FROM QDB TO FEATURE PROFILING

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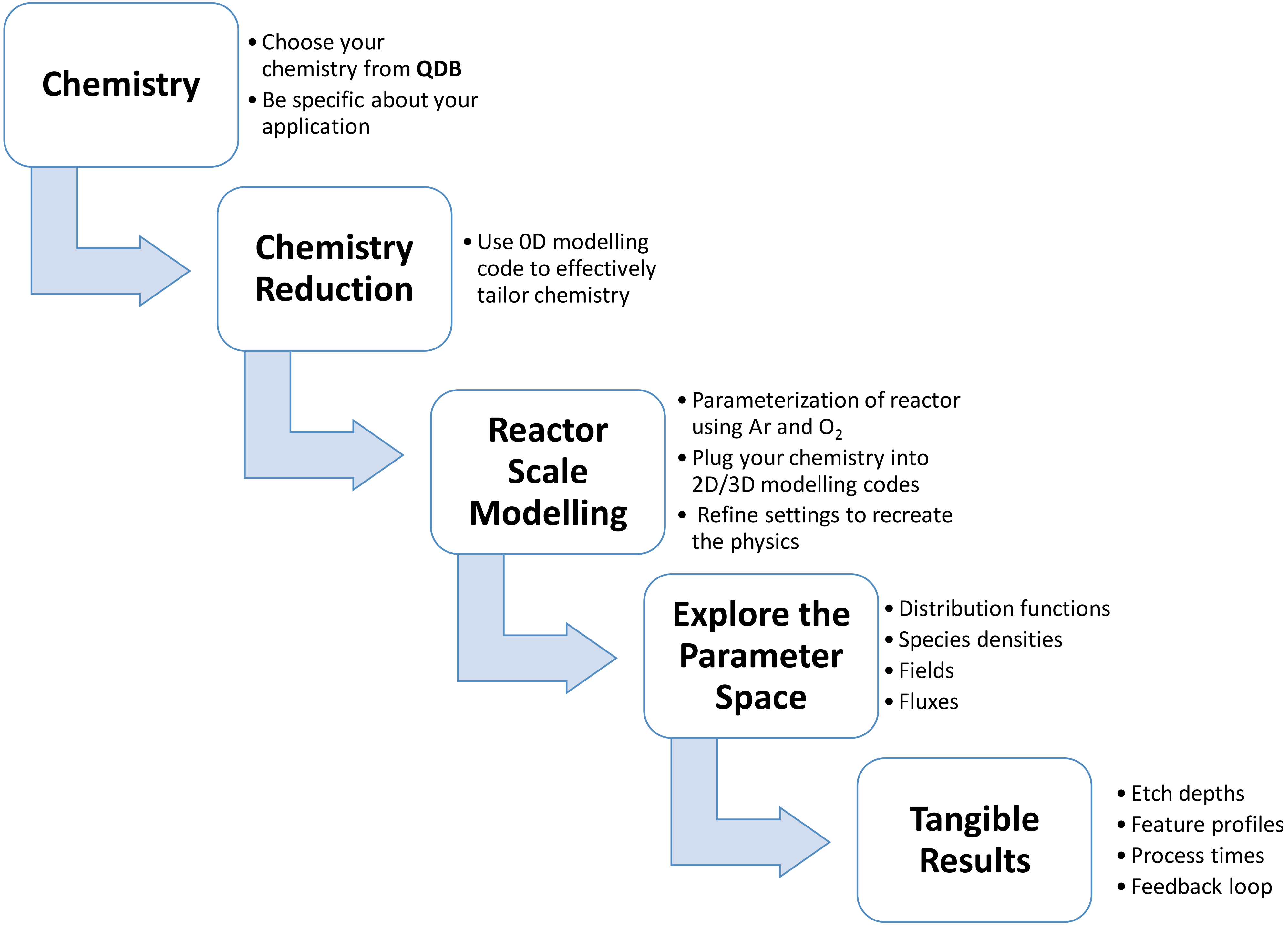
Quantemol

Understanding the workflow in a typical plasma physics related investigation



Chemistry

- Choose your chemistry from **QDB**
- Be specific about your application

Chemistry Reduction

- Use 0D modelling code to effectively tailor chemistry

Reactor Scale Modelling

- Parameterization of reactor using Ar and O_2
- Plug your chemistry into 2D/3D modelling codes
- Refine settings to recreate the physics

Explore the Parameter Space

- Distribution functions
- Species densities
- Fields
- Fluxes

Tangible Results

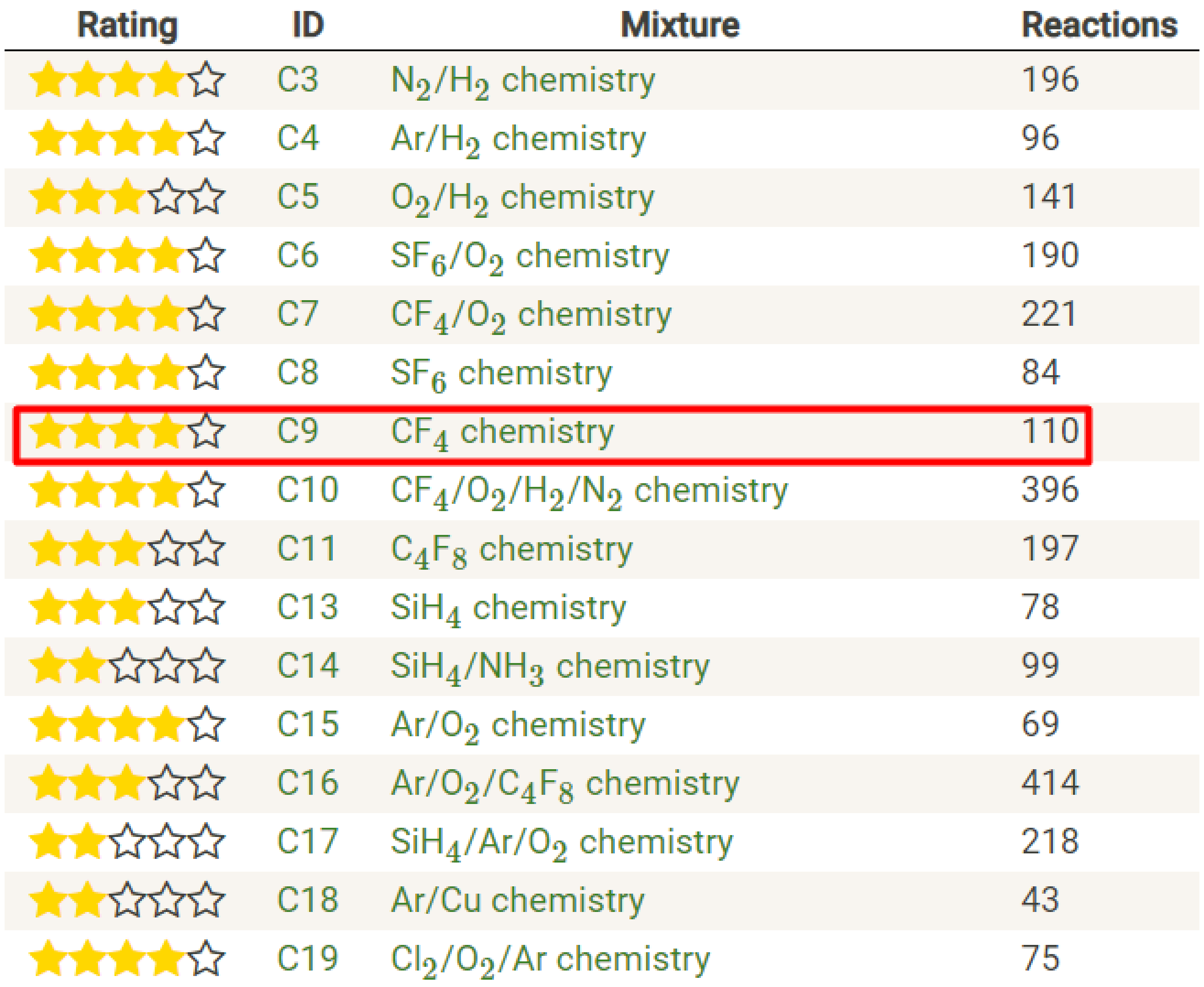
- Etch depths
- Feature profiles
- Process times
- Feedback loop

Choosing a Chemistry and Application using QDB

QDB
plasma chemistry

Quantemol

www.quantemolDB.com



Rating	ID	Mixture	Reactions
★★★★☆	C3	N_2/H_2 chemistry	196
★★★★☆	C4	Ar/H_2 chemistry	96
★★★☆☆	C5	O_2/H_2 chemistry	141
★★★★☆	C6	SF_6/O_2 chemistry	190
★★★★☆	C7	CF_4/O_2 chemistry	221
★★★★☆	C8	SF_6 chemistry	84
★★★★☆	C9	CF_4 chemistry	110
★★★★☆	C10	$CF_4/O_2/H_2/N_2$ chemistry	396
★★★☆☆	C11	C_4F_8 chemistry	197
★★★☆☆	C13	SiH_4 chemistry	78
★★☆☆☆	C14	SiH_4/NH_3 chemistry	99
★★★★☆	C15	Ar/O_2 chemistry	69
★★★☆☆	C16	$Ar/O_2/C_4F_8$ chemistry	414
★★☆☆☆	C17	$SiH_4/Ar/O_2$ chemistry	218
★★☆☆☆	C18	Ar/Cu chemistry	43
★★★★☆	C19	$Cl_2/O_2/Ar$ chemistry	75

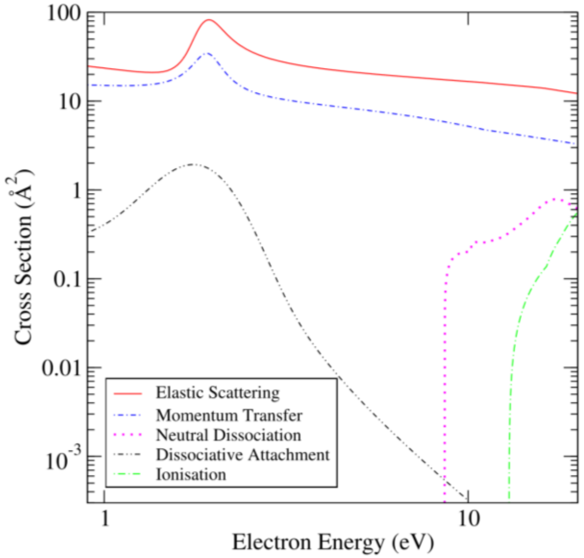
Application of interest: Etching

Pressure range: 1 – 30 mTorr

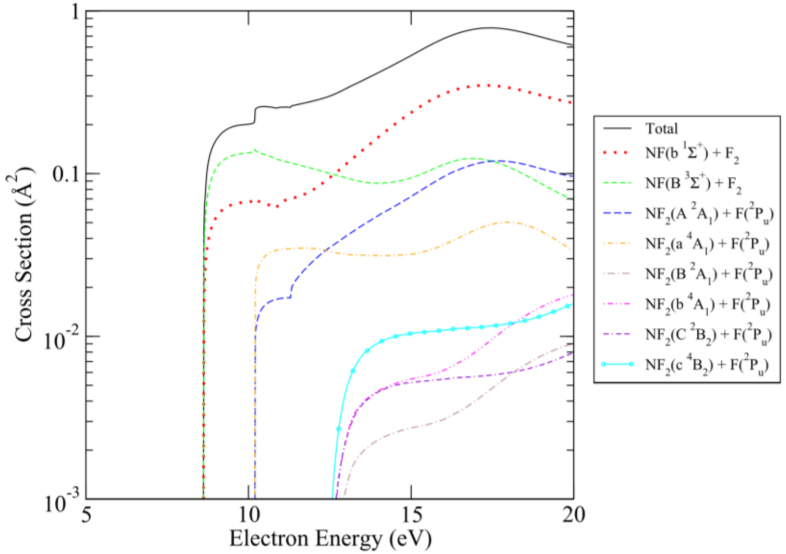
Power range: ~ 1000 W

What about more Novel Chemistries?

