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SIMULATIONS OF REMOTE AR/O_2 PLASMAS FOR OXIDE GROWTH AND INTERFACE TREATMENTS

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AGENDA

- Introduction
- Plasma and reactor model
- Effects of plasma parameters on :
    - Production of radicals and ions
    - Reactant fluxes to the substrate
- Conclusion

INTRODUCTION

- RPACVD provides a mean to deposit thin dielectric films with low ion bombardment, while having high selectivity in generating precursors.

- In RPACVD of SiO_2, it has been found that the fluxes of SiH_2O, SiH_3O, and SiH_n, directly scale in the same manner as the experimental precursor rates.

- The production and uniformity of these precursors largerly depends on the rate of oxidation of SiH_4. Reactions of O atoms with SiH_4 proceed by a series of H abstraction and elimination reactions.

- Since the fluxes of O atoms (and $O_2(^1\Delta)$) are large, and not rate limiting, this scaling supports the proposal that the surface catalyzed reactions between O (or $O_2(^1\Delta)$) and SiH_n are deposition precursors.

MODEL EQUATIONS FOR HPEM OPTIONS

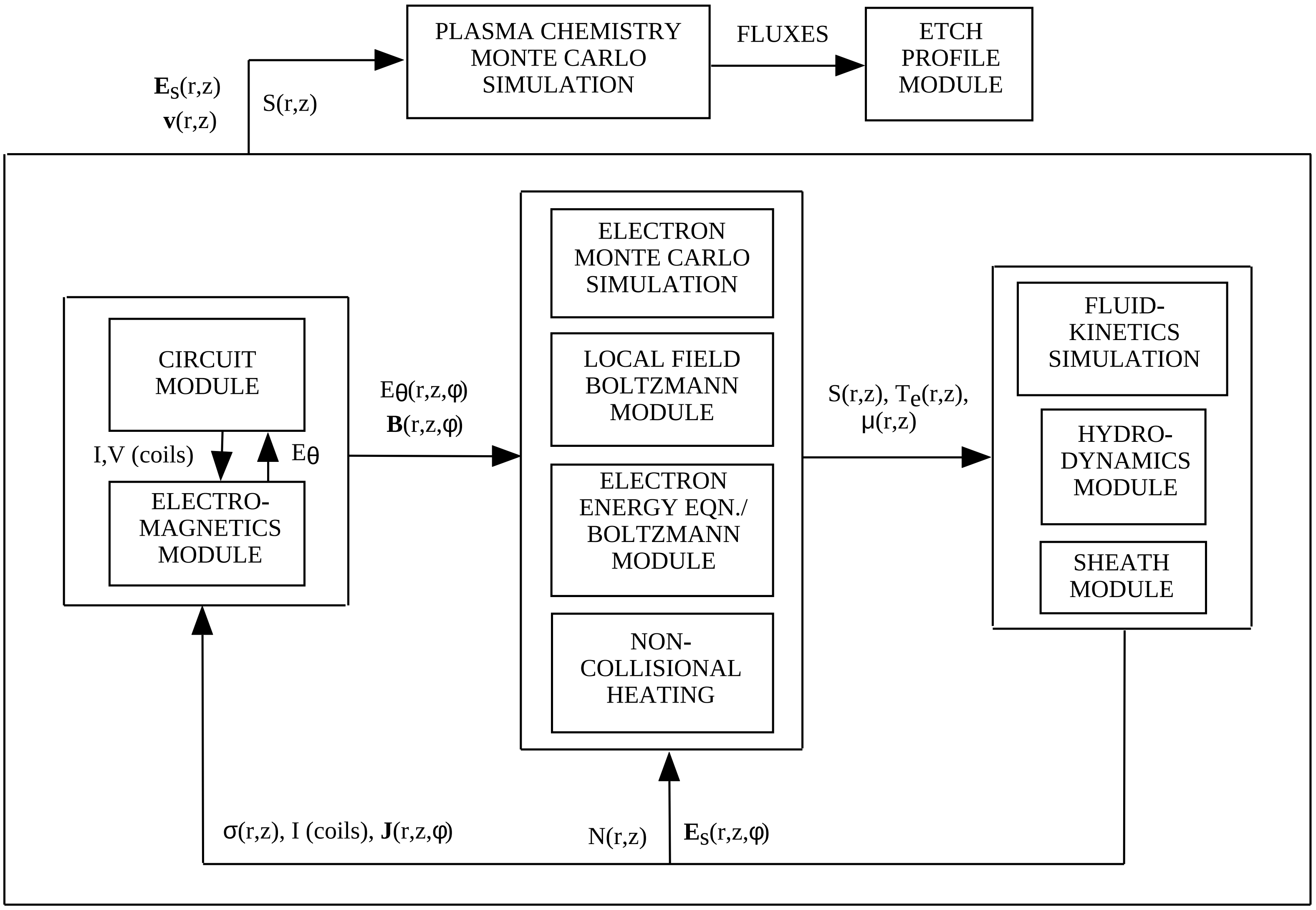
- To investigate the reaction pathways and to identify deposition precursors, a model has been developed to simulate production and transport of such precursors (mainly $O(^3P)$ and $O_2(^1\Delta)$).

- Ion transport was calculated by time integrating the drift diffusion equations. While electron energy transport was determined by time integrating the electron energy conservation equation.

- Neutral transport was determined by solving the neutral momentum equation.

- An ambipolar approximation was used to solve a Poisson-like equation for Φ. Due to the vastly different kinetic time scales for the kinetic reactions compared to convection, such an approximation, allowed for the use of larger time steps during each iteration.

THE HYBRID PLASMA EQUIPMENT MODEL



PLASMA CHEMISTRY
MONTE CARLO
SIMULATION

FLUXES

ETCH
PROFILE
MODULE

$\mathbf{E}_S(r,z)$
$\mathbf{v}(r,z)$

$S(r,z)$

CIRCUIT
MODULE

I,V (coils)

