1. 2D Fluid Reactor Models using COMSOL

Develop fast 2D TCP Fluid Reactor Model using COMSOL (portable, user-friendly, numerical finite elements simulation tool):

- Both inductive and capacitive coupling.
- Bulk Fluid Plasma is coupled with analytic sheath model.
- Gas flow, temperature and pressure model with reactive gas chemistries (e.g., O_2 or Cl_2).
- Verify model by comparing to experimental data (i.e., Malyshev and Donnelly 2000-2001).

Compare Fluid CCP with 1D PIC CCP to verify analytic sheath model:

- Vacuum sheath of varying thickness is modeled with fixed width sheath of varying dielectric constant.
- A dissipative term is added to the sheath dielectric constant.
- Sheath Ohmic and stochastic heating are energy fluxes entering the plasma-sheath boundary in the electron energy balance equation.

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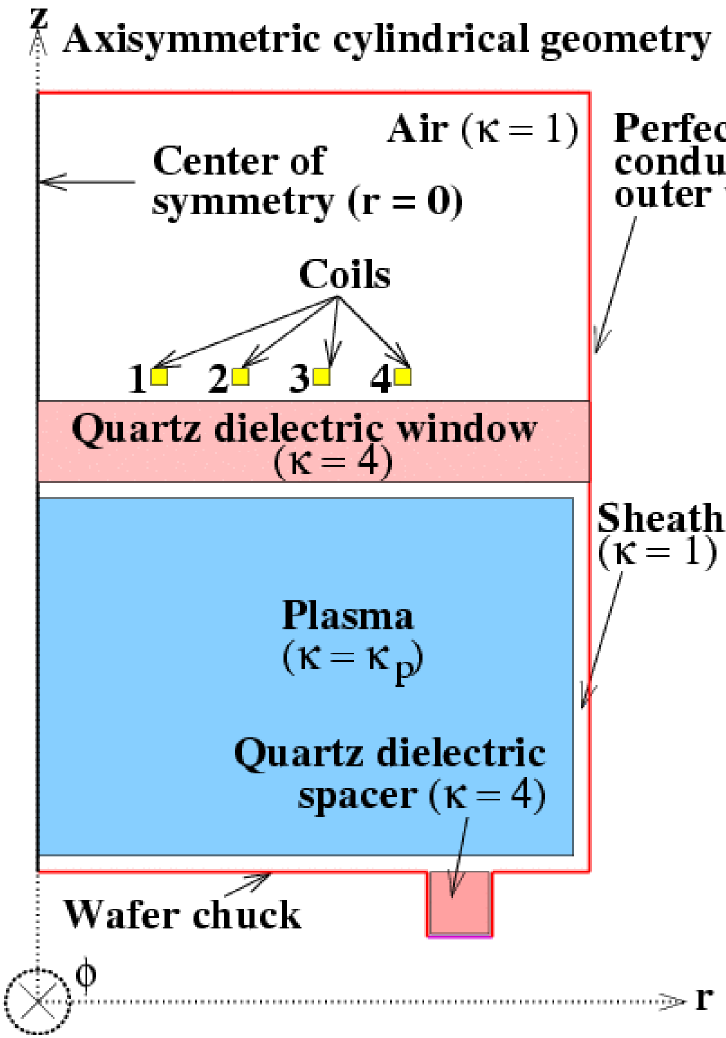
2. Geometry of TCP Reactor



- Similar to Malyshev and Donnelly (2000-2001) geometry.
- Axisymmetric cylindrical geometry with center of symmetry at $r = 0$.
- Outer surface is a perfect conductor.
- Wafer chuck insulated from outer walls by a quartz dielectric spacer.
- 4-turn stove-top coil set {1, 2, 3, 4} placed on top of quartz dielectric window.
- Plasma surrounded by thin vacuum sheath. K_p depends on n_e, T_e, p and applied RF frequency.
- Fields produced by coils separate into inductive TE fields (E_ϕ, H_r, H_z) & capacitive TM fields (E_r, E_z, H_ϕ).

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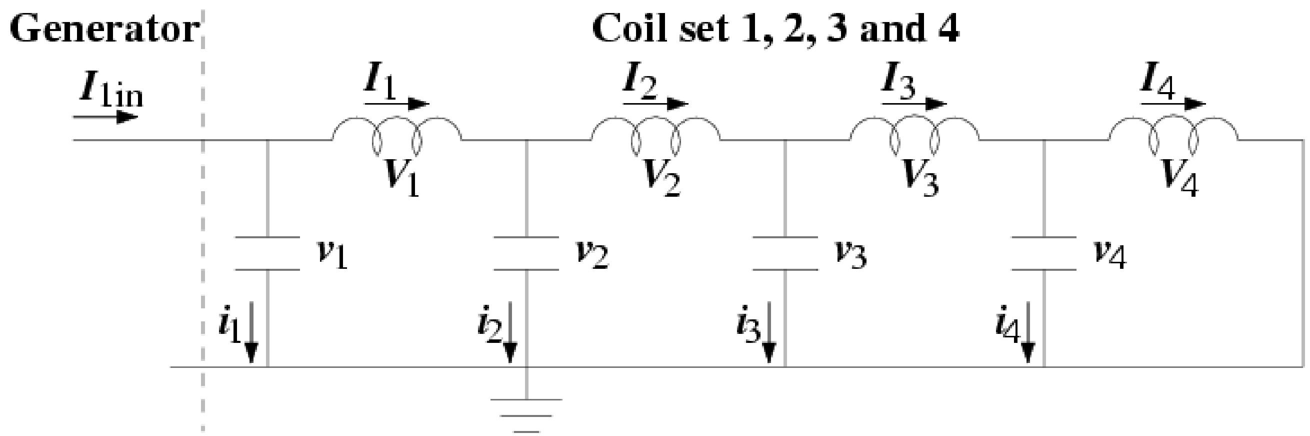
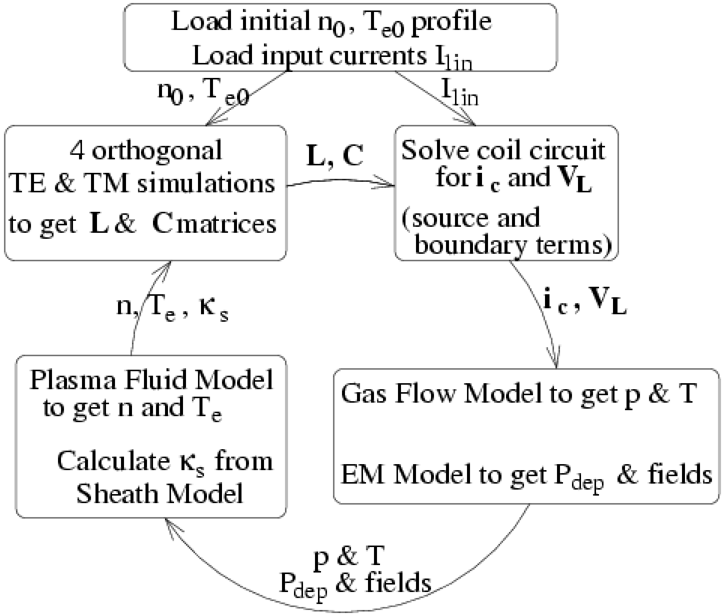
3. Coupling of TE and TM coil fields



