NON-EQUILIBRIUM ION AND NEUTRAL TRANSPORT IN LOW-PRESSURE PLASMA PROCESSING REACTORS*

Vivek Vyas and Mark J. Kushner*****

****Department of Materials Science and Engineering**

*****Department of Electrical and Computer Engineering**

University of Illinois,

Urbana IL 61801

http://uigelz.ece.uiuc.edu

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AGENDA

- **Simulation of low pressure plasmas.**
- **Description of the Ion/Neutral Monte Carlo Simulation (IMCS) and the Hybrid Plasma Equipment Model.**
- **Validation of the model**
- **Comparative study of results obtained using fluid equations and IMCS**
  - **Ar: Temperatures and Densities**
  - **Ar-Cl_2: Temperatures and Densities**
  - **Ar-Cu: Temperatures and Sputter Profiles**
- **Concluding Remarks**

SIMULATION OF LOW PRESSURE PLASMAS

- **Low pressure (1-10 mTorr), weakly ionized plasmas are used extensively for processing of electronic materials.**
- **At these pressures, conventional continuum simulations are questionable as transport is highly non-equilibrium and a kinetic approach may be warranted.**
- **In principle, continuum equations are simply moments of the Boltzmann's equation. If the distribution functions are known, the equations should be valid at low pressures.**
- **In this regard, a hybrid modeling approach has been developed in which the ion and neutral temperatures are kinetically derived and implemented in fluid equations.**

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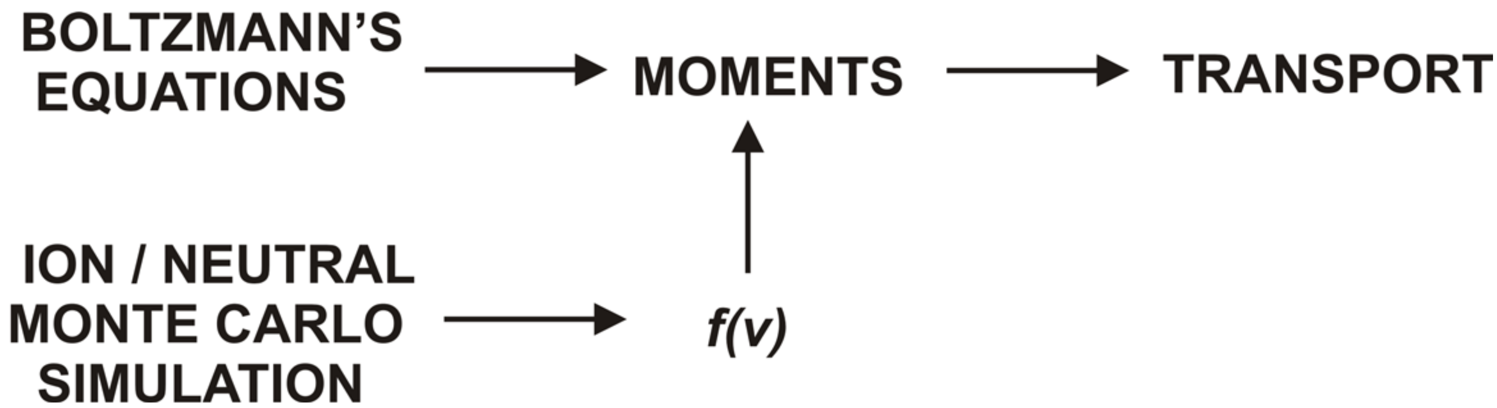
DESCRIPTION OF HYBRID METHOD



- **An ion/neutral Monte Carlo simulation is used to compute the transport coefficients for computing moments of the Boltzmann's equation.**

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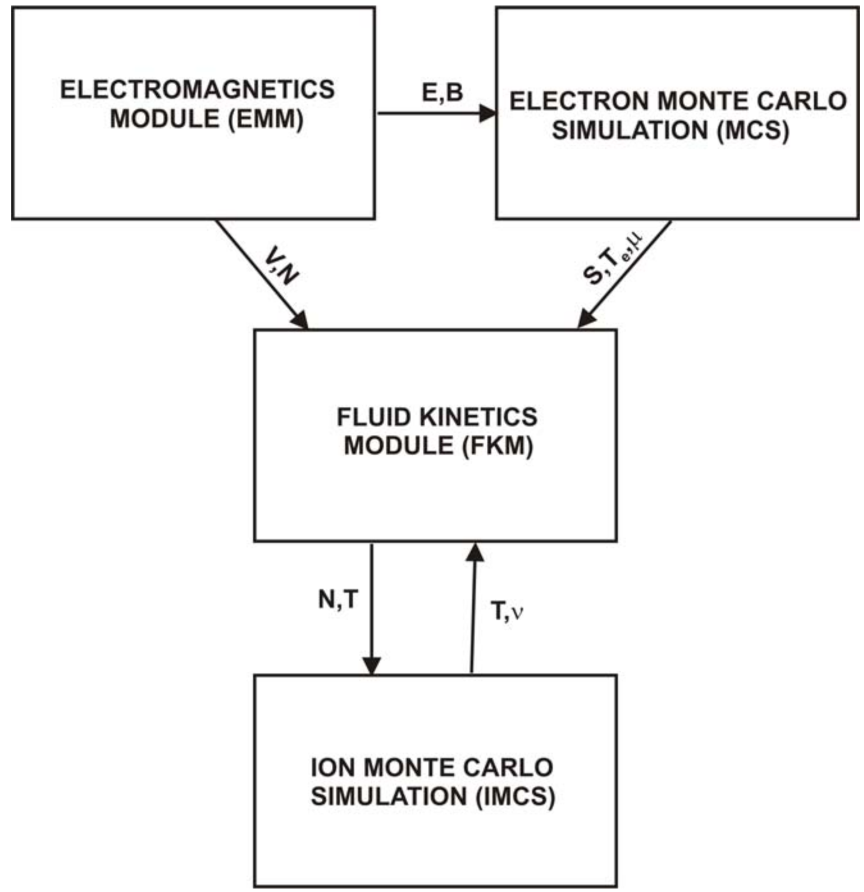
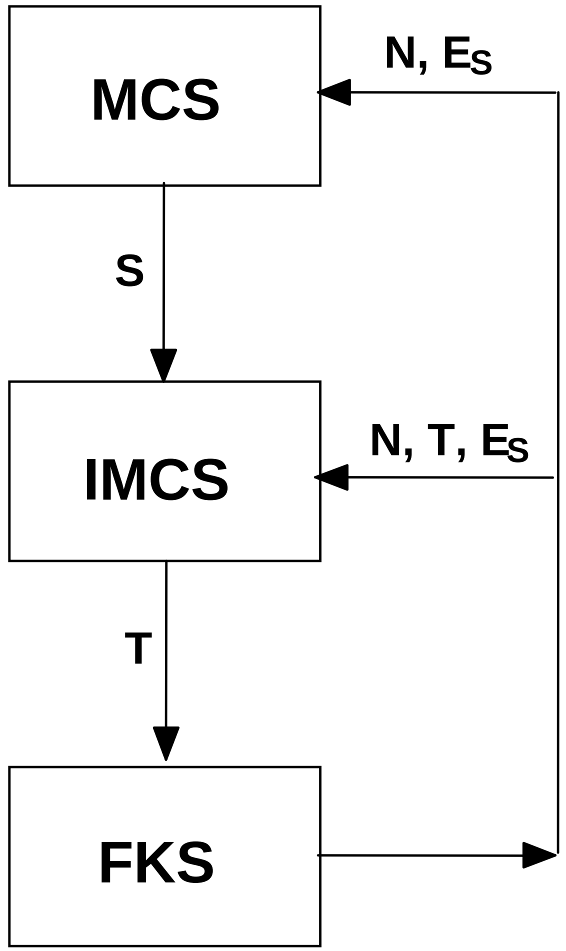
HYBRID PLASMA EQUIPMENT MODEL (HPEM)

