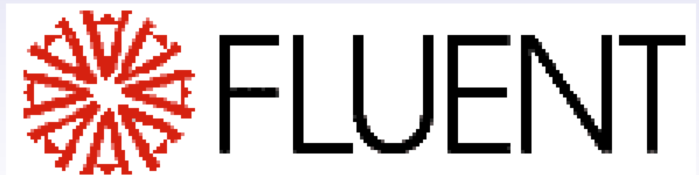
3D SIMULATION

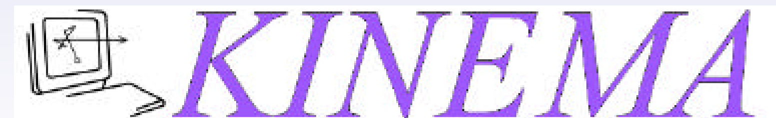
OF

PLASMA DISCHARGES

IN THE

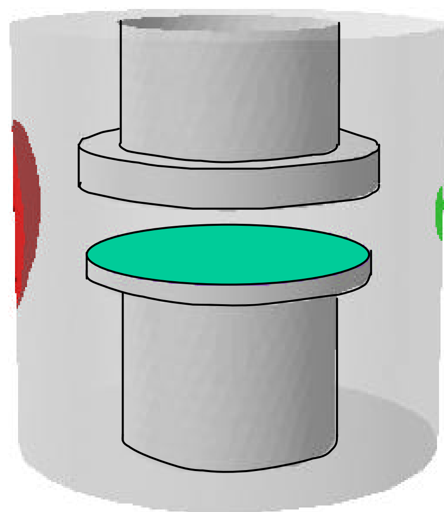
GEC REFERENCE CELL





COMPUTATIONAL METHOD:

CODE COUPLING: PLASMATOR Computes the Electron Energy and Distribution and Passes Them on to FLUENT



PLASMATOR

Full plasma chemistry is utilized to compute:

- electron energy and distribution
- ion transport and distribution

N_e, T_e

$\mathbf{r}_{neut}(x,y,z)$

FLUENT

A reduced chemistry set is utilized along with the equilibrium electrons to compute:

- neutral species composition
- 3-Dimensional transport

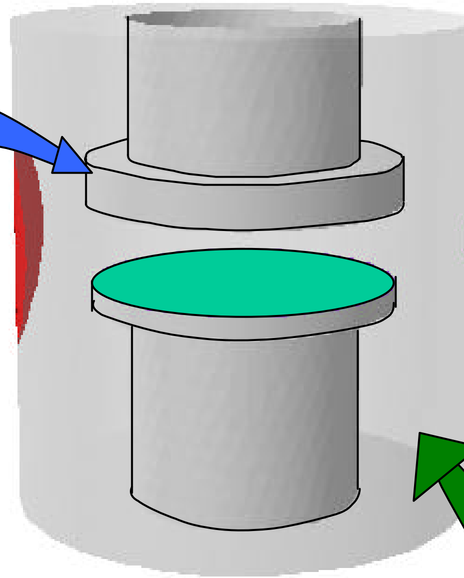
CODE STRENGTHS: Each Code is Utilized in the Physical Regime Where it Excels

PLASMATOR

Plasma Model:

- **Continuity**
- **Ion Transport**
  - -full momentum equations
  - -electric field body force
- **Electron Energy & Transport**
- **Chemistry**
  - -electron impact
    - -excitation
    - -ionization
  - -meta-Stable quenching
  - -ion neutralization

Typical Model: 40 species
100 reactions



FLUENT

Flow Model:

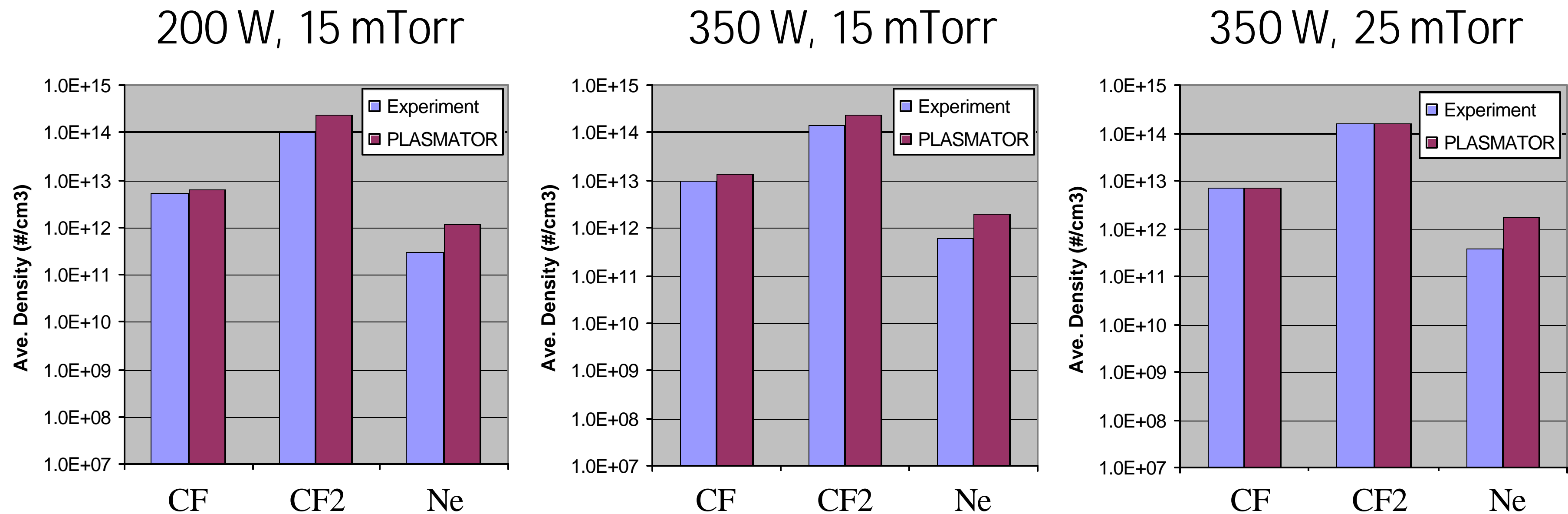
- **Continuity**
- **Neutral Transport**
  - -convection
  - -diffusion
- **Ion Transport**
  - -ambipolar model
- **Chemistry**
  - -electron impact
    - -excitation
    - -ionization
  - -meta-Stable quenching
  - -ion neutralization
  - -deposition

Typical Model: 10 species
15 reactions

Reduced chemistry model allows fast 3D simulation with minimal loss in accuracy

CODE VALIDATION: PLASMATOR is a Mature, Robust, and Accurate Plasma Simulation Code

GEC Reference Cell C_4F_8 ICP Discharge*

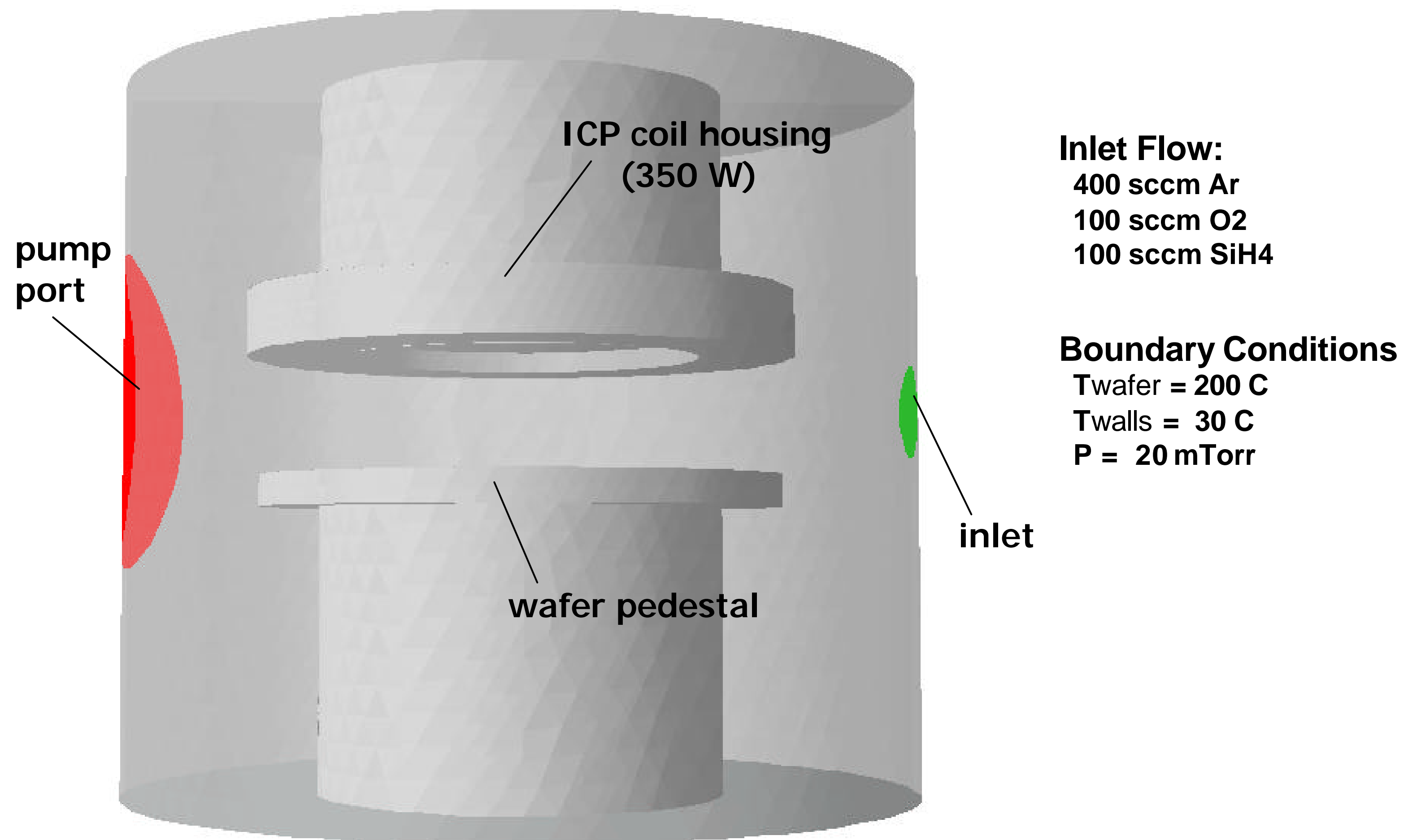


* Measurements courtesy of Karla Waters & Harold Anderson at the University of New Mexico