E_θ

ELECTRO-
MAGNETICS
MODULE

$E_\theta(r,z,\varphi)$
$\mathbf{B}(r,z,\varphi)$

ELECTRON
MONTE CARLO
SIMULATION

LOCAL FIELD
BOLTZMANN
MODULE

ELECTRON
ENERGY EQN./
BOLTZMANN
MODULE

NON-
COLLISIONAL
HEATING

$S(r,z)$, $T_e(r,z)$,
$\mu(r,z)$

FLUID-
KINETICS
SIMULATION

HYDRO-
DYNAMICS
MODULE

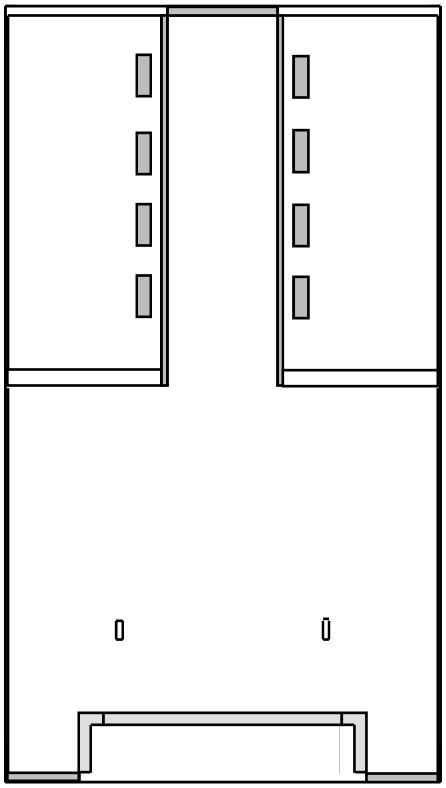
SHEATH
MODULE

$\sigma(r,z)$, I (coils), $\mathbf{J}(r,z,\varphi)$

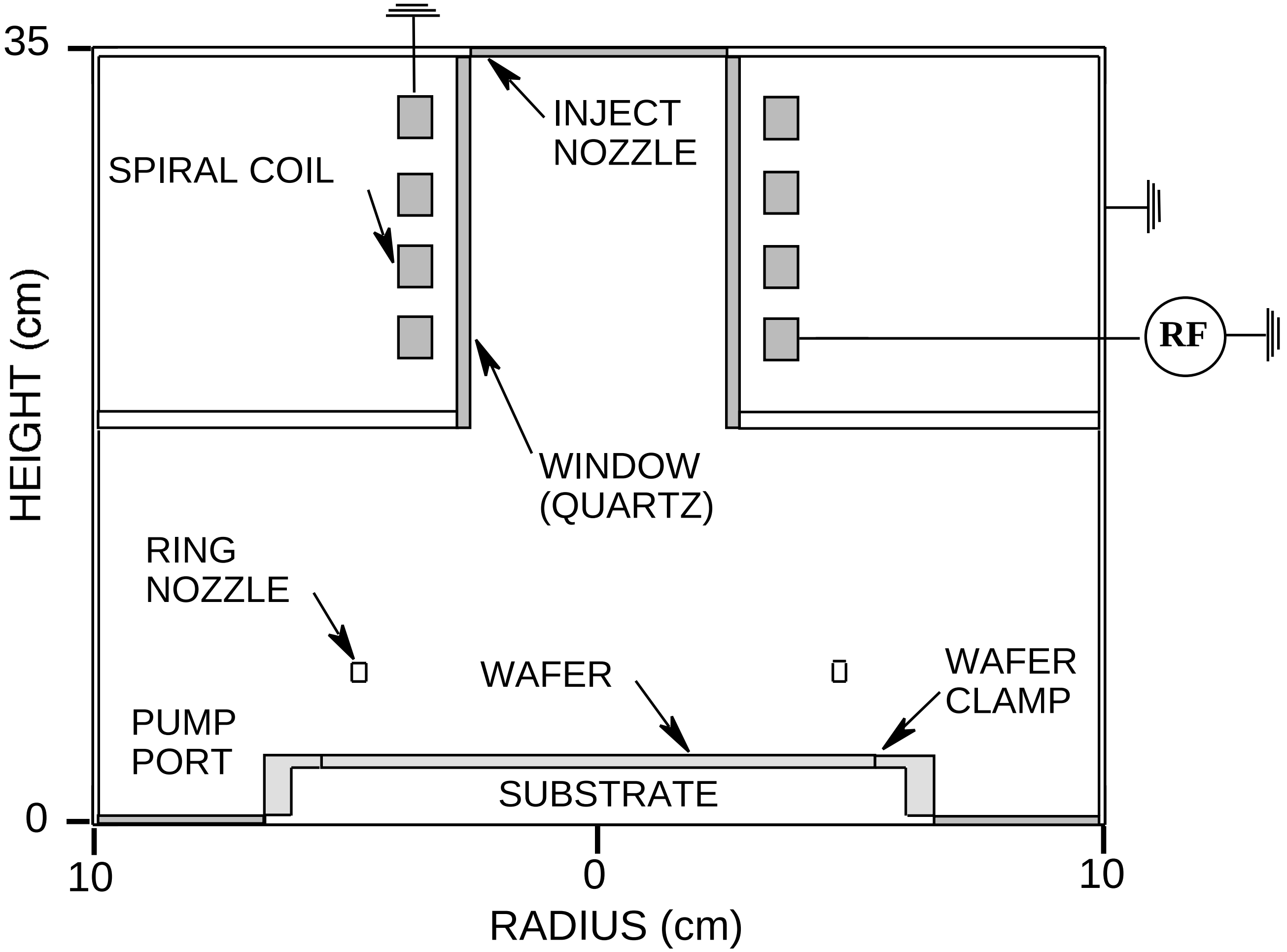
