COMSOL CONFERENCE BOSTON 2011

Effect of Gas Flow Rate and Gas Composition in Ar/CH_4 Inductively Coupled Plasmas

Keisoku Engineering System Co., Ltd., JAPAN

Dr. Lizhu Tong

October 14, 2011

Contents

Plasma processing and nonequilibrium discharge (1)

Plasma processing has been used for fabricating semiconductors. In order to make a hyperfine feature on the wafer, a high aspect-ratio etching is needed.

↓

The energy of ions incident on the wafer must be controlled to realize an accurate and reliable processing.

↓

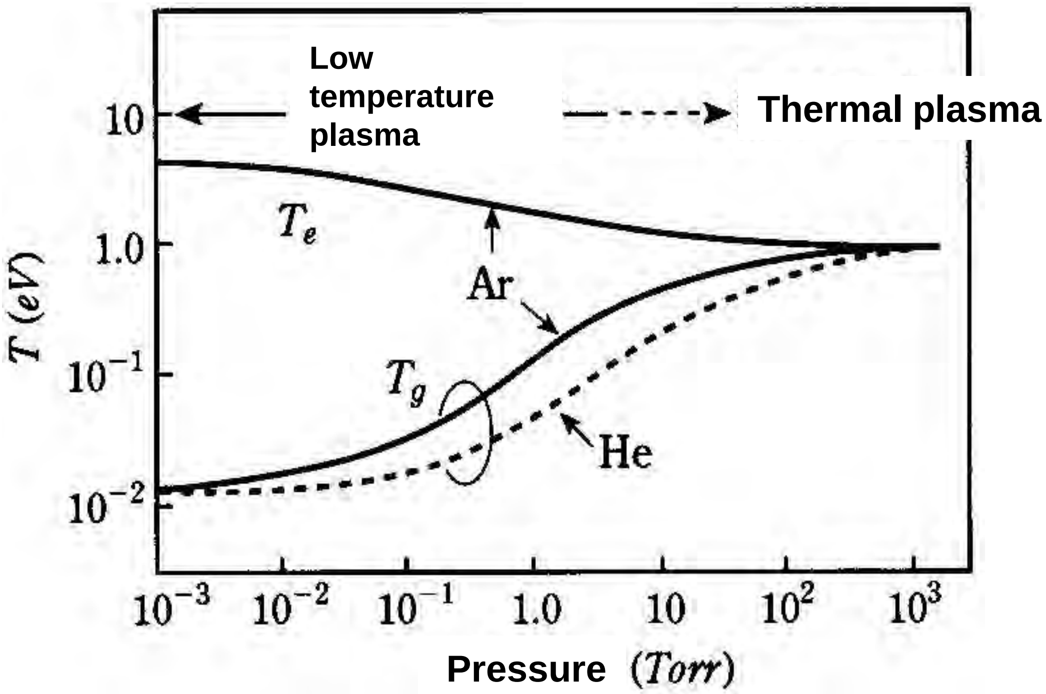
Low gas pressure in etching

↓

Nonequilibrium discharge

Plasma processing and nonequilibrium discharge (2)

- For low pressure discharges the plasma is not in thermal equilibrium.
- In the bulk plasma, the electron temperature T_e greatly exceeds the ion temperature T_i and neutral gas temperature T_g.



Types of plasma involved in COMSOL Multiphysics

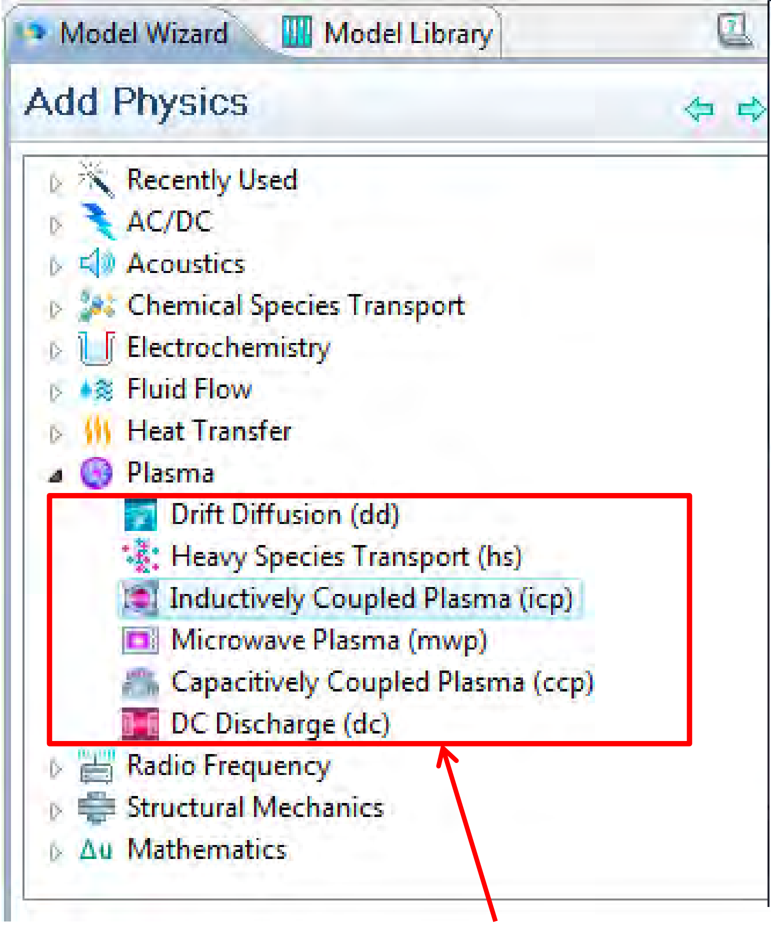
The common types of plasma:

- Inductively coupled plasma (ICP)
- DC discharge
- Microwave plasma
- Electrical breakdown
- Capacitively coupled plasma (CCP)
- Combined ICP/CCP reactor

