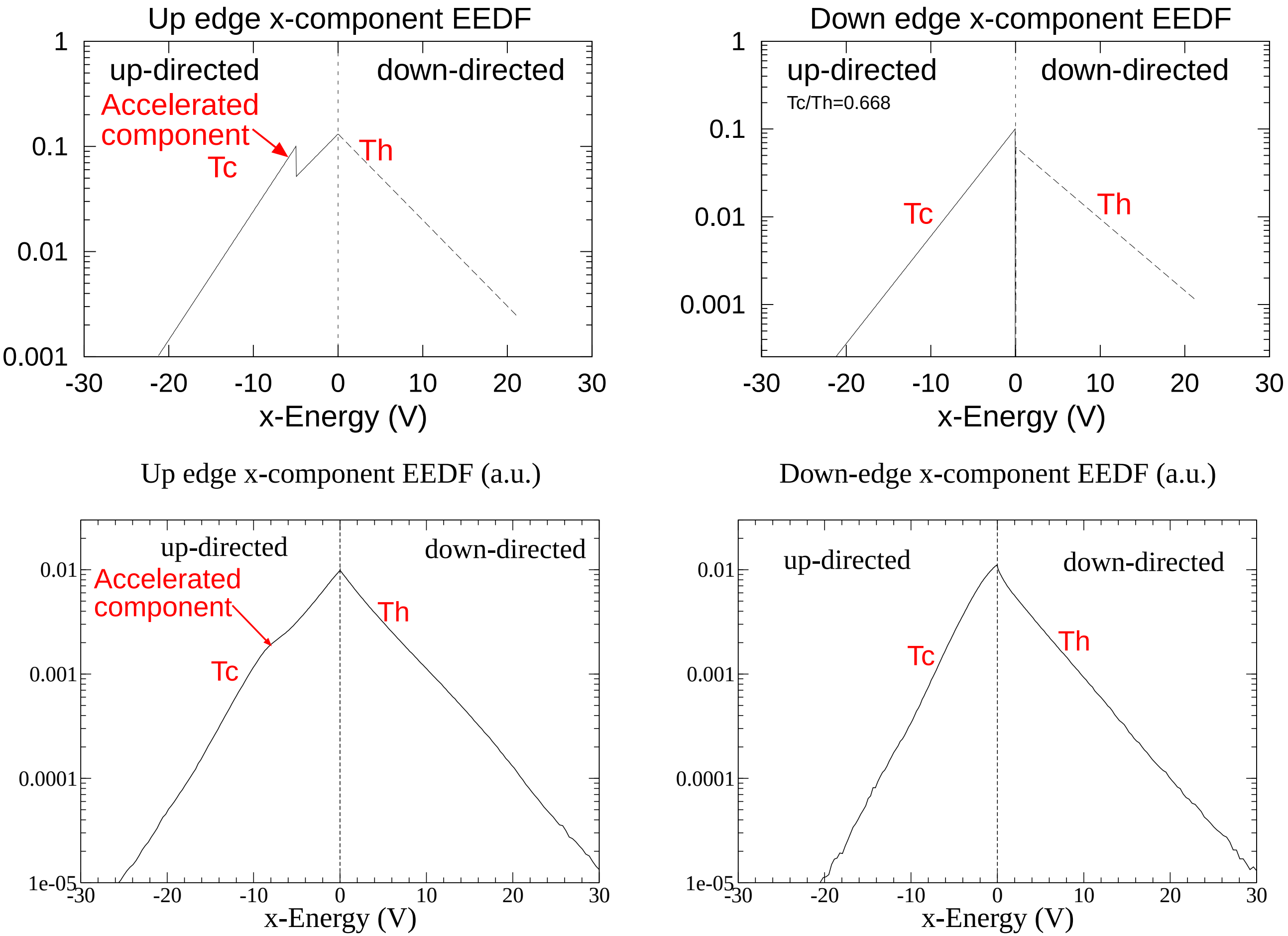
- Charge density ρ and potential V within the DL are found by solving Poisson's equation
- Six types of particles contribute to ρ:
  — thermal positive ions, negative ions, and electrons
  — positive ions accelerated downstream
  — negative ions and electrons accelerated upstream
- The particle motions 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