- Inductive voltages $\mathbf{V_L}=(V_1, V_2, V_3, V_4)$ give *boundary conditions* for TE solve. Capacitive currents $\mathbf{i_c}=(i_1, i_2, i_3, i_4)$ give *external source terms* for TM solve.
- An Inductance Matrix **L** relates inductive currents $\mathbf{I_L}=(I_1, I_2, I_3, I_4)$ to inductive coil voltages: $\mathbf{V_L} = j\omega \mathbf{L} \mathbf{I_L}$. Find **L** by conducting 4 *orthonormal TE* simulations in which $V_n=1$ for one coil and $V_n=0$ for the other 3 coils.
- A Capacitance Matrix **C** relates capacitive voltages $\mathbf{v_c}=(v_1, v_2, v_3, v_4)$ to capacitive currents: $\mathbf{i_c}=j\omega \mathbf{C} \mathbf{v_c}$. Find **C** by conducting 4 *orthonormal TM* simulations in which $i_n=1$ for one coil while $i_n=0$ for the other 3 coils.
- Given input current I_{1in}, we can solve the coil circuit to determine all the values of the coil currents and voltages.

4. Outline of TCP Reactor Model



- **EM Model**: Solves for the inductive and capacitive coupling of power from TCP coils to plasma via a dielectric window. Assumes harmonic time dependence: Fields ~ exp($j\omega t$).

- **Plasma Fluid Model**: Solves the 2D time-dependent plasma fluid equations for ion continuity and electron energy balance. Assumes a quasineutral and ambipolar plasma.

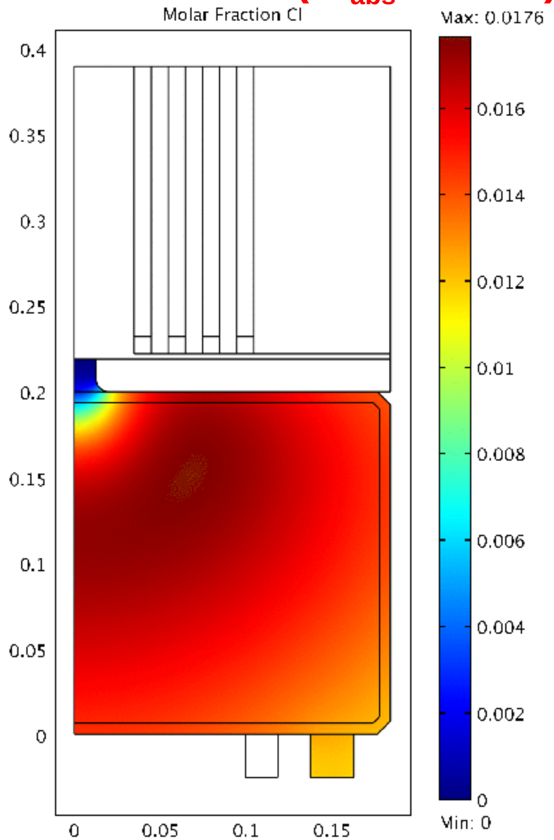
- **Sheath Model**: Models a vacuum sheath of variable sheath thickness with a fixed width sheath of varying dielectric constant (Insook Lee et al, 2008). Changes: Stochastic and sheath Ohmic heating treated as incoming energy flux at plasma-sheath boundary. Dissipative term added to sheath dielectric constant to get correct power balance.

- **Gas Flow Model**: Solves for steady-state gas pressure, temperature, velocity, and neutral species mass fractions of a reactive gas (Hsu et al 2006).