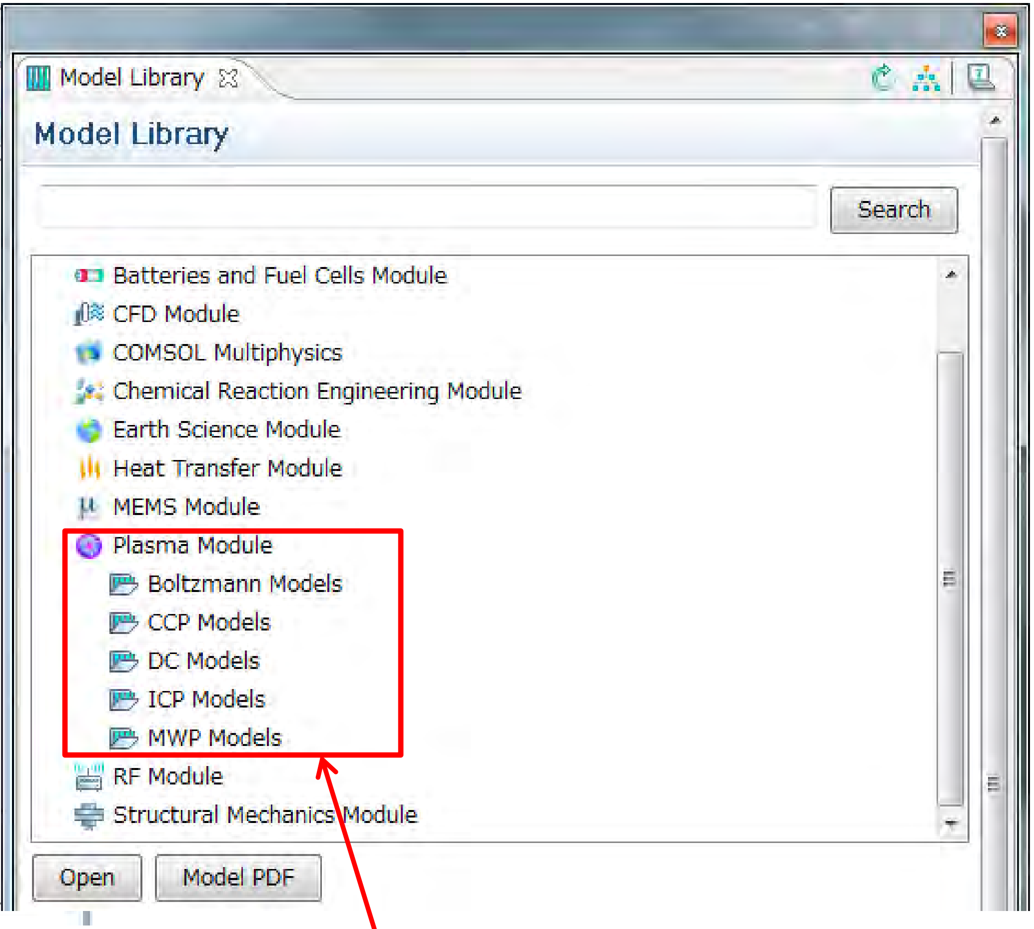
Plasma module physics interfaces

- The drift diffusion interface
- The heavy species transport interface
- The Boltzmann equation, Two-term approximation interface
- The inductively coupled plasma interface (ICP)
- The microwave plasma interface
- The capacitively coupled plasma interface (CCP)
- The DC discharge interface

Plasma module format in COMSOL Multiphysics



Plasma interfaces



Plasma model library

Plasma chemistry (1)

Neutrals (7)
CH_4
$C_2H_2, C_2H_4, C_2H_6, C_3H_8$
H_2, Ar

Ions (13)
$CH^+, CH_2^+, CH_3^+, CH_4^+, CH_5^+$
$C_2H_2^+, C_2H_4^+, C_2H_5^+, C_2H_6^+$
H^+, H_2^+, Ar^+, ArH^+

Radicals (5)
CH, CH_2, CH_3, CH_5
H

Excited species (5)
$CH_4^*(2vib.)$, $H(2p,3p)$, Ar^*

Electron reactions included in the model

No.	Reaction
1	$Ar + e^- \rightarrow Ar^* + e^-$
2	$Ar^* + e^- \rightarrow Ar + e^-$
3	$Ar + e^- \rightarrow Ar^+ + 2e^-$
4	$Ar^* + e^- \rightarrow Ar^+ + 2e^-$
5	$CH_4 + e^- \rightarrow CH_4^* + e^- (2\ vib.)$
6	$CH_4 + e^- \rightarrow CH_4^+ + 2e^-$
7	$CH_4 + e^- \rightarrow CH_3^+ + H + 2e^-$
8	$CH_4 + e^- \rightarrow CH_3 + H + e^-$
9	$CH_4 + e^- \rightarrow CH_2 + 2H + e^-$
10	$CH_4 + e^- \rightarrow CH + 3H + e^-$
11	$CH_4 + e^- \rightarrow CH + 3H + e^-$
12	$H_2 + e^- \rightarrow H_2^+ + 2e^-$
13	$H_2 + e^- \rightarrow 2H + e^-$
14	$H + e^- \rightarrow H(2p, 3p) + e^-$
15	$H(2p, 3p) + e^- \rightarrow H + e^-$
16	$H + e^- \rightarrow H^+ + 2e^-$
17	$C_2H_2 + e^- \rightarrow C_2H_2^+ + 2e^-$
18	$C_2H_4 + e^- \rightarrow C_2H_2 + 2H + e^-$
19	$C_2H_4 + e^- \rightarrow C_2H_4^+ + 2e^-$
20	$C_2H_5 + e^- \rightarrow C_2H_4 + H + e^-$
21	$C_2H_5 + e^- \rightarrow C_2H_5^+ + 2e^-$
22	$C_2H_5 + e^- \rightarrow C_2H_4^+ + H + 2e^-$
23	$C_2H_6 + e^- \rightarrow C_2H_5 + H + e^-$
24	$C_2H_6 + e^- \rightarrow C_2H_4 + 2H + e^-$
25	$C_2H_6 + e^- \rightarrow C_2H_6^+ + 2e^-$
26	$C_2H_6 + e^- \rightarrow C_2H_5^+ + H + 2e^-$
27	$CH_3 + e^- \rightarrow CH_2 + H + e^-$
28	$CH_3 + e^- \rightarrow CH + 2H + e^-$
29	$CH_3 + e^- \rightarrow CH_3^+ + 2e^-$
30	$CH_2 + e^- \rightarrow CH + H + e^-$
31	$CH_2 + e^- \rightarrow CH_2^+ + 2e^-$
32	$CH + e^- \rightarrow CH^+ + 2e^-$
33	$ArH^+ + e^- \rightarrow Ar + H$

Plasma chemistry (2)

Reactions of ion and neutral species

No.	Reaction
34	$CH_4 + CH_3^+ \rightarrow CH_4^+ + CH_3$
35	$CH_4 + CH_3^+ \rightarrow C_2H_5^+ + H_2$
36	$CH_4 + CH_4^+ \rightarrow CH_5^+ + CH_3$
37	$H_2 + CH_4^+ \rightarrow CH_5^+ + H$
38	$C_2H_6 + CH_5^+ \rightarrow C_2H_5^+ + CH_4 + H_2$
39	$CH_4 + Ar^+ \rightarrow CH_3^+ + H + Ar$
40	$H_2 + Ar^+ \rightarrow ArH^+ + H$
41	$H_2 + Ar^+ \rightarrow Ar + H_2^+$

