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# Simulation of an Atmospheric Pressure Direct Current Microplasma Discharge in He/$N_2$

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    - Effect of cathode temperature
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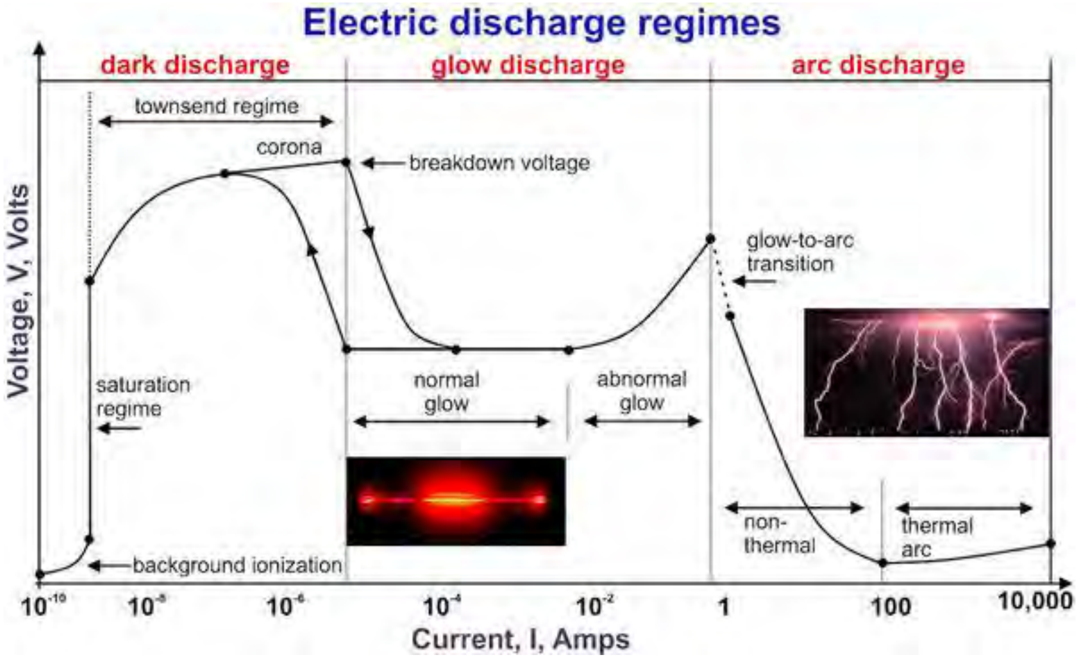
# Atmospheric pressure glow discharge (1)

- Recently, interest has grown toward atmospheric pressure plasmas to reduce the cost by moving away from vacuum equipment.
- Microplasmas are characterized by their small size (characteristic dimensions, of tens to hundreds of microns) and high gas pressure (100 Torr–1 atm), yielding nonequilibrium plasmas.

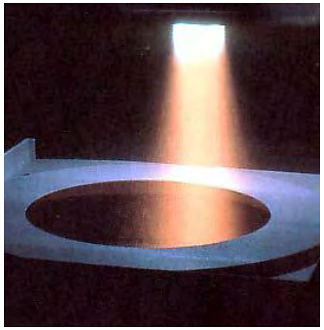


# Atmospheric pressure glow discharge (2)

## Application fields

- Etching for semiconductor devices
- Formation of Diamonds
- Formation of carbon nanotube

- Control of physicochemical properties on substrate



- Flue gas treatment
- Ozone formation
- Sterilization, etc.

- Biocompatibility granted to medical materials

**In this work,**

**The atmospheric pressure direct current (dc) microdischarge, one of the easy methods of generating an atmospheric pressure nonequilibrium plasma, is studied.**

# Types of plasma involved in COMSOL Multiphysics

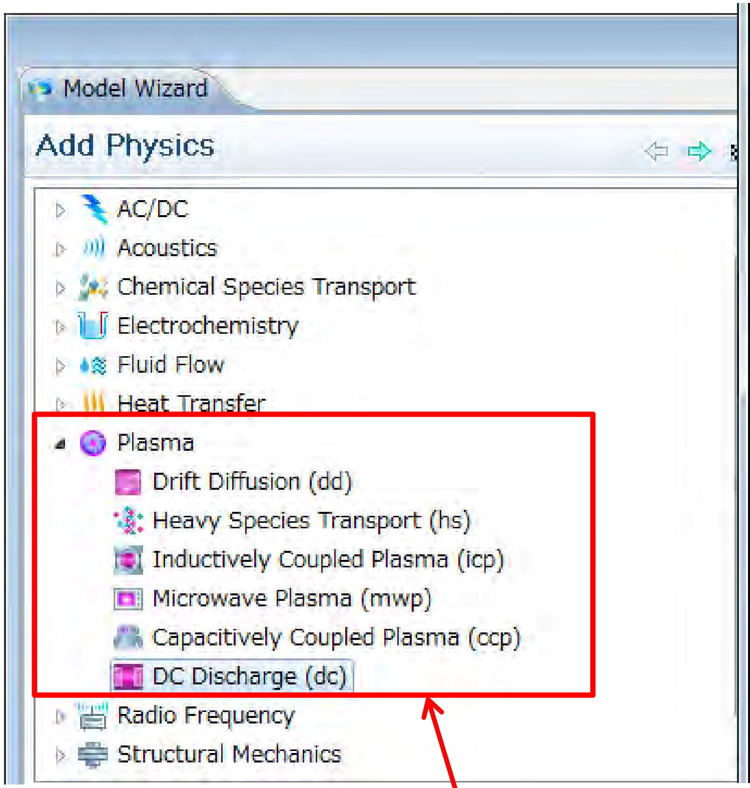
The common types of plasma:

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

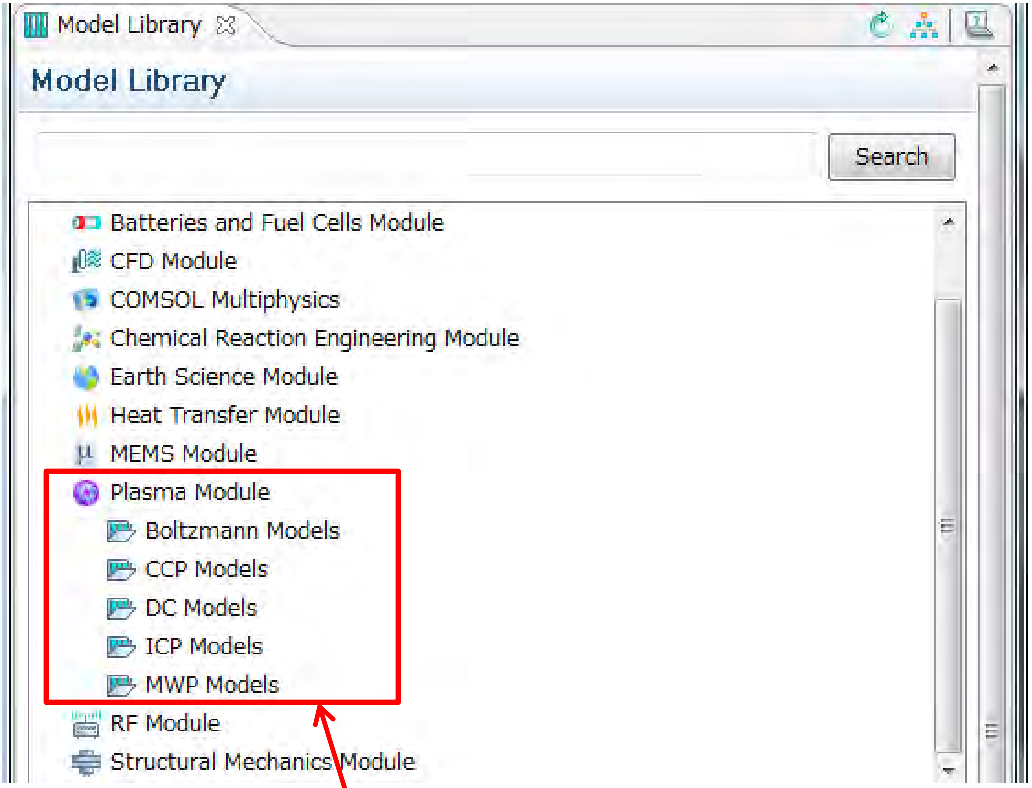
# Plasma module physics interfaces

- 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

| Neutrals (2) |
|---|
| He, $N_2$ |

| Ions (3) |
|---|
| $He^+$, $He_2^+$, $N_2^+$ |

| Excited species (3) |
|---|
| $He(2^1S)$, $He(2^3S)$, $He^*$ |

The reactions included in the model

| No. | Reaction |
|---|---|
| 1 | $e^- + He \rightarrow e^- + He(2^1S)$ |
| 2 | $e^- + He \rightarrow e^- + He(2^3S)$ |
| 3 | $e^- + He \rightarrow 2e^- + He^+$ |
| 4 | $e^- + He(2^1S) \rightarrow 2e^- + He^+$ |
| 5 | $e^- + He(2^3S) \rightarrow 2e^- + He^+$ |
| 6 | $2e^- + He^+ \rightarrow e^- + He$ |
| 7 | $2e^- + He^+ \rightarrow e^- + He^*$ |
| 8 | $e^- + He_2^+ \rightarrow He + He^*$ |
| 9 | $e^- + N_2 \rightarrow 2e^- + N_2^+$ |
| 10 | $e^- + N_2^+ \rightarrow N_2$ |
| 11 | $He^+ + 2He \rightarrow He_2^+ + He$ |
| 12 | $He(2^1S) + He \rightarrow 2He + hv$ |
| 13 | $He(2^3S) + 2He \rightarrow He_2 + He$ |
| 14 | $He(2^3S) + He(2^3S) \rightarrow He^+ + He + e^-$ |
| 15 | $He^+ + N_2 \rightarrow N_2^+ + He$ |
| 16 | $He_2^+ + N_2 \rightarrow N_2^+ + 2He$ |
| 17 | $He^+ + N_2 + He \rightarrow N_2^+ + 2He$ |
| 18 | $He_2^+ + N_2 + He \rightarrow N_2^+ + 3He$ |
| 19 | $He(2^3S) + N_2 \rightarrow N_2^+ + He + e^-$ |
| 20 | $He(2^1S) + N_2 \rightarrow N_2^+ + He + e^-$ |
| 21 | $He(2^3S) + N_2 + He \rightarrow N_2^+ + 2He + e^-$ |

