$O_2(^1\Delta)$ PRODUCTION IN HIGH PRESSURE FLOWING He/O_2 PLASMAS: SCALING AND QUENCHING

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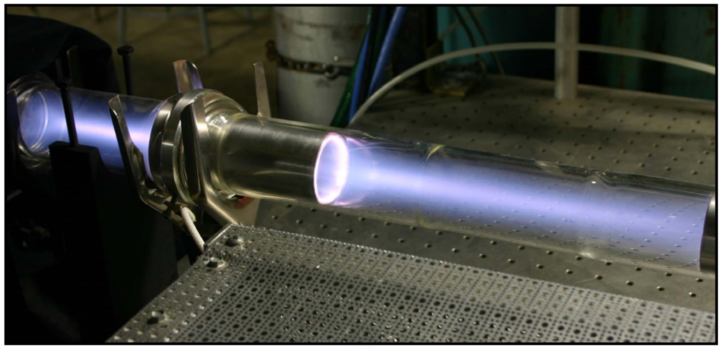
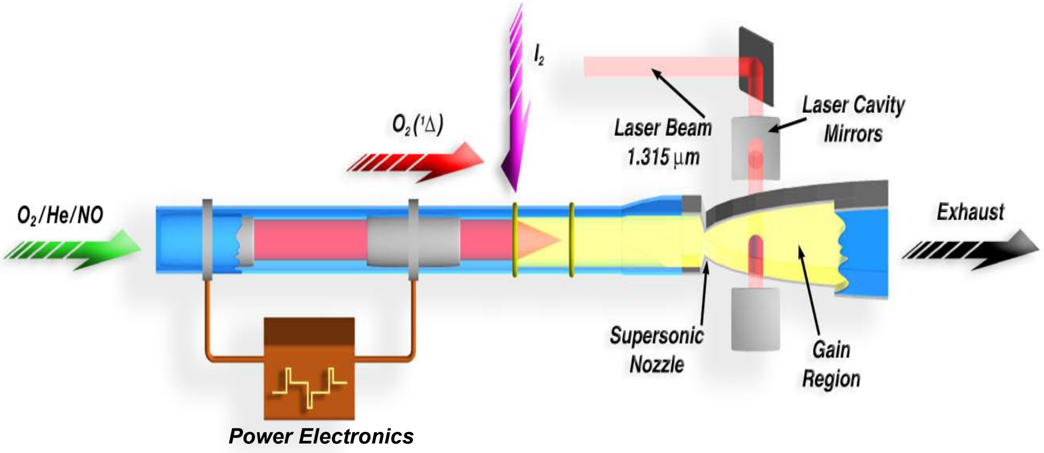
AGENDA

- Introduction to eCOIL
- Description of the models (GlobalKIN, 2-d nonPDPSIM)
- Performance at high pressures
  - Sublinear scaling of $O_2(^1\Delta)$ with pressure
  - Main quenchers of $O_2(^1\Delta)$
  - Gas heating and discharge stability
  - CW vs Spiker-Sustainer excitation
- Concluding Remarks

ELECTRICALLY EXCITED OXYGEN-IODINE LASERS

- In chemical oxygen-iodine lasers (COILs), oscillation at 1.315 µm $I(^2P_{1/2}) \rightarrow I(^2P_{3/2})$ occurs by excitation transfer of $O_2(^1\Delta)$ to I_2 and I.
- Plasma production of $O_2(^1\Delta)$ in electrical COILs (eCOILs) eliminates liquid phase generators.





- I_2 injection and supersonic expansion (to lower T_{gas} for inversion) occurs downstream of the plasma zone.

- Ref: CU Aerospace

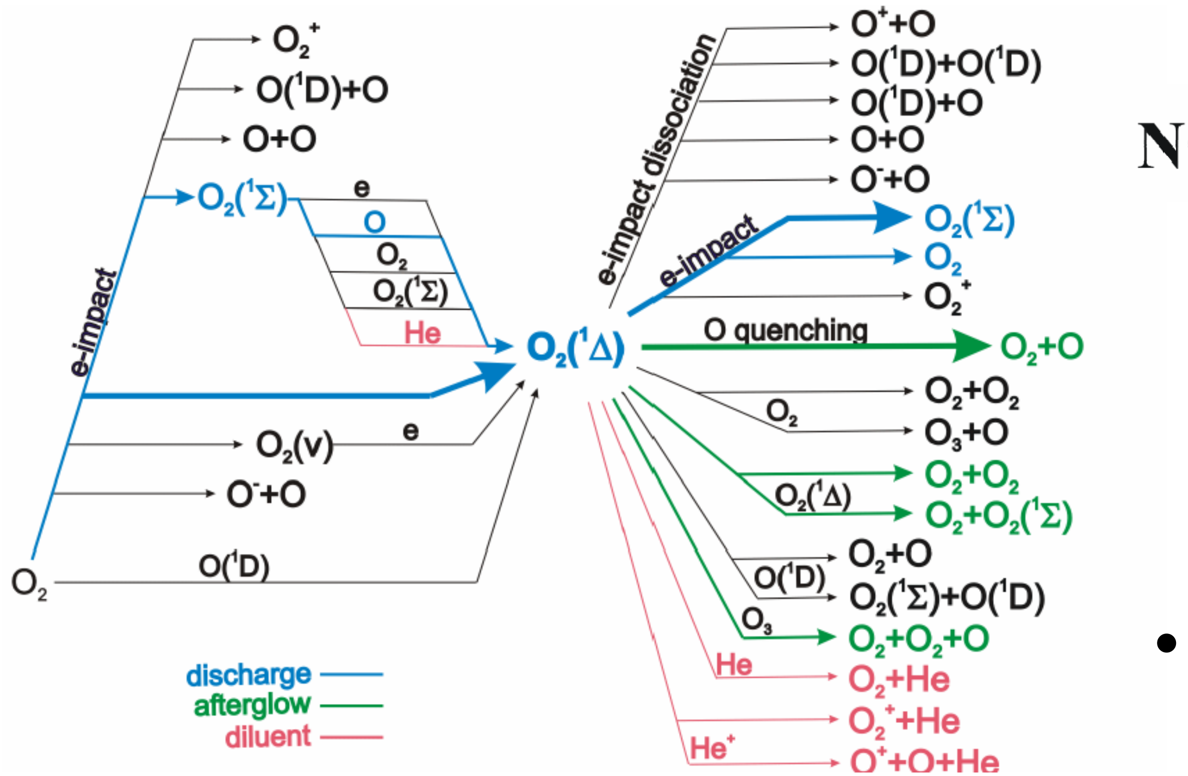
HIGH PRESSURE ISSUES FOR $O_2(^1\Delta)$ PRODUCTION

- Motivation for operating eCOIL at higher pressures
  - Larger absolute density of $O_2(^1\Delta)$ for a given yield (fraction of O_2 in excited state).
  - Higher back pressure for expansion.
- If there are no second order effects….
  - If Power ~ pressure and flowrate ~ pressure then eV/molecule is a constant.
  - $O_2(^1\Delta)$ production scales linearly with pressure.
  - Yield remains constant.
- Electron temperature and gas temperature weakly depend upon pressure.

