Technical meeting on emerging applications of plasma science and technology

ML-aided plasma source and process simulation for semiconductor fabrication processes

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PEI Convergence Research Center for Plasma Equipment Intelligence

KRISS

Contents

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Introduction

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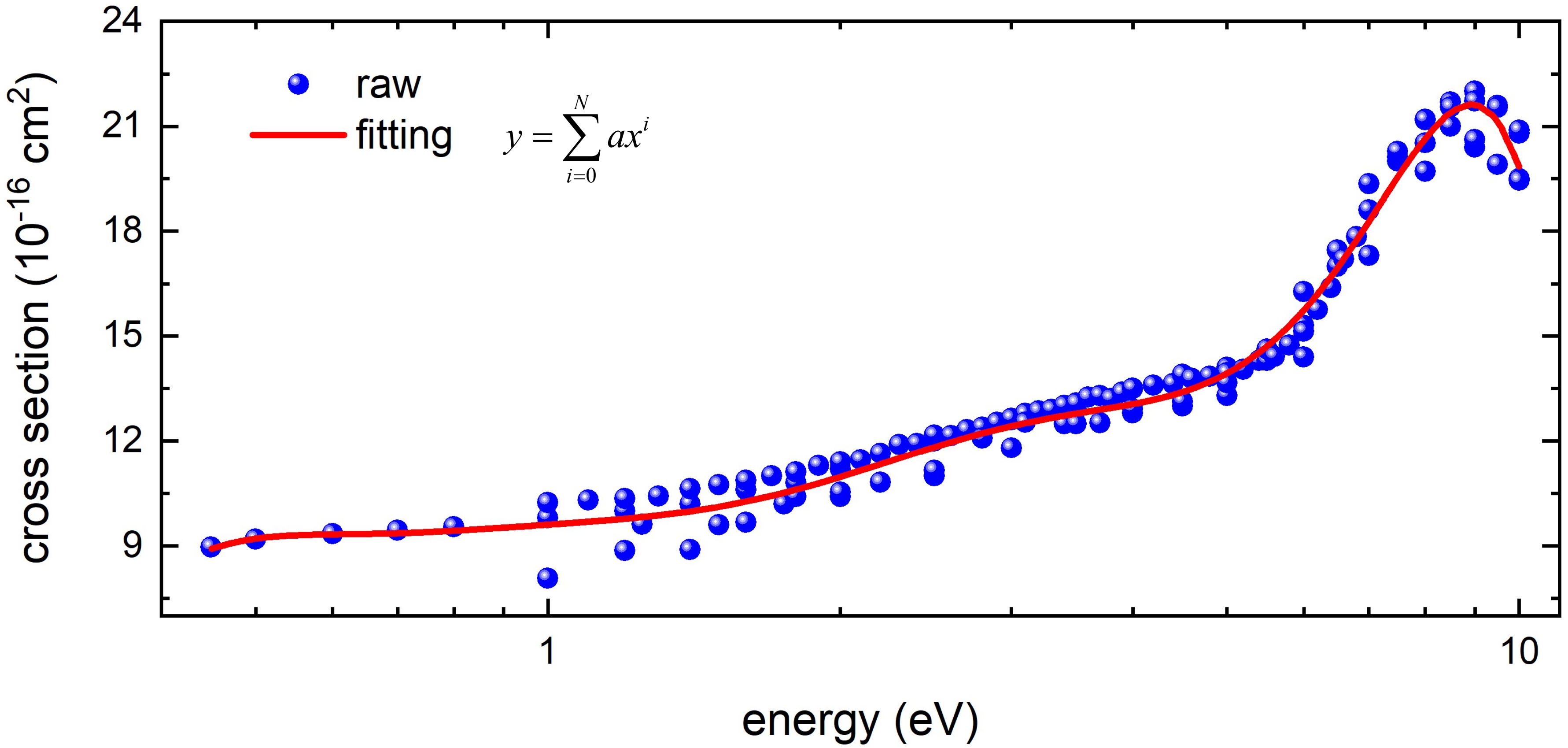
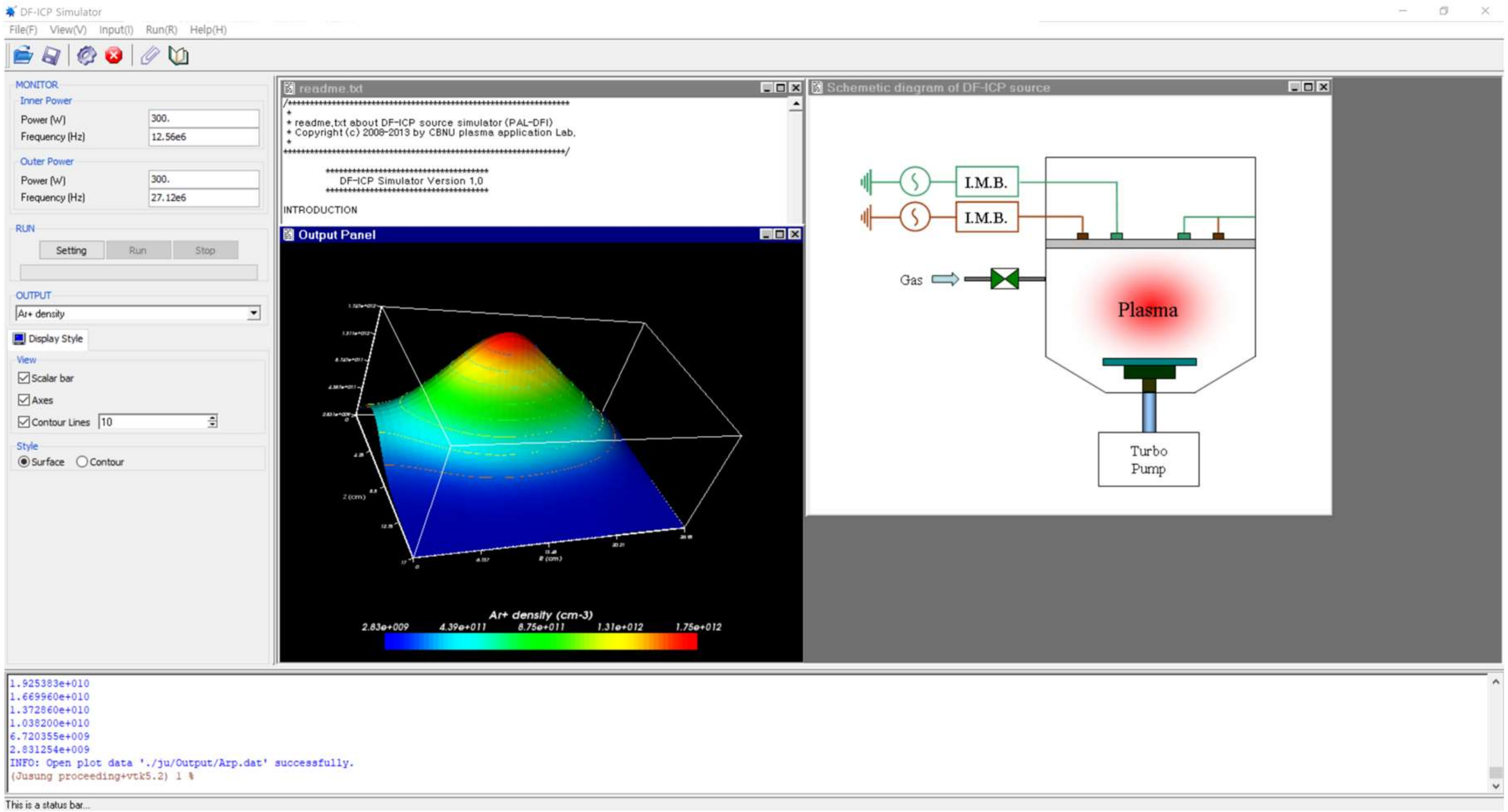
1. Introduction

Motivation & Need for development



1. Introduction

Motivation & Need for development

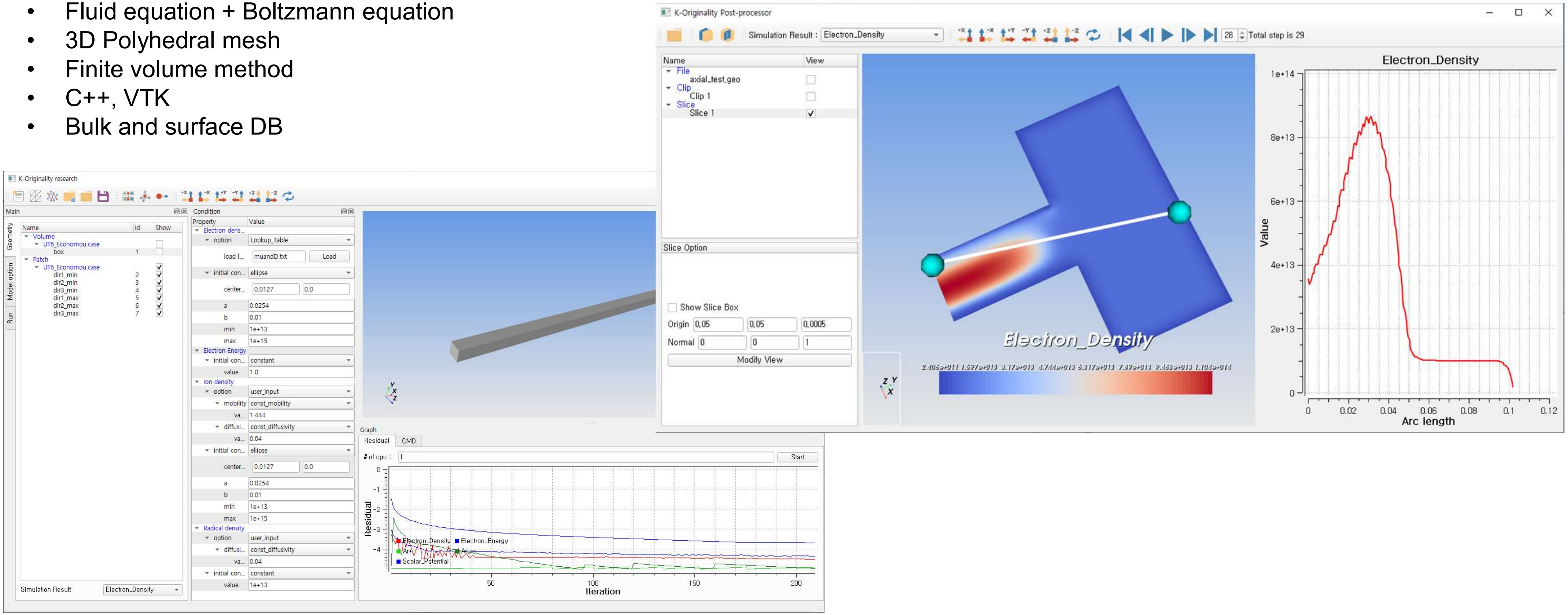


- Language : C, Tcl/TK, VTK
- Source : TCP/ICP
- Model :
  - Fluid model
  - Non-local heating model
  - Cylindrical 2D geometry
  - Ar plasma

1. Introduction

Developed 3D simulator

- Fluid equation + Boltzmann equation
- 3D Polyhedral mesh
- Finite volume method
- C++, VTK
- Bulk and surface DB



2

Plasma Modeling

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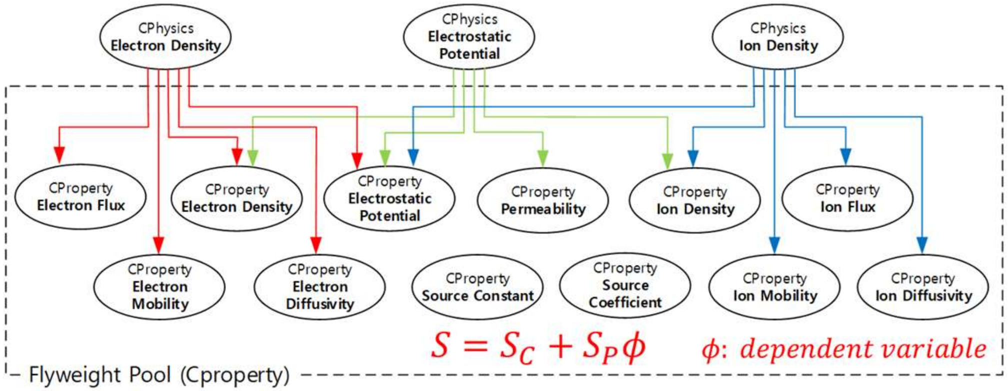
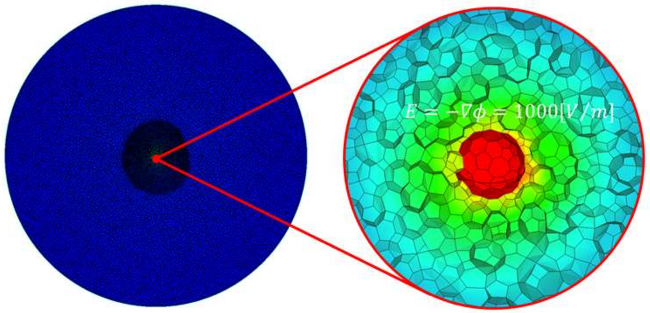
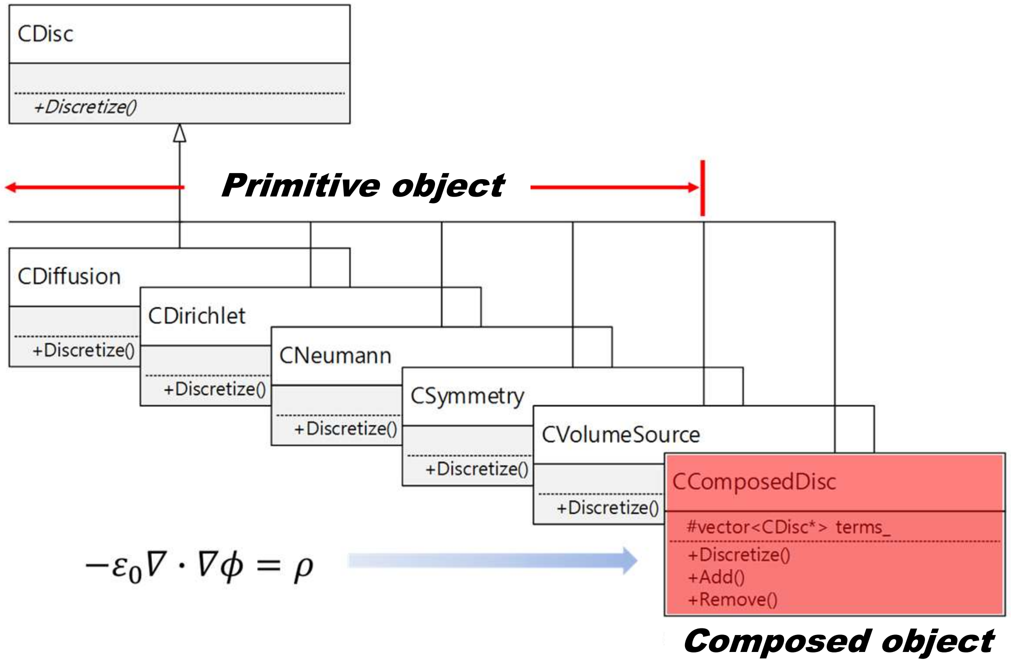
2. Plasma Modeling

Flyweight pool and composite pattern





$E = -\nabla\phi = 0.0998\ [V/m]$

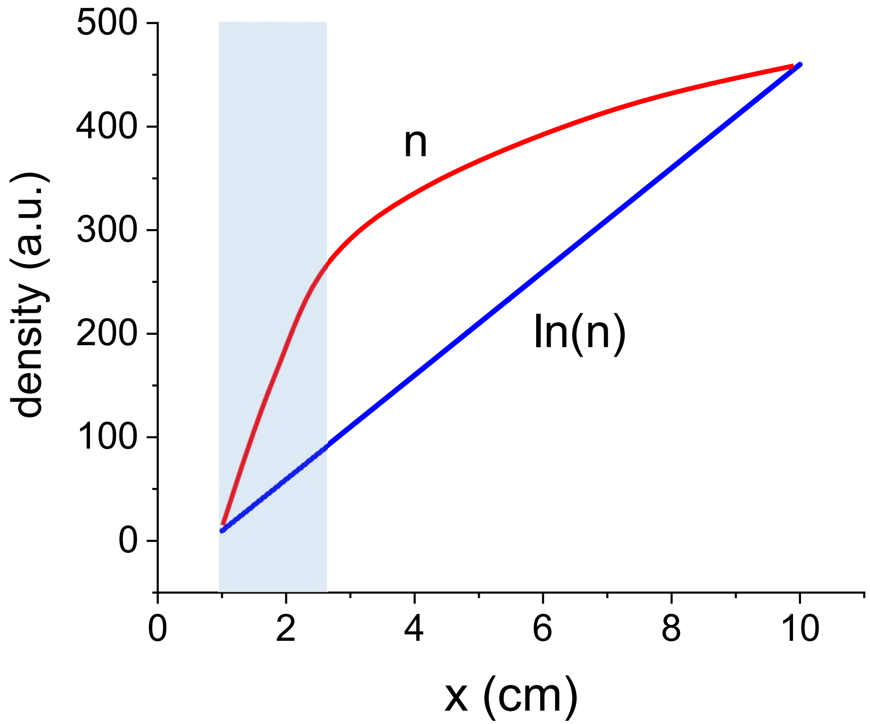


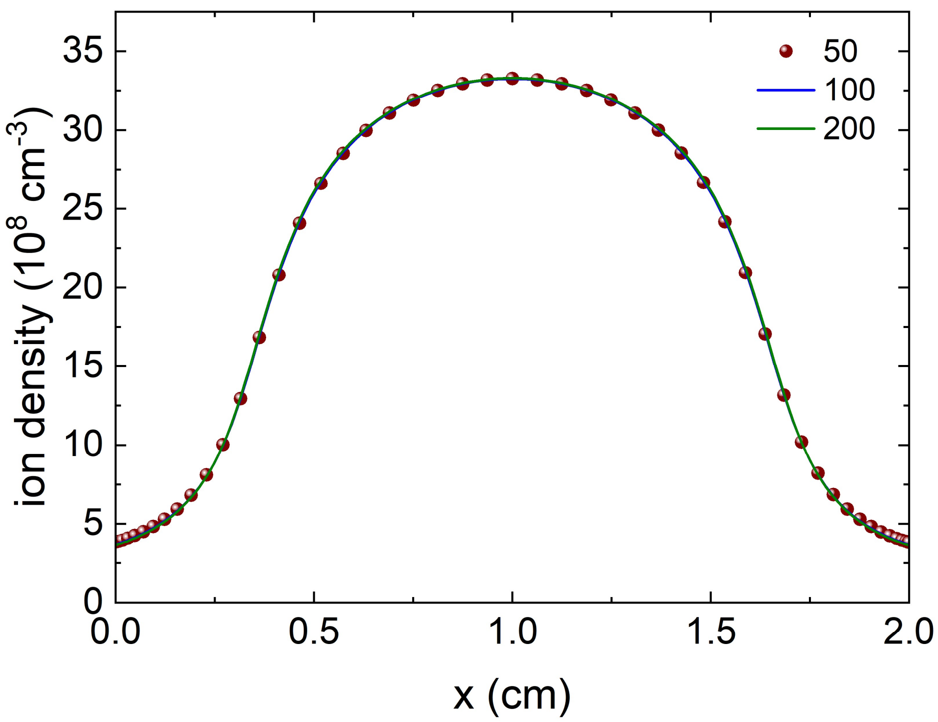
2. Plasma Modeling

Log transformation

- Improves linearity between independent and dependent variables
- CCP 1D discharge → reduce grid dependence of results

$$\frac{\partial n_e}{\partial t} = \frac{n_e}{n_e}\frac{\partial n_e}{\partial t} = n_e \frac{\partial(\ln n_e)}{\partial t} = n_e \frac{\partial N_e}{\partial t}$$

