MODELING PLASMA PROCESSING DISCHARGES

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OUTLINE

- Fast computation of atmospheric pressure rf capacitive discharges
- Fluid model of E-H transition instability in electronegative inductive discharge

ATMOSPHERIC PRESSURE
CAPACITIVE RF DISCHARGE

MOTIVATION

- Biomedical — example of reactive oxygen species

  (Review article: H.W. Lee et al, J. Phys. D **44**, 053001, 2011)

  — Applications to sterilization, cancer cell treatment, blood coagulation, wound healing

- Unique materials — example of anatase crystalline TiO_2

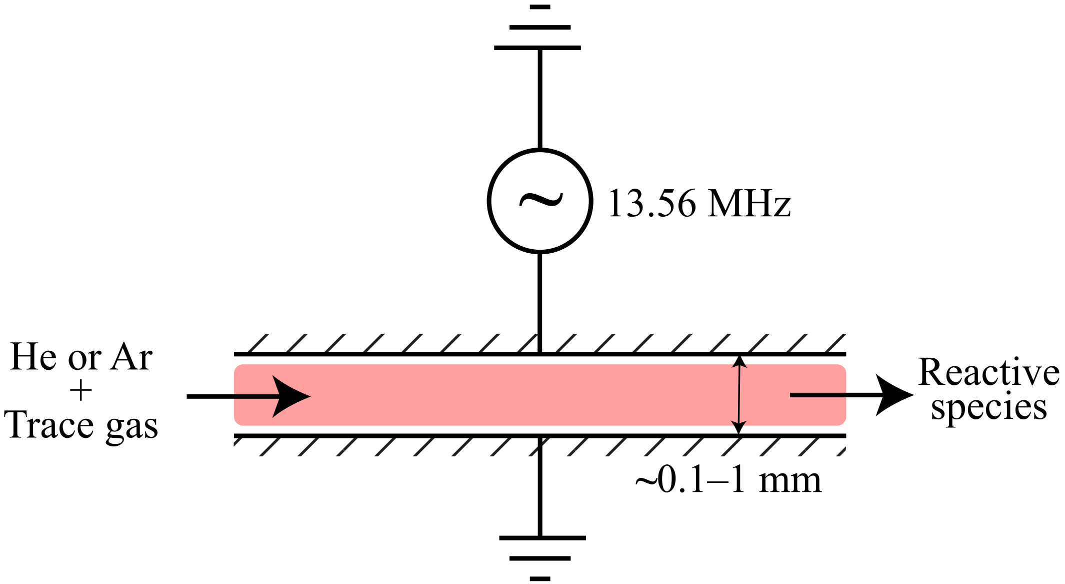
  (Review article: D. Mariotti and R.M. Sankaran, J. Phys. D, 323001, 2010)

  (Anatase TiO_2: H.G. Yang et al, Nature **453**, 638, 2008)

  — Applications to photonics crystals, photo/electrochromic devices, gas sensors, spintronic devices, anticancer or gene therapies, solar cells for electric energy or hydrogen production

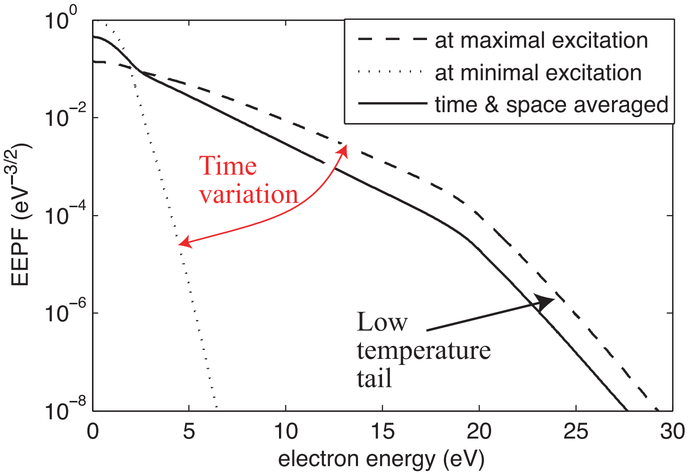
DISCHARGE CONFIGURATION

- Atmospheric pressure
- He or Ar with trace reactive gases
- 1D plane-parallel geometry (∼0.2–2 mm gap)
- RF-driven (nominal 13.56 MHz)



