Two-dimensional Simulation of RF CF_4 Discharge Using the Particle-in-Cell/Monte Carlo Method

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OUTLINE

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Introduction

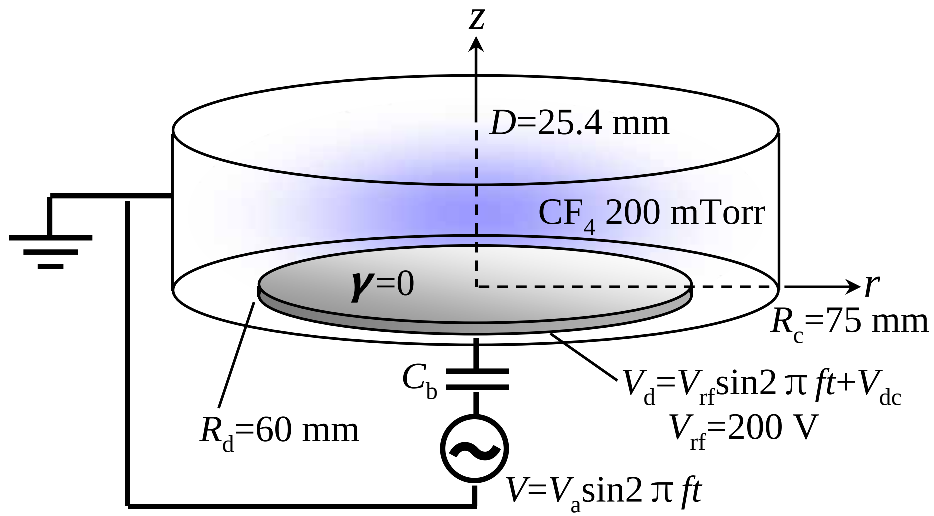
- Fluorocarbon gases(CF_4, C_2F_6, C_4F_8, ...) are widely used in plasma-assisted etching processes.

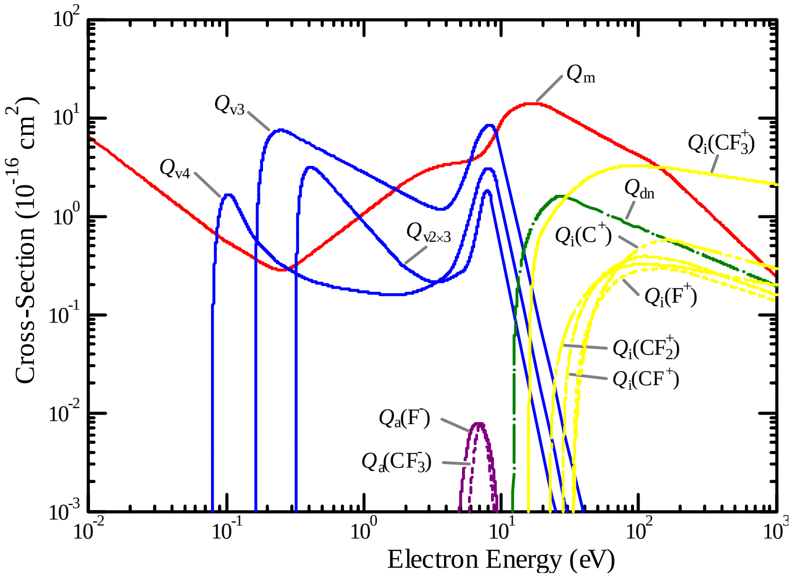
- In previous work, we were successful in 1-D simulation of rf CF_4 plasma using PIC/MC method.
  - 1-D discharge structure (density, temperature, reaction rate, etc...)
  - sustaining mechanism
  - effects of secondary electron emission and electrode spacing

- In this work, the 1-D PIC/MC code is extended to axisymmetric plasma.
  - 2-D discharge structure
  - Energy/Angular distribution functions

Modeling of RF CF_4 Plasma

- **Species**
  - CF_4
  - electron
  - CF_3^+, CF_2^+, CF^+, C^+, F^+
  - F^-, CF_3^-
- **Collision**
  - electron-CF_4
  - ion-CF_4
  - positive-negative ion recombination
    $k = 5.5\times10^{-13}$ $(m^{-3}s^{-1})$
  - electron-CF_3^+ recombination
    $k = 3.95\times10^{-9}\, T_e^{-0.5} T_i^{-1}$ $(m^{-3}s^{-1})$