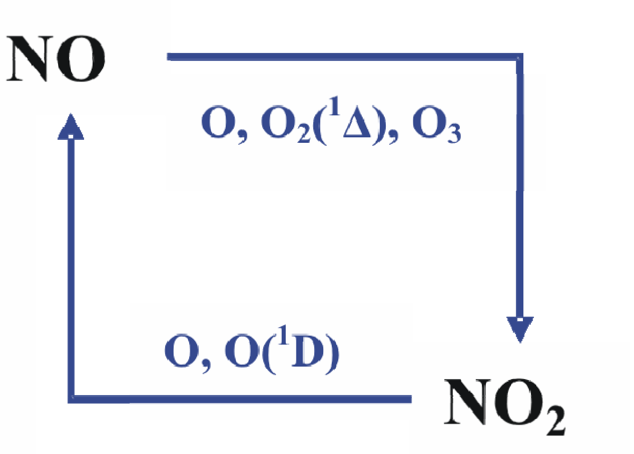
SECOND ORDER EFFECTS

- Second order effects may dominate the scaling of $O_2(^1\Delta)$ at higher pressures
- Three-body reactions produce quenchers of $O_2(^1\Delta)$, primarily O_3
- Quenching rates by O may increase with pressure with 3-body enhancement.
- Reactions $A + B + M \rightarrow AB + M$ are usually exothermic - significant heating source.
- Maintaining stability of discharge becomes more difficult at higher pressures.
- In this talk, we report on computational investigation of importance of second order effects in pressure scaling.

$O_2(^1\Delta)$ KINETICS IN He/O_2 DISCHARGES



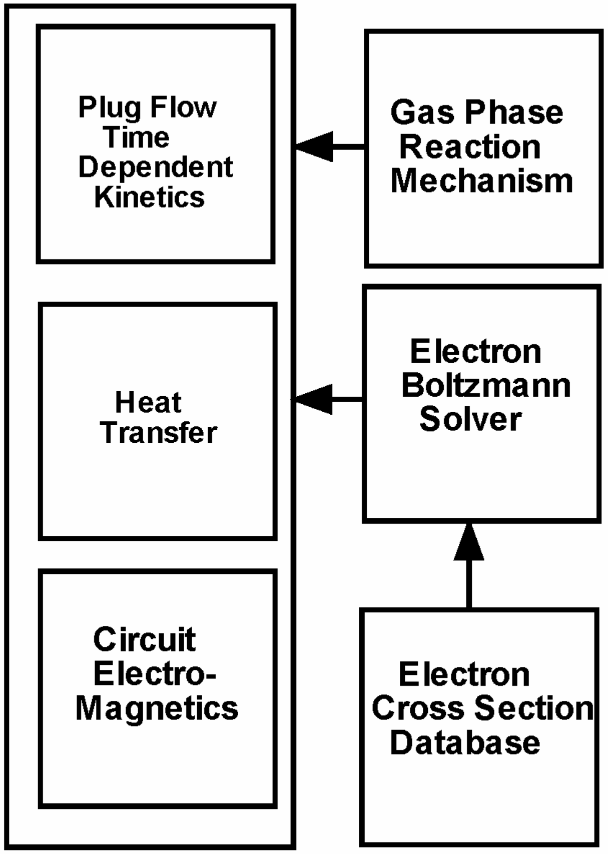
- Direct electron impact of O_2 and excitation of $O_2(^1\Sigma)$ (quenching) are main channels of $O_2(^1\Delta)$ production.
- O and O_3 quench $O_2(^1\Delta)$.



- NO/NO_2 recycling chain scavenges O atoms:

$$NO + O + M \rightarrow NO_2 + M$$
$$NO_2 + O \rightarrow NO + O_2$$

DESCRIPTION OF GlobalKIN



- Global model utilized in a plug flow mode.
- Boltzmann’s equation solved for electron energy distribution.
- Ion transport linked to database.
- Electric field obtained from circuit model or electro-magnetics power balance.
- Plug flow model includes enthalpy induced change in flow speeds.

DESCRIPTION OF 2d-nonPDPSIM: CHARGED PARTICLES, SOURCES

- **Poisson's equation, continuity equations and surface charge are simultaneously solved using a Newton iteration technique.**

$$-\nabla \cdot \varepsilon \nabla \Phi = \sum_j N_j q_j + \rho_s$$

$$\frac{\partial N_j}{\partial t} = -\nabla \cdot \vec{\phi}_j + S_j$$

$$\frac{\partial \rho_s}{\partial t} = \sum_j -q_j (\nabla \cdot \vec{\phi}_j + S_j) - \nabla \cdot (\sigma(-\nabla \Phi))$$

- **Electron energy equation:**

$$\frac{\partial (n_e \varepsilon)}{\partial t} = \vec{j} \cdot \vec{E} - n_e \sum_i \Delta\varepsilon_i N_i \kappa_i - \nabla \cdot \left(\frac{5}{2} \varepsilon \varphi - \lambda \nabla T_e \right), \quad \vec{j} = q \vec{\phi}_e$$

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DESCRIPTION OF 2d-nonPDPSIM: NEUTRAL PARTICLE TRANSPORT

- **Fluid averaged values of mass density, mass momentum and thermal energy density obtained using unsteady algorithms.**

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \vec{v}) + (inlets, pumps)$$

$$\frac{\partial (\rho \vec{v})}{\partial t} = \nabla (NkT) - \nabla \cdot (\rho \vec{v}\vec{v}) - \nabla \cdot \bar{\mu} + \sum_i q_i N_i \vec{E}_i$$