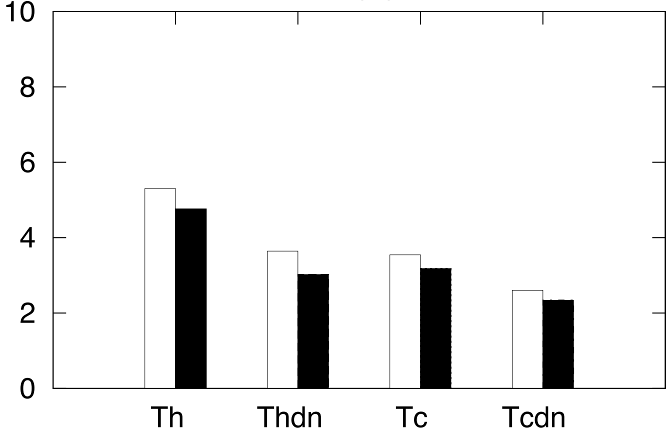


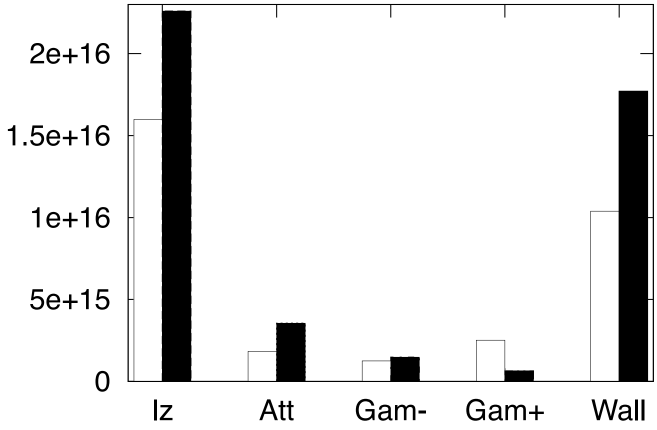
- We use a 2D rectangular geometry
- To determine the equilibrium quantities we use
  — global particle balance upstream
  — global particle balance downstream
  — global energy balance downstream
- Upstream energy balance (which determines the upstream electron density) depends on the input power; we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

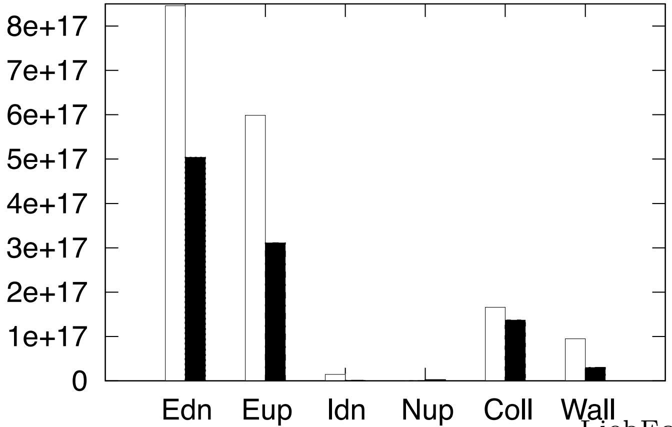
MODEL (TOP) and PIC (BOTTOM) EEDF'S (6 mTorr O_2)

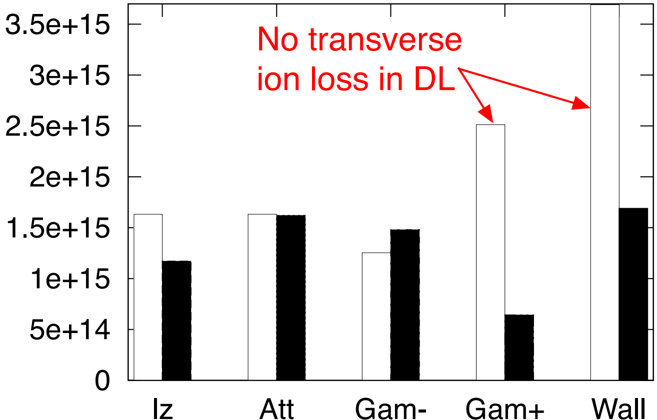


MODEL (WHITE) AND PIC (BLACK) FOR 6 mTorr O_2


Te (V)

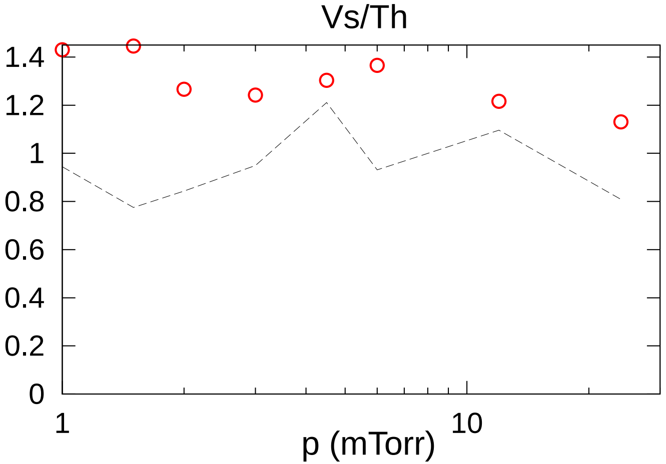

Up elec bal (#/s)