- Ab initio methods to calculate electron scattering; Elastic scattering, Electronic excitation, Quenching, Rotational excitation, Electron impact ionization and more!
- The Dissociative Electron Attachment mechanism can be modelled and cross-sections calculated.
- Branching ratios for neutral dissociation and ionization



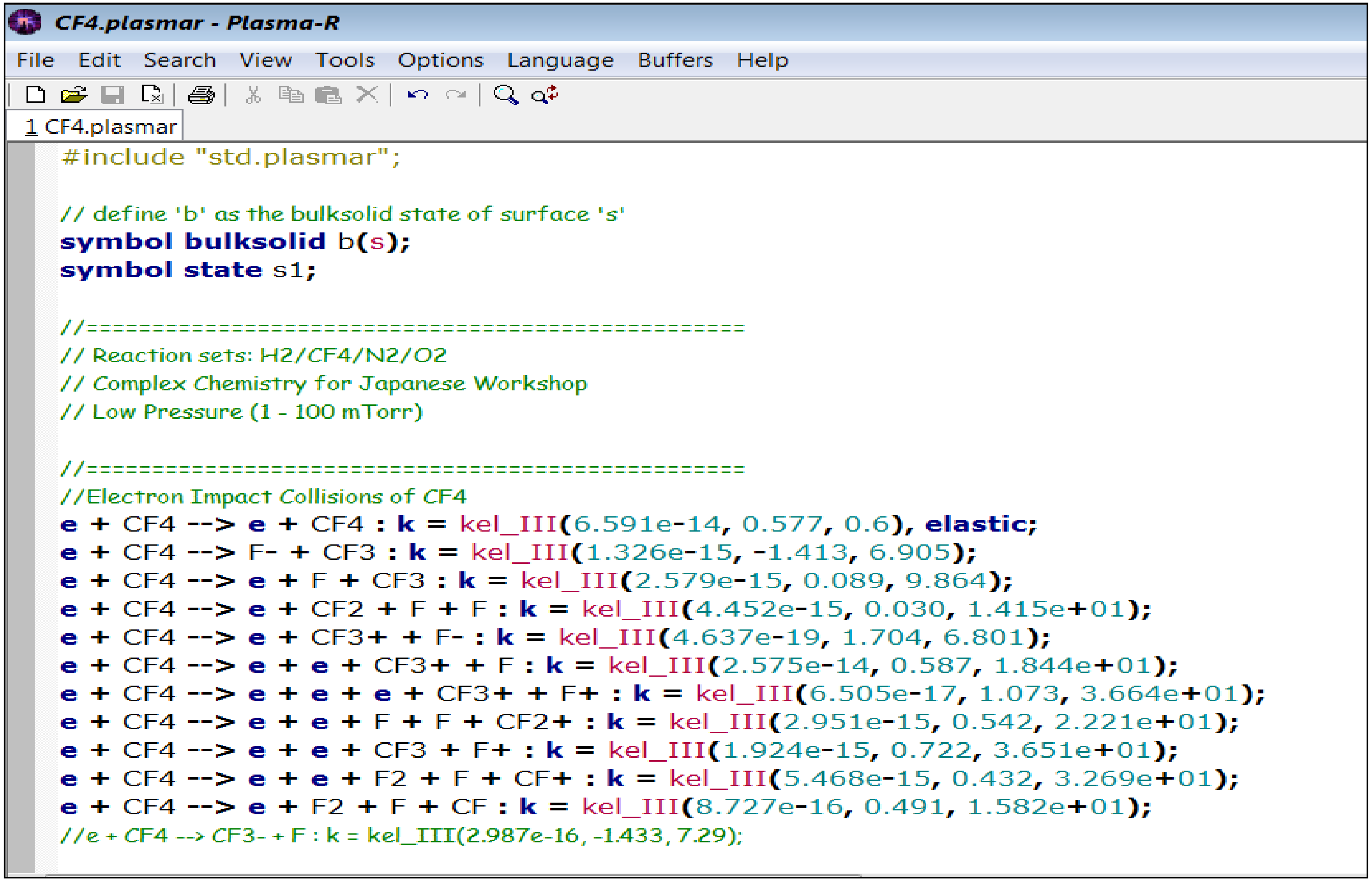
Overview of NF_3 Cross-sections at low electron collision energies



NF_3 Electron Impact Dissociation Cross-sections

J. R. Hamilton et al 2017, *"Calculated cross sections for electron collisions with NF3, NF2 and NF with applications to remote plasma sources"* Plasma Sources Sci. Technol. 26 065010

Chemistry Reduction



```
#include "std.plasmar";

// define 'b' as the bulksolid state of surface 's'
symbol bulksolid b(s);
symbol state s1;

//==================================================
// Reaction sets: H2/CF4/N2/O2
// Complex Chemistry for Japanese Workshop
// Low Pressure (1 - 100 mTorr)

//==================================================
//Electron Impact Collisions of CF4
e + CF4 --> e + CF4 : k = kel_III(6.591e-14, 0.577, 0.6), elastic;
e + CF4 --> F- + CF3 : k = kel_III(1.326e-15, -1.413, 6.905);
e + CF4 --> e + F + CF3 : k = kel_III(2.579e-15, 0.089, 9.864);
e + CF4 --> e + CF2 + F + F : k = kel_III(4.452e-15, 0.030, 1.415e+01);
e + CF4 --> e + CF3+ + F- : k = kel_III(4.637e-19, 1.704, 6.801);
e + CF4 --> e + e + CF3+ + F : k = kel_III(2.575e-14, 0.587, 1.844e+01);
e + CF4 --> e + e + e + CF3+ + F+ : k = kel_III(6.505e-17, 1.073, 3.664e+01);
e + CF4 --> e + e + F + F + CF2+ : k = kel_III(2.951e-15, 0.542, 2.221e+01);
e + CF4 --> e + e + CF3 + F+ : k = kel_III(1.924e-15, 0.722, 3.651e+01);
e + CF4 --> e + e + F2 + F + CF+ : k = kel_III(5.468e-15, 0.432, 3.269e+01);
e + CF4 --> e + F2 + F + CF : k = kel_III(8.727e-16, 0.491, 1.582e+01);
//e + CF4 --> CF3- + F : k = kel_III(2.987e-16, -1.433, 7.29);
```

Πlasma-R modelling using Arrhenius Coefficients

$$R = AT_e{}^n e^{-\frac{c}{T_e}}$$

Pressure: 10 mTorr
Power: 1000 W

CF_3^- removed
F_2^+ removed

Species	Reduced Set	Full Set
CF_4	1.47E+20 m^{-3}	1.46E+20 m^{-3}
F^-	1.98E+16 m^{-3}	2.14E+16 m^{-3}
CF_3	4.41E+19 m^{-3}	4.45E+19 m^{-3}
F	1.60E+20 m^{-3}	1.62E+20 m^{-3}
CF_2	3.20E+19 m^{-3}	3.22E+19 m^{-3}
CF_3^+	3.05E+17 m^{-3}	3.02E+17 m^{-3}
F^+	8.71E+15 m^{-3}	8.81E+15 m^{-3}
CF_2^+	1.99E+17 m^{-3}	2.01E+17 m^{-3}
F_2	2.55E+18 m^{-3}	2.58E+18 m^{-3}
CF^+	8.60E+16 m^{-3}	8.63E+16 m^{-3}
CF	1.24E+19 m^{-3}	1.25E+19 m^{-3}
C	4.80E+18 m^{-3}	4.87E+18 m^{-3}
F^*	2.39E+15 m^{-3}	3.80E+15 m^{-3}
C^+	5.98E+15 m^{-3}	6.04E+15 m^{-3}
T_e	3.29 eV	3.29 eV
n_e	5.85E+17 m^{-3}	5.84E+17 m^{-3}

Reaction set reduced from 110 to 51

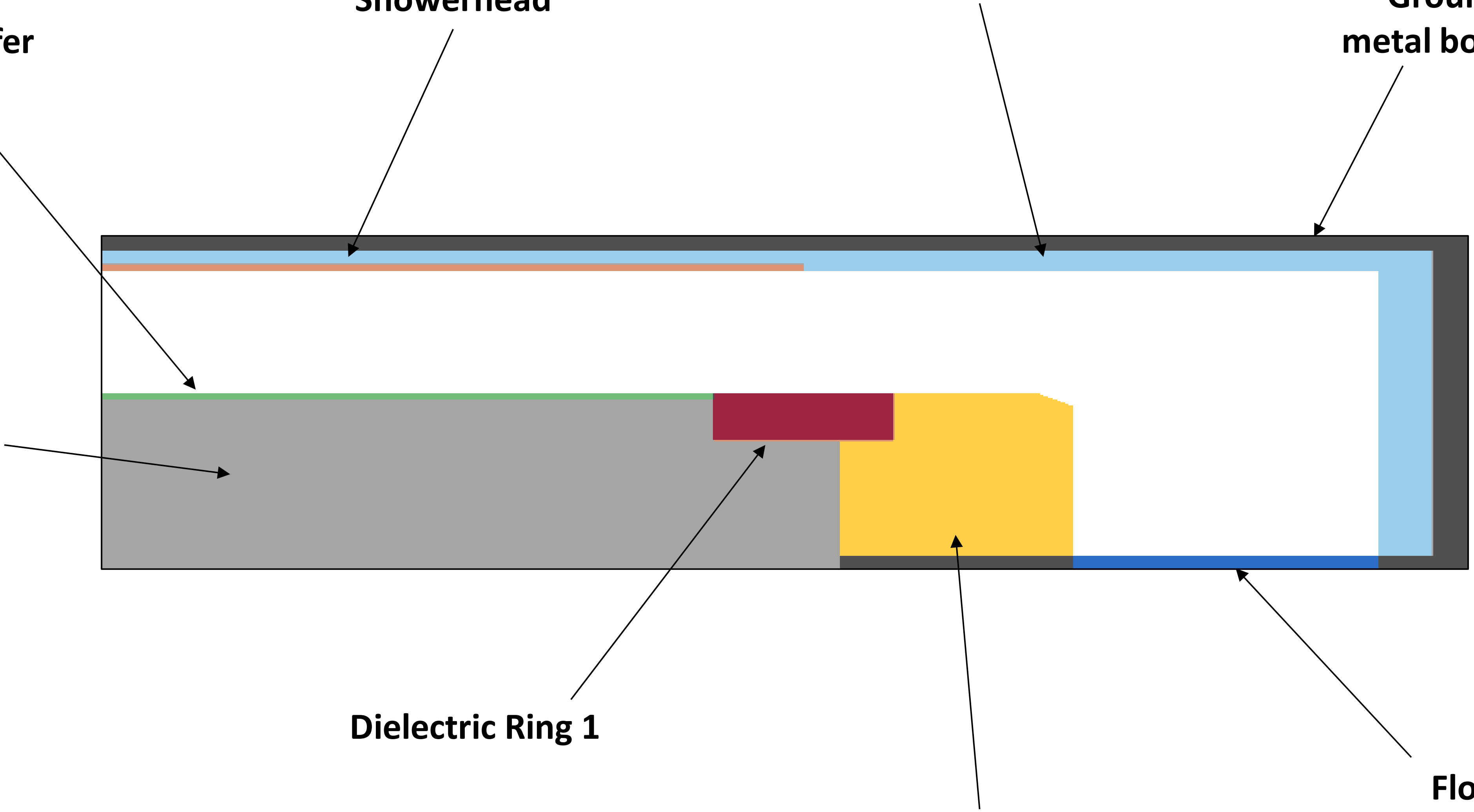
Much easier to integrate into reactor scale modelling!

