Simulations of Ar/H_2 and H_2 Microwave Plasma

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Outline

1. Motivation
2. Geometry
3. Challenges
4. The model
5. Results and Outlook

Motivation

- Growing importance of plasma torches and jets
- Microwave plasma torch (MPT) in doc. Zajíčková's group - fast CNT and iron NP deposition
- Grant cooperation with the Institute of Physics, ASCR (dr. Bonaventura)
- Complex, challenging problem
- Software simulation available - COMSOL, Matlab

Geometry

The atmospheric-pressure microwave plasma torch - CNT, iron NP synthesis (here at DPE)

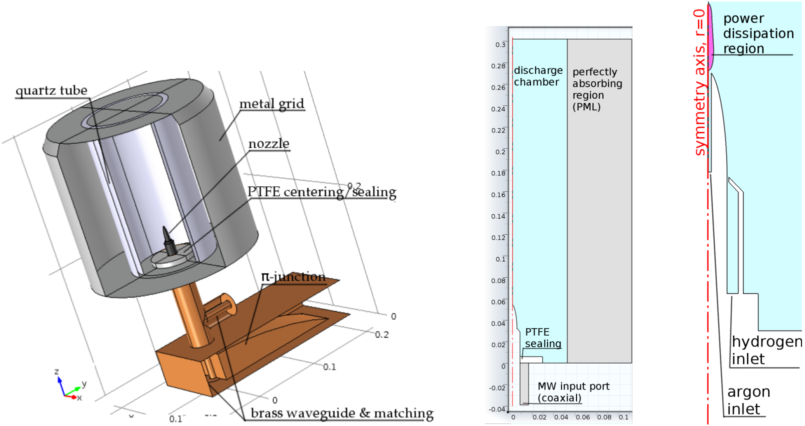


Figure: The geometry - MPT

Geometry

Linear antenna microwave reactor - low pressure, NCD synthesis (FZU AV CR)

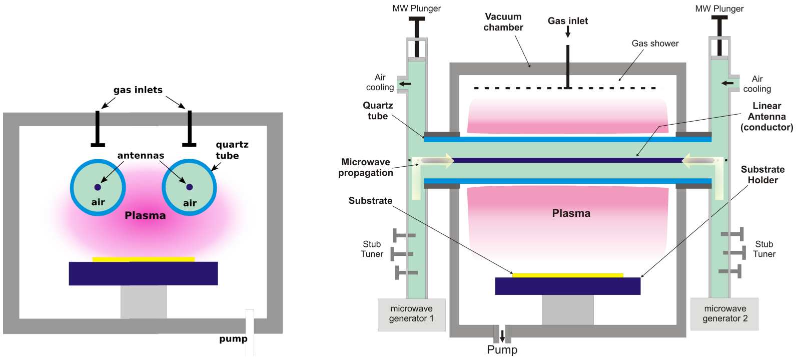


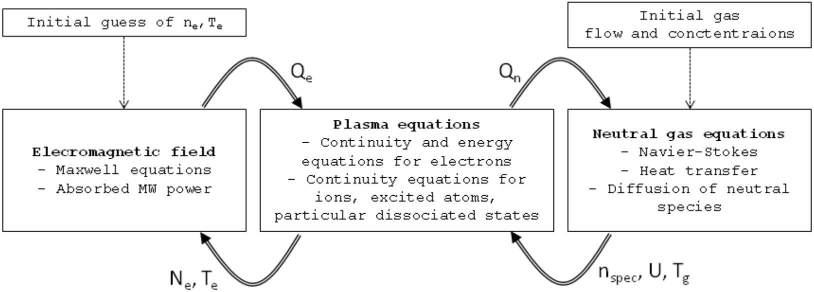
Figure: The geometry - Ak400

Challenges

- Very complex problem
  - Turbulent flow ($\mathrm{Re} \approx 60\,000$ near main inlet)
  - Highly inhomogeneous, non-isothermal gas mixture
  - Relatively small plasma region $\Rightarrow$ very steep velocity/temperature gradients
  - Minimum 11 species and 16 plasma reactions
  - All must be solved at least in 2D axial symmetry
- Necessary input data (cross sections, gas properties at very high temperatures) scarcely available
- Out-of-the-box solutions (COMSOL Plasma Module, Fluent), usually insufficient for such a complex problem (unstable, only for DC, Maxwellian EEDFs, etc...)