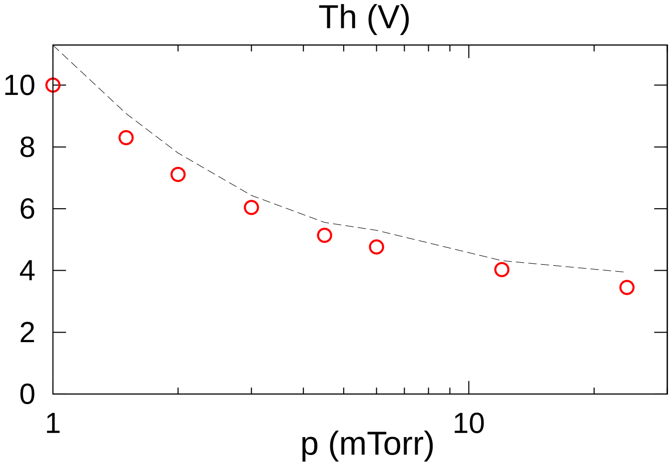

Down energy bal (eV/s)

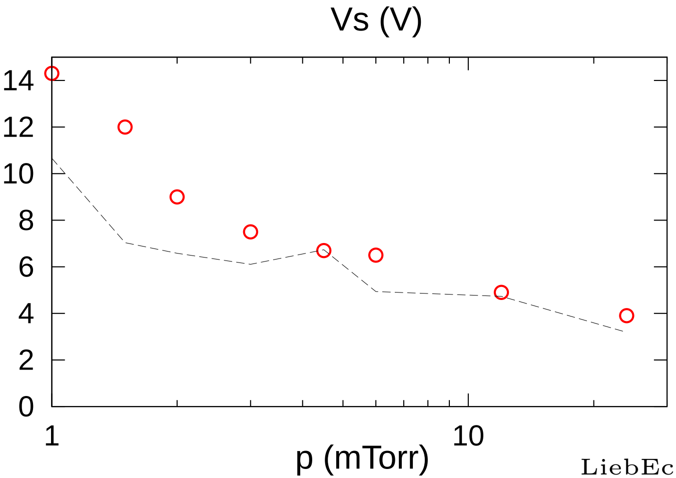

Down elec balance (#/s)

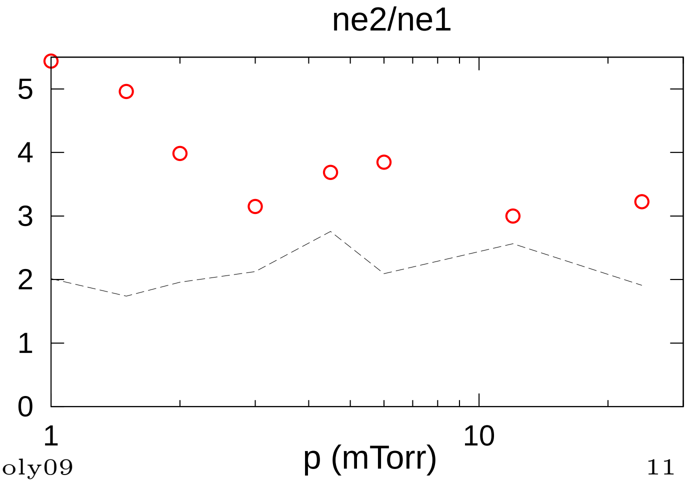
No transverse ion loss in DL

MODEL (DASH) AND PIC (CIRCLES) VS PRESSURE

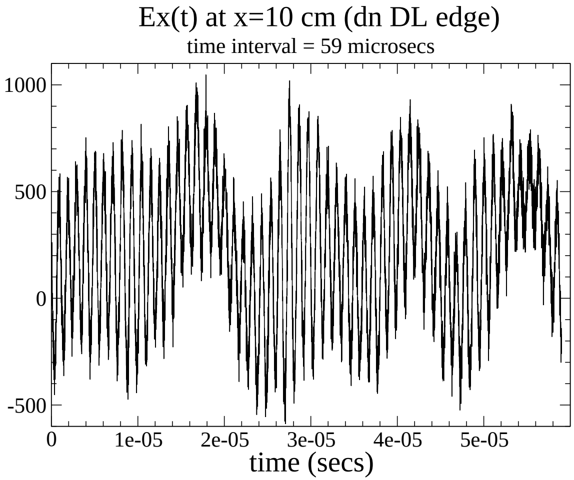

Vs/Th


Th (V)