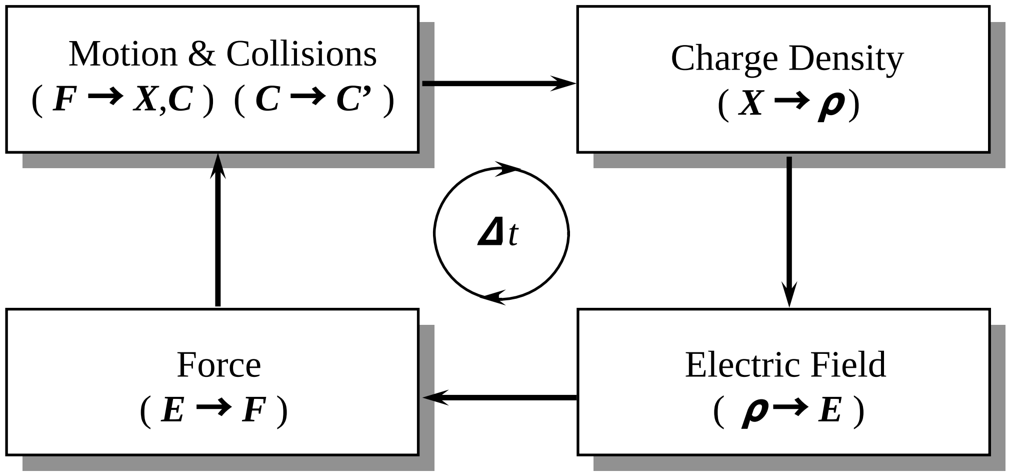
Ion-CF_4 Collision Model

- The RRK theory is adopted to describe unimolecular decomposition of activated complex.
- Elastic collision and 183 endothermic reactions (dissociation, electron detachment).

No.	Reactions			ΔE (eV)
1.1	$CF_3^+ + CF_4$	$\longrightarrow$	$CF_3^+ + CF_3 + F$	5.621
1.2			$CF_2^+ + CF_4 + F$	5.843
1.3			$CF^+ + CF_4 + F_2$	7.546
2.1	$CF_2^+ + CF_4$	$\longrightarrow$	$CF^+ + CF_4 + F$	3.303
2.2			$CF_2^+ + CF_3 + F$	5.621
2.3			$CF^+ + CF_3 + F_2$	7.324
3.1	$CF^+ + CF_4$	$\longrightarrow$	$CF^+ + CF_3 + F$	5.621
3.2			$CF^+ + CF_2 + F_2$	7.598
3.3			$CF^+ + CF_2 + 2F$	9.198
4.1	$C^+ + CF_4$	$\longrightarrow$	$C^+ + CF_3 + F$	5.621
4.2			$C^+ + CF_2 + F_2$	7.598
4.3			$C^+ + CF_2 + 2F$	9.198
5.1	$F^+ + CF_4$	$\longrightarrow$	$F^+ + CF_3 + F$	5.621
5.2			$F^+ + CF_2 + F_2$	7.598
5.3			$F^+ + CF_2 + 2F$	9.198
6.1	$F^- + CF_4$	$\longrightarrow$	$CF_4 + F + e$	3.521
6.2			$F^- + CF_3 + F$	5.621
6.3			$CF_3 + F_2 + e$	7.542
7.1	$CF_3^- + CF_4$	$\longrightarrow$	$CF_4 + CF_3 + e$	1.871
7.2			$F^- + CF_4 + CF_2$	1.927
7.3			$CF_4 + CF_2 + F + e$	5.448