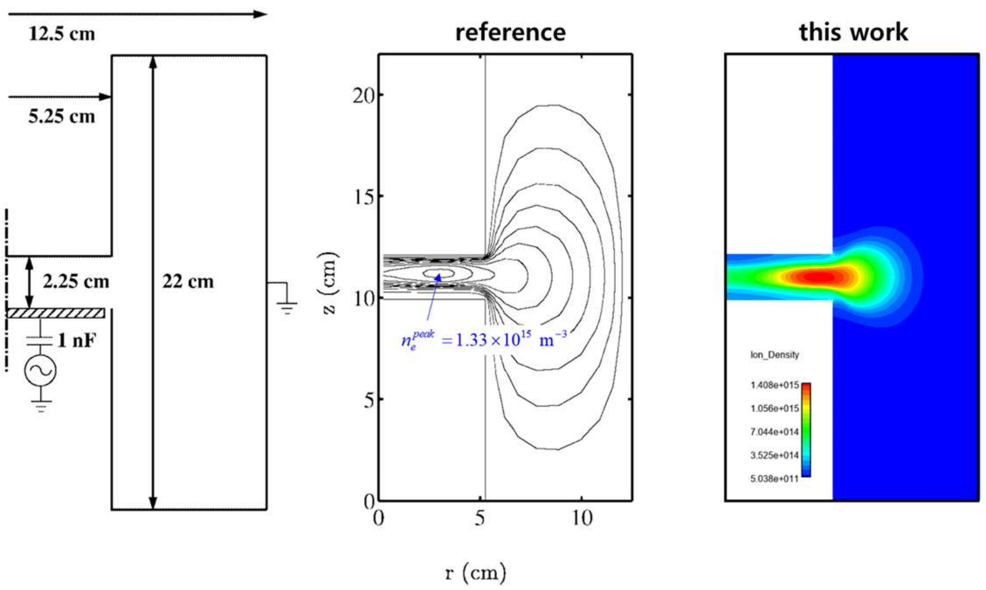


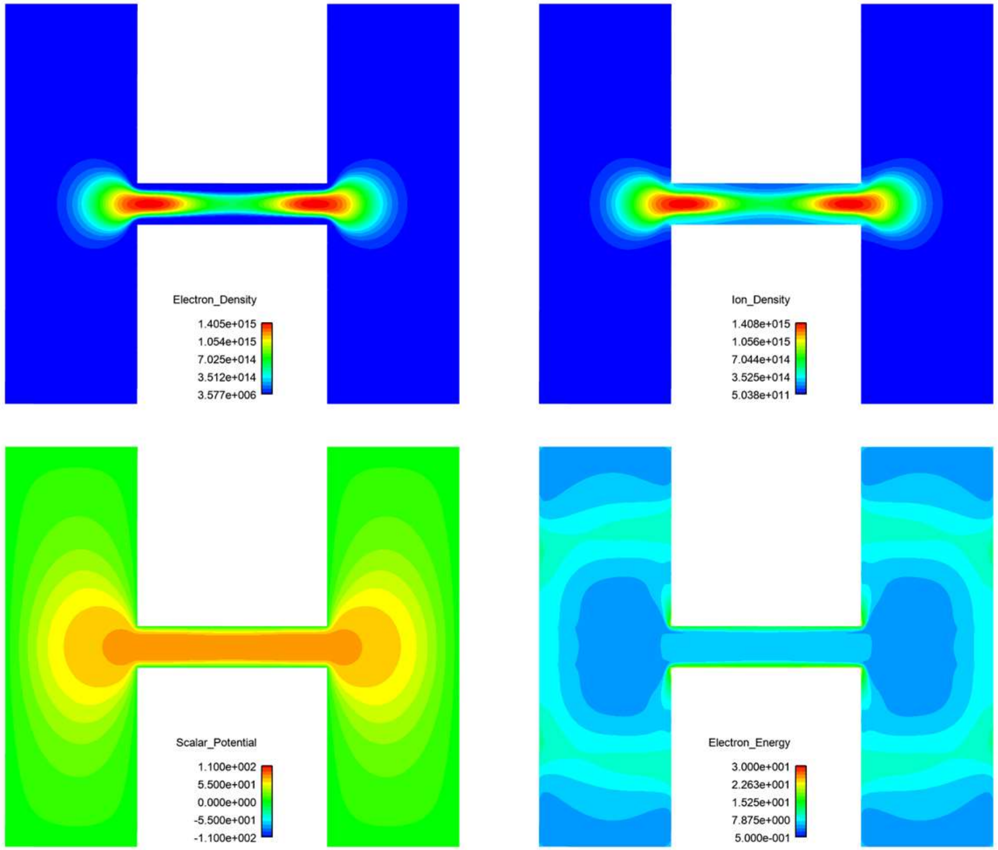


COMSOL Multiphysics Plasma module user's guide 5.2a

2. Plasma Modeling

K-PLASMA unit test



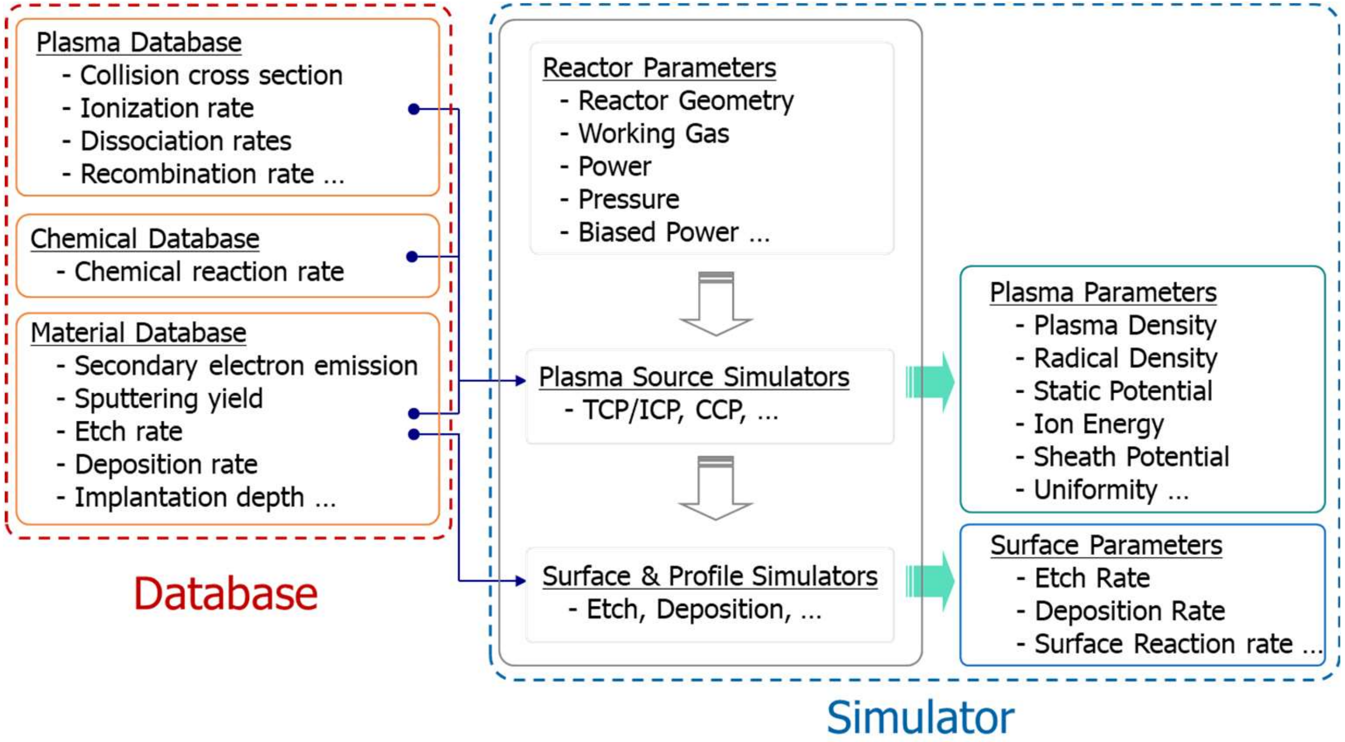


Hammond et al, J. Comp. Phys. **176**, 402 (2002)

2. Plasma Modeling

Database development

- Bulk and surface chemistry data base (DB) **are necessarily required** to compute the plasma parameters.
- **High reliable DB is closely related with accuracy enhancement of simulations.**



2. Plasma Modeling

Database development

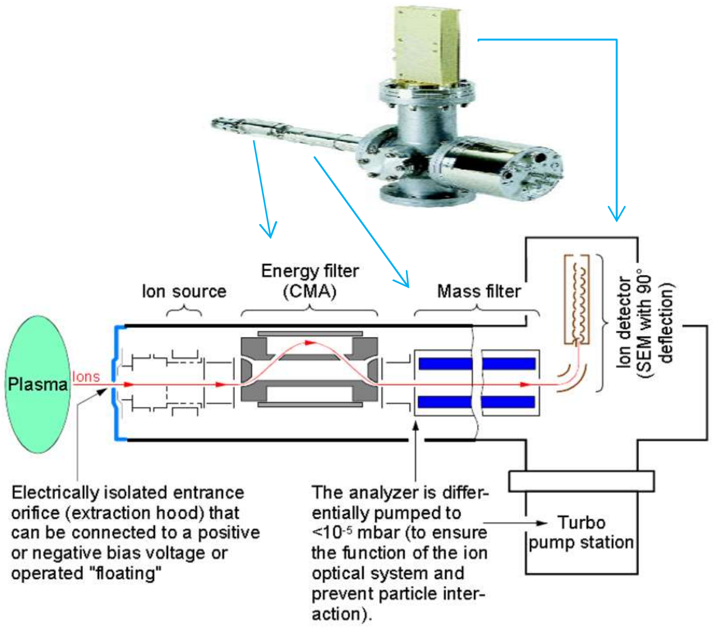
Software	Key DB
CFD-ACE+	Ar, $SiH_4/O_2/Ar$, NF_3/Ar, C_2F_6/O_2, CF_4, Cl_2, He, Ne, N_2, O_2, Xe, SF_6/O_2
COMSOL	Ar, He, Hg, O_2
VizGlow	Ar, He, Xe, H_2, N_2, O_2, Ar/O_2, $Ar/O_2/H_2$, CF_4, C_2F_6, C_4F_8, CHF_3, $CF_4/O_2/He$, C_2H_2/Ar, HBr, SiH_4/N_2, NF_3, $NH_3/N_2/H_2/Ar$, NF_3, NF_3/O_2, SF_6/O_2, BF_3/Ar
QuantemolDB	N_2/H_2, Ar/H_2, O_2/H_2, SF_6/O_2, CF_4/O_2, CF_4, $CF_4/O_2/H_2/N_2$, C_4F_8, SiH_4, SiH_4/NF_3, Ar/O_2, $Ar/O_2/C_4F_8$, $SiH_4/Ar/O_2$, Ar/Cu, $Cl_2/O_2/Ar$, $Ar/BCl_3/Cl_2$, Ar/NF_3, CH_4/H_2, C_2H_2/H_2, CH_4/NF_3, H_2/O_2, $CF_4/CHF_3/H_2/Cl_2/O_2/HBr$, $SF_6/CF_4/O_2$, Ar/Cu/He, Ar/NF_3, $SF_6/CF_4/N_2/H_2$
K-SPEED	$C_{x1}F_{y1}/C_{x2}F_{y2}/CH_xF_y/O_2/Ar$, NF_3/Ar, $SiH_4/O_2/Ar$

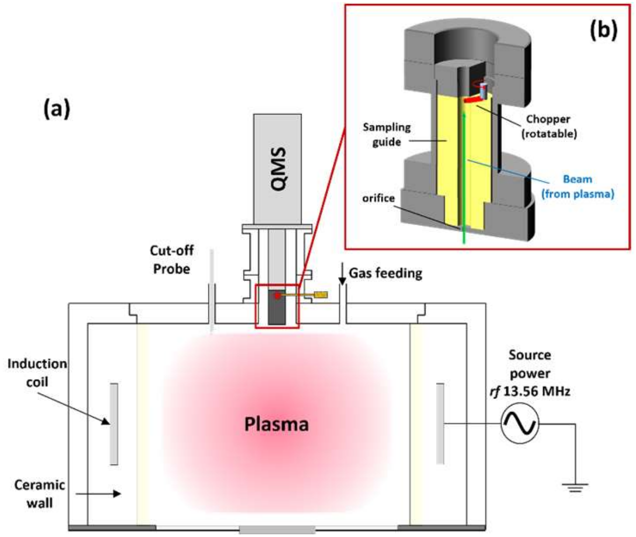
https://www.quantemoldb.com/chemistries/all-chemistries, http://esgeetech.com *This information may have been updated

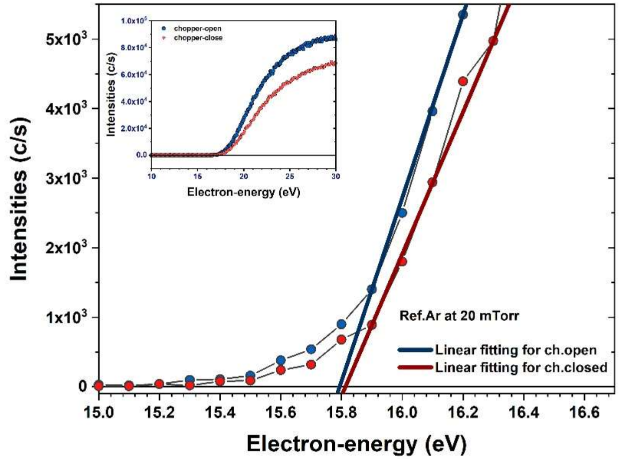
2. Plasma Modeling

Database development

- APMS (appearance potential mass spectrometry) method and the microwave cut-off probe
- Reducing the back-ground noise inside the QMS by using a chopper (W. S. Chang et al, **to be published**)







Singh et al, J. Vac. Sci. Technol. A **18**, 299 (2000)

2. Plasma Modeling

Global model

$$\frac{\partial n_i}{\partial t} = \sum_j R_{g,j} + \frac{Q_i}{\Omega} - \sum_j R_{l,j} - n_i\left(\frac{V_{pump}}{\Omega} + \nu_l^i\right)$$

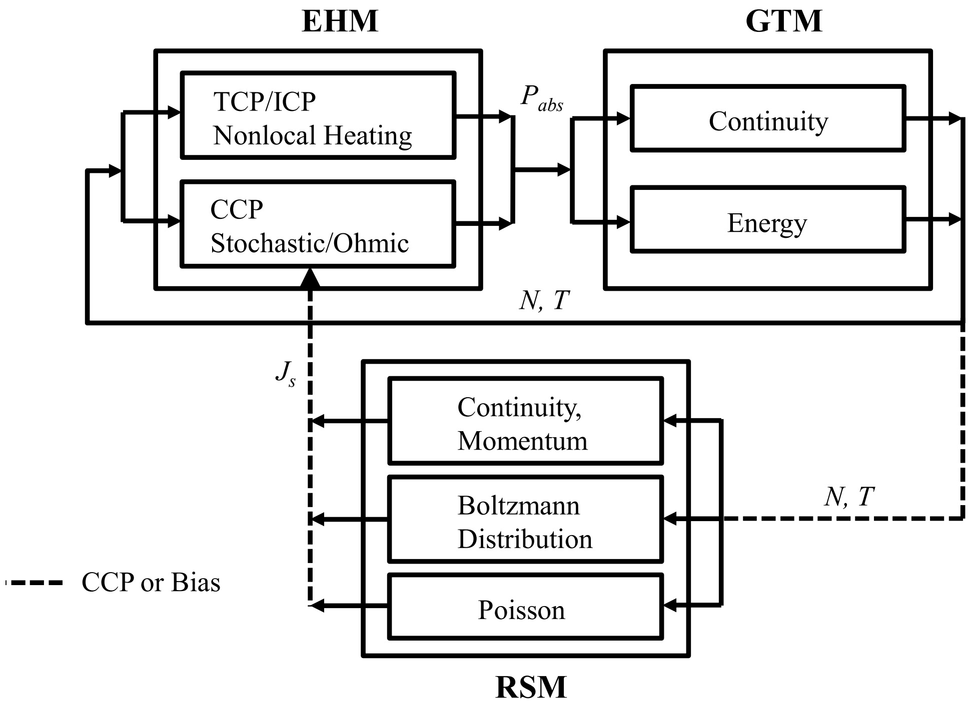
$$\frac{\partial}{\partial t}\left(Nc_pT_g\right) = \sum_i 3n_e\nu_m\left(\frac{m_e}{m_i}\right)k_B\left(T_e - T_g\right) + \sum_j n_e k_j n_j \Delta E_j - \sum_j \Delta H_j - \frac{h_{tc}A}{\Omega}\left(T_g - T_w\right)$$

When the EEDF is given,

$$\frac{\partial}{\partial t}\left(\frac{3}{2}n_eT_e\right) = \frac{P_{abs}}{\Omega} - E_e - n_e\varepsilon_l^e\nu_l^e$$

When the EEDF is solved in a self-consistent manner,

$$T_e = \frac{2}{3}\langle\varepsilon\rangle = \frac{2}{3n_e}\int_0^\infty \varepsilon^{3/2} f_0(\varepsilon)\,d\varepsilon$$



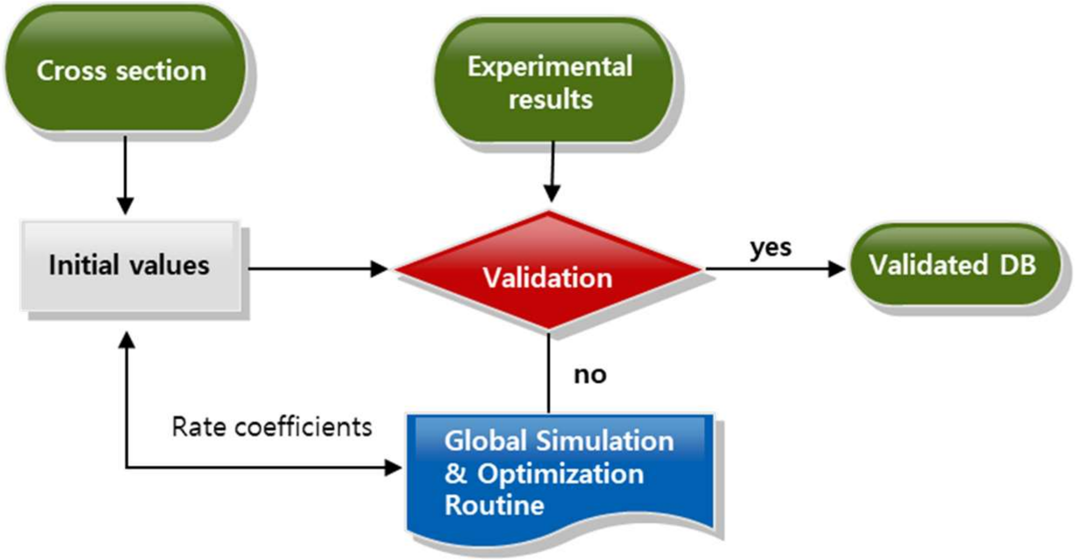
$$k = \int_0^\infty f_0(\varepsilon)\sigma(\varepsilon)\upsilon\,d\varepsilon,\ R = k\times\prod_j n_{r,j},\ \nu_l^i = \frac{A_{eff}}{\Omega}\sqrt{\frac{k_BT_e(1+\alpha_s)}{m_i(1+\alpha_s\gamma_-)}},\ A_{eff} = 2\pi\left(R_p^2h_L + R_pL_ph_R\right)$$

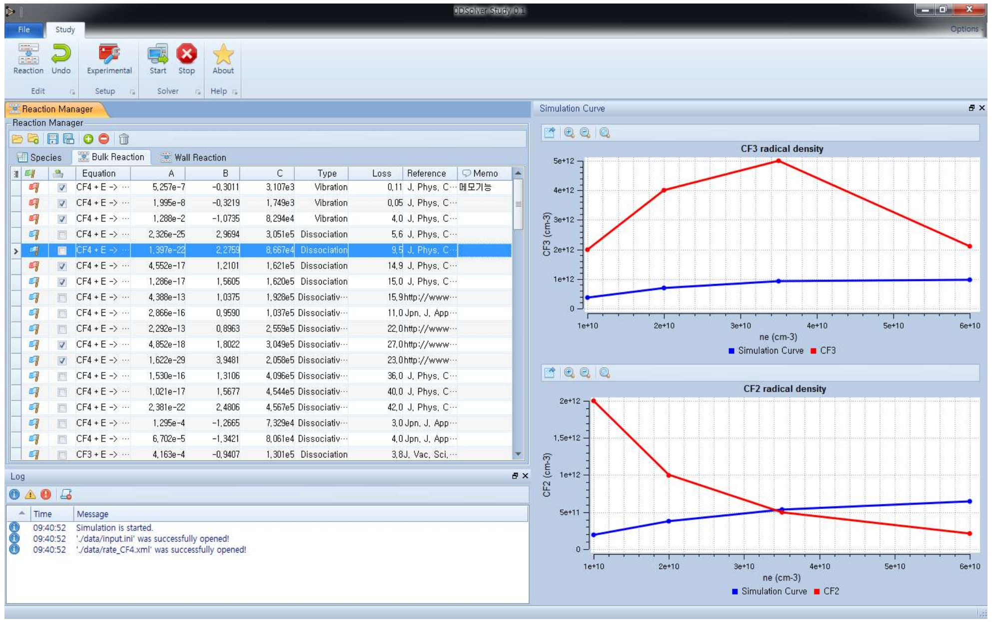
D. C. Kwon et al, J. Appl. Phys. **109**, 073311 (2011), S. S. Kim et al, J. Korean Phys. Soc. **52**, 300 (2008)

2. Plasma Modeling

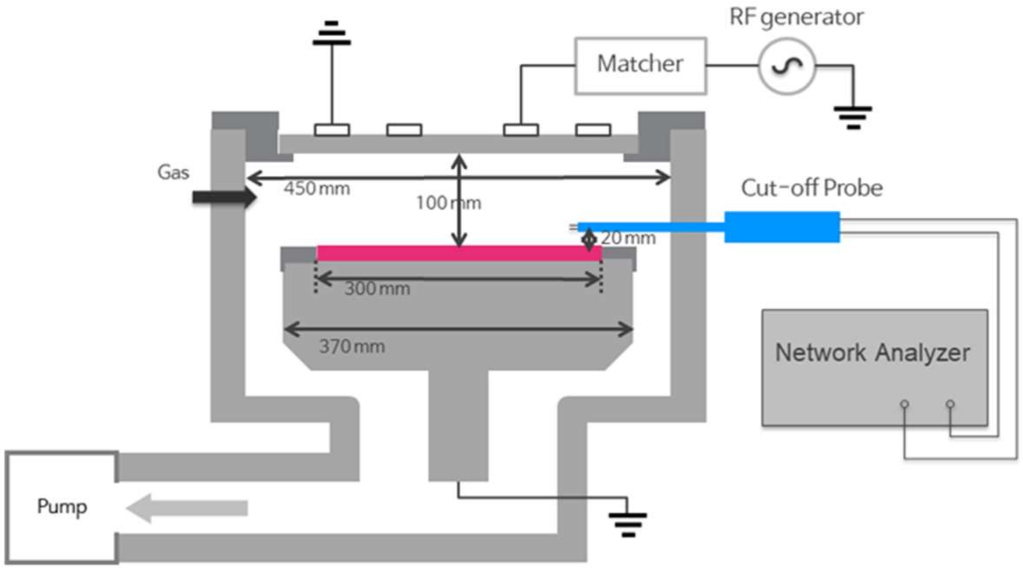
Global model

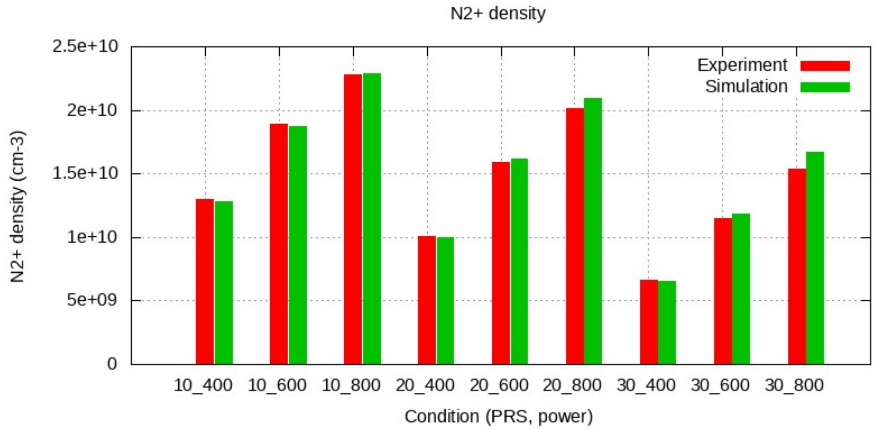
- Optimized the rate coefficients for heavy particle reactions excluding electron collisions.
- Numerical optimization (Random sampling, Newton, Secan, Broyden-Fletcher-Goldfarb-Shanno, etc.)

