Including Convective Flows in a Self-Consistent Hydrogen-Based Microwave PACVD Reactor Model

C. S. Meierbachtol[1], **T. A. Grotjohn**[1], **B. Shanker**[1,2]

[1]Department of Electrical & Computer Engineering, Michigan State University, East Lansing, MI

[2]Department of Physics & Astronomy, Michigan State University, East Lansing, MI

meierbac@egr.msu.edu,grotjohn@egr.msu.edu,bshanker@egr.msu.edu

Motivation

- Higher pressures for Microwave PACVD reactors result in:[1]
  1. Faster growth rates
  2. Better quality diamond
- Development of multi-physics simulations at higher pressures will:
  - Help understand underlying mechanisms
  - Aid in development of new reactors

Governing Equations

Electromagnetics (FDFD)

$$\left[\nabla \times \frac{1}{\hat{\epsilon}_{\mathbf{r}}}\nabla \times - \left(\frac{\omega}{c}\right)^2\right]\vec{H} = 0 \quad (1)$$

Absorbed Power

$$\mathcal{P} = \frac{1}{2}\Re\{\sigma_e\}\left(\vec{E}\cdot\vec{E}^*\right) \quad (2)$$

Plasma

$$\nabla\left(\rho\frac{M_s}{M}D_s\nabla x_s\right) = W_s - \nabla\cdot(\rho_s\vec{v}) \quad (3)$$

$$-\frac{\partial v_r}{\partial t} = v_r\frac{\partial v_r}{\partial r} + v_z\frac{\partial v_r}{\partial z} + \frac{1}{r\rho}\frac{\partial p}{\partial r} + \frac{1}{r\rho}\frac{\partial(r\tau_{rr})}{\partial r} + \frac{1}{\rho}\frac{\partial\tau_{rz}}{\partial z} \quad (4a)$$

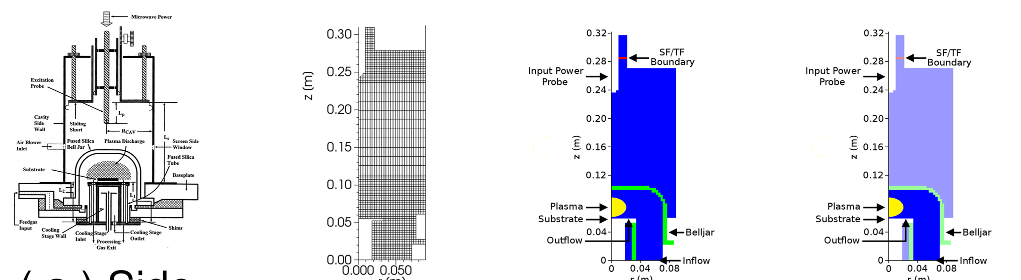
$$-\frac{\partial v_z}{\partial t} = v_r\frac{\partial v_z}{\partial r} + v_z\frac{\partial v_z}{\partial z} + \frac{1}{r\rho}\frac{\partial p}{\partial z} + \frac{1}{r\rho}\frac{\partial(r\tau_{rz})}{\partial r} + \frac{1}{\rho}\frac{\partial\tau_{zz}}{\partial z} - g \quad (4b)$$

$$\nabla\cdot\lambda_g\nabla T_g = \nabla\cdot\left[\rho\vec{v}\left(\frac{1}{2}v^2 + \frac{3}{2}\frac{k_B T_g}{m_0}\right)\right] = \nabla\cdot\left(\lambda_e\nabla T_e + \lambda_v\nabla T_v + \sum_{s=1}^{N_s}\rho h_s D_s\nabla x_s\right) - \nabla\cdot(p\vec{v}) + \nabla\cdot\hat{\tau} + \mathcal{P}_{abs} - Q_{rad} + n\vec{g} \quad (5)$$

Conductivity

$$\sigma = \frac{q_e^2 n_e}{m_e}\left(\frac{\nu_{eff} - j\omega}{\nu_{eff}^2 + \omega^2}\right) \quad (6)$$