EEPF TIME VARIATIONS

- He/N_2 fluid simulation with kinetic (Bolsig+) EEPF calculation



(J. Waskoenig, PhD Thesis, Queens U Belfast, 2010)

- Conclusions used in modeling
  — The EEPF oscillates in time with the rf electron power absorbed
  — The EEPF is Maxwellian below a break energy $\mathcal{E}_b \approx 20$ V (metastable He excitation energy)
  — The EEPF has a low temperature tail above the break energy

HYBRID DISCHARGE MODEL

- Numerical solution of particle balances for each species

$$\frac{\mathrm{d}n_j}{\mathrm{d}t} = G_j - L_j$$

G_j = volume creation rate (2-body, 3-body and surfaces)
L_j = volume loss rate (2-body, 3-body, and surfaces)

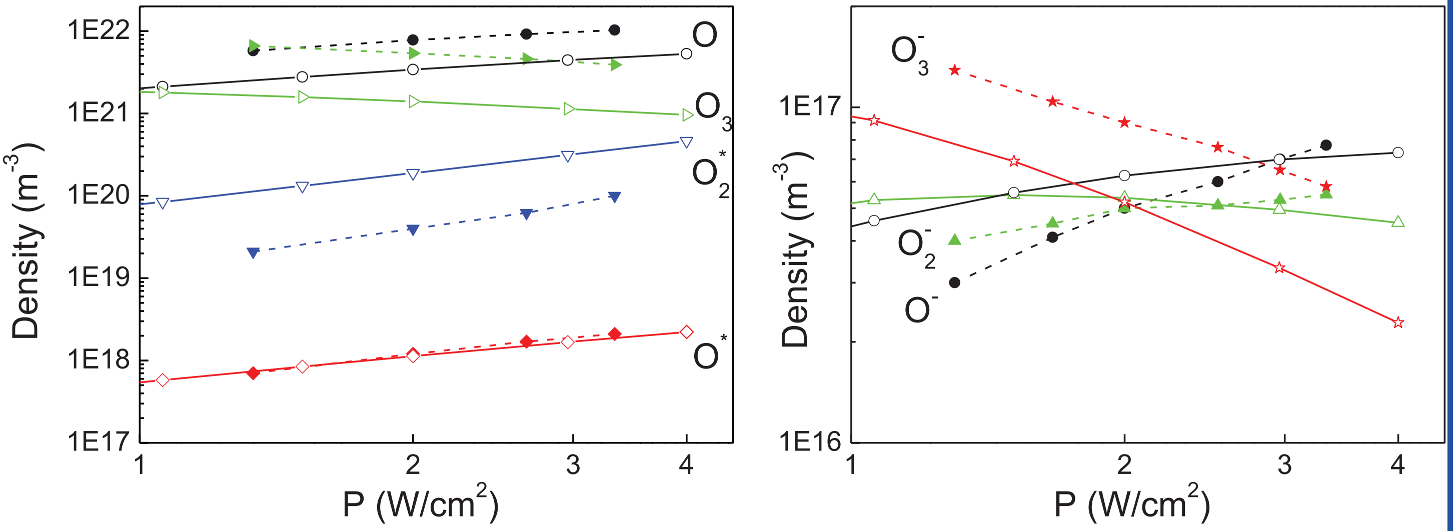
- Analytical solutions of
— the discharge dynamics (homogeneous model)
— the time-varying $\mathrm{T}_e(t)$
— the effective rate coefficients $\langle K \rangle$

- Coupling the analytical and numerical solutions

$$\boxed{\Longrightarrow \text{ fast solution of the discharge equilibrium}}$$

COMPARISON TO FLUID SIMULATION

- He/0.5%O_2 (16 species), 1mm gap, 13.56 MHz
- Neutral (left) and charged (right) densities versus power



(open symbols — global model; solid symbols — fluid results, Waskoenig, 2010)

- ⇒ Reasonable agreement of model and fluid simulations
  40 sec simulation time on fast laptop