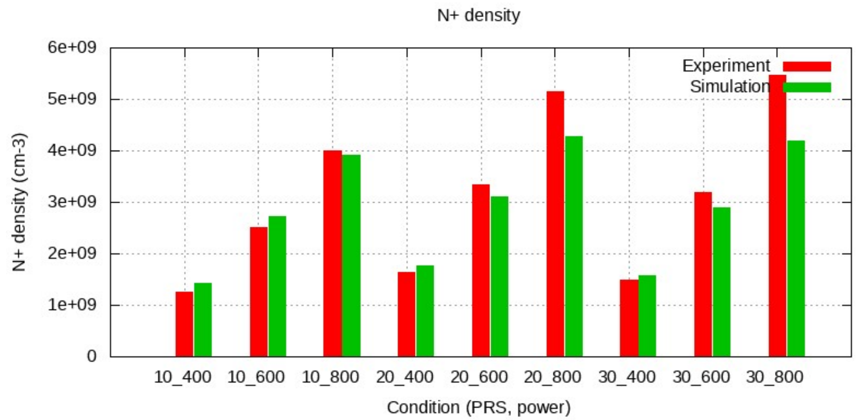




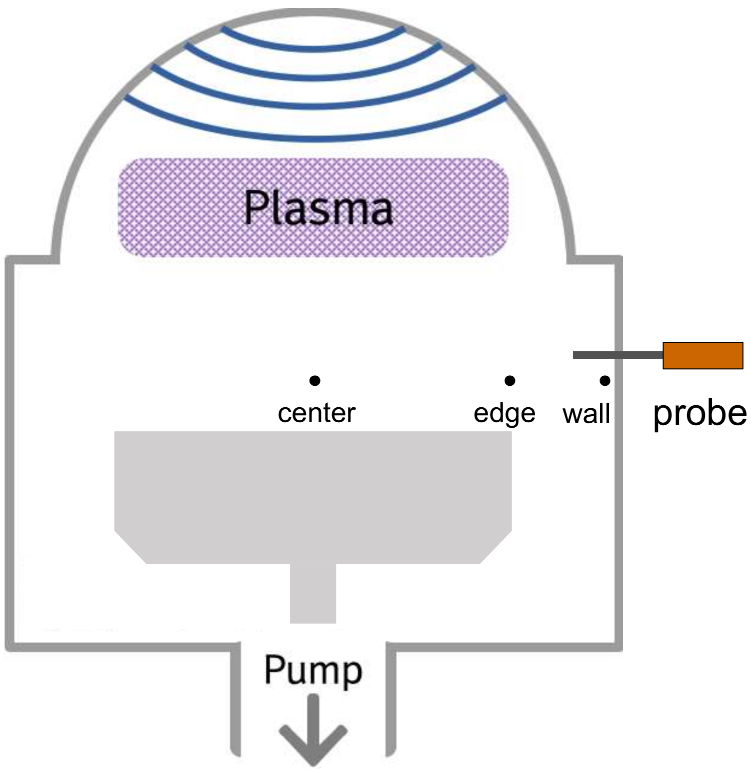
Global model @ N_2 discharges

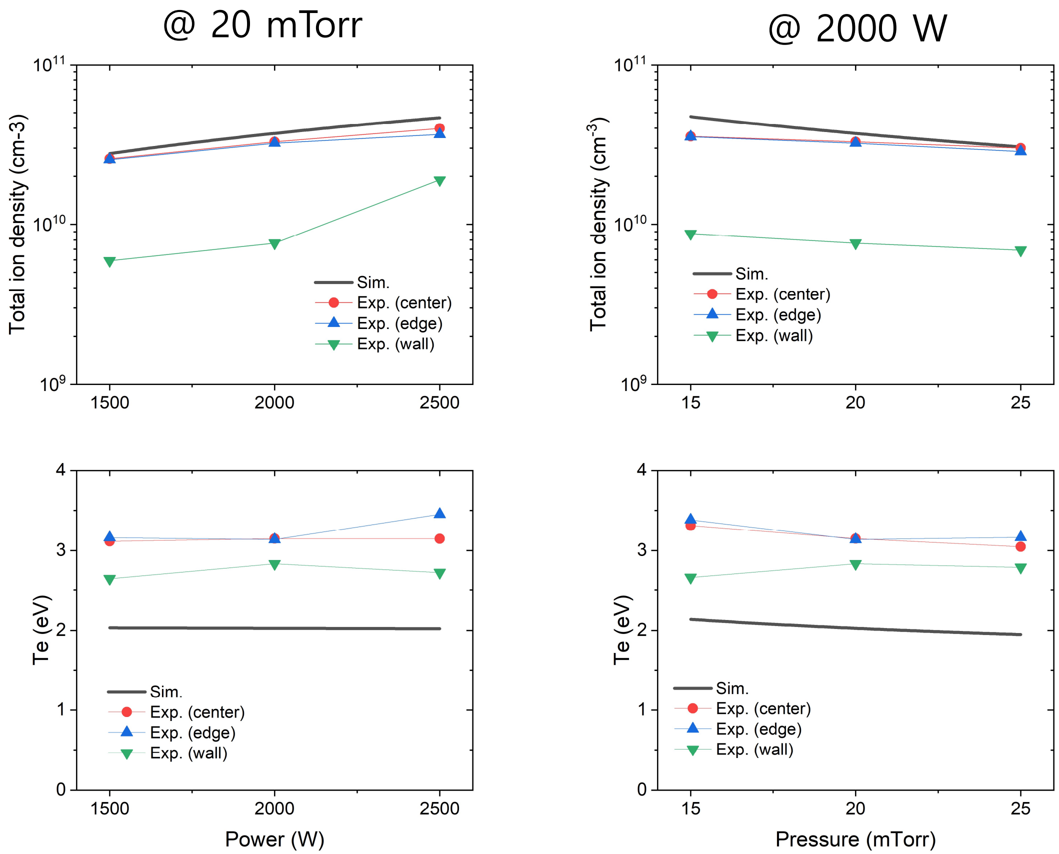






Global model @ commercial source

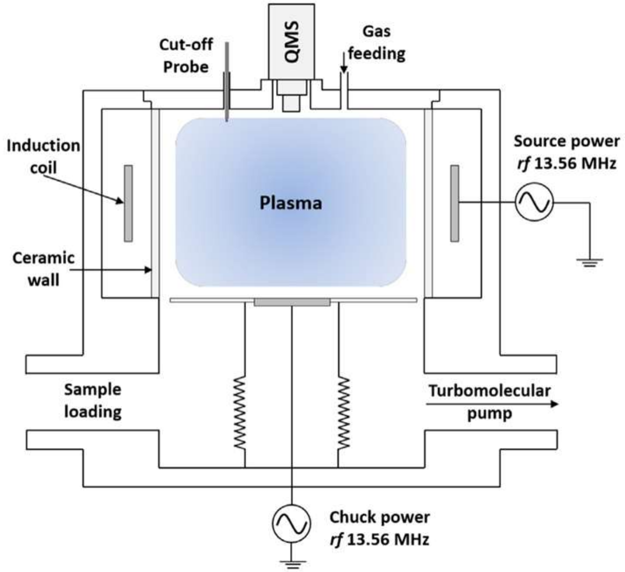


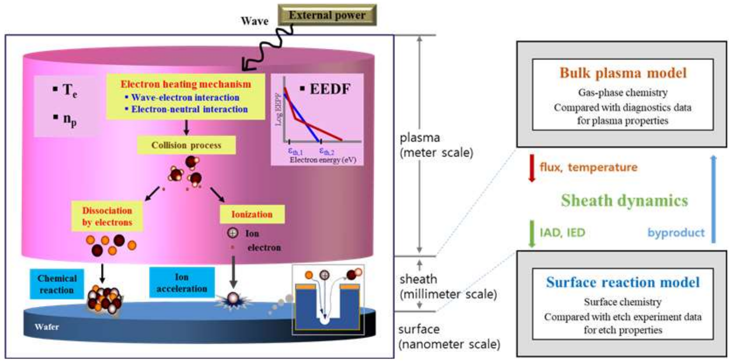


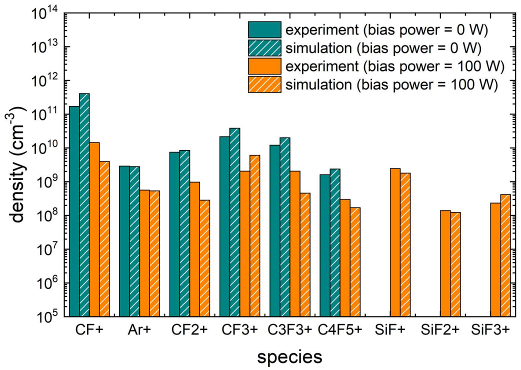
2. Plasma Modeling

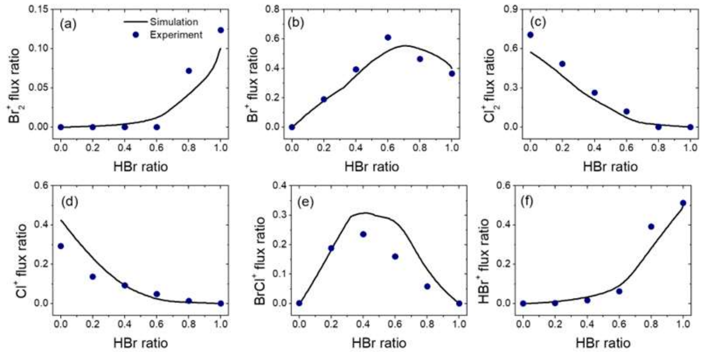
Global model

6 inch oxide wafer

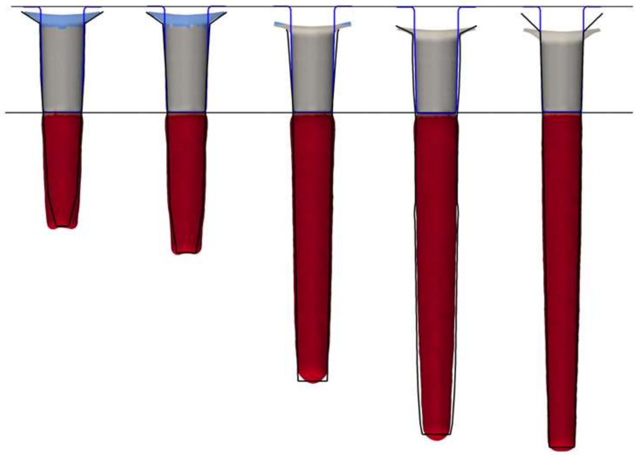






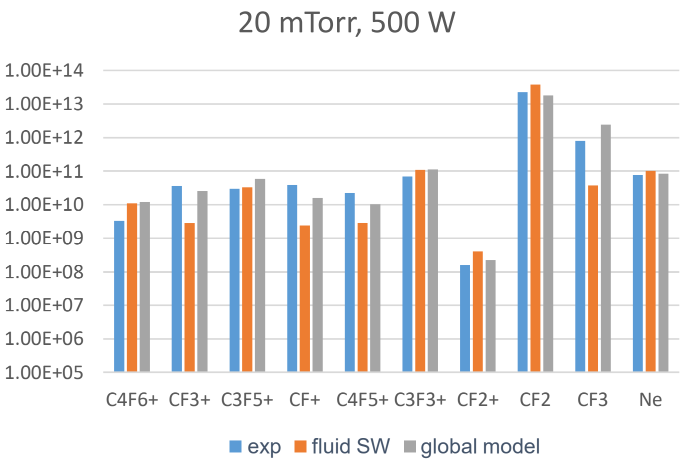


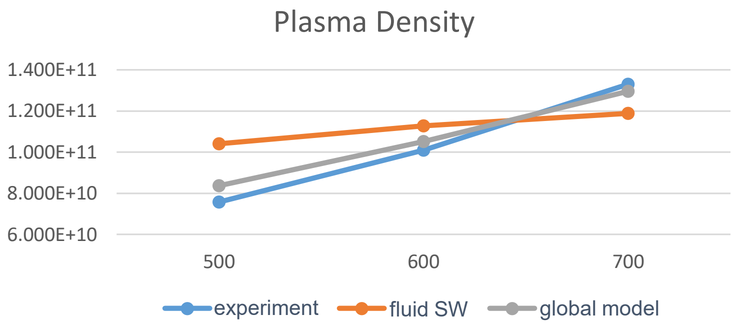
Cl2	0	10	20	30	40
HBr	40	30	20	10	0

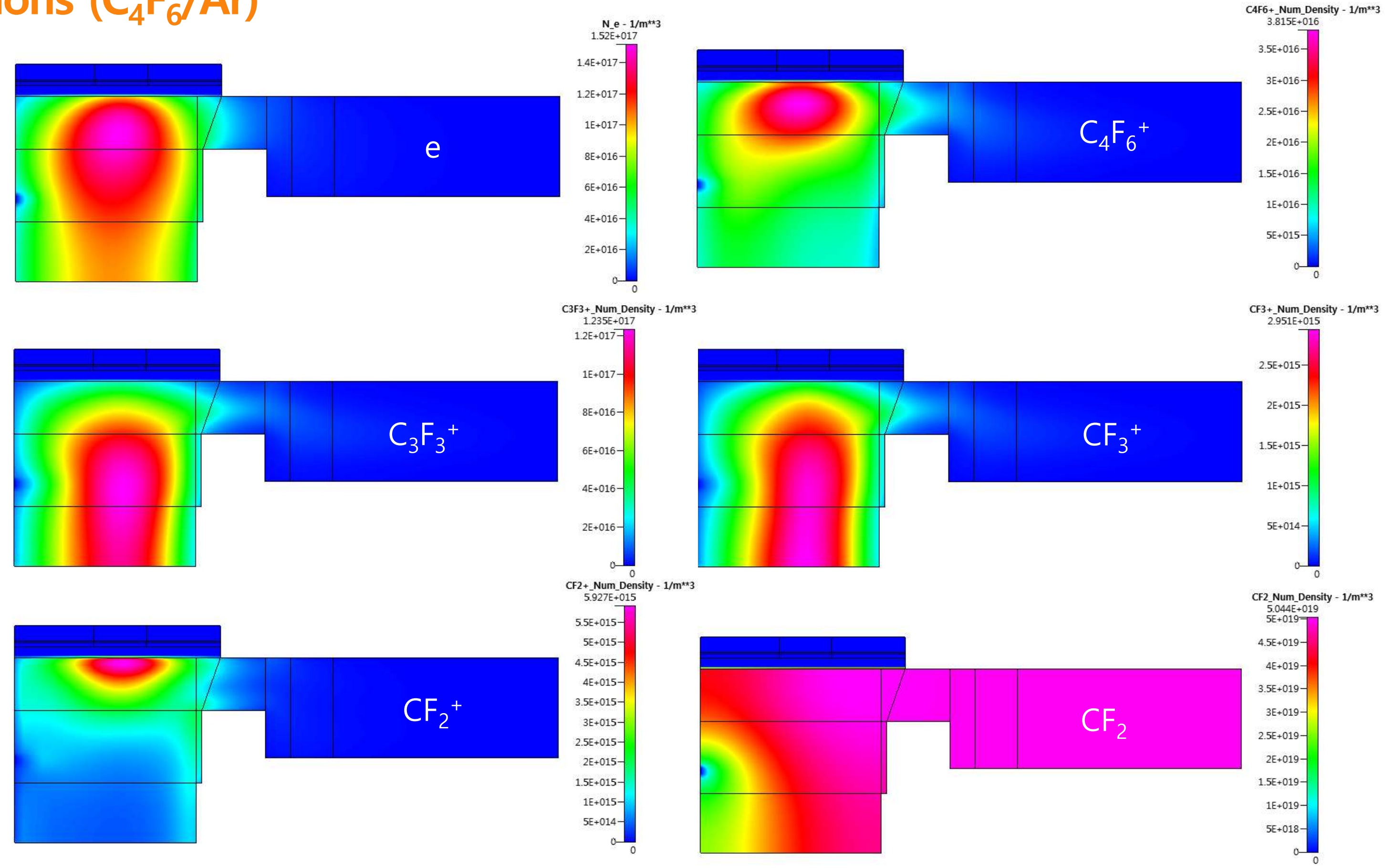


S. Y. Chung et al. (**KISM2022, Busan**), Y. G. Yook et al. (**KISM2022, Busan**)

Comparison with 2D simulations (C_4F_6/Ar)







Developed bulk databae

Gas	DB	experiment	validated
C_4F_6/Ar	O	O	O
C_4F_6/Cl_2/Ar	O	O	O
C_4F_8/Ar	O	O	O
C_4F_6/C_4F_8/Ar	O	O	O
C_4F_6/O_2/Ar	O	O	O
C_4F_6/C_4F_8/O_2	O	O	O
C_4F_6/C_4F_8/CH_2F_2/O_2	O	O	O
C_4F_6/C_4F_8/CH_2F_2/O_2/Ar	O	O	O
C_4F_6/C_4F_8/CH_2F_2/Ar	O	O	O
C_4F_6/C_4F_8/CHF_3/Ar	O	O	O
C_4F_6/C_4F_8/CH_3F/Ar	O	O	O
C_4F_6/C_4F_8/C_3F_8/Ar	O	O	O
CHF_3/Ar	△	X	△
C_2HF_5/Ar	O	O	O
CH_2F_2/Ar	O	O	O
SiH_4/Ar	O	O	O
SiH_4/NH_3/Ar	O	O	O

Gas	DB	experiment	validated
N_2	O	O	O
Ar	O	O	O
CF_4/O_2	O	△	O
CF_4/Cl_2	△	X	△
PF_3	△	X	△
SF_6	△	X	△
WF_6	△	X	△
Kr	△	X	△
Xe	△	X	△
CBr_2F_2	△	X	△
NF_3/O_2/Ar	O	O	O
HBr/Cl_2	O	△	O
C_4F_8/CHF_3/Kr	O	O	O
C_4F_8/CH_2F_2/O_2/Xe	O	O	O
C_4F_8/CH_2F_2/O_2/Ar(Kr)	O	O	X
SiH_4/H_2/Ar	O	O	X
Etc	△	△	△

3

ML-aided Modeling

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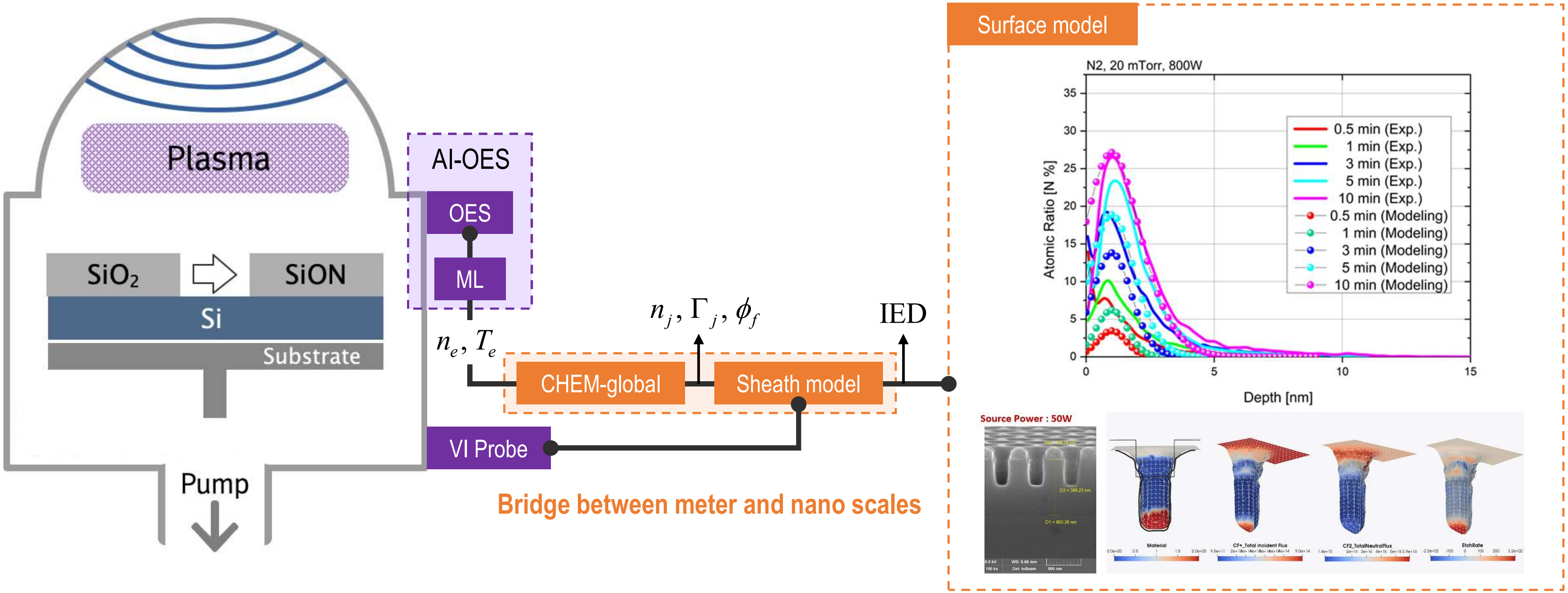
3. ML-aided Modeling

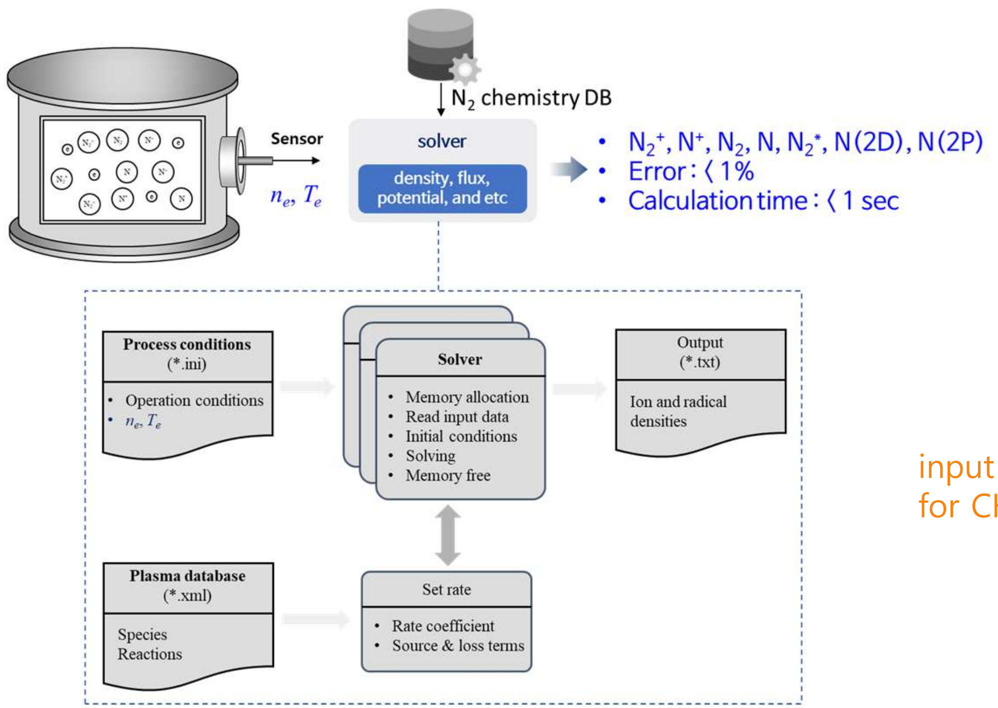
Sensor-bulk-surface coupling model



3. ML-aided Modeling

CHEM-global (chemical reaction analyzer using a global model)

- Quasi-neutrality
  - Assuming the quasi-neutrality, the continuity equation is solved using the electron density and temperature.