Geometry



(a) Side view (b) Mesh (c) E/M (d) Plasma

Figure 1: *(a) Schematic of MSU Microwave PACVD reactor, (b) discretized mesh, (c) electromagnetics and (d) plasma simulation domains.*

Solution Process

- **Electromagnetics**: Direct (sparse)
- **Plasma (Scalar)**: Gauss-Seidel Line Relaxation
- **Plasma (Flows)**: Implicit direct solver [2]

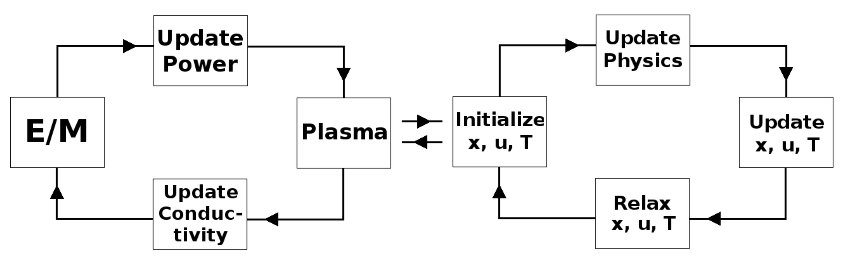


Figure 2: *Solution process for (left) complete system and (right) plasma convergence.*

Validation

Electron Density

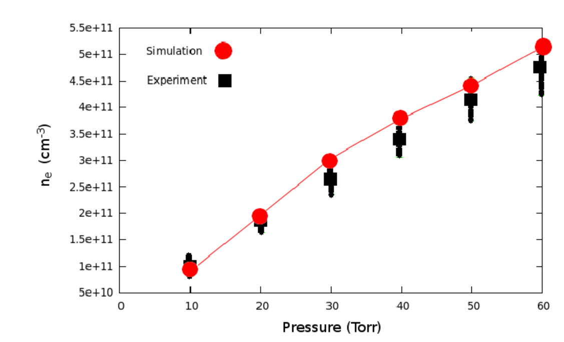
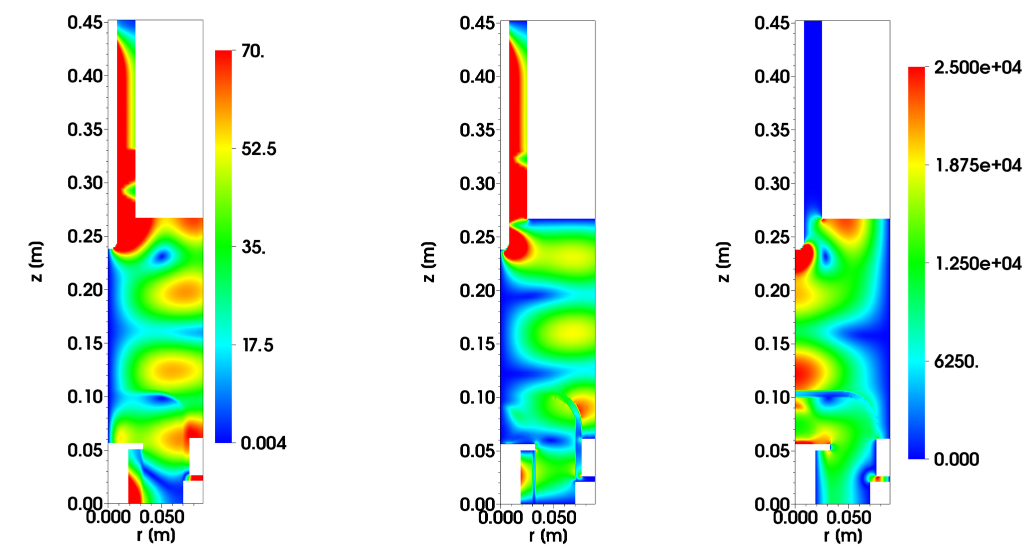


Figure 3: *Simulated (red) and experimentally measured (black) electron density versus pressure at constant power of 600 Watts. Experimental data from Grotjohn et. al., 2000.*