$N(r,z)$

$\mathbf{E}_S(r,z,\varphi)$

REMOTE PLASMA ENHANCED CVD TOOL

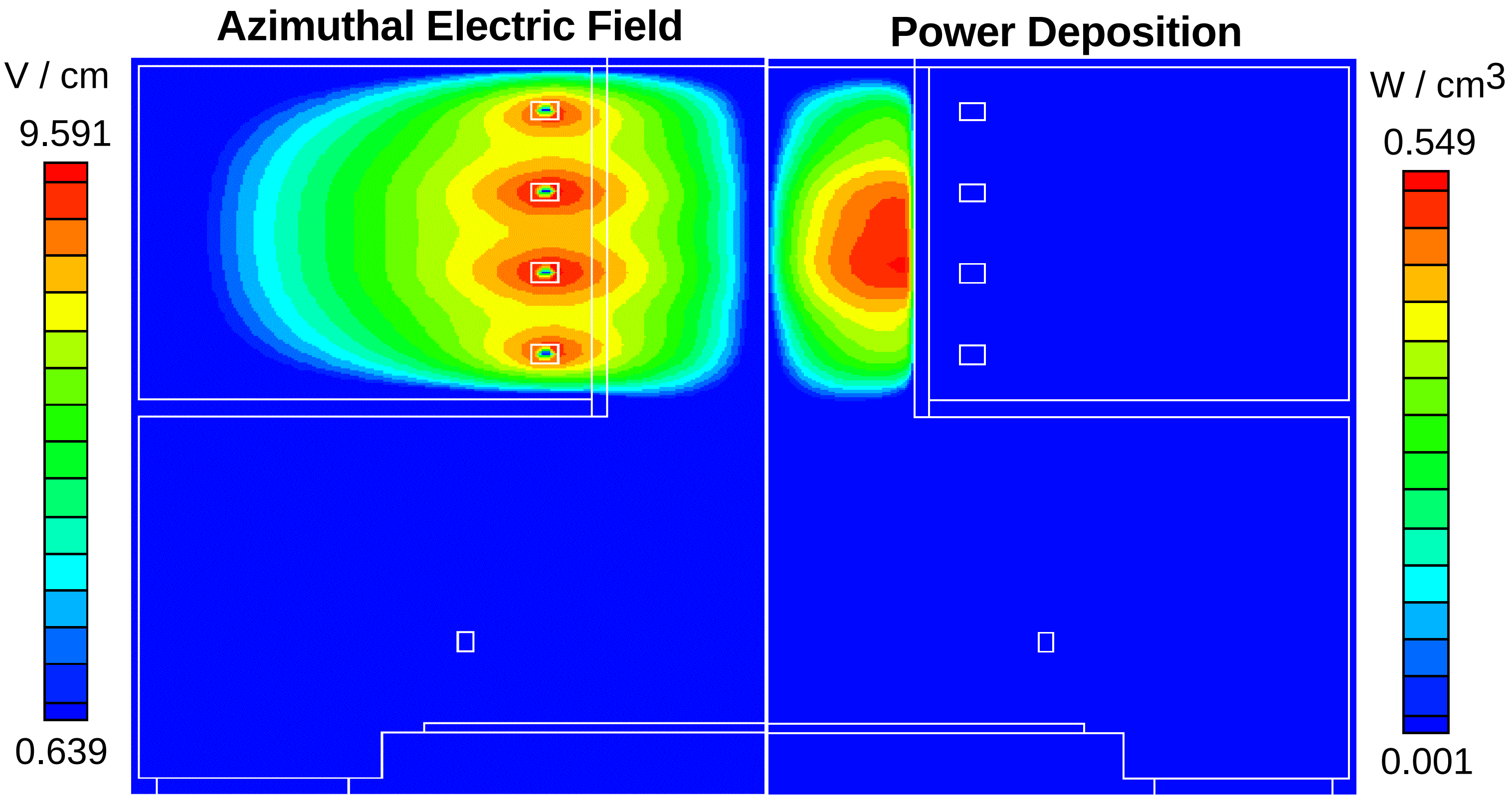


* Size to Scale



Operating Conditions: 50 - 100 mTorr, 20 - 50 Watts (IC), 100 - 120 sccm, $Ar/O_2/O$ = 90/10/5, No Substrate Bias

ELECTRIC FIELD AND POWER DEPOSITION

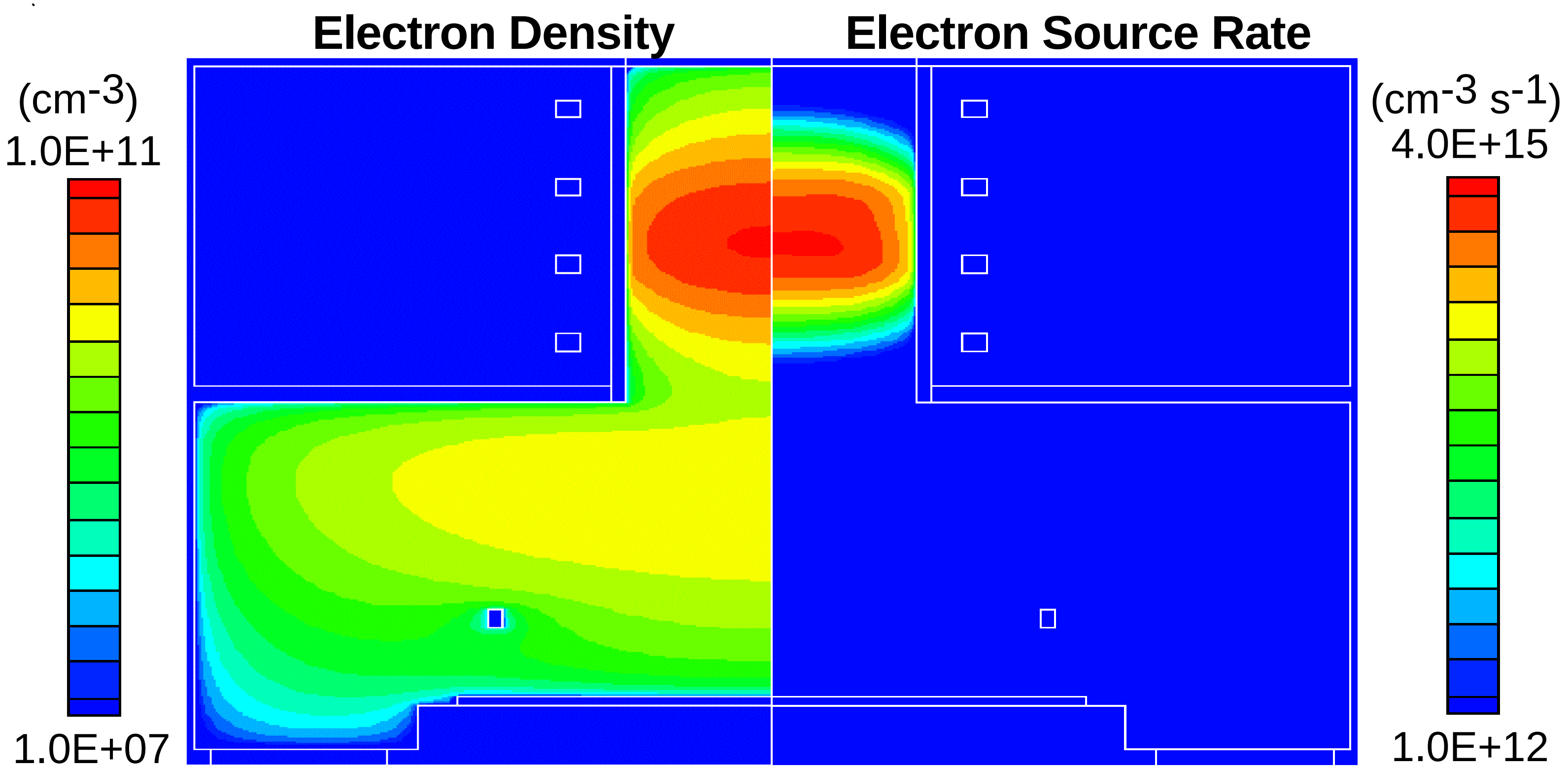


- 75 mTorr, 40 Watts, Ar/O_2 = 9/1

- At the pressures of interest the skin depth exceeds the throat radius.