INDUCTIVELY COUPLED PLASMA

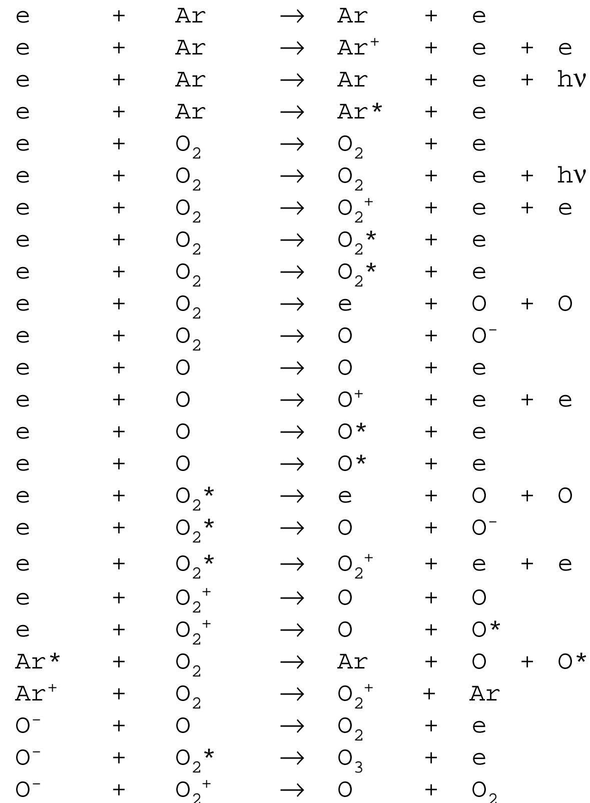
OXIDE DEPOSITION

ICP SIMULATION: The Standard GEC Reference Cell Geometry is Computed During Oxide Deposition



ICP SIMULATION: PLASMATOR Utilizes a Comprehensive Chemistry Model to Characterize the Equilibrium Electrons

Plasma Reactions



$e + Ar \rightarrow Ar + e$

$e + Ar \rightarrow Ar^+ + e + e$

$e + Ar \rightarrow Ar + e + h\nu$

$e + Ar \rightarrow Ar^* + e$

$e + O_2 \rightarrow O_2 + e$

$e + O_2 \rightarrow O_2 + e + h\nu$

$e + O_2 \rightarrow O_2^+ + e + e$

$e + O_2 \rightarrow O_2^* + e$

$e + O_2 \rightarrow O_2^* + e$

$e + O_2 \rightarrow e + O + O$

$e + O_2 \rightarrow O + O^-$

$e + O \rightarrow O + e$

$e + O \rightarrow O^+ + e + e$

$e + O \rightarrow O^* + e$

$e + O \rightarrow O^* + e$

$e + O_2^* \rightarrow e + O + O$

$e + O_2^* \rightarrow O + O^-$

$e + O_2^* \rightarrow O_2^+ + e + e$

$e + O_2^+ \rightarrow O + O$

$e + O_2^+ \rightarrow O + O^*$

$Ar^* + O_2 \rightarrow Ar + O + O^*$

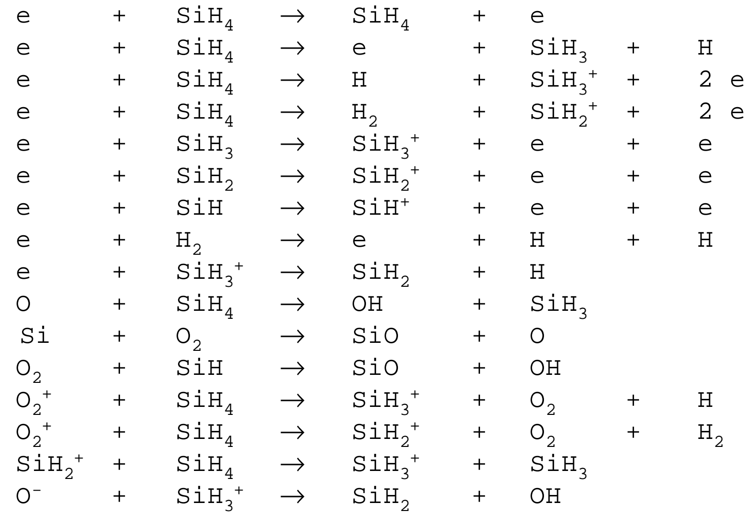
$Ar^+ + O_2 \rightarrow O_2^+ + Ar$

$O^- + O \rightarrow O_2 + e$

$O^- + O_2^* \rightarrow O_3 + e$

$O^- + O_2^+ \rightarrow O + O_2$

Plasma Reactions (continued)



$e + SiH_4 \rightarrow SiH_4 + e$

$e + SiH_4 \rightarrow e + SiH_3 + H$

$e + SiH_4 \rightarrow H + SiH_3^+ + 2e$

$e + SiH_4 \rightarrow H_2 + SiH_2^+ + 2e$

$e + SiH_3 \rightarrow SiH_3^+ + e + e$

$e + SiH_2 \rightarrow SiH_2^+ + e + e$

$e + SiH \rightarrow SiH^+ + e + e$

$e + H_2 \rightarrow e + H + H$

$e + SiH_3^+ \rightarrow SiH_2 + H$

$O + SiH_4 \rightarrow OH + SiH_3$

$Si + O_2 \rightarrow SiO + O$

$O_2 + SiH \rightarrow SiO + OH$

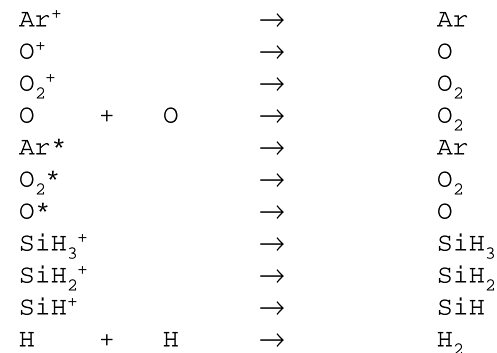
$O_2^+ + SiH_4 \rightarrow SiH_3^+ + O_2 + H$

$O_2^+ + SiH_4 \rightarrow SiH_2^+ + O_2 + H_2$

$SiH_2^+ + SiH_4 \rightarrow SiH_3^+ + SiH_3$

$O^- + SiH_3^+ \rightarrow SiH_2 + OH$

Surface Reactions



$Ar^+ \rightarrow Ar$

$O^+ \rightarrow O$

$O_2^+ \rightarrow O_2$

$O + O \rightarrow O_2$

$Ar^* \rightarrow Ar$

$O_2^* \rightarrow O_2$

$O^* \rightarrow O$

$SiH_3^+ \rightarrow SiH_3$

$SiH_2^+ \rightarrow SiH_2$

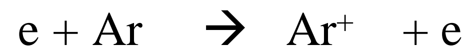
$SiH^+ \rightarrow SiH$

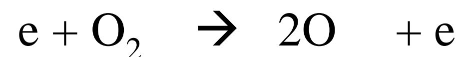
$H + H \rightarrow H_2$

ICP SIMULATION: FLUENT Utilizes a Reduced Chemistry Model to Allow Fast 3D Simulation