Reaction Scheme

Charge	**Species**	**Reactions**
Positive	CF_3^+ CF_2^+ CF^+ F^+ C^+	Ionization Charge Exchange Charge Neutralization
Negative	e F^-	Dissociation Charge Neutralization
Neutral	CF_4 CF_3 CF_2 CF F F^* F_2 C	Ionization Dissociation Recombination Charge Exchange

$$F + s \rightarrow F(s)$$
$$CF_{\mathrm{X}} + F(s) \rightarrow CF_{\mathrm{X+1}} + s$$
$$\mathrm{X}^{+} + s \rightarrow \mathrm{X}^{0} + \mathrm{s}$$

Reactor Scale Modelling Using Q-VT (HPEM)



Input Nozzle / Showerhead

Dielectric Vessel

Grounded metal boundary

Silicon Wafer

Powered Electrode

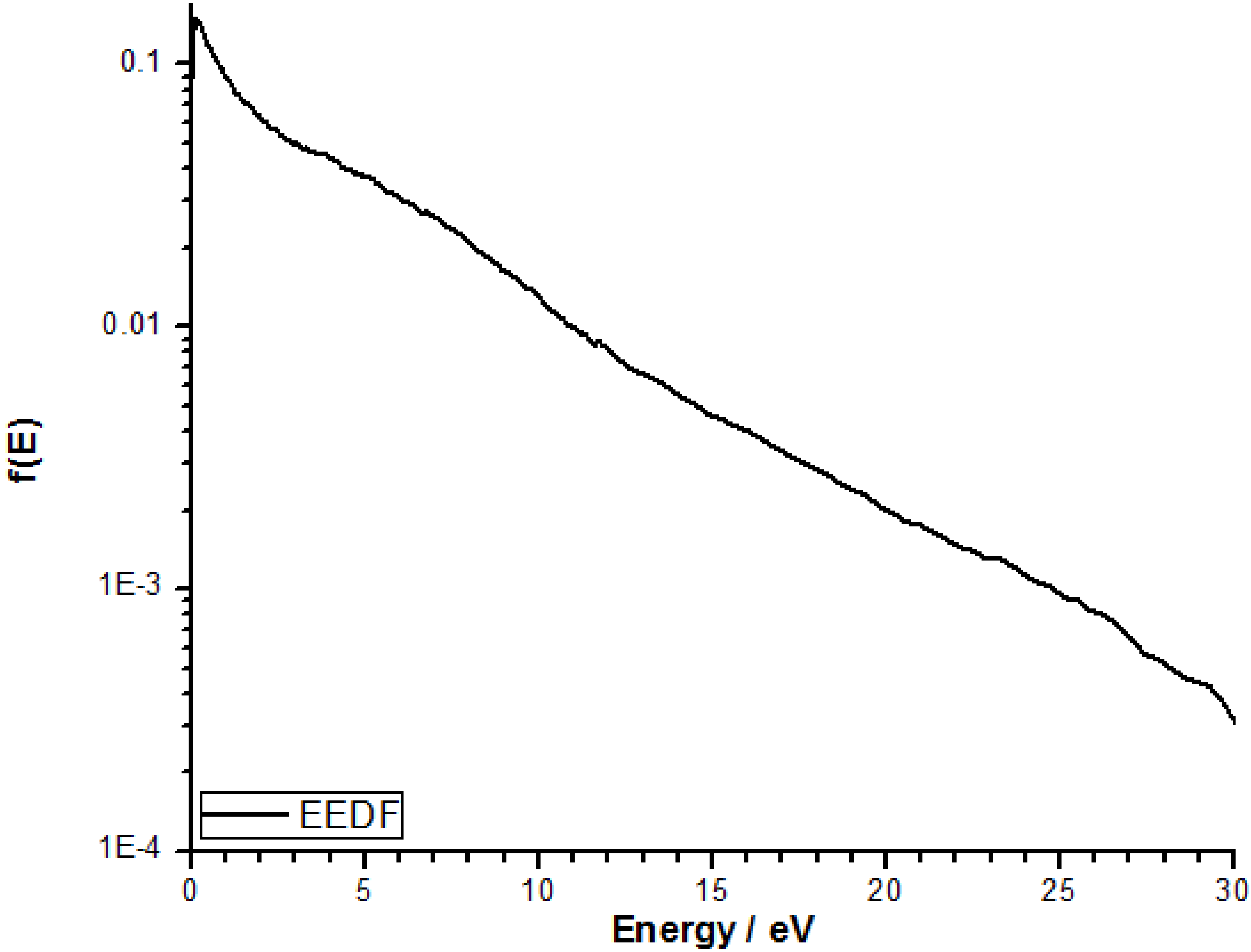
Dielectric Ring 1

Dielectric Ring 2

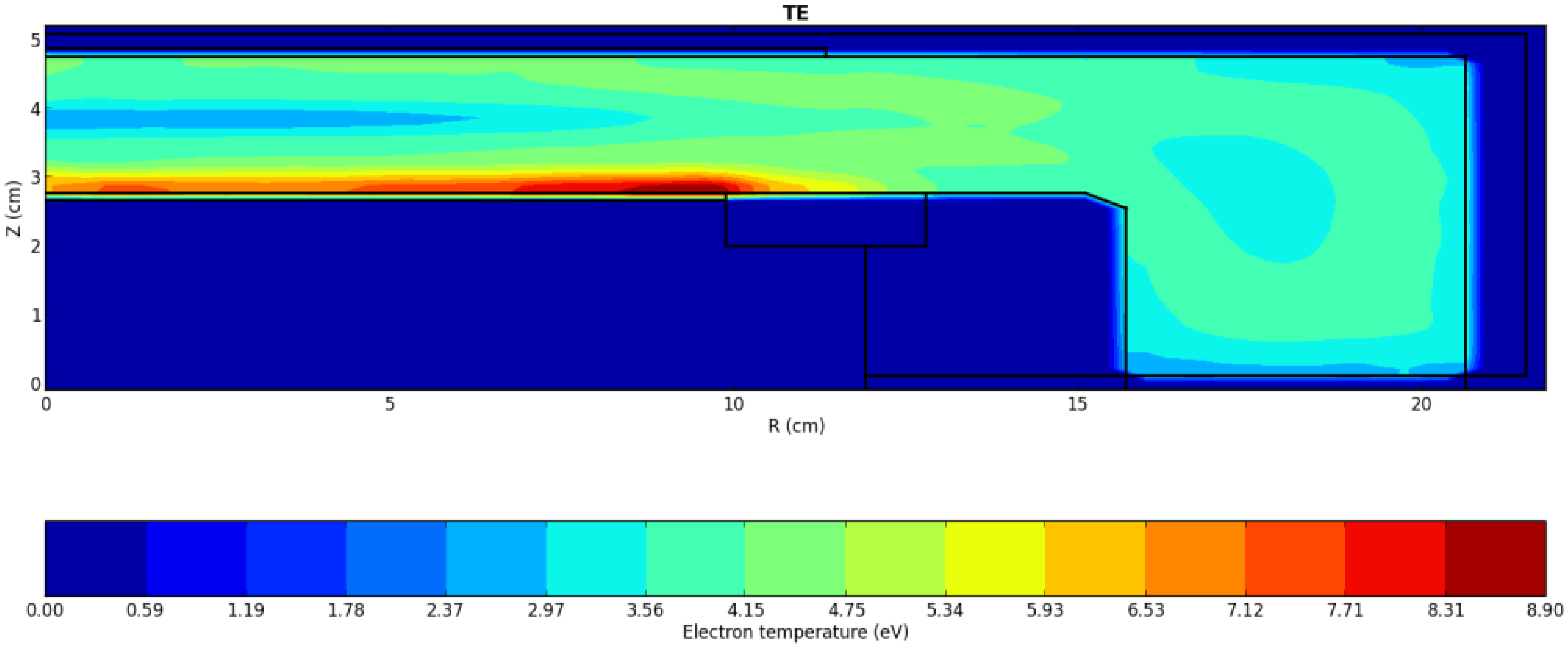
Flow Output

Dual-frequency Powered electrode
High Frequency: 60 MHz, 500 W
Low Frequency: 2 MHz, 500 V