- **HPEM is a modular simulator of low pressure plasmas.**
- **EMM: inductively coupled electric and magnetic fields.**
- **MCS: EEDs, transport coefficients and source functions.**
- **FKS:**
  Ions: Continuity, Momentum, Energy
  Neutrals: Continuity,Momentum,Energy
  Electrons: Drift Diffusion, Energy
  Electric Potentials: Poisson's Equation
- **IMCS: ion/neutrals transport coefficients.**



ION/NEUTRAL MONTE CARLO SIMULATION (IMCS)

- **MCS provides the transport coefficients and source functions at low pressures.**
- **The IMCS uses electron impact source functions; and electric /magnetic fields to advance trajectories of ions/neutrals and collisions are treated using a particle-mesh approach.**
- **The ion and neutral velocity distributions obtained are used to compute temperatures which are, in turn, used in the continuum equations.**



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CONTINUUM EQUATIONS

- **Continuity (heavy species) :**

$$\frac{\partial N_i}{\partial t} = \nabla \cdot \left(N_i \vec{v}_i\right) + S_i$$

- **Momentum (heavy species) :**

IMCS

$$\frac{\partial\left(N_i \vec{v}_i\right)}{\partial t} = \frac{q_i}{m_i} N_i\left(\vec{E}_s + \vec{v}_i \times \vec{B}_s\right) - \frac{1}{m_i}\nabla P_i + \sum_j N_i N_j k_{ij}\left(\vec{v}_j - \vec{v}_i\right) - \nabla \cdot \overline{\overline{\tau}}_i - \nabla \cdot \left(N_i \vec{v}_i \vec{v}_i\right)$$

- **Energy (heavy species) :**

IMCS

OR

$$\frac{\partial N_i c_v T_i}{\partial t} = \nabla \cdot \kappa_i \nabla T_i - P_i \nabla \cdot \vec{v}_i - \nabla \cdot (\vec{\varphi}_i \varepsilon_i) + \frac{N_i q_i^2}{m_i \nu_i} E_s^2 + \frac{N_i q_i^2 \nu_i}{m_i (\nu_i^2 + \omega^2)} E^2 + \sum_j 3 \frac{m_{ij}}{m_i + m_j} N_i N_j R_{ij} k (T_j - T_i)$$

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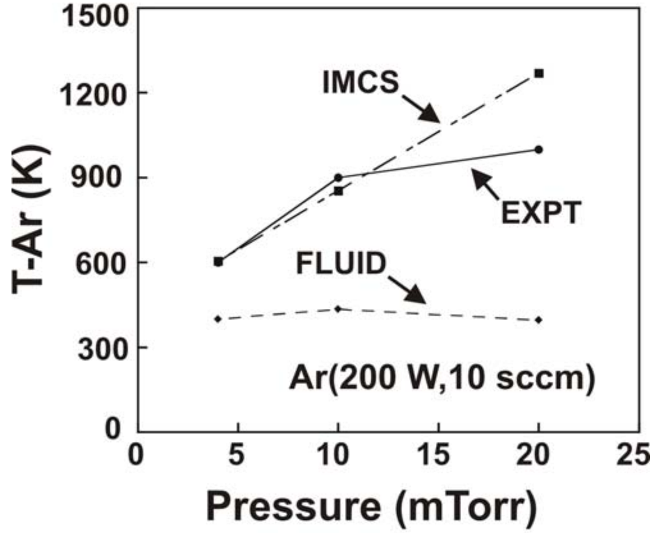
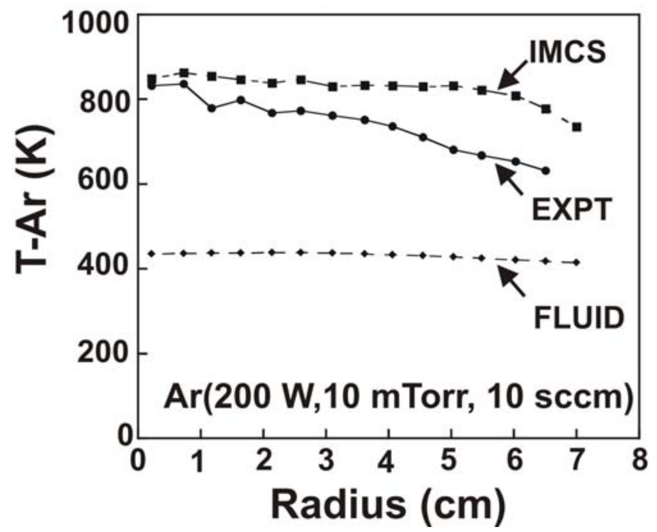
MODEL VALIDATION- T-Ar

- The model was validated by comparison with experiments performed in a GEC Reference cell reactor by Hebner.*

- T-Ar increases with pressure due to a higher charge exchange reaction rate.