@ N_2 80 SCCM, 15 mTorr, 500 W

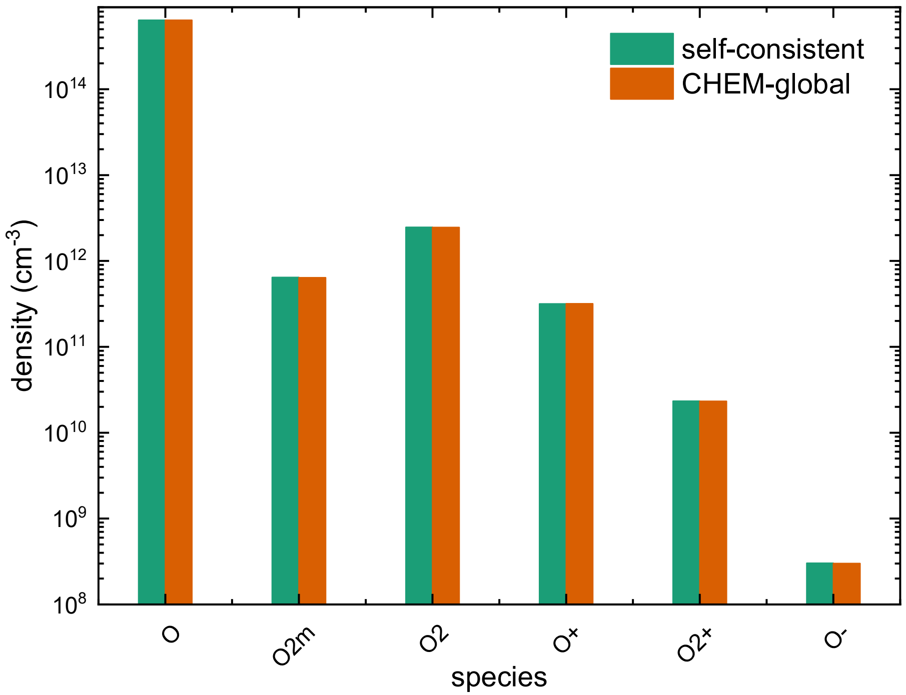
species	Self-consistent	CHEM-global
N	1.5166×10^{13} cm^{-3}	1.5164×10^{13} cm^{-3}
N_2^*	7.3827×10^{12} cm^{-3}	7.3815×10^{12} cm^{-3}
N_2	4.6440×10^{14} cm^{-3}	4.6432×10^{14} cm^{-3}
N(2P)	6.9623×10^{11} cm^{-3}	6.9603×10^{11} cm^{-3}
N(2D)	1.3143×10^{12} cm^{-3}	1.3141×10^{12} cm^{-3}
N_2^+	6.0594×10^{10} cm^{-3}	6.0595×10^{10} cm^{-3}
N^+	2.4852×10^{9} cm^{-3}	2.4850×10^{9} cm^{-3}
e	6.3080×10^{10} cm^{-3}	
T_e	2.9531 eV	
Calculation time	161 sec	0.001 sec

input parameters for CHEM-global

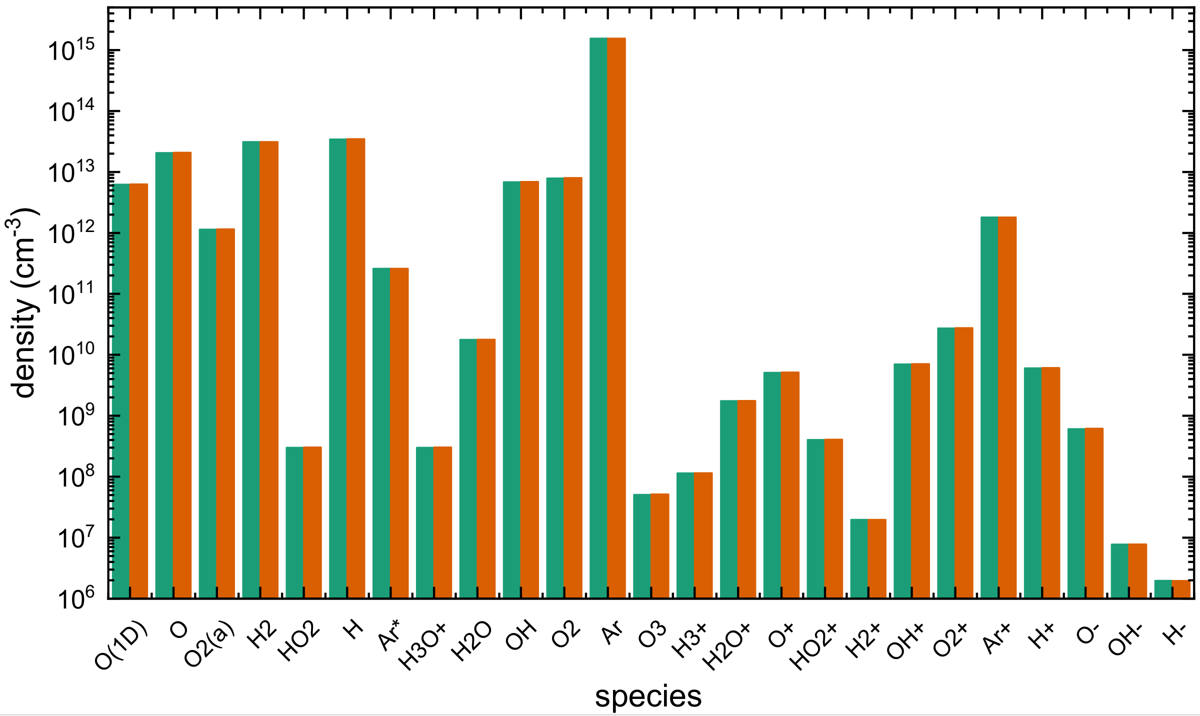
3. ML-aided Modeling

CHEM-global

- O_2 plasma
  - 7 species and 25 reactions
  - O_2 80 SCCM, 10 mTorr, 500 W → 0.5% mean error

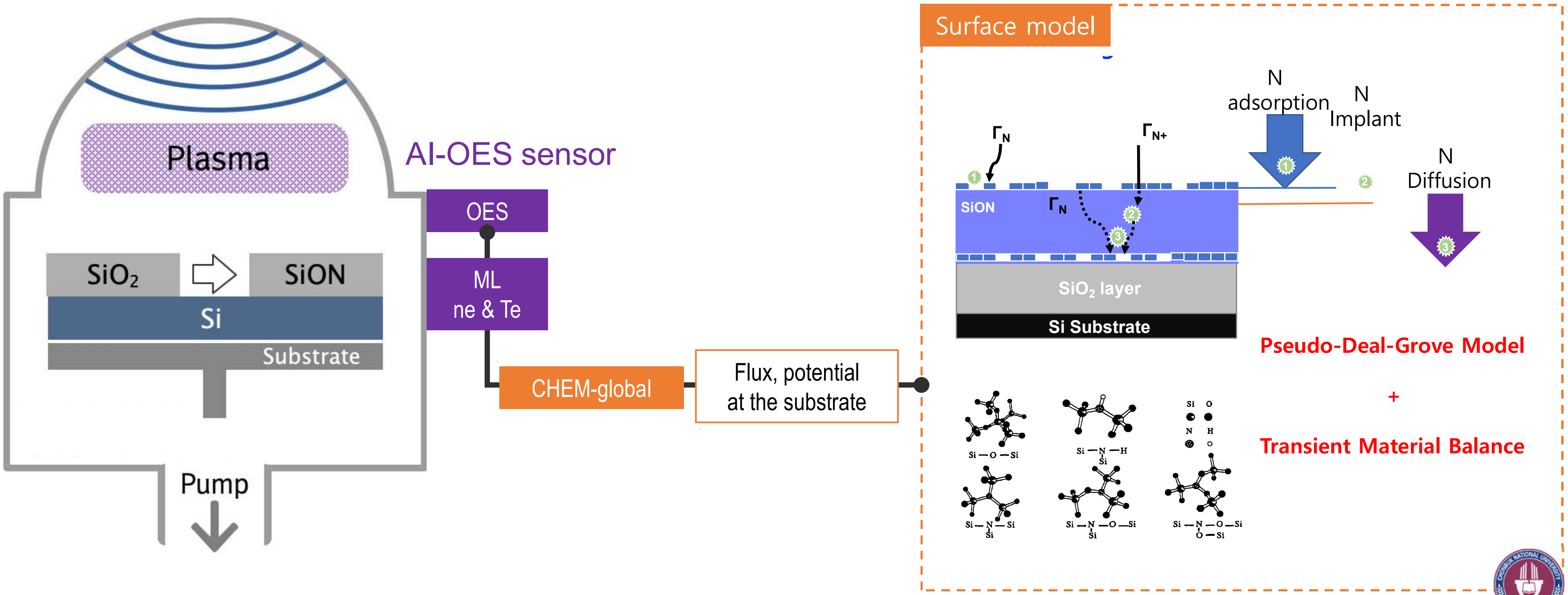


- H_2O/Ar plasma
  - 26 species and 153 reactions
  - H_2O 1 SCCM, Ar 30 SCCM, 50 mTorr, 1500 W → 0.8% mean error



3. ML-aided Modeling

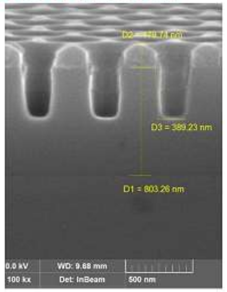
Bulk-surface coupling model

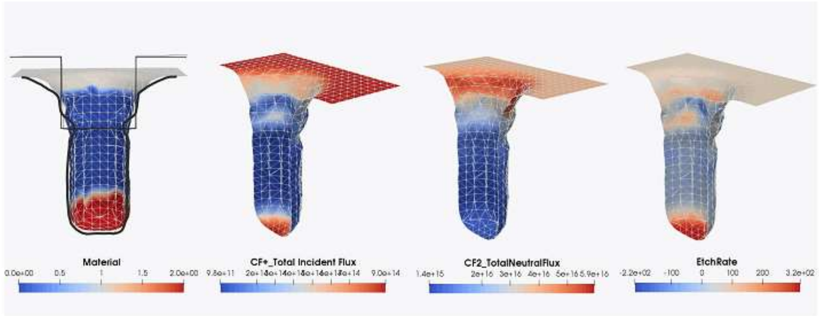


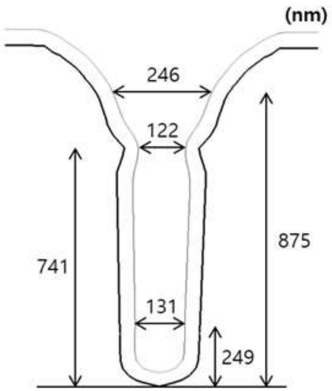
3. ML-aided Modeling

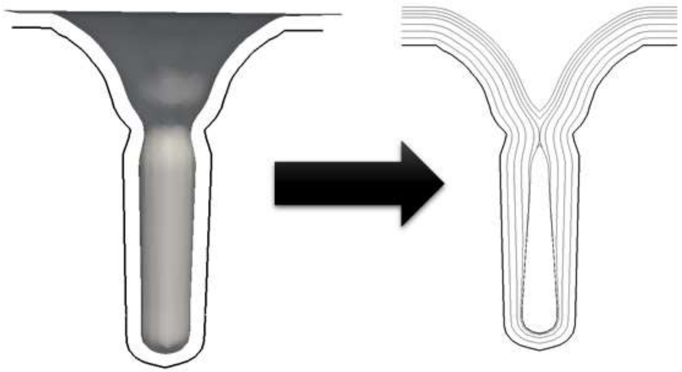
Bulk-surface coupling model

Source Power : 50W

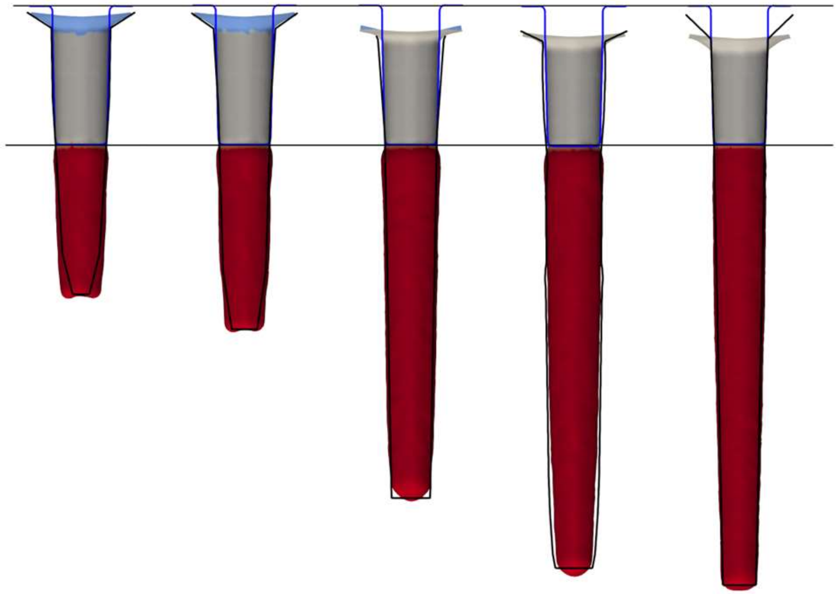






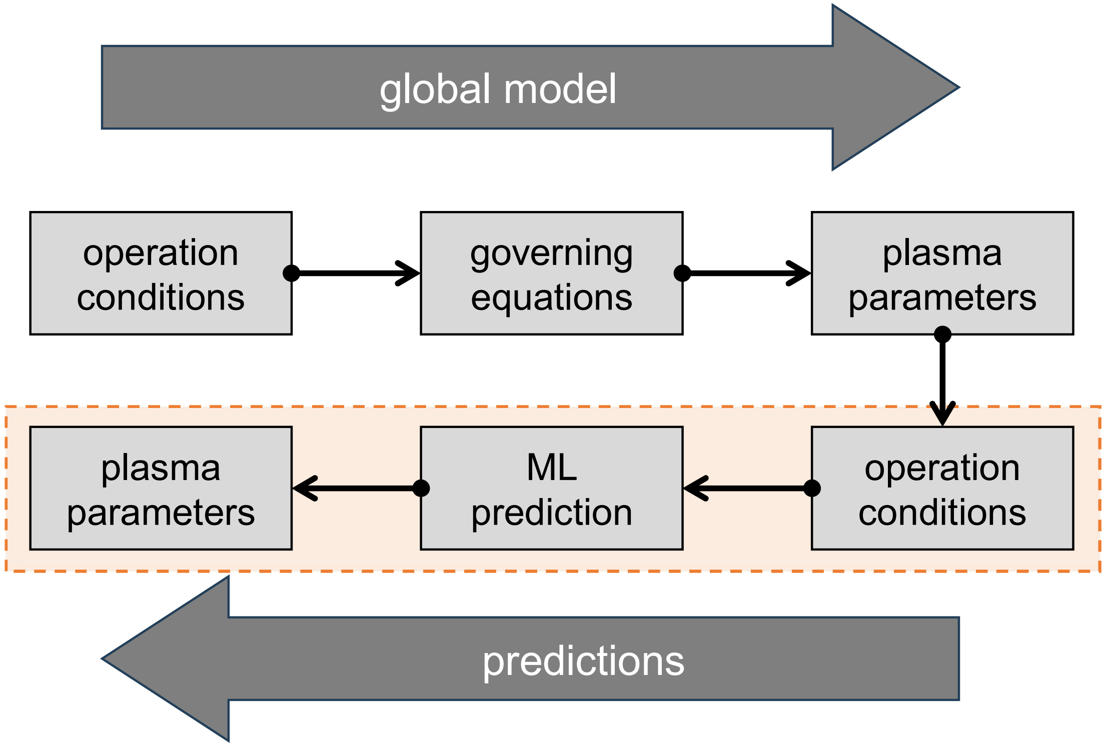


Cl2	0	10	20	30	40
HBr	40	30	20	10	0

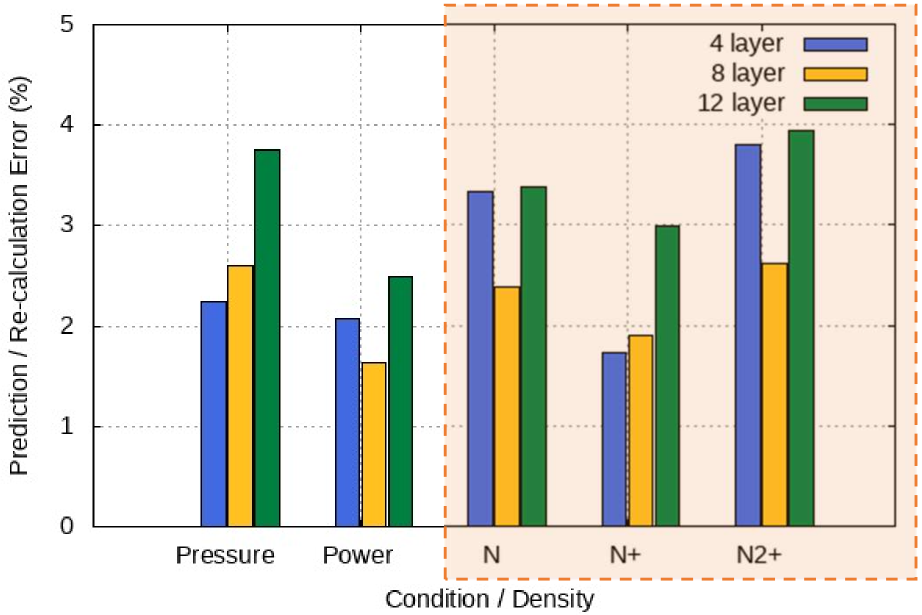


3. ML-aided Modeling

Global model + Machine learning

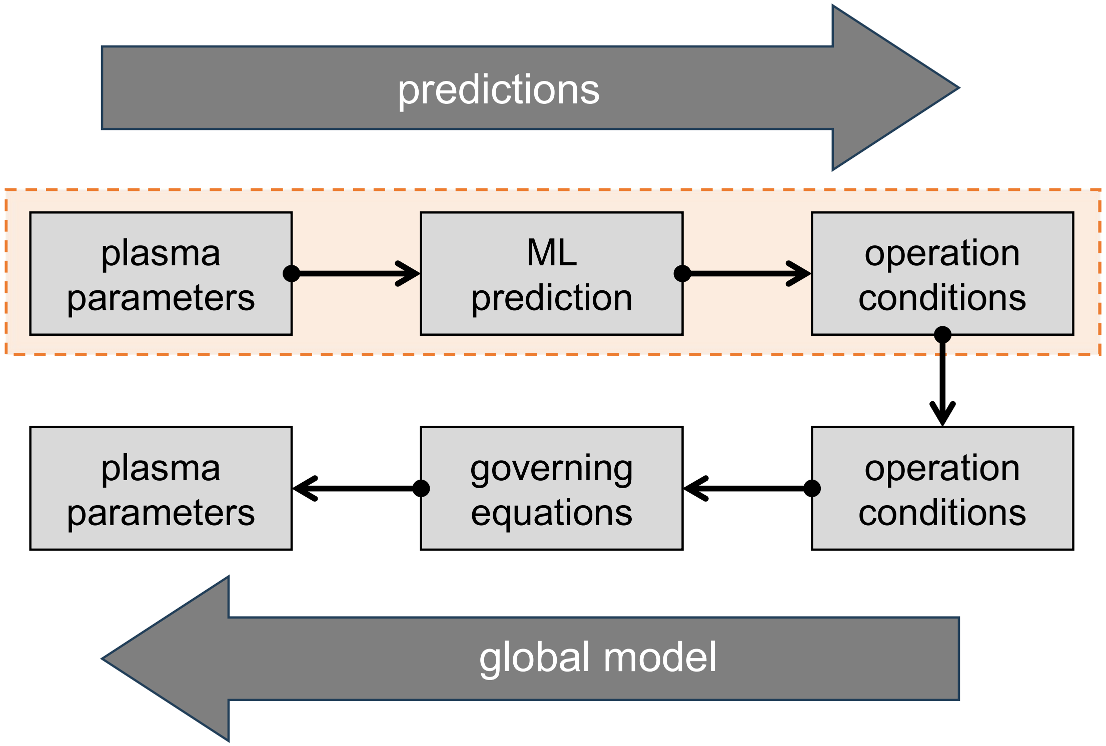


- Training plasma parameters on operations → prediction of plasma parameters
- Accuracy is not always proportional to the number of hidden layers