Reactions among neutral species

No.	Reaction
42	$CH_3 + CH_3 \rightarrow C_2H_6$
43	$CH_3 + H \rightarrow CH_4$
44	$C_2H_5 + H \rightarrow CH_3 + CH_3$
45	$C_2H_5 + CH_3 \rightarrow C_3H_8$
46	$CH_2 + H \rightarrow CH + H_2$
47	$CH + CH_4 \rightarrow C_2H_5$
48	$CH_2 + CH_4 \rightarrow CH_3 + CH_3$
49	$CH_2 + CH_4 \rightarrow C_2H_4 + H_2$
50	$CH_4 + CH \rightarrow C_2H_4 + H$
51	$CH_3 + CH_2 \rightarrow C_2H_4 + H$
52	$C_2H_5 + H \rightarrow C_2H_4 + H_2$
53	$CH_2 + CH_2 \rightarrow C_2H_2 + H_2$
54	$Ar^* + Ar^* \rightarrow Ar^+ + Ar + e^-$
55	$Ar^* + Ar \rightarrow Ar + Ar$
56	$Ar^* + H_2 \rightarrow Ar + H + H$

Electron transport

COMSOL Multiphysics solves a pair of drift diffusion equation for the electron density and electron energy density.

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e \qquad \Gamma_e = -n_e(\mu_e \mathbf{E}) - D_e \nabla n_e$$

$$\frac{\partial}{\partial t}(n_\varepsilon) + \nabla \cdot \Gamma_\varepsilon + \mathbf{E} \cdot \Gamma_e = R_\varepsilon \qquad \Gamma_\varepsilon = -n_\varepsilon(\mu_\varepsilon \mathbf{E}) - D_\varepsilon \nabla n_\varepsilon$$

Source term

$$R_e = \sum_{j=1}^{M} x_j k_j N_n n_e$$

Source term

$$R_\varepsilon = \sum_{j=1}^{P} x_j k_j N_n n_e \Delta\varepsilon_j$$

Rate coefficient $k_j = \gamma \int_0^\infty \varepsilon \sigma_j(\varepsilon) f(\varepsilon) d\varepsilon$ $\gamma = (2q/m)^{1/2}$

Electron transport boundary conditions

- There are a variety of boundary conditions available for the electrons:
  - Wall which includes the effects of :
    - Secondary electron emission
    - Thermionic emission
    - Electron reflection
  - Flux which allows you to specify an arbitrary influx for the electron density and electron energy density.
  - Fixed electron density and mean electron energy
  - Insulation

Heavy species transport

- Transport of the heavy species (non-electron species) is determined from solving a modified form of the Maxwell-Stefan equations :

$$\rho \frac{\partial}{\partial t}(w_k) + \rho(\mathbf{u} \cdot \nabla) w_k = \nabla \cdot \mathbf{j}_k + R_k$$

where

$$\mathbf{j}_k = \rho \omega_k \mathbf{V}_k \qquad \mathbf{V}_k = \sum_{j=1}^{Q} \widetilde{D}_{kj} \mathbf{d}_k - \frac{{D_k}^T}{\rho \omega_k} \nabla lnT$$

$$\mathbf{d}_k = \frac{1}{cRT}\left[\nabla p_k - \omega_k \nabla p - \rho_k \mathbf{g}_k + \omega_k \sum_{j=1}^{Q} \rho_j \mathbf{g}_j\right]$$

- The multiphysics interfaces contain an integrated reaction manager to keep track of the electron impact reactions, reactions, surface reactions and species.

Gas flow transport

- The neutral gas flow is determined by the Navier-stokes equations :

Conservation of mass

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

Conservation of momentum

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \tau] + \mathbf{F}$$

where

$$\tau = 2\mu \underset{\uparrow}{\mathbf{S}} - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I}$$

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)$$

Electrostatic field

- The plasma potential is computed from Poisson's equation:

$$-\nabla \cdot \varepsilon_0 \varepsilon_r \nabla V = \rho$$

- The space charge is computed from the number densities of electrons and other charged species.

$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

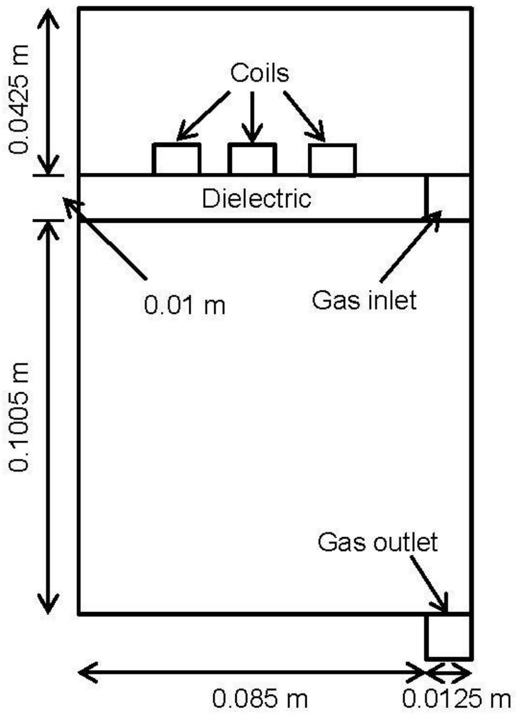
Electromagnetic field

- For inductive discharges we solve the magnetic field in the frequency domain:

$$(j\omega\sigma - \omega^2 \varepsilon_0 \varepsilon_r)\mathbf{A} + \nabla \times ({\mu_0}^{-1} \nabla \times \mathbf{A}) = \mathbf{J}^e$$

Ar/CH_4 ICP plasma model (1)

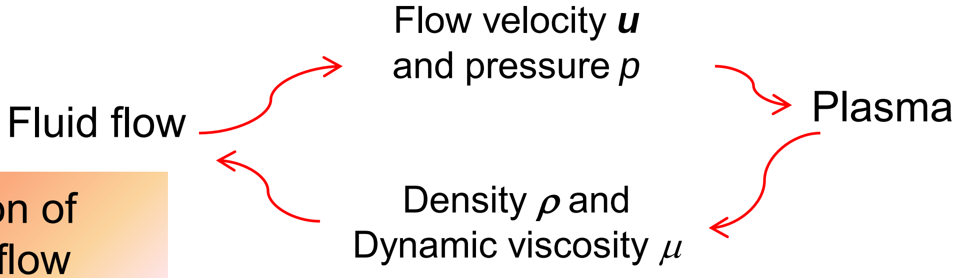
ICP plasma model



Computational conditions

- Gas: Ar/CH_4 mixtures
- RF frequency: 13.56 MHz
- Operating pressure: 20 mTorr
- Temperature: 300 K
- Input power: 300 W
- Fluid flow: laminar
- Gas flow rate: 20–1000 sccm
- Ar fractions: 0–1
- EEDF (Electron energy distribution function): Druyvesteynian