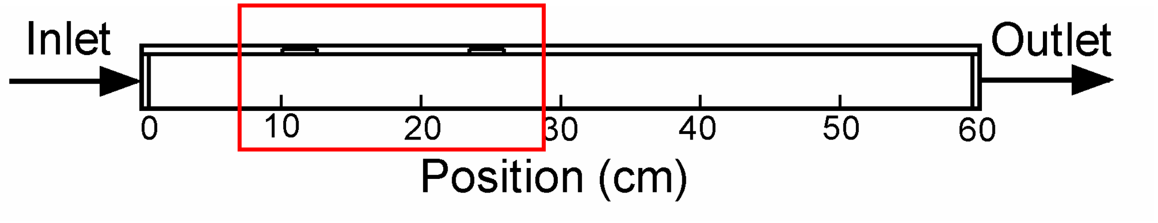
$$\frac{\partial (\rho c_p T)}{\partial t} = -\nabla \left(-\kappa \nabla T + \rho \vec{v} c_p T \right) + P_i \nabla \cdot v_f - \sum_i R_i \Delta H_i + \sum_i \vec{j}_i \cdot \vec{E}$$

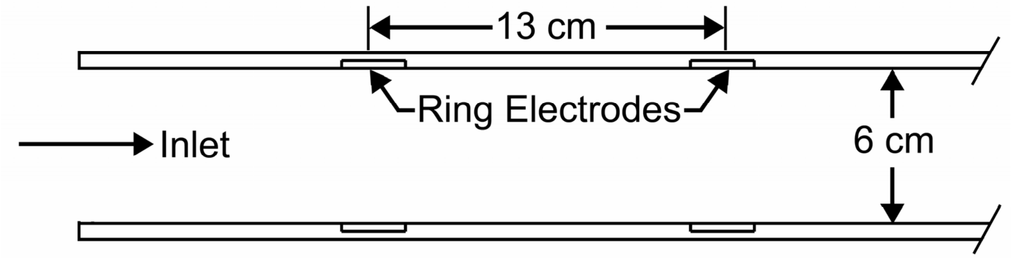
- **Individual fluid species diffuse in the bulk fluid.**

$$N_i(t + \Delta t) = N_i(t) - \nabla \cdot \left(\vec{v}_f - D_i N_T \nabla \left(\frac{N_i(t + \Delta t)}{N_T} \right) \right) + S_V + S_S$$

GEOMETRY FOR CAPACITIVE EXCITATION

$He/O_2/NO$



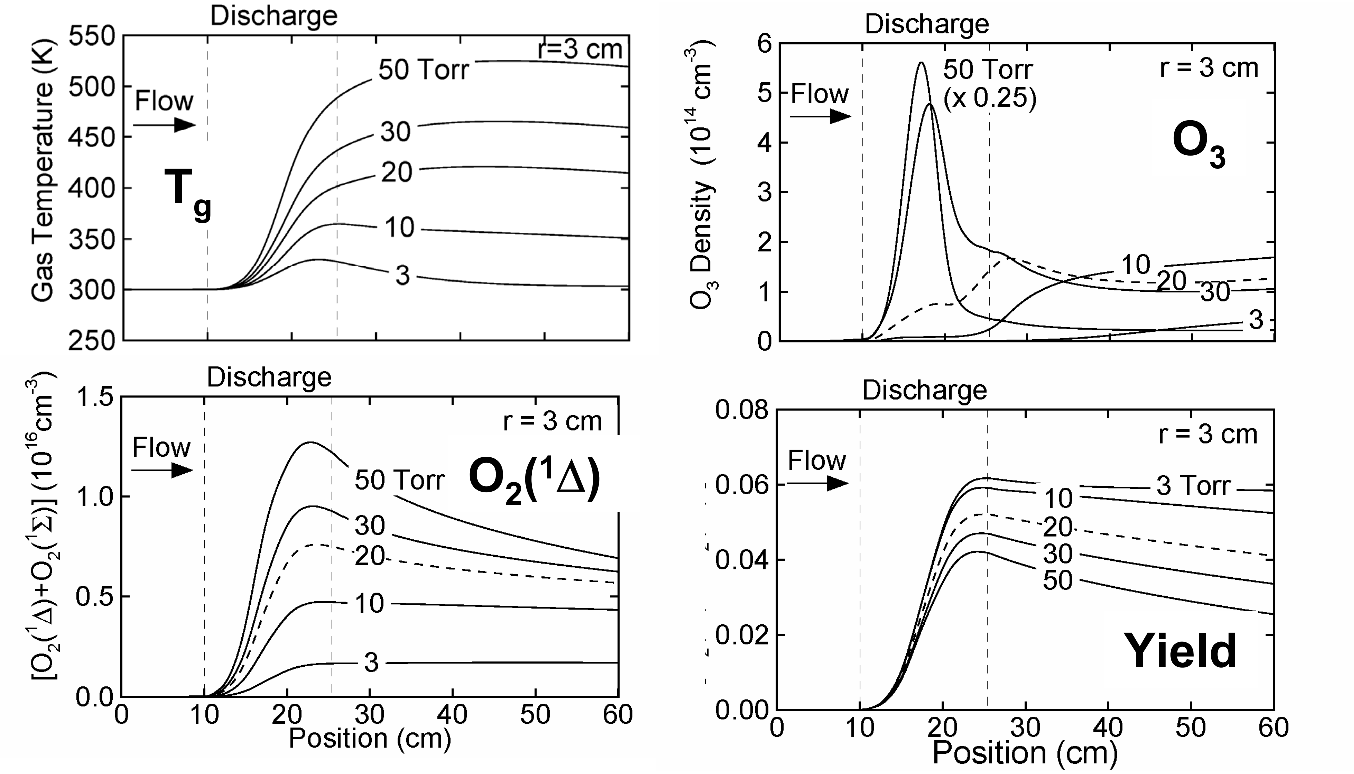


- **Cylindrical tube (2 and 6 cm diameter)**
- **Capacitive excitation (10-25 MHz).**
- **Constant eV/molecule and residence time.**
- **He/O_2=70/30, 3-50 Torr, 10's to 2000 W**
- **NO injection to control O atom inventory.**