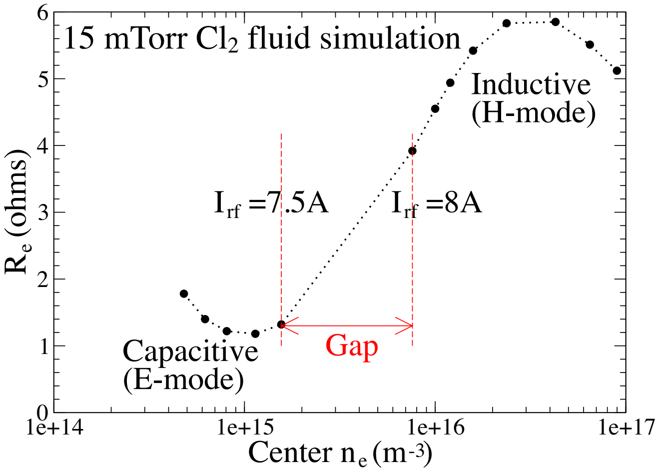
E/H (CAPACITIVE/INDUCTIVE) MODE TRANSITION INSTABILITY IN ELECTRONEGATIVE DISCHARGE

MOTIVATION

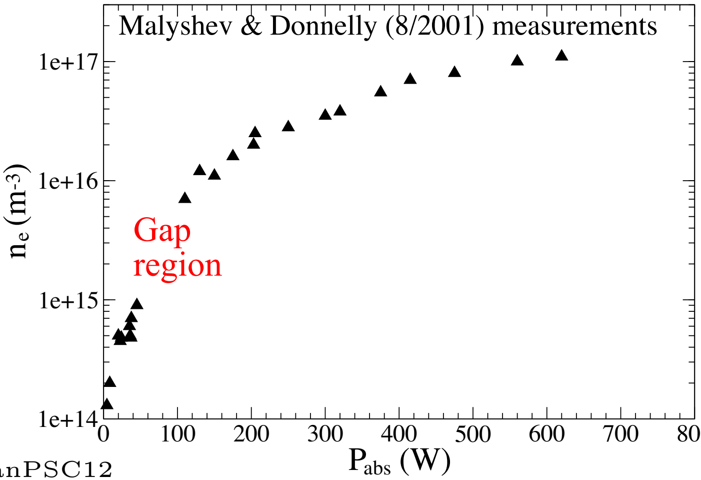
- Low pressure inductive reactors for thin film processing
  - Example: fabrication of CMOS transistors for microprocessors/memory
  - Inductive reactors often operate near the E/H transition with electronegative feedstock gases
  - Macroscopic instabilities observed in both commercial and research reactors

E/H MODE TRANSITION

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

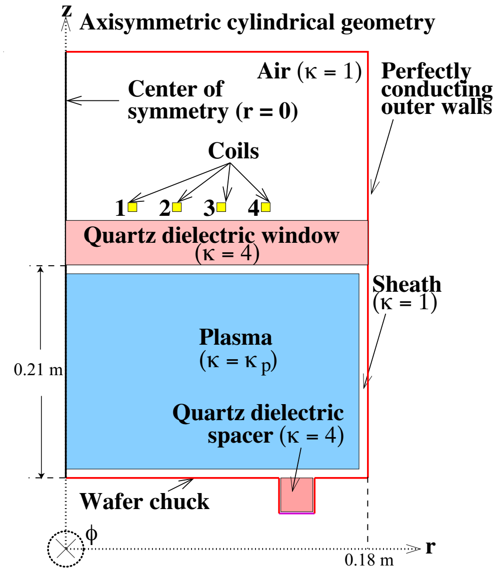


- Measurements at 10 mTorr Cl_2 show "gap region"
- Previous measurements (many) and global models (many) indicate instability
- First calculation of E/H instability in fluid simulations



BULK-FLUID/ANALYTIC-SHEATH MODEL

- Inductive reactor (Malyshev and Donnelly, 2000–01)