Ar/CH$_4$ ICP plasma model (2)

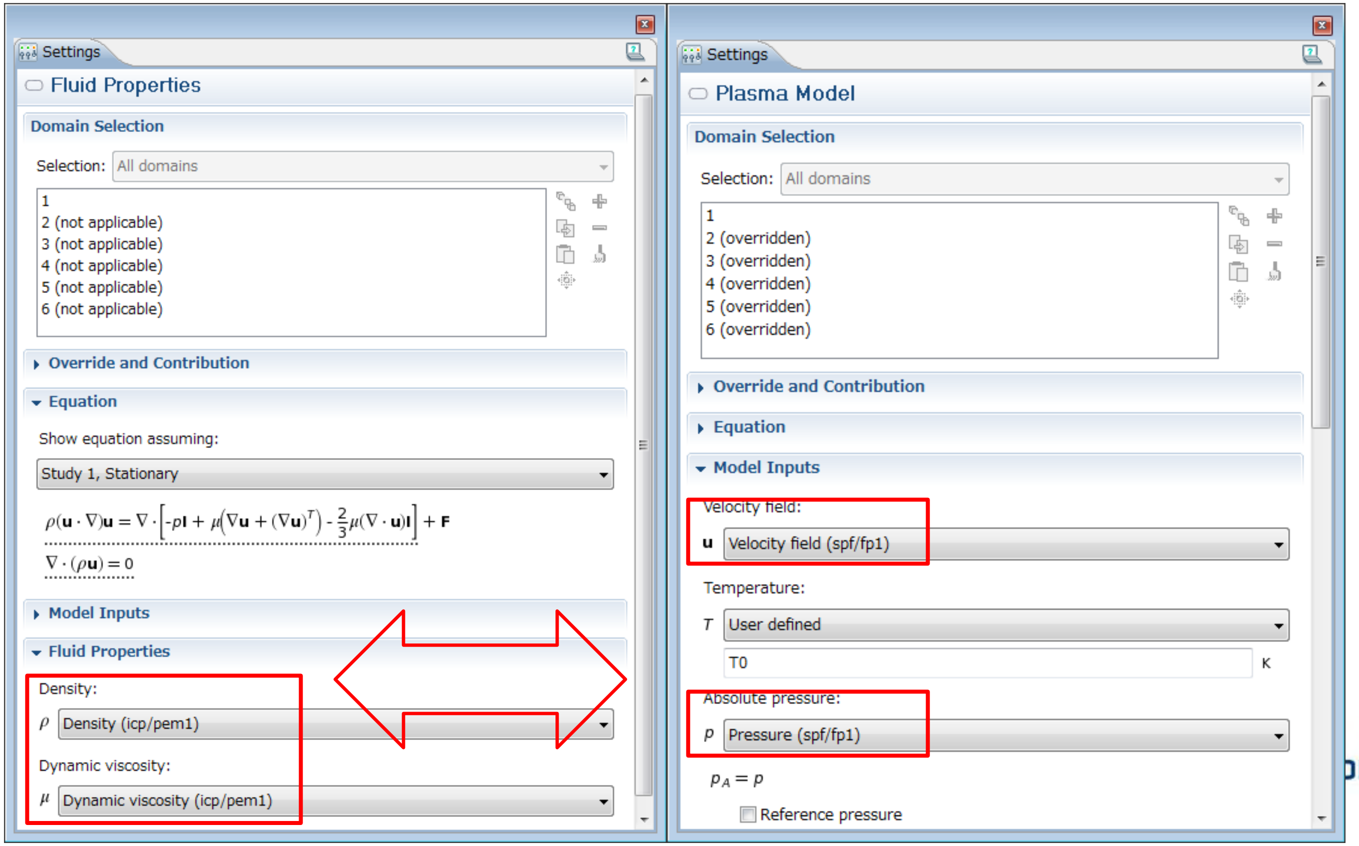

Fluid flow

Flow velocity ***u*** and pressure *p*

Plasma

Density ρ and Dynamic viscosity μ

Coupled simulation of plasma and fluid flow


Settings

Fluid Properties

Domain Selection

Selection: All domains

1
2 (not applicable)
3 (not applicable)
4 (not applicable)
5 (not applicable)
6 (not applicable)

Override and Contribution

Equation

Show equation assuming: Study 1, Stationary

$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot\left[-p\mathbf{I} + \mu\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) - \frac{2}{3}\mu(\nabla\cdot\mathbf{u})\mathbf{I}\right] + \mathbf{F}$$

$$\nabla\cdot(\rho\mathbf{u}) = 0$$

Model Inputs

Fluid Properties

Density:
ρ: Density (icp/pem1)

Dynamic viscosity:
μ: Dynamic viscosity (icp/pem1)

Settings

Plasma Model

Domain Selection

Selection: All domains

1
2 (overridden)
3 (overridden)
4 (overridden)
5 (overridden)
6 (overridden)

Override and Contribution

Equation

Model Inputs

Velocity field:
u: Velocity field (spf/fp1)

Temperature:
T: User defined
T0 K

Absolute pressure:
p: Pressure (spf/fp1)