# Electron transport

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

$$\frac{\partial}{\partial t}(n_e) + \nabla \cdot \Gamma_e = R_e$$

$$\Gamma_e = -n_e(\mu_e \mathbf{E}) - D_e \nabla n_e$$

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

$$\Gamma_\varepsilon = -n_\varepsilon(\mu_\varepsilon \mathbf{E}) - D_\varepsilon \nabla n_\varepsilon$$

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.

# Heat transfer

- Heat transfer inside the computational domain is modeled by the below equation:

$$\underset{\substack{\uparrow\\ \text{Accumulation}}}{\rho C_p \frac{\partial T}{\partial t}} + \overbrace{\nabla\cdot(-k\nabla T)}^{\text{Conduction}} = \underset{\substack{\uparrow\\ \text{Heat source}}}{Q} + \underset{\substack{\uparrow\\ \text{Temperature-dependent heat source}}}{q_s T} - \overbrace{\rho C_p \mathbf{u}\cdot\nabla T}^{\text{Advection}} + \underset{\substack{\uparrow\\ \text{Viscous heating}}}{\tau : \mathbf{S}} + \overbrace{\frac{T}{\rho}\left(\frac{\partial \rho}{\partial T}\right)_p \left(\frac{\partial p_a}{\partial t} + \mathbf{u}\cdot\nabla p_a\right)}^{\text{Pressure Work}}$$

# 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.

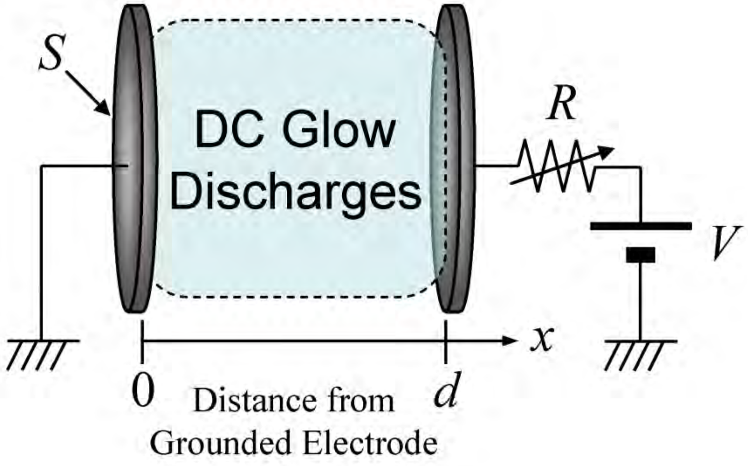
$$\rho = q\left(\sum_{k=1}^{N} Z_k n_k - n_e\right)$$

# Discharge voltage

$$\underset{\substack{\uparrow \\ \text{Discharge voltage}}}{V_d} = \underset{\substack{\uparrow \\ \text{Supplied voltage}}}{V} - \underset{\substack{\uparrow \\ \text{Current density}}}{j}\overset{\substack{\text{Electrode area} \\ \downarrow}}{A}\underset{\substack{\uparrow \\ \text{Ballast resistor}}}{R_b}$$

# He/$N_2$ dc microplasma model (1)

DC microplasma model



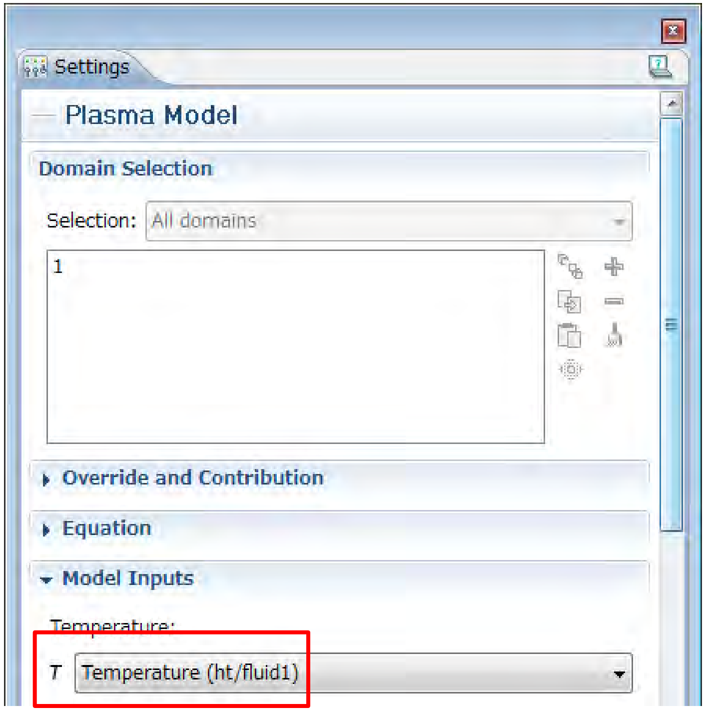
Computational conditions

- Gas: pure He and He/$N_2$ mixtures
- $N_2$ fractions: 0.002–0.02%
- Pressure: 760 Torr
- Power source: DC
- Operating voltage: 232–450V
- Ballast resistor: 10 k$\Omega$
- Electrode area: 0.006 $cm^2$
- Cathode temperature: 350, 450, 550 K
- Anode temperature: 350 K

