MODELING AND SIMULATION OF LOW TEMPERATURE PLASMA DISCHARGES

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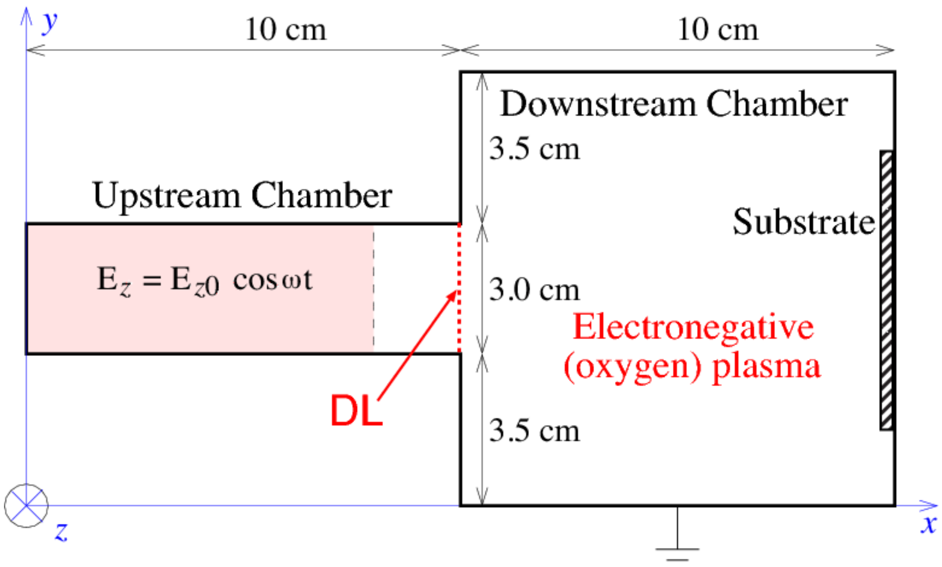
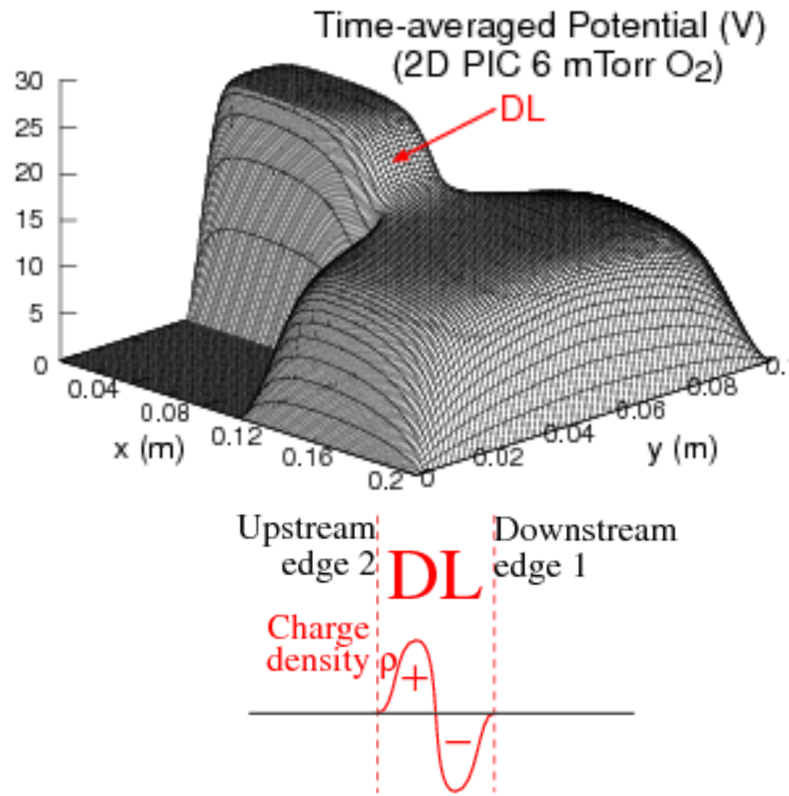
LOW PRESSURE DISCHARGES

- 1D and 2D particle-in-cell (PIC) kinetic simulations
- 2D bulk-fluid/analytic-sheath simulations
- Theory

Motivations: plasma processing of materials; plasma thrusters

2D PIC SIMULATIONS OF DOUBLE LAYERS

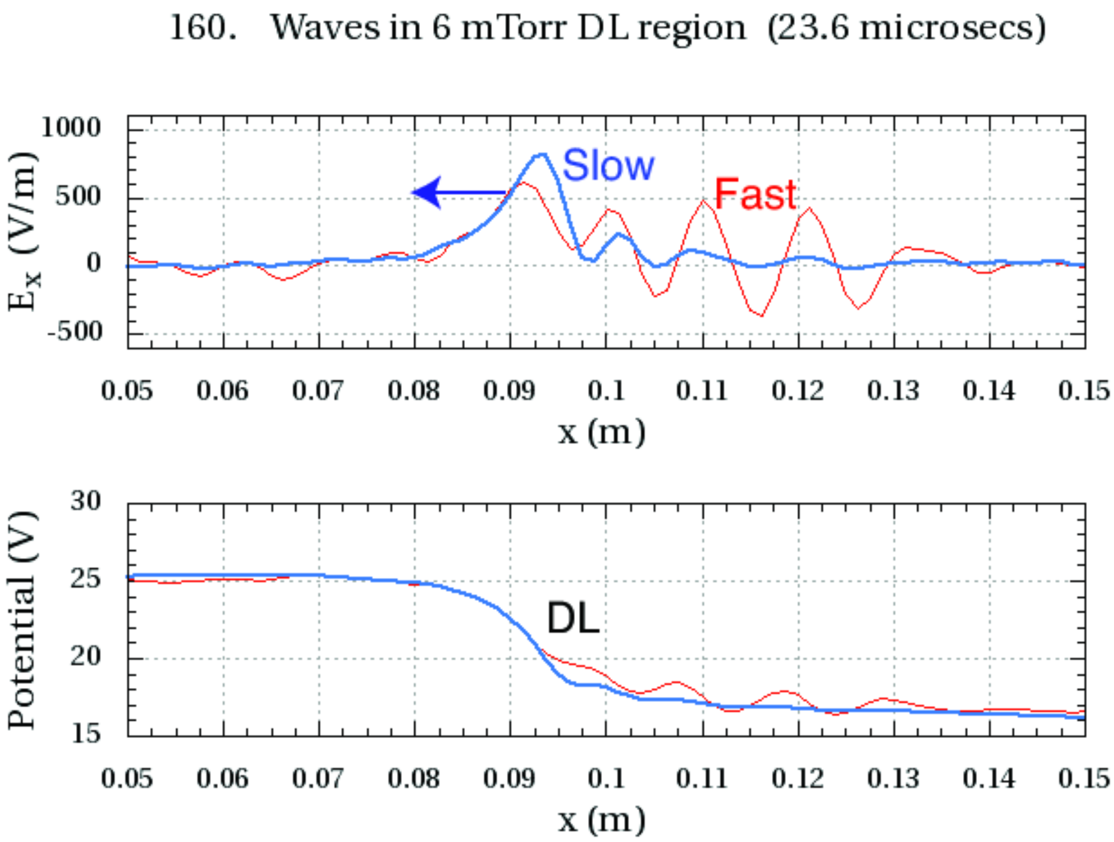




- **DL's observed over a wide range (1–24 mTorr) of pressures (Kawamura et al, Phys. Fluids, 2009)**
- **DL's typically have time-varying (wave) structures**

