

SCALING OF PLASMA SOURCES FOR $O_2(^1\Delta)$ GENERATION FOR CHEMICAL OXYGEN-IODINE LASERS

**D. Shane Stafford and Mark J. Kushner
University of Illinois**

**Department of Electrical and Computer Engineering
Urbana, IL 61801**

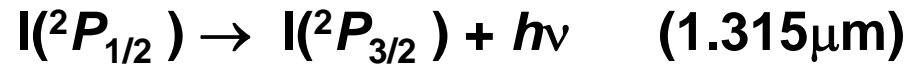
<http://uigelz.ece.uiuc.edu> mjk@uiuc.edu

June 2004

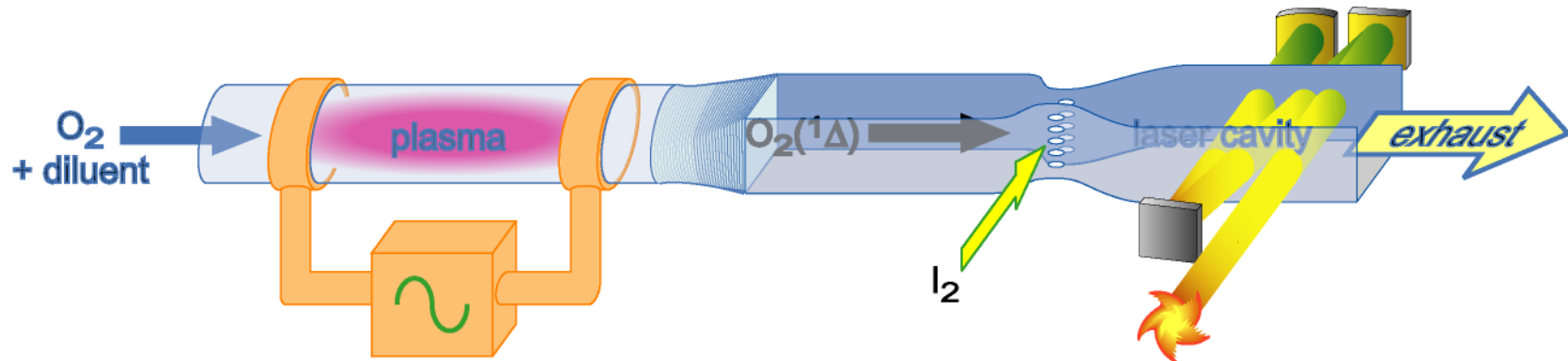
*** Work supported by Air Force Office of Scientific Research and Air Force Research Laboratories**

OXYGEN-IODINE LASERS

- $O_2(^1\Delta)$ dissociates I_2 and pumps I which lases on the $^2P_{1/2} \rightarrow ^2P_{3/2}$ electronic transition.



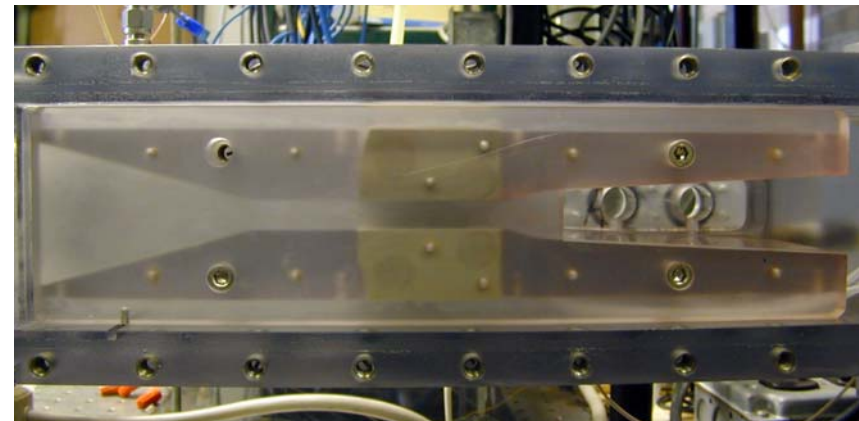
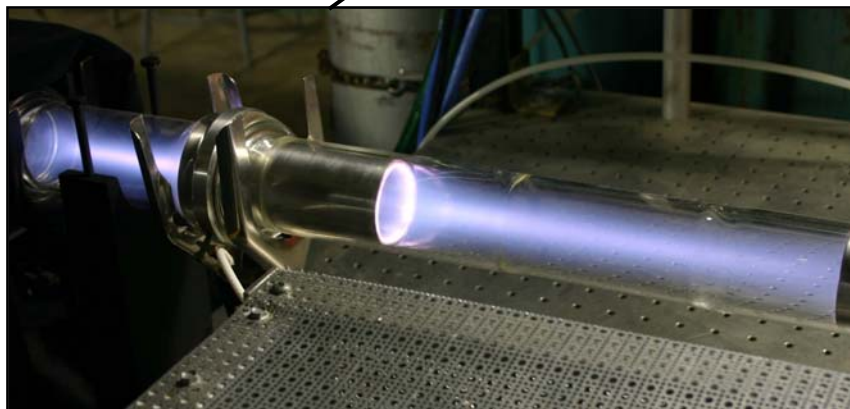
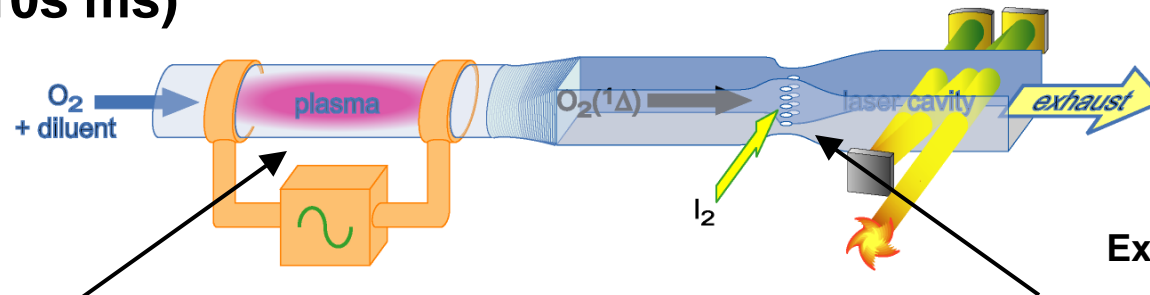
- Conventional COILs obtain $O_2(^1\Delta)$ from a liquid phase reaction.
- Electrical COILs obtain $O_2(^1\Delta)$ by exciting O_2 in discharge.