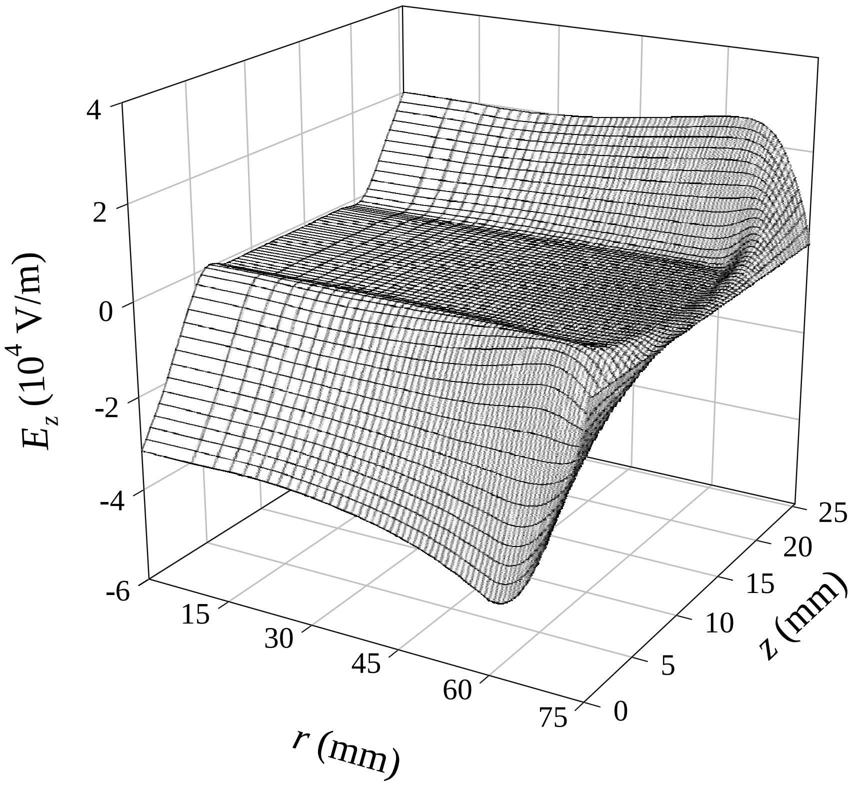
Particle-in-Cell / Monte Carlo Method

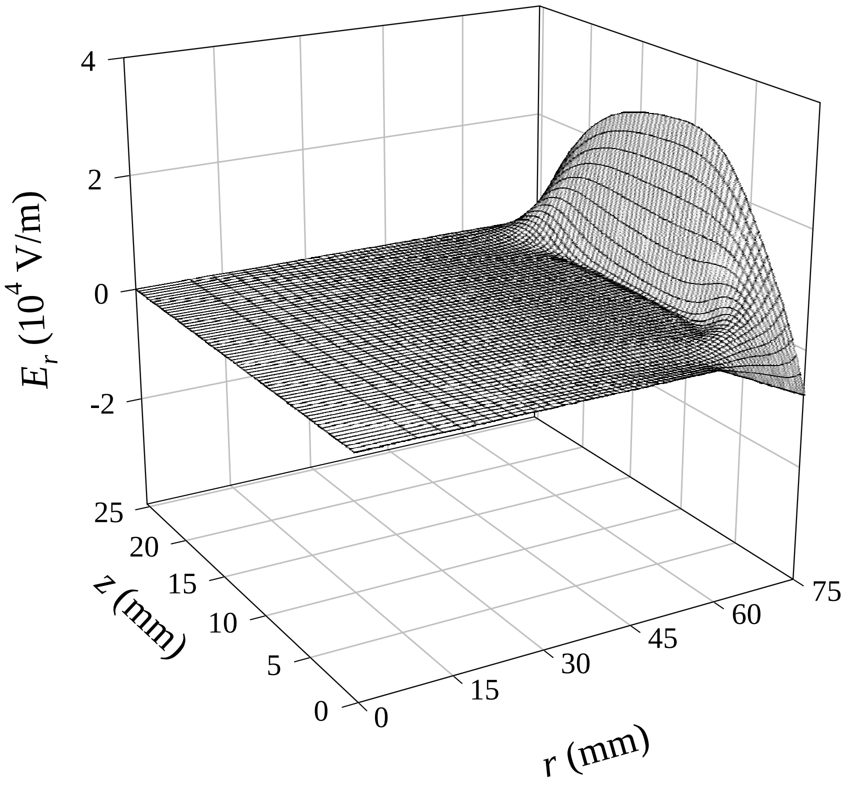
- Poisson equation: ADI with multi-grid method
- Equation of motion: Leap-frog scheme
- Collisions: Monte Carlo



Electric Field ($2\pi f t = \pi$)