- **Yield**

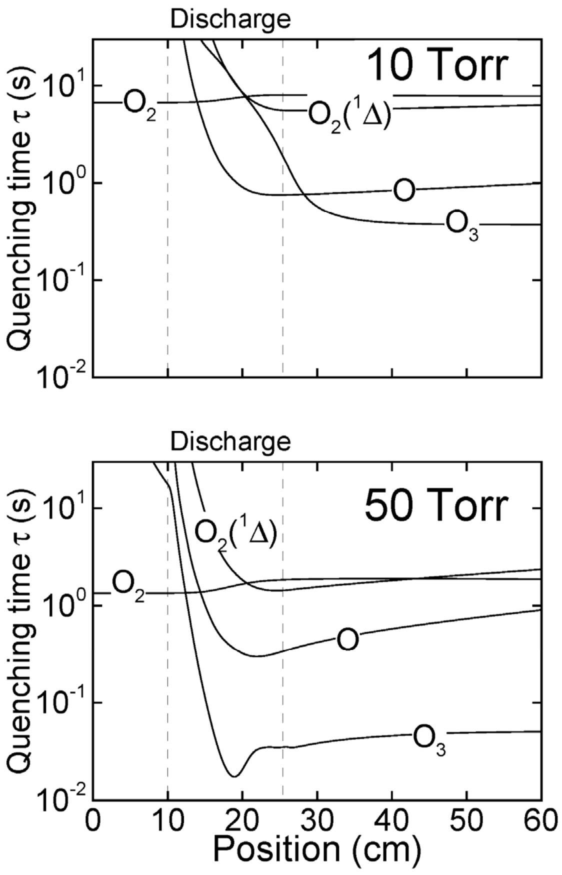
$$Y = \frac{[O_2(^1\Delta)] + [O_2(^1\Sigma)]}{([O_2] + [O_2(v)] + [O_2(^1\Delta)] + [O_2(^1\Sigma)] + 0.5[O] + 1.5[O_3])}$$

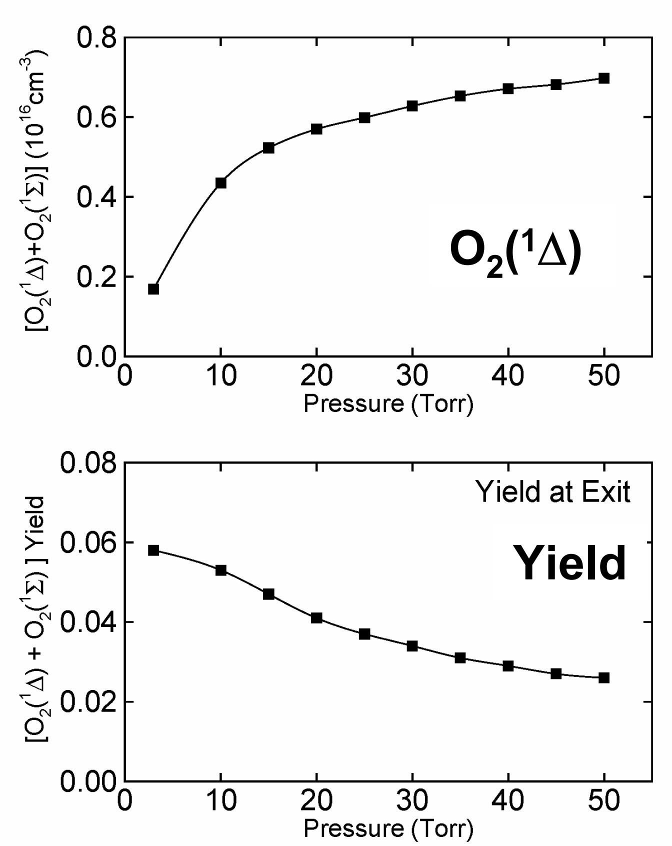
2nd ORDER EFFECT: 3-BODY REACTIONS AND O_3



- **Gas heating due to exothermic 3-body reactions.**
- **Peak O_3 density downstream at low pressure; in discharge region at higher pressures due to O_3 destruction with increase of T_g**
- **Sub-linear scaling of $O_2(^1\Delta)$ yield due to quenching by O_3.**
  - **GlobalKin: 3-50 Torr, 40-670 W, 0.3 eV/molecule**

MAIN QUENCHERS OF $O_2(^1\Delta)$: OZONE



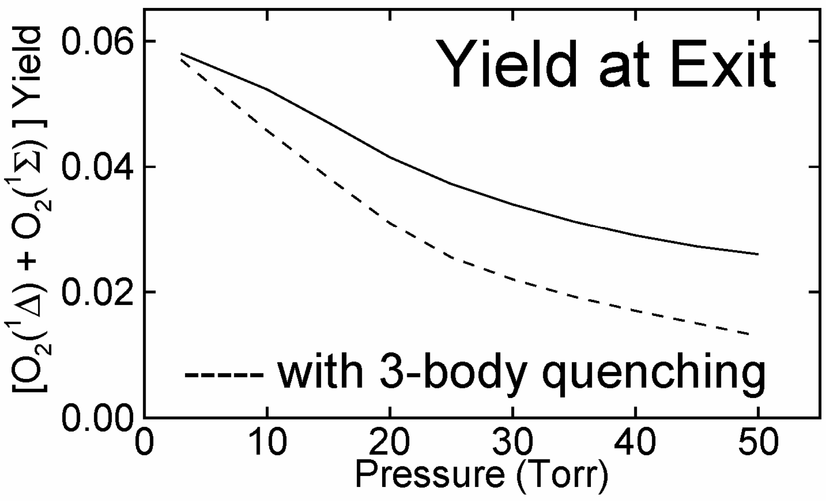


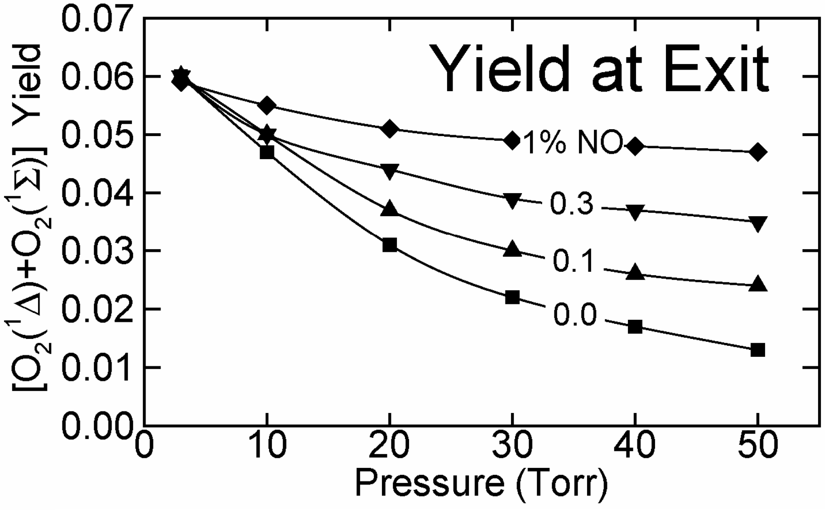
- **O_3 is the primary quencher > 10 Torr**

- **Sublinear $O_2(^1\Delta)$ scaling and decrease of yield with pressure.**

- **GlobalKin: 3-50 Torr, 40-670 W, 0.3 eV/molecule**

MAIN QUENCHERS OF $O_2(^1\Delta)$: ATOMIC OXYGEN





- **Yields decrease by a factor of 2 at 50 Torr when including three-body quenching:**

  $O_2(^1\Delta) + O + O_2 \rightarrow O_2 + O_2 + O$.