- T-Ar peaks in the center of the reactor due to higher Ar^+ density.

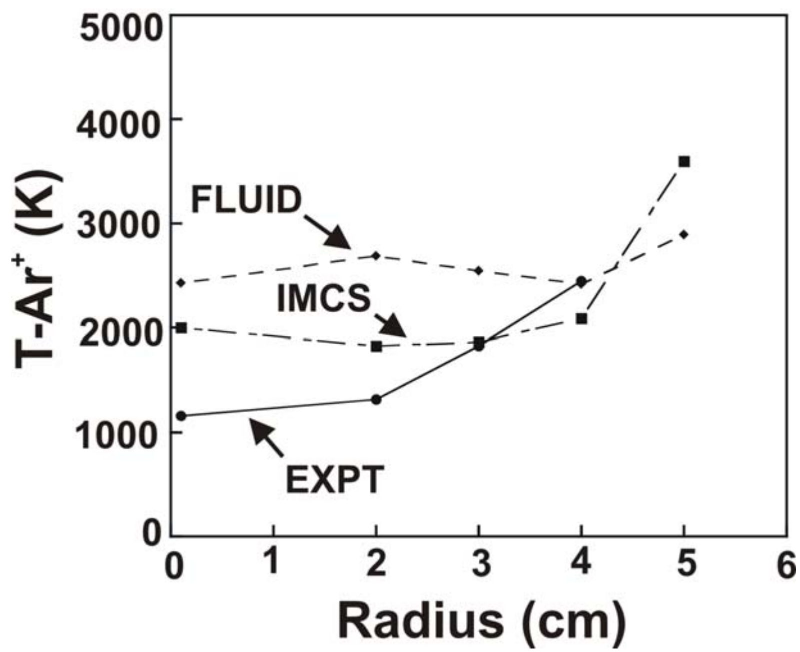




[1]G. A. Hebner, J. Appl. Phys. 80 (5), 2624 (1996)

MODEL VALIDATION- T-Ar^+

- **T-Ar^+ increases with radius due to the larger electric fields at the periphery of the reactor.**



Ar (200 W, 10 mTorr, 10 sccm)

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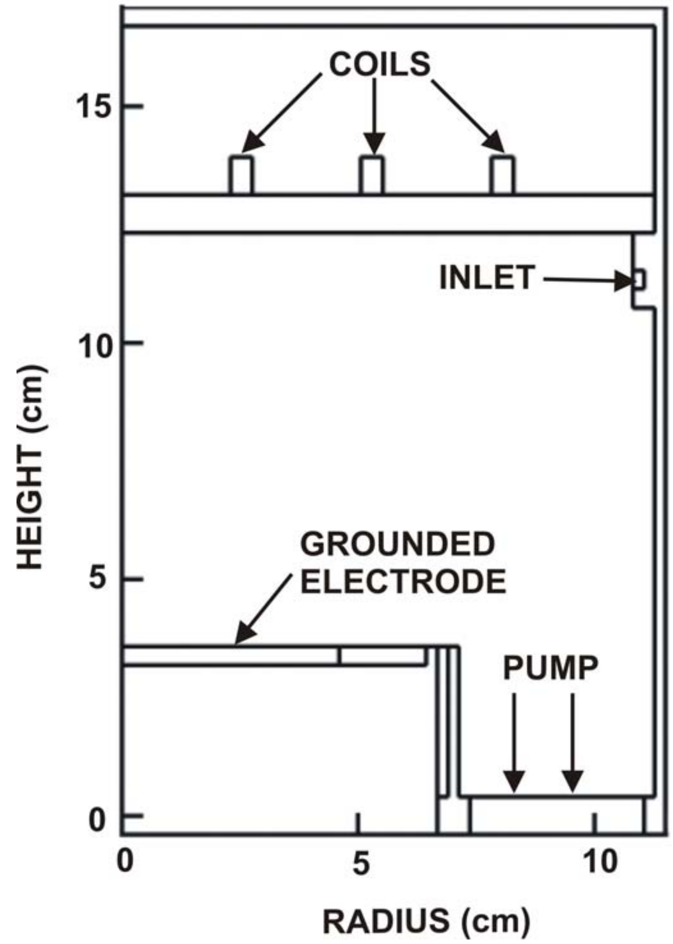
OPERATING CONDITIONS

- **Pressure : 1 - 20 mTorr**
- **ICP Power: 100 – 300 W, 10 MHz**
- **Chemistries: Ar, Ar-Cl_2**
- **Flow: 100 sccm**