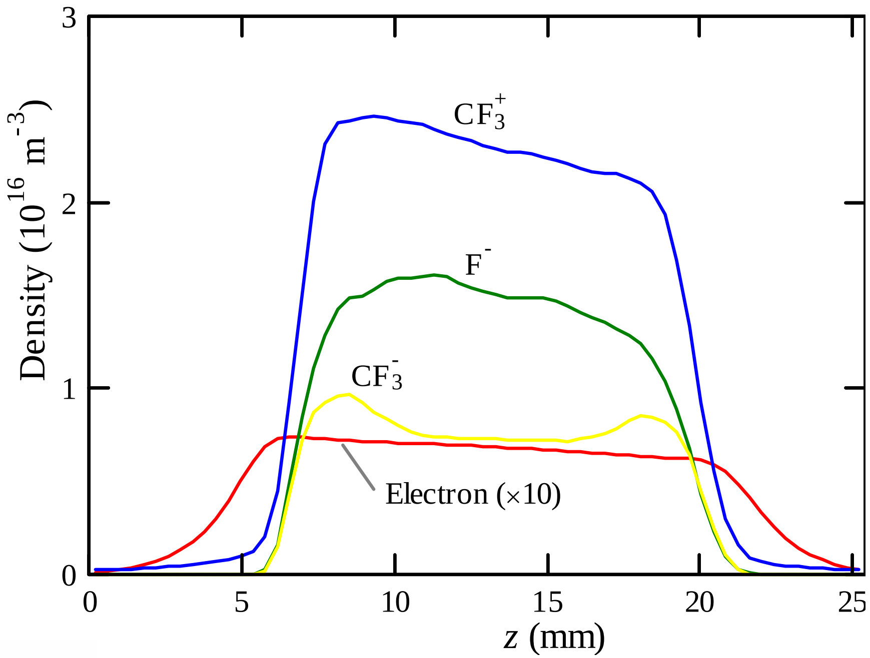
- Double-layer can be observed in both E_z and E_r.
- Electric field is strengthened around the edge of powered electrode.