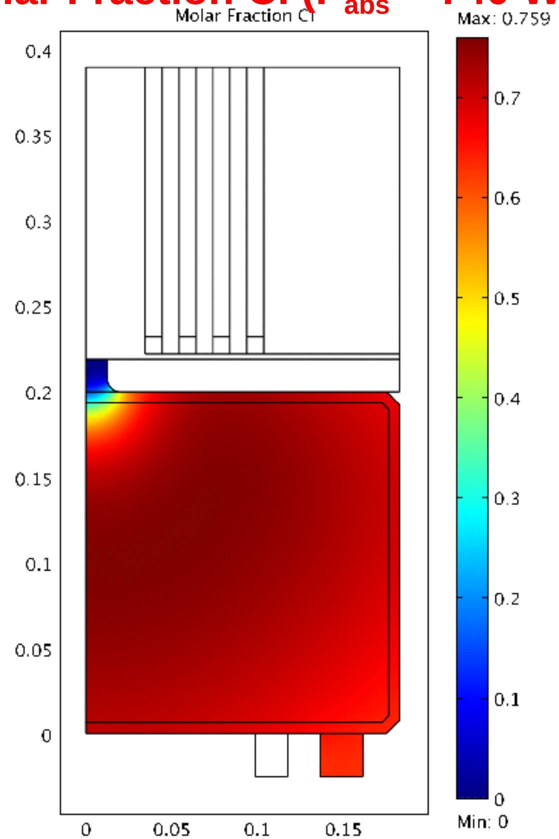
5. TCP Chlorine Reactor Simulations

- 13.56 MHz, 100 sccm, 10 mTorr , I_{1in} =18-70 A, and P_{abs}=5.8-800 W. (Cl_2 reaction set from E.G. Thorsteinsson and J.T. Gudmundsson 2009.)
- Total Simulation time ~ 70 min. on a 2.2 GHz CPU, 4GB RAM system.

Molar Fraction Cl(P_{abs} = 5.8W)



Molar Fraction Cl (P_{abs} = 740 W)



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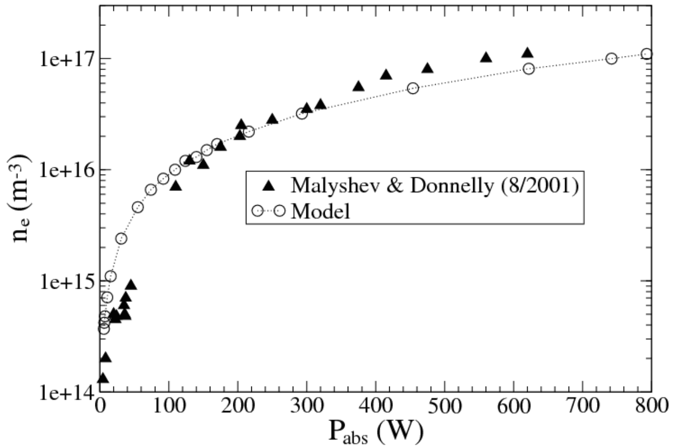
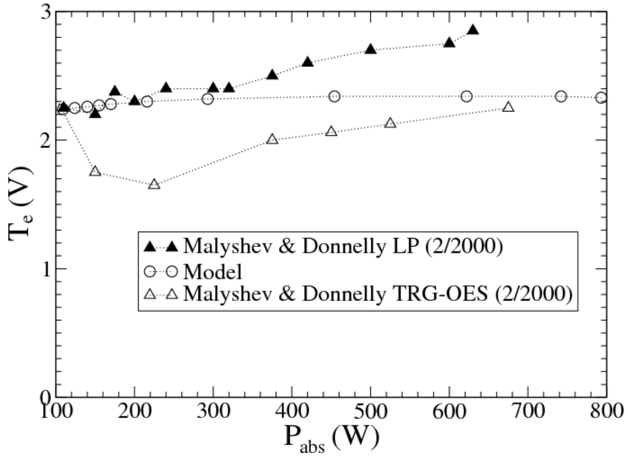
6. Model vs. Experiment