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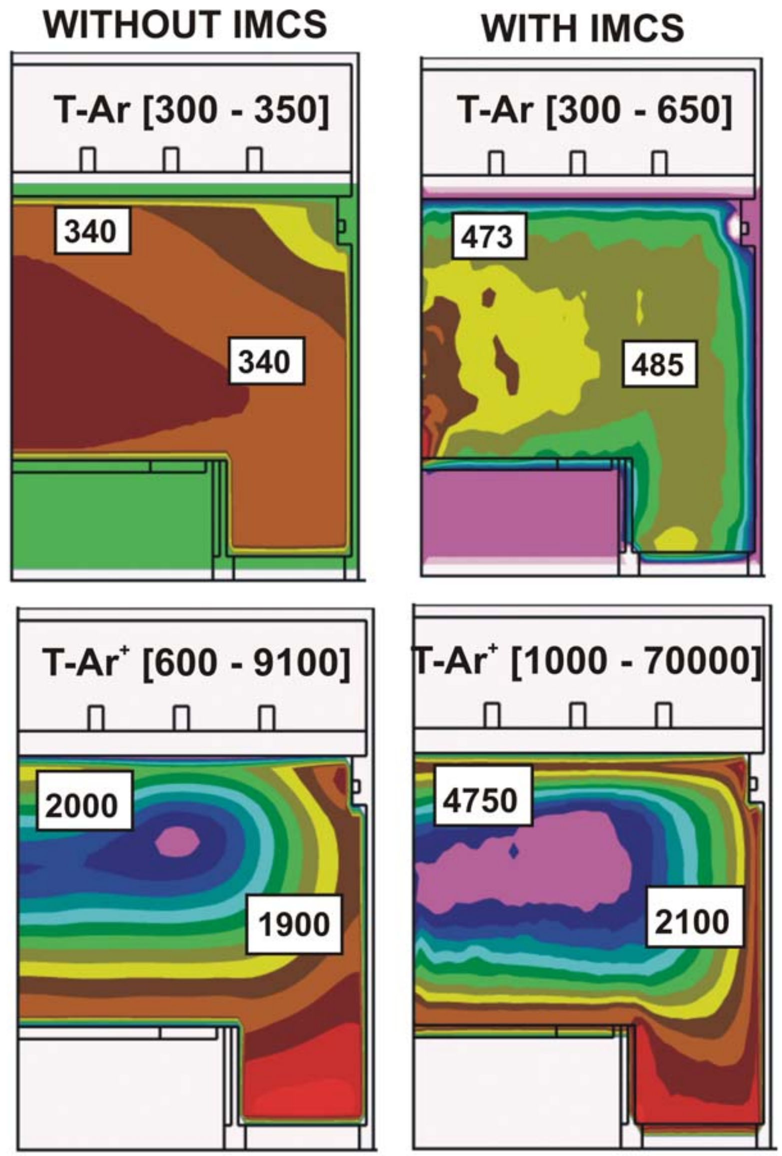
PLASMA PROPERTIES: T-Ar AND T-Ar^+

- **Temperatures computed using fluid equations and IMCS are compared.**
- **T-Ar peaks in the center of the reactor and T-Ar^+ at the periphery.**
- **IMCS predicts higher temperatures for Ar and Ar^+.**
- **A higher T-Ar results in a lower Ar density at a constant pressure.**

- **Ar (300 W, 2 mTorr, 100 sccm)**



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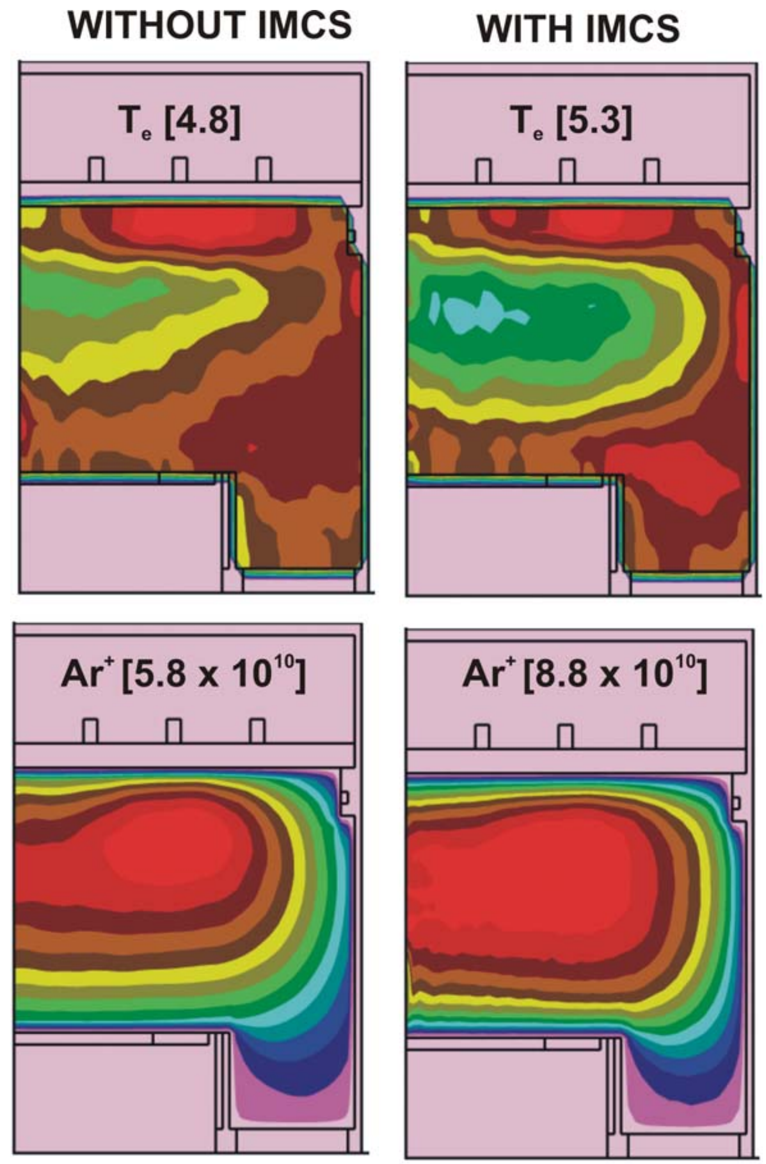
ELECTRON TEMPERATURE AND Ar^+ DENSITY

- The lower Ar density, with IMCS, translates into a higher electron temperature.
- A larger T_e results in more ionization, hence Ar^+ density is higher with IMCS.
- [Ar^+] is more uniform with IMCS because of a flatter T_e profile in the center of the reactor.