Ar / SiH4 / O2 FLUENT Oxide Deposition Chemistry

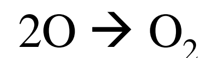
Electron Impact Chemistry

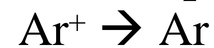

$e + Ar \rightarrow Ar^{+} + e$

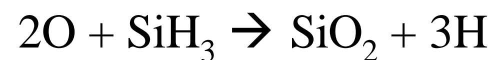

$e + O_2 \rightarrow 2O + e$

$e + SiH_4 \rightarrow SiH_3 + H + e$

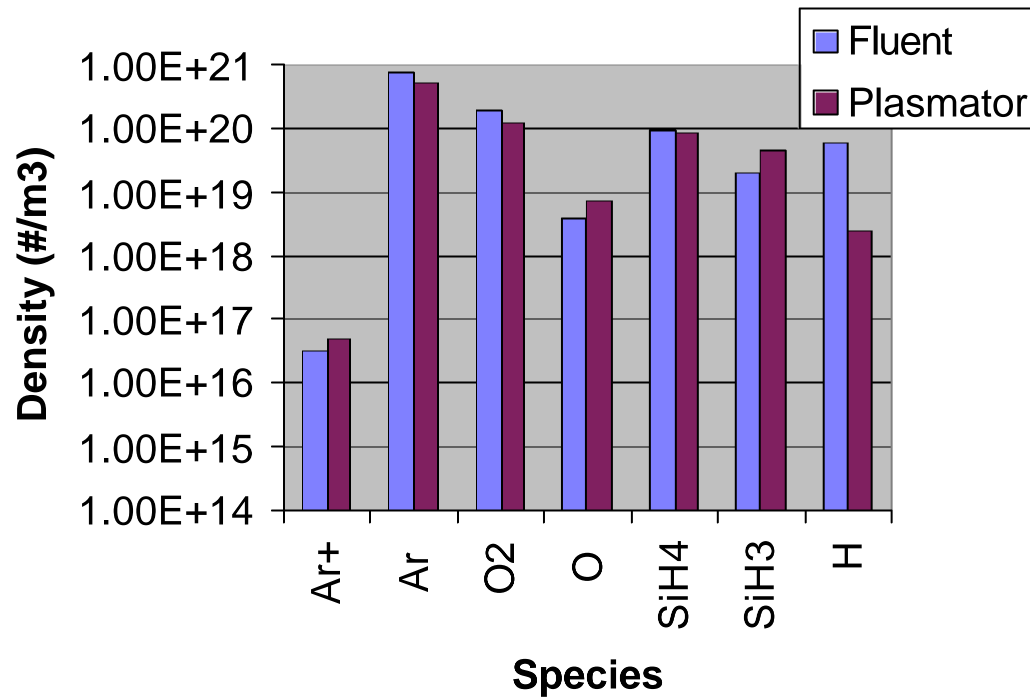
Surface Chemistry


$2O \rightarrow O_2$


$Ar^{+} \rightarrow Ar$


$2O + SiH_3 \rightarrow SiO_2 + 3H$

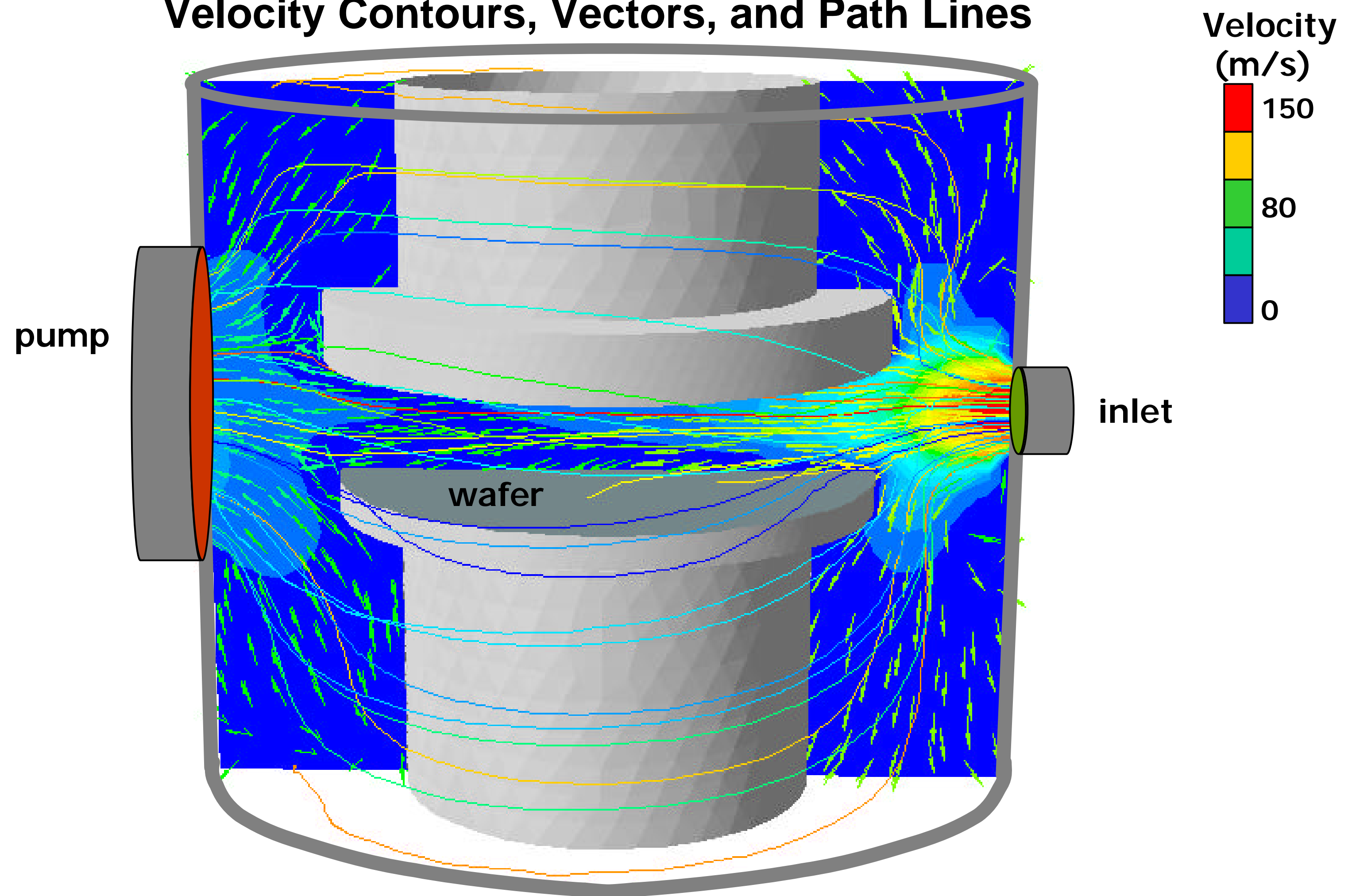
ICP SIMULATION: The Reduced Chemistry Model is Constructed so it Reproduces the Results from the Comprehensive Model