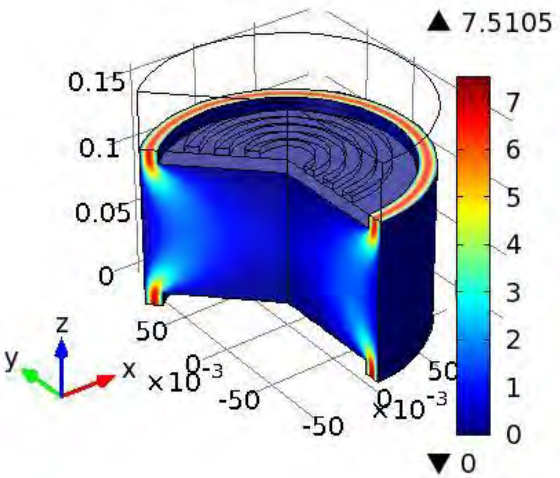
$p_A = p$

☐ Reference pressure

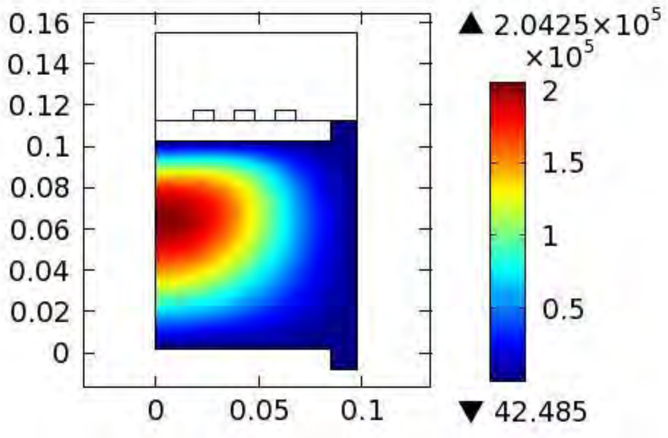
Results (1)

Discharge structure in a 95%Ar/5%CH_4 ICP plasma at a gas flow of 50 sccm

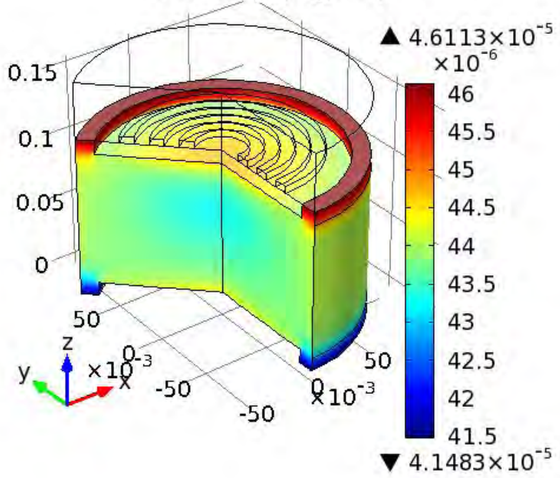
Velocity magnitude (m/s)



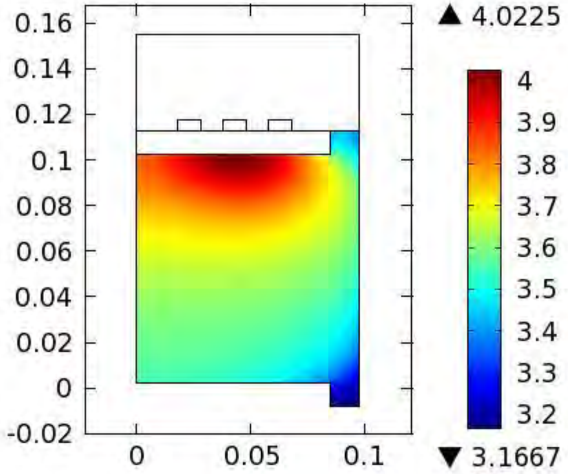
Collisional power loss (W/m³)



Density (kg/m³)

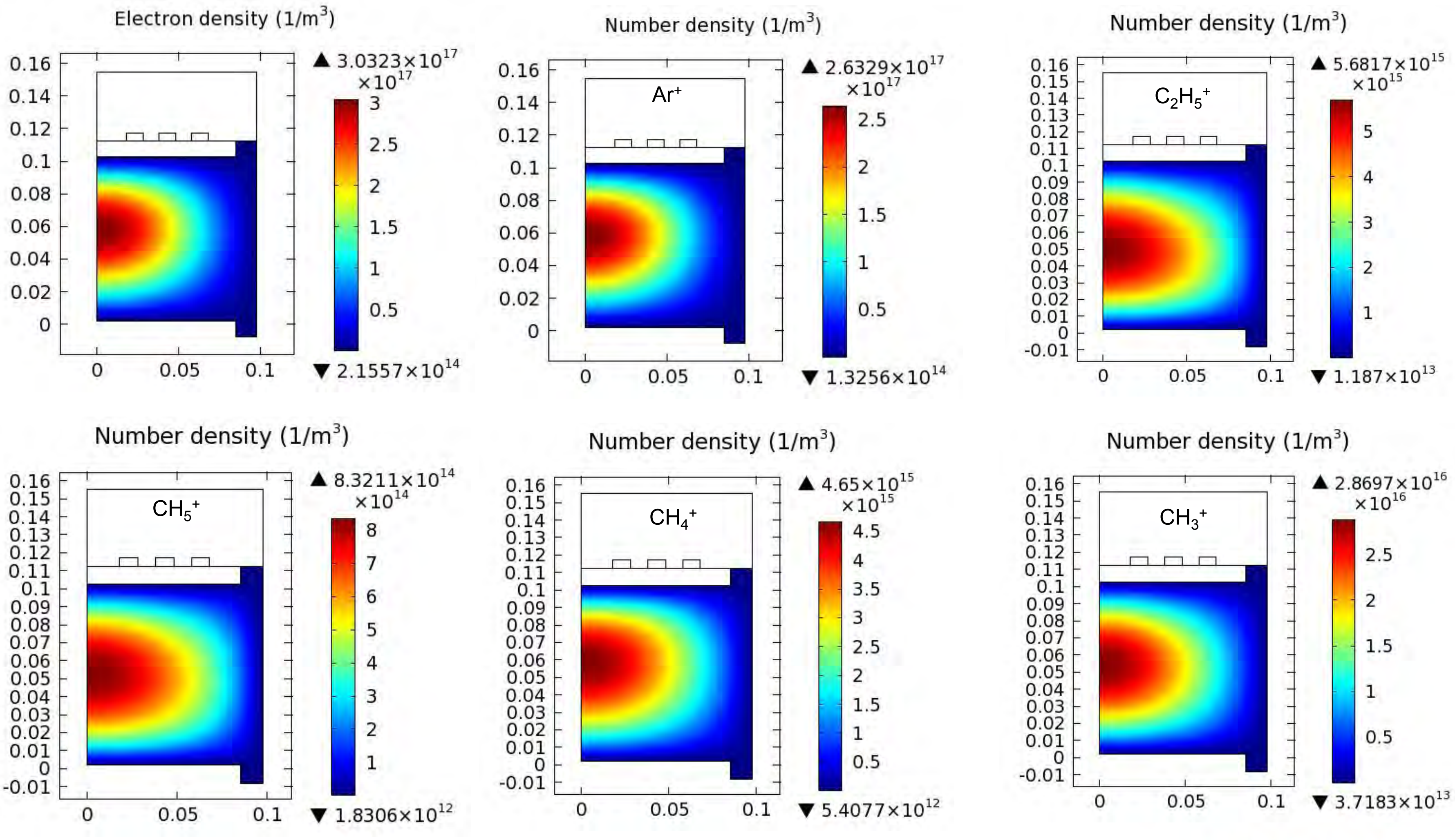


Electron temperature (V)