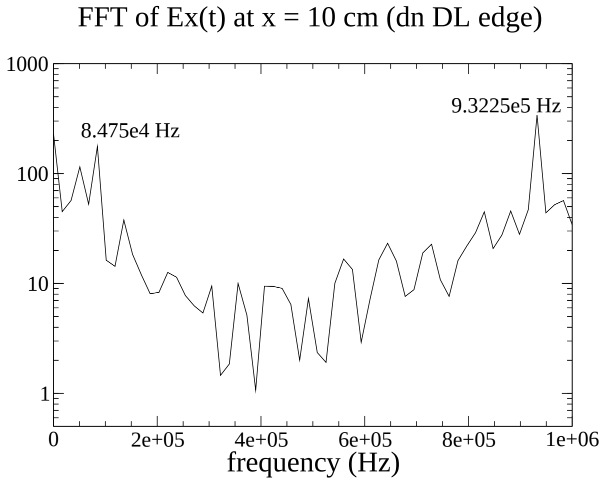

Vs (V)


ne2/ne1

SLOW AND FAST WAVES: INSTABILITIES (6 mTorr O_2)


Ex(t) at x=10 cm (dn DL edge)

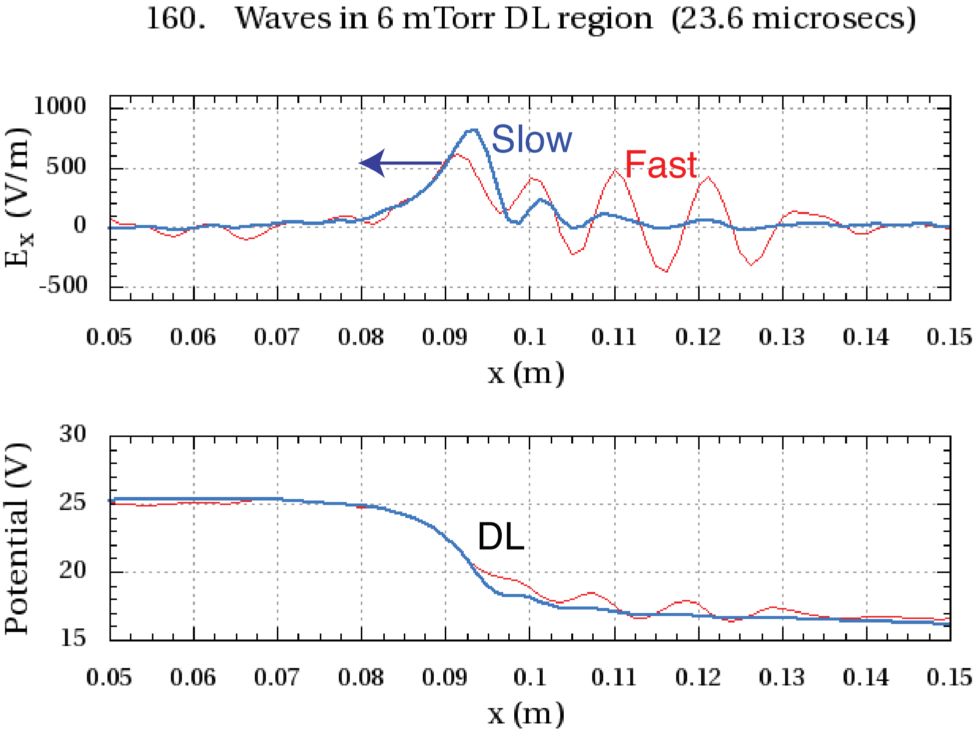
time interval = 59 microsecs


FFT of Ex(t) at x = 10 cm (dn DL edge)

- 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 ∼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 μs intervals
Blue solid line: slow waves averaged over 1.18 μs intervals



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

PART 2:

TRANSPORT IN A MAGNETIZED DISCHARGE

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OUTLINE

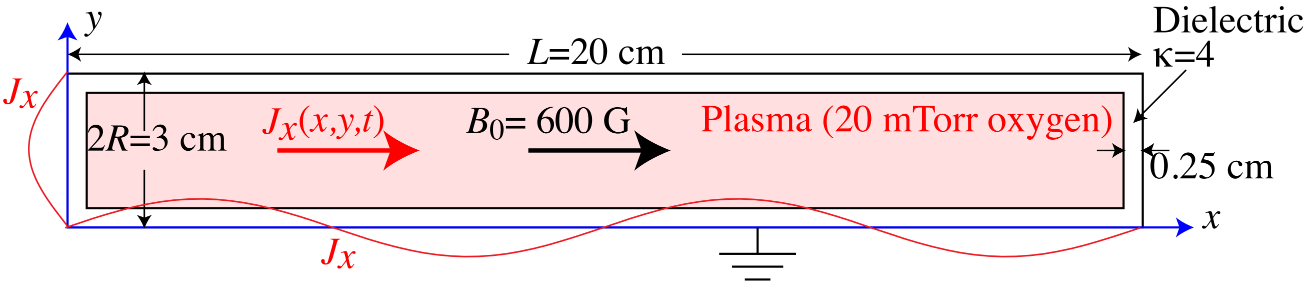
- Introduction

- “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 $T_e \approx$ const

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

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

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

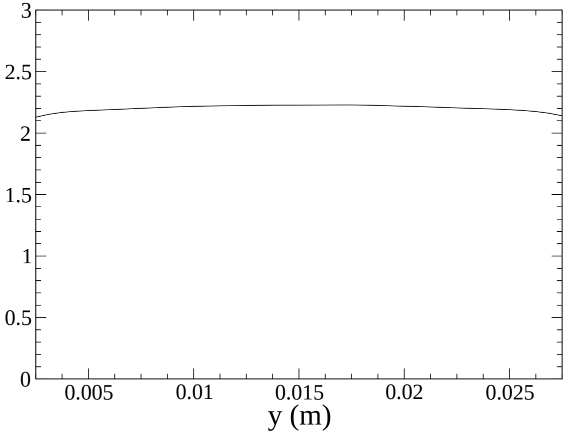
- Due to low density, rescaled oxygen cross sections were used:

  Positive-negative ion recombination ↑ ×20, ×100, etc

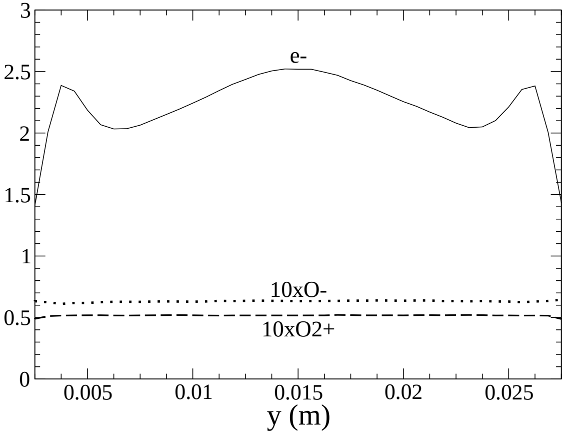
- A typical simulation takes 1–2 weeks

PIC RESULTS FOR $100 \times \mathrm{K}_{\mathrm{rec}}$ O_2 DISCHARGE

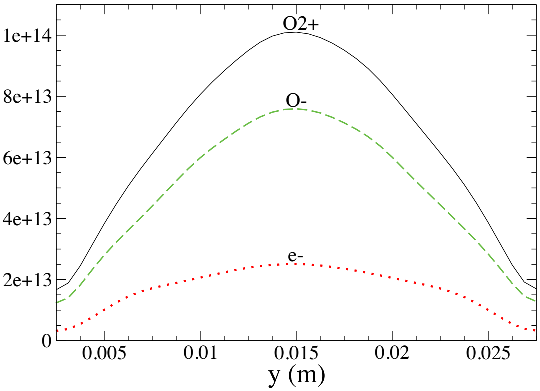
Radial Potential (V)



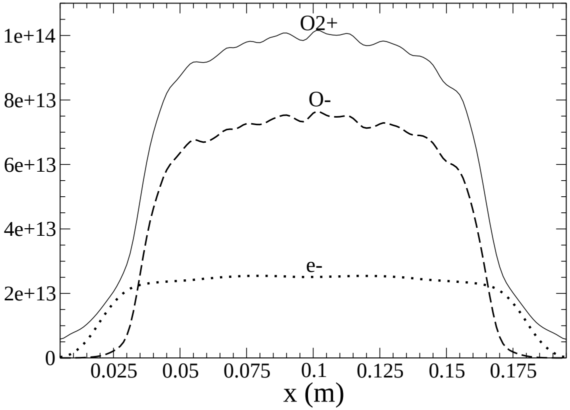
Radial T (eV)



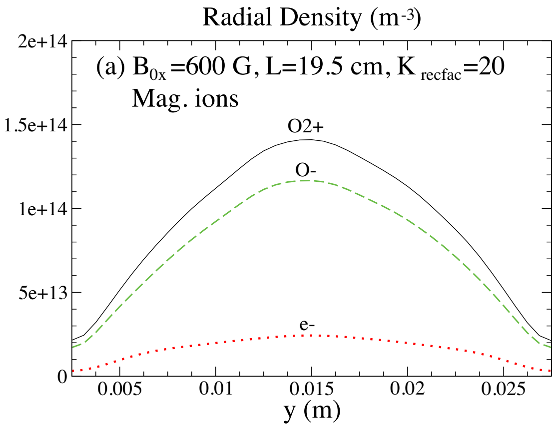
Radial Density (m^{-3})