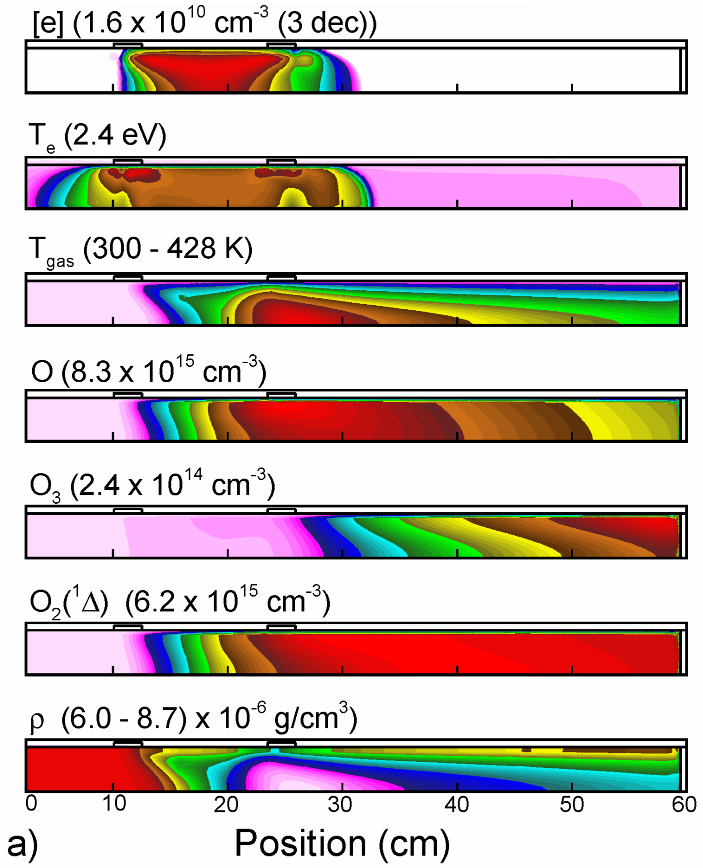
- **Addition of small amounts (< 1%) of NO in inlet scavenges O atoms and restores yield.**

A. N. Vasilieva et. al.
JPD 37, 2455 (2004)

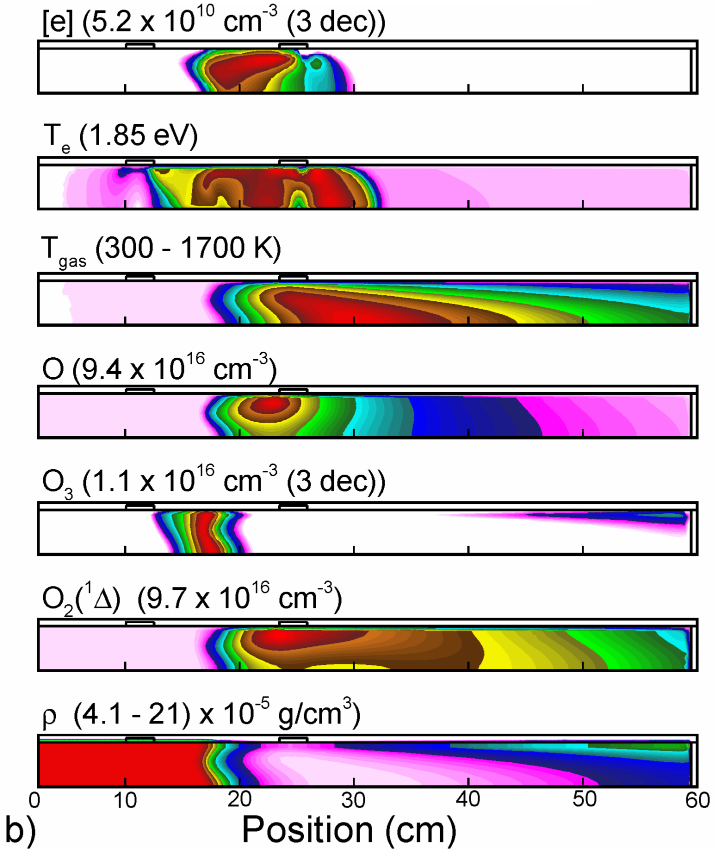
- **GlobalKin: 3-50 Torr, 40-670 W, 0.3 eV/molecule**