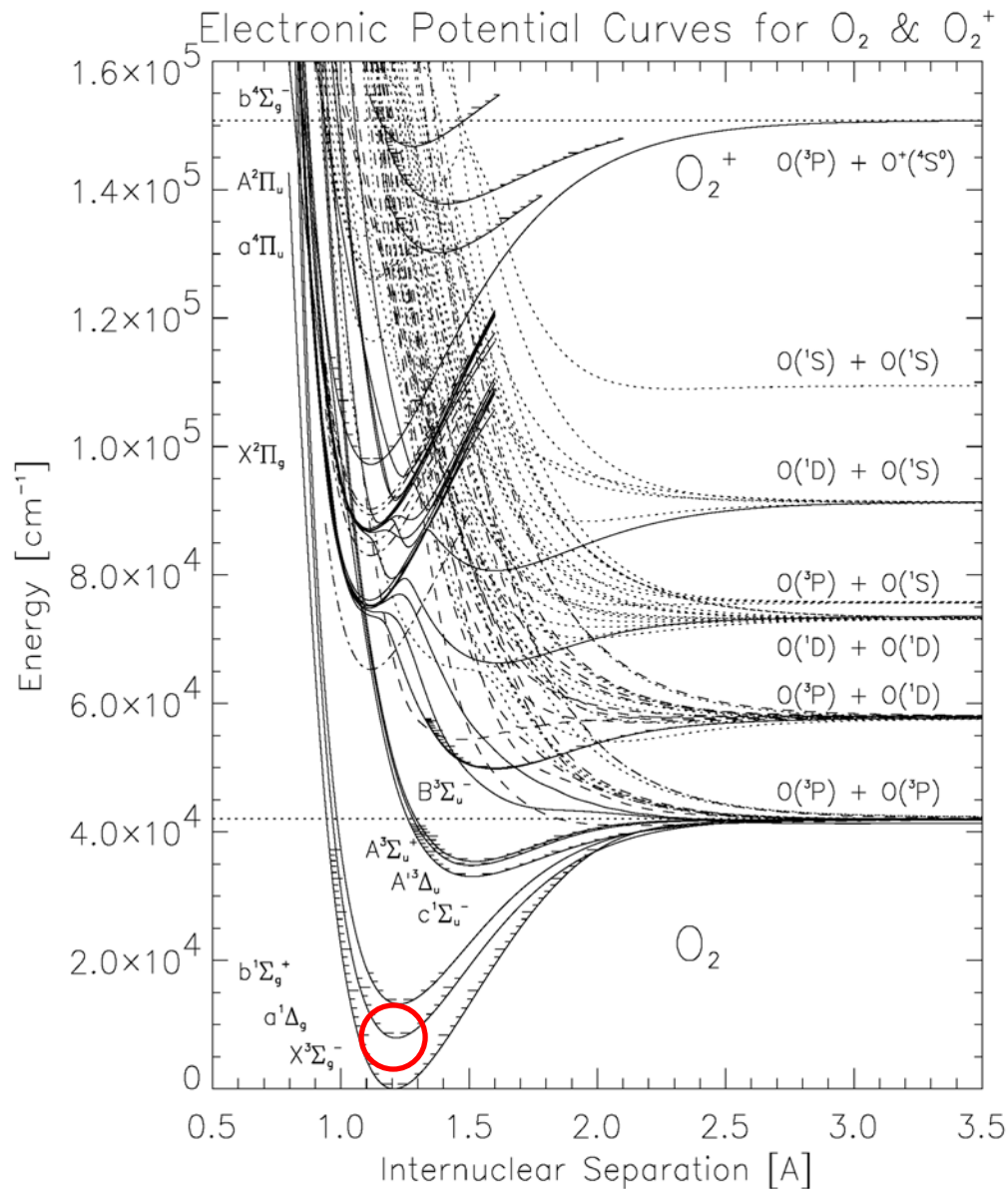
University of Illinois
Optical and Discharge Physics

TYPICAL CONDITIONS

- Pressures: a few to 10s Torr (Higher is better to provide back pressure for expansion)
- Mixtures: He/O₂ , f(O₂) = 10's – 50% (Need He for discharge stability, tailoring E/N, high thermal conductivity).
- Size: Flow tube 3-10 cm diameter (pump limited?)
- Flow speeds: 10s m/s (plasma residence time many ms, flow times 10s ms)



O₂ ENERGY POTENTIAL ENERGY DIAGRAM