- The deposition of power peaks where the electric field is highest.

ELECTRON DENSITY DISTRIBUTION AND SOURCE RATE


Electron Density

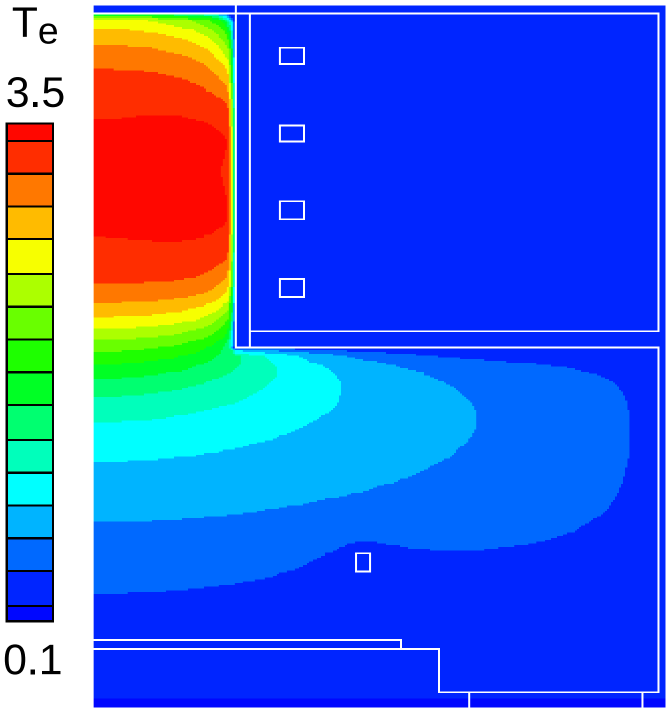
Electron Source Rate

- 75 mTorr, 40 Watts, Ar/O_2 =9/1

- The electron density peaks inside the throat region and falls of by a factor of three in the downstream region.
- Ionization, within the reactor, is localized inside the throat region.

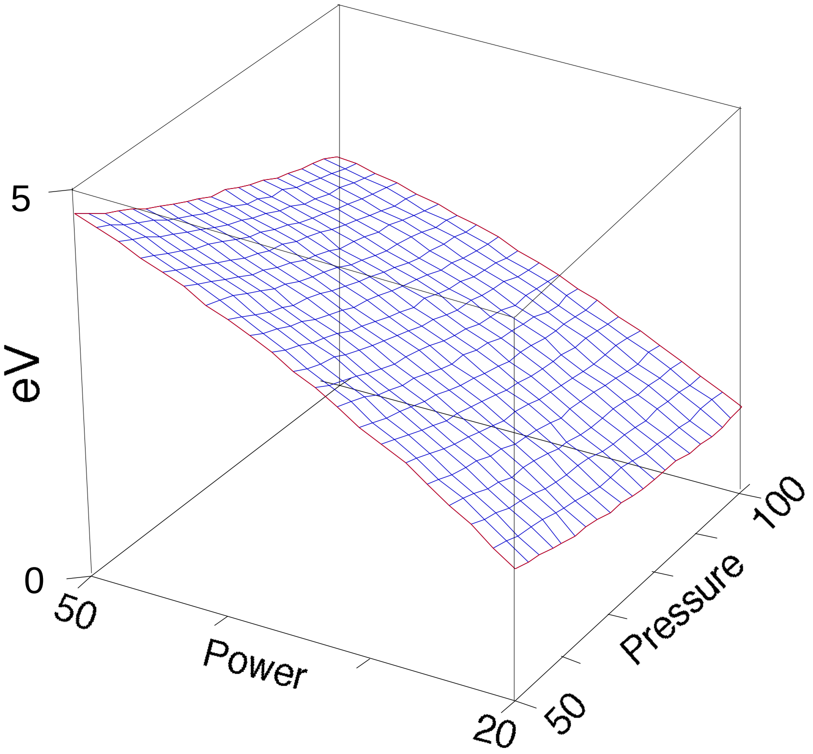
REACTOR AVERAGE ELECTRON TEMPERATURE

Temperature Distribution



- 75 mTorr, 40 Watts, Ar/O_2=9/1

Average T_e in the Source Region

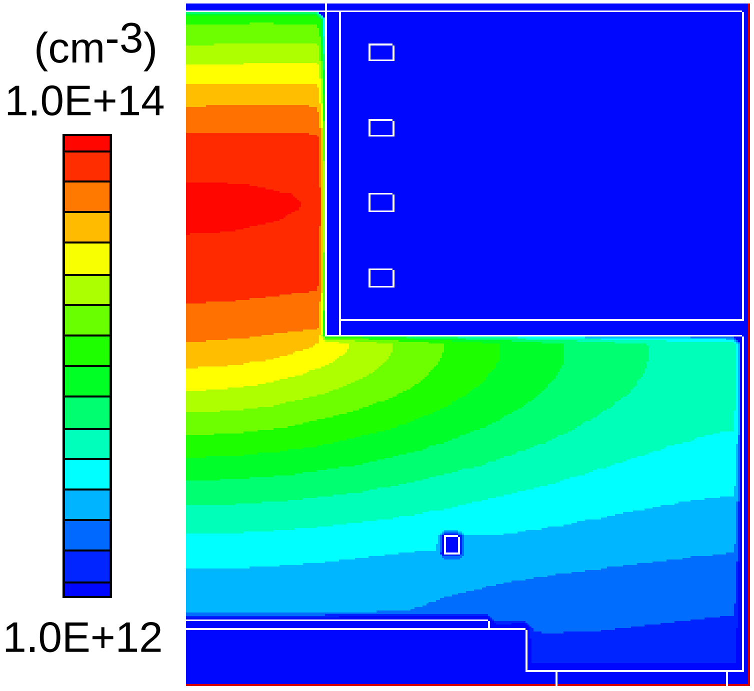


- The decrease in average T_e with increase in pressure is due to reduced diffusion losses and subsequent electron thermalization at higher pressures.
- Average T_e increases nearly linearly with power. (e.g. $P \sim \sigma E^2$)

AVERAGE REACTOR DENSITY OF O(^{3}P)