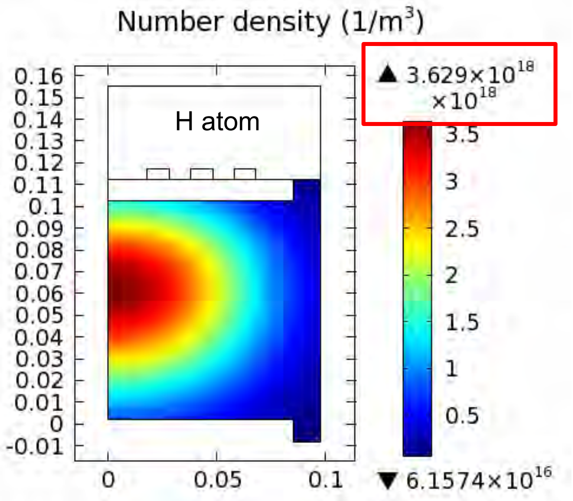
Results (2)

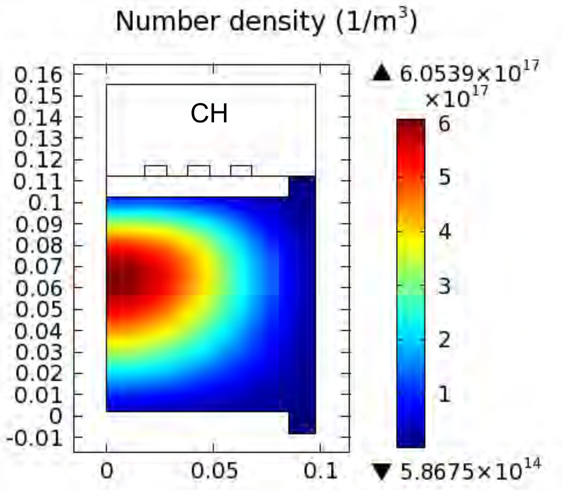
Electron and ion densities

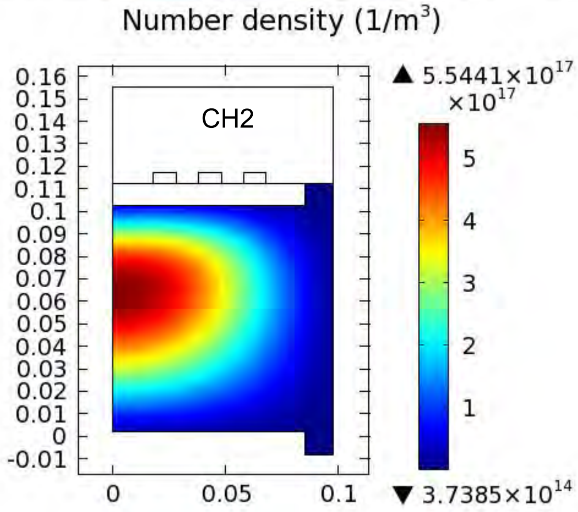


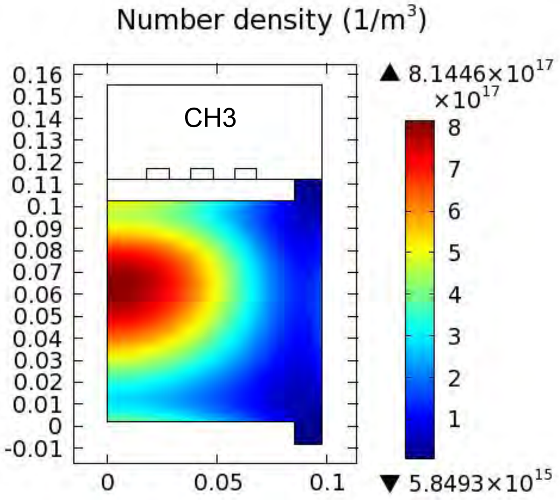
Results (3)

Radical number density





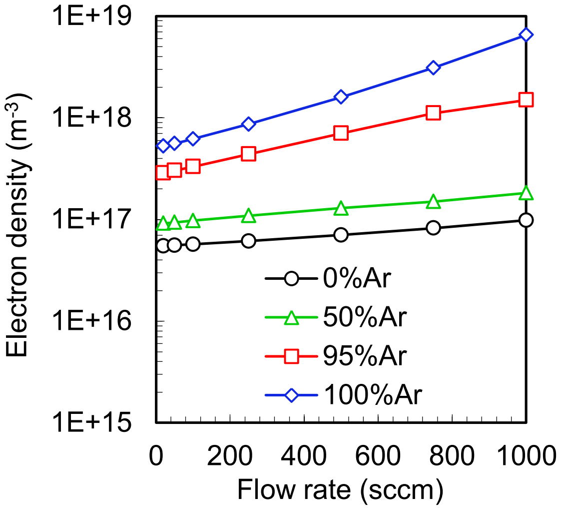




Results (4)

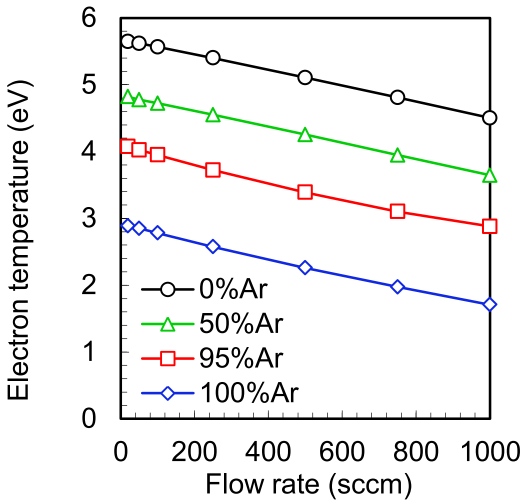
Electron density

(Gas flow rate: 20-1000 sccm)