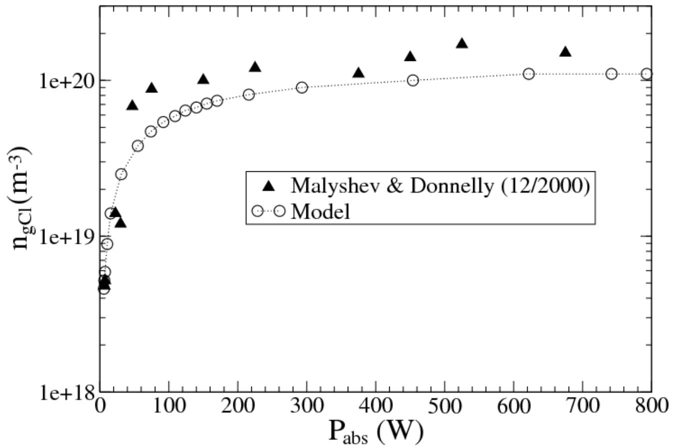
n_e vs. P_{abs} at Discharge Center



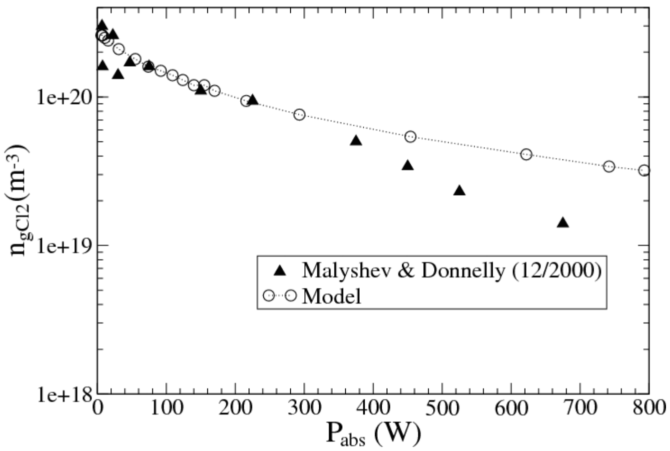
T_e vs. P_{abs} at Discharge Center



n_{gCl} vs. P_{abs} at Discharge Center



n_{gCl2} vs. P_{abs} at Discharge Center



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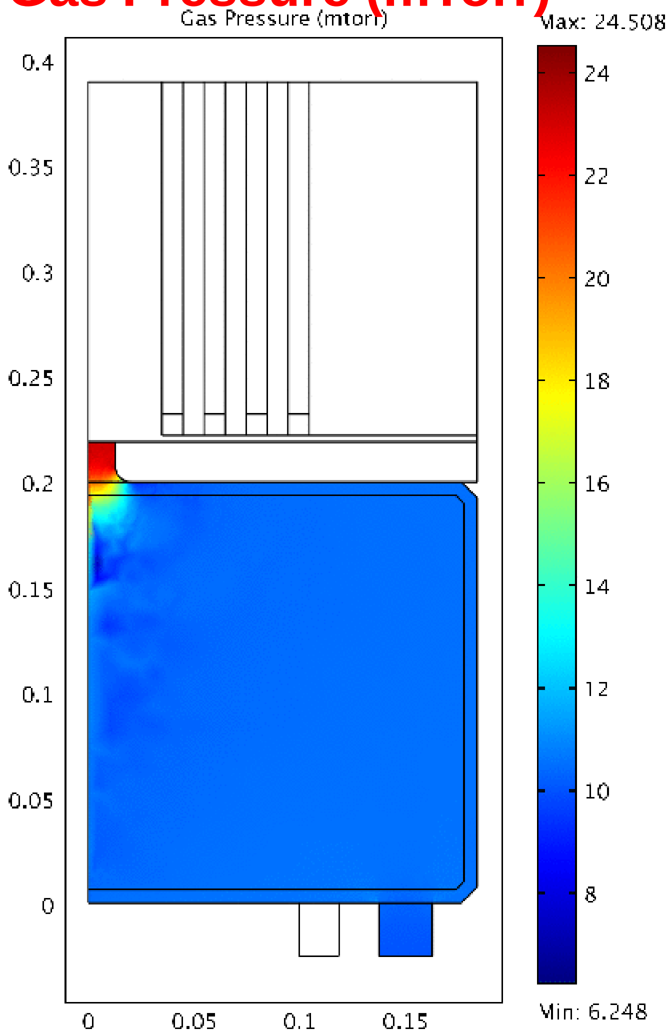
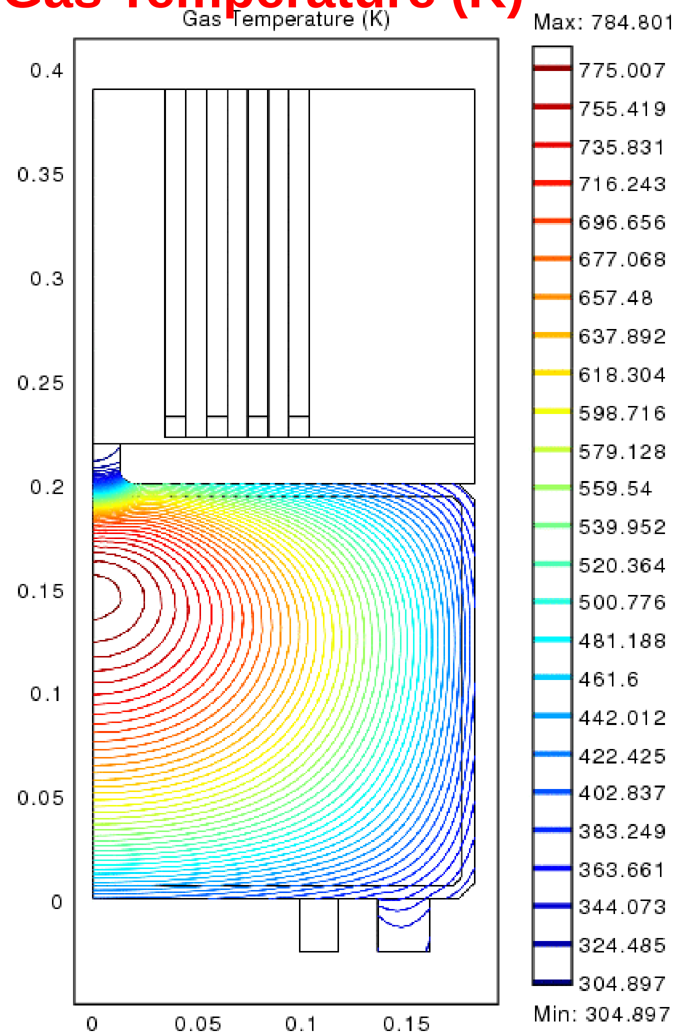
7. Gas Pressure and Temperature (P_{abs}=740 W)

Gas Pressure (mTorr)



Gas Temperature (K)