EXCITATION OF SLOW AND FAST WAVES

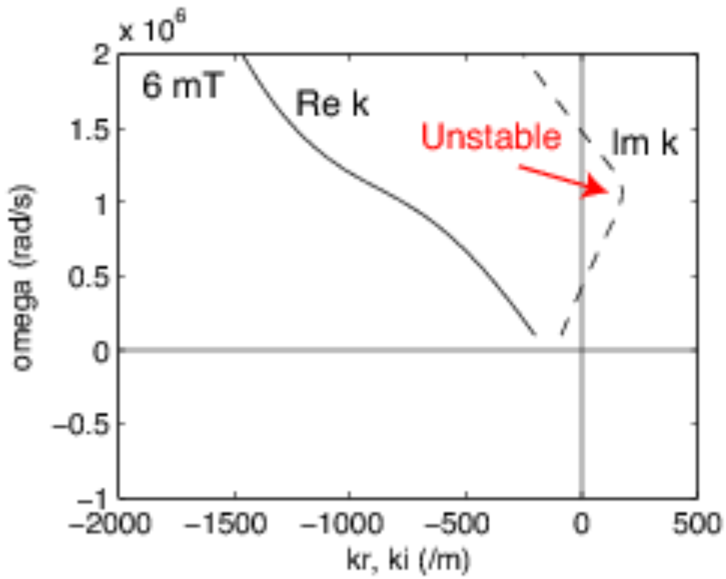
- **Red: 900 kHz fast waves averaged over 0.1475 μs intervals**
- **Blue: 85 kHz slow waves averaged over 1.18 μs intervals**



KINETIC THEORY OF UNSTABLE WAVES

- Waves produce 20% oscillations in DL potential and position
- Electron and ion kinetic effects are important
- Most unstable slow wave at λ = 0.7 cm at 173 kHz (PIC simulation gives λ = 1 cm at 85 kHz)
- Fast wave weakly damped at λ=0.7 cm; excitation from non-uniformities and nonlinearities

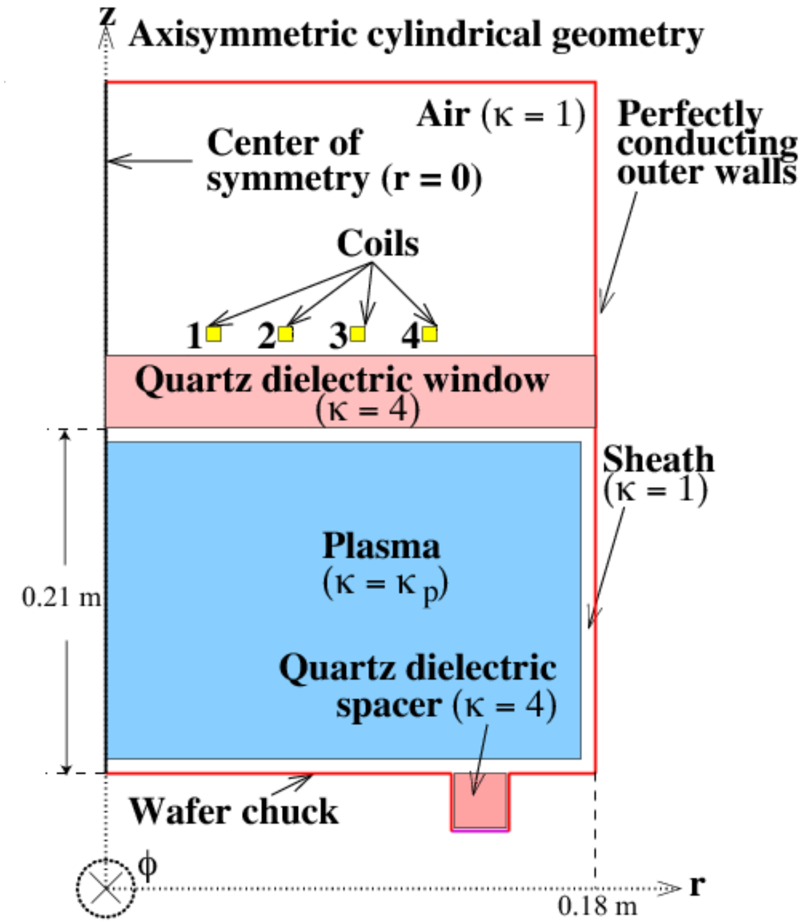
(Kawamura et al, JAP 2010)



2D BULK-FLUID/ANALYTIC-SHEATH MODELS

- Inductive reactor (Malyshev and Donnelly, 2000–01)
  - Electromagnetic field solve
  - Fluid bulk plasma model
  - Analytical sheath model
  - Flow model of reactive gas
  - Commercial software (COMSOL)

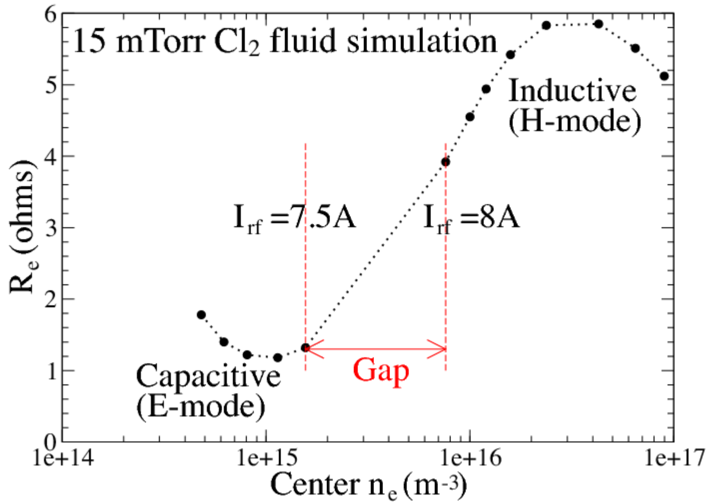
  (Kawamura et al, PSST 2012)



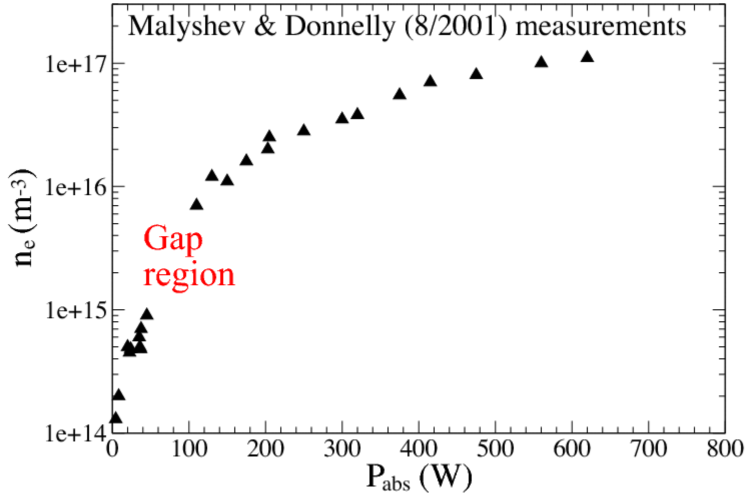
  - Low density capacitive (E-mode)
  - High density inductive (H-mode)
  - Attaching gas ➔negative ions ➔E/H instability