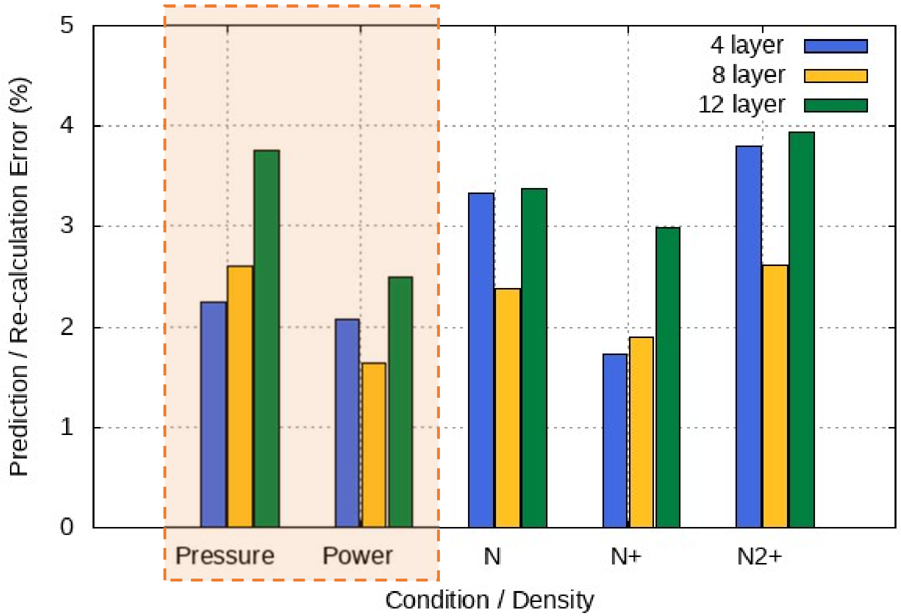


3. ML-aided Modeling

Global model + Machine learning



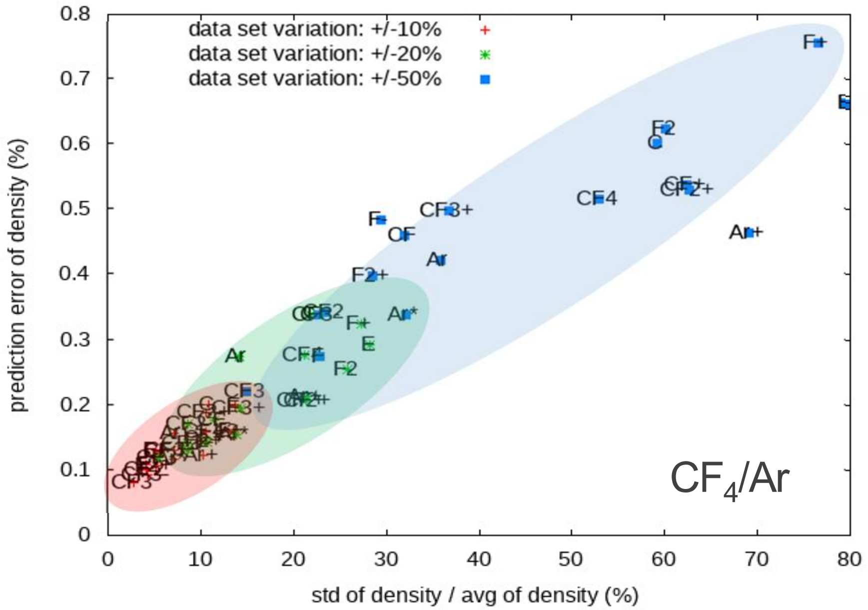
- Inversely, training operation conditions on plasma parameters
- Prediction of operation conditions for a target plasma



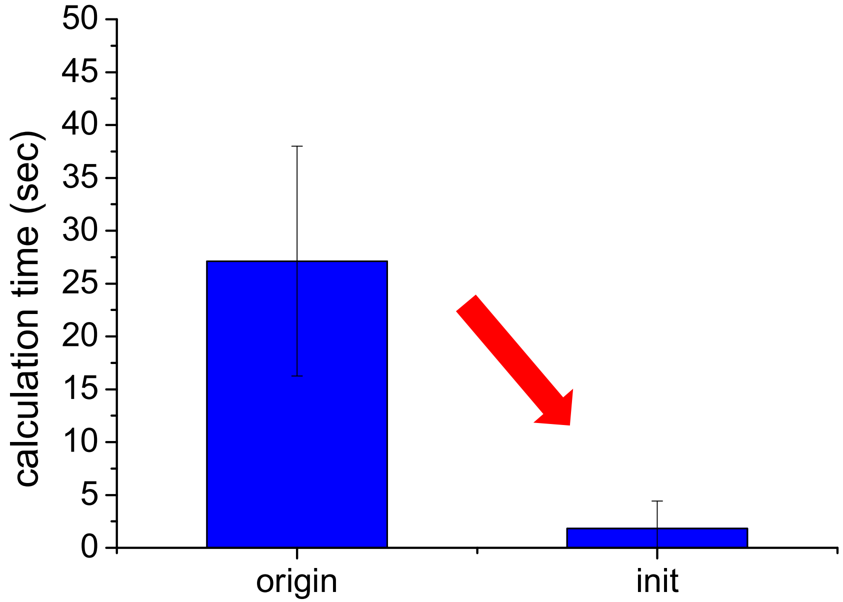
3. ML-aided Modeling

Global model + Machine learning

- Global model → training → prediction
  - Prediction errors ∝ data set variation
  - Sensitive species on input conditions → error ↑



- ML prediction → global model
  - Predicted values → set to be initial values
  - Improved computational efficiency



Neural network for ICP sources

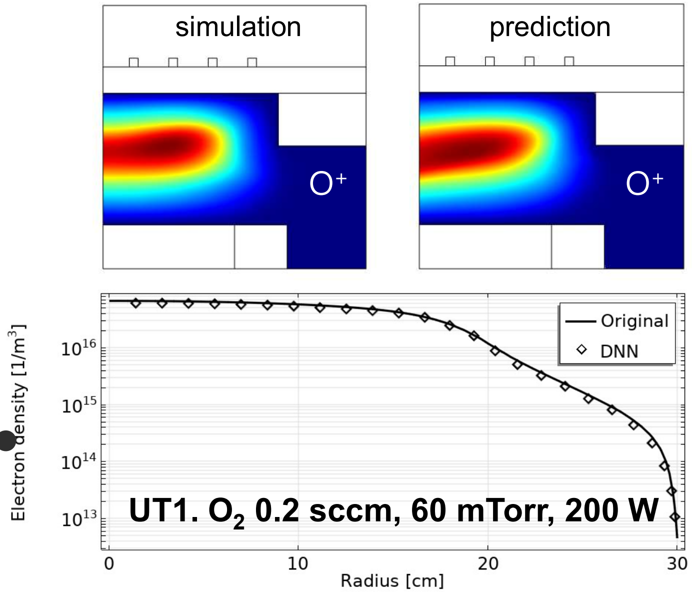
DNN model optimization

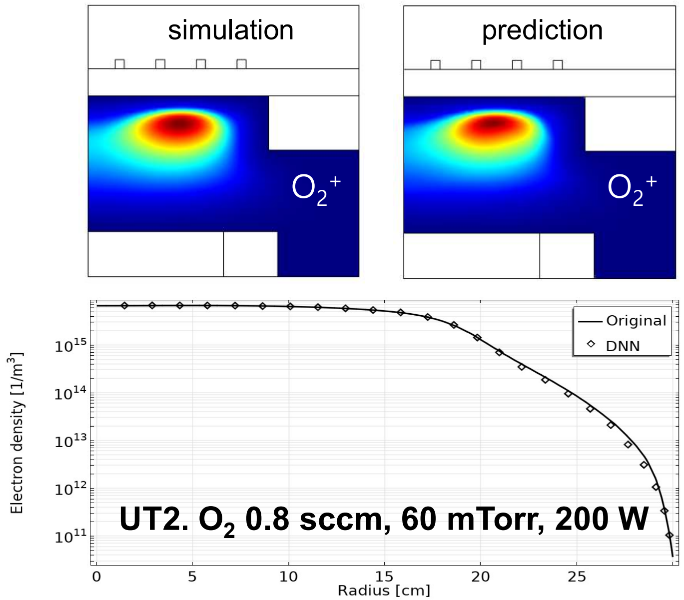
@ out of training range

- Z-score normalization for input data
- Log normalization for output data
- Train type : Bayesian regulation (Trainbr)
- Train network : feedforward net
- Activate function type : rectified linear unit (ReLU)
- Hidden layer : $n^{[1]} = 20$, $n^{[2]} = 20$, $n^{[3]} = 20$

Conditions :

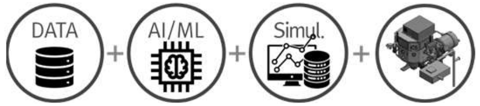
- Ar/O_2 total 250 sccm
- O_2 flow rate = 0.3, 0.4, 0.5, 0.6, 0.7 scccm
- Power = 100, 120, 140, 160, 180 W
- Pressure = 10, 20, 30, 40, 50 mTorr



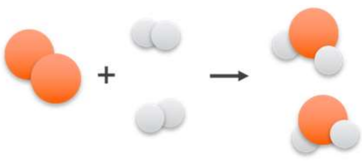


Choe et al., ASCT (to be published)

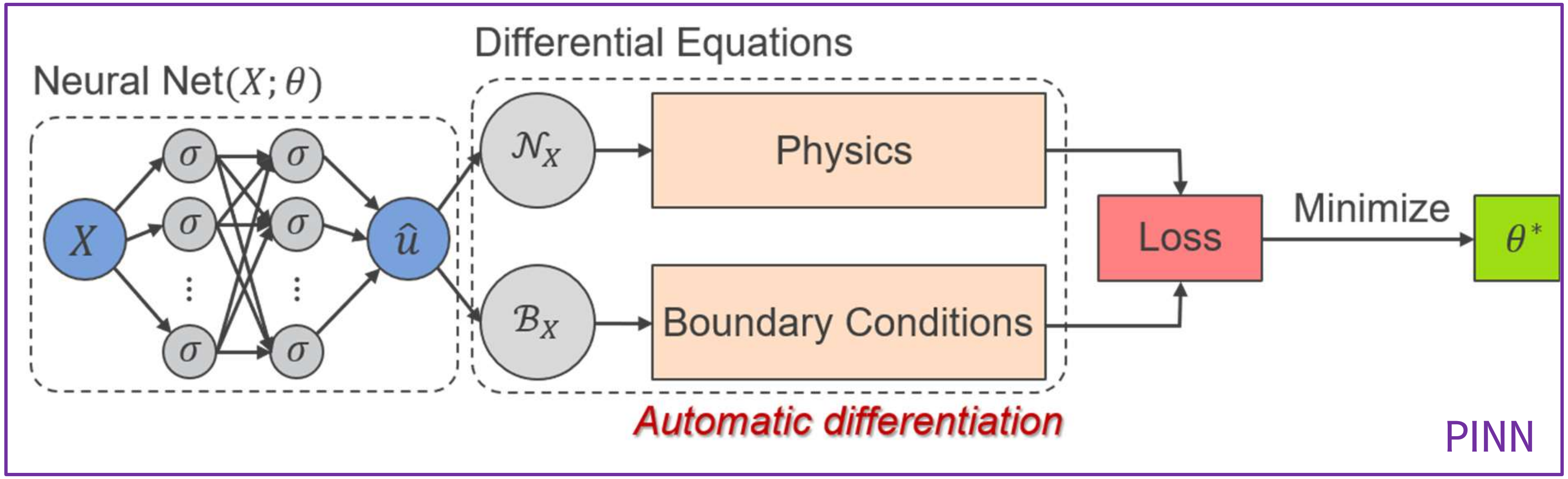
Physics-informed neural networks (PINNs)



- Intersection of the traditional physics model and the purely data-driven neural network approach.
- Physical parameters are can be obtained without solving governing equations directly.
- DB (required), discretization (partially unnecessary) → lower barriers to entry into simulations



DB & conditions

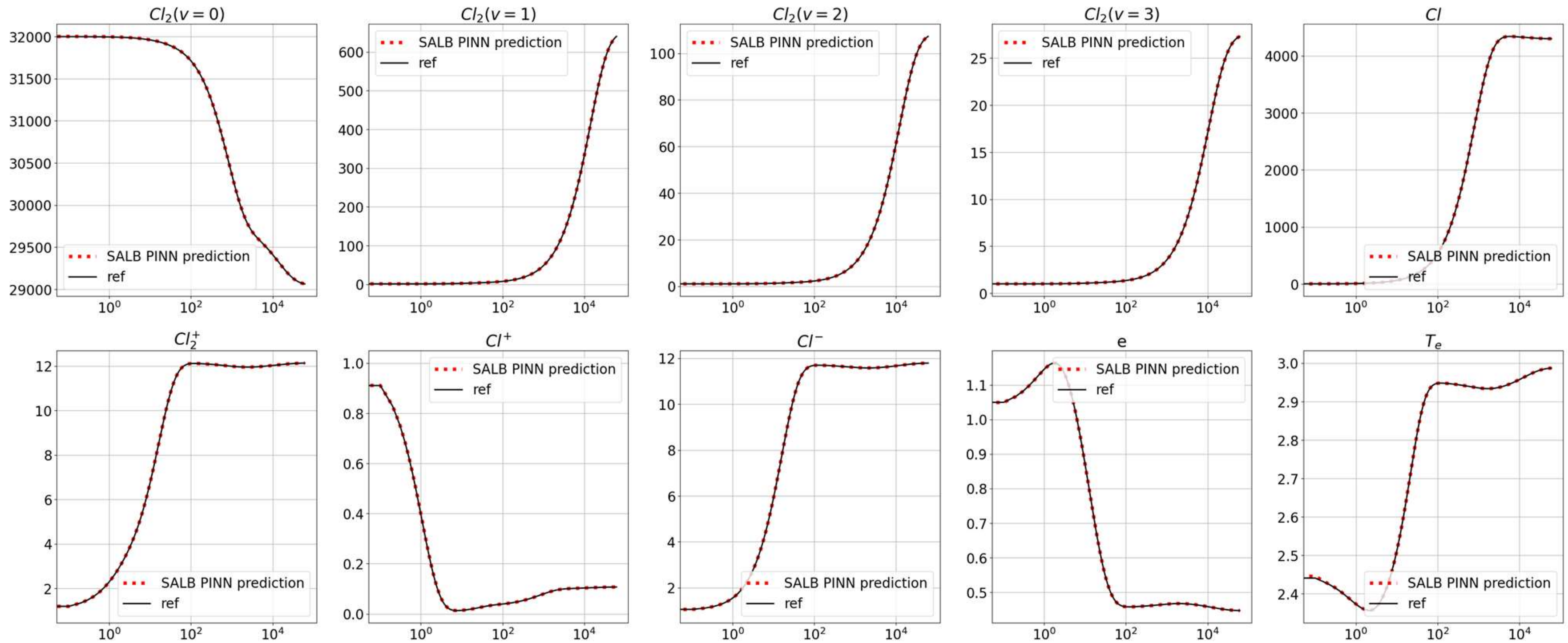


M. Raissi et al, J. Comput. Phys. **378**, 686 (2019), Lu Lu et al, arXiv:1907.045202, https://towardsdatascience.com/, https://en.wikipedia.org

3. ML-aided Modeling

Physics-informed neural networks (PINNs)

- Forward problem, Normalization
- Naive PINNs → Learn only some variable → SALB (self adaptive loss balance) loss function



E. G. Thorsteinsson and J. T. Gudmundsson, Plasma Sources Sci. Technol. **19**, 015001 (2010), Z. Xiang et al, Neurocomputing **496**, 11 (2022)

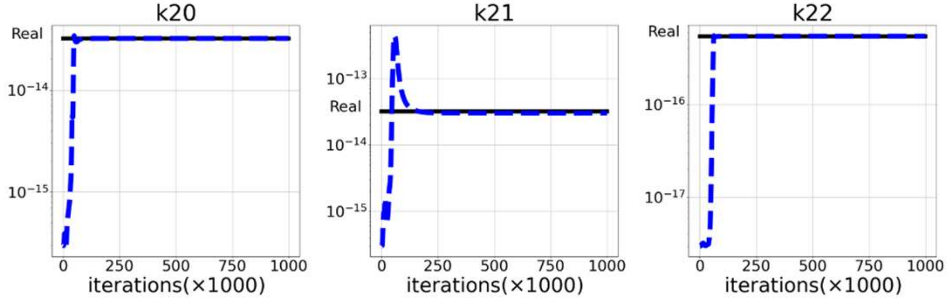
3. ML-aided Modeling

Physics-informed neural networks (PINNs)

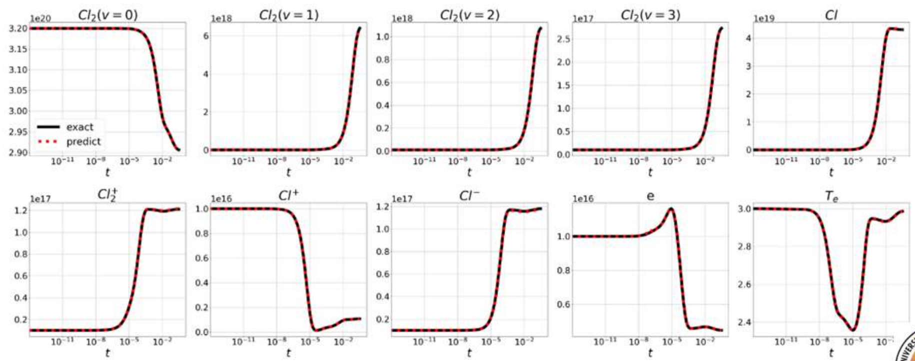
- Inverse problem to find rate coefficients

	Reaction	Rate coefficient ($m^3\,s^{-1}$ or $m^6\,s^{-1}$)
(R1)	$e + Cl_2(v=0) \rightarrow Cl + Cl + e$	$6.67 \times 10^{-14} T_e^{-0.10} e^{-8.67/T_e}$
(R2)	$e + Cl_2(v=0) \rightarrow Cl_2^+ + e + e$	$4.87 \times 10^{-14} T_e^{0.50} e^{-12.17/T_e}$
(R3)	$e + Cl_2(v=0) \rightarrow Cl + Cl^+ + 2e$	$1.79 \times 10^{-13} e^{-24.88/T_e}$
(R4)	$e + Cl_2(v=0) \rightarrow Cl^+ + Cl^+ + 3e$	$1.46 \times 10^{-16} T_e^{2.16} e^{-21.42/T_e}$
(R5)	$e + Cl_2(v=0) \rightarrow Cl + Cl^-$	$(22.5 T_e^{-0.46} e^{-2.82/T_e} - 12.1\, e^{-0.99/T_e} + 6.54) \times 10^{-16}$
(R6)	$e + Cl_2(v=1) \rightarrow Cl + Cl^-$	$(9.29 T_e^{-0.47} e^{-2.83/T_e} - 4.96\, e^{-0.99/T_e} + 2.70) \times 10^{-15}$
(R7)	$e + Cl_2(v=2) \rightarrow Cl + Cl^-$	$(20.1 T_e^{-0.47} e^{-2.83/T_e} - 10.8\, e^{-0.97/T_e} + 5.92) \times 10^{-15}$
(R8)	$e + Cl_2(v=3) \rightarrow Cl + Cl^-$	$(30.5 T_e^{-0.46} e^{-2.82/T_e} - 16.3\, e^{-0.99/T_e} + 8.81) \times 10^{-15}$
(R9)	$e + Cl_2(v=0) \rightarrow Cl^+ + Cl^- + e$	$3.45 \times 10^{-16} T_e^{0.13} e^{-19.70/T_e}$
(R10)	$e + Cl_2(v=0) \rightarrow Cl_2(v=1) + e$	$4.35 \times 10^{-16} T_e^{-1.48} e^{-0.76/T_e}$
(R11)	$e + Cl_2(v=0) \rightarrow Cl_2(v=2) + e$	$8.10 \times 10^{-17} T_e^{-1.48} e^{-0.68/T_e}$
(R12)	$e + Cl_2(v=0) \rightarrow Cl_2(v=3) + e$	$2.39 \times 10^{-17} T_e^{-1.49} e^{-0.64/T_e}$
(R13)	$e + Cl_2(v=1) \rightarrow Cl_2(v=2) + e$	$1.04 \times 10^{-15} T_e^{-1.48} e^{-0.73/T_e}$
(R14)	$e + Cl_2(v=1) \rightarrow Cl_2(v=3) + e$	$2.98 \times 10^{-16} T_e^{-1.48} e^{-0.67/T_e}$
(R15)	$e + Cl_2(v=2) \rightarrow Cl_2(v=3) + e$	$1.04 \times 10^{-15} T_e^{-1.48} e^{-0.73/T_e}$
(R16)	$e + Cl \rightarrow Cl^+ + e + e$	$2.48 \times 10^{-14} T_e^{0.62} e^{-12.76/T_e}$
(R17)	$e + Cl^- \rightarrow Cl + e + e$	$2.33 \times 10^{-15} T_e^{1.45} e^{-2.48/T_e}$
(R18)	$e + Cl^- \rightarrow Cl^+ + 3e$	$3.38 \times 10^{-15} T_e^{0.75} e^{-25.28/T_e}$
(R19)	$e + Cl_2^+ \rightarrow Cl + Cl$	$9.00 \times 10^{-14} T_e^{-0.50}$
(R20)	$Cl_2^+ + Cl^- \rightarrow Cl + Cl + Cl$	$5.00 \times 10^{-14}\,(300/T_g)^{0.50}$
(R21)	$Cl^+ + Cl^- \rightarrow Cl + Cl$	$5.00 \times 10^{-14}\,(300/T_g)^{0.50}$
(R22)	$Cl_2 + Cl^+ \rightarrow Cl_2^+ + Cl$	5.40×10^{-16}
(R23)	$2Cl + Cl_2 \rightarrow Cl_2(v=0) + Cl_2$	$3.50 \times 10^{-45} e^{810/T_g}$
(R24)	$2Cl + Cl \rightarrow Cl_2(v=0) + Cl$	$8.75 \times 10^{-46} e^{810/T_g}$