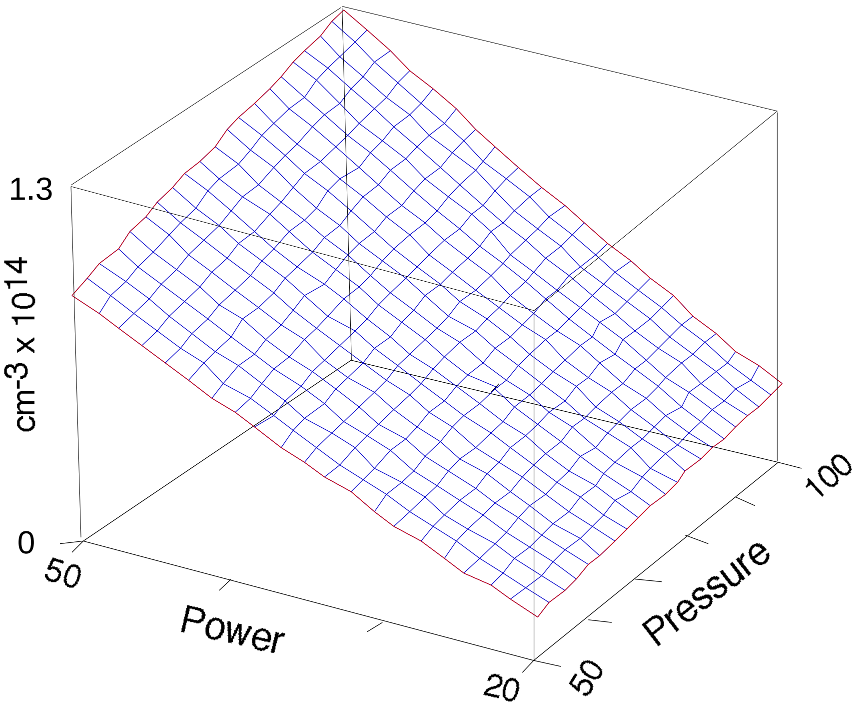
- The reactor density of O(^{3}P) is determined by the source production rate.
- Production of atomic oxygen occurs by the dissociation of $O_2(^3\Sigma_g)$. While the main loss mechanism is wall recombination. (i.e $O + O_{wall} + O_2 \text{ --> } 2\,O_2$)

Reactor O(^{3}P) Distribution



• 75 mTorr, 40 Watts, Ar/O_2 =9/1

Average Reactor Density of O(^{3}P)



MECHANISMS FOR THE PRODUCTION OF O(^{3}P)