E/H MODE TRANSITION IN CHLORINE

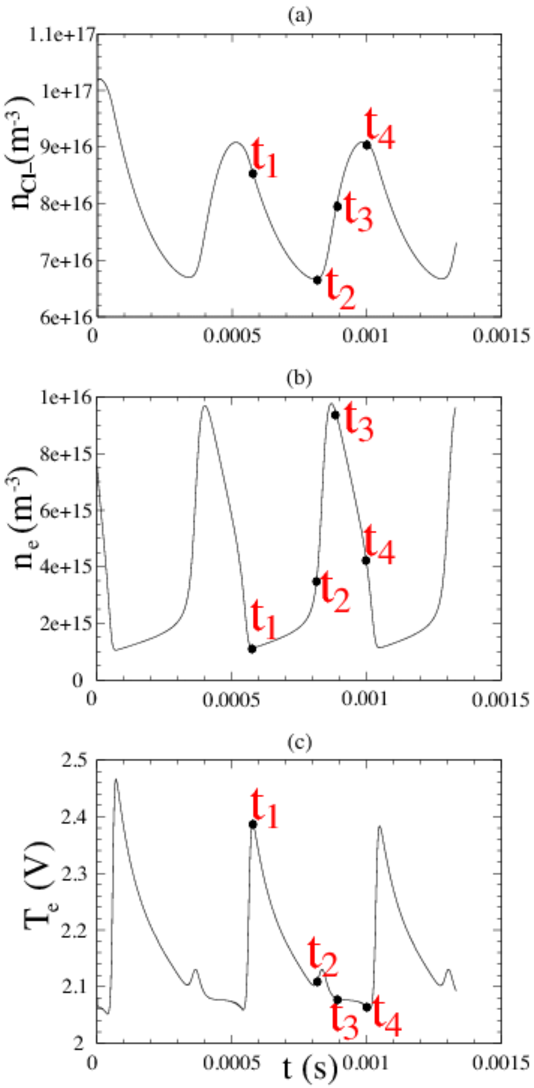
- Plasma resistance R_e versus n_e as I_{rf} is varied
- A "gap" occurs between I_{rf} = 7.5 and 8 A



- Measurements at 10 mTorr Cl_2 show "gap region"
- Previous measurements (many) and global models (many) indicate instability
- First calculation of E/H instability in fluid simulations



E/H TRANSITION INSTABILITY



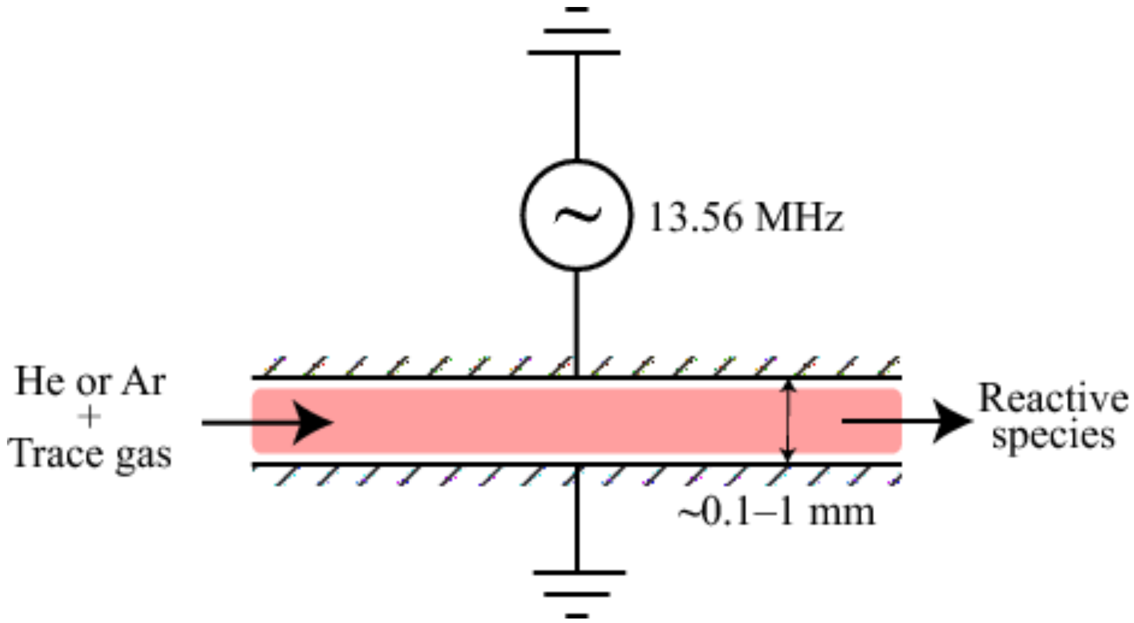
- **Example: 2.2 kHz instability in 15 mTorr Cl_2 at I_{rf} = 7.75 A, showing (a) $n_{Cl^-}(t)$, (b) $n_e(t)$, and (c) $T_e(t)$**
  - **At time t_1 the discharge enters capacitive mode**
  - **From t_1–t_2 the discharge is in capacitive mode**
  - **From t_2–t_3 the discharge makes a transition to inductive mode**
  - **From t_3–t_4 the discharge is in inductive mode**
  - **From t_4–t_1 the discharge makes a transition back into capacitive mode**

ATMOSPHERIC PRESSURE DISCHARGES

- 1D particle-in-cell (PIC) kinetic simulations
- 1D bulk-fluid/analytic-sheath hybrid simulations
- Theory

Motivations: biomedical plasmas; plasma processing of materials

DISCHARGE CONFIGURATION



- Atmospheric pressure
- He or Ar with trace reactive gases
- 1D plane-parallel geometry (~0.1–1 mm gap)
- RF-driven (6.78–54.24 MHz)