Model - schematic view

- Implemented in Matlab with COMSOL API
- Solved in 2D axial symmetry



A schematic overview of the iterative loop

Model - Equations

- Reynolds-averaged Navier-Stokes equations with the $k-\varepsilon$ model

$$\rho\frac{\partial \mathbf{U}}{\partial t}+\rho\left(\mathbf{U}\cdot\nabla\right)\mathbf{U}-\nabla\cdot\langle\rho(\mathbf{u}_\mathrm{T}\otimes\mathbf{u}_\mathrm{T})\rangle=-\nabla\cdot\hat{P}-\nabla\cdot\mu\left[\nabla\otimes\mathbf{U}+(\nabla\otimes\mathbf{U})^T\right]+\mathbf{F}.$$

- Heat equation, diffusion equation for the neutral gas
- Continuity equation for electrons, energy equation for electrons

$$\frac{\partial n_j}{\partial t}+\nabla\cdot\mathbf{\Gamma}_j+(\vec{u}\cdot\nabla)n_j=R_j,\qquad \mathbf{\Gamma}_j=-\mu_i\mathbf{E}n_i-D_i\nabla n_i$$

- 9 continuity equations for ionized and excited species
- EM field equation (time-harmonic approximation), plasma as a lossy dielectric

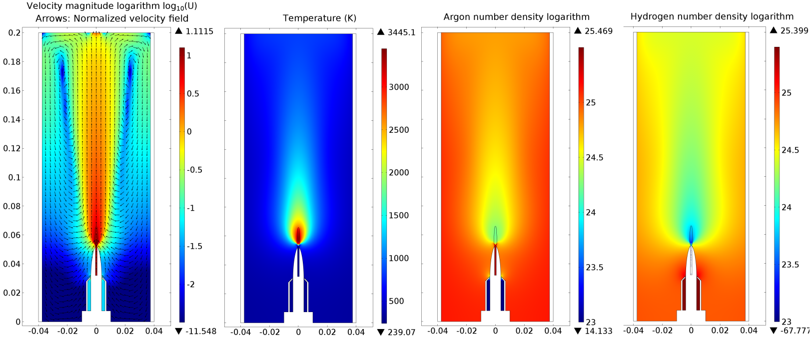
$$\varepsilon=\varepsilon_0-\frac{\varepsilon_0\omega_{\mathrm{pe}}^2}{\nu_{\mathrm{en}}^2+\omega^2}+i\frac{\varepsilon_0\omega_{\mathrm{pe}}^2\nu_{\mathrm{en}}}{\omega\left(\nu_{\mathrm{en}}^2+\omega^2\right)}$$

Model - Reactions

The following reactions were considered (+ rotational and vibrational H_2 excitations)

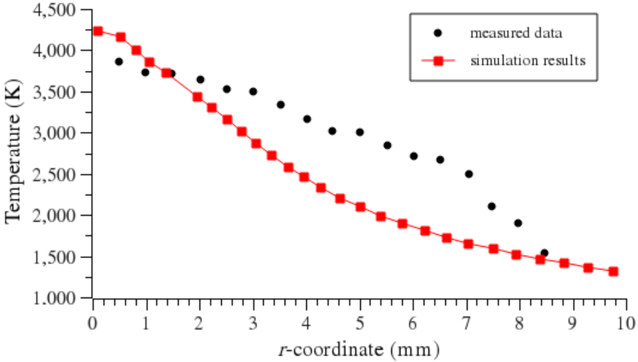
$$
\begin{aligned}
&e^- + Ar \rightarrow 2e^- + Ar^+ \\
&e^- + Ar \rightarrow e^- + Ar^* \\
&e^- + Ar^+ \rightarrow Ar \\
&e^- + H_2 \rightarrow 2e^- + H_2^+ \\
&e^- + H_2 \rightarrow e^- + H + H(n = 2) \\
&e^- + H_2 \rightarrow e^- + H + H(n = 3) \\
&e^- + H \rightarrow e^- + H^+ \\
&e^- + H \rightarrow e^- + H(n = 2) \\
&e^- + H \rightarrow e^- + H(n = 3) \\
&H_2 + H(n = 2) \rightarrow H_3^+ + e^- \\
&H_2 + H(n = 3) \rightarrow H_3^+ + e^- \\
&H_2 + H_2^+ \rightarrow H_3^+ + H \\
&e^- + H^+ \rightarrow H(n = 2) \\
&e^- + H^+ \rightarrow H(n = 3) \\
&e^- + H_3^+ \rightarrow H_2 + H(n = 3) \\
&2H + H_2 \rightarrow H_2 + H_2 \\
&3H \rightarrow H_2 + H
\end{aligned}
$$