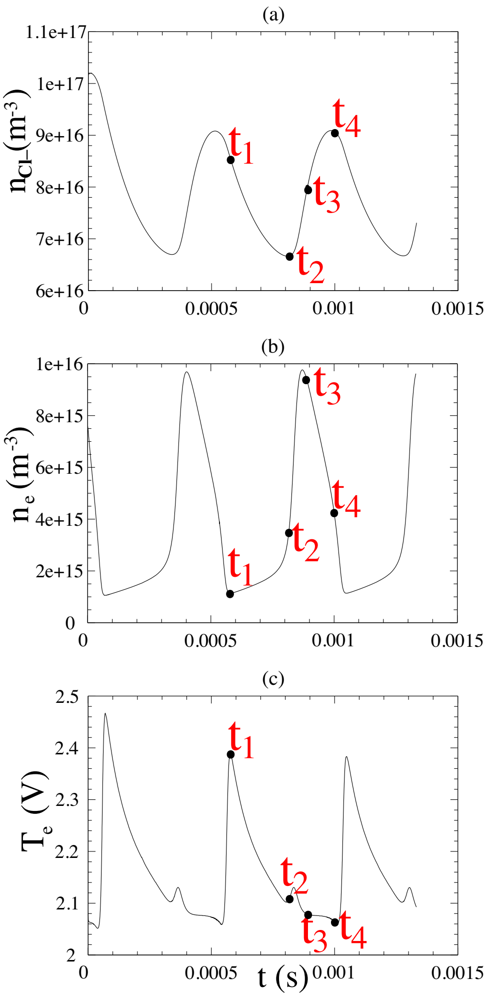


  — Electromagnetic field solve
  — Fluid bulk plasma model
  — Analytical sheath model
  — Flow model of reactive gas
  — Commercial software (COMSOL)

(Kawamura et al, PSST 2011)

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



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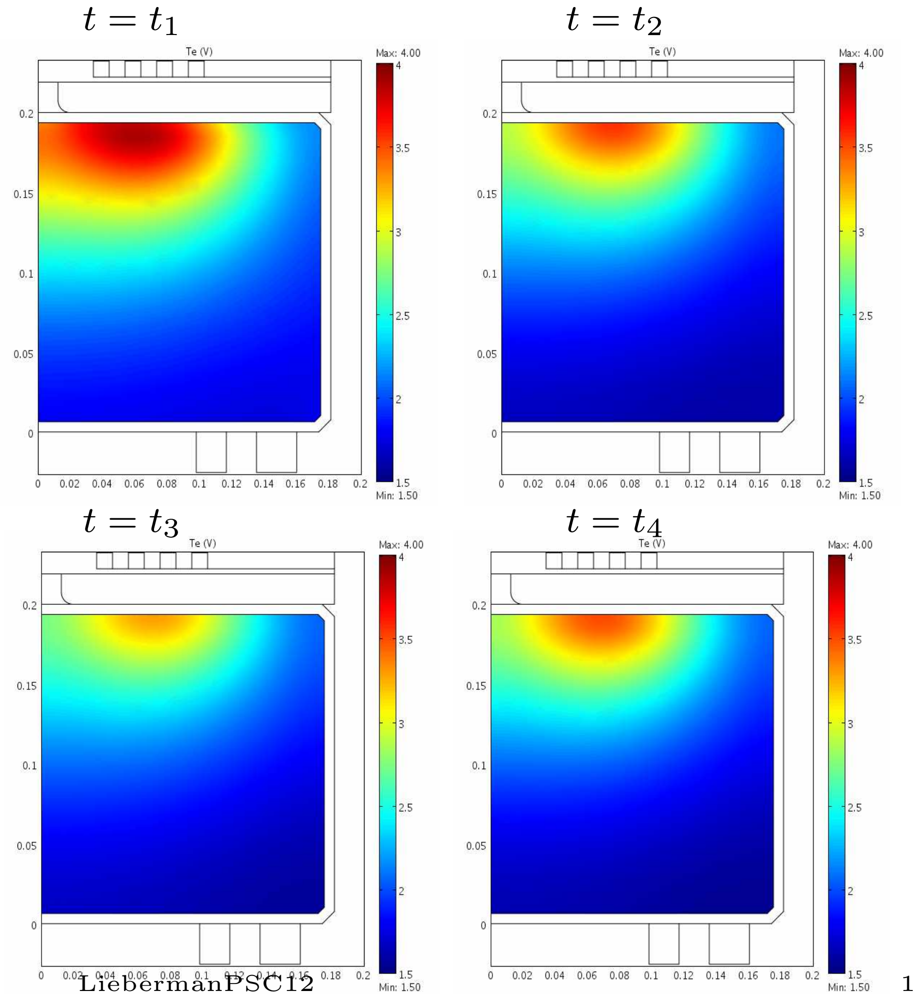
$\mathbf{T_e(r,z)}$ VERSUS t

- T_e strongly localized near coil
- t_1 (enter E-mode): Te jumps to highest value