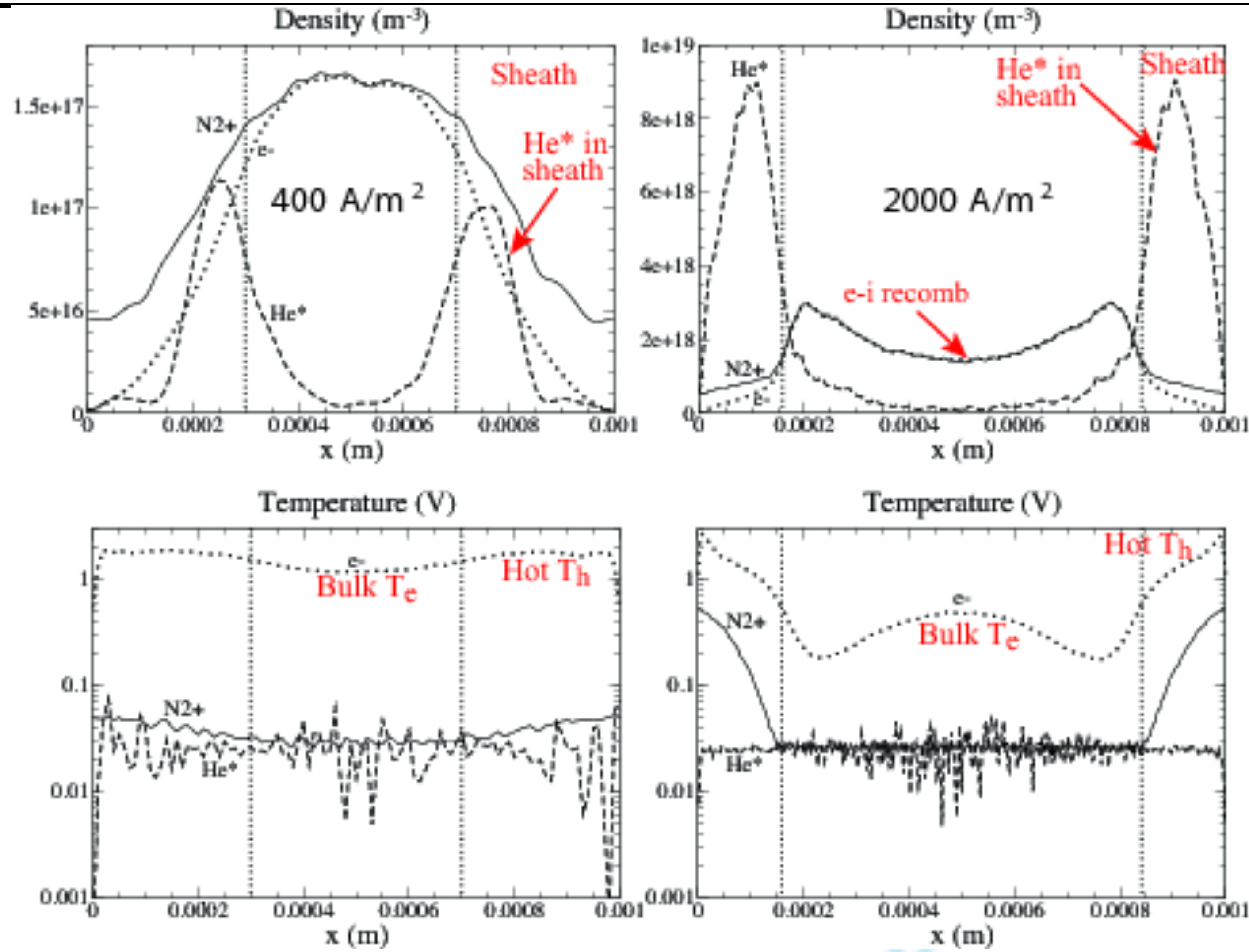
TWO-TEMPERATURE HYBRID DISCHARGE MODEL

- **Numerical solution of particle balances for each species**
  - $\mathrm{d}n_j/\mathrm{d}t = G_j - L_j$
  - G_j = volume creation rate (2-body, 3-body and surfaces)
  - L_j = volume loss rate (2-body, 3-body and surfaces)
- **Numerical solution of Penning/secondary electron multiplication in sheaths ⇒ hot $T_h(t)$, $n_h(t)$**
- **Analytical solutions of**
  - the discharge dynamics (homogeneous model)
  - the time-varying warm $T_e(t)$
  - the effective rate coefficients $\langle K \rangle$
- **Coupling the analytical and numerical solutions**
  - ⇒ fast solution of the discharge equilibrium

(Kawamura et al, PSST 2014; Ke Ding et al, JPD 2014)

PIC RESULTS (27.12 MHz, 1 mm gap, He/0.1%N_2)