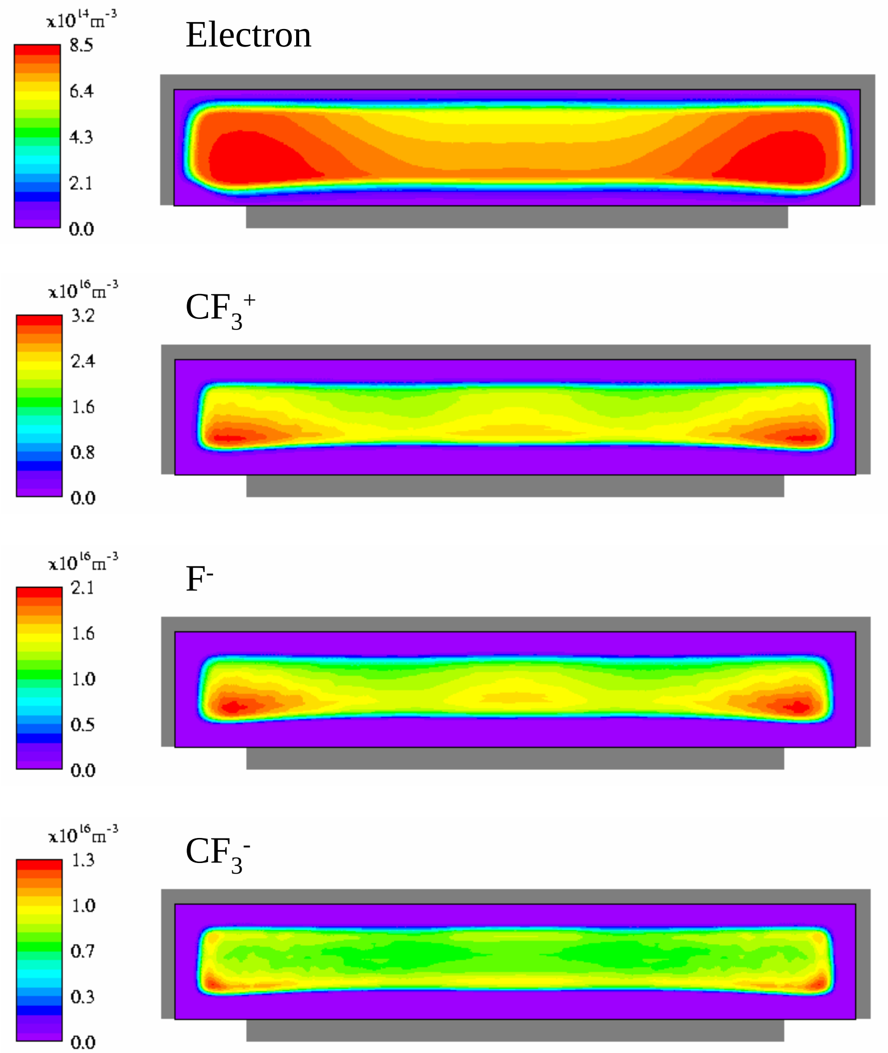




Electron and Ion Densities

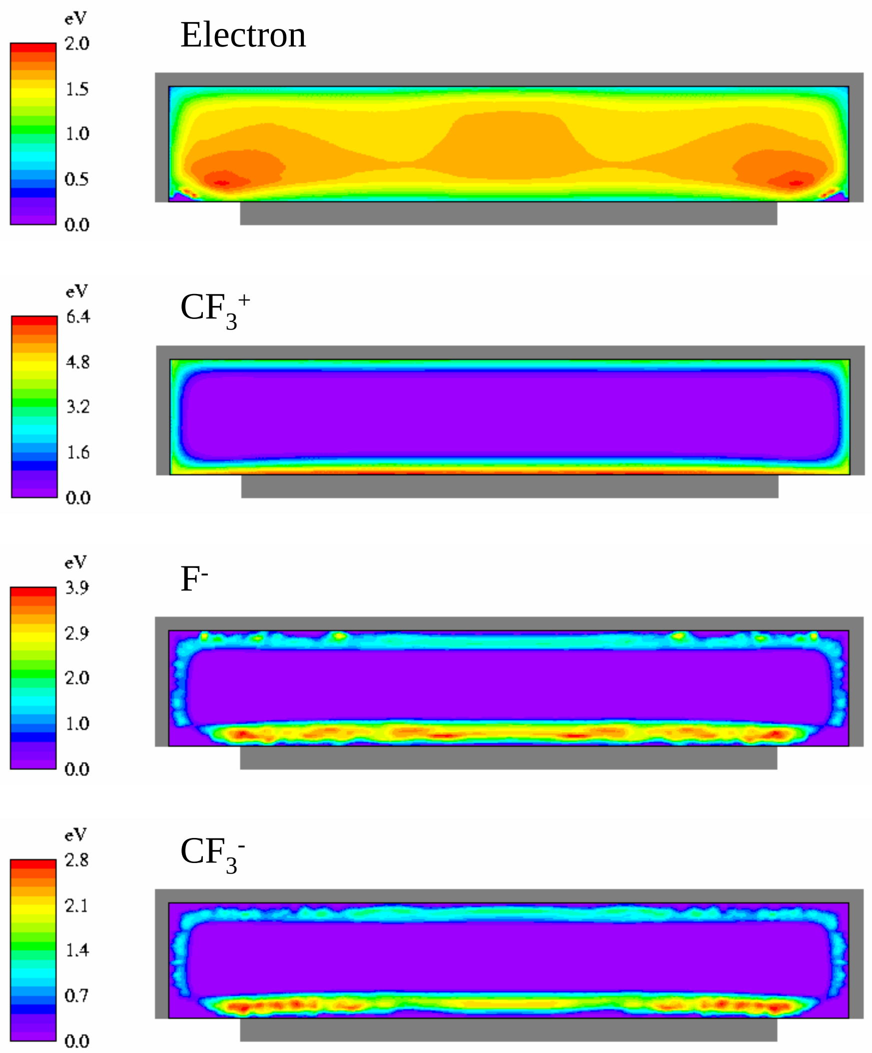
- CF_3^+, F^-, and CF_3^- are dominant ions in the discharge.
- Negative ion density is about 30 times greater than electron density.
- Densities have maxima around the edge of powered electrode.