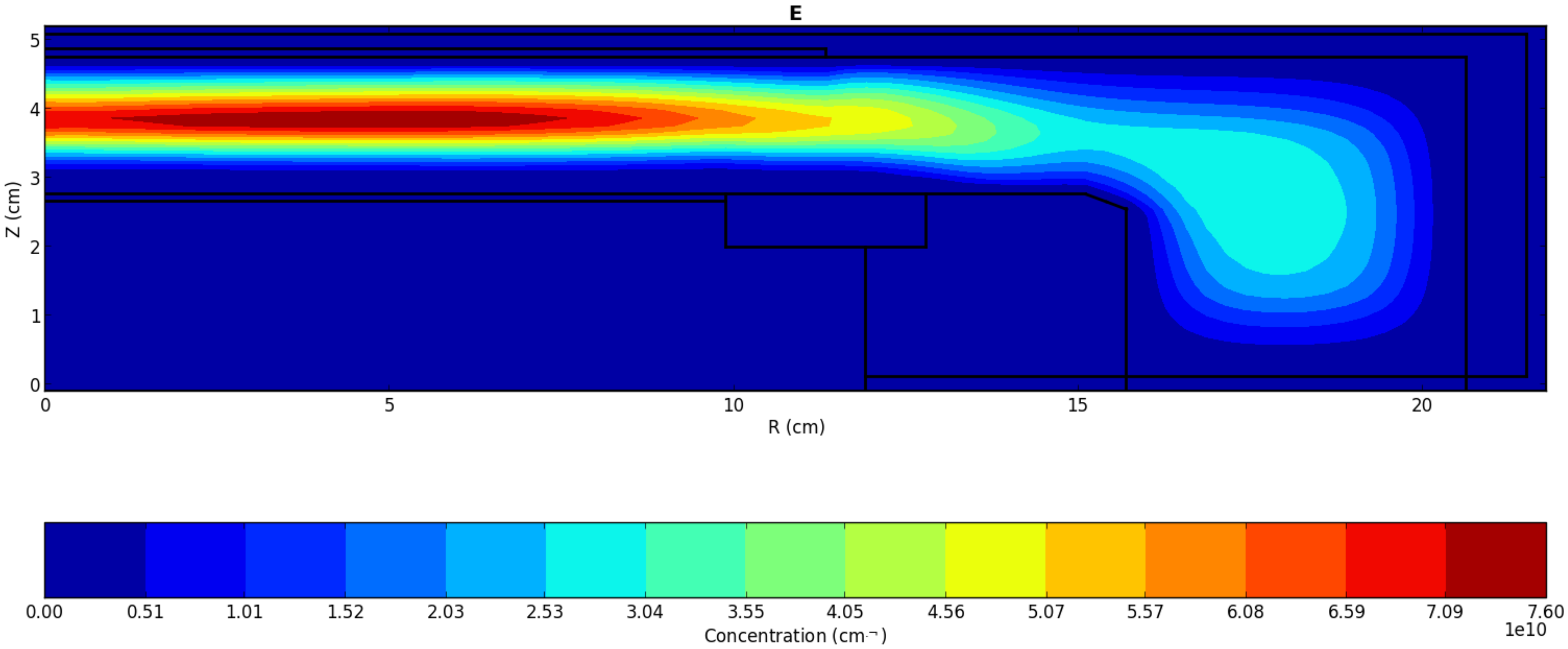
Plasma Discharge Parameter Results



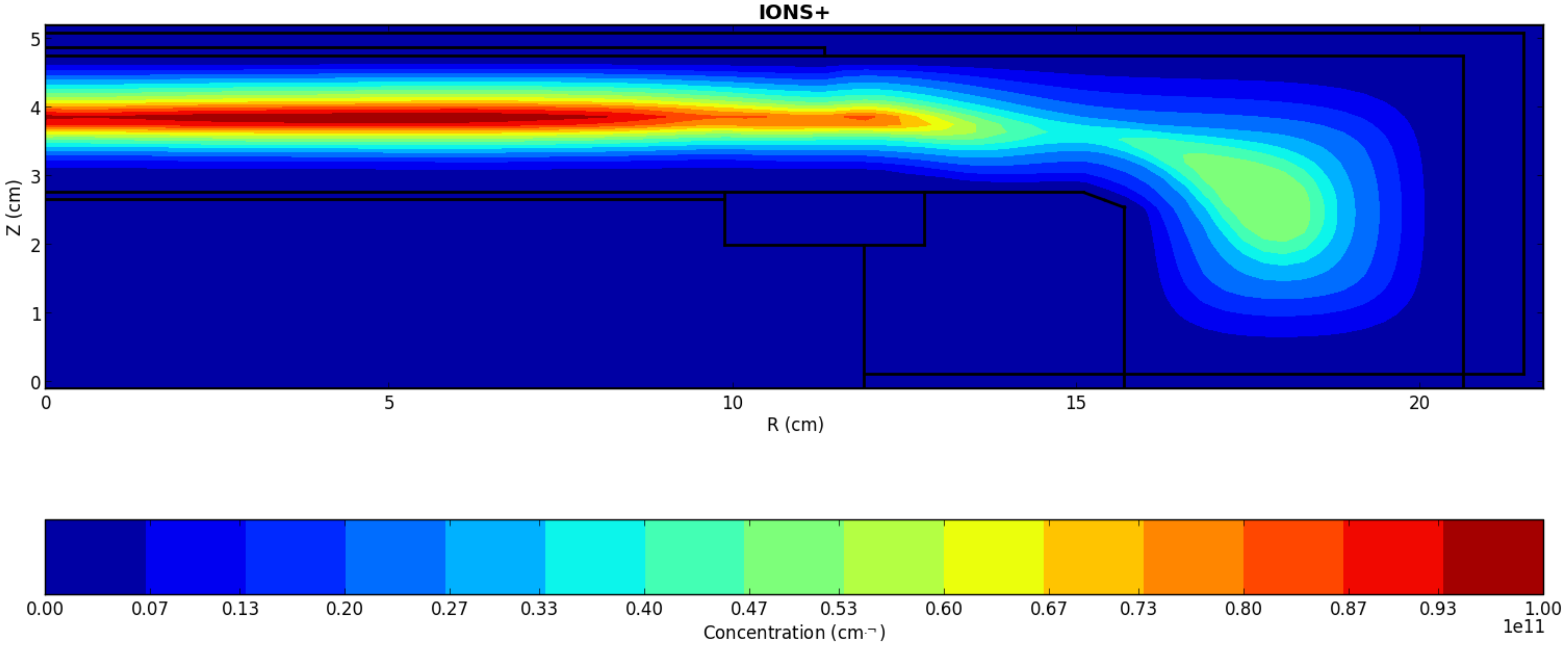
1D Electron Energy Distribution Function