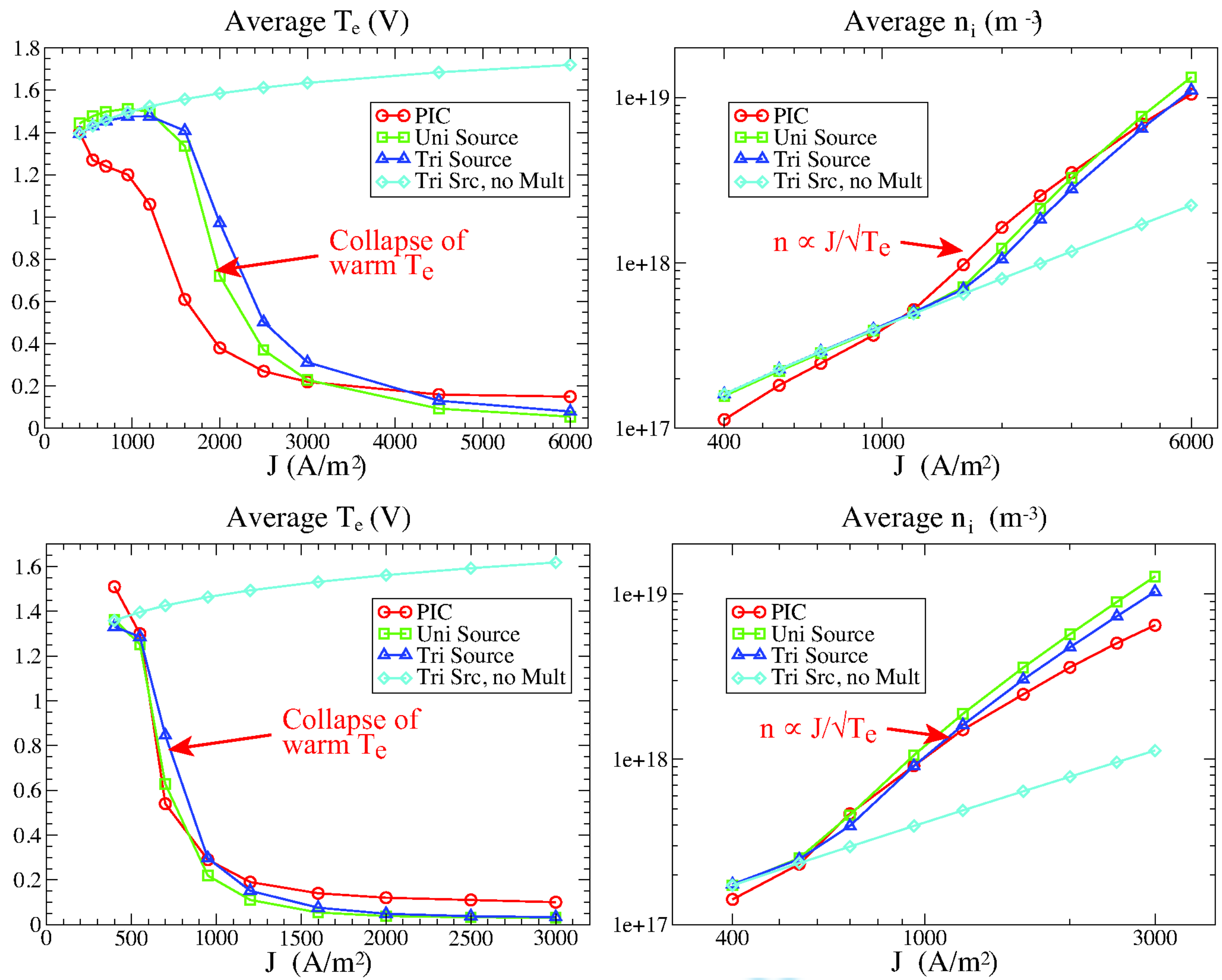
α-mode γ-mode



He/0.1%N_2 HYBRID – PIC COMPARISON

27.12 MHz

13.56 MHz



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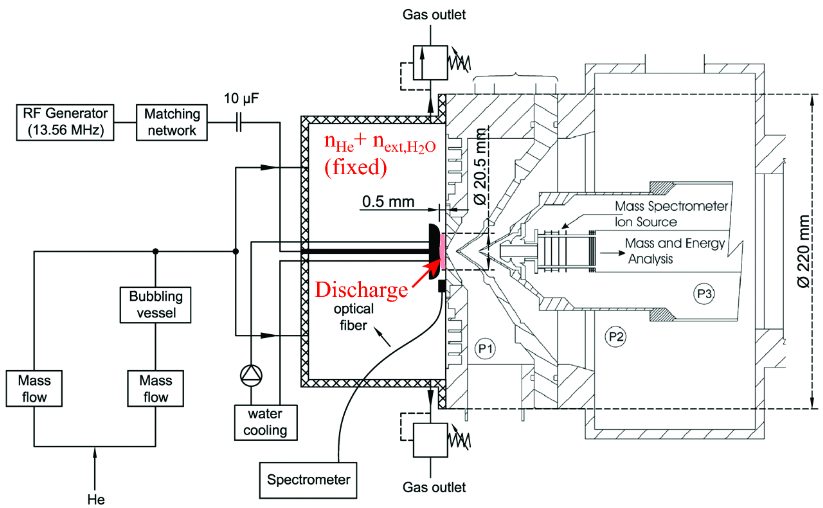
He/H_2O ATMOSPHERIC PRESSURE DISCHARGE MODELING

- In an experiment, a 1 cm radius 0.5 mm gap discharge was embedded in a large chamber with fixed H_2O concentration

(P. Bruggeman et al, J. Phys. D 43, 012003, 2010)



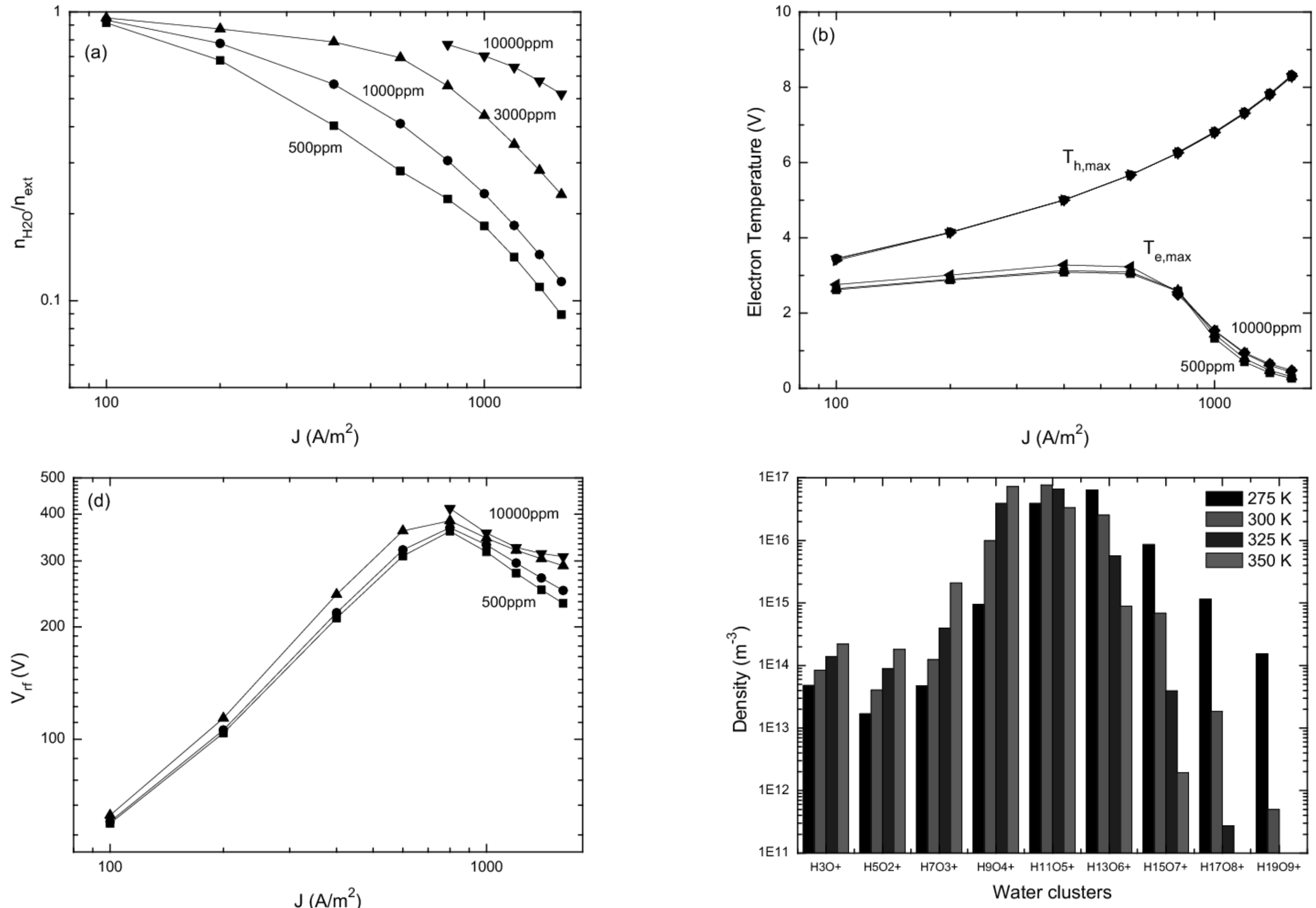
- In a global model (46 species, 577 reactions), particle and energy balance were solved to determine the discharge equilibrium

(D.X. Liu et al, PSST 19, 025018, 2010)

- Discharge depletes external H2O density, reaction products diffuse to axial and radial walls, sheaths cause α-to-γ transition

SOME HYBRID MODEL RESULTS

- **He/0.1%H_2O discharge, 0.5 mm gap, 13.56 MHz, γ_{se} = 0.25 (209 reactions among 43 species with clusters up to $H_{19}O_9^+$)**