High Pressure Results

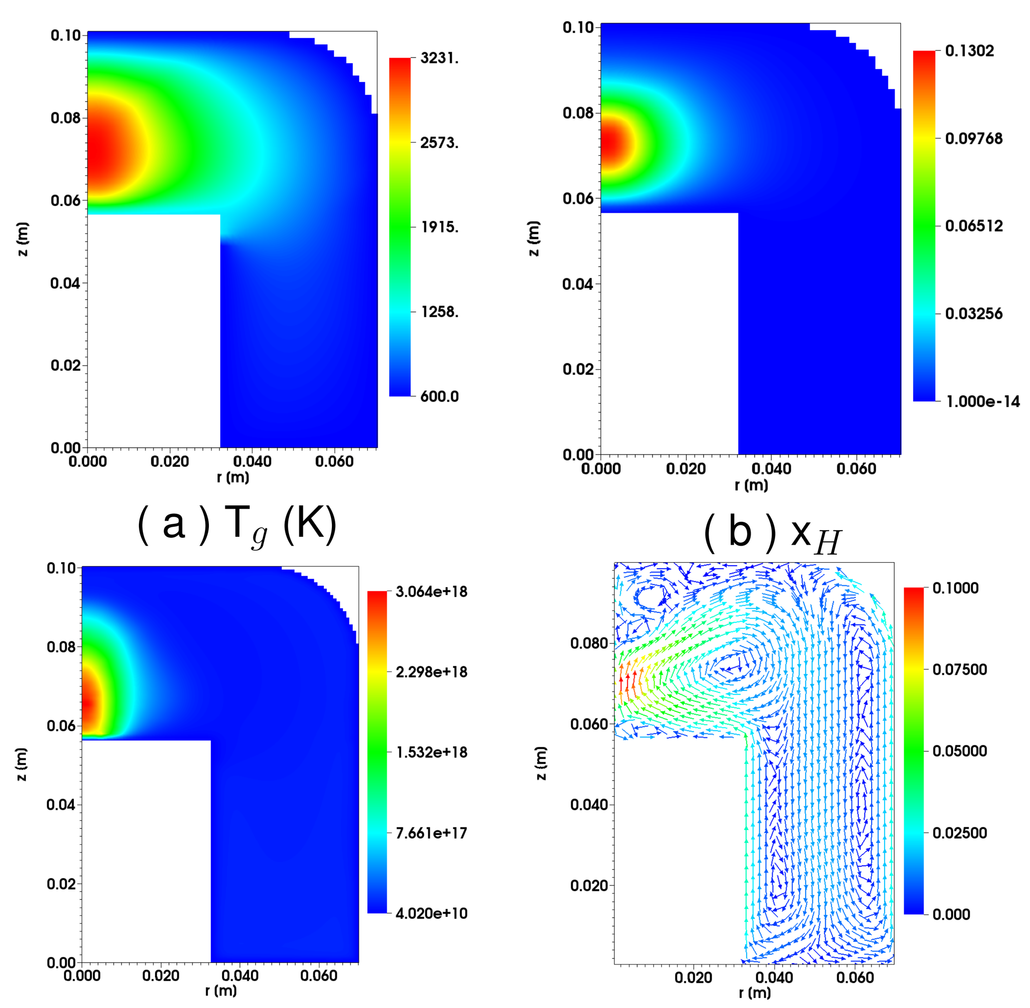
Electromagnetic Module



(a) $|H_\phi|$ (A/m) (b) $|E_r|$ (V/m) (c) $|E_z|$ (V/m)

Figure 4: *(a) $|H_\phi|$, (b) $|E_r|$, and (c) $|E_z|$ solutions when operating at 250 Torr and 3 kW. The same scale is used in both electric field plots.*