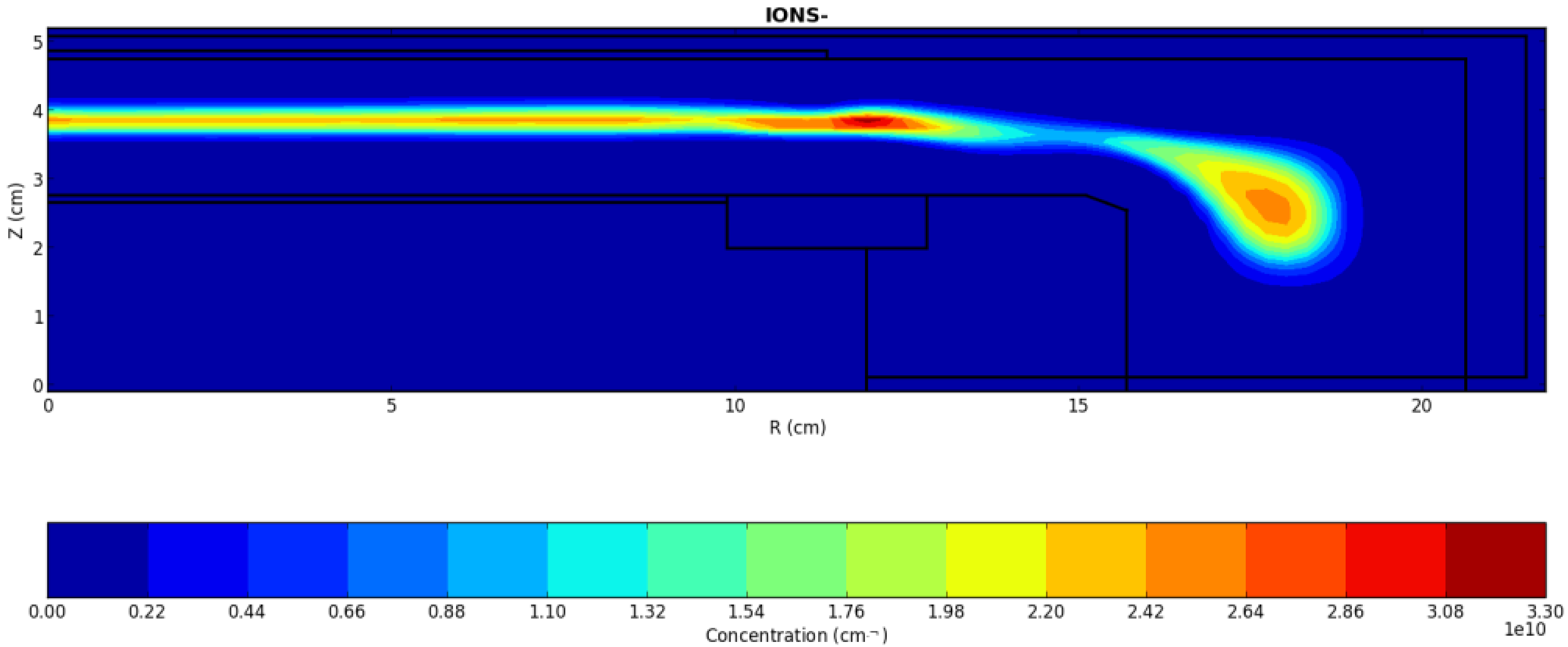
Electron Temperature 2D Distribution



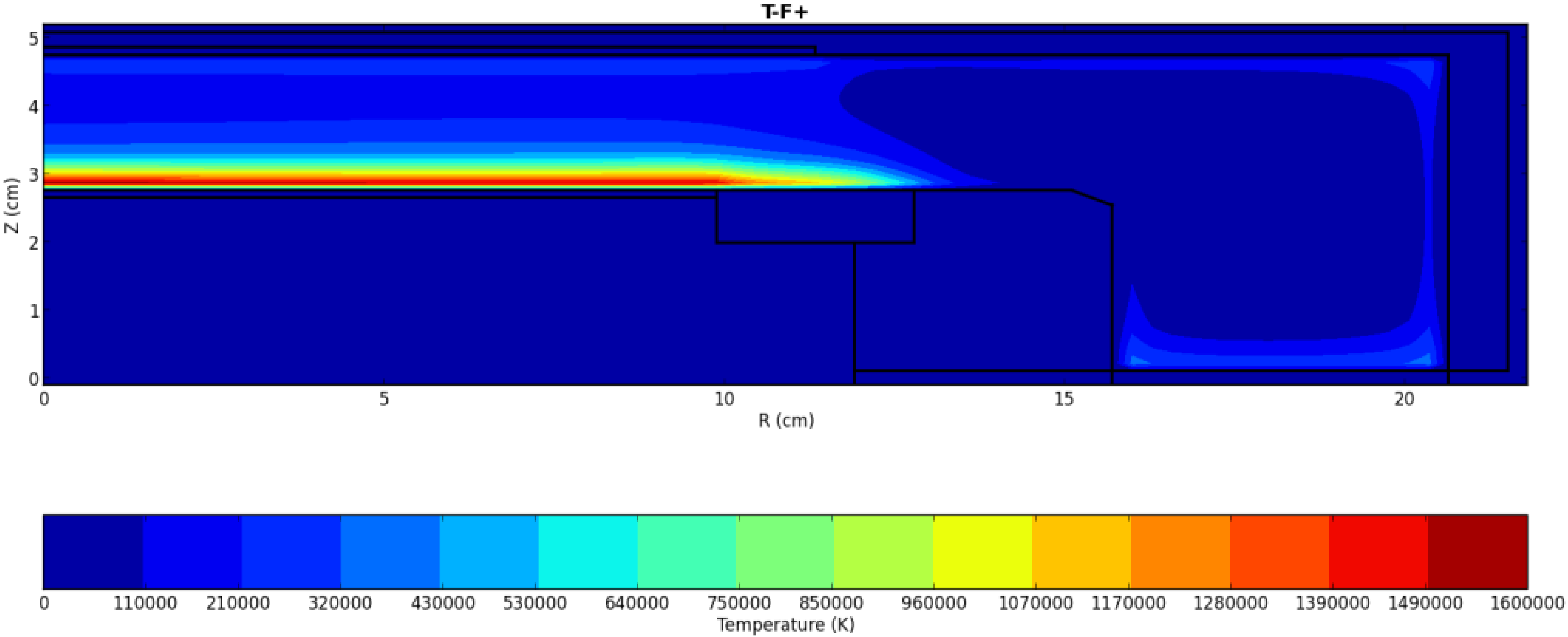
Electron Density 2D Distribution



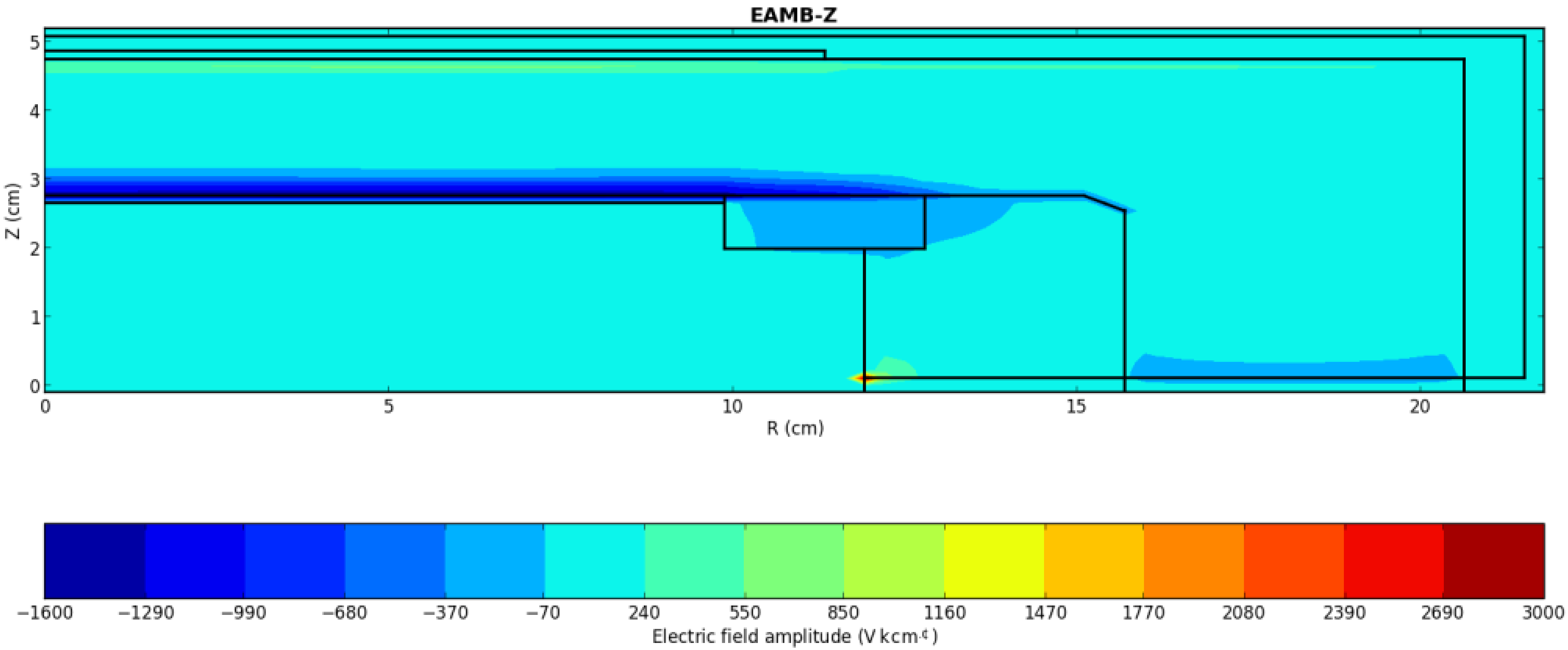
Positive Ion Density 2D Distribution



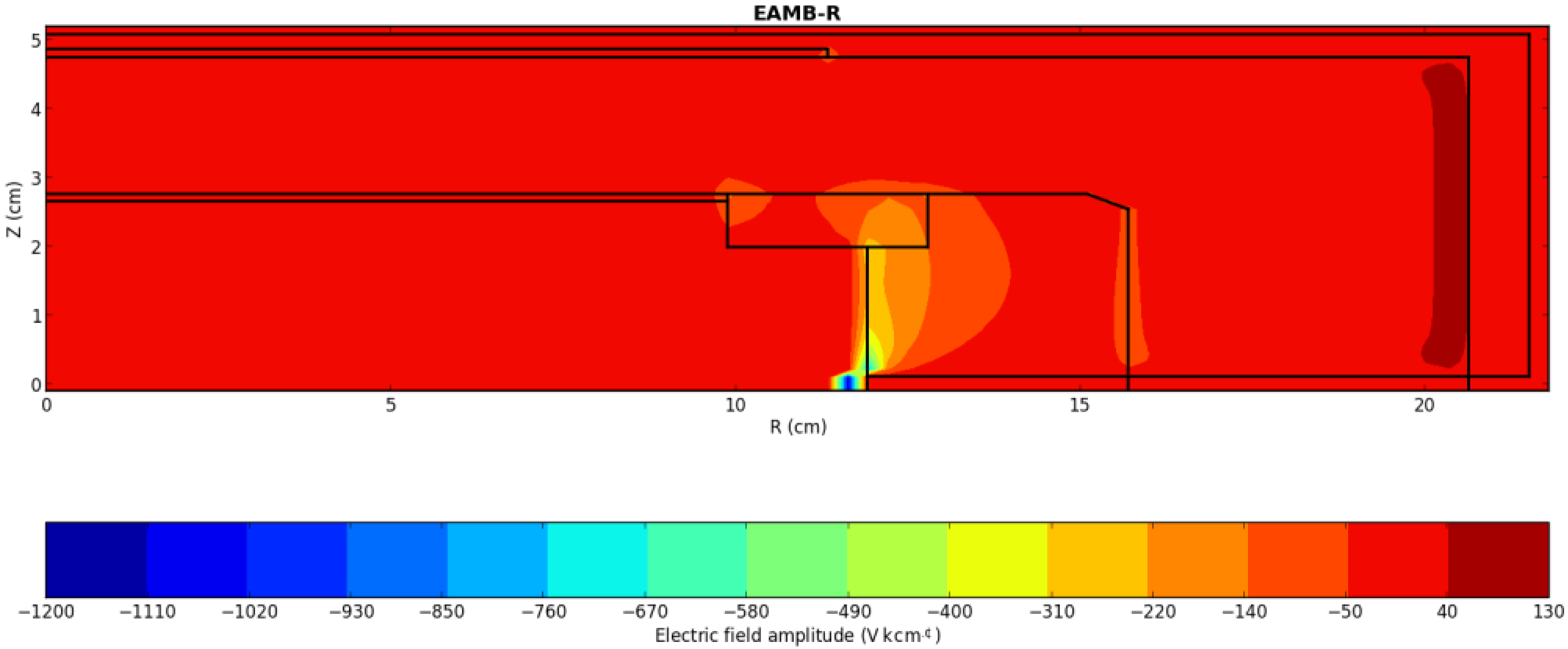
Negative Ion Density 2D Distribution



F^+ Ion Temperature 2D Distribution

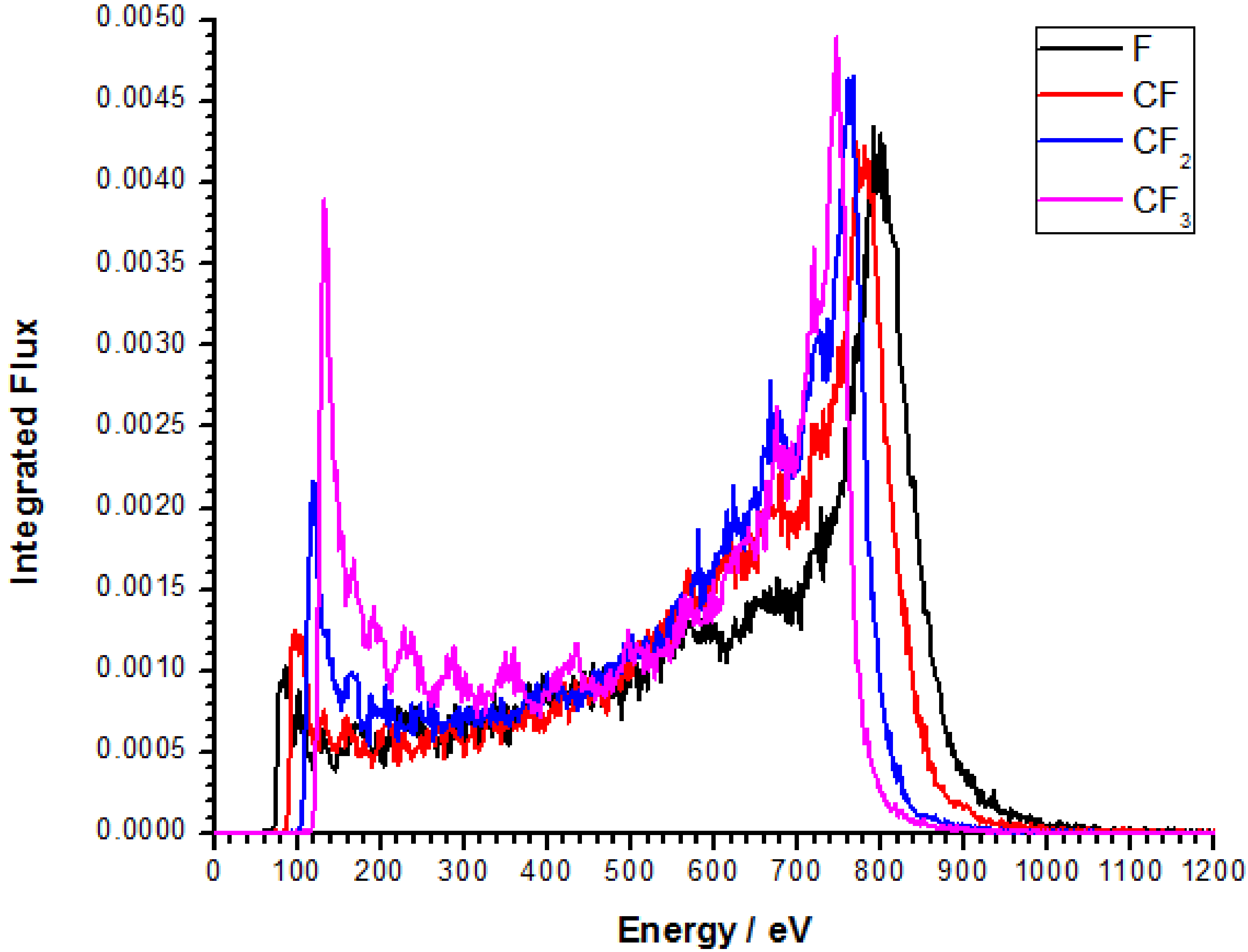


Axial Electric Field 2D Distribution

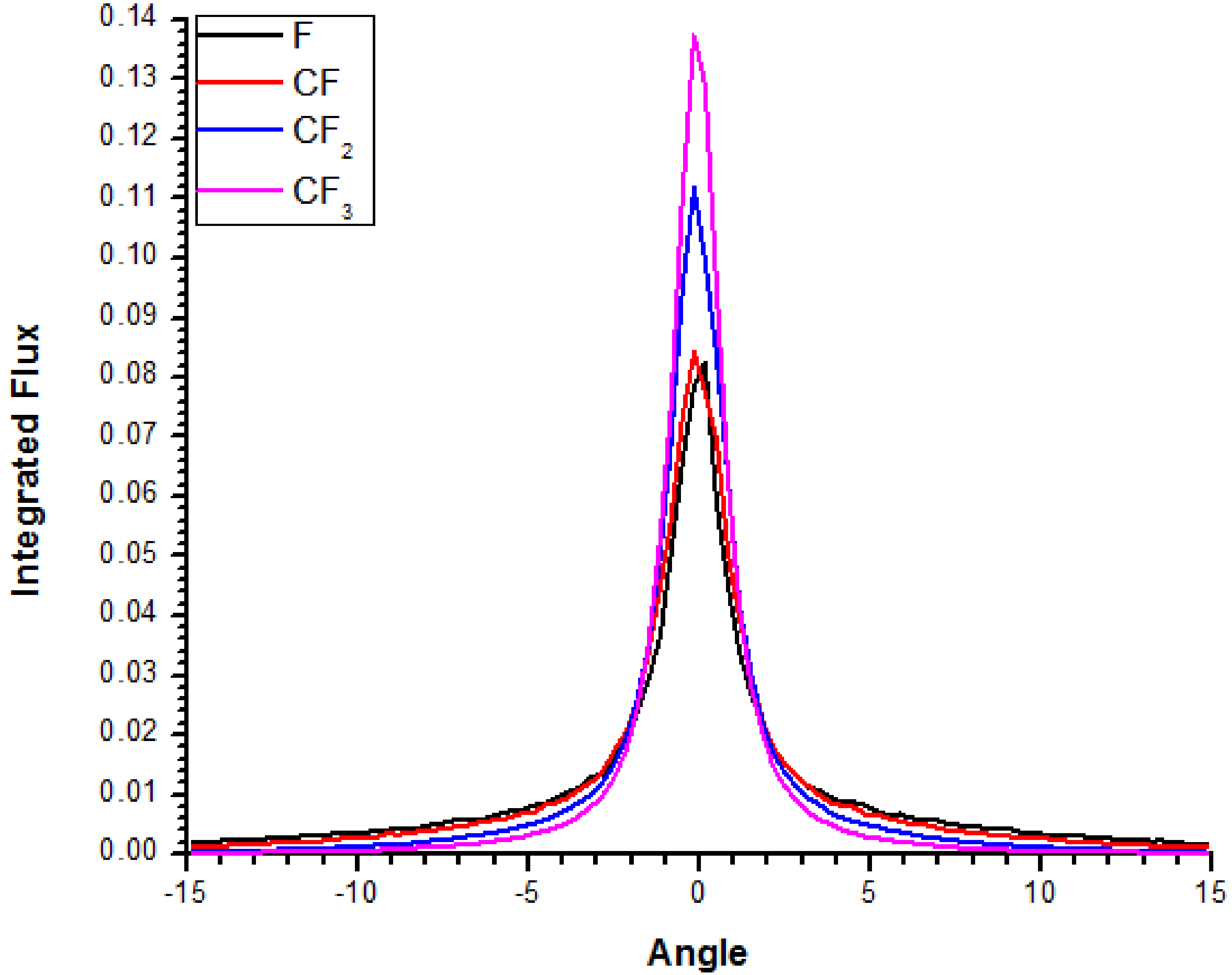