YEAR 6 RESEARCH

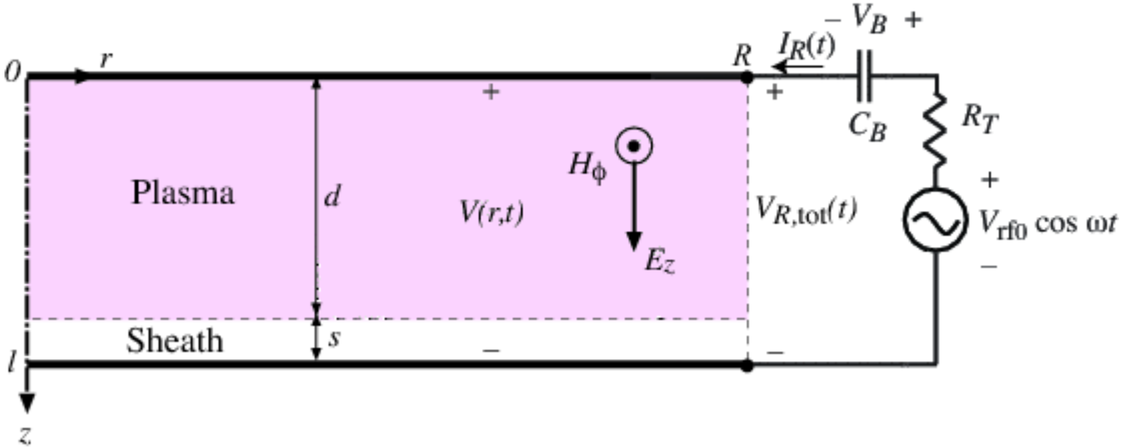
- **Low Pressure Discharges**
  - Fast 2D Fluid-Analytical Simulation of Ion Energies and EM Effects in Multi-Frequency Capacitive Discharges
  - Electron Heating in Capacitive Discharges
  - Metastables in Capacitively Coupled Oxygen Discharges
  - Nonlinear Standing Wave Excitation by Series-Resonance Enhanced Harmonics in Capacitive Discharges
- **Atmospheric Pressure Discharges**
  - Comparison of a Hybrid Model with Experiments in Helium and Argon Discharges
  - Reaction Pathways for Bio-Active Species in He/H2O Discharges
  - Analytic Model of Helium/Trace Gas Penning Discharges
  - PIC Simulations of He/H2O Plasma Near a Water Interface

CENTRAL PLASMA NONUNIFORMITY IN LOW PRESSURE CAPACITIVE DISCHARGES

- **Asymmetric argon capacitive discharge (2.5 cm gap, driven at 60 MHz), showing ne(r)**

  (Sawada et al, JJAP, 2014)

- **Investigate coupling of series-resonance enhanced harmonics of driving frequency to standing waves using a radial transmission line model**



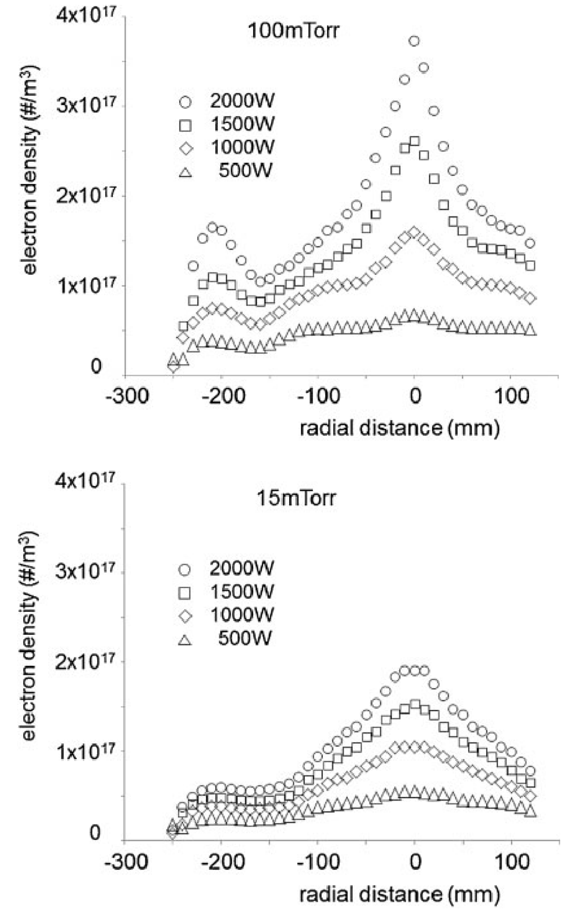
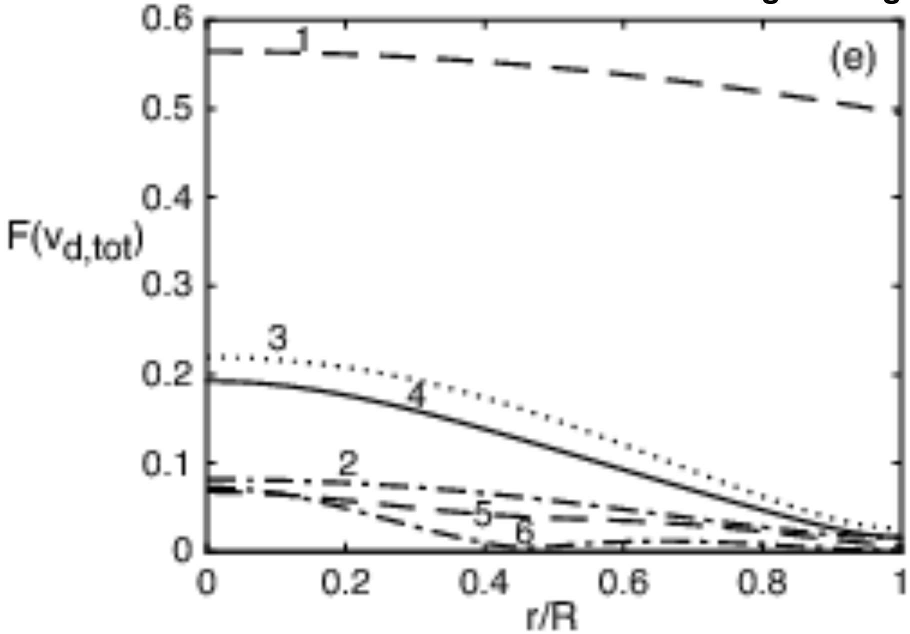


Fig. 3. Experimentally measured electron density profiles along the test-bench A reactor midgap for argon plasma driven at 60 MHz. Top: 100 mTorr. Bottom: 15 mTorr.

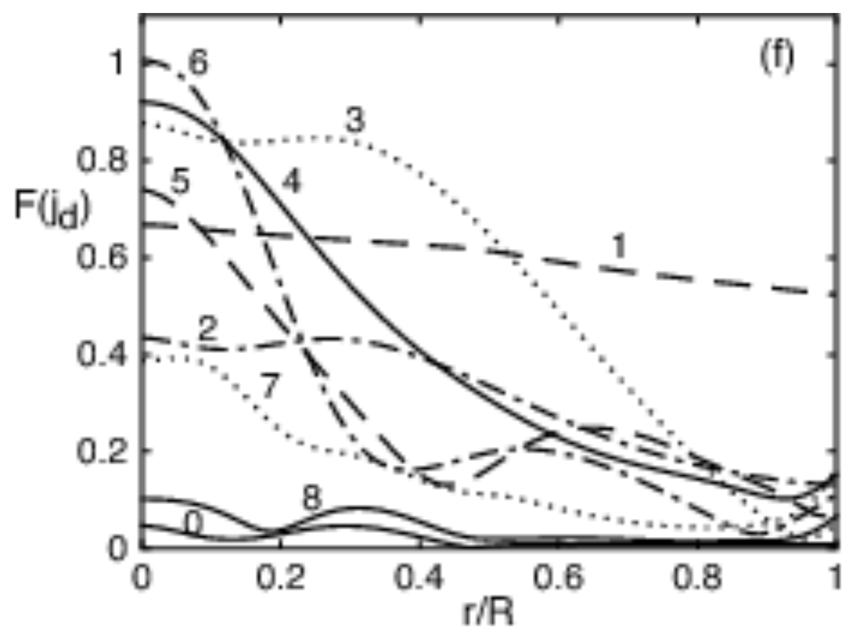
TRANSMISSION LINE MODEL RESULTS

- **Series resonances:** $\omega_{SR} = N\omega = (s/d)^{1/2}\omega_{pe}$
- **Standing wave resonances:** $\omega_{wave} = M\omega = (s/d)^{1/2}\chi_{01}c/R$