- ***Electron Impact Dissociation***

  $e + O_2\ (^3\Sigma_g) \rightarrow O\ (^3P) + O\ (^3P)$

- ***Electron Impact Dissociative***

  $e + O_2\ (^3\Sigma_g) \rightarrow O\ (^1D) + O\ (^3P)$

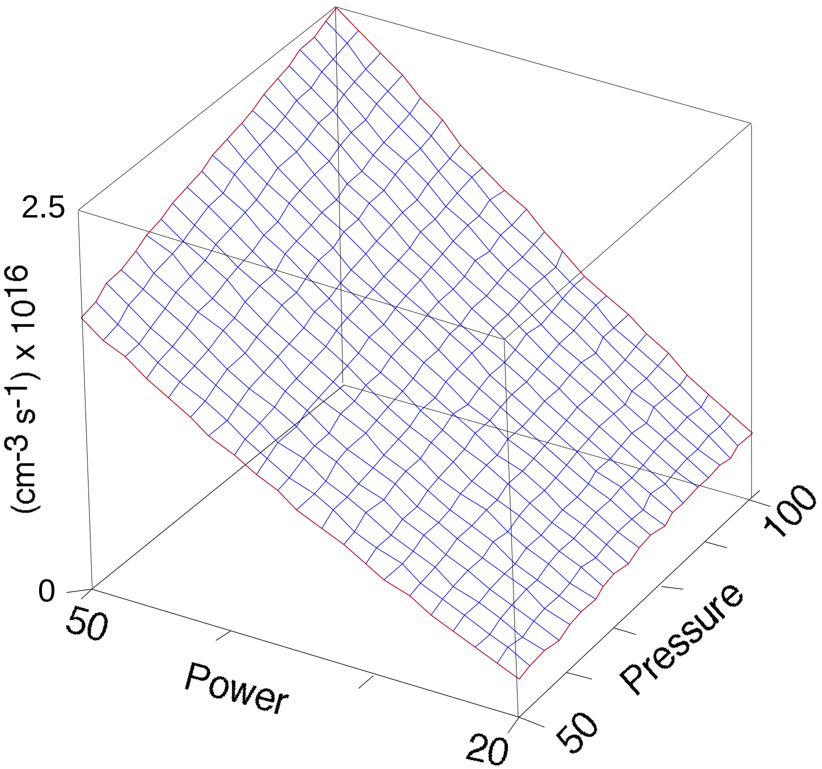
- ***Collisional De-Excitation***

  $O\ (^1D) + O_2\ (^3\Sigma_g) \rightarrow O_2\ (^3\Sigma_g) + O\ (^3P)$

- ***Dissociation by Excited Argon***

  $Ar\ (^4S) + O_2\ (^3\Sigma_g) \rightarrow Ar\ (^3P) + 2\ O\ (^3P)$

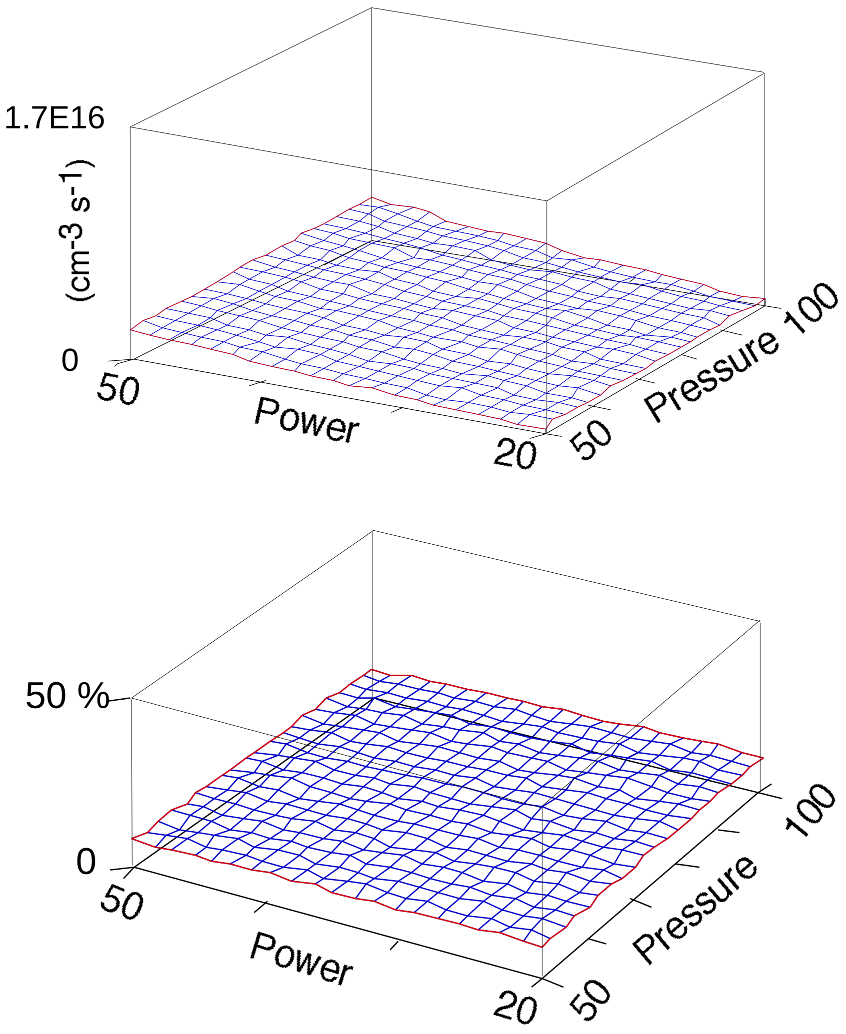
Average Production Rate of O(^{3}P)



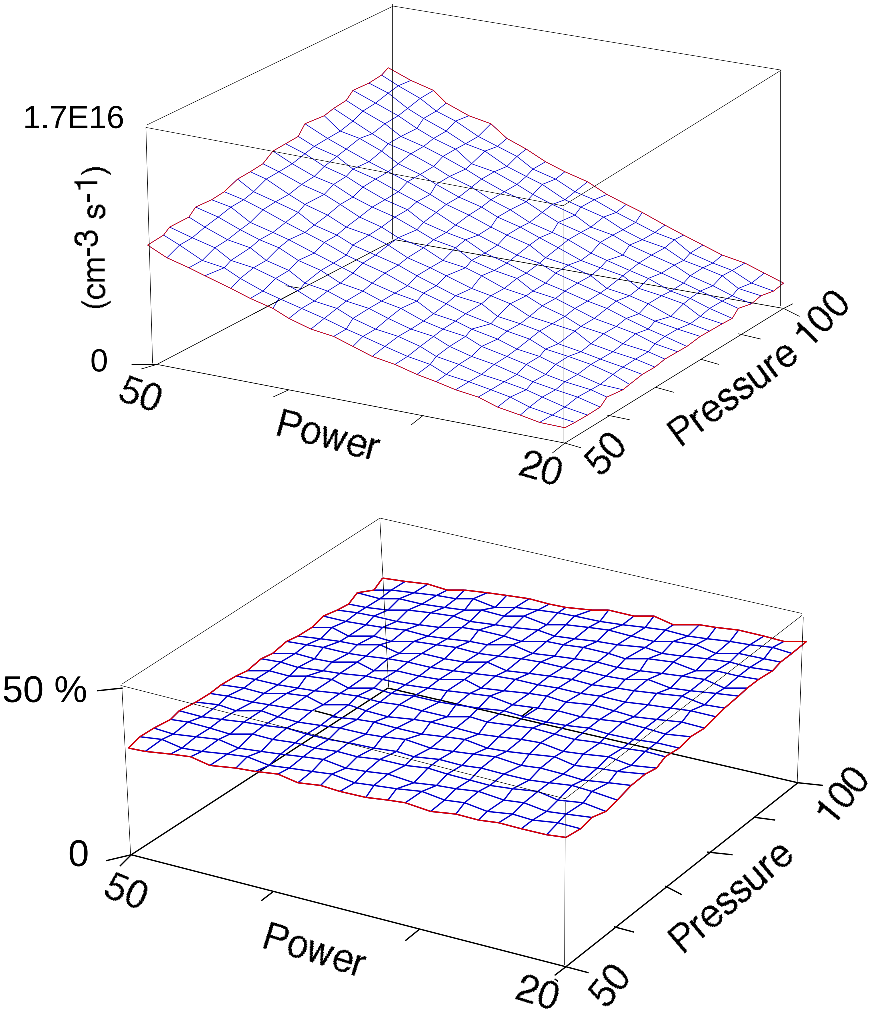
- The loss mechanism of : $O + O + O_2 \rightarrow 2\ O_2$ can be diregarded, since at low pressures the effective two-body reaction rate coefficient is small.

AVERAGE REACTOR PRODUCTION RATE OF O(^{3}P)

e + O_2 ($^3\Sigma_g$) --> O (^{3}P) + O (^{3}P)