Radial Electric Field 2D Distribution

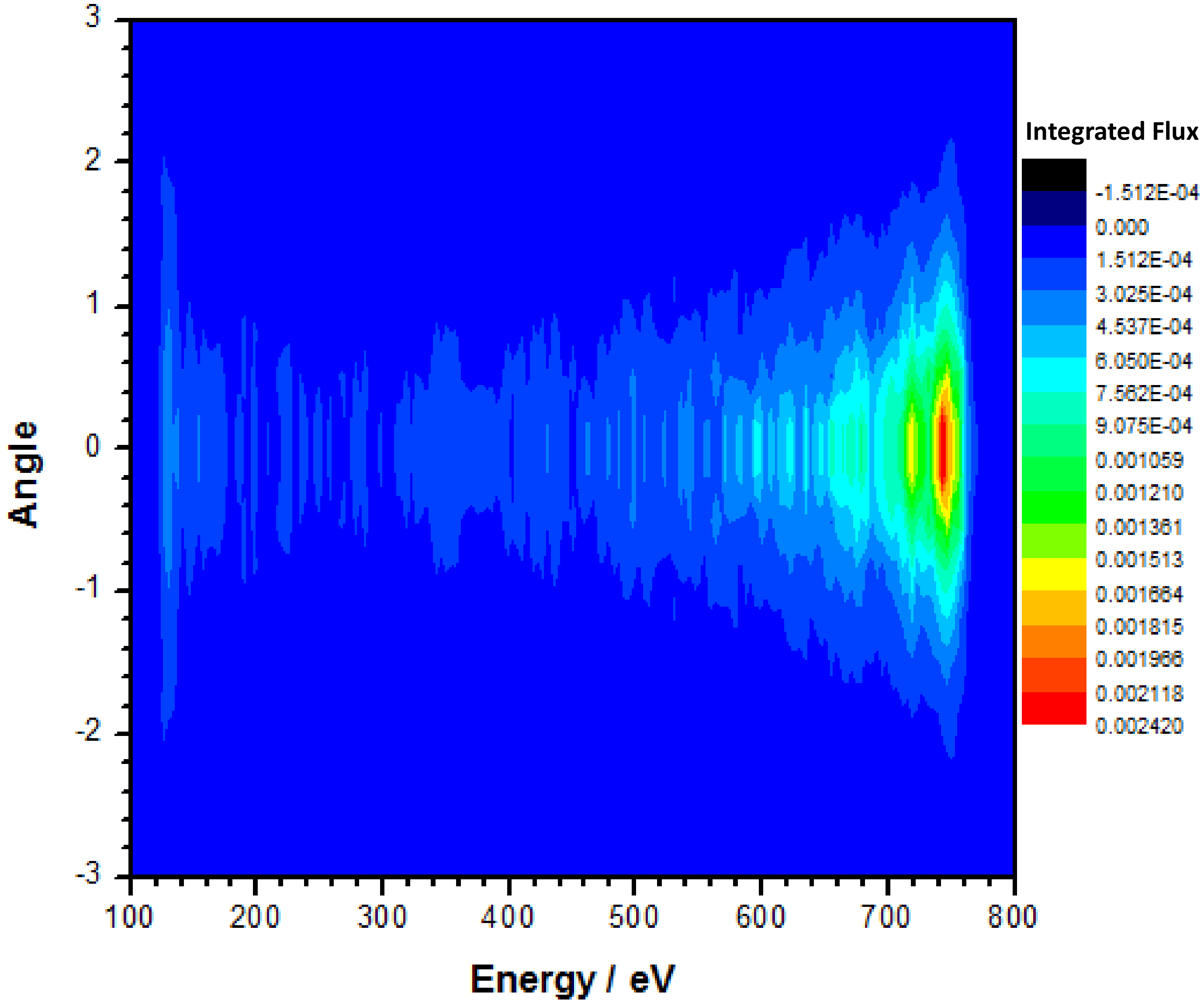
Surface Results using the Plasma Chemistry Monte Carlo (PCMC) Module



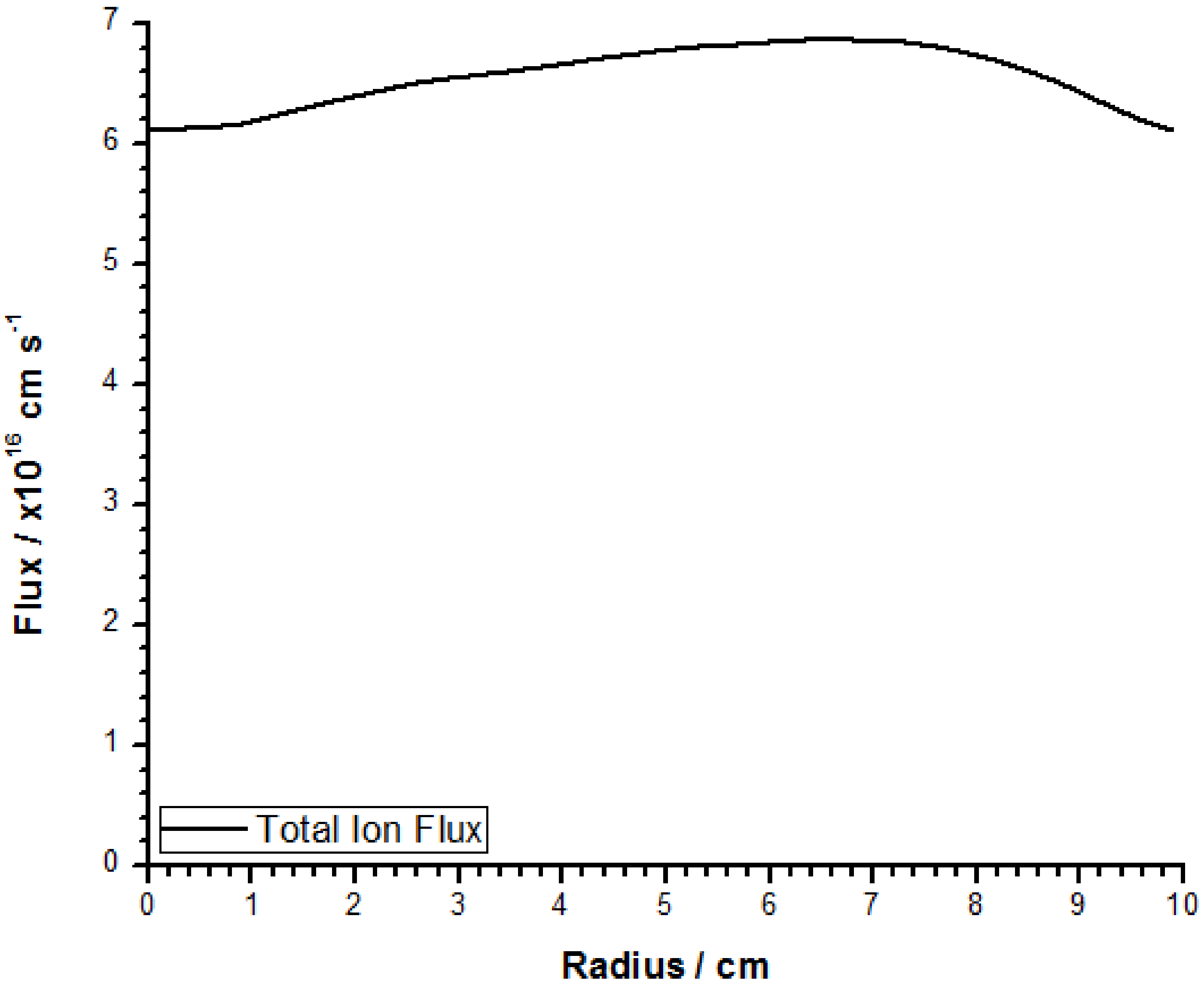
1D Ion Energy Distributions



1D Ion Angle Distributions



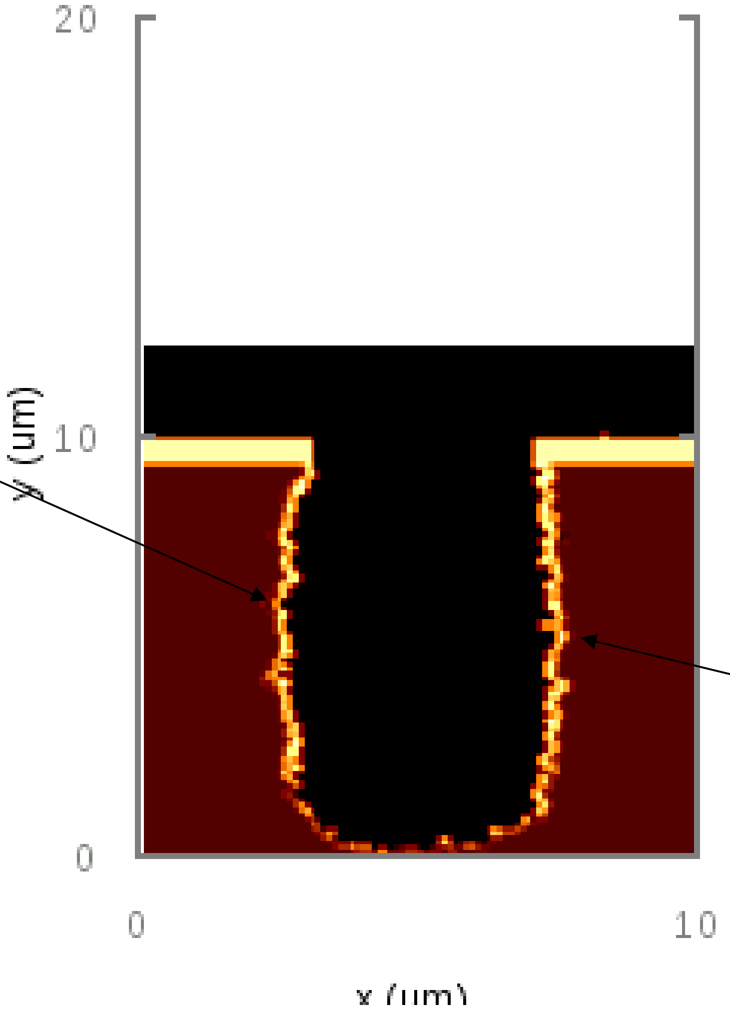
2D Total Ion Angle/Energy Distribution



Total Ion Flux to the Wafer

Feature Profile Modelling using the Monte Carlo Feature Profile Modeller (MCFPM)