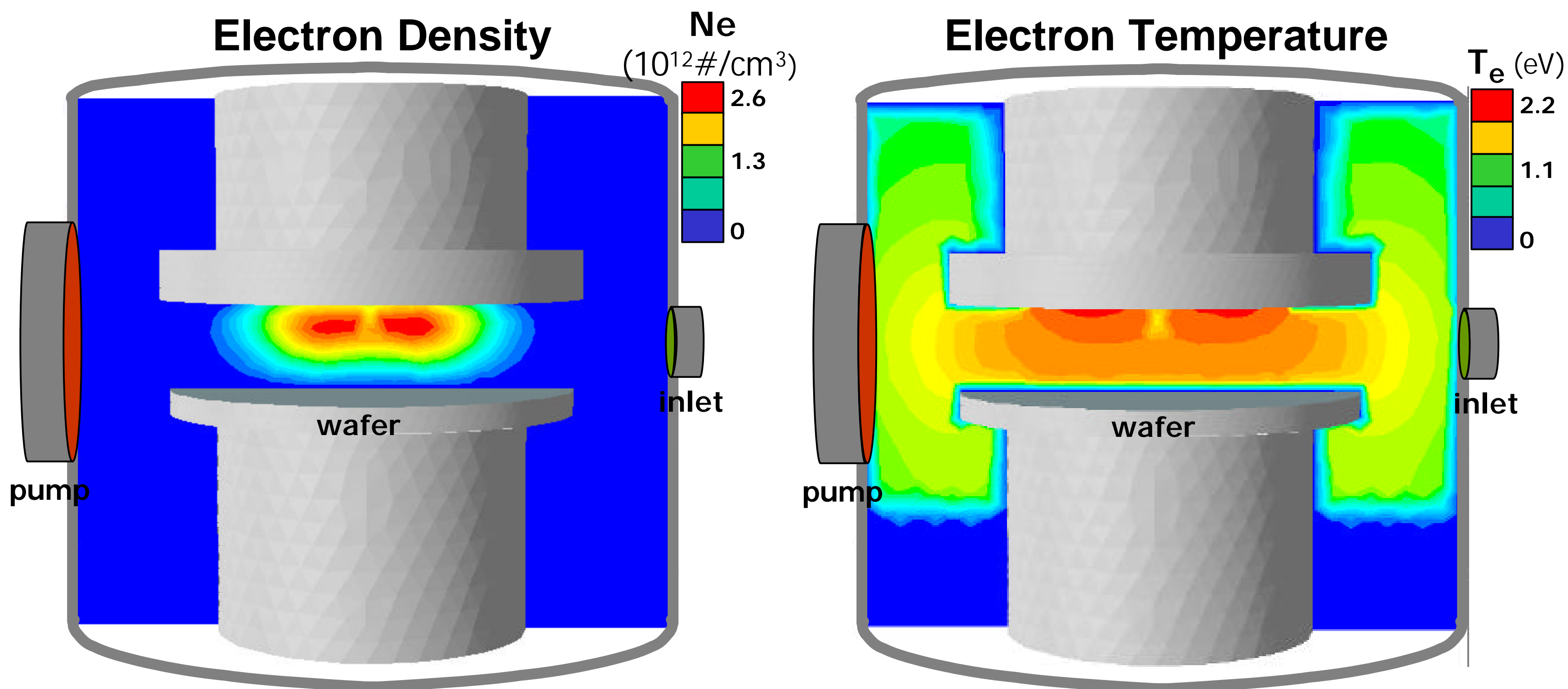
INDUCTIVELY COUPLED PLASMA

RESULTS

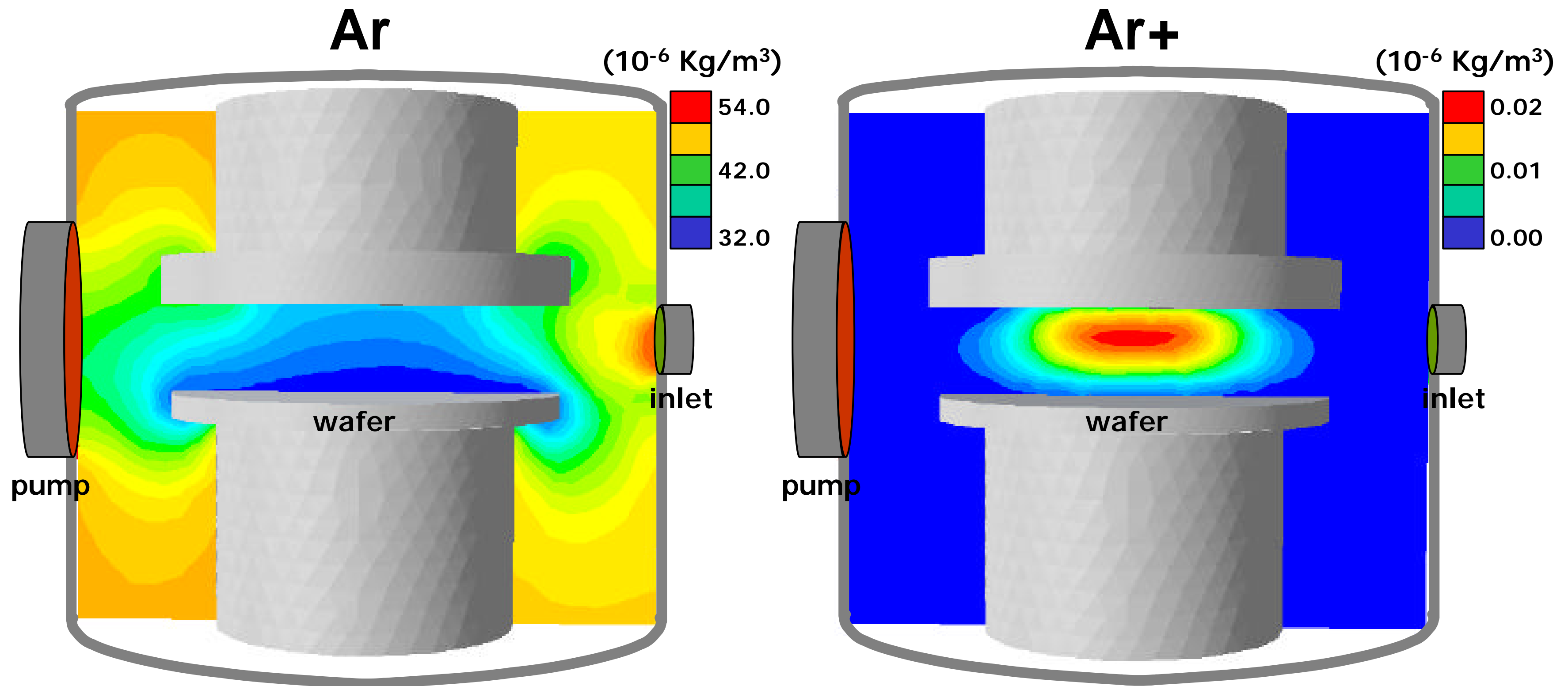
ICP SIMULATION: The GEC Cell Produces a Unique Cross-Wafer Flow Pattern



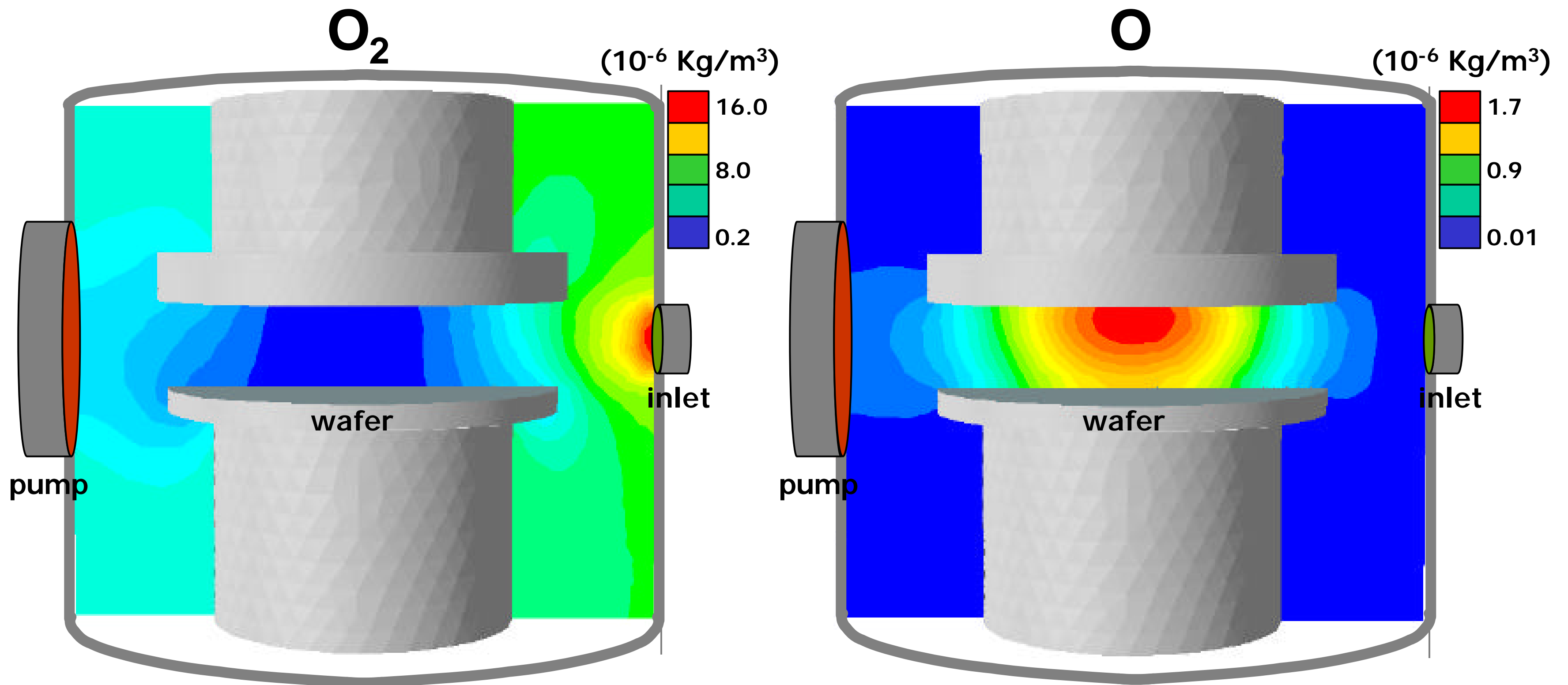
ICP SIMULATION: PLASMATOR Accurately Calculates the Electron Energy and Distribution



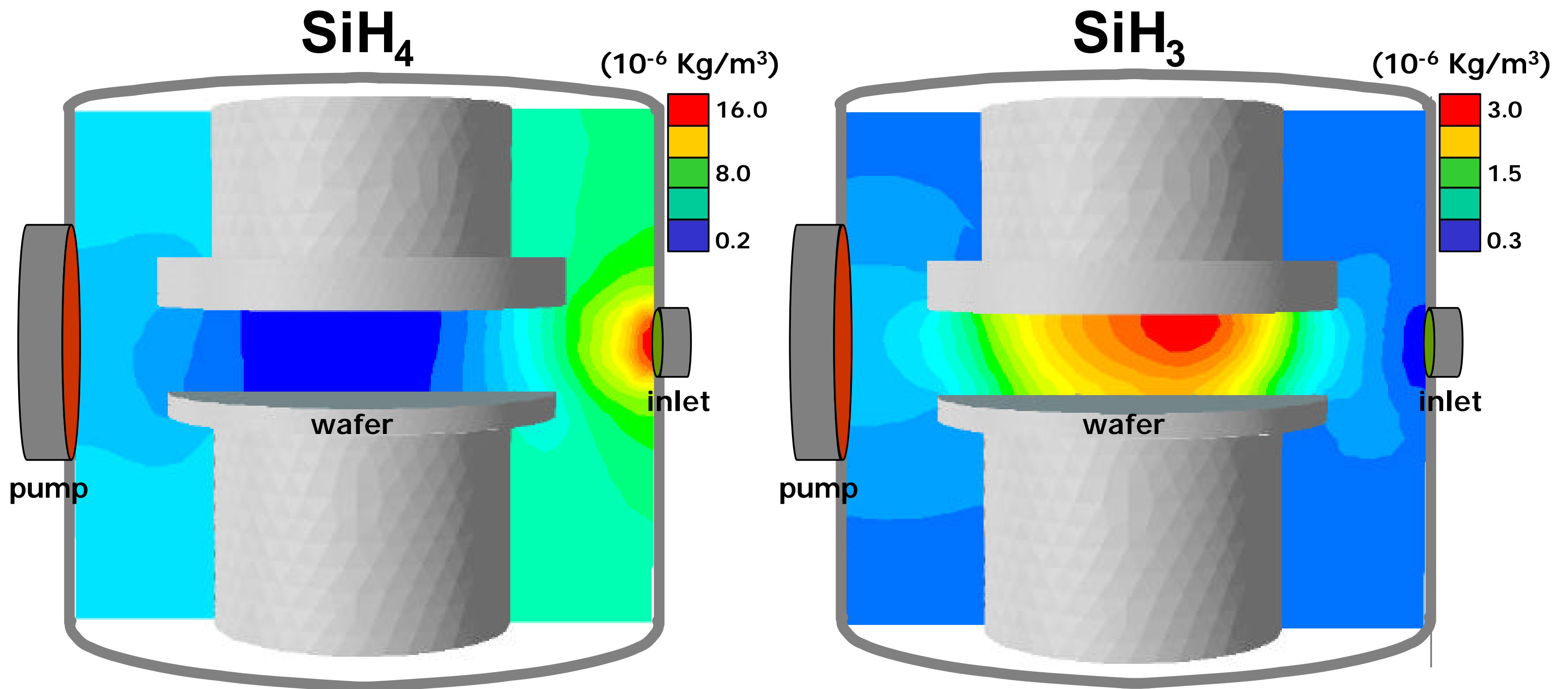
ICP SIMULATION: FLUENT - PLASMATOR Captures Argon Ionization in the GEC Reactor