Fourier transform normalized discharge voltage



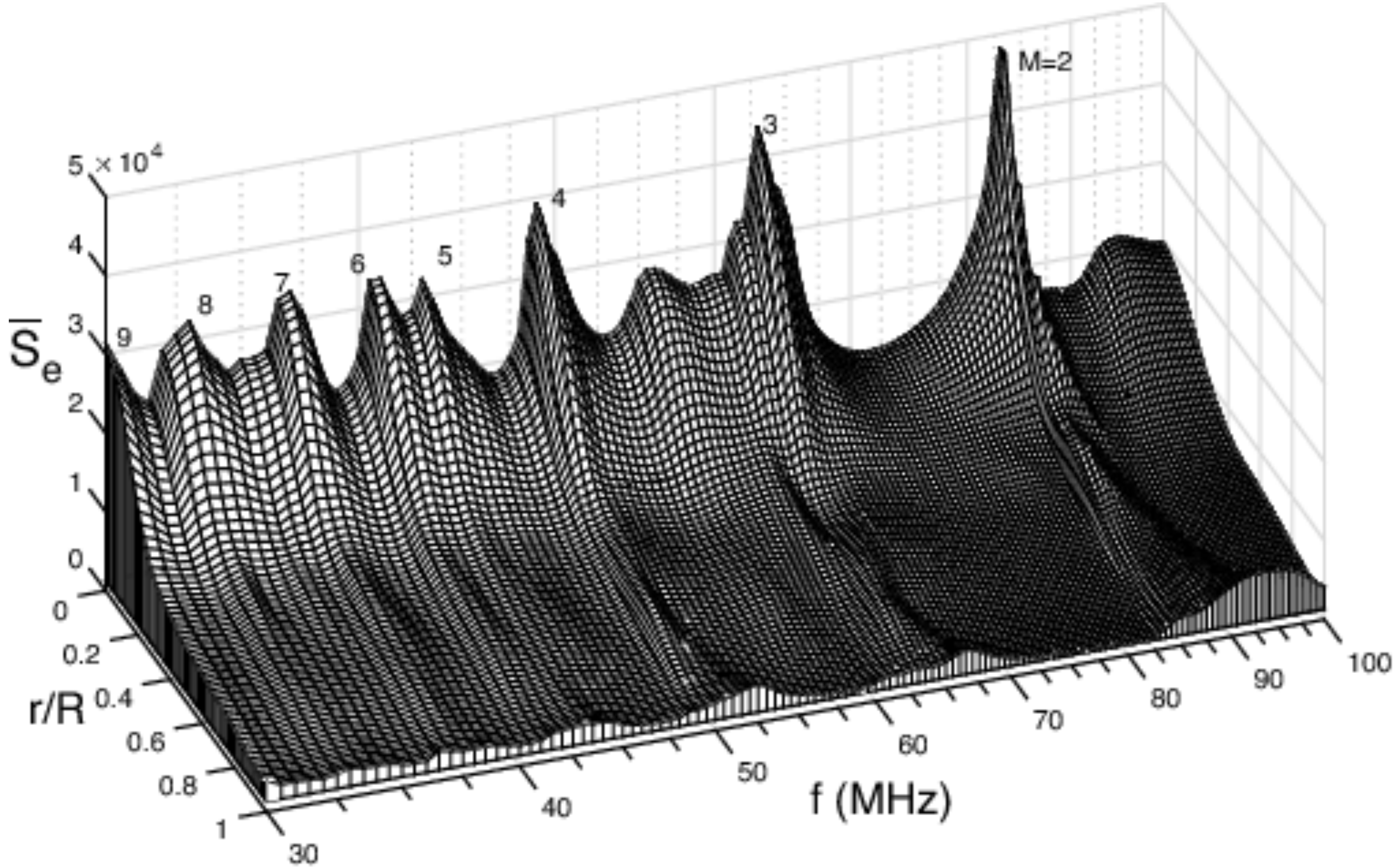
Fourier transform normalized discharge current density



- **Example: 10 mTorr argon driven at 60 MHz and 500 V through 0.5 Ω, 15 cm radius, 2 cm gap, $n_e = 2 \times 10^{16}$ m^{-3}**

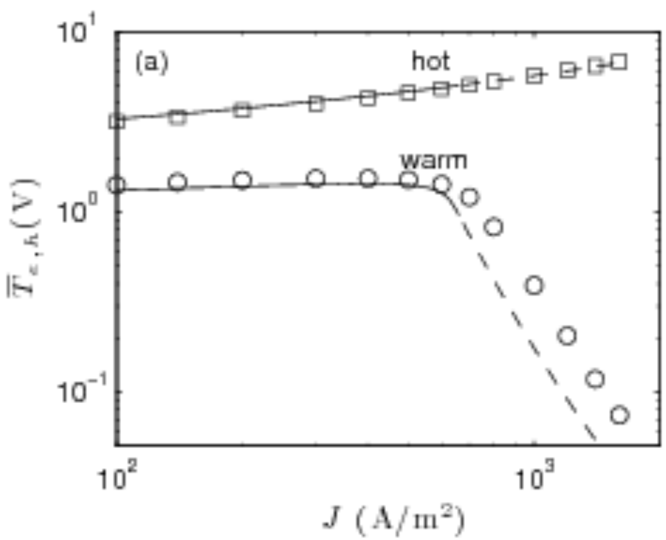
DISCHARGE ELECTRON POWER/AREA

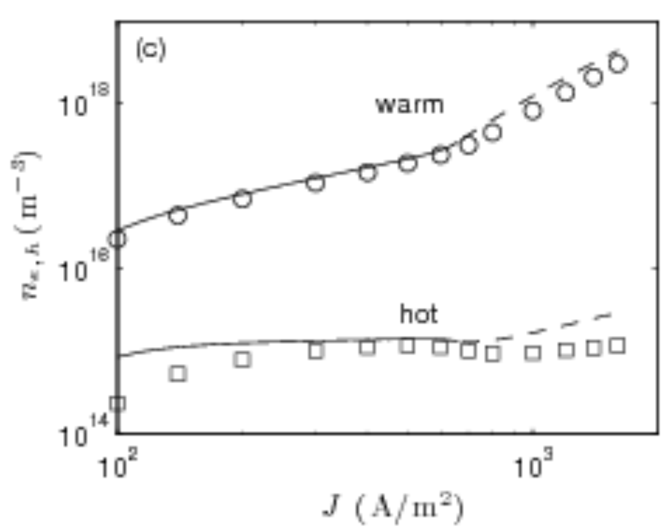
- 10 mTorr argon discharge driven through 0.5 Ω, 15 cm radius, 2 cm gap
- Voltage rescaled as $\omega^2 V_{rf}$ = const to keep $n_e = 2 \times 10^{16}$ m^{-3}