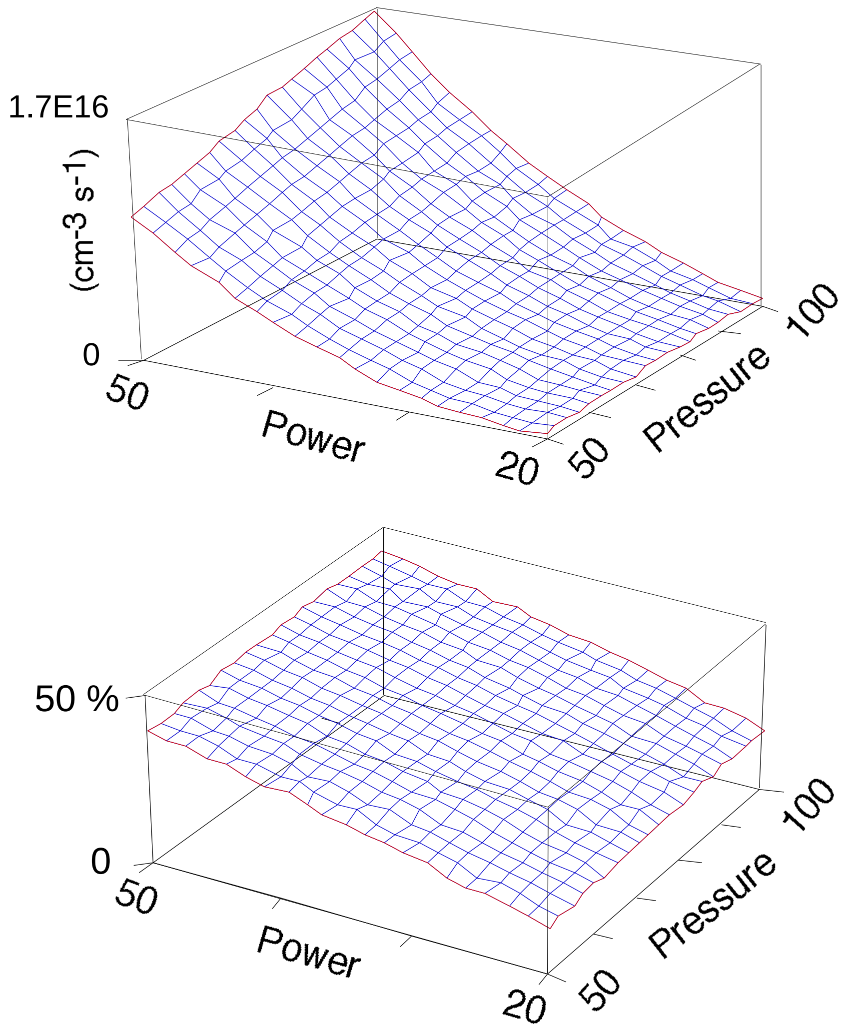


e + O_2 ($^3\Sigma_g$) --> O (^{1}D) + O (^{3}P)