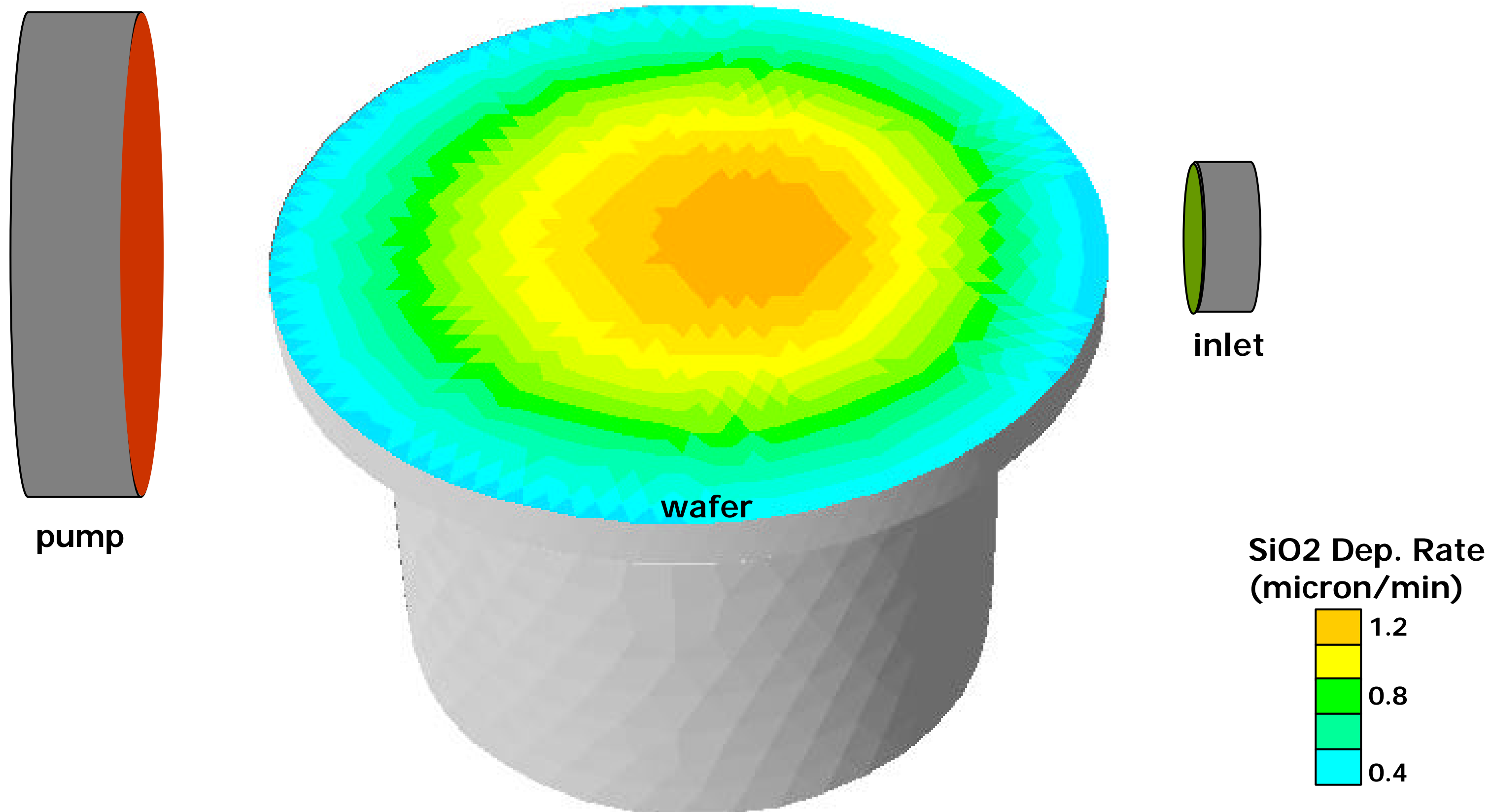
ICP SIMULATION: FLUENT - PLASMATOR Models the Oxygen Dissociation Distribution



ICP SIMULATION: FLUENT - PLASMATOR Captures the 3-D Silane Dissociation Asymmetry



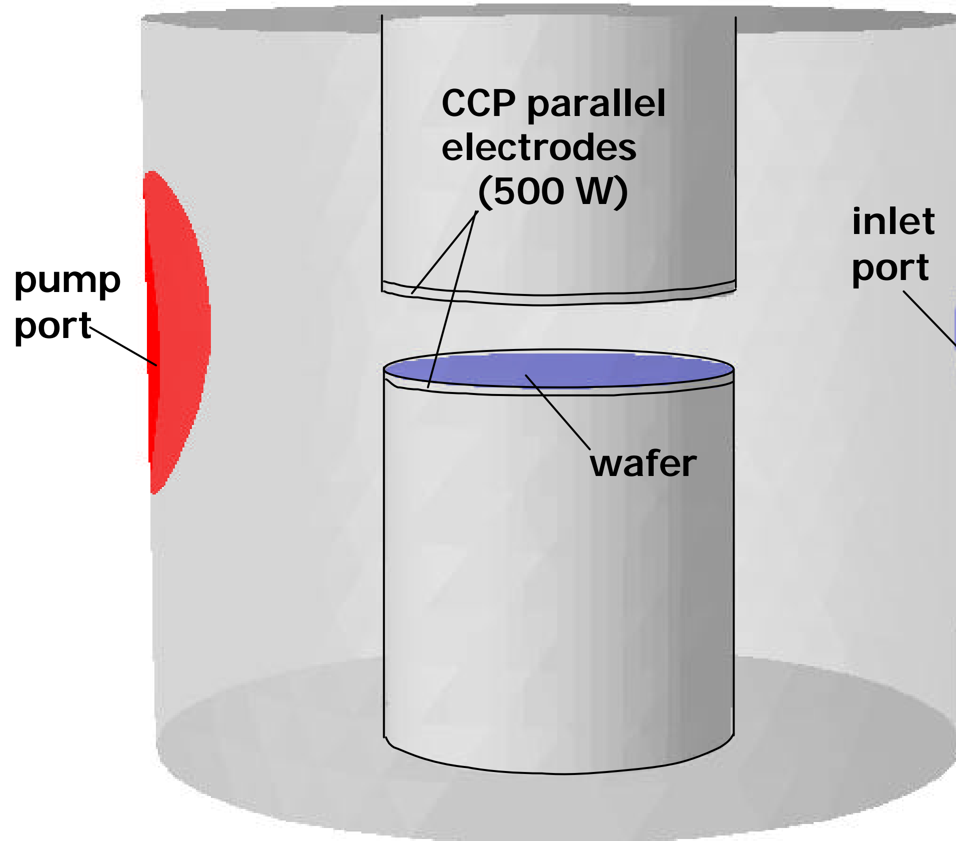
ICP SIMULATION: FLUENT - PLASMATOR Reveals the Oxide Deposition Asymmetry



CAPACITIVELY COUPLED PLASMA

OXIDE ETCHING

CCP SIMULATION: The Standard GEC Reference Cell Geometry is Computed During Oxide Etching

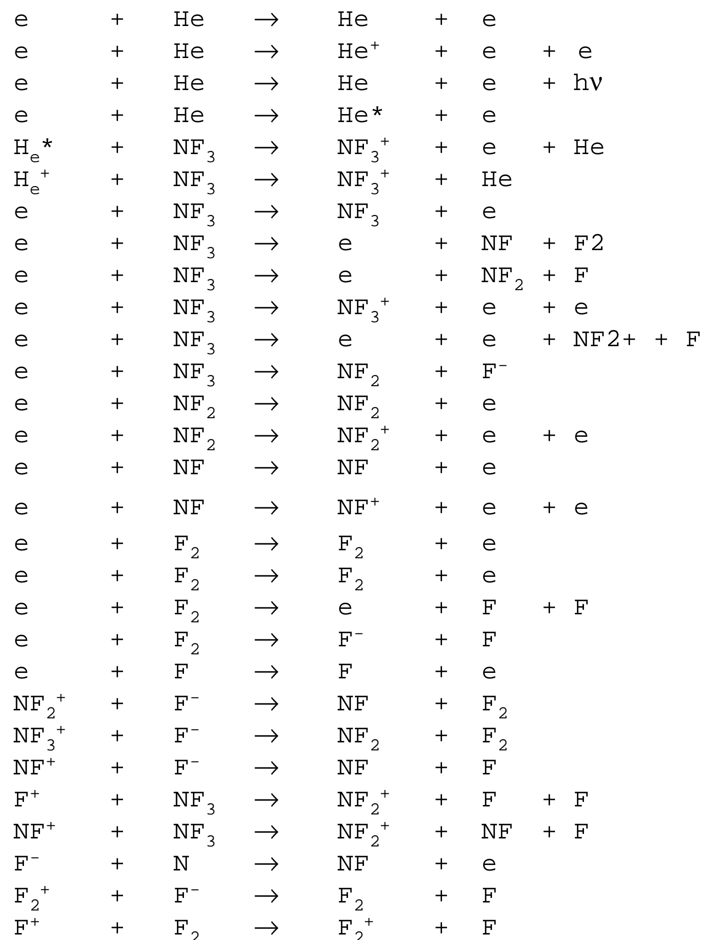


Inlet Flow:
400 sccm He
100 sccm NF3

Boundary Conditions
Twafer = 200 C
Twalls = 30 C
P = 2 Torr

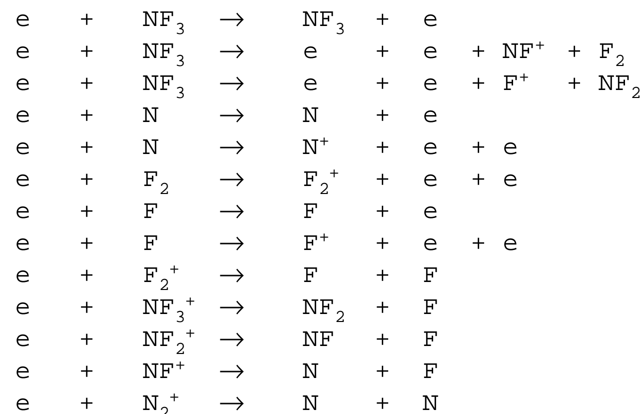
CCP SIMULATION: PLASMATOR Utilizes a Comprehensive Chemistry Model to Characterize the Equilibrium Electrons