• Ar (300 W, 2 mTorr, 100 sccm)

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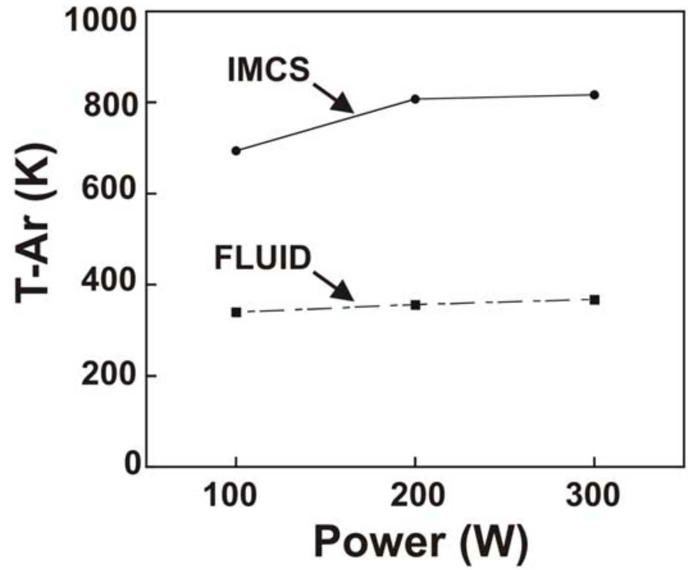
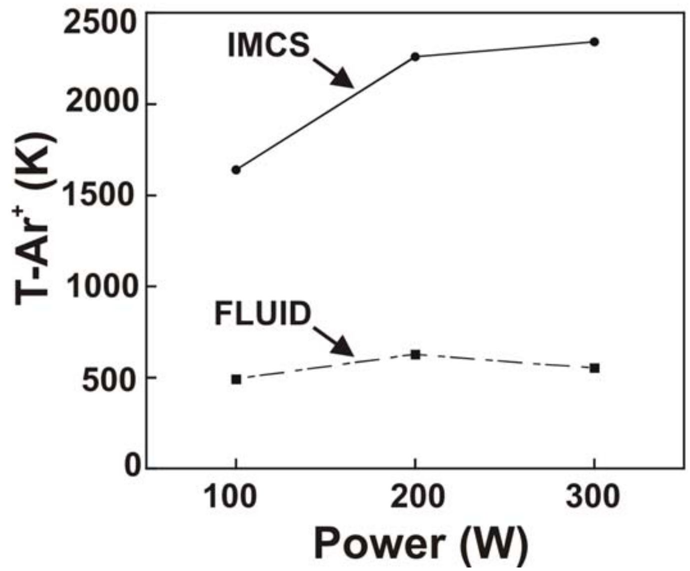
TEMPERATURES: POWER

- T-Ar increases with power as the rate of symmetric charge exchange increases.

- T-Ar^+ in the center of the reactor increases with power because of larger electric fields.





- Ar (300 W, 10 mTorr, 100 sccm)

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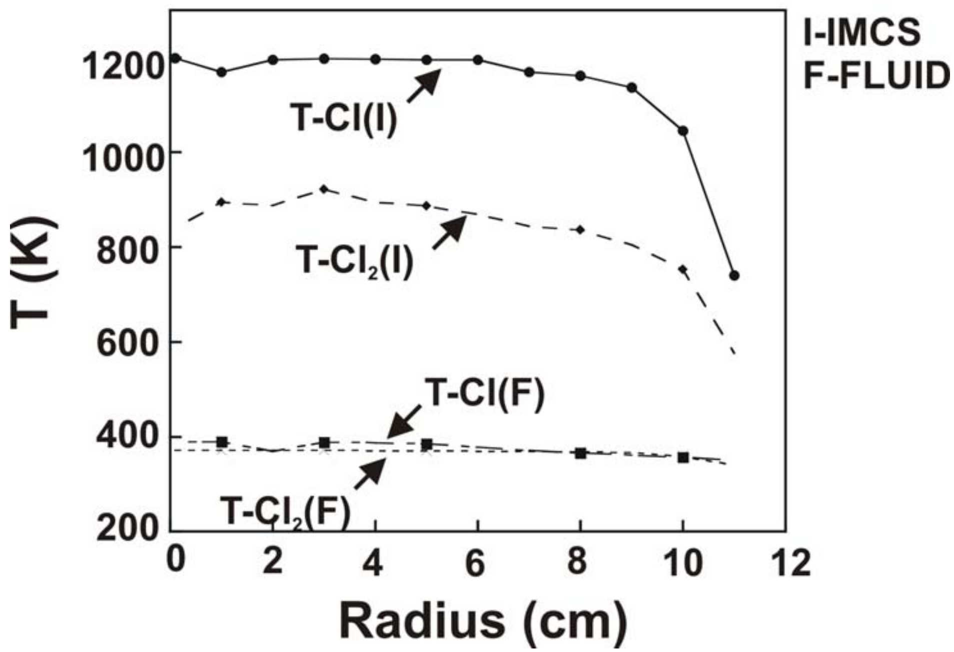
PLASMA PROPERTIES: Ar/Cl_2

- **A higher symmetric charge exchange rate causes neutral temperatures to peak in the center of the reactor.**
- **IMCS predicts larger values for T-Cl and T-Cl_2 than the fluid equations.**
- **T-Cl is higher than T-Cl_2 because of a higher charge exchange collision frequency independent of Frank Condon heating.**