# He/$N_2$ dc microplasma model (2)

Coupled simulation of plasma and heat transfer

Plasma



Plasma Model

Domain Selection

Selection: All domains

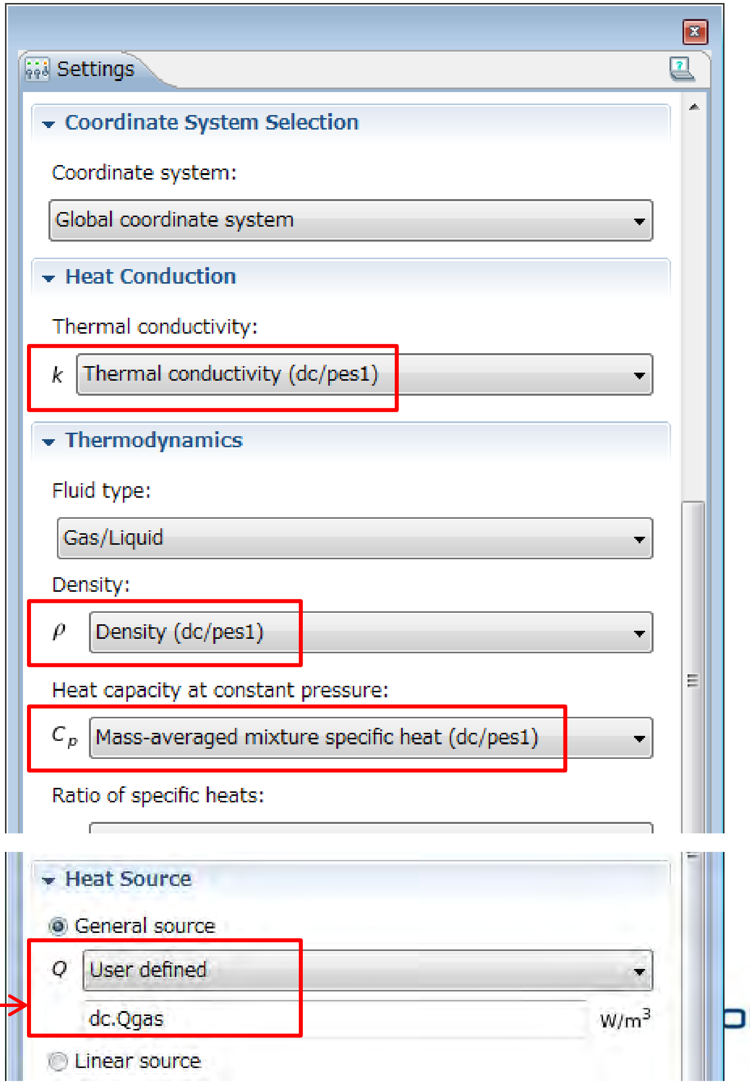
1

Model Inputs

Temperature:

T Temperature (ht/fluid1)

Heat transfer



Coordinate System Selection

Coordinate system: Global coordinate system

Heat Conduction

Thermal conductivity:

k Thermal conductivity (dc/pes1)

Thermodynamics

Fluid type: Gas/Liquid

Density:

ρ Density (dc/pes1)

Heat capacity at constant pressure:

$C_p$ Mass-averaged mixture specific heat (dc/pes1)

Ratio of specific heats:

Heat Source

● General source

Q User defined

dc.Qgas W/$m^3$

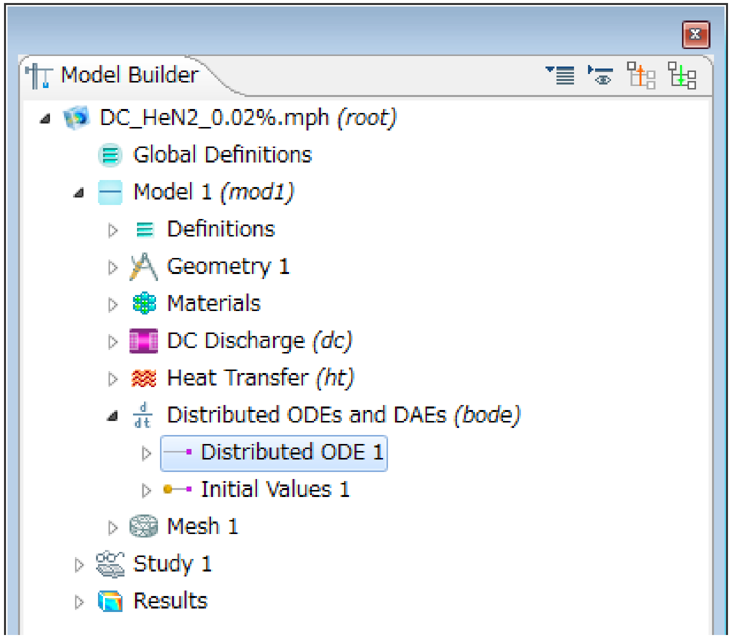
○ Linear source

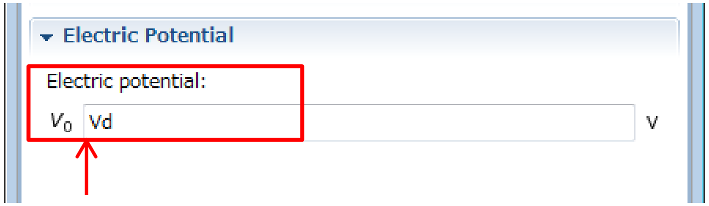
Heat source →

# He/N$_2$ dc microplasma model (3)

PDE equation

Plasma



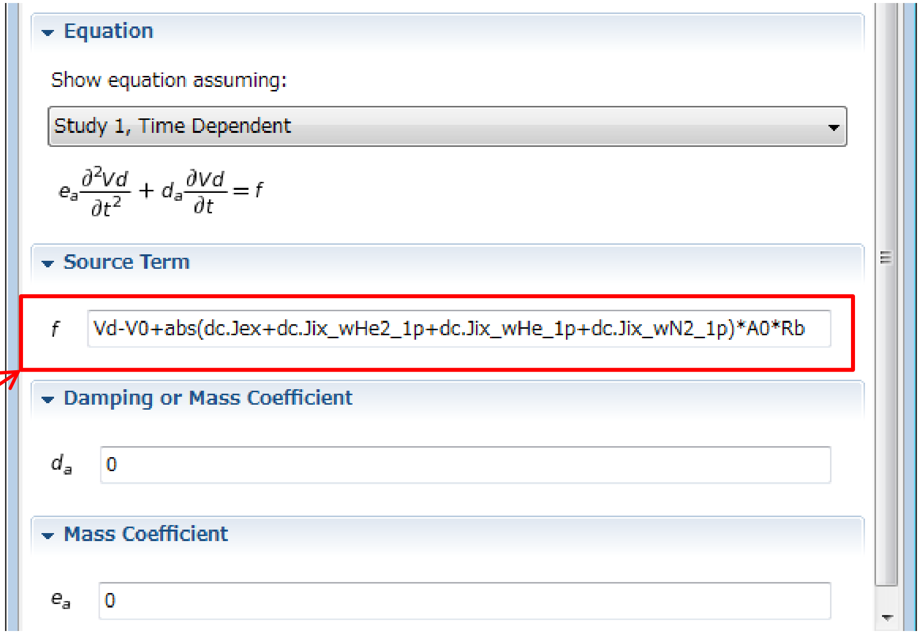


**Electric Potential**

Electric potential:

$V_0$ Vd V

Discharge voltage



**Equation**

Show equation assuming:

Study 1, Time Dependent

$$e_a \frac{\partial^2 Vd}{\partial t^2} + d_a \frac{\partial Vd}{\partial t} = f$$