Plasma Reactions



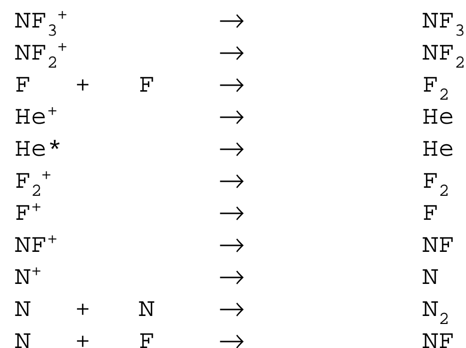
e	+	He	→	He	+	e				
e	+	He	→	He^+	+	e	+	e		
e	+	He	→	He	+	e	+	hv		
e	+	He	→	He*	+	e				
H_e^*	+	NF_3	→	NF_3^+	+	e	+	He		
H_e^+	+	NF_3	→	NF_3^+	+	He				
e	+	NF_3	→	NF_3	+	e				
e	+	NF_3	→	e	+	NF	+	F2		
e	+	NF_3	→	e	+	NF_2	+	F		
e	+	NF_3	→	NF_3^+	+	e	+	e		
e	+	NF_3	→	e	+	e	+	NF2+	+	F
e	+	NF_3	→	NF_2	+	F^-				
e	+	NF_2	→	NF_2	+	e				
e	+	NF_2	→	NF_2^+	+	e	+	e		
e	+	NF	→	NF	+	e				
e	+	NF	→	NF^+	+	e	+	e		
e	+	F_2	→	F_2	+	e				
e	+	F_2	→	F_2	+	e				
e	+	F_2	→	e	+	F	+	F		
e	+	F_2	→	F^-	+	F				
e	+	F	→	F	+	e				
NF_2^+	+	F^-	→	NF	+	F_2				
NF_3^+	+	F^-	→	NF_2	+	F_2				
NF^+	+	F^-	→	NF	+	F				
F^+	+	NF_3	→	NF_2^+	+	F	+	F		
NF^+	+	NF_3	→	NF_2^+	+	NF	+	F		
F^-	+	N	→	NF	+	e				
F_2^+	+	F^-	→	F_2	+	F				
F^+	+	F_2	→	F_2^+	+	F				

Plasma Reactions (continued)



e	+	NF_3	→	NF_3	+	e				
e	+	NF_3	→	e	+	e	+	NF^+	+	F_2
e	+	NF_3	→	e	+	e	+	F^+	+	NF_2
e	+	N	→	N	+	e				
e	+	N	→	N^+	+	e	+	e		
e	+	F_2	→	F_2^+	+	e	+	e		
e	+	F	→	F	+	e				
e	+	F	→	F^+	+	e	+	e		
e	+	F_2^+	→	F	+	F				
e	+	NF_3^+	→	NF_2	+	F				
e	+	NF_2^+	→	NF	+	F				
e	+	NF^+	→	N	+	F				
e	+	N_2^+	→	N	+	N				

Surface Reactions

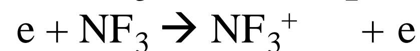


NF_3^+			→	NF_3
NF_2^+			→	NF_2
F	+	F	→	F_2
He^+			→	He
He*			→	He
F_2^+			→	F_2
F^+			→	F
NF^+			→	NF
N^+			→	N
N	+	N	→	N_2
N	+	F	→	NF

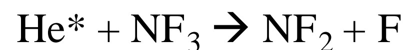
CCP SIMULATION: FLUENT Utilizes a Reduced Chemistry Model to Allow Fast 3D Simulation

He / NF3 FLUENT Oxide Etch Chemistry

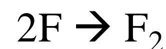
Electron Impact Chemistry

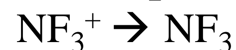


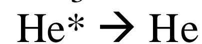
Flow Field Chemistry

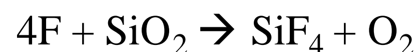


Surface Chemistry



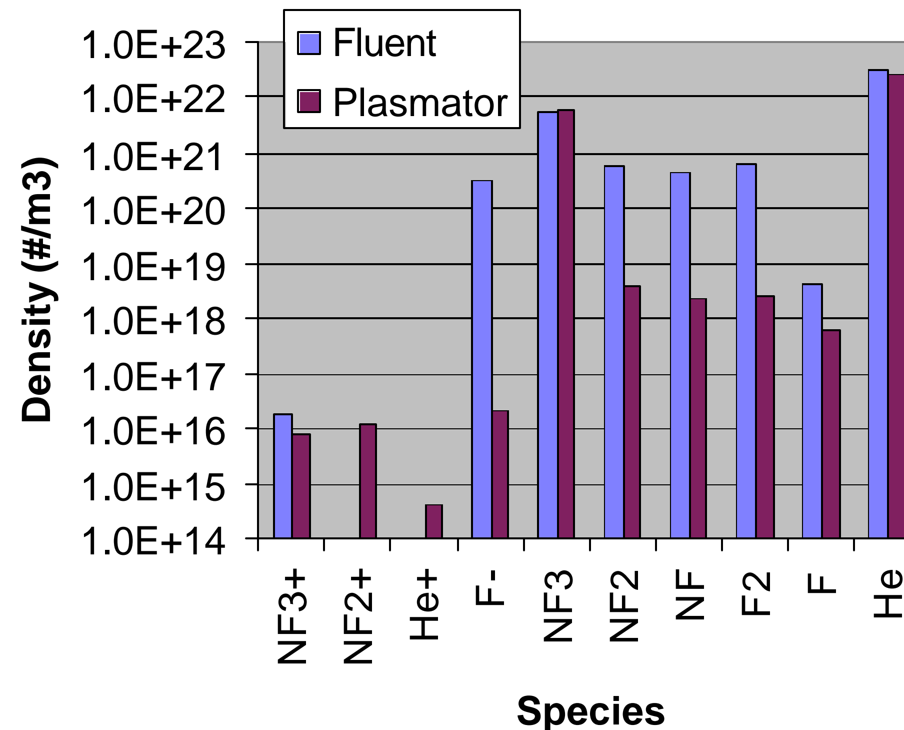






CCP SIMULATION: The Reduced Chemistry Model is Constructed so it Reproduces the Results from the Comprehensive Model

He / NF3 Average Density Results

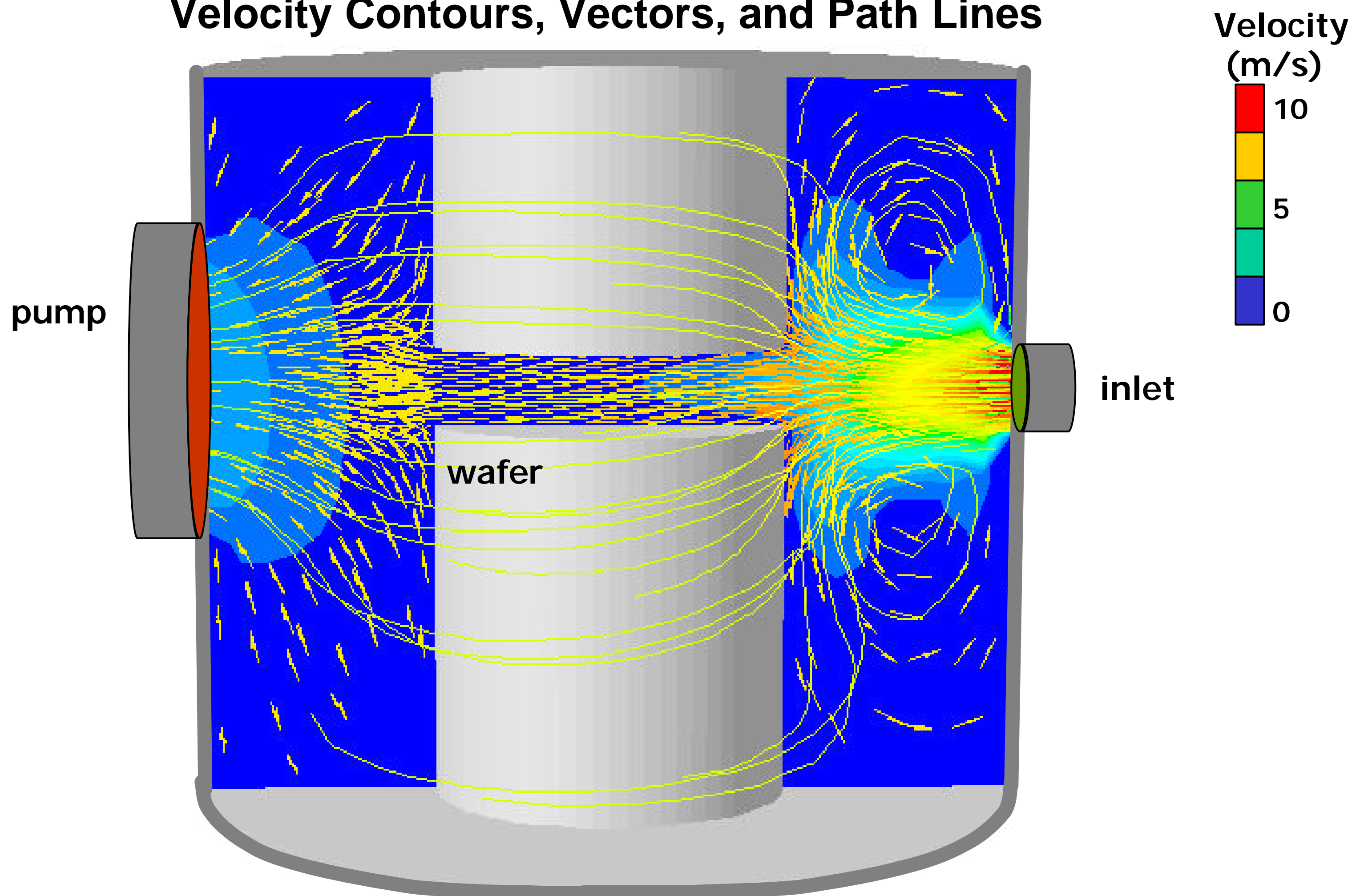


While the FLUENT and PLASMATOR models generally agree –especially in the characterization of the etch gas F, further refinement is necessary in the FLUENT reduced chemistry set.