- **Ar/Cl_2 (80:20), 10 mTorr, 300 W, 100 sccm**

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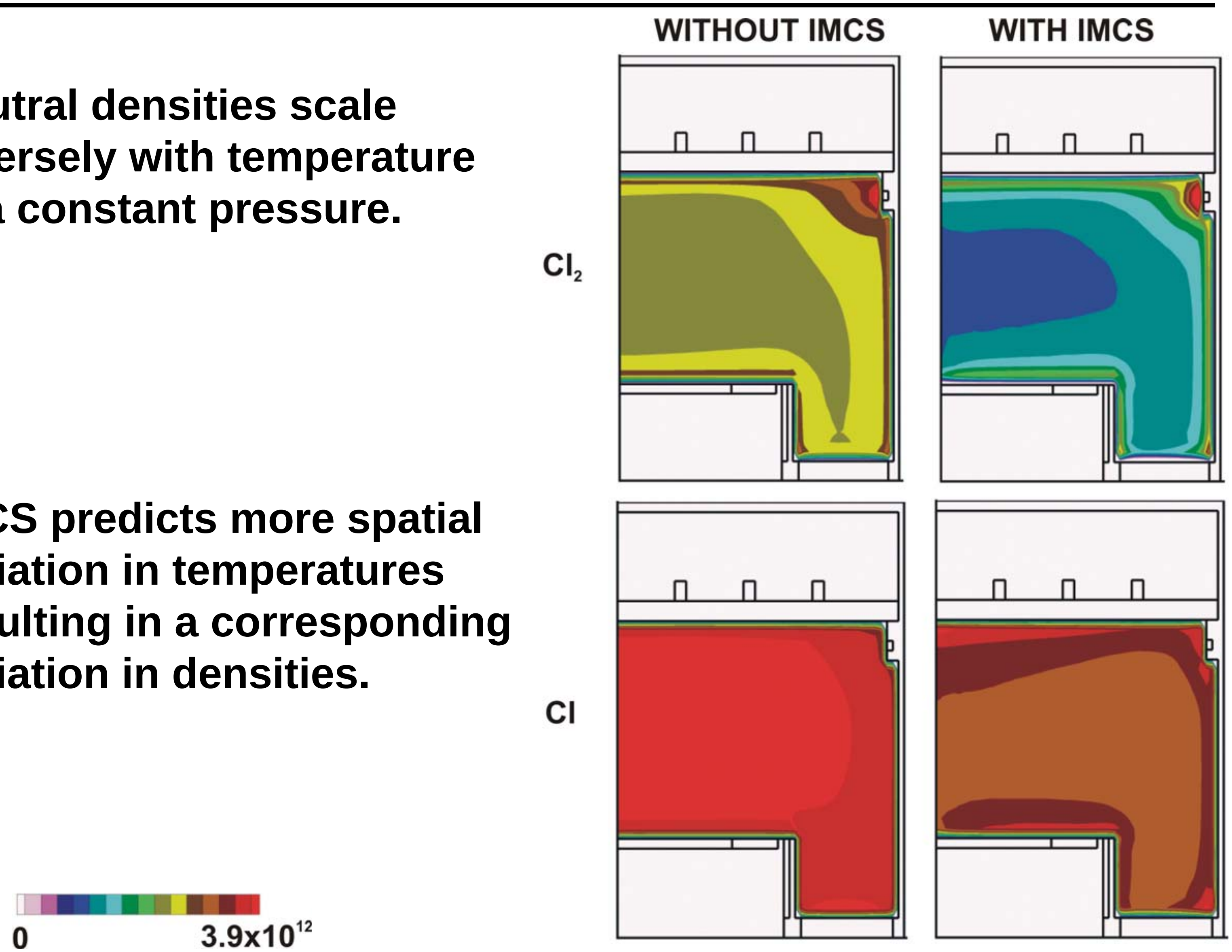
PLASMA PROPERTIES: NEUTRAL DENSITY

- **Neutral densities scale inversely with temperature at a constant pressure.**

- **IMCS predicts more spatial variation in temperatures resulting in a corresponding variation in densities.**



- **Ar/Cl_2 (80:20), 10 mTorr, 300 W, 100 sccm**

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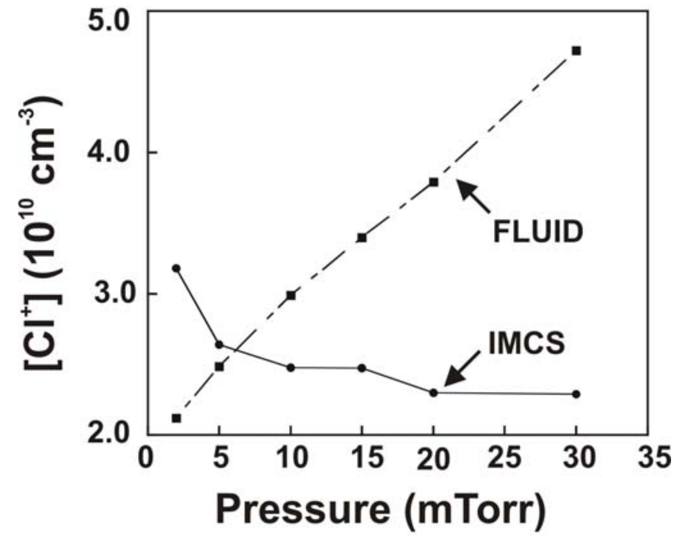
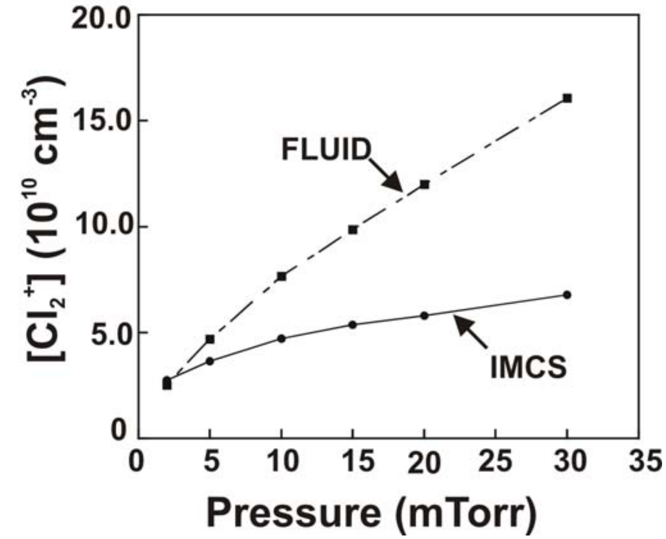
Cl^+ DENSITY: PRESSURE

- $[Cl^+]$ was compared at different pressures for a constant power.
- With fluid equations, $[Cl^+]$ increases with increase in pressure.
- With IMCS, $[Cl^+]$ decreases with increase in pressure in agreement with experimental observations.*
- $[Cl_2^+]$ increases with pressure in both cases.
  - Ar/Cl_2 (80:20), 300 W, 100 sccm