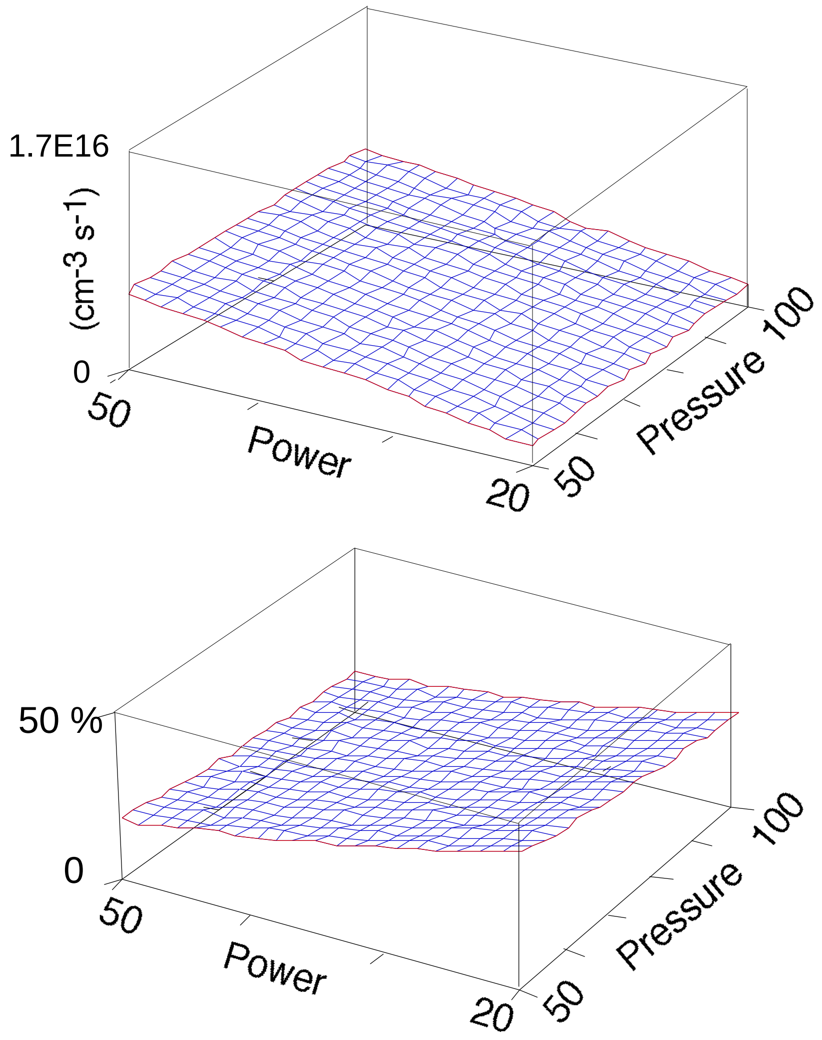


AVERAGE REACTOR PRODUCTION RATE OF $O(^3P)$

$O(^1D) + O_2(^3\Sigma_g)$ --> $O_2(^3\Sigma_g) + O(^3P)$



$Ar(^4S) + O_2(^3\Sigma_g)$ --> $Ar(^3P) + 2\,O(^3P)$

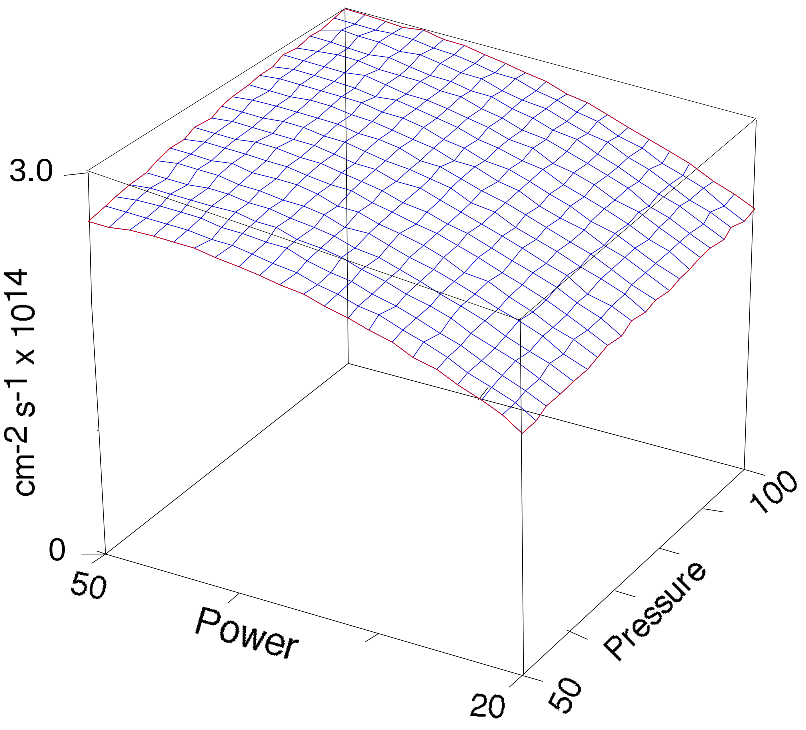


n/a

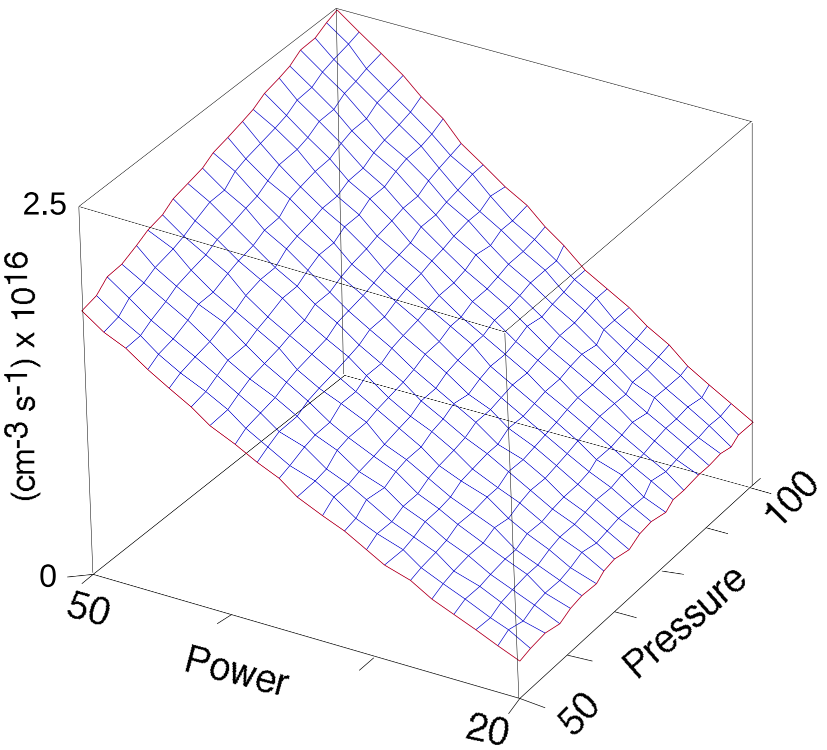
AVERAGE FLUX TO THE SUBSTRATE OF O(^{3}P)

At lower pressures, the flux of O(^{3}P) is significantly higher than expected when comparing the trends for average reactor densities and production rates for O(^{3}P).

Average Flux to Substrate O(^{3}P)

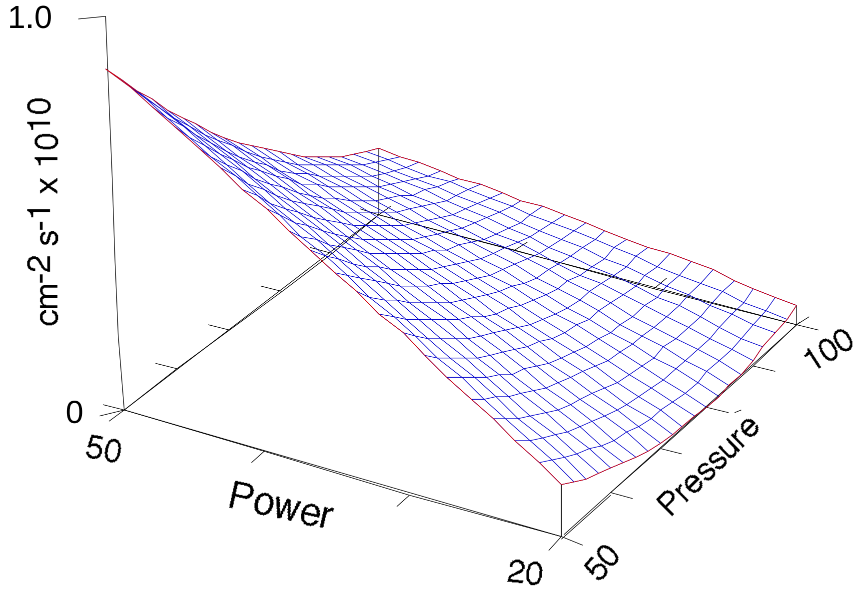


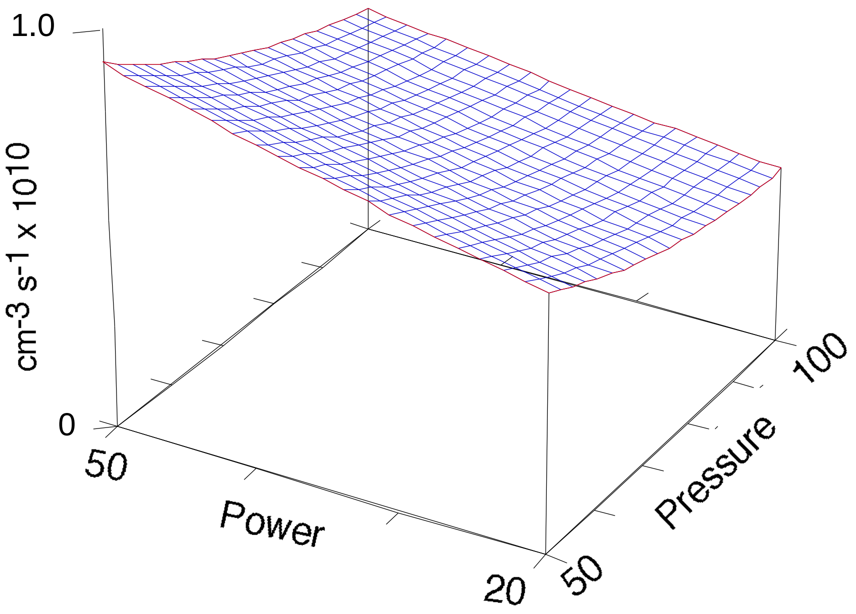
Average Production Rate of O(^{3}P)



AVERAGE FLUX TO THE SUBSTRATE OF O(^{1}D) AND Ar(^{4}S)

- Both species scale linearly with the power depositon.
- The greater dependence of Ar(^{4}S) on pressure, reflects the shorter reactive path length (quenching) of the excited radical.


Average Flux to Substrate of Ar(^{4}S)


Average Flux to Substrate of O(^{1}D)

- At lower pressures, the higher temperature produces a greater excitation of radicals. Combining with a larger diffusivity, allows for the production of O(^{3}P) downstream.

CONCLUSIONS

- RPACVD provides high selectivity in generating and controlling the transport of precursors within the reactor.

- The majority of chemical reactions occur within the throat of the reactor, but diffusion of metastable products still induce reactions downstream.

- The flux of precursors to the substrate is sensitive to pressure and gas flow rates, and highly depends on the chemical kinetics that occur close to the substrate.

- For the simulations shown, it was seen that the flux of atomic oxygen has high correlation to the local density of metastable products.