PLASMA PARAMETERS 10 - 50 TORR

- **10 Torr,133 W**

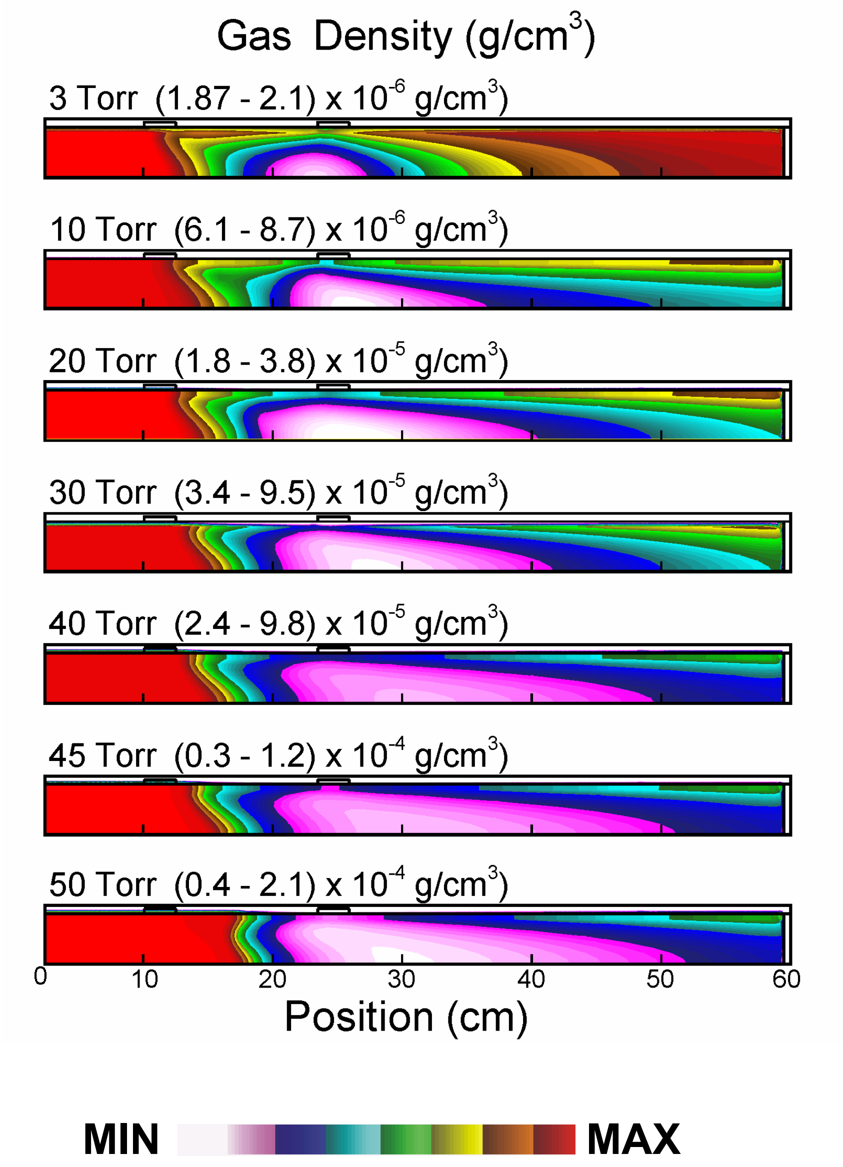


- **50 Torr,670 W**



- **Gas heating increases with pressure due to 3-body reactions resulting in non-uniform power deposition.**

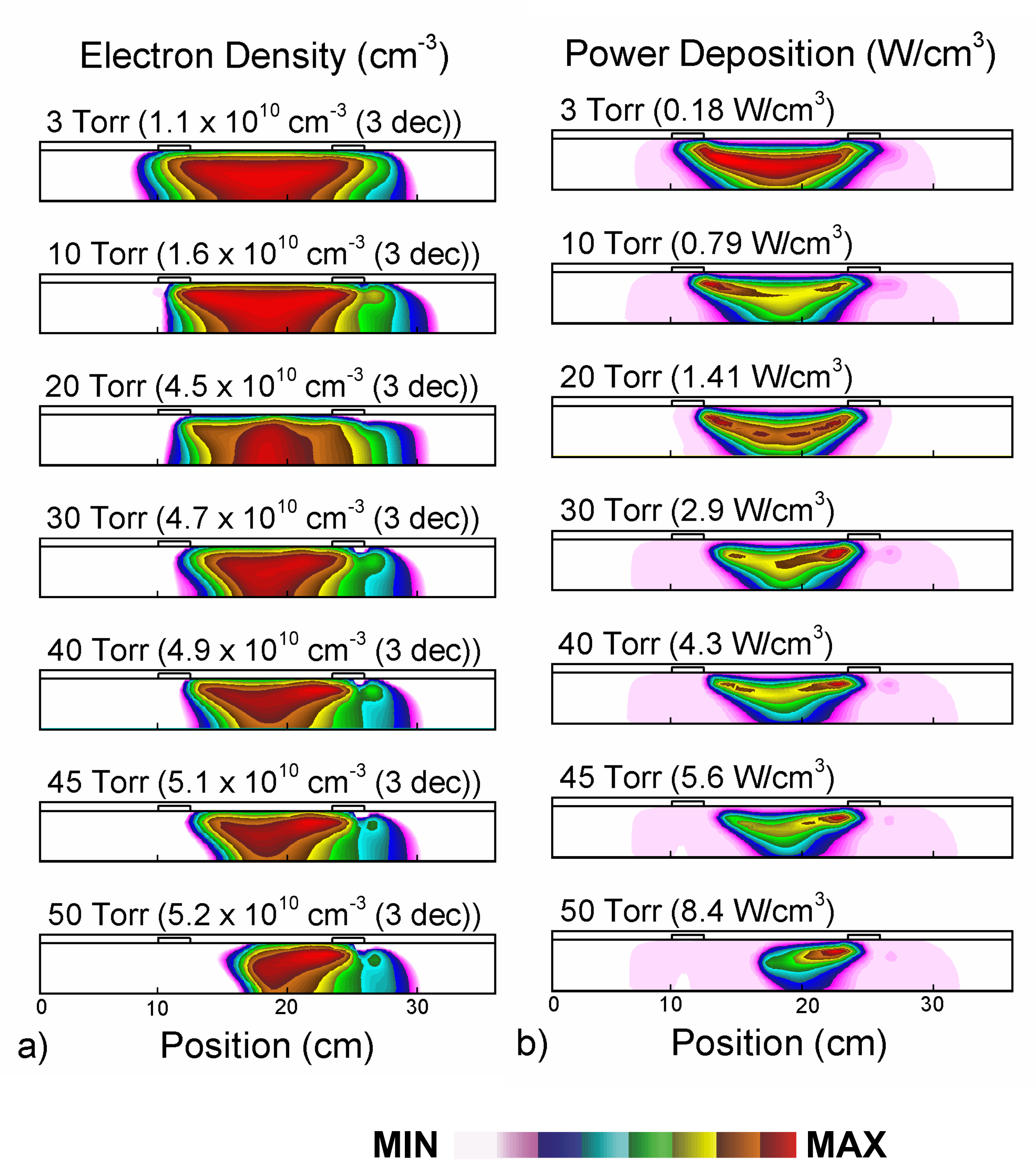
RAREFACTION DUE TO 3-BODY ENTHALPY CHANGES



- **Change in enthalpy from 3-body reactions increases with pressure.**
- **Heating accumulates in moving downstream.**
- **Rarefaction increases with pressure**
- **Localized rarefaction near downstream electrode where power is maximum.**