- t_2–t_4 (E-mode followed by transition to H-mode): T_e decays in time



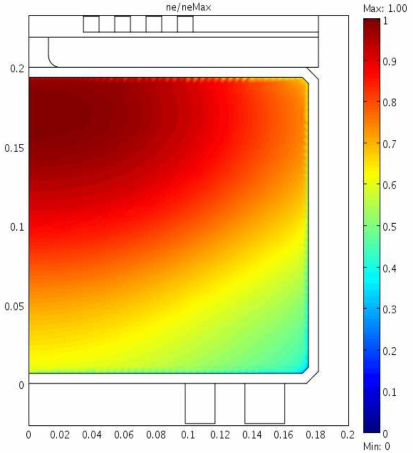
$t = t_1$ $t = t_2$

$t = t_3$ $t = t_4$

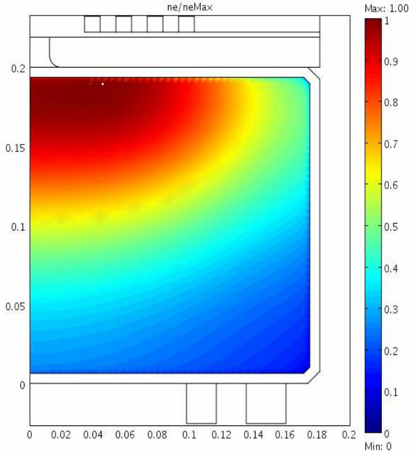
$\mathbf{n_e(r,z)/n_{emax}}$ VERSUS t

- n_e weakly localized near coil
- t_1 (enter E-mode): n_e rapidly decays with time