**Source Term**

$f$ Vd-V0+abs(dc.Jex+dc.Jix_wHe2_1p+dc.Jix_wHe_1p+dc.Jix_wN2_1p)*A0*Rb

**Damping or Mass Coefficient**

$d_a$ 0

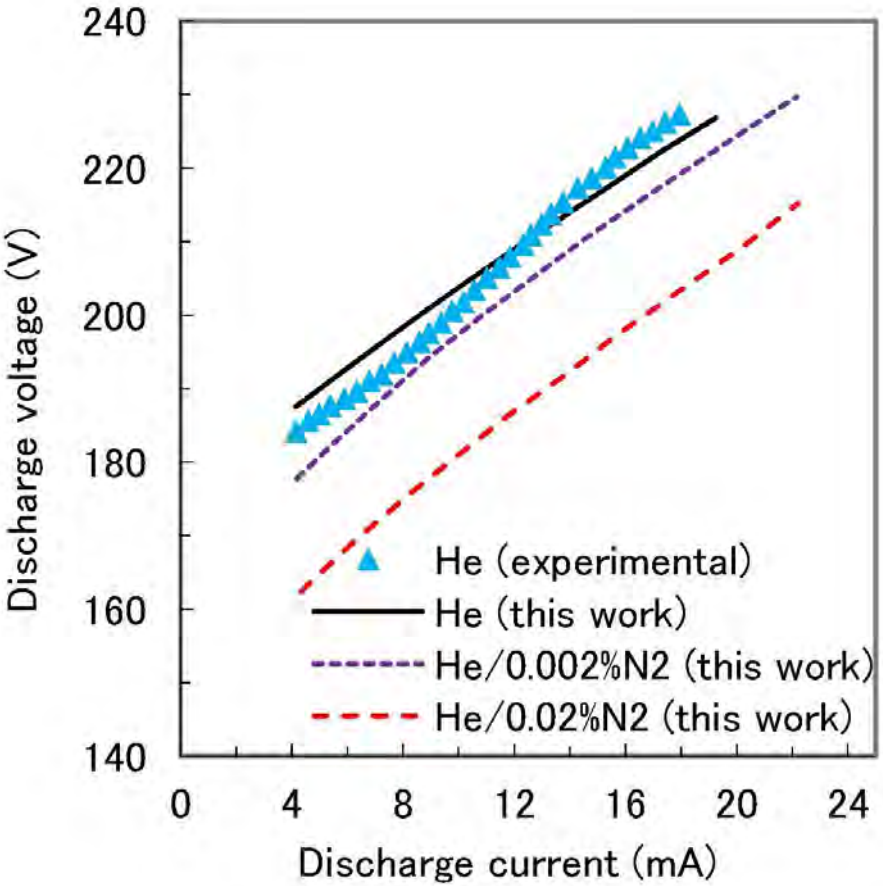
**Mass Coefficient**

$e_a$ 0

$$V_d = V - jAR_b$$

# Results (1)

**Current-voltage (*I*-*V*) characteristics**:

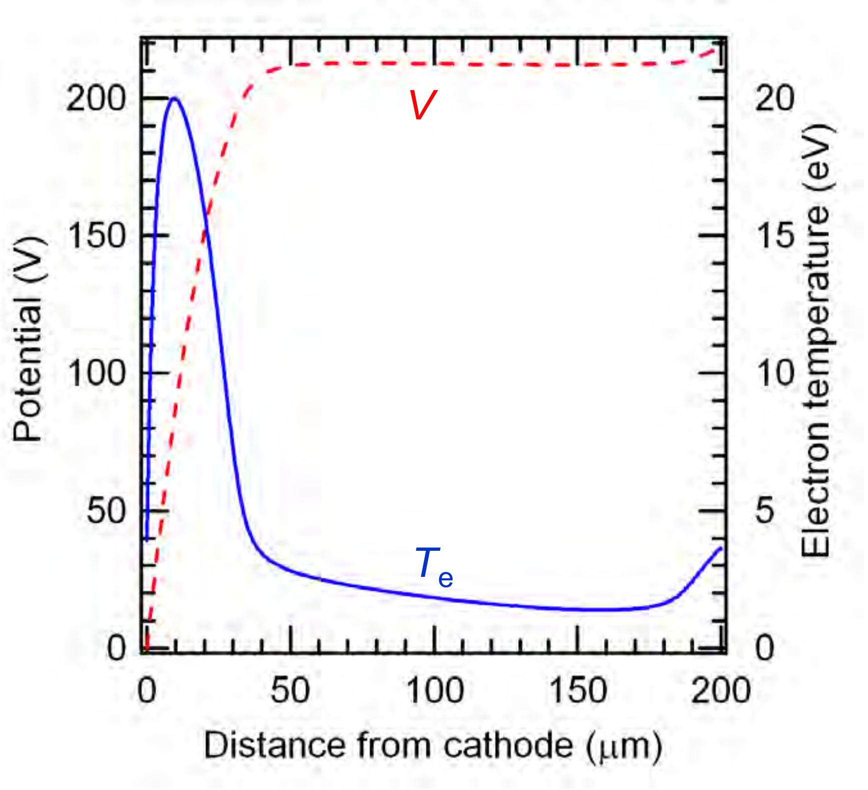


The boundary condition for electric field calculation is specified as $V_c = 0$ on the cathode and $V_a = V_d$ on the anode.

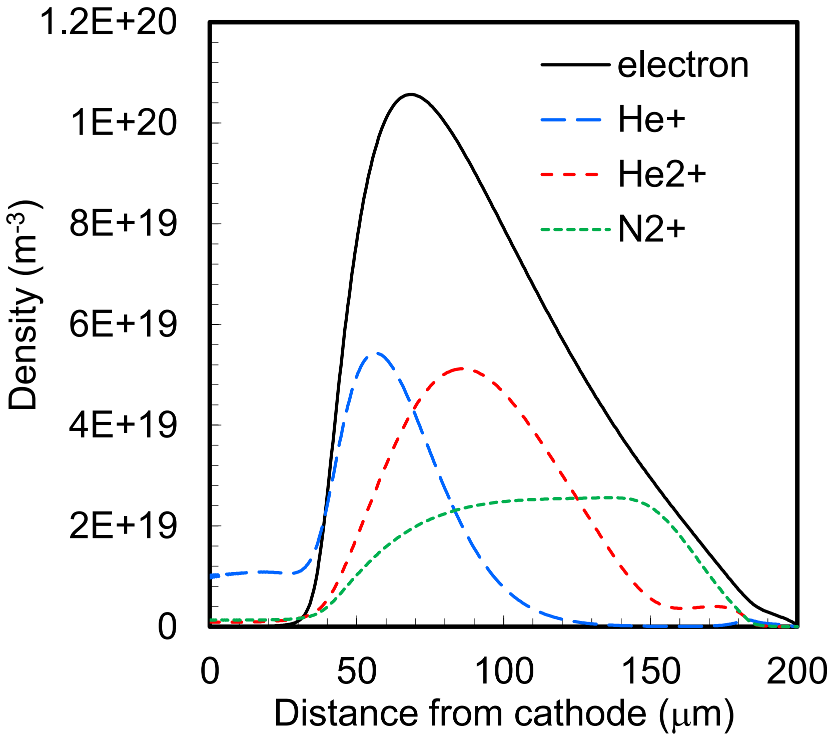
# Results (2)