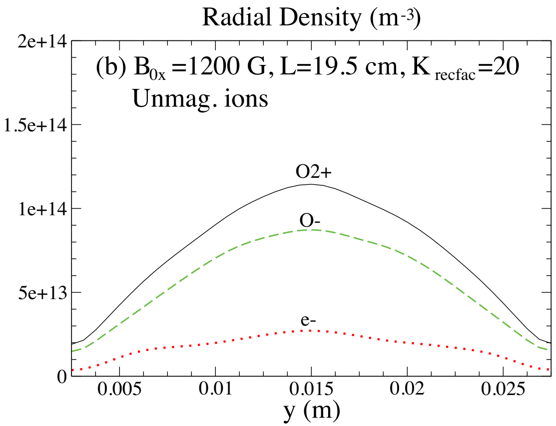


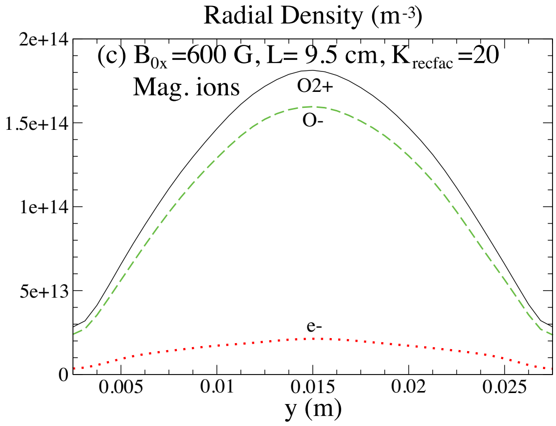
Axial Density (m^{-3})

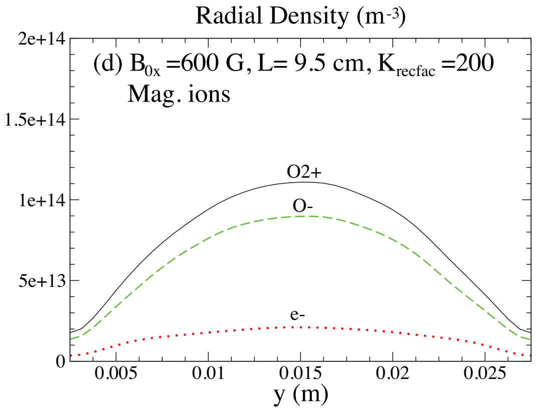


PIC RESULTS FOR OTHER O_2 DISCHARGES



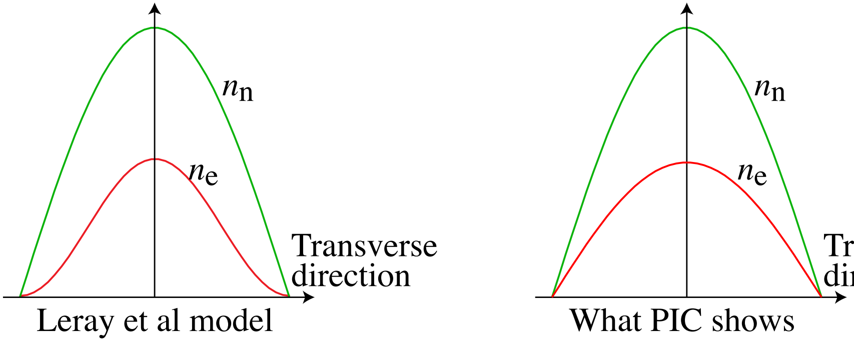






CONCLUSIONS FROM PIC SIMULATIONS

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



Leray et al model

What PIC shows

- 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

$$-D^*_{\perp e}\frac{\mathrm{d}^2 n_e}{\mathrm{d}y^2} = (\nu_{\mathrm{iz}} - \nu_{\mathrm{att}})n_e - \nu_L(n_e + n_n)$$

- Negative ion balance

$$-D^*_{\perp n}\frac{\mathrm{d}^2 n_n}{\mathrm{d}y^2} = \nu_{\mathrm{att}} n_e - K_{\mathrm{rec}} n_n(n_e + n_n)$$

- $D^*_{\perp e}$ 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

$$\boxed{\Rightarrow \text{good agreement with PIC results}}$$

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:

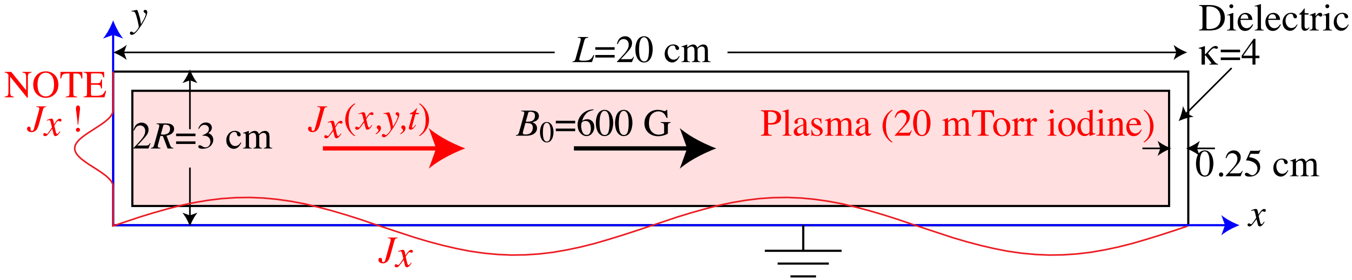
$$\frac{4R}{\pi}\nu_{\mathrm{att}} = \frac{\pi}{R} D^*_{\perp n} \alpha_0 + K_{\mathrm{rec}} n_{e0} \alpha_0 (1 + \alpha_0)$$

- Range of solutions:

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

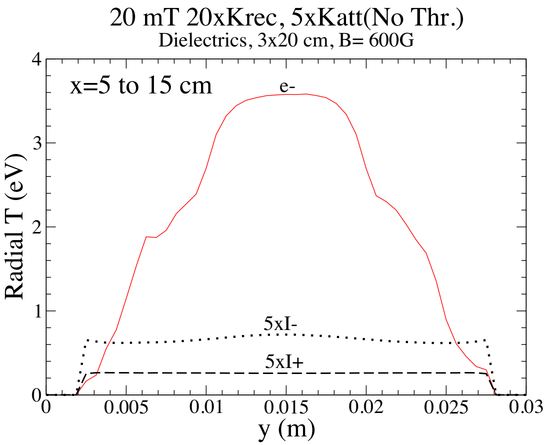
TWO-REGION IODINE SIMULATIONS

- 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

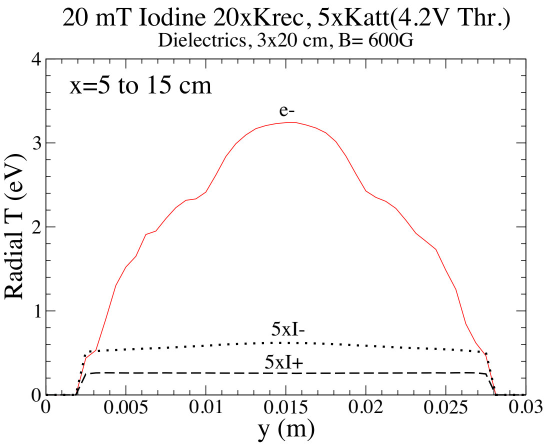


- Rescaled oxygen cross sections were used:
  — Positive-negative ion recombination ↑ ×20
  — Attachment ↑ ×5 (w/wo 4.2 V threshold energy)
- Iodine masses were used

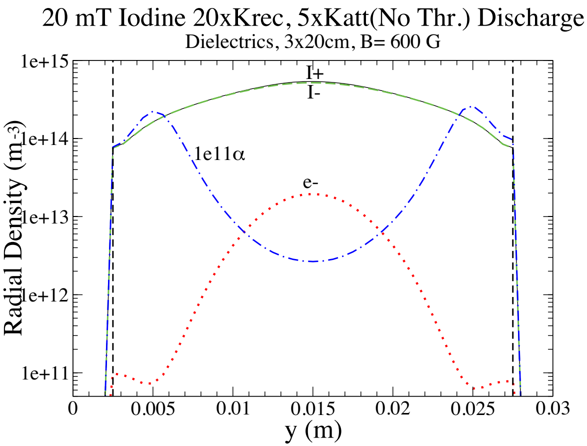
PIC RESULTS FOR IODINE DISCHARGE



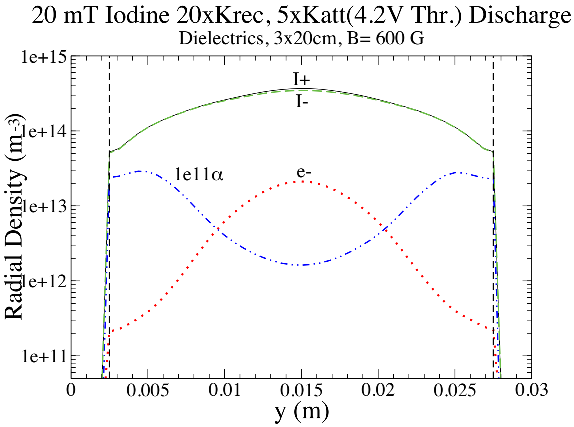
20 mT 20xKrec, 5xKatt(No Thr.)
Dielectrics, 3x20 cm, B= 600G