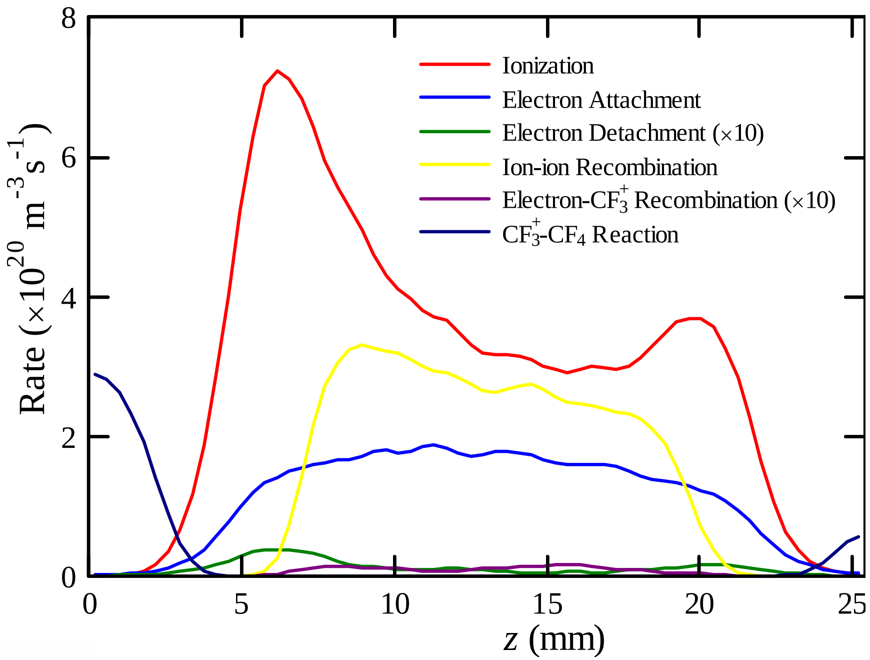
Electron and Ion Temperatures

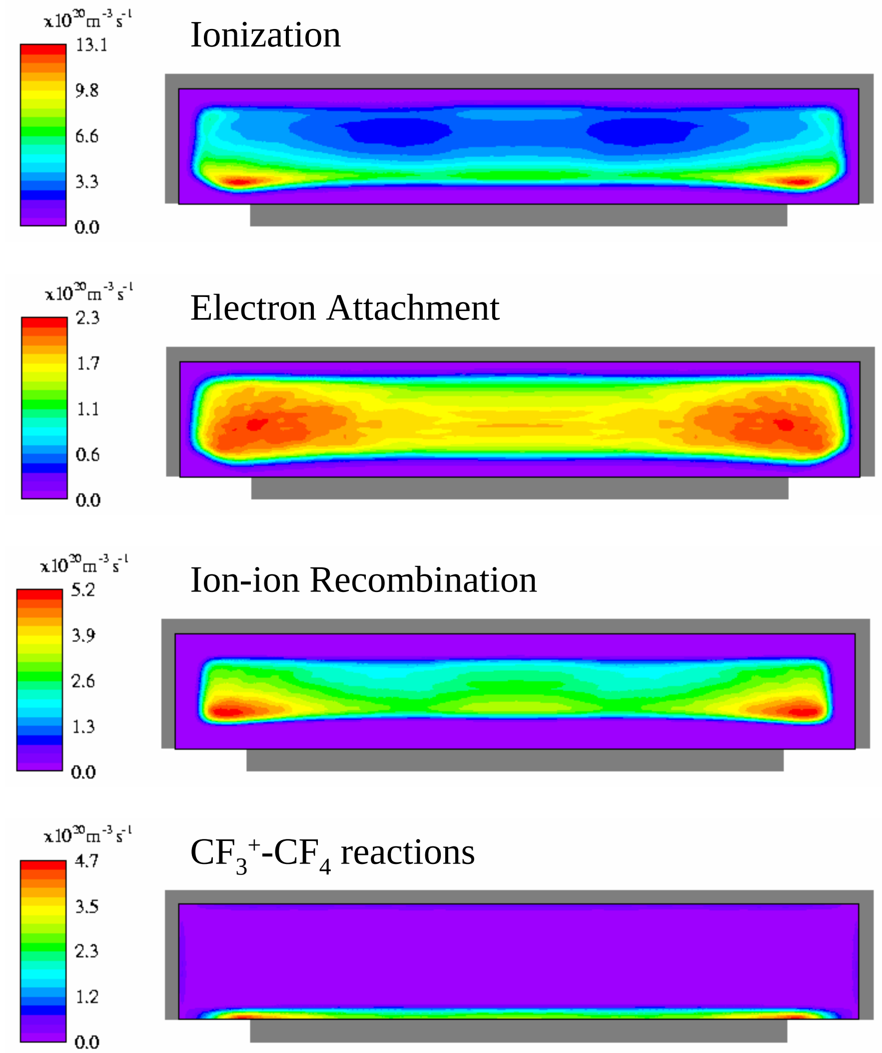
- Bulk electron temperature is about 1.7 eV.
- High temperature region
  - Electron: around the edge of powered electrode
  - CF_3^+: on the powered electrode
  - F^- and CF_3^-: in the middle of sheath near the powered electrode