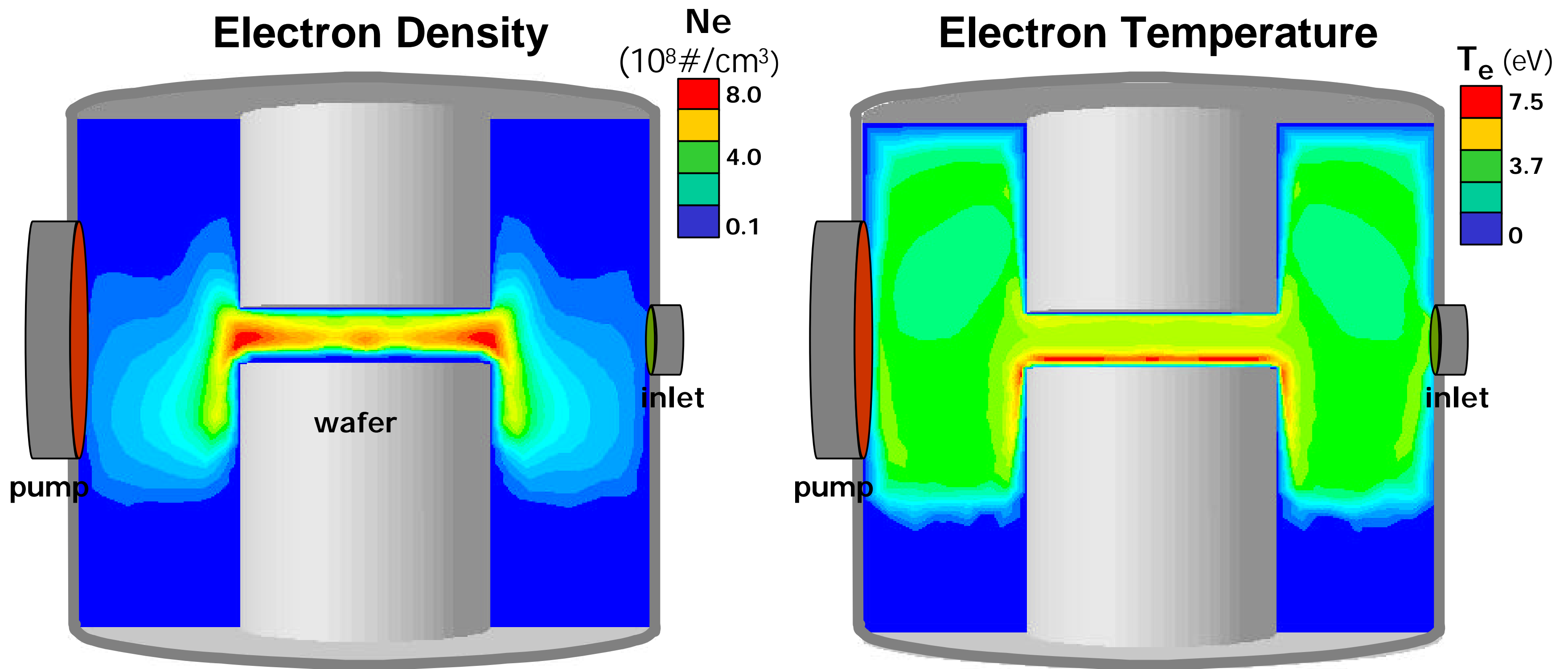
CAPACITIVELY COUPLED PLASMA

RESULTS

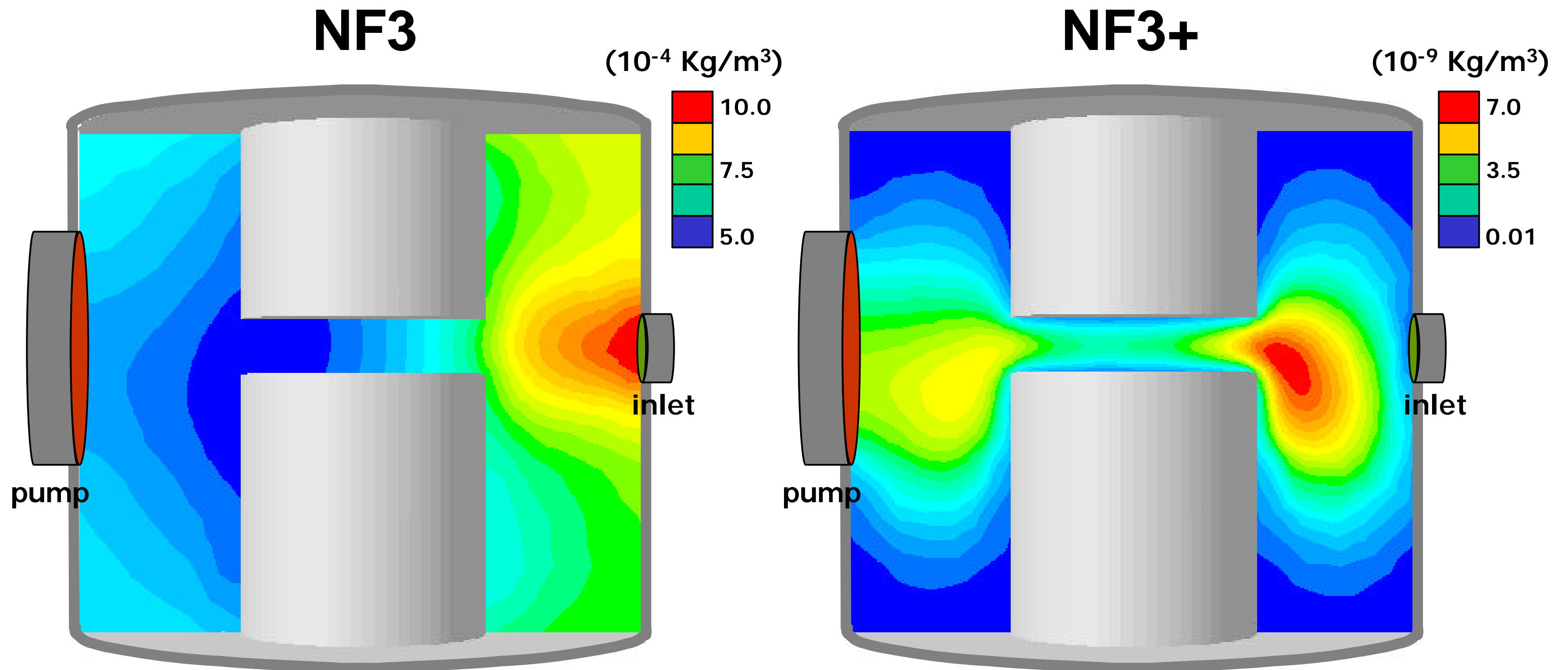
CCP SIMULATION: The GEC Cell Produces a Unique Cross-Wafer Flow Pattern



CCP SIMULATION: PLASMATOR Accurately Calculates the Electron Energy and Distribution