$n_{emax} = 1.29 \times 10^{15}\ \mathrm{m}^{-3}$ at t_1

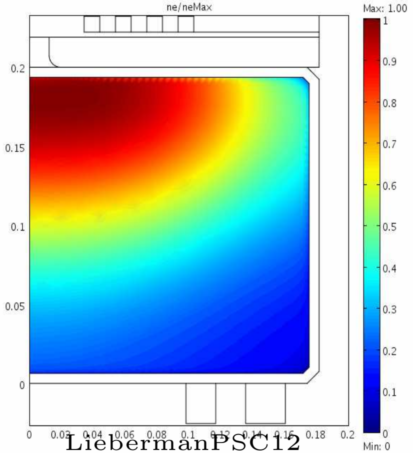


$n_{emax} = 5.73 \times 10^{15}\ \mathrm{m}^{-3}$ at t_2

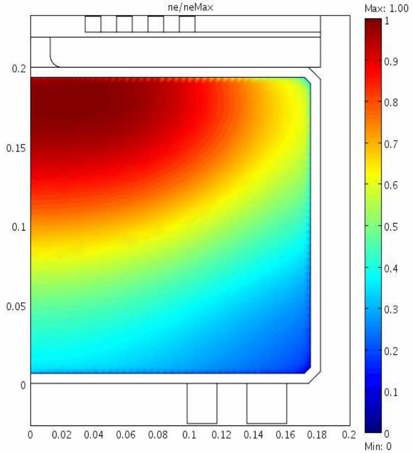


- t_3 (enter H-mode): n_e rapidly increases with time

$n_{emax} = 15.6 \times 10^{15}\ \mathrm{m}^{-3}$ at t_3

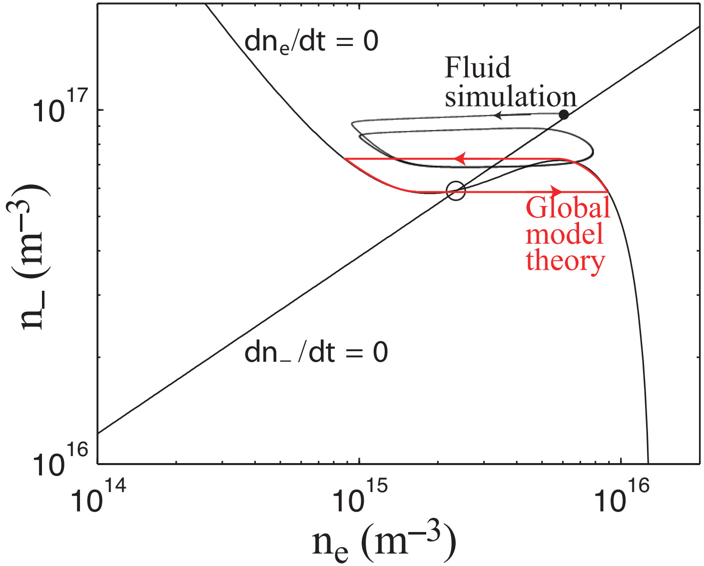


$n_{emax} = 5.86 \times 10^{15}\ \mathrm{m}^{-3}$ at t_4



FLUID AND GLOBAL MODEL COMPARISON

- Intersection of $\mathrm{d}n_e/\mathrm{d}t = 0$ and $\mathrm{d}n_-/\mathrm{d}t = 0$ curves $\Rightarrow$ equilibrium
- Slope $\mathrm{d}n_-/\mathrm{d}n_e$ of $\mathrm{d}n_e/\mathrm{d}t = 0$ curve positive $\Rightarrow$ unstable

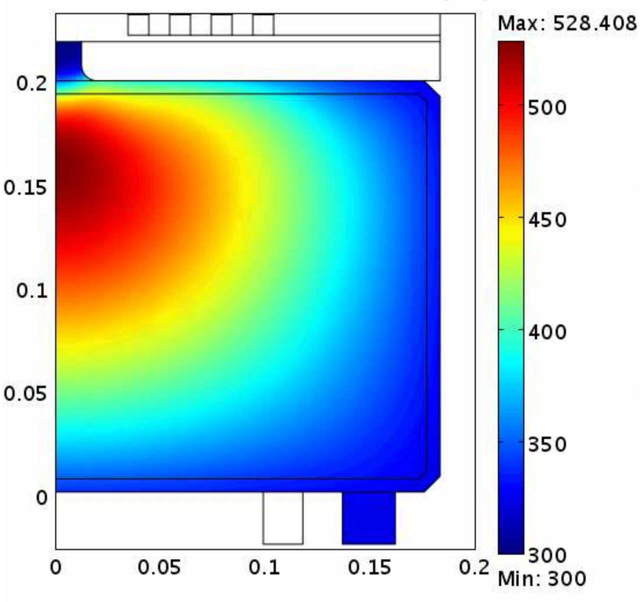


- Good agreement of fluid calculation and analytical global model

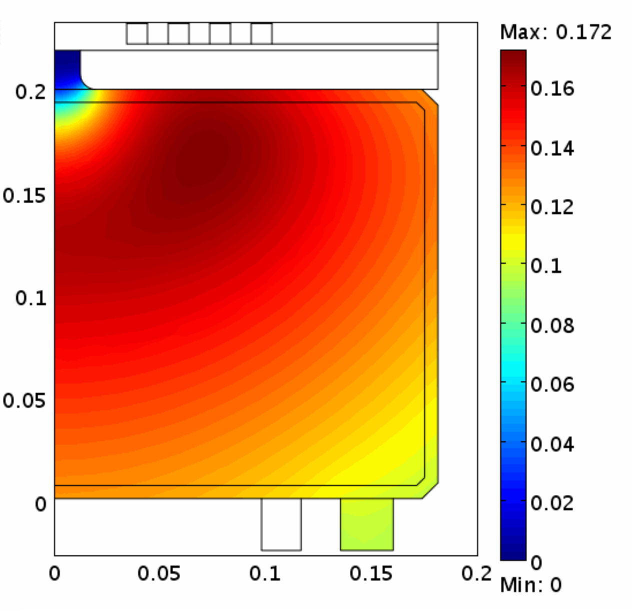
NEUTRAL TIME AVERAGES OVER INSTABILITY

- Neutral species time variations are very small
- Time averages:

Gas Temperature (K)



Molar Cl Fraction



- T_g rises to 530 K inside discharge
- Chlorine density varies significantly with radius

SUMMARY

- A one-dimensional hybrid analytical-numerical global model of atmospheric pressure, rf-driven capacitive discharges was developed
- Coupling analytical solutions of the time-varying discharge and EEPF dynamics, and numerical solutions of the discharge chemistry, allows for a fast solution of the discharge equilibrium

  (Lazzaroni et al, to appear in PSST, 2012)
- The E/H transition instability has been found and studied in 2D fluid simulations
- The fluid instability dynamics is in good agreement with an analytical global model

  (Kawamura et al, submitted to PSST, 2012)

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