Discharge structure in a He/0.02%$N_2$ microdischarge at $V$ = 420 V

Electrical potential and electron temperature

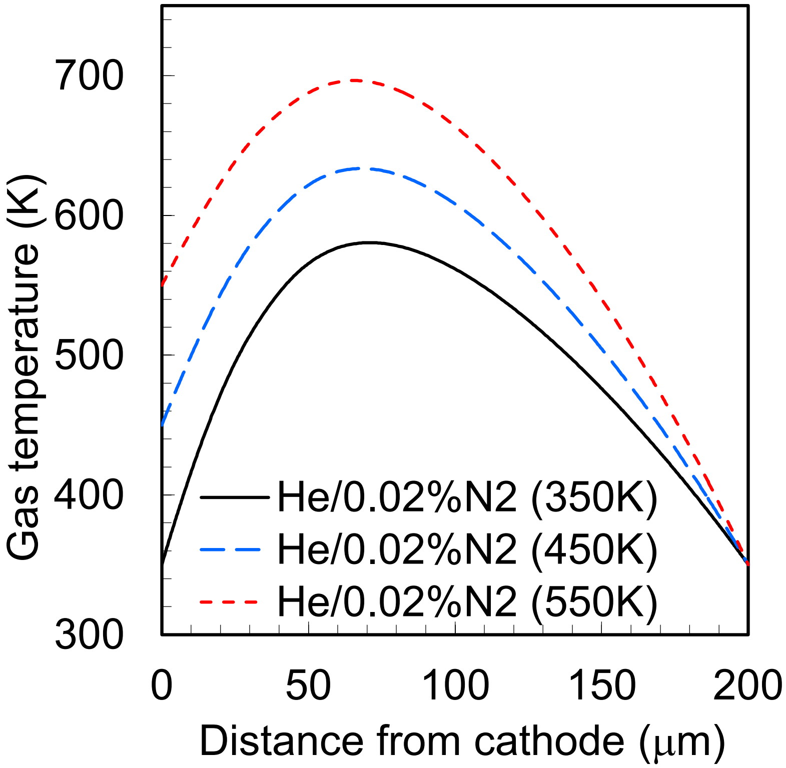


Number density



# Results (3)

The effect of cathode temperature in He/0.02%$N_2$ microdischarges



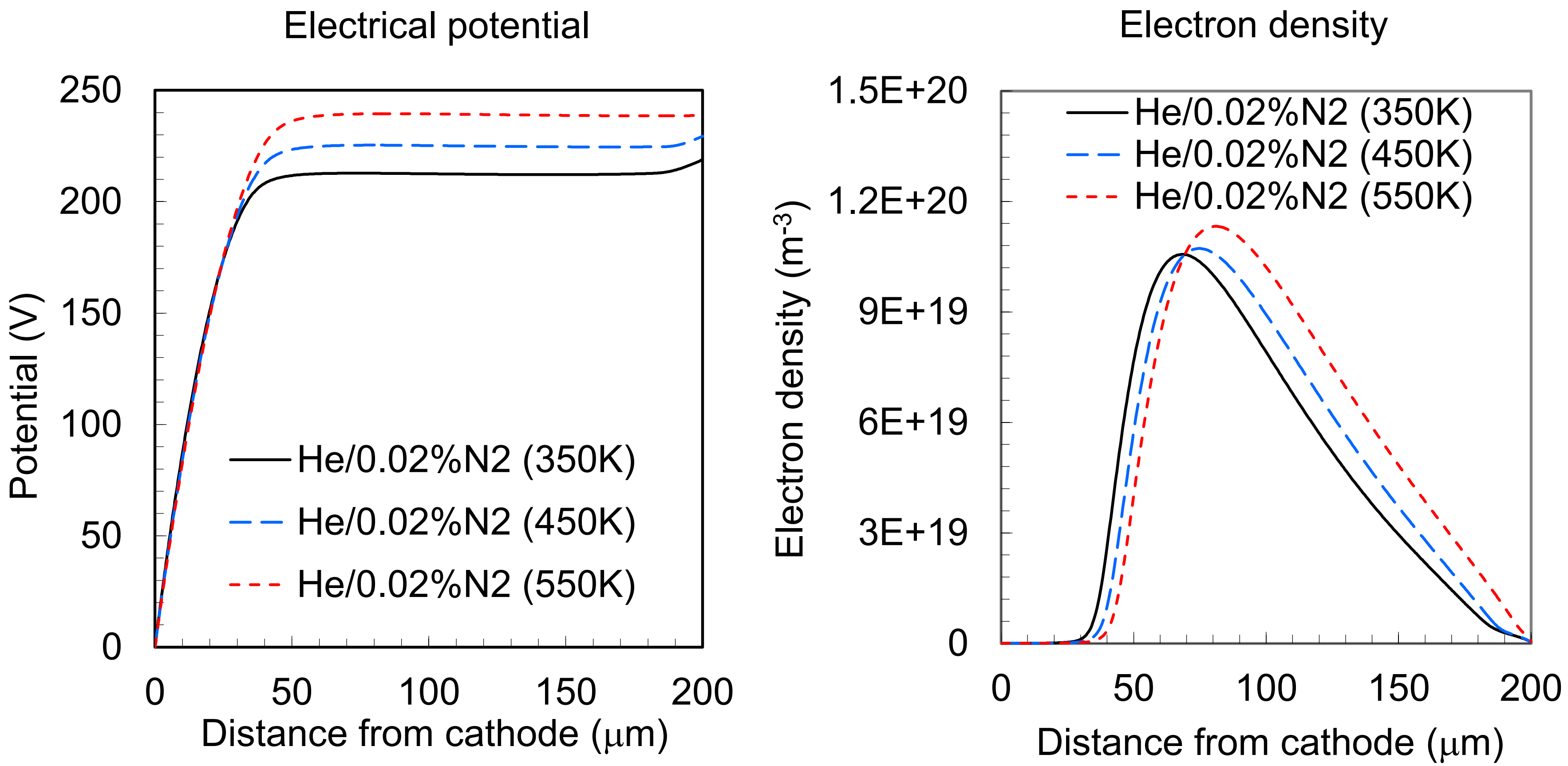
Gas temperature

The electrical conductivity $\sigma$ is strongly dependent on temperature, which can be approximated by

$$\sigma = \frac{1}{\rho_0[1+\alpha(T-T_0)]}$$

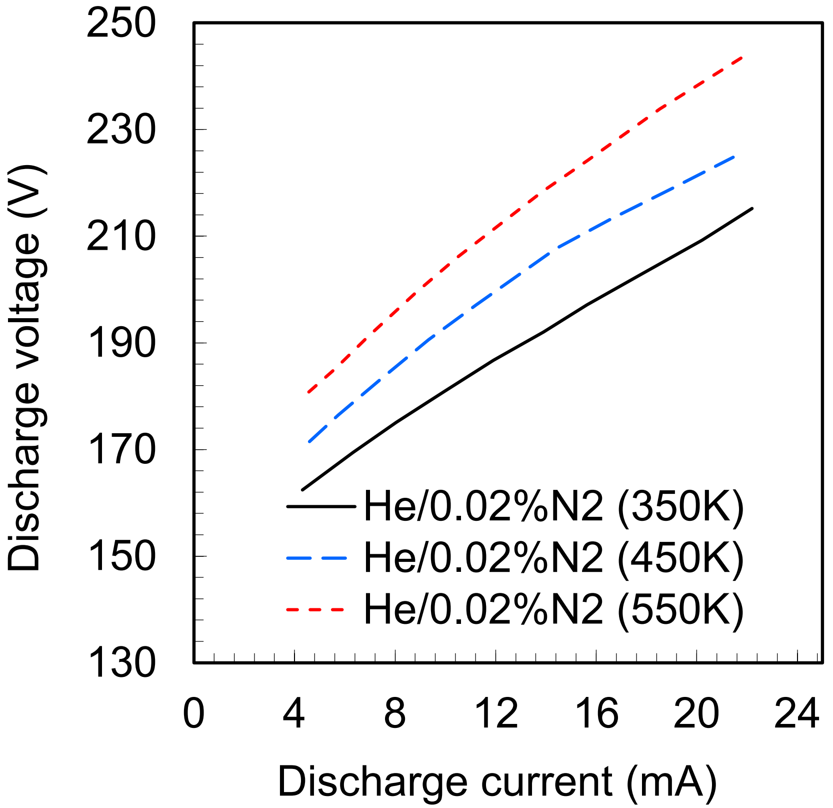
# Results (4)

Discharge structure in He/0.02%$N_2$ microdischarges at different cathode temperatures



# Results (5)

*I-V* characteristics in He/0.02%$N_2$ microdischarges at different cathode temperatures



# Conclusions

- The simulations of atmospheric pressure direct current micro-plasma discharges in He/$N_2$ were performed by coupling plasma simulation with heat transfer calculation.
- A simple circuit model was used to obtain the discharge voltage regarded as the boundary potential condition in the plasma simulation.
- The effect of a small amount of $N_2$ added to He as well as the effect of cathode temperature on the *I*-*V* characteristics were studied.
- It could be concluded that by using COMSOL Multiphysics, the simulations would be very beneficial in finding the design parameters of atmospheric pressure plasma sources for surface modification.

# Thank you for your attention