Results of k's values over iterations



Predict results about each species

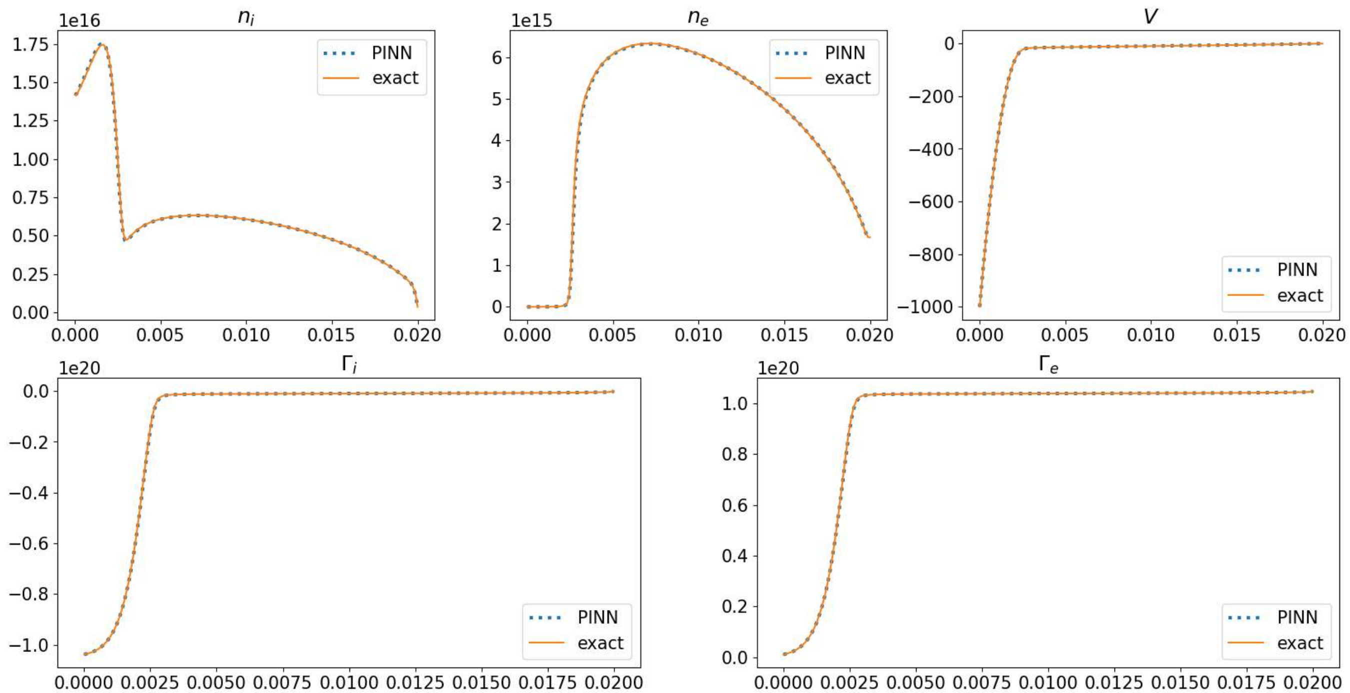


E. G. Thorsteinsson and J. T. Gudmundsson, Plasma Sources Sci. Technol. **19**, 015001 (2010)

3. ML-aided Modeling

Physics-informed neural networks (PINNs)

- Normalization, SALB + PINNs
- 1D DC discharge problem



H. J. Kim et al, J. Krean Phys. Soc. **51**, 633 (2007)

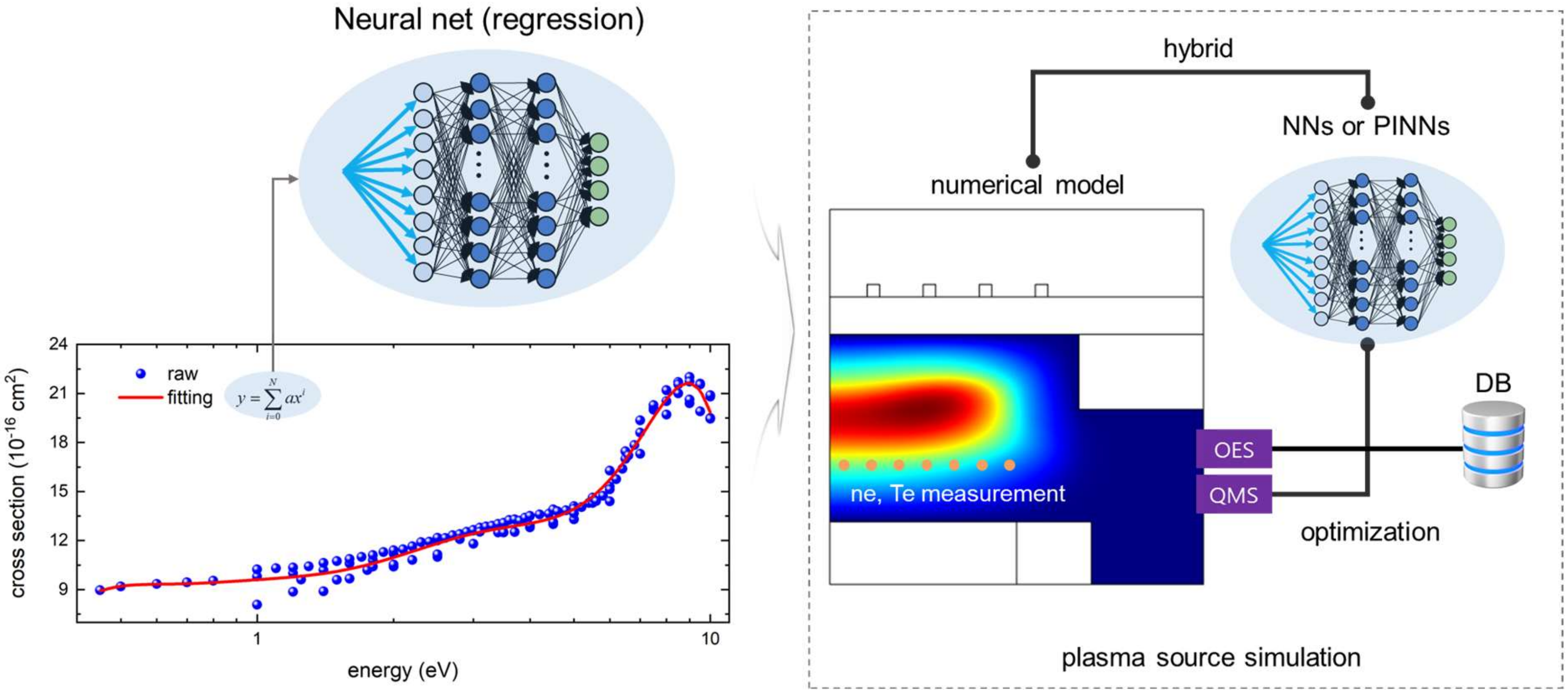
4

Summary & Future works

KFE KOREA INSTITUTE OF FUSION ENERGY

4. Summary & Future works

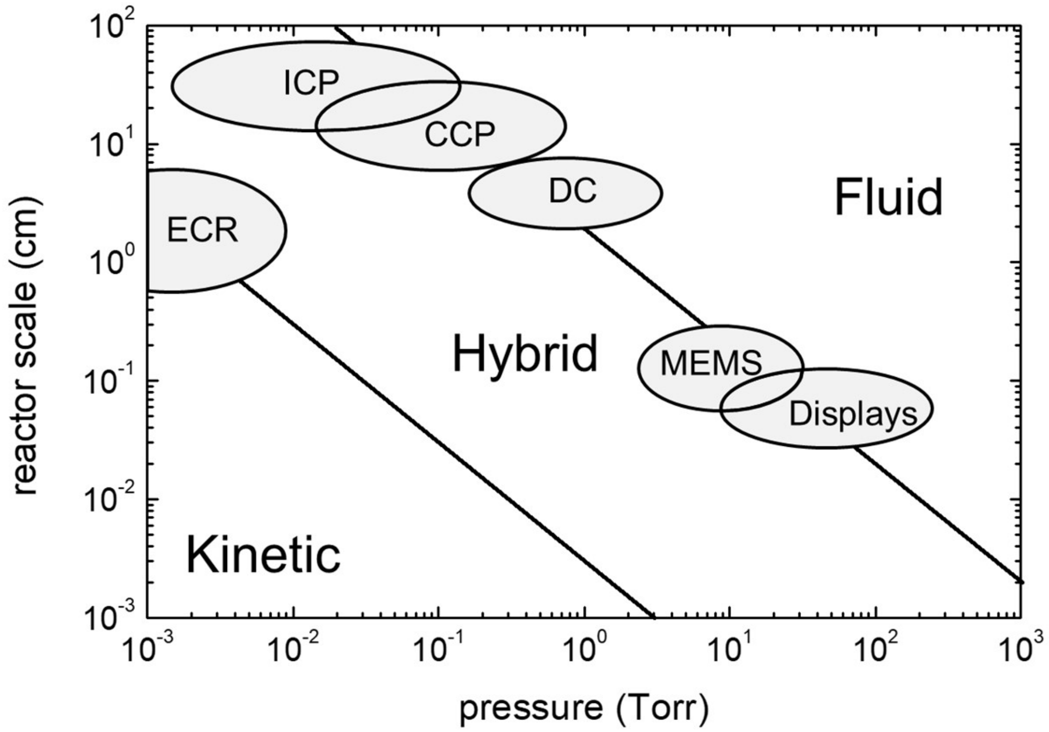
- This talk introduces our group's simulator and database development status and the results of applying machine learning technology to plasma source monitoring and simulations
- Get helps from NNs when prediction and optimization are needed
- Fill in the blank with NNs

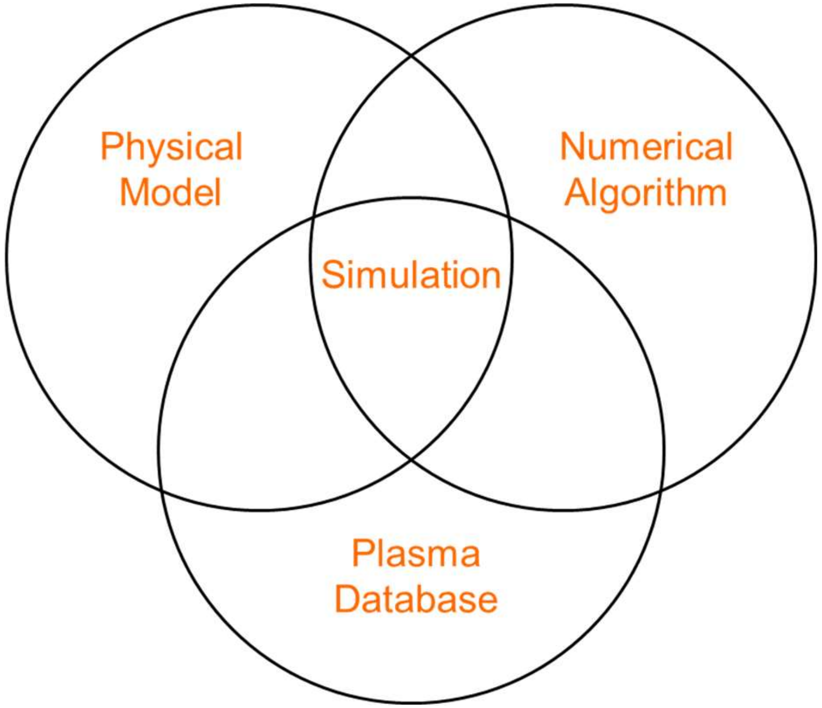


Thank you for your attention

5. Supplementary

Kinetic, Hybrid, and Fluid models



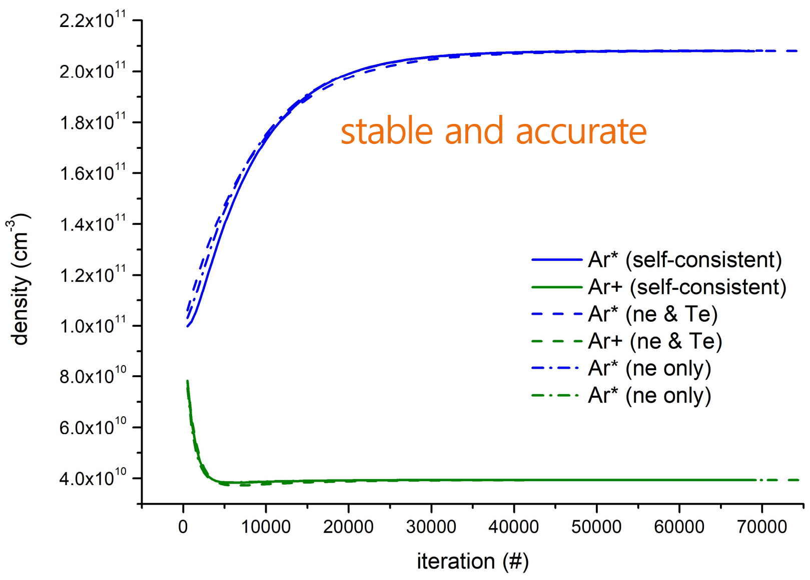


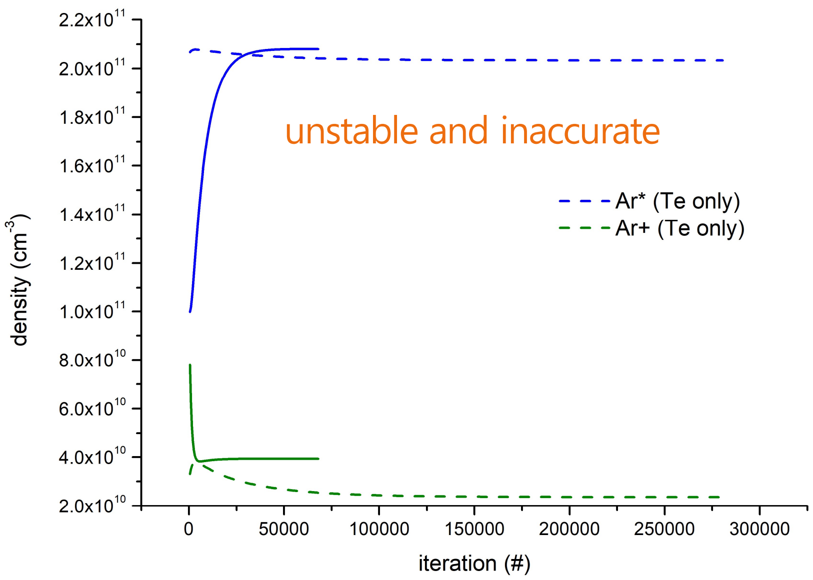
V. I. Kolobov, Comput. Material Sci. **28**, 302 (2003)

5. Supplementary

CHEM-global (chemical reaction analyzer using a global model)

- Quasi-neutrality
  - In some cases, the quasi-neutrality condition was not satisfied → after solving the continuity equation, densities are normalized





normalization

$$\sum_i n_i^+ = \sum_j n_j^- + n_e$$

$$\rightarrow \sum_i n_i^+ - \sum_j n_j^- = n_e$$

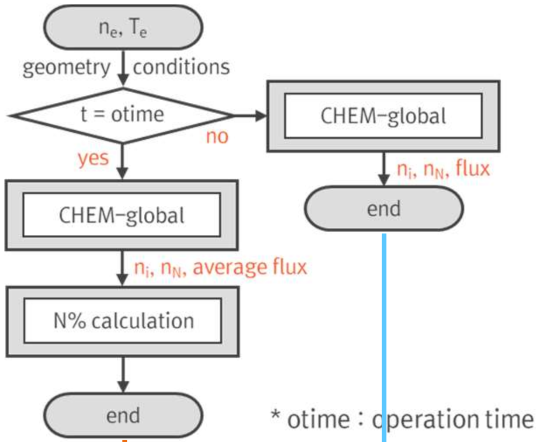
Step 1. $\hat{n} = \sum_i n_i^+ - \sum_i n_i^-$

Step 2. $\kappa = \frac{n_e}{\hat{n}}$

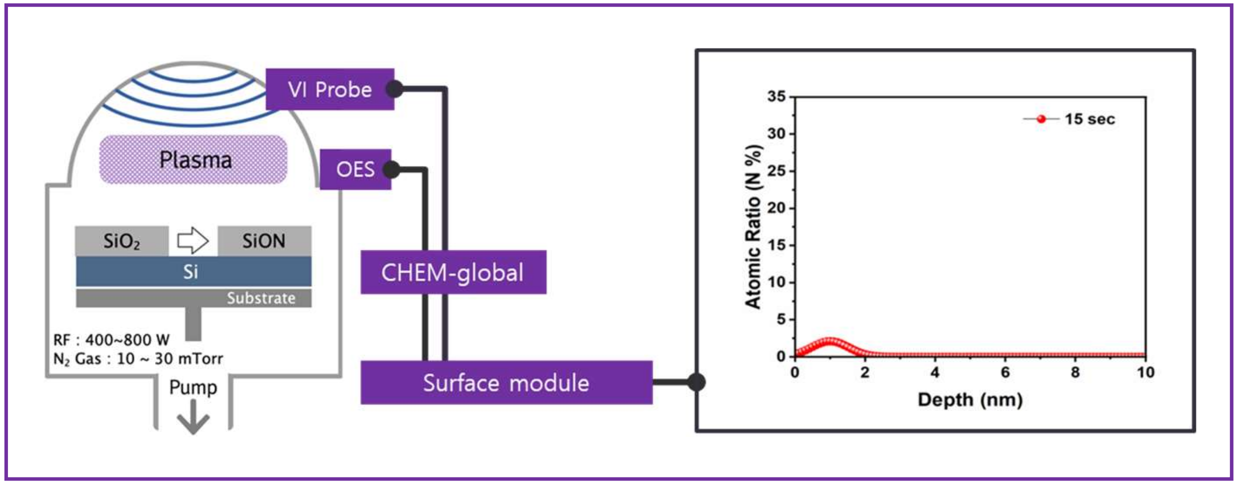
Step 3. $n_i = \kappa n_i$

5. Supplementary

Sensor-bulk-surface coupling model



* otime : operation time



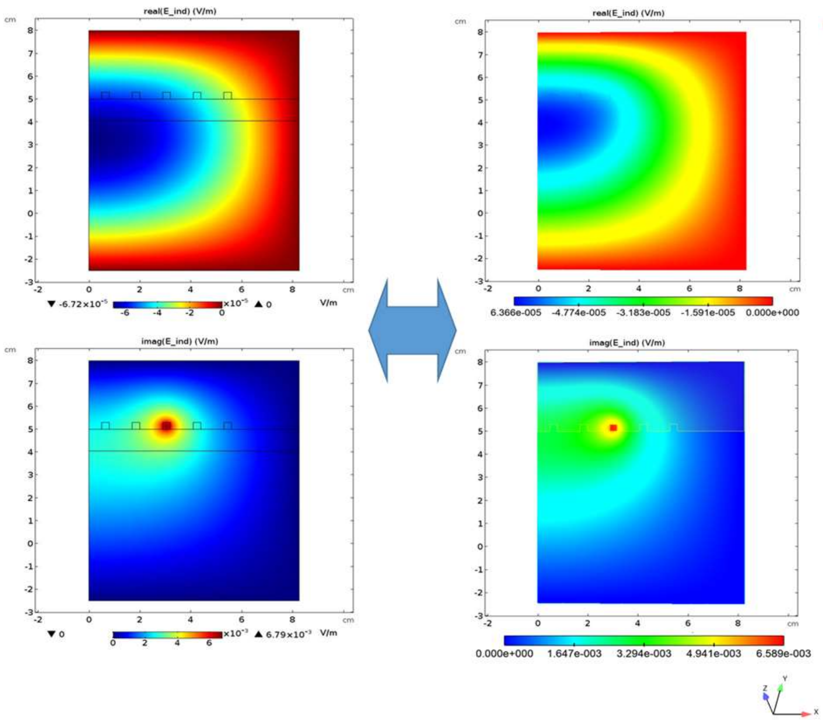

```
~/Code/NT_8.6.8  ./CHEM-global -n 6.31e10 -t 2.96 -s 600. -d 20. -v 2.0 -c 60. -f 5.e16 -x 1
N2+:6.065187e+10 N+:2.448126e+09 N:1.533671e+13 N2*:7.423527e+12 N2:4.641126e+14 N(2P):7.076060e+11 N(2D):1.330500e+12
3.805098e+16
```

```
~/Code/NT_8.6.8  ./CHEM-global -n 6.31e10 -t 2.96 -s 600. -d 20. -v 2.0 -c 600. -f 5.e16 -x 1
N2+:6.065187e+10 N+:2.448126e+09 N:1.533671e+13 N2*:7.423527e+12 N2:4.641126e+14 N(2P):7.076060e+11 N(2D):1.330500e+12
3.805098e+16
2.000000e+00 4.529994e+01
4.000000e+00 6.137989e+00
6.000000e+00 1.510557e-01
8.000000e+00 9.260711e-04
1.000000e+01 1.406361e-06
1.200000e+01 5.106815e-10
1.400000e+01 4.336434e-14
1.600000e+01 8.488942e-19
1.800000e+01 3.794496e-24
2.000000e+01 3.847017e-30
```