ANALYTIC MODEL OF HELIUM/TRACE GAS ATMOSPHERIC PRESSURE DISCHARGES

- Rf capacitive-driven with Penning ionization
- Reduced chemical complexity: helium monomer metastable, one kind of positive ion, and hot and warm electrons
- He/0.1%H_2O discharge, 0.5 mm gap, driven at 13.56 MHz
- Compare analytic model (solid and dashed lines) to hybrid simulations (symbols)
  (209 reactions, 43 species, clusters up to $H_{19}O_9^+$)





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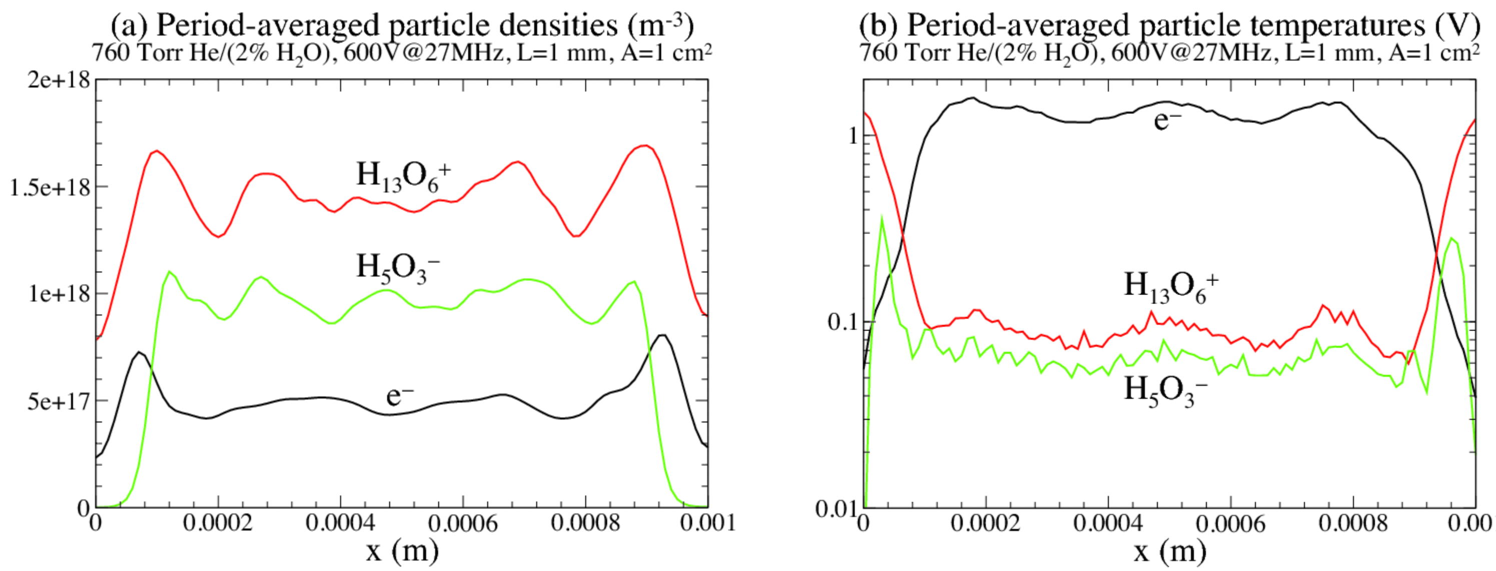
1D PIC SIMULATIONS OF ATMOSPHERIC PLASMA NEAR A WATER INTERFACE

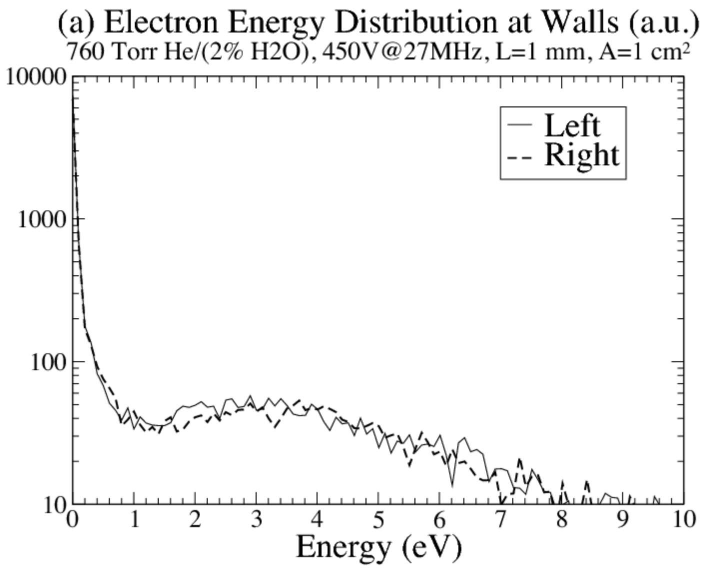
- 1 mm gap He/2%H_2O atmospheric pressure discharge in series with an 0.5 mm H_2O liquid layer and a 1 mm quartz dielectric
- Hybrid model used to determine the most important species and reactions used in the PIC simulations of the discharge
- Example of 600 V at 27.12 MHz, γ_{se} = 0.15

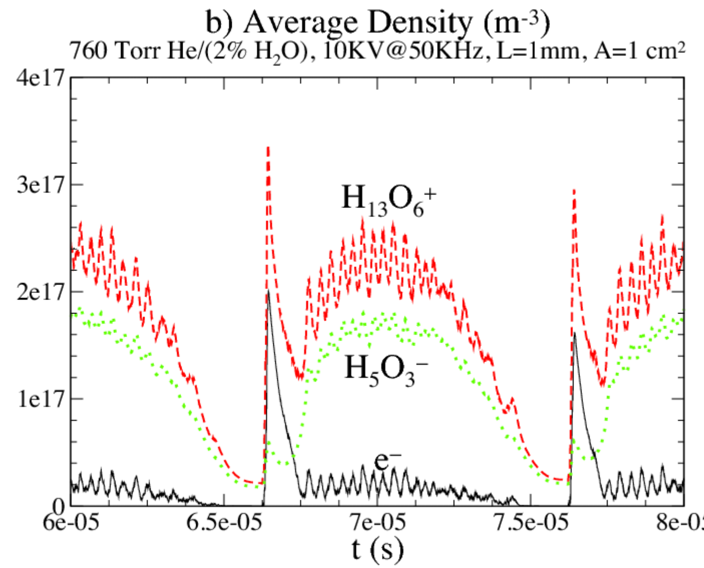


- WHAT ARE THE OSCILLATIONS IN THE BULK?

1D PIC SIMULATIONS OF PLASMA NEAR A WATER INTERFACE (CONT'D)

- **H_2O vibrational and rotational energy losses are so high that most electrons reach the walls at thermal energies**
- **Low frequency simulations: 10 kV at 50 kHz, γ_{se} = 0.15**





- **Low frequency discharge runs in a pure γ-mode**
- **A dc argon simulation is being used to model a solvated electron experiment (David Go, to appear in Nature Communications, 2015)**