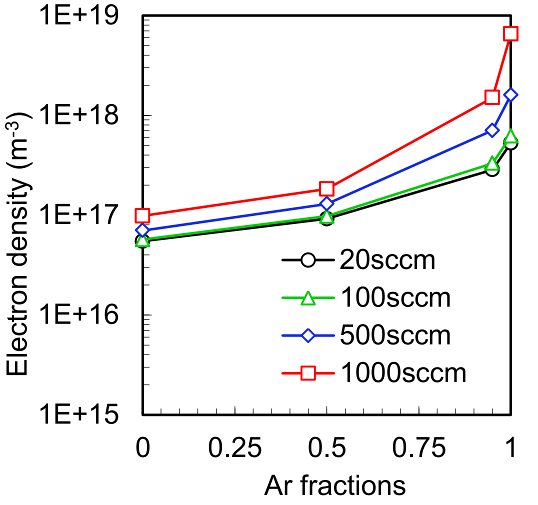
Electron temperature

(Gas flow rate: 20-1000 sccm)



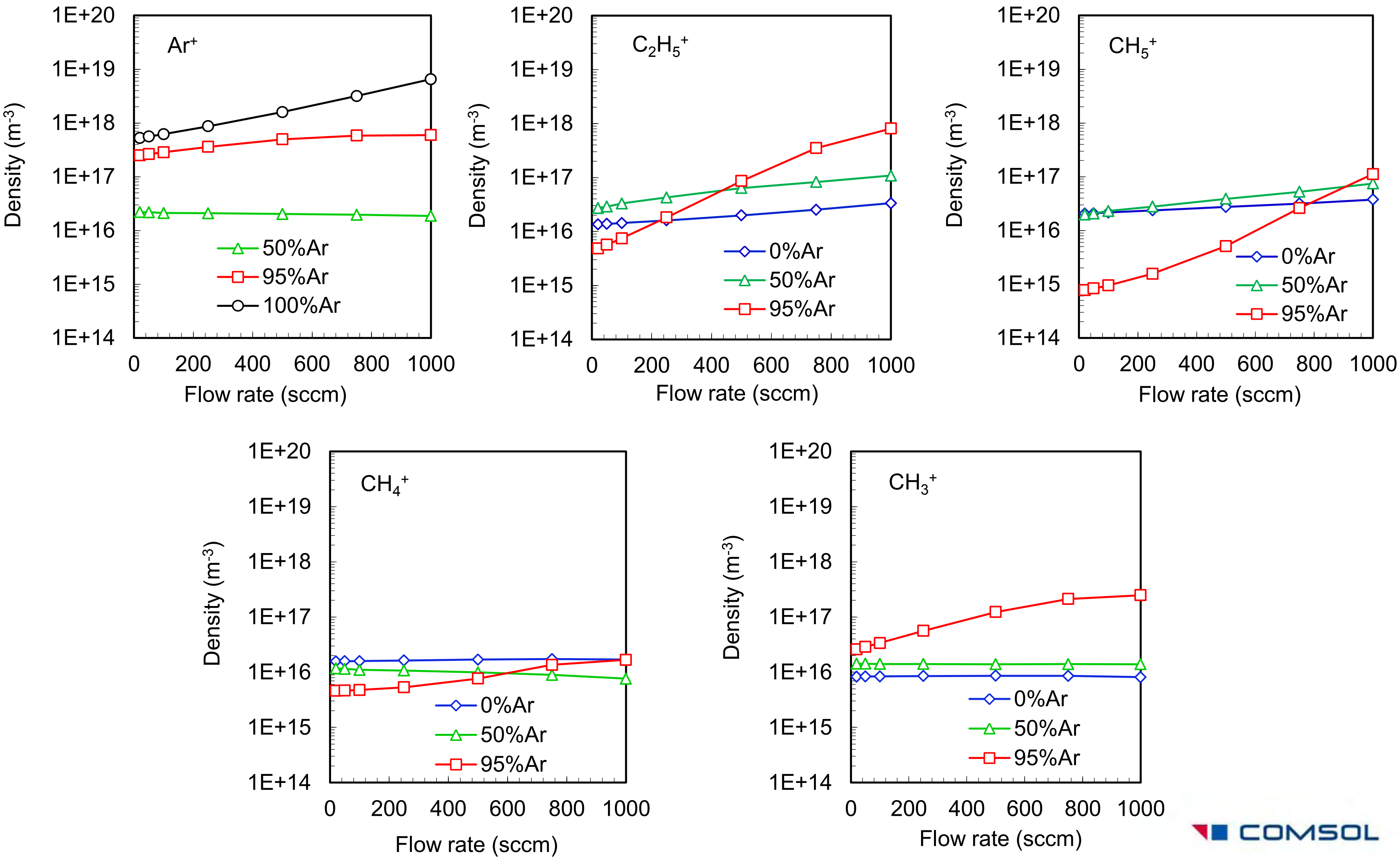
Electron density

(Ar fractions: 0 -1)



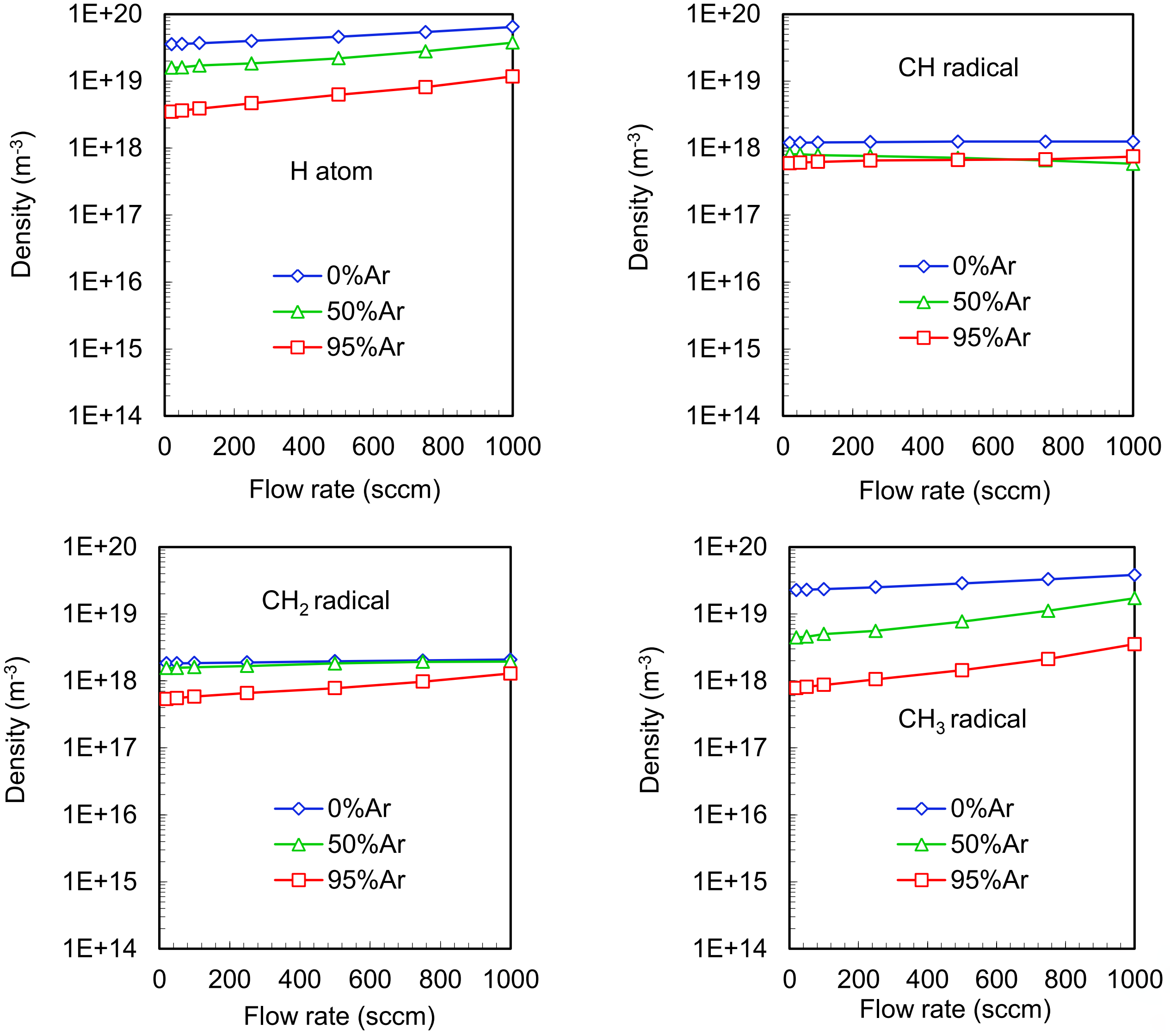
Results (5)