Results - gas flow



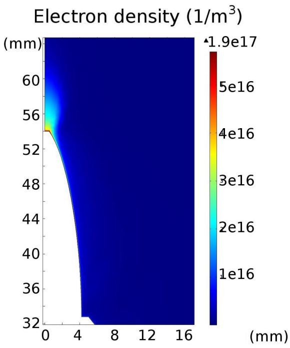
Neutral gas properties - simplified fluid dynamics simulations without the plasma

Results - gas flow (MPT)



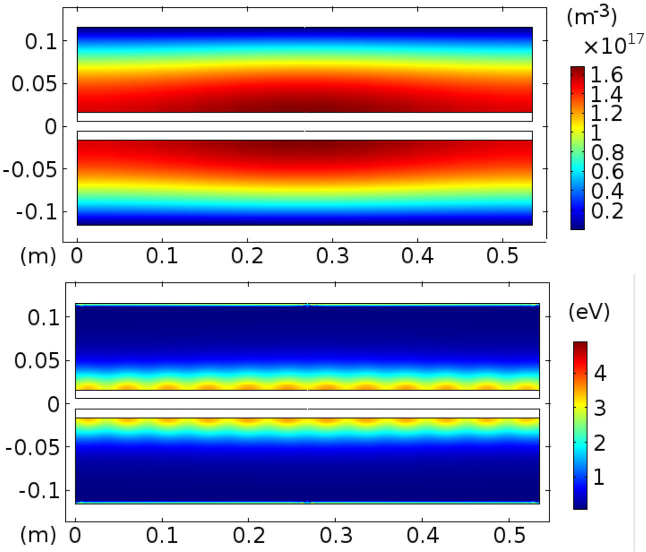
Experimental verification - fluid dynamics

Results - with plasma (MPT)



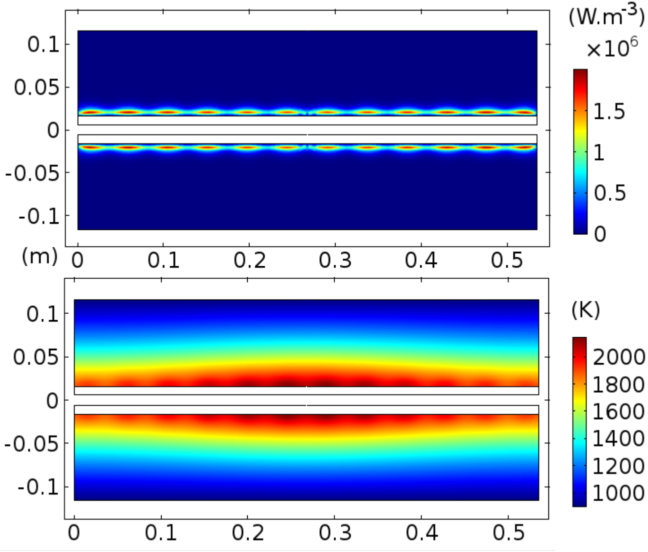
Basic plasma characteristics

Results - with plasma (linear antenna MW reactor)



Electron concentration (above), electron temperature (below)

Results - with plasma (linear antenna MW reactor)



Power deposition (above), neutral temperature (below)

Conclusion

1. A very promising algorithm for simulations of complex plasmas developed and implemented using Matlab and COMSOL Multiphysics API
2. Takes into account both the plasma kinetics and neutral gas dynamics
3. Good results for the Linear Antenna MW Plasma source, not so good for the MW plasma torch
4. Future experimental verification necessary

Conclusion

Thank you for your attention.