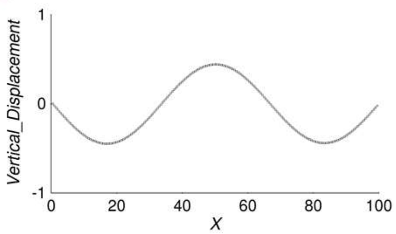
5. Supplementary

K-PLASMA unit test 1

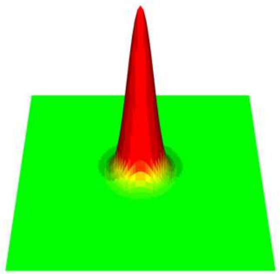
COMSOL CAP



3rd standing wave

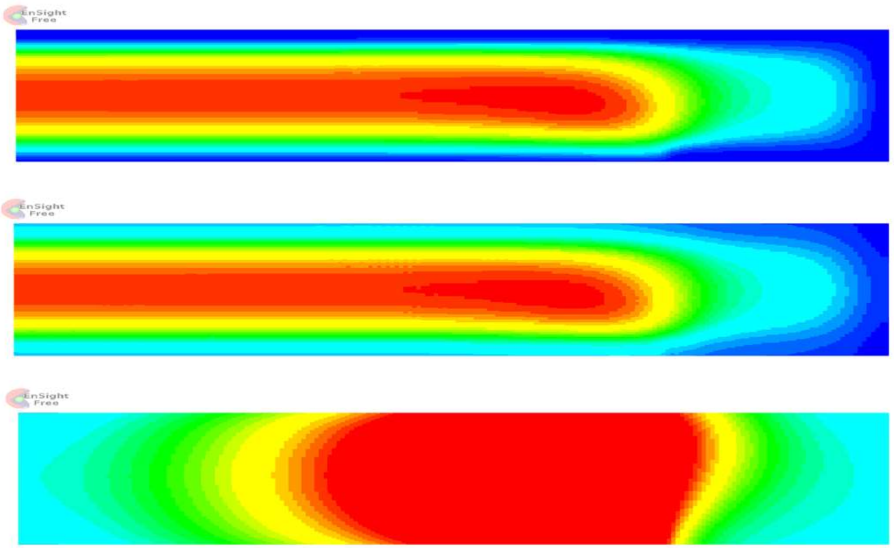


Gaussian function wave source

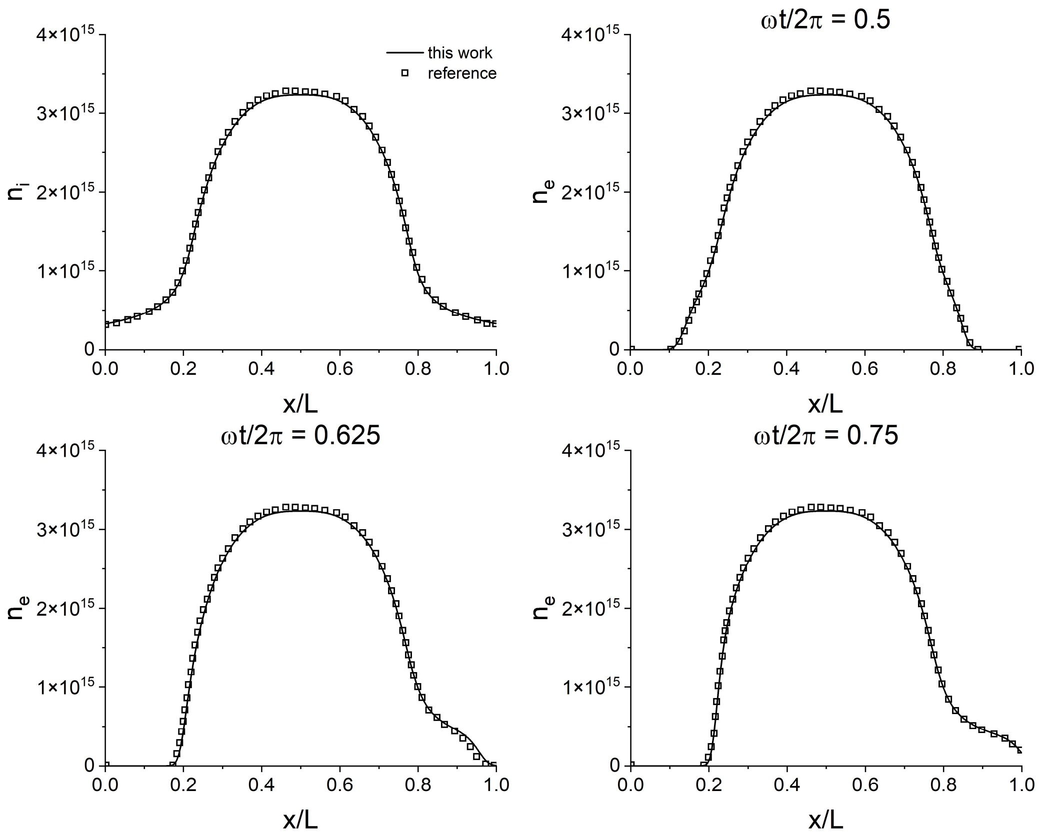


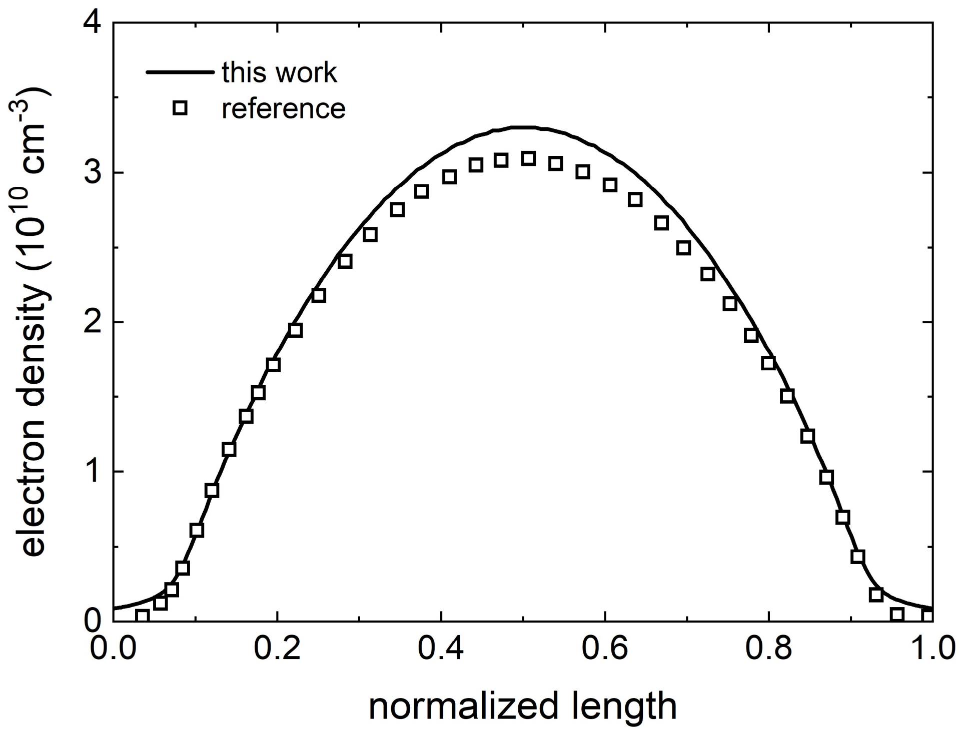
vortex extric field $\mathbf{E}_t = -\frac{\partial \mathbf{A}}{\partial t}$

$$-\nabla^2\left(-\frac{\partial \mathbf{A}}{\partial t}\right) = -\mu_0\varepsilon_0\frac{\partial^2}{\partial t^2}\left(-\frac{\partial \mathbf{A}}{\partial t}\right) - \frac{\partial}{\partial t}\left\{\mu_0\left[\mathbf{J} + \varepsilon_0\frac{\partial}{\partial t}(-\nabla\phi)\right]\right\}$$



K-PLASMA unit test 2





K-PLASMA – algorithm

$$\frac{\partial n_e}{\partial t} + \nabla \cdot \boldsymbol{\Gamma}_e = R_e$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2} n_e k_B T_e\right) + \nabla \cdot \mathbf{Q}_e = P_{ind} - e\mathbf{E} \cdot \boldsymbol{\Gamma}_e + E_e$$

$$N_e = \ln n_e$$

$$n_\varepsilon = \frac{3}{2} n_e k_B T_e$$

$$E_n = \ln n_\varepsilon$$

$$\frac{\partial n_e}{\partial t} = \frac{n_e}{n_e}\frac{\partial n_e}{\partial t} = n_e \frac{\partial\left(\ln n_e\right)}{\partial t} = n_e \frac{\partial N_e}{\partial t}$$

$$\frac{\partial}{\partial t}\left(\frac{3}{2} n_e k_B T_e\right) = \frac{\partial n_\varepsilon}{\partial t} = \frac{n_\varepsilon}{n_\varepsilon}\frac{\partial n_\varepsilon}{\partial t} = n_\varepsilon \frac{\partial\left(\ln n_\varepsilon\right)}{\partial t} = n_\varepsilon \frac{\partial E_\varepsilon}{\partial t}$$

$$\boldsymbol{\Gamma}_e = -\frac{q n_e}{m_e \nu_{eN}}\mathbf{E} - \frac{n_e}{m_e \nu_{eN}}\nabla T_e - \frac{T_e}{m_e \nu_{eN}}\nabla n_e$$

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

$$\rightarrow \boldsymbol{\Gamma}_e = -\mu_e n_e \mathbf{E} - n_e \nabla D_e - n_e D_e \nabla N_e$$

$$\Rightarrow n_e \frac{\partial N_e}{\partial t} + \nabla \cdot \left[-\mu_e n_e \mathbf{E} - n_e \nabla D_e - n_e D_e \nabla N_e\right] = R_e$$

$$\mathbf{Q}_e = \frac{5}{2}\boldsymbol{\Gamma}_e k_B T_e - \frac{5}{2}\frac{n_e k_B T_e}{m_e \nu_{eN}} \nabla\left(k_B T_e\right)$$

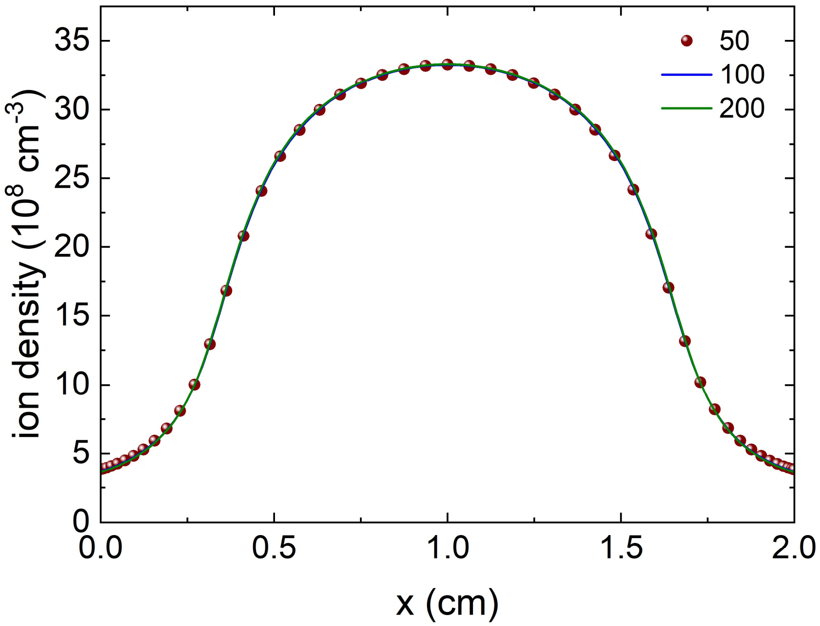
$$\rightarrow \mathbf{Q}_e = -\mu_\varepsilon \mathbf{E} n_\varepsilon - D_\varepsilon n_\varepsilon \nabla E_\varepsilon - n_\varepsilon \nabla D_\varepsilon$$

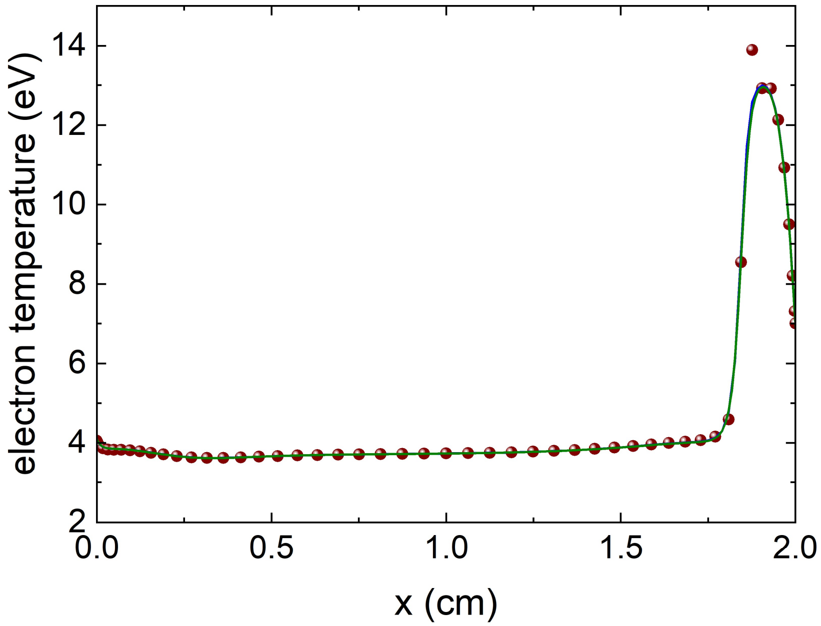
$$\Rightarrow n_\varepsilon \frac{\partial E_\varepsilon}{\partial t} + \nabla \cdot \left[-\mu_\varepsilon n_\varepsilon \mathbf{E} - n_\varepsilon D_\varepsilon \nabla E_\varepsilon - n_\varepsilon \nabla D_\varepsilon\right] = P_{ind} - e\mathbf{E} \cdot \boldsymbol{\Gamma}_e + E_e$$

COMSOL Multiphysics Plasma module user's guide 5.2a

5. Supplementary

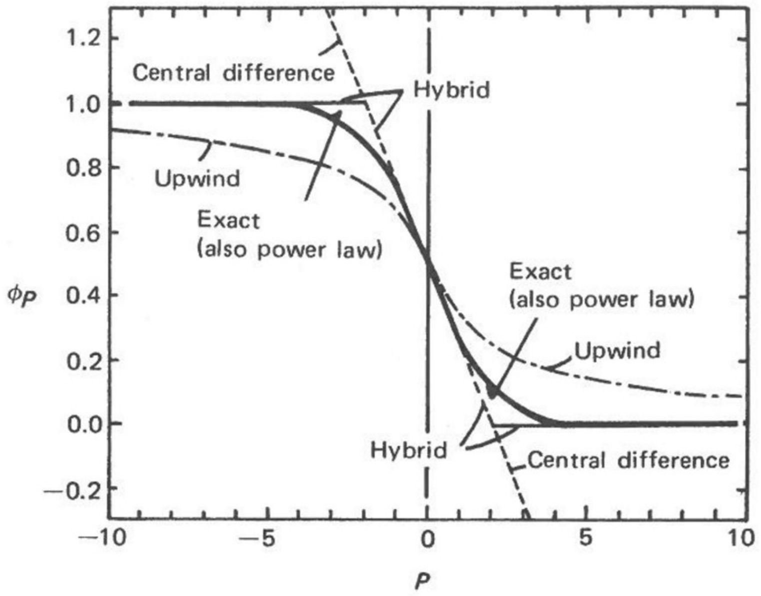
K-PLASMA – algorithm

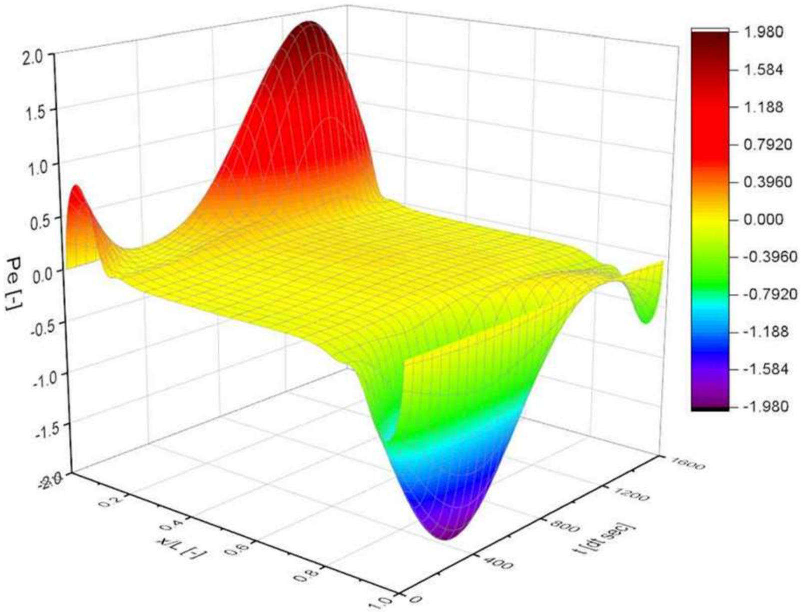




5. Supplementary

K-PLASMA – algorithm





S. V. Patankar, *Numerical heat transfer and fluid flow*

5. Supplementary

K-PLASMA – algorithm

$$\begin{cases} \dfrac{\partial \boldsymbol{\Gamma}_i}{\partial t} + \nabla\cdot(\boldsymbol{\Gamma}_i \mathbf{u}_i) = \dfrac{en_i}{m_i}\mathbf{E} - \dfrac{1}{m_i}\nabla(n_i k_B T_i) - \nu_{iN}\boldsymbol{\Gamma}_i \\ \boldsymbol{\Gamma}_i = \dfrac{en_i}{\nu_{iN} m_i}\mathbf{E}_{eff} - \dfrac{1}{\nu_{iN} m_i}\nabla(n_i k_B T_i) \end{cases}$$

$$\text{assuming } \frac{\partial}{\partial t}\left[\frac{1}{\nu_{iN} m_i}\nabla(n_i k_B T_i)\right] \approx 0,\ \nu_{iN} = const$$

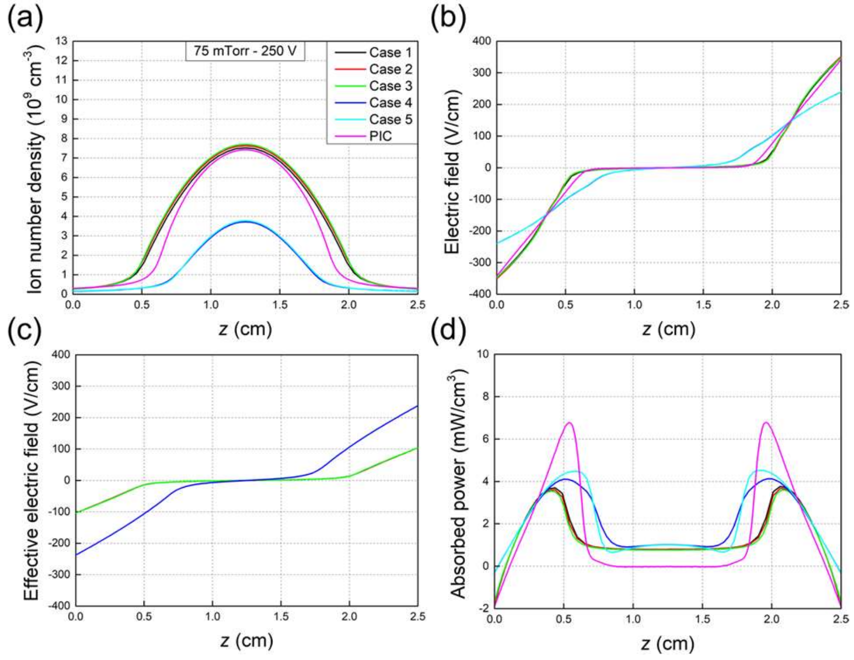
$$\frac{\partial}{\partial t}\left(\frac{en_i}{\nu_{iN} m_i}\mathbf{E}_{eff}\right) = \frac{e}{\nu_{iN} m_i}\left(n_i\frac{\partial \mathbf{E}_{eff}}{\partial t} + \mathbf{E}_{eff}\frac{\partial n_i}{\partial t}\right) = \frac{e}{\nu_{iN} m_i}\left[n_i\frac{\partial \mathbf{E}_{eff}}{\partial t} + \mathbf{E}_{eff}(R_i - \nabla\cdot\boldsymbol{\Gamma}_i)\right]$$

$$\rightarrow \frac{en_i}{\nu_{iN} m_i}\frac{\partial \mathbf{E}_{eff}}{\partial t} = -\nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i) + \frac{en_i}{m_i}\mathbf{E} - \frac{1}{m_i}\nabla(n_i k_B T_i) - \nu_{iN}\left[\frac{en_i}{\nu_{iN} m_i}\mathbf{E}_{eff} - \frac{1}{\nu_{iN} m_i}\nabla(n_i k_B T_i)\right] - \frac{e}{\nu_{iN} m_i}\mathbf{E}_{eff}(R_i - \nabla\cdot\boldsymbol{\Gamma}_i)$$

$$= -\nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i) + \frac{en_i}{m_i}\mathbf{E} - \frac{1}{m_i}\nabla(n_i k_B T_i) - \frac{en_i}{m_i}\mathbf{E}_{eff} + \frac{1}{m_i}\nabla(n_i k_B T_i) - \frac{e}{\nu_{iN} m_i}\mathbf{E}_{eff}(R_i - \nabla\cdot\boldsymbol{\Gamma}_i)$$

$$\rightarrow \frac{\partial \mathbf{E}_{eff}}{\partial t} = -\frac{\nu_{iN} m_i}{en_i}\nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i) + \nu_{iN}\mathbf{E} - \nu_{iN}\mathbf{E}_{eff} - \frac{1}{n_i}\mathbf{E}_{eff}(R_i - \nabla\cdot\boldsymbol{\Gamma}_i)$$

$$\Rightarrow \frac{\partial \mathbf{E}_{eff}}{\partial t} = \nu_{iN}(\mathbf{E} - \mathbf{E}_{eff}) - \frac{\nu_{iN} m_i}{en_i}\nabla\cdot(\boldsymbol{\Gamma}_i\mathbf{u}_i) - \frac{1}{n_i}\mathbf{E}_{eff}(R_i - \nabla\cdot\boldsymbol{\Gamma}_i)$$



Case 1; full momentum equation
Case 2; full effective electric field
Case 3; Ignoring the third term on RHS
Case 4; Ignoring the second and third terms on RHS
Case 5; without the effective electric field

Y. Lee et al, Curr. Appl. Phys. **42**, 31 (2022)

Equivalent circuit of dielectric wall ICP sources

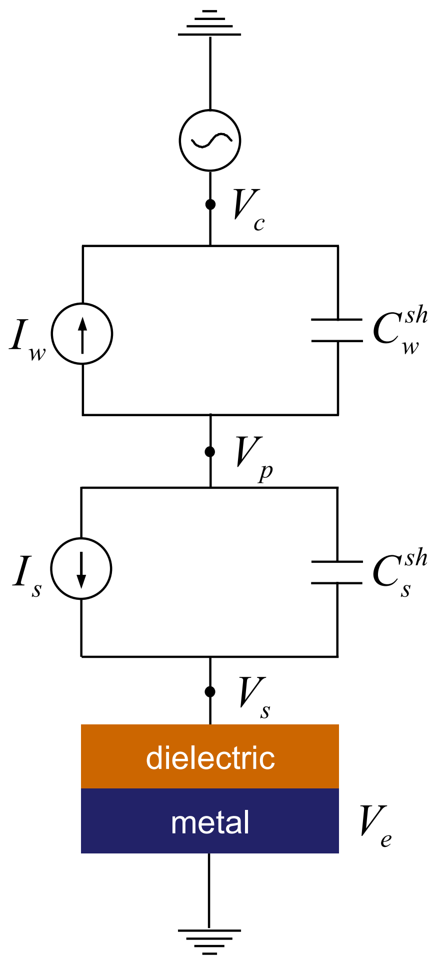
$$\begin{cases} C_w^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_c\right) + I_w + C_s^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_s\right) + I_s = 0 \\ \dfrac{\partial V_s}{\partial t} = \dfrac{1}{C_{eff}}\left(\underbrace{I_i - I_e}_{} + I_d\right) = \dfrac{1}{C_{eff}} I_s + \dfrac{1}{C_{eff}} C_s^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_s\right) \end{cases}$$

$I_s = I_i - I_e$ $\quad$ $I_d = C_s^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_s\right)$

$$\Rightarrow \begin{cases} C_w^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_c\right) + I_w + C_s^{sh}\dfrac{\partial}{\partial t}\left(V_p - V_s\right) + I_s = 0 \\ \dfrac{\partial V_s}{\partial t} = \dfrac{1}{C_{eff}} I_s + \dfrac{C_s^{sh}}{C_{eff}}\dfrac{\partial}{\partial t}\left(V_p - V_s\right) \end{cases}$$

where $C_{eff} = \dfrac{\varepsilon_r \varepsilon_0 A_w}{d_f}$, A_w is the surface area of the dielectric wall,

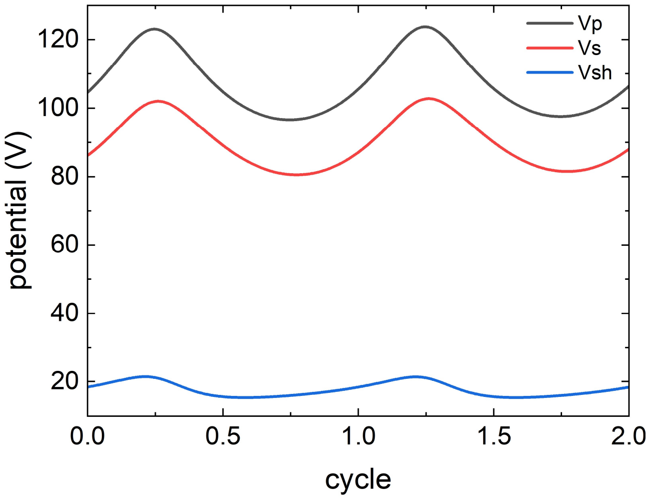
ε_r and d_f are the dielectric constant and thickness of the dielectric material.