Reaction Rates

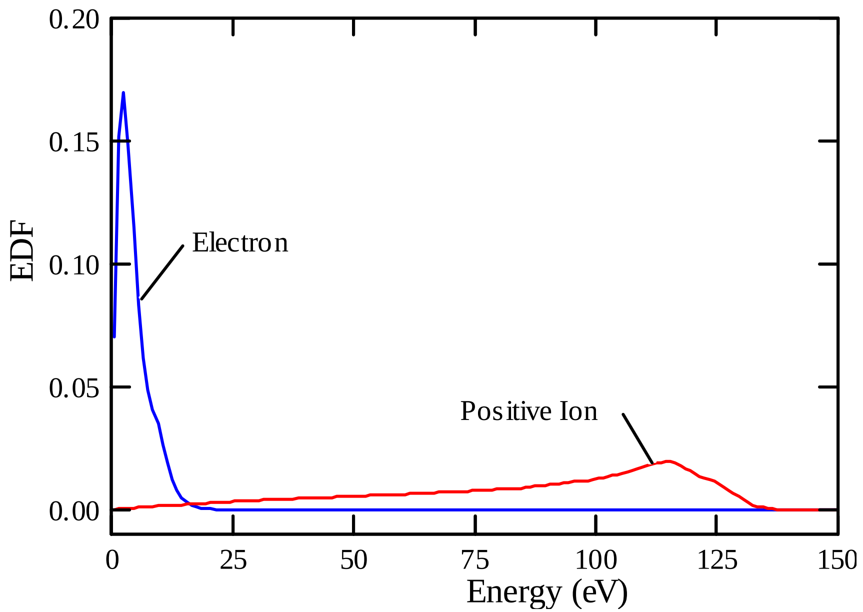
- Discharge is sustained by electrons produced in ionization.
- Major loss process of negative ions is ion-ion recombination.
- CF_3^+-CF_4 reactions are remarkable in the sheath.