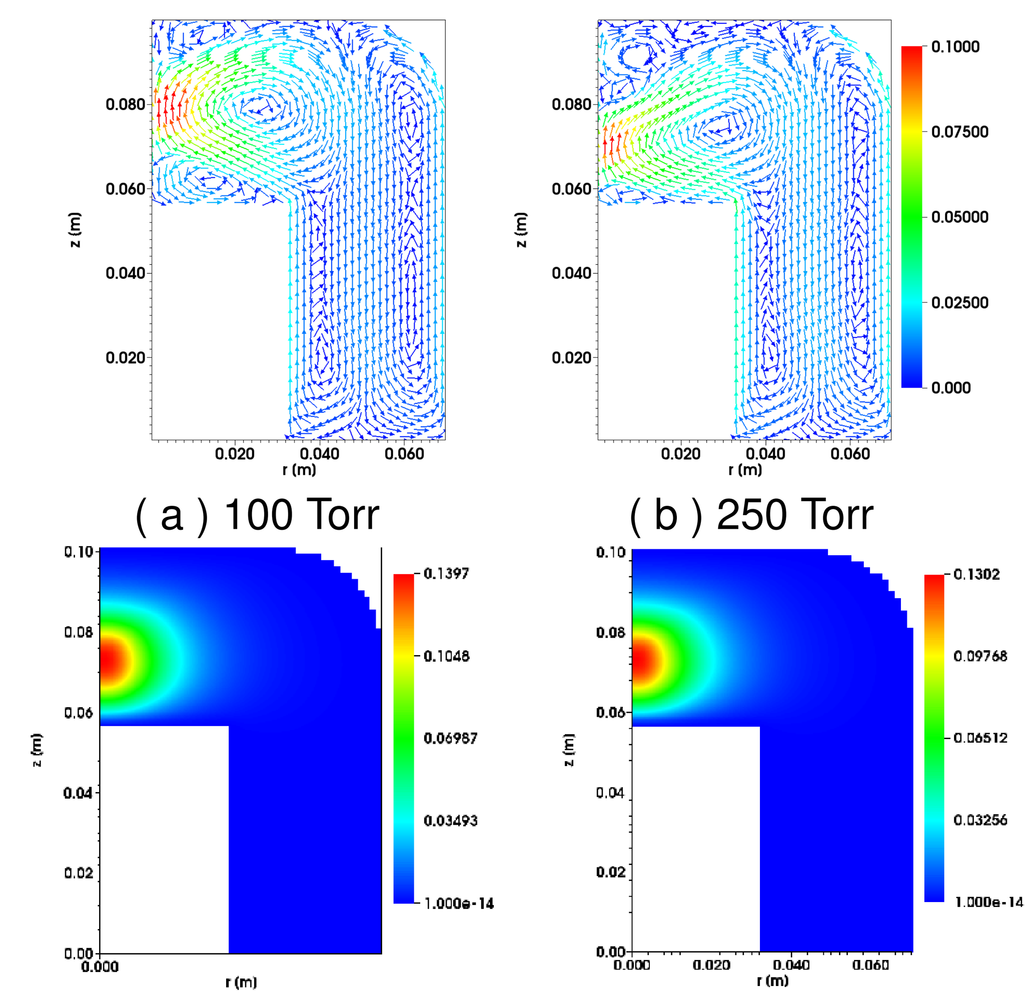
Plasma Flow Module



(a) T_g (K) (b) x_H (c) n_{e^-} (m^{-3}) (d) $|\vec{v}|$ (m/s)

Figure 5: *MSU reactor (a) gas temperature, (b) H molar fraction, (c) electron denisty, and (d) vector gas flow for $\mathcal{P}_{abs}$ of 3 kW and pressure of 250 Torr.*

Convective Flow



(a) 100 Torr (b) 250 Torr (c) No Flow (d) Flow Included

Figure 6: *Average gas flow vector at (a) 100 Torr, 1.5 kW and (b) 250 Torr, 3 kW, and atomic hydrogen mole fraction for (c) no flow and (d) flow included at 250 Torr, 3 kW.*

Conclusions

- Self-consistent multi-physics Microwave PACVD diamond reactor simulation accurate at higher pressures
  - **Convective forces significant above 150 Torr**
  - Influence primarily in mole fractions
- Future work:
  - Substrate temperature
  - Hydrocarbons

References

[1] K.W. Hemawan, T.A. Grotjohn, D.K. Reinhard, and J.Asmussen, Diam. Rel. Mater. **19**, 1446-1452 (2010).

[2] Gilbert Strang, *Computational Science and Engineering* (2007).