- **10 to 50 Torr, 133 to 670 W, 25 MHz, 0.3 eV/molecule**

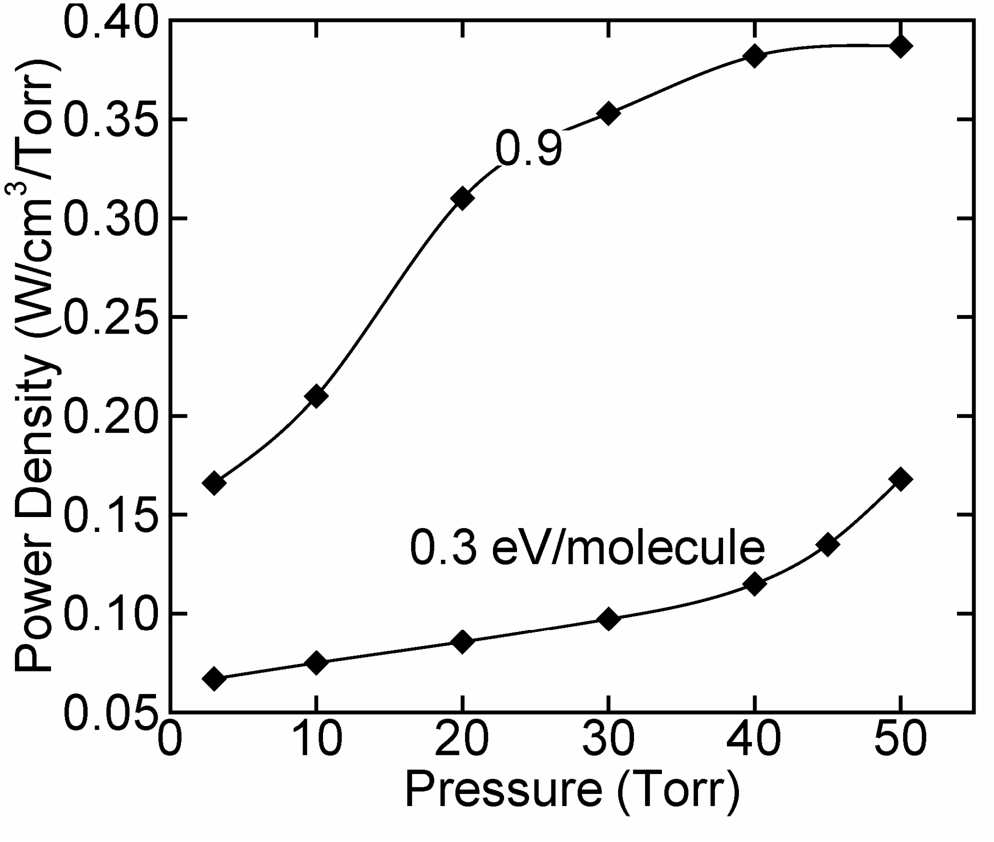
DIFFUSIVE TO CONSTRICTED DISCHARGE



- **Power deposition and electron density gradually constrict due to rarefaction of the gas.**

- **10 to 50 Torr, 133 to 670 W, 25 MHz, 0.3 eV/molecule**

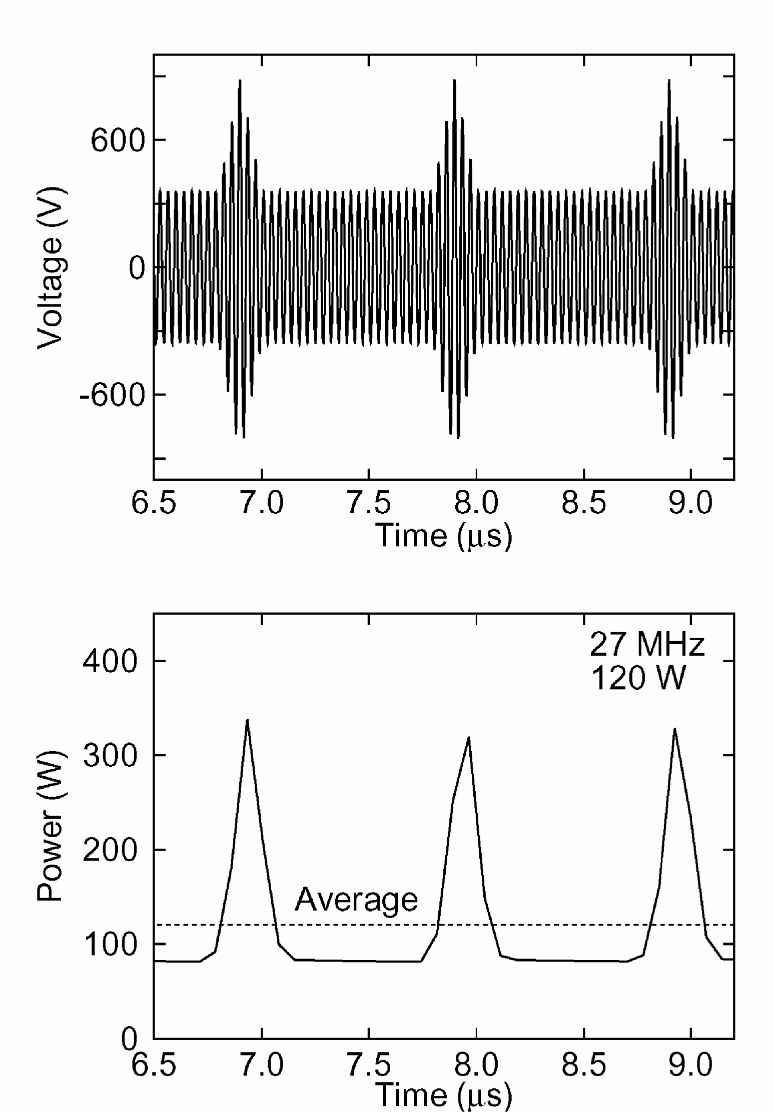
POWER DEPOSITION



- **Rapid increase in pressure normalized power deposition indicates a discharge constriction.**