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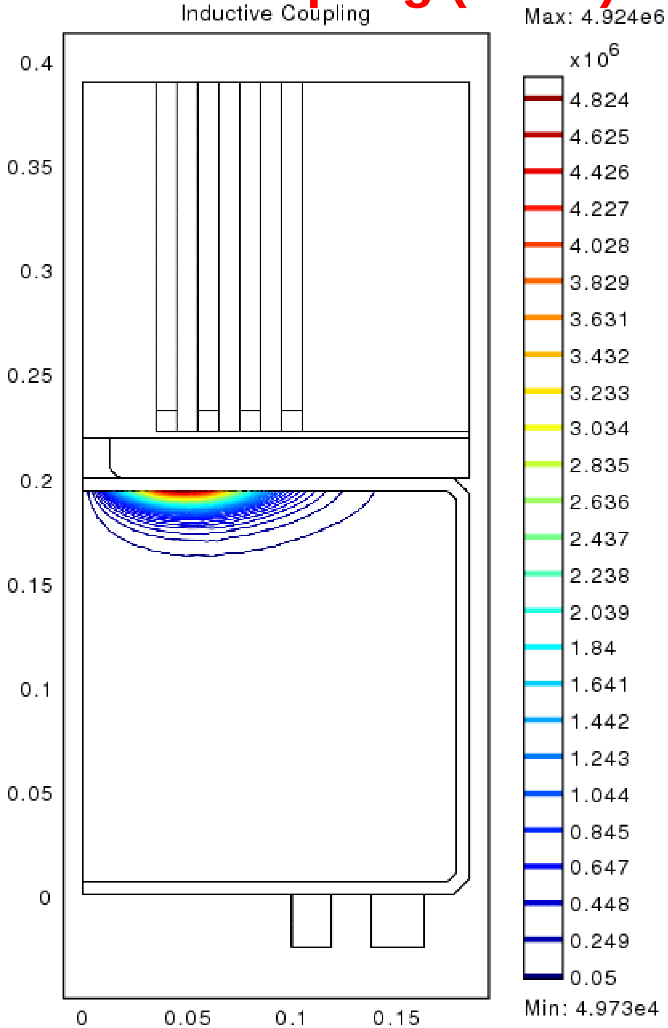
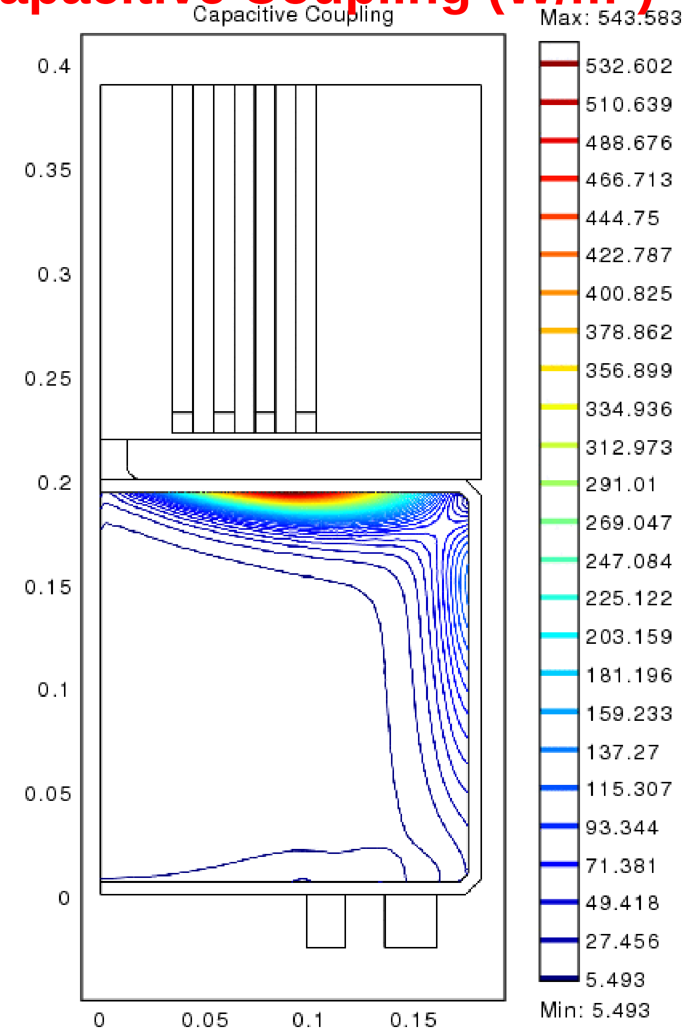
8. Inductive and Capacitive Power (P_{abs}=740 W)

Inductive Coupling (W/m³)



Capacitive Coupling (W/m³)