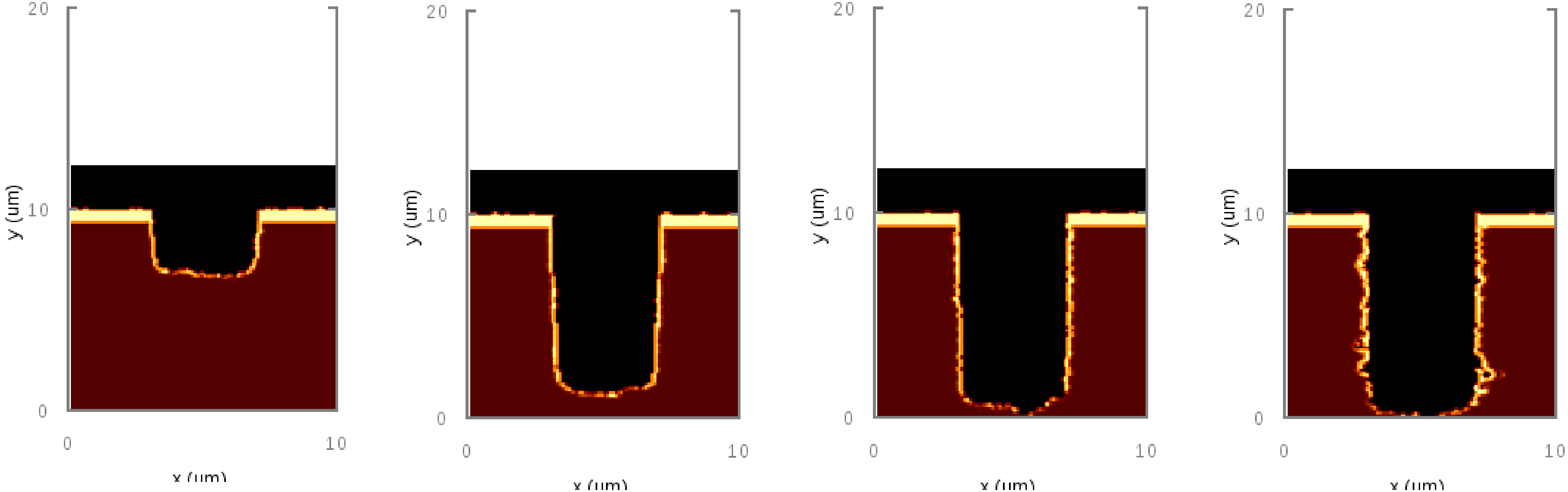
Etch Profile Obtained from Reactor Simulation Output



Rough sidewalls due to incomplete anisotropy and total ion flux

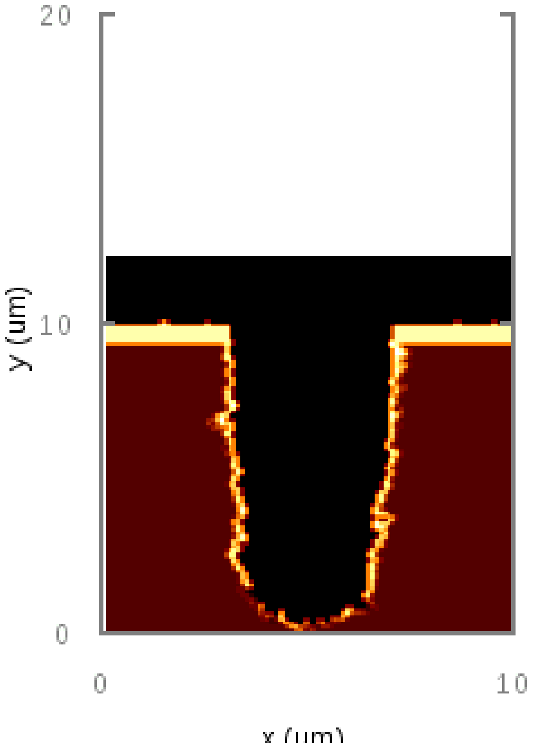
Bowing due to neutral scattering in the trench