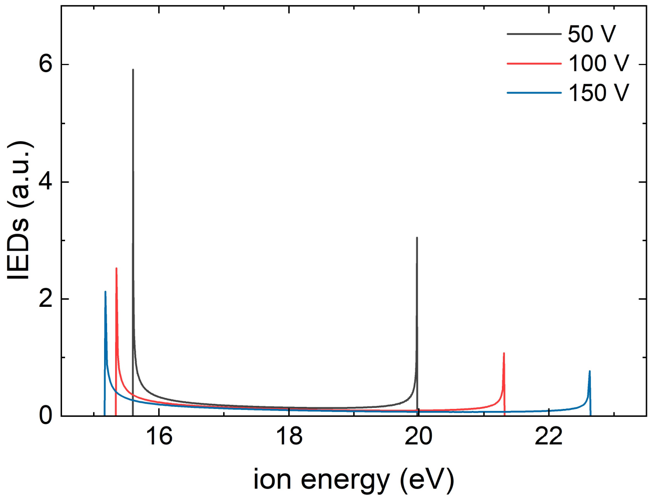


5. Supplementary

Equivalent circuit of dielectric wall ICP sources

$$\begin{cases} \dfrac{\partial V_p}{\partial t} = \dfrac{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh}}{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh} + C_s^{sh}C_{eff}}\dfrac{\partial V_c}{\partial t} - \dfrac{C_{eff} + C_s^{sh}}{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh} + C_s^{sh}C_{eff}}\left[I_w + I_s - \dfrac{C_s^{sh}}{C_{eff} + C_s^{sh}}I_s\right] \\ \dfrac{\partial V_s}{\partial t} = \dfrac{1}{C_{eff} + C_s^{sh}}I_s + \dfrac{C_s^{sh}}{C_{eff} + C_s^{sh}}\left\{\dfrac{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh}}{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh} + C_s^{sh}C_{eff}}\dfrac{\partial V_c}{\partial t} - \dfrac{C_{eff} + C_s^{sh}}{C_w^{sh}C_{eff} + C_w^{sh}C_s^{sh} + C_s^{sh}C_{eff}}\left[I_w + I_s - \dfrac{C_s^{sh}}{C_{eff} + C_s^{sh}}I_s\right]\right\} \end{cases}$$





$$\frac{d\chi}{dx}\left(\frac{\partial f}{\partial \chi} + \frac{\partial f}{\partial y}\right) = -q(y)f(\chi, y) + C(\chi)\delta(y)$$

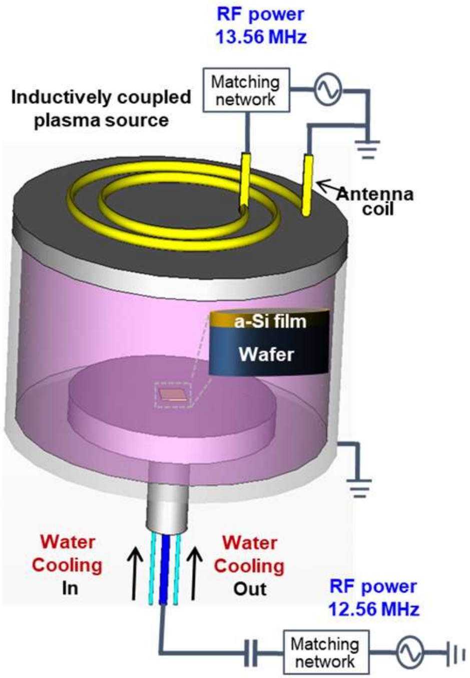
$$\text{where } \chi = \frac{-e\phi}{k_B T_i},\ x = \frac{z}{L},\ y = \frac{m_i \upsilon^2}{2k_B T_i},\ q(y) = \frac{L}{\lambda(y)}$$

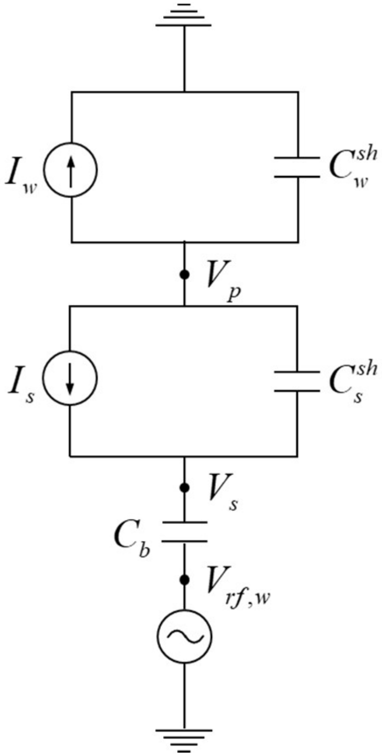
Riemann obtained the IEDs at the chamber wall by solving the Boltzmann equation

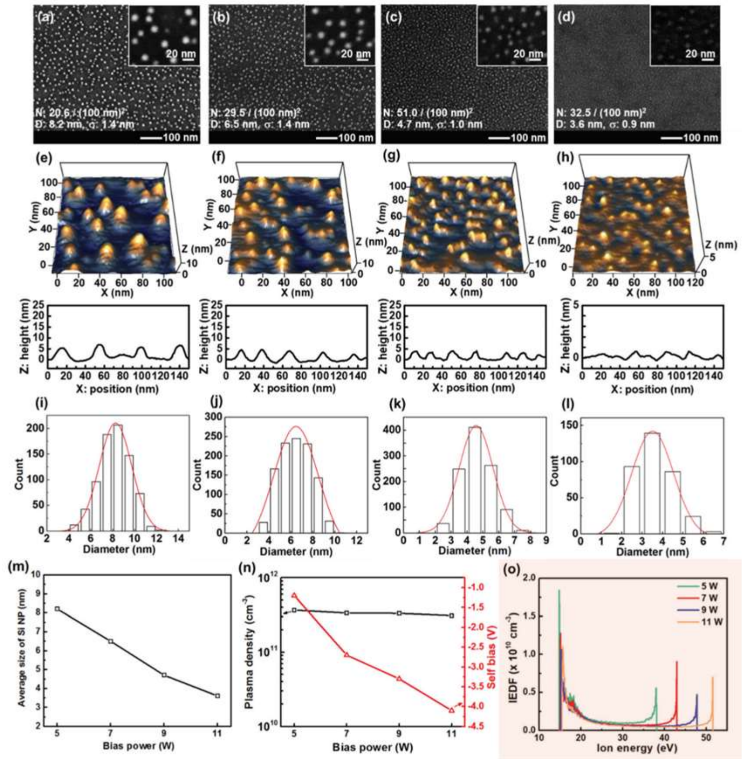
K.-U. Riemann, Phys. Fluids **24**, 2163 (1981)

5. Supplementary

Equivalent circuit for rf-biased sheath



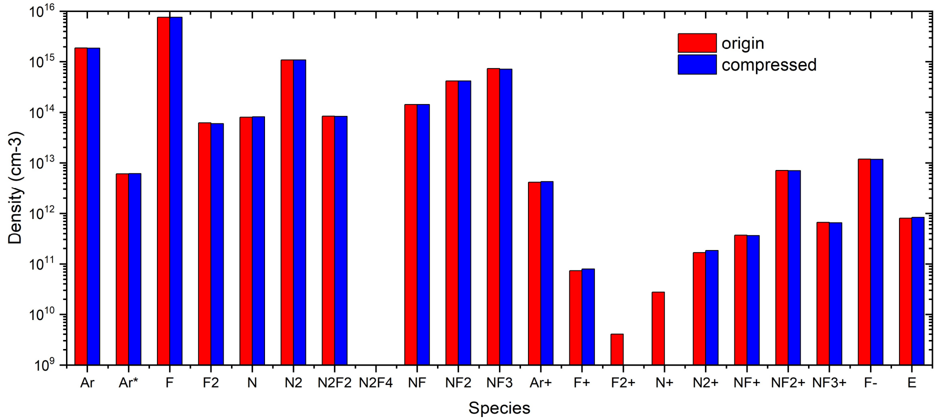


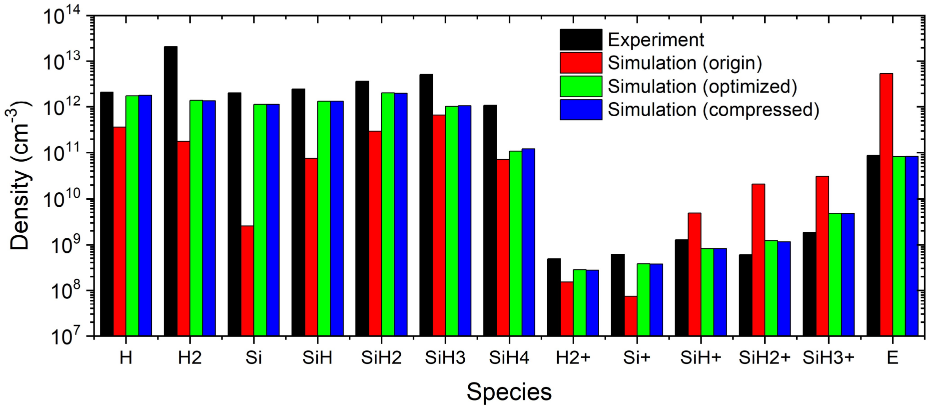


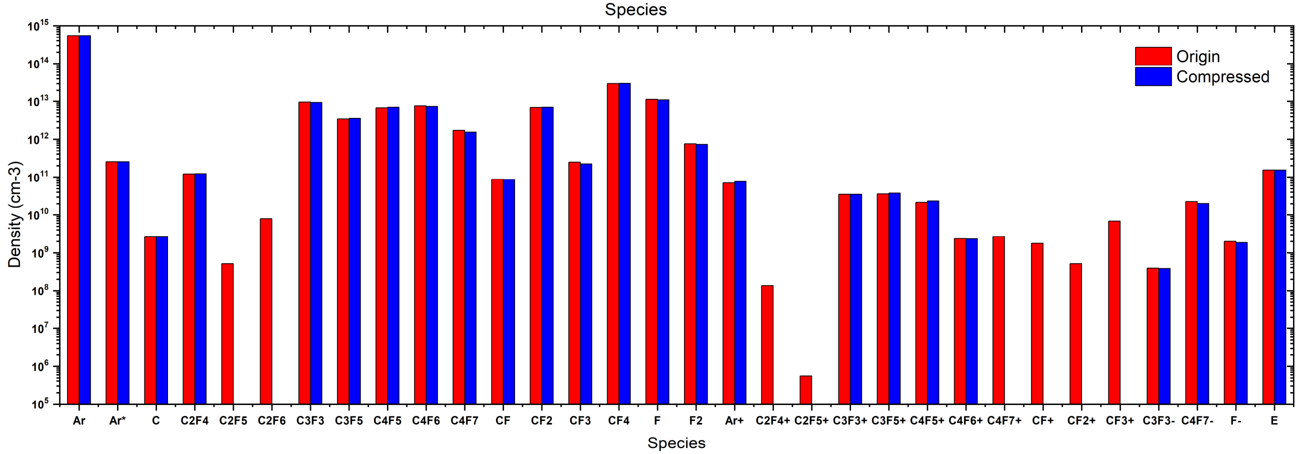
D. Choi et al., Nanoscale **13**, 10356 (2021)

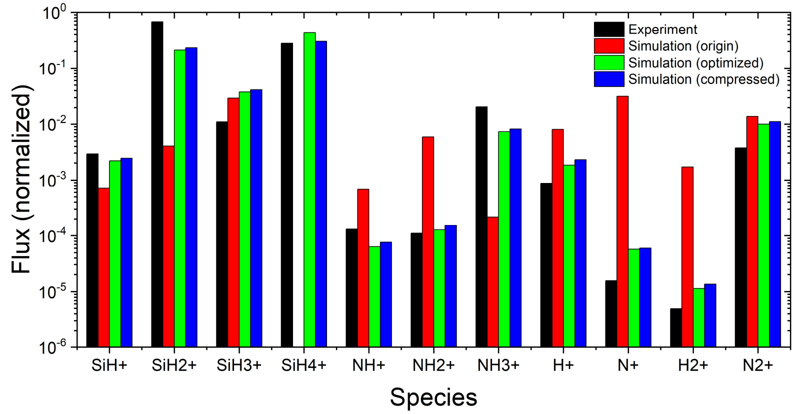
5. Supplementary

Database development



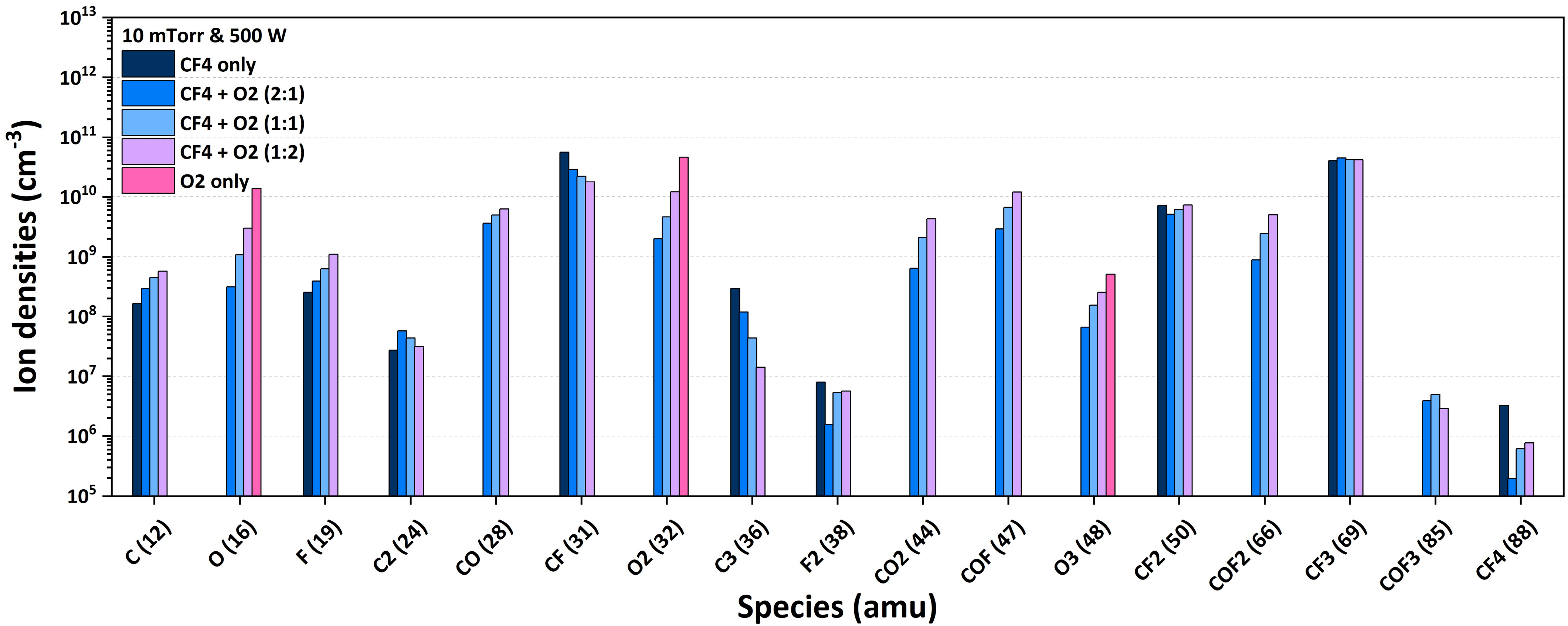






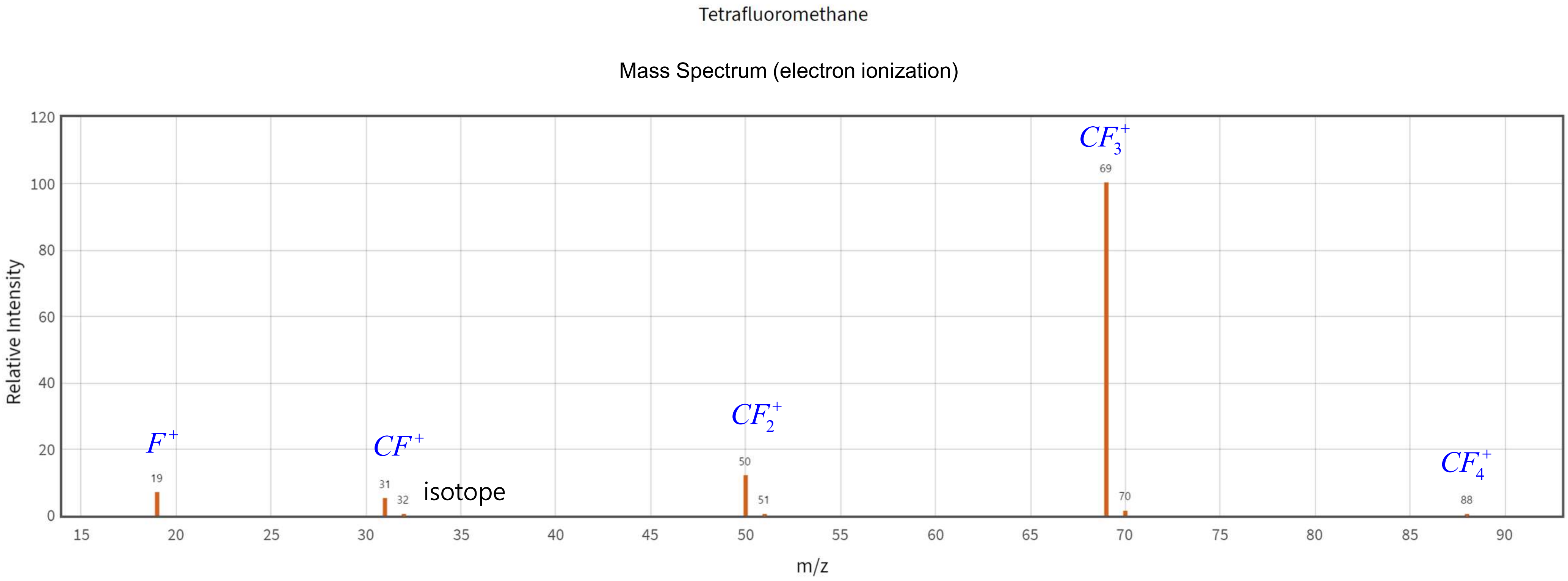
5. Supplementary

Database development (CF_4/O_2 mixture)



5. Supplementary

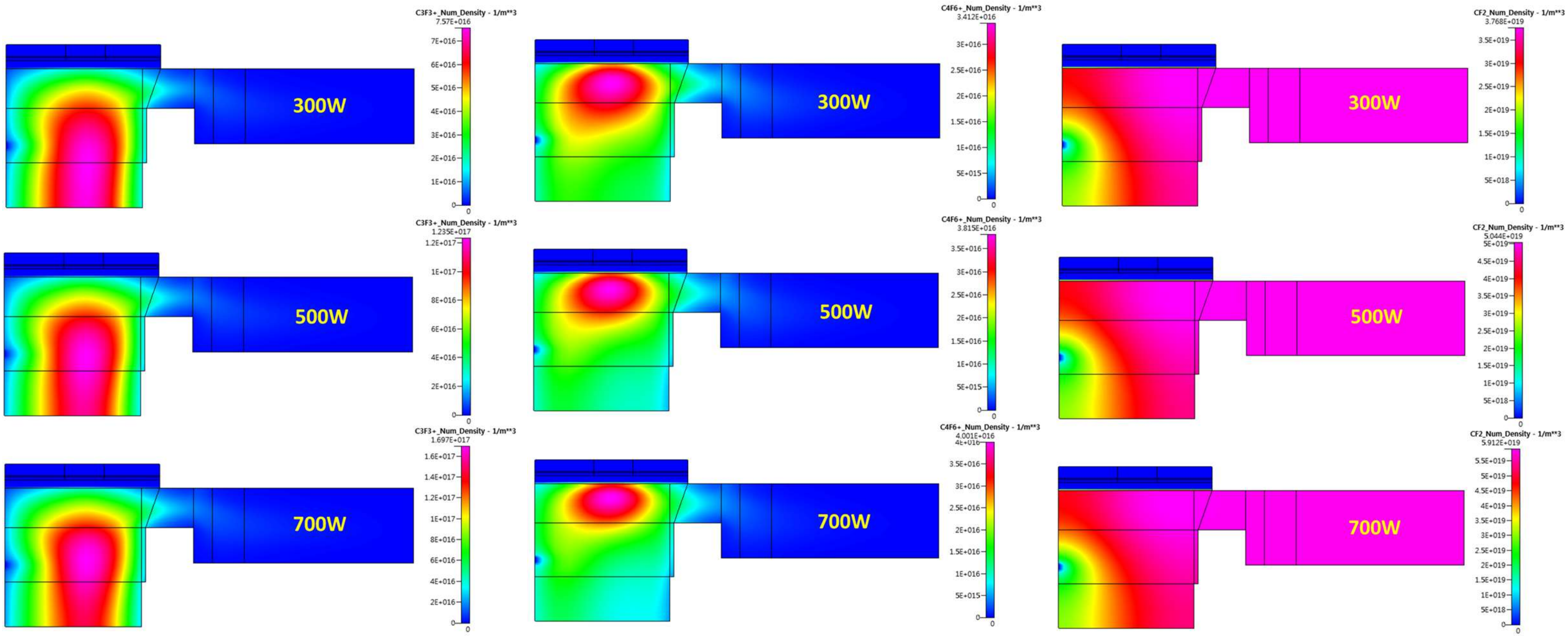
Database development (CF_4/O_2 mixture)



https://webbook.nist.gov/cgi/inchi?ID=C75730&Mask=200#Mass-Spec

5. Supplementary

2D simulations at 20 mTorr



4. Summary & Future works