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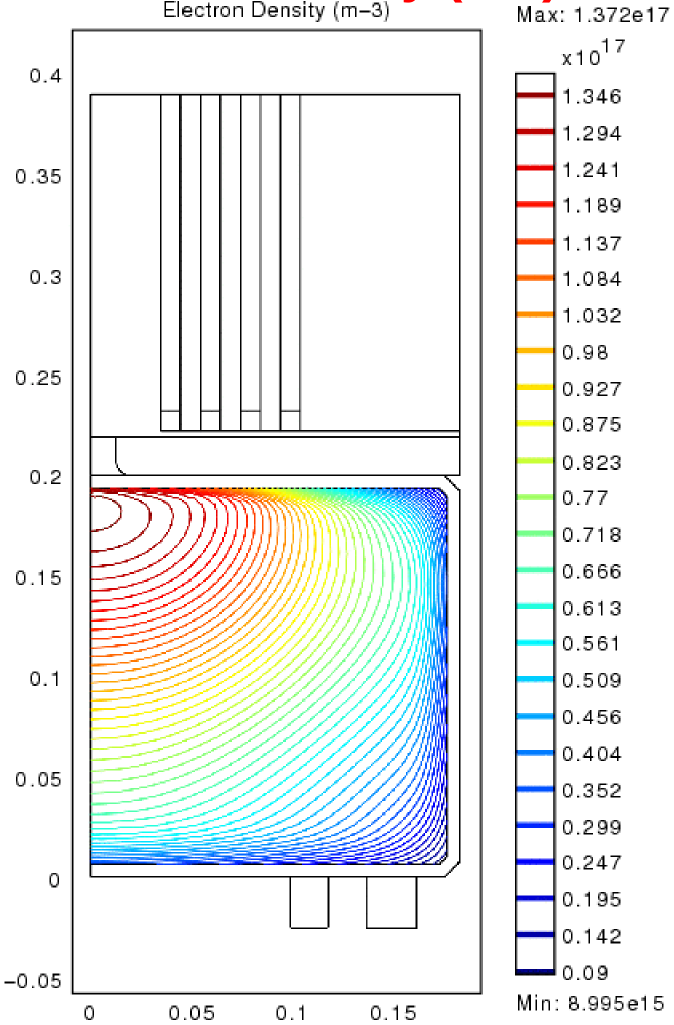
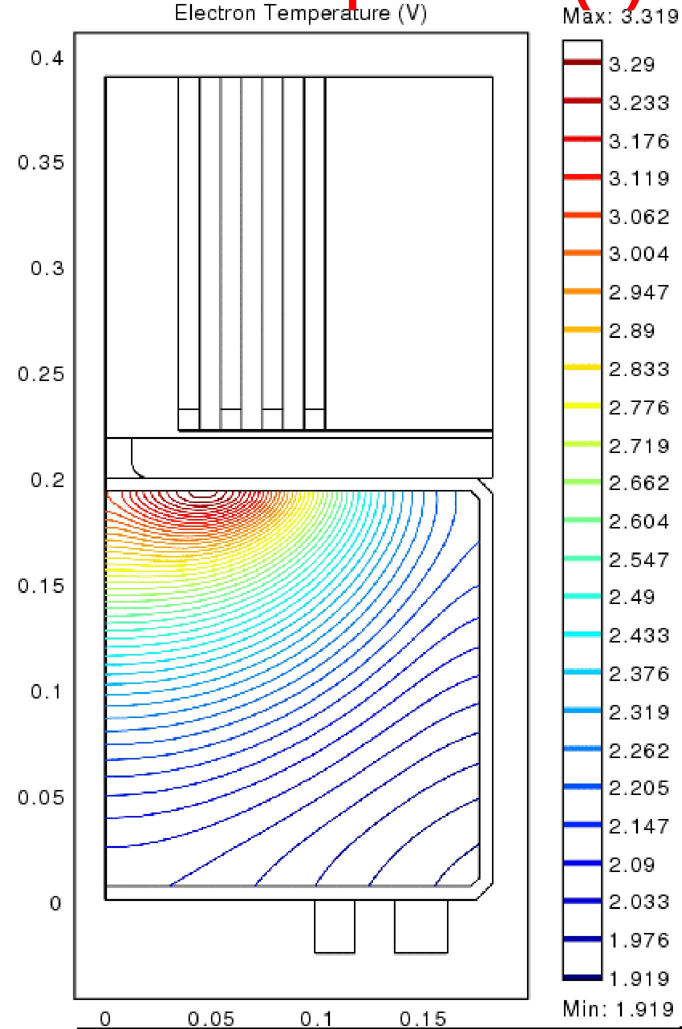
9. Electron density and Temperature (P_{abs}=740 W)

Electron Density (m^{-3})



Electron Temperature (V)



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10. Power Balance Results

	I_{1in} = 18 A	I_{1in} = 67 A
Peak n_e (m^{-3})	4.8e14	1.4e17
Peak T_e (V)	3.3	3.3
P_{coll} (W)	4.3	626
P_{amb} (W)	0.05	9.4
P_{ewall} (W)	0.13	22.7
P_{iwall} (W)	1.3	83.6
P_{loss} (W)	5.8	741
$P_{plasCap}$(W)	3.2	0.82
$P_{plasInd}$ (W)	2.6	740
P_{abs} (W)	5.8	741
$P_{CoilCap}$ (W)	3.2	1.0
$P_{CoilInd}$ (W)	2.6	724
P_{Coil} (W)	5.8	725

11. Bulk Plasma Fluid Model

Ion Continuity Equation:

$$\partial n_i / \partial t + \nabla \cdot \boldsymbol{\Gamma}_\mathbf{i} = \nu_{iz} n_e$$

boundary conditon: $\boldsymbol{\Gamma}_\mathbf{i} \cdot \mathbf{n} = 0$, at r = 0

$\boldsymbol{\Gamma}_\mathbf{i} \cdot \mathbf{n} = n_i u_B$ at plasma sheath boundary

Electron Energy Balance Equation:

$$1.5\, e\, \partial(n_e T_e)/\partial t + \nabla \cdot \mathbf{Q_e} = -e\, \mathbf{E_a} \cdot \boldsymbol{\Gamma}_\mathbf{e} + p_{dep} - p_{coll}$$

boundary condition: $\mathbf{Q_e} \cdot \mathbf{n} = 0$, at $r = 0$

$\mathbf{Q_e} \cdot \mathbf{n} = (2eT_e + eV_{float} - S_{stoc} - S_{ohmSh})(\boldsymbol{\Gamma}_\mathbf{e} \cdot \mathbf{n})$ at plasma sheath boundary,

Electron heat flux: $\mathbf{Q_e} = 2.5\, \boldsymbol{\Gamma}_\mathbf{e}\, eT_e - 2.5\, n_e e^2 T_e\, \nabla T_e/(m_e \nu_m)$

Ambipolar electric field: $\mathbf{E_a} = -T_e\, \nabla n_e / n_e$

Ion Flux: $\boldsymbol{\Gamma}_\mathbf{i} = -D_i\, (1 + T_e/T_i)\, \nabla n_{i,,}$ and $D_i = eT_i/(M_i \nu_m)$

Bulk power deposition: $p_{dep} = 0.5\, \mathrm{Re}(\sigma_p)|\mathbf{E}|^2$

Assumptions: Quasineutral, ambipolar plasma, constant uniform T_i , neglect ion and electron inertia.