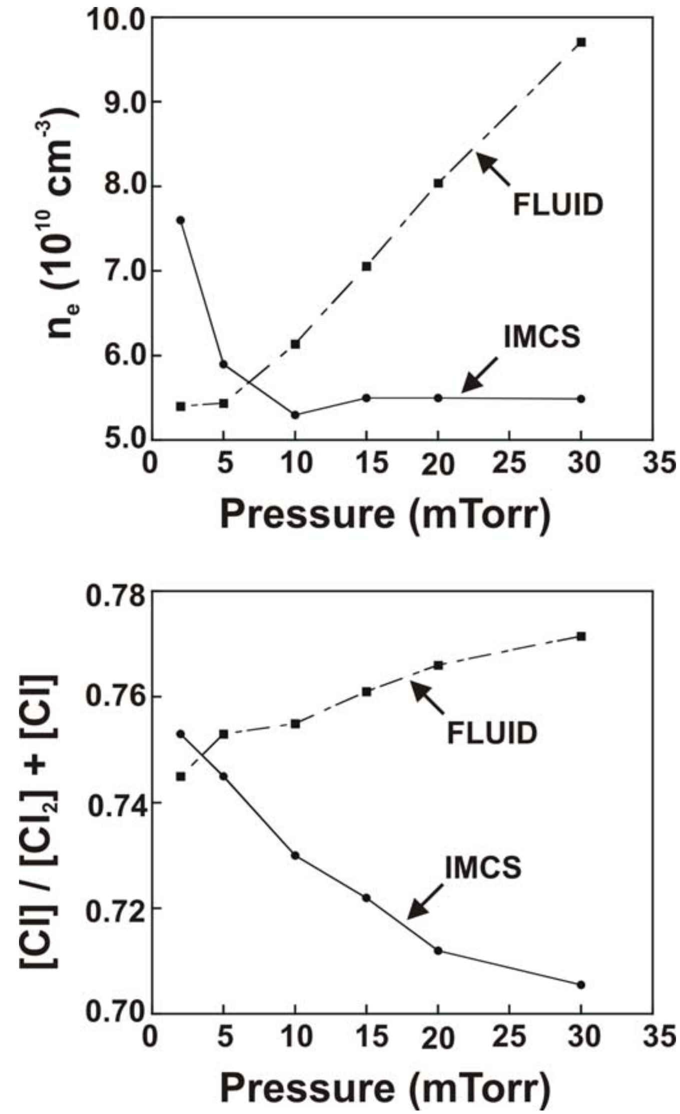




*Hebner et al., J. Vac. Sci. Technol. 15 (5), 2698 (1997)

Cl^+ DENSITY: PRESSURE

- **With IMCS, n_e decreases with increasing pressure.**
- **A lower n_e results is lesser production of [Cl], and consequently a smaller [Cl^+].**
- **With IMCS, [Cl_2^+] increases with pressure because of reduced dissociation of [Cl_2].**



• **Ar/Cl_2 (80:20), 300 W, 100 sccm**

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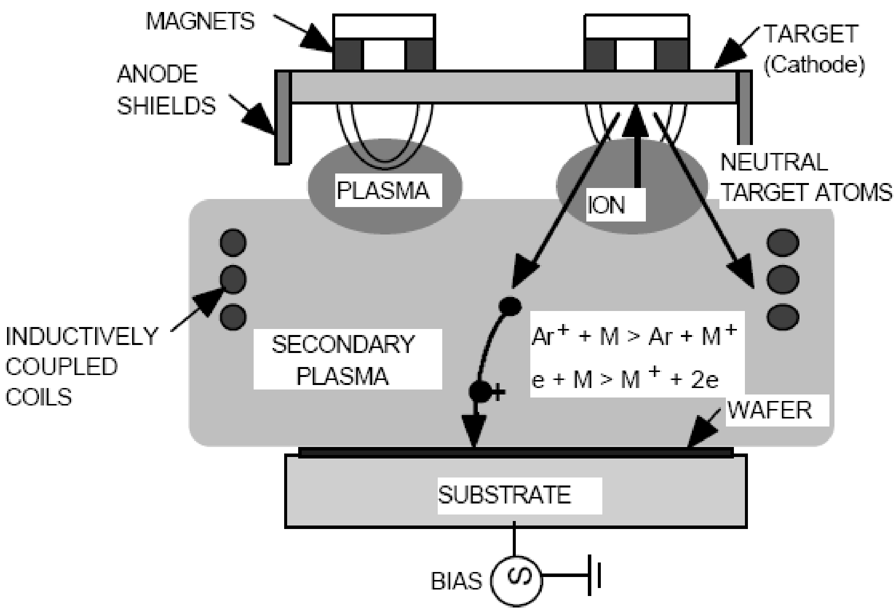
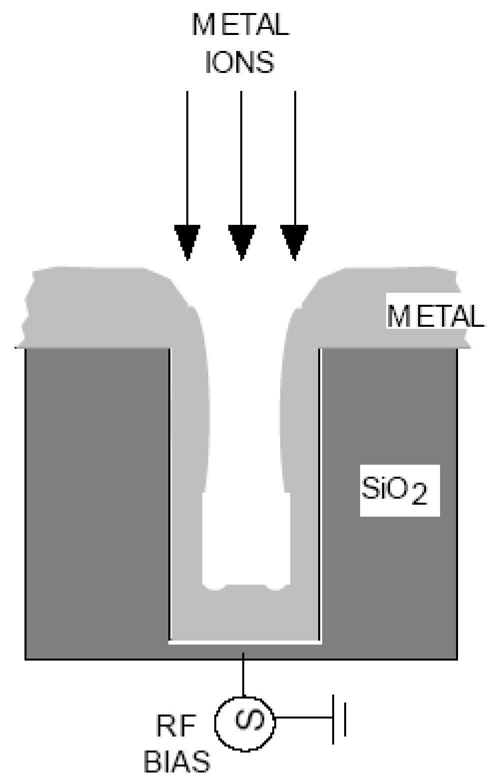
IONIZED METAL PHYSICAL VAPOR DEPOSITION