Ion number density



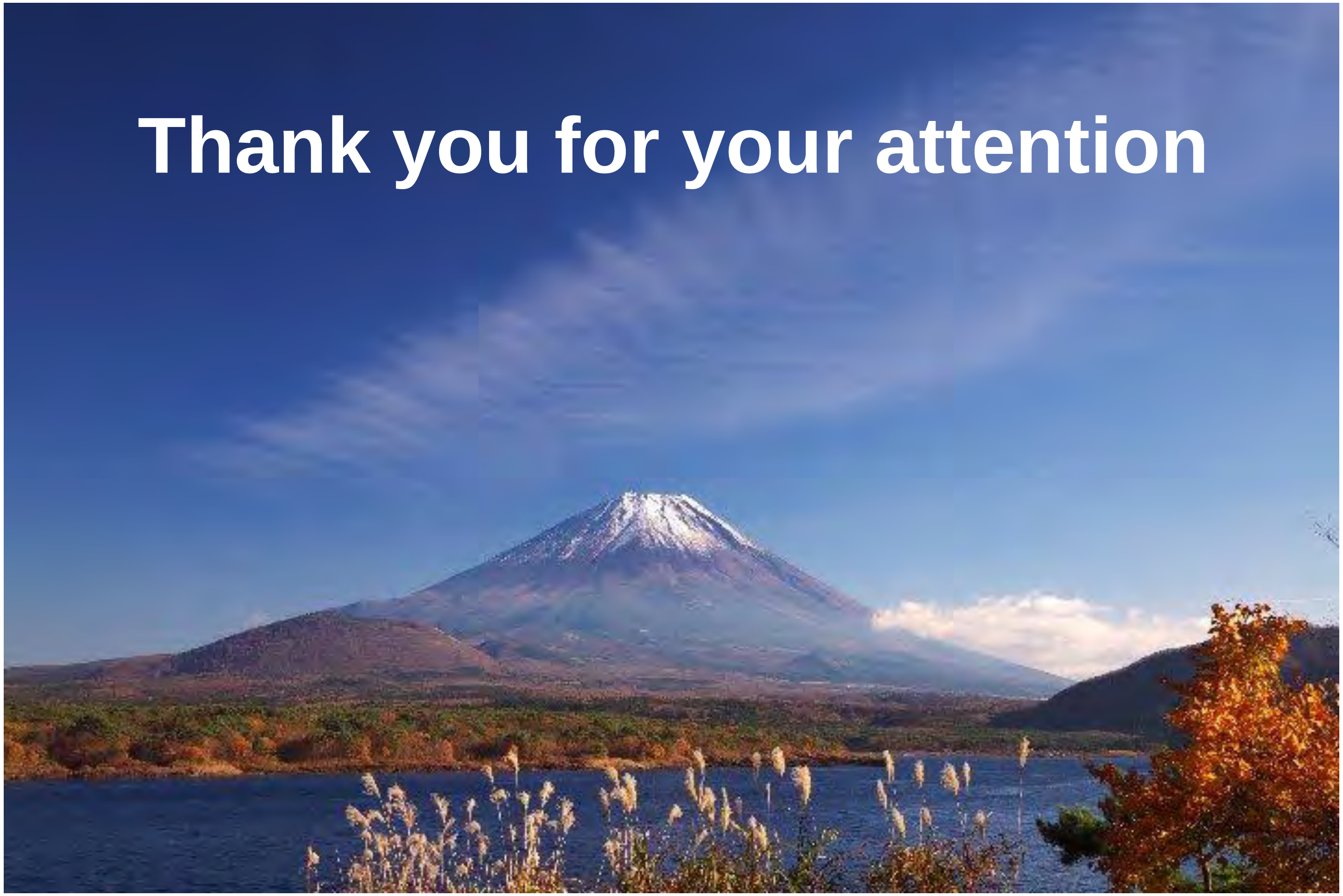
Results (6)

Radical number density



Conclusions

- The simulations of low-pressure inductively coupled rf plasmas in Ar/CH_4 were performed by coupling plasma simulation with fluid dynamics calculation.
- It is found that the electron densities increased and electron temperatures decreased with a rise in gas flow rate for the different Ar fractions. The radicals CH_3, CH_2, CH, and H appeared the high densities over all the gas flow rates and different Ar fractions.
- The gas flows presented the largest influence on plasma properties at a small amount (5%mol) of CH_4 added to Ar.
    - From 20 to 1000 sccm, the densities of CH_3^+ ions increased one order and those of CH_5^+ and $C_2H_5^+$ increased over two orders.
- The control of gas flow rate and gas composition would be very beneficial in obtaining the deposition of good quality thin films.
- It could be concluded that by using COMSOL Multiphysics, the simulations in actual plasma reactors could be realized by coupling with the calculations of CFD, heat transfer, electromagnetic field and etc..



Thank you for your attention