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12. Sheath Heating Models

- In ν_{eff} method, a dissipative term ν_{sh} is added to ν_{coll} so that $\nu_{eff} = \nu_{coll} + \nu_{sh}$. This increases σ_p and the bulk Ohmic heating term $p_{dep} = 0.5\,\mathrm{Re}(\sigma_p)|\mathbf{E}|^2$.
- In B.C. model, sheath Ohmic and stochastic heating is treated as an incoming energy flux at the plasma sheath boundary.
- The K_{sh} model extends the B.C. model by adding a dissipative (imaginary) term to the sheath dielectric constant. Then, the EM model can give the correct phase relation between V_{rfin} and I_{rfin} so that $P_{abs} = P_{source}$.
- We tested the sheath heating models on a 250 mTorr, 13.56 MHz parallel plate CCP with a 20 cm radius and 16 cm gap. A current source with $I_{rfin} = 10$ A was attached to the bottom plate. Sheath heating was turned on only for the top plate at z=16 cm.

13. Sheath Heating Model Comparison

Argon CCP with sheath heating only on Top Plate:
250 mTorr, 13.56 MHz, radius=20 cm, gap=16 cm, I_{rfin} = 10 A.

	K_{sh}	B.C.	ν_{eff}
n_{epeak} (m-3)	1.3e17	1.3e17	1.5e17
T_{epeak} (V)	2.99	2.99	2.5
V_{rfin} (V)	10.25-1.3e3j	6.24-1.3e3j	10.23-1.4e3j
P_{source} (W)	51.2	31.2	51.2
P_{bulk} (W)	31.2	31.2	51.2
P_{sheath} (W)	18.8	18.8	0
P_{abs} (W)	50.0	50.0	51.2
P_{loss} (W)	50.0	50.0	50.0
	$P_{source}=P_{abs}$	$P_{source}=P_{bulk}$	$P_{source}=P_{abs}$

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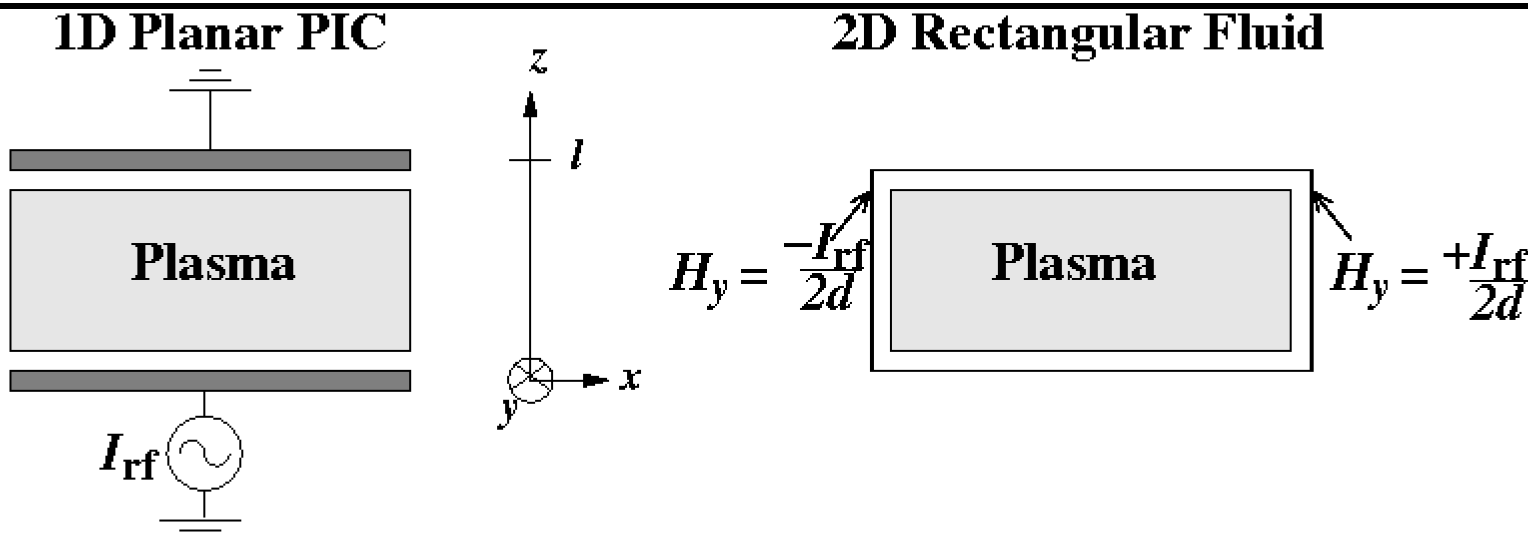
14. 1D Planar PIC vs. 2D Rectangular Fluid



•1D planar electrostatic PIC code tracks (z, v_x, v_y, v_z) of particles. Poisson's equation solves for E_z. No assumptions about particle velocity distributions.

•2D rectangular fluid model solves for TM fields (H_y, E_x, E_z), $n(x,z)$ and $T_e(x,z)$. Assumes ambipolar, quasineutral plasma and Maxwellian EEDF.

•l = discharge gap = 5 cm. Each plate area = 100 cm^2.
d = depth of discharge in y-direction = 10 cm.

•Current-source driven argon CCP with f=27.12 MHz, I_{rf} = 1 A at 15 and 30 mTorr.
Goal: Test analytical collisionless sheath model with PIC.