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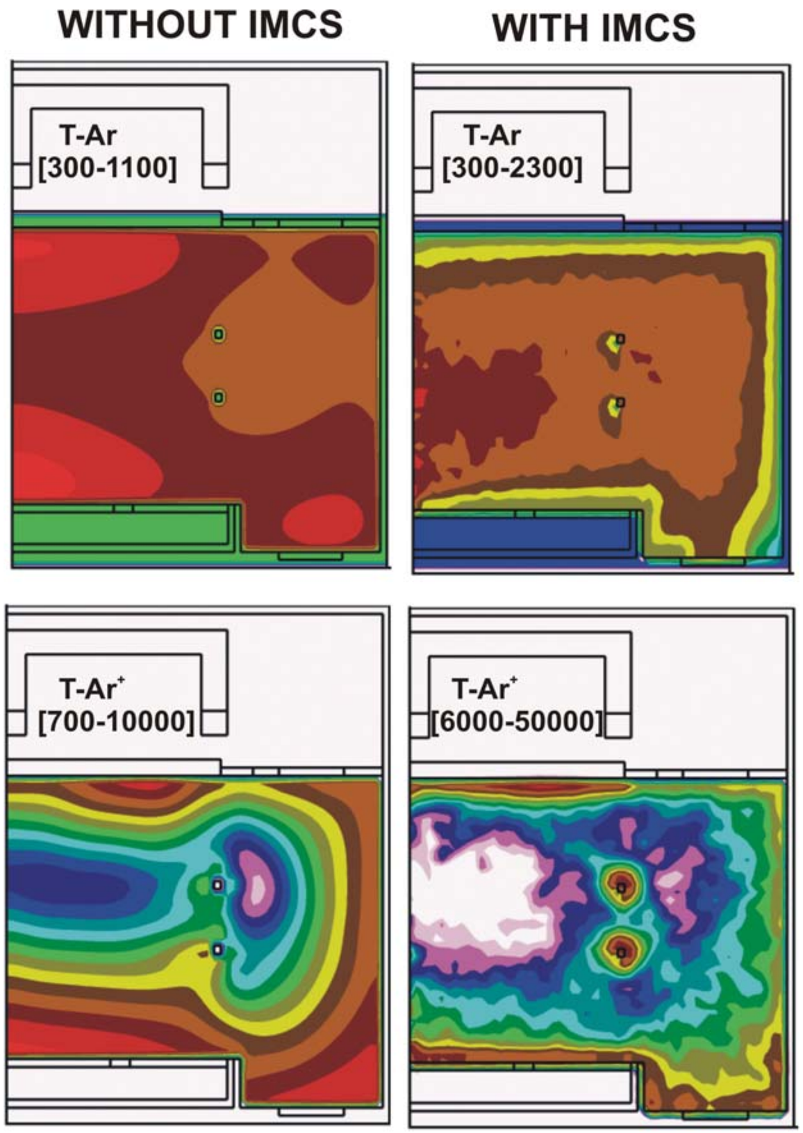
IMPVD REACTOR: TEMPERATURES

- **With IMCS, T-Ar peaks in the center of the reactor because of higher collisional heating.**

- **IMCS predicts higher T-Ar^+ than fluid equations.**

- **A higher ion temperature results in a smaller voltage drop in the sheath region.**



• **Ar (1 kW ICP, 300 W MAGNETRON, 10 mTorr)**

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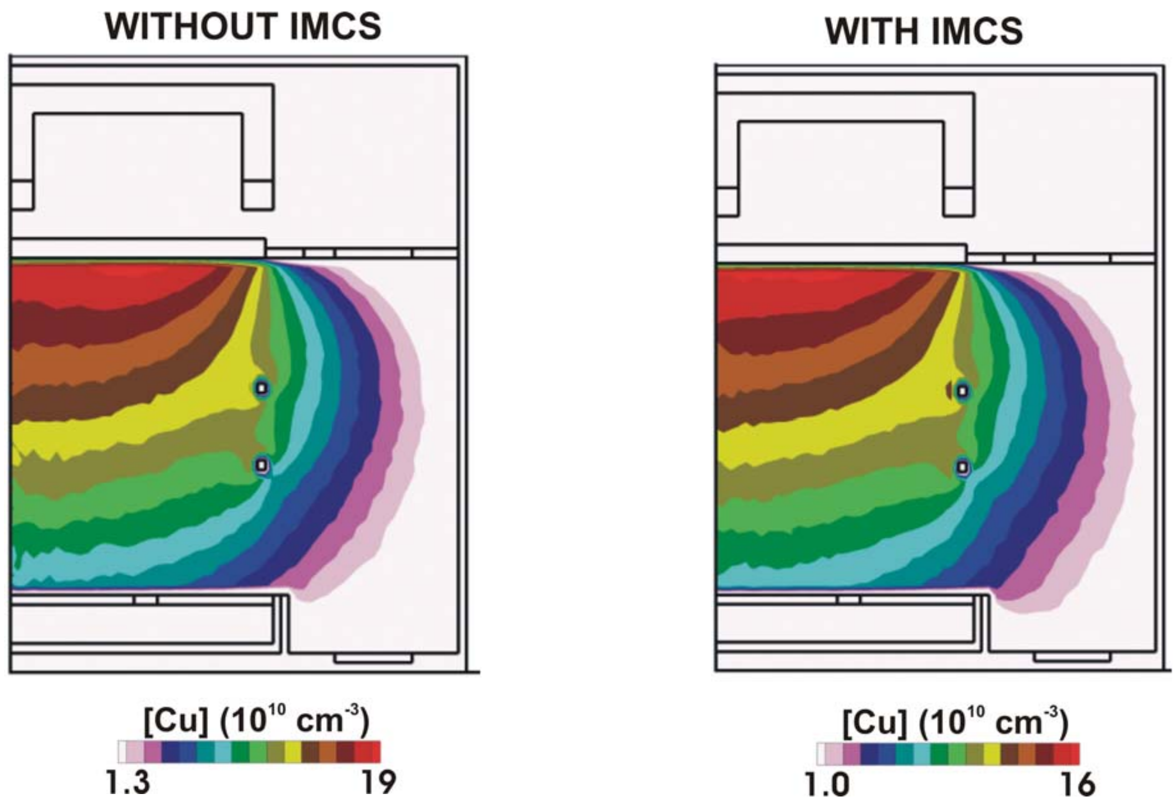
IMPVD REACTOR: Cu DENSITIES

- **A lower sheath voltage with IMCS results in less sputtering and smaller in-flight [Cu].**



- **Ar (1 kW ICP, 300 W MAGNETRON, 10 mTorr)**

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CONCLUDING REMARKS

- A hybrid modeling approach has been developed in which the ion and neutral transport coefficients are kinetically derived and implemented in fluid equations.
- IMCS predicts higher temperatures for ions and neutrals than the fluid equations; this results in lower neutral densities and higher electron temperatures.
- Neutral and ion temperatures increase with power and pressure.
- [Cl^+] decreases with increase in pressure because of reduced electron density.
- IMCS predicts lower sheath voltages than fluid equations and consequently reduced sputtering.

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