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



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

No attachment threshold

4.2 V attachment threshold

TWO-REGION 1D MODEL

- Electron balance

$$-D^*_{\perp e}\frac{\mathrm{d}^2 n_e}{\mathrm{d}y^2} = (\nu_{\mathrm{iz}} - \nu_{\mathrm{att}})n_e - \nu_L(n_e + n_n)$$

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

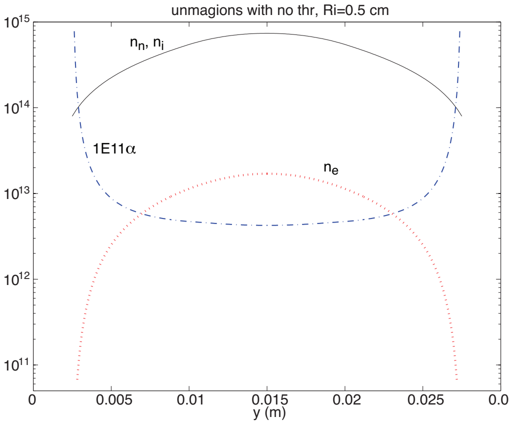
- Negative ion balance

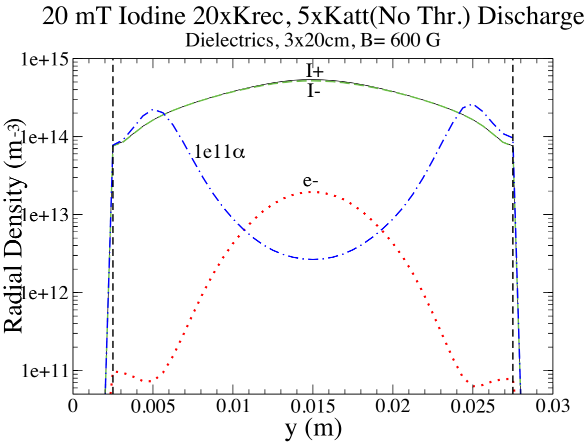
$$-D^*_{\perp n}\frac{\mathrm{d}^2 n_n}{\mathrm{d}y^2} = \nu_{\mathrm{att}} n_e$$

  (Neglect recombination compared to negative ion transverse loss)

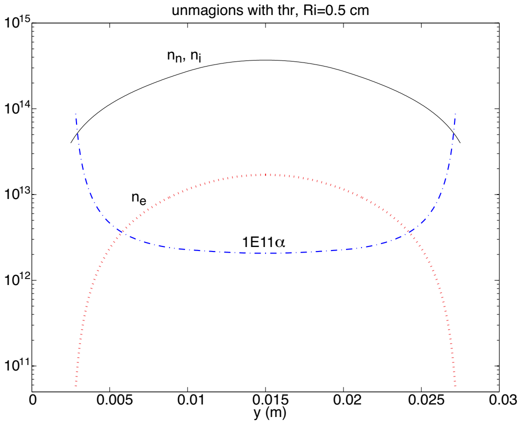
- Match densities and fluxes at the core-periphery transition
- Boundary conditions $n_e = n_n = 0$ at transverse wall
- This linear system can be solved exactly

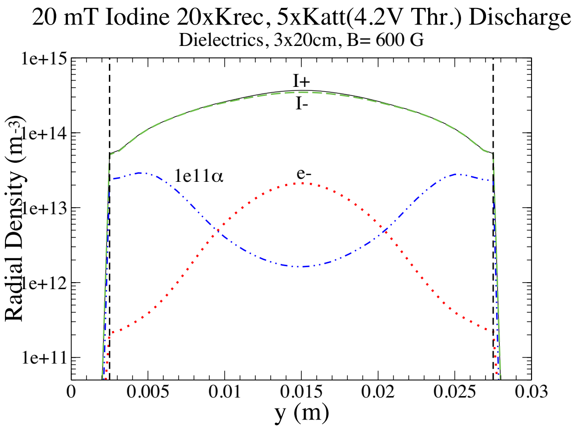
COMPARISON OF MODEL WITH PIC





No attachment threshold





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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