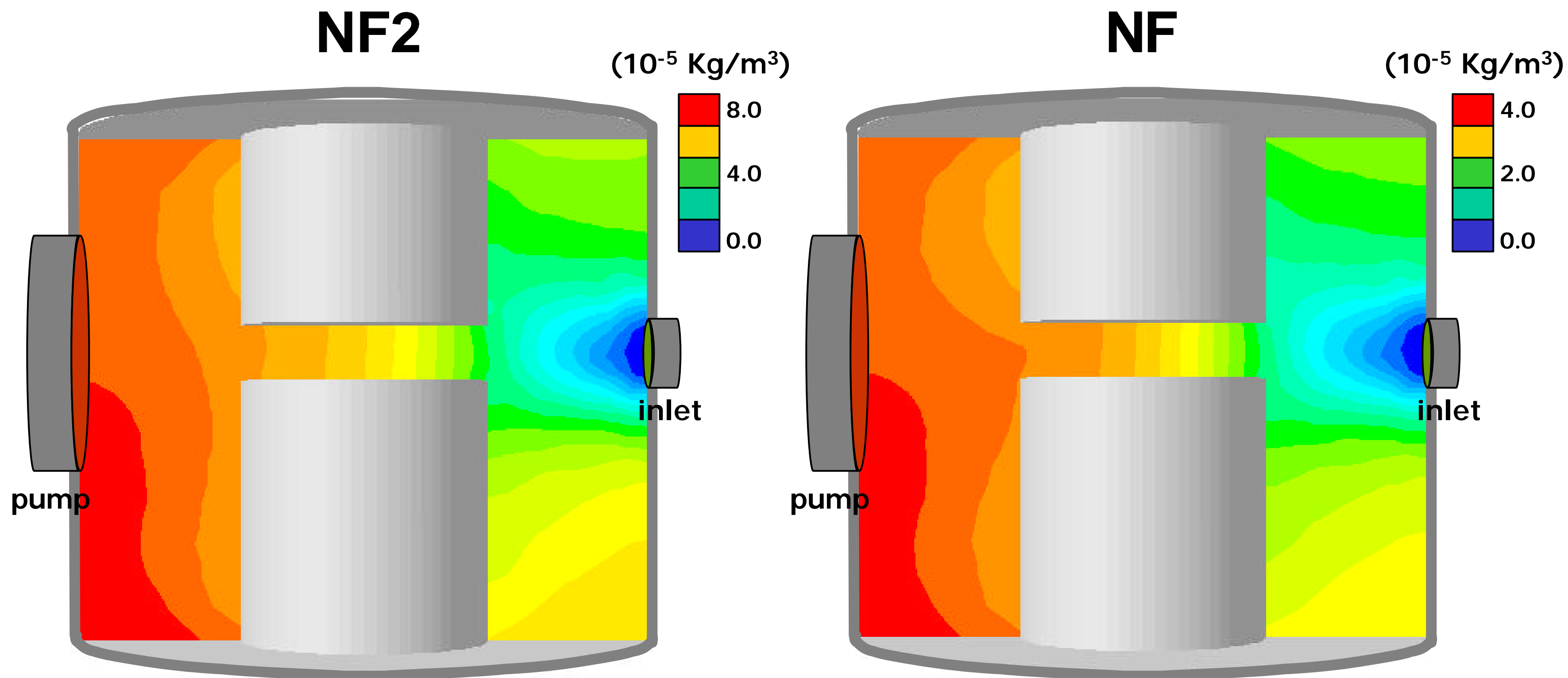


CCP SIMULATION: FLUENT - PLASMATOR Captures NF3 Ionization in the GEC Reactor

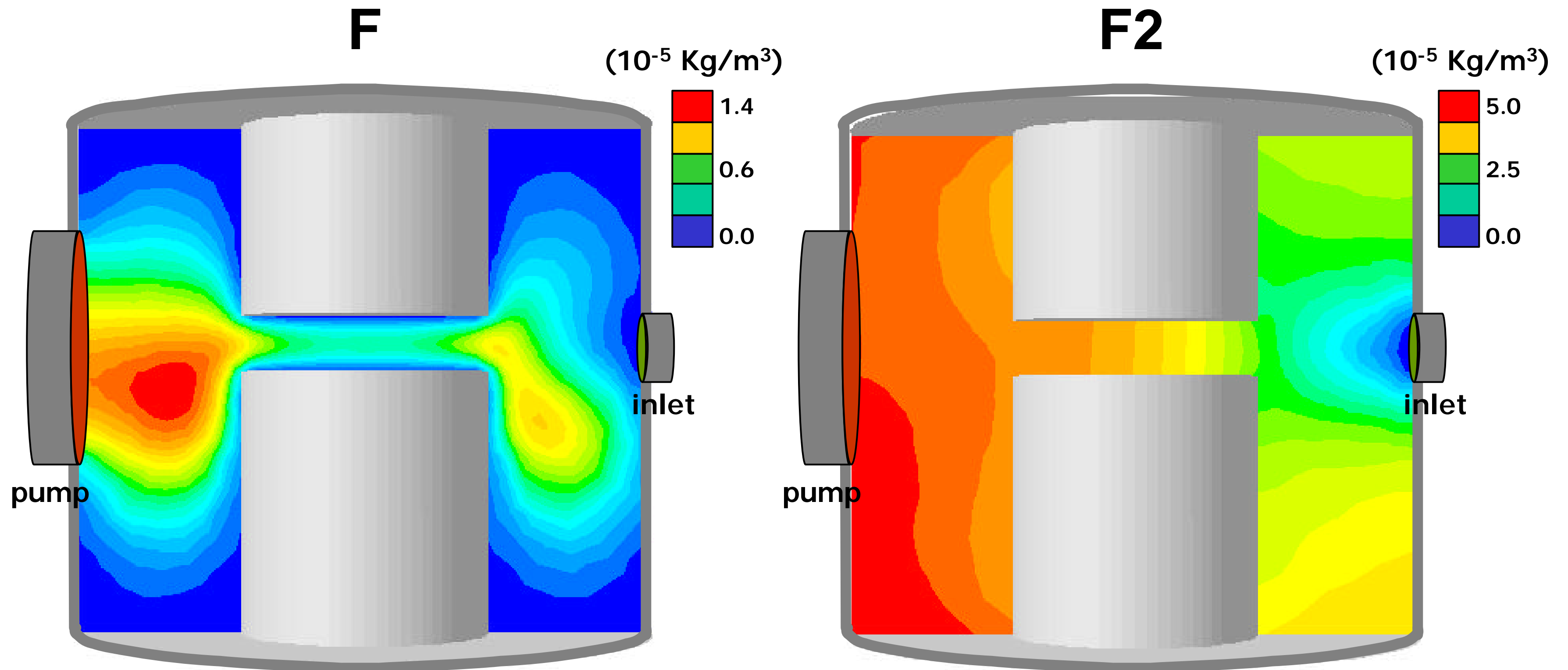


CCP SIMULATION: FLUENT - PLASMATOR

Demonstrates the Progressive Dissociation of NF3

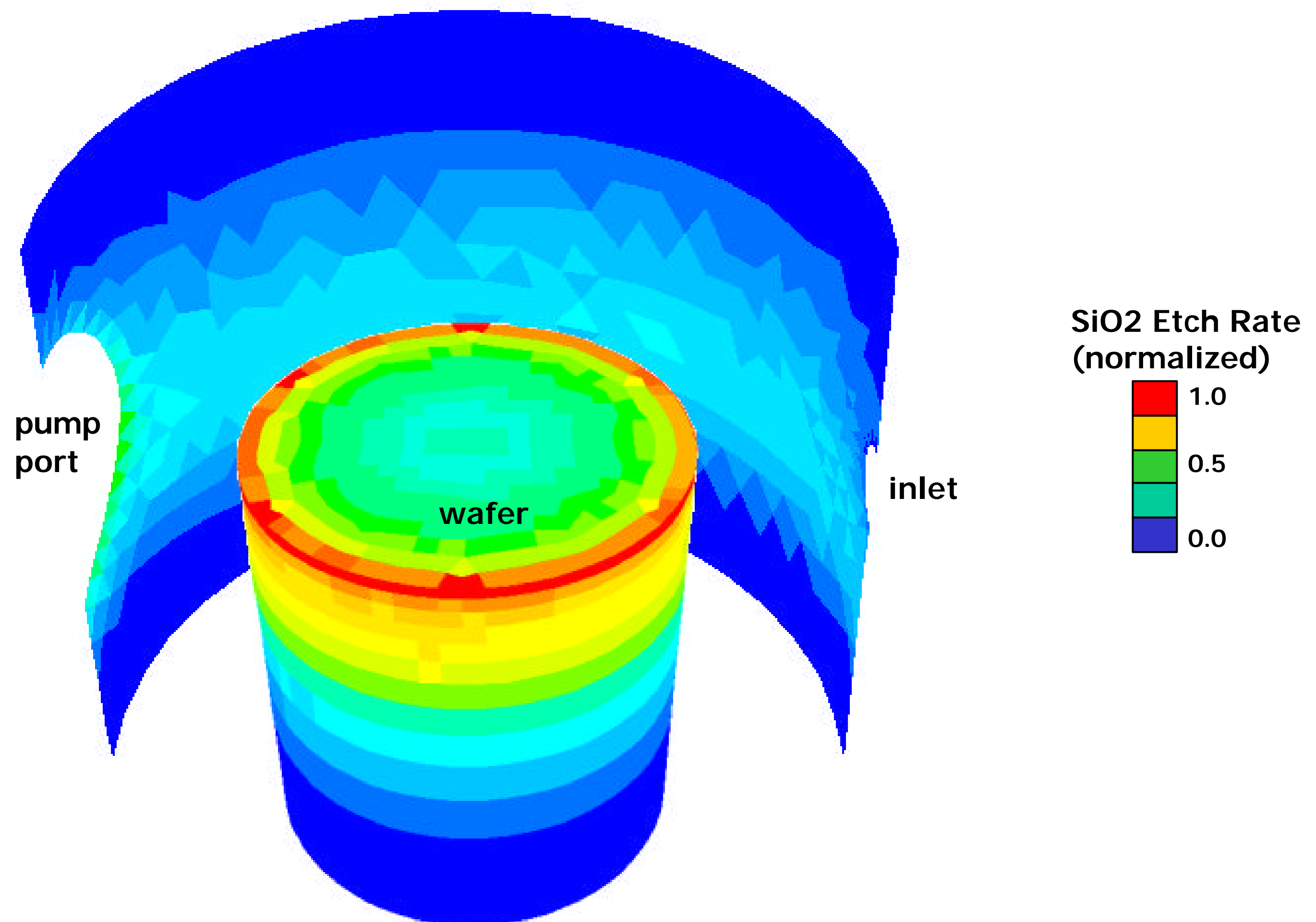


CCP SIMULATION: FLUENT - PLASMATOR
Calculates the Production of Etch Gasses



CCP SIMULATION: FLUENT - PLASMATOR

Calculates Etch Rate Throughout the Reactor



PLASMA DISCHARGE SIMULATION: CONCLUSIONS

- The linked FLUENT-PLASMATOR codes provide an accurate method for fast 3D plasma discharge simulations.
- The package is capable of robustly handling diverse geometries and complicated chemistries.