Variation of F:CF Ratio

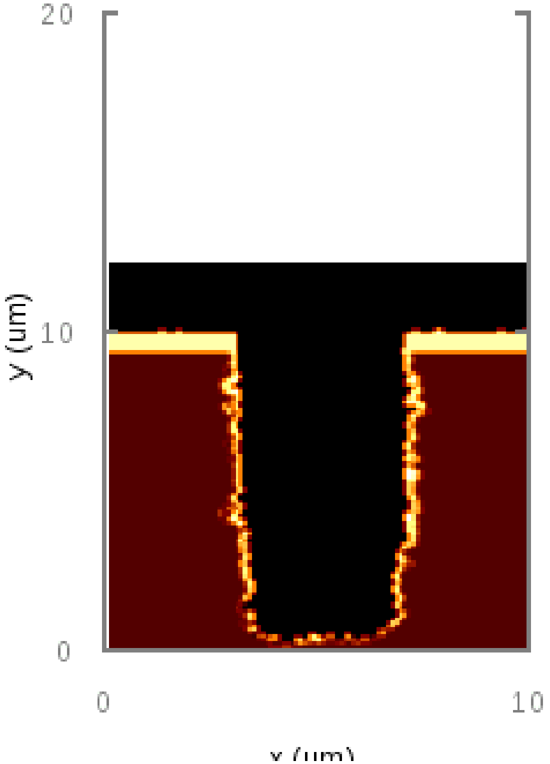


1:1 **4:1** **10:1** **20:1**

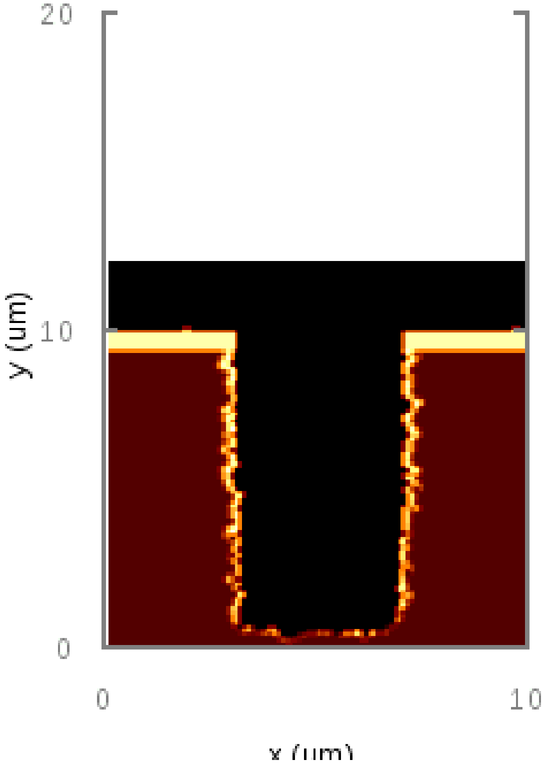
Variation of Energy Range



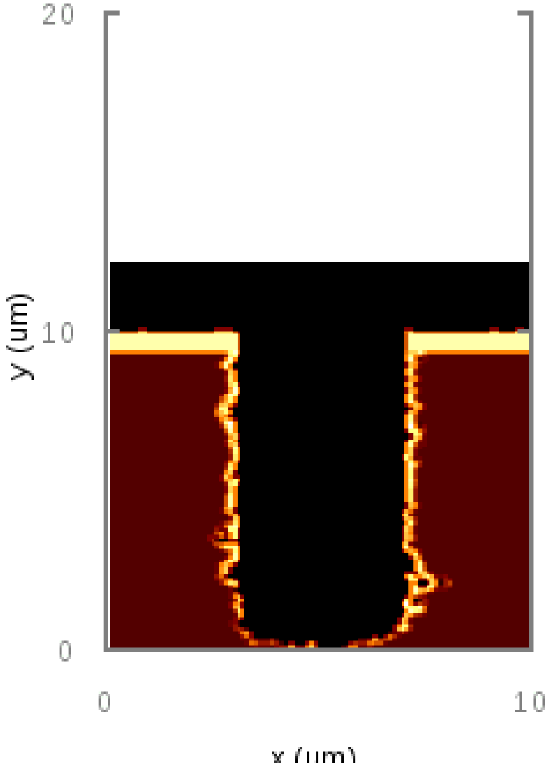
1.5 – 12.5 eV



6.25 – 50 eV

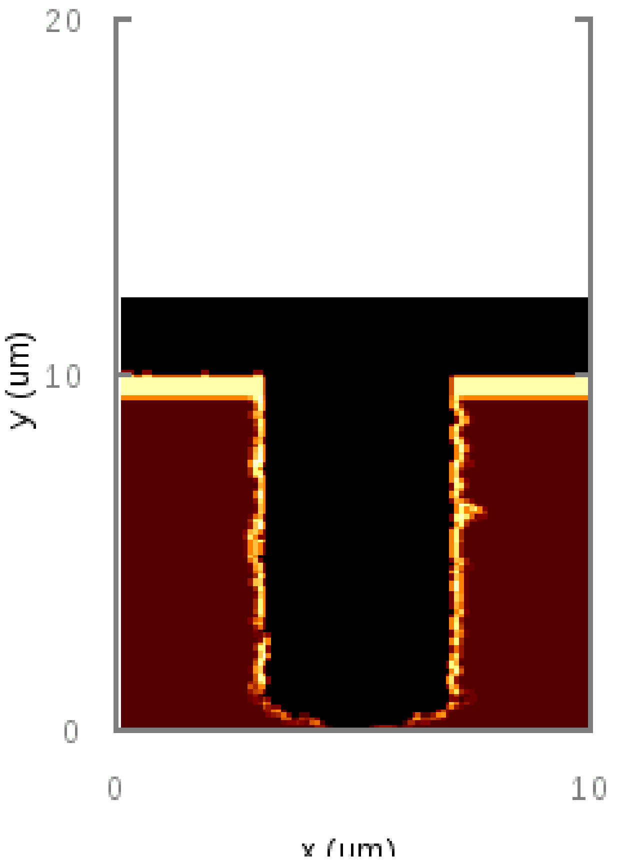


25 – 200 eV

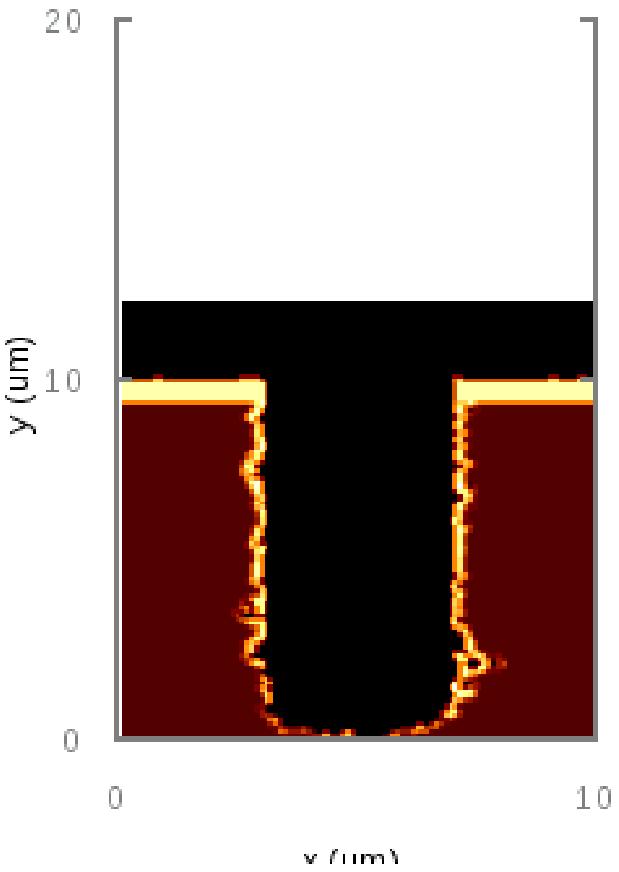


100 – 800 eV

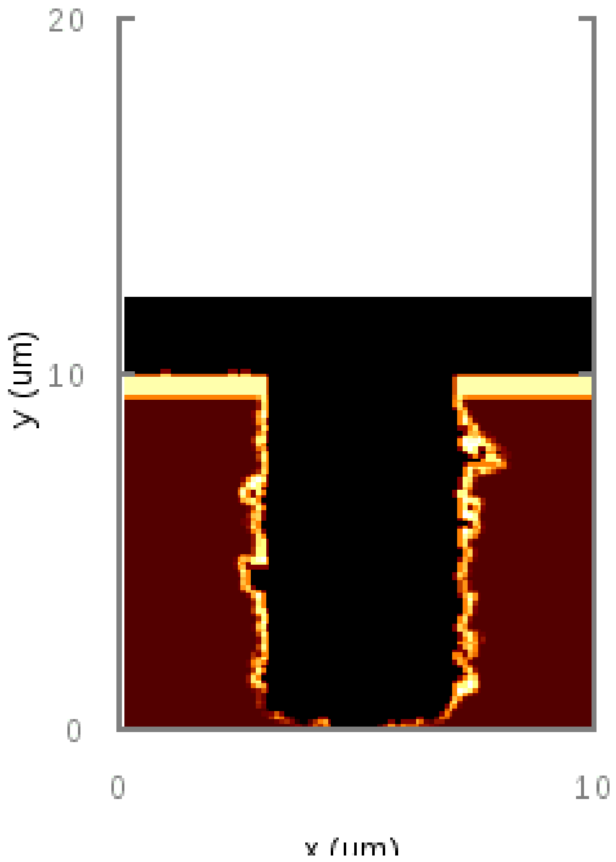
Variation of Angular Spread



Δ 0.5°



Δ 1°

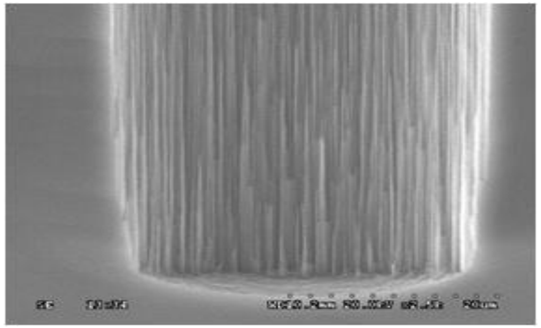


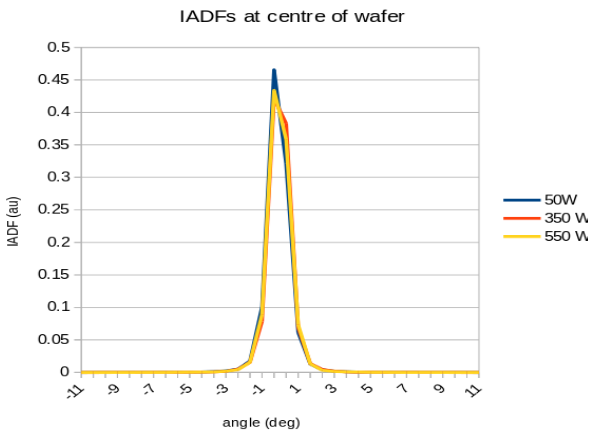
Δ 2°

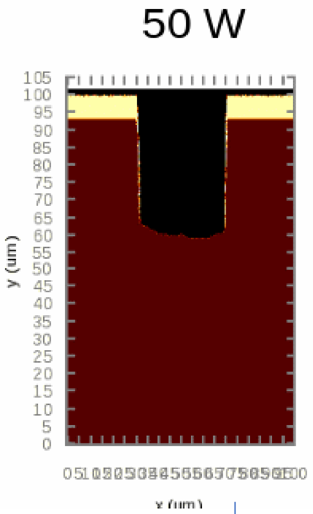
Further Profile Modelling

Tilt

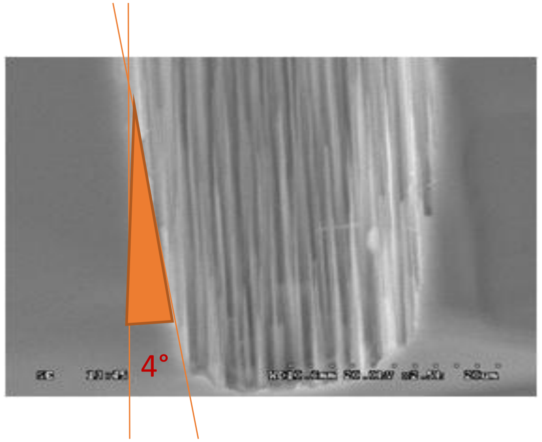
Middle of the wafer

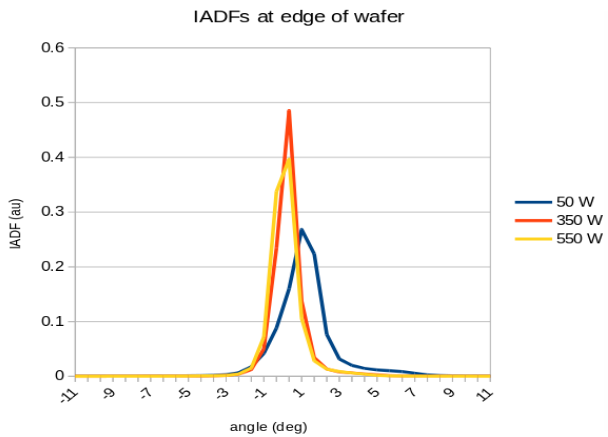


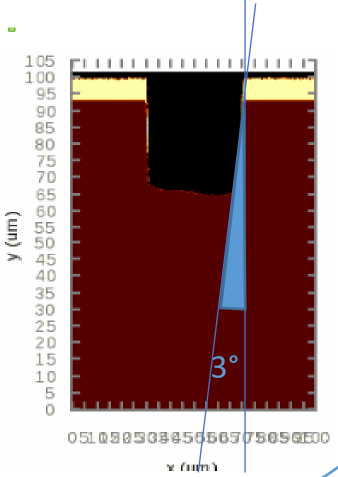




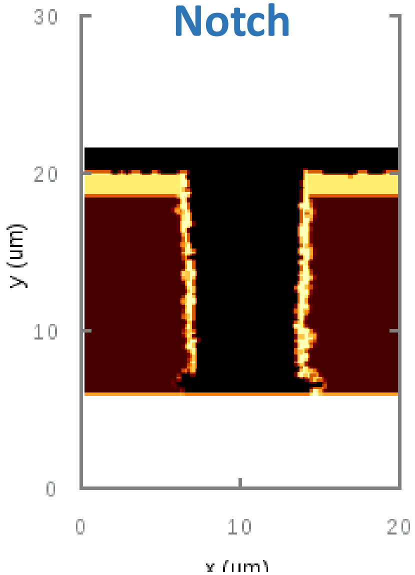
Edge of the wafer

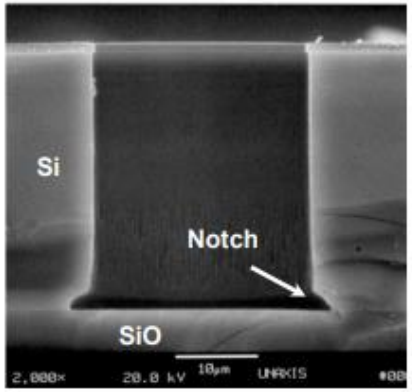


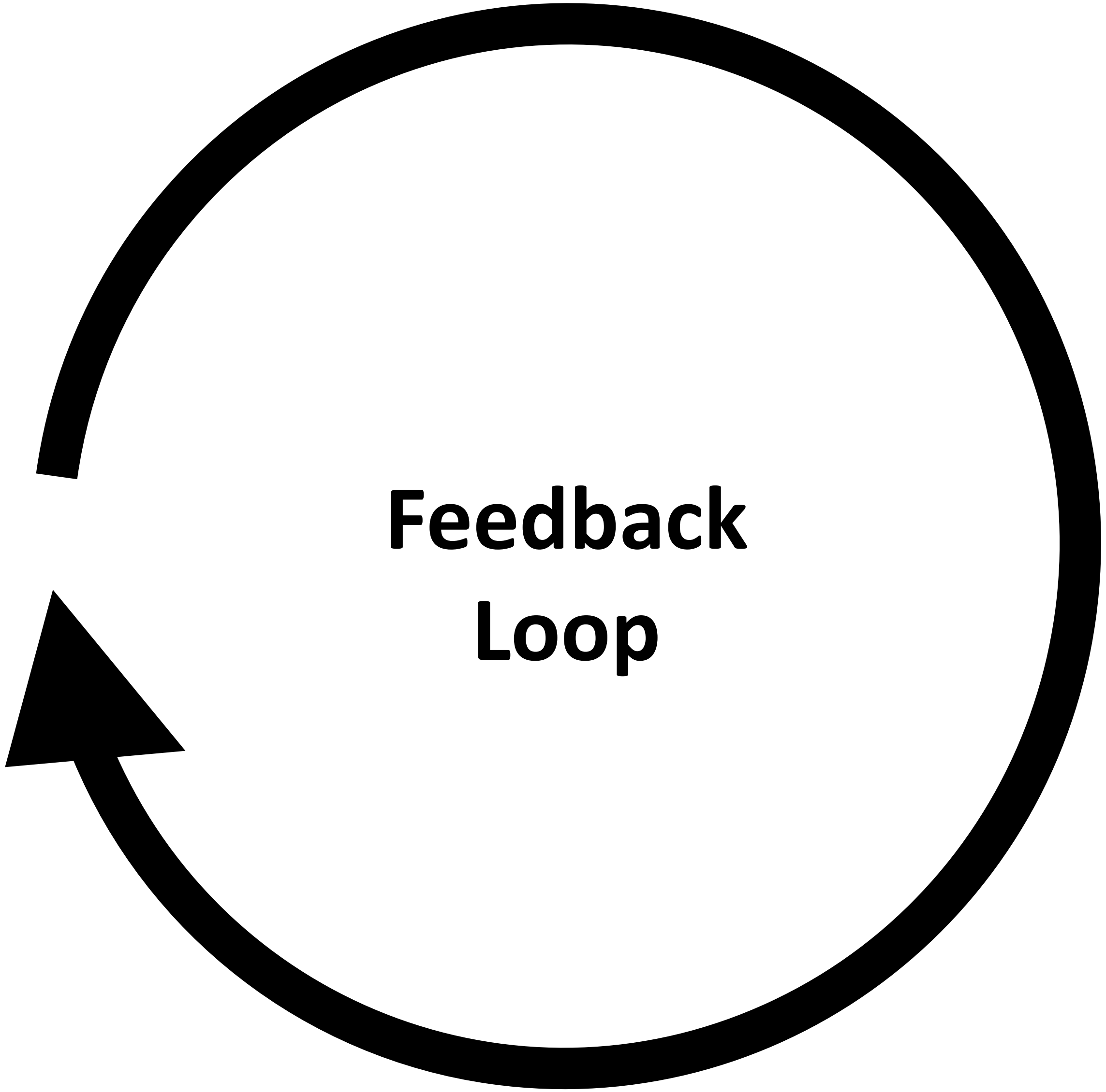




Notch







Feedback Loop

Theoretically, can have the opportunity to first run the MCFPM to look for favourable fluxes and distributions and then use the QVT (HPEM) reactor model to find the parameter settings yielding these parameters

Conclusions

- The work flow of innovation and progress in plasma physics should aim to connect the plasma behaviour to the final substrate
- This can be done in a modular fashion; using separate but relevant tools to tackle specific parts of the whole problem
    - Breaking a problem down into its constituents!
- At each step, full control over the evolution of the problem and its solution is enabled by modelling techniques
- More complex problems such as chemical vapour deposition, the study of different discharges such as ECR's, sputtering deposition of multi-compound substrates can be tackled this way
- Experts at **Quantemol Ltd** are able to provide a step by step investigation of many physical processes by using a wide variety of techniques as shown