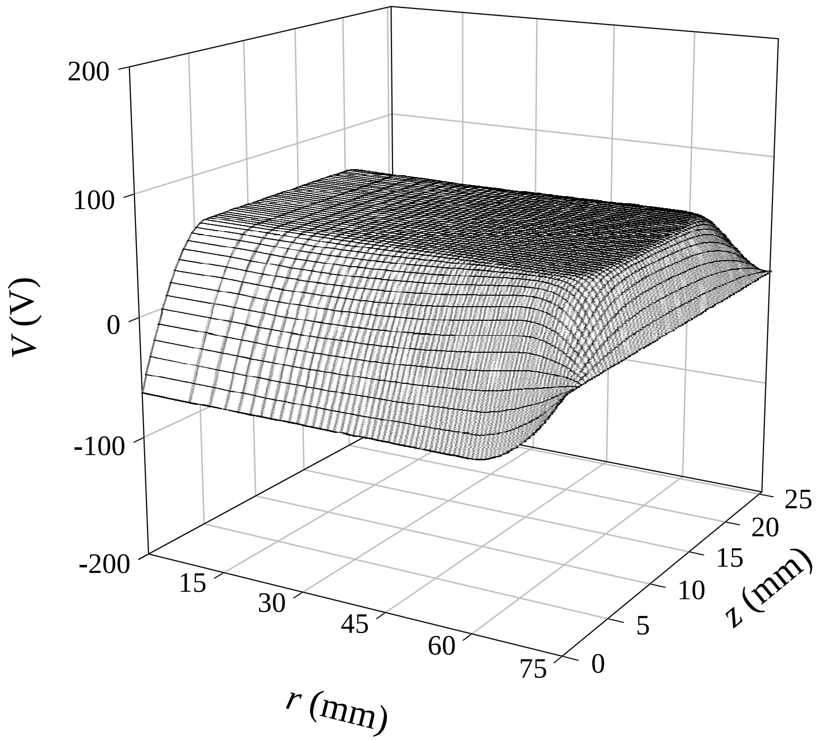




EEDF, IEDF and Time-Averaged Potential

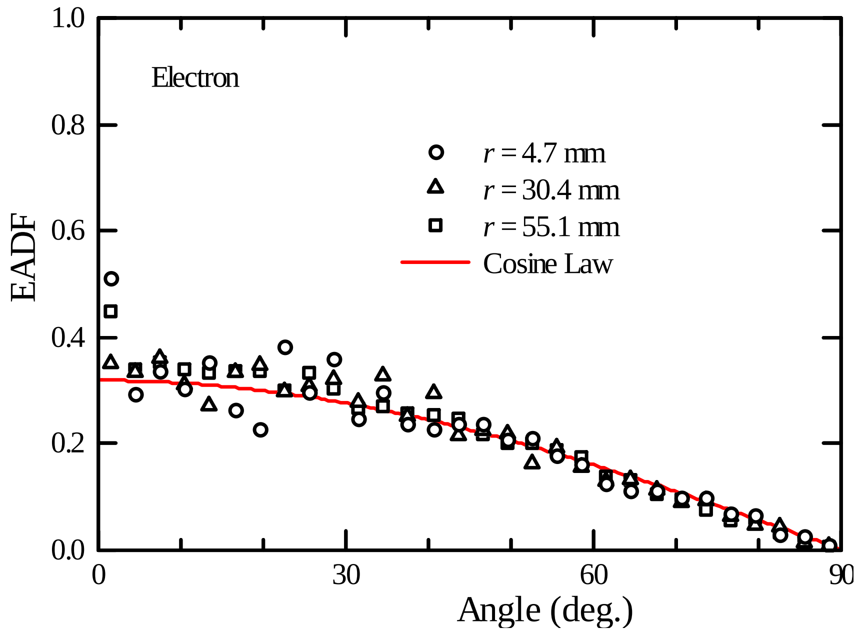
- Negative-ion flux onto powered electrode is 0.
- The ion energy at maximum IEDF agrees with potential fall from V_p to V_{dc}. (Plasma potential V_p is 61 V. Self-bias V_{dc} is -62 V.)

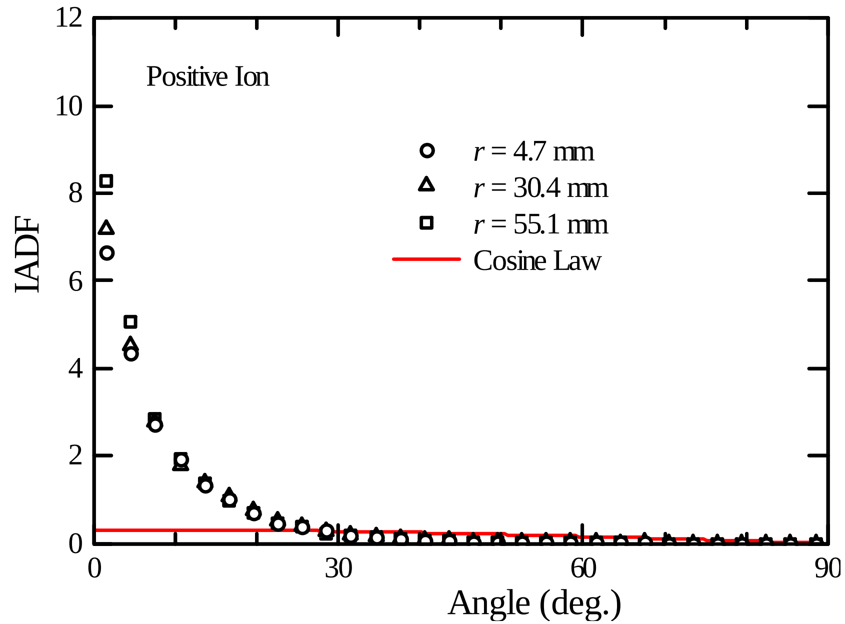




EADF and IADF

- IADF is directional as expected.
- EADF can be described as Cosine Law.





Summary

- Axisymmetric PIC/MC code for rf CF_4 discharge has been developed.
- Discharge structure is characterized by an enhanced electric field around the edge of powered electrode.
- Double-layer appears also in radial component of electric field near cylindrical reactor wall.
- We also investigate the energy/angular distribution functions of charged species arriving at the powered electrode.