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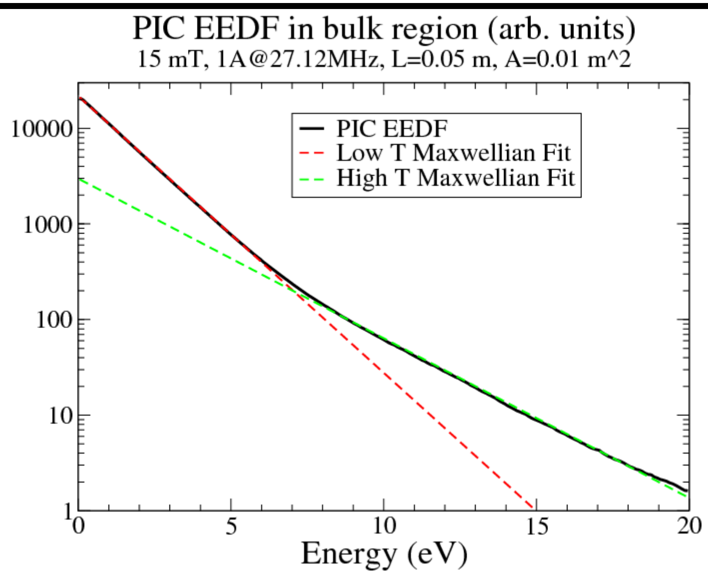
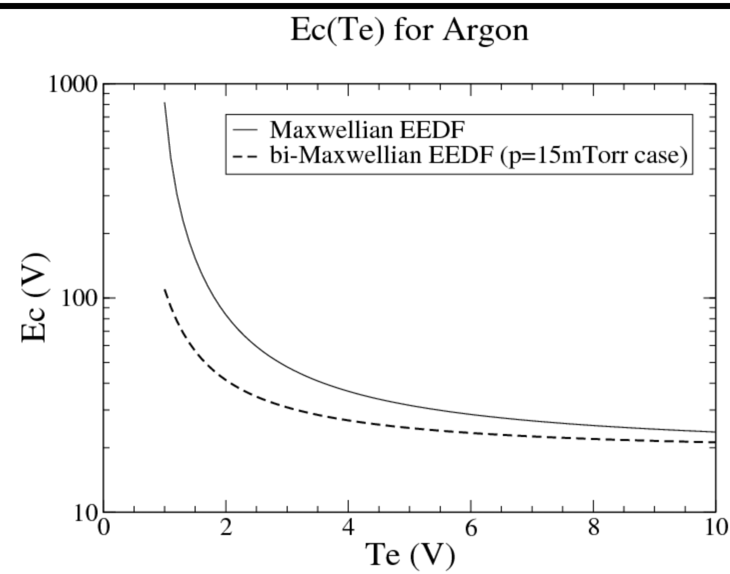
15. Maxwellian vs. Bi-Maxwellian EEDF





- PIC EEDFs were bi-Maxwellian at 15 and 30 mTorr.
- Fluid and PIC bulk parameters should match better when Fluid code uses bi-Maxwellian EEDFs from PIC.
- Fluid and PIC sheath parameters should match better at lower pressures since Fluid code uses an analytical collisionless sheath model.
- Fluid and PIC bulk parameters should match better at higher pressures due to Fluid code's assumption of constant ion diffusion coefficient.

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16. Fluid vs. PIC at 15 mTorr

	PIC	Fluid Maxw	Fluid bi-Maxw
n_{mid} (m-3)	3.1e16	1.2e16	1.7e16
T_{emid} (V)	1.62	2.72	1.81
Γ_i (m^{-2}/s)	1.19e19	1.04e19	1.00e19
V_{rfin} (V), ϕ (deg)	511, -87.7	490, -87.8	487, -88.0
P_{source} (W)	10.3	9.23	8.46
P_{e-} (W)	1.76	2.00	1.62
P_{ion} (W)	8.16	7.60	7.19
P_{loss} (W)	9.93	9.60	8.81
P_{ohm} (W)	0.171	0.369	0.186
P_{stoc} (W)	1.63	1.94	1.63
V_{rfSh} (V)	255	252	251
V_{dcSh} (V)	215	218	214

17. Fluid vs. PIC at 30 mTorr

	PIC	Fluid Maxw	Fluid bi-Maxw
n_{mid} (m-3)	4.1e16	2.2e16	2.9e16
T_{emid} (V)	1.48	2.25	1.67
Γ_i (m^{-2}/s)	9.99e18	9.25e18	9.18e18
V_{rfin} (V), ϕ (deg)	495, -88.0	533, -88.0	515, -88.1
$P_{sourcel}$ (W)	10.3	9.23	8.46
P_{e-} (W)	1.84	2.23	1.78
P_{ion} (W)	6.55	7.36	6.97
P_{loss} (W)	8.39	9.60	8.75
P_{ohm} (W)	0.269	0.479	0.266
P_{stoc} (W)	1.57	1.99	1.68
V_{rfSh} (V)	249	274	265
V_{dcSh} (V)	208	235	225

18. Conclusions

- The TCP Fluid reactor model shows good agreement with Malyshev and Donnelly's experimental data for n_e, T_e, n_{gCl}, n_{gCl2} at discharge center.
- Treating the sheath heating as an incoming heat flux at the plasma-sheath boundary correctly captures the local nature of the sheath heating.
- A dissipative term to the sheath dielectric constant is needed to get correct power balance between the driving circuit and the plasma.
- Analytical sheath model was verified by PIC at 15 and 30 mTorr.
- Hybrid fluid-analytical model allows fast computation of chemically active plasmas with flow and allows predictions of inductive, capacitive (and even wave) plasma sustaining mechanisms. Codes can be shared quickly among COMSOL users with ability to change geometry fairly easily.
- Next steps include incorporating matching network/ power generator models into the coil/circuit model, adding a multi-frequency sheath model and adding more chemistries (currently, $Ar/O_2/Cl_2$) . We would also like to couple particle codes to our fluid models to obtain the IEDS and IADs at the substrate.

19. References

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