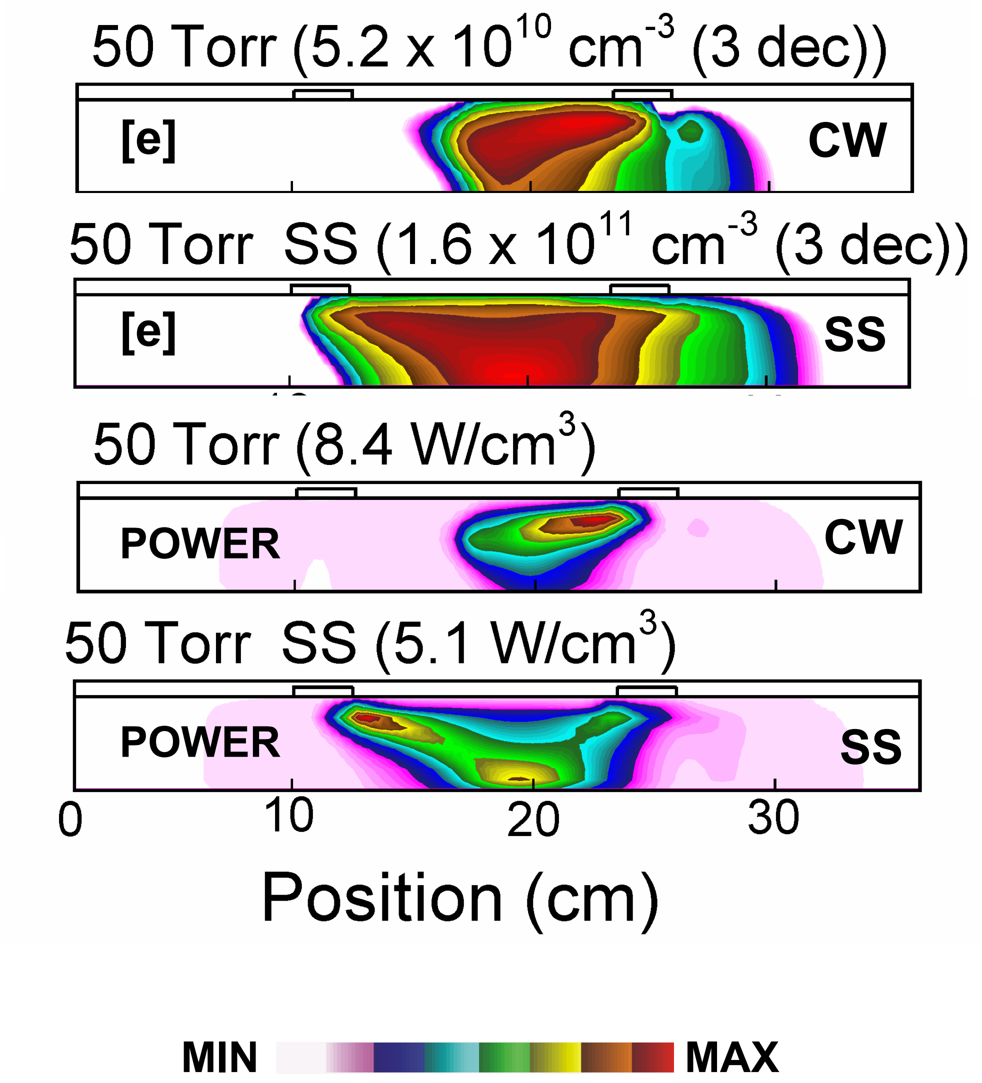
- **For high energy loadings constriction occurs at lower pressure.**

NON-SELF SUSTAINED DISCHARGES: SPIKER SUSTAINER



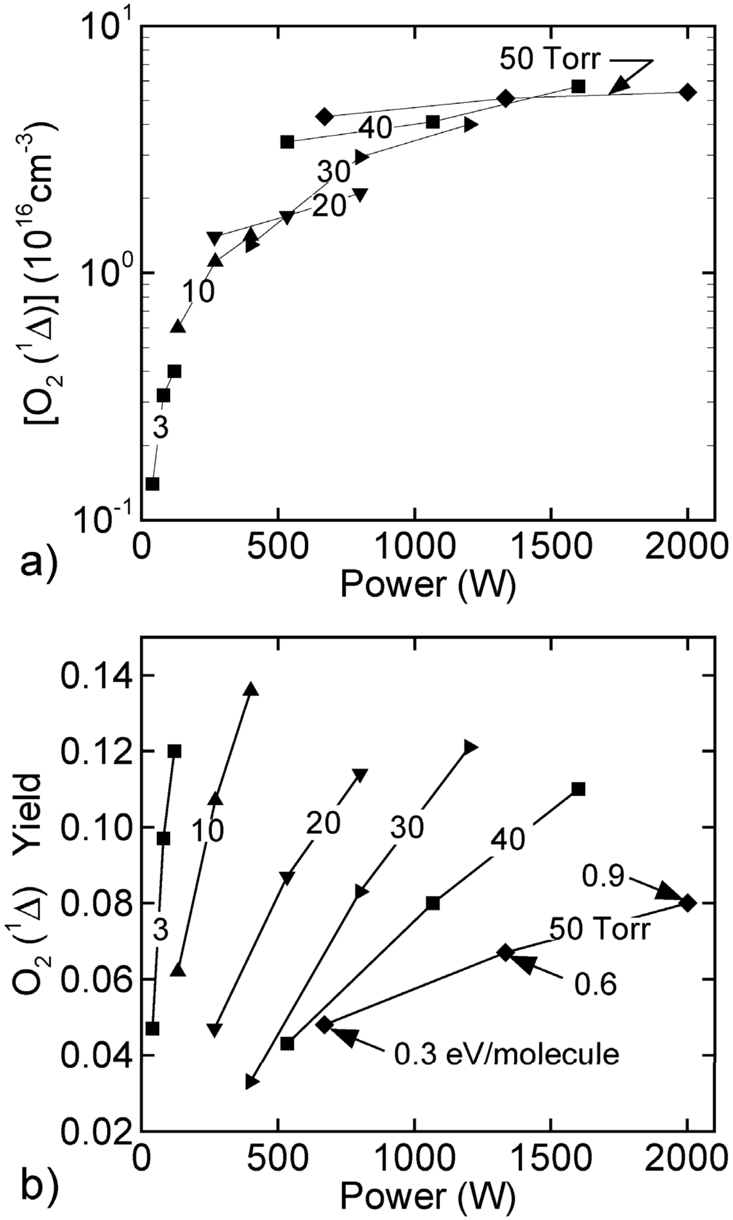
- **Short high power (spiker) pulse is followed by plateau of lower power (sustainer). Excess ionization in "afterglow".**
- **Spiker sustainer (SS) consists of modulated rf excitation.**
- **27 MHz, He/O_2 = 70/30, 3 Torr**

IMPROVEMENT WITH SPIKER-SUSTAINER (SS)



- **CW discharge becomes inhomogeneous at high pressures and high energy loading.**
- **In SS discharges, ionization is produced by a high-voltage pulse, which is turned off before ionization instabilities develop.**
- **SS discharge remains stable to higher pressures and power inputs.**

$O_2(^1\Delta)$ and Yield



SUMMARY OF PRESSURE SCALING

- **Absolute $O_2(^1\Delta)$ production increases with power for any given pressure.**
- **Yield increases with power for any given pressure.**
- **Yield at a given power generally decreases with pressure.**

- **He/O_2=70/30, 6 lpm, 25 MHz, 3-50 Torr, 0.3, 0.6, 0.9 eV/molecule**

CONCLUDING REMARKS

- Oxygen-iodine kinetics in flowing afterglows for eCOIL has been computationally investigated.
- High pressure operation should produce larger densities of $O_2(^1\Delta)$ but densities and yields usually scale sub-linearly with pressure (or decrease).
- Careful management is required:
  - O_3 and atomic oxygen densities: Left unchecked, quenching at high pressure is a rate limiting step
  - Influence of O-atom quenching can be minimized by NO injection.
  - Gas temperature: Active cooling increases O_3 formation
  - Stability: Asymmetries in excitation due to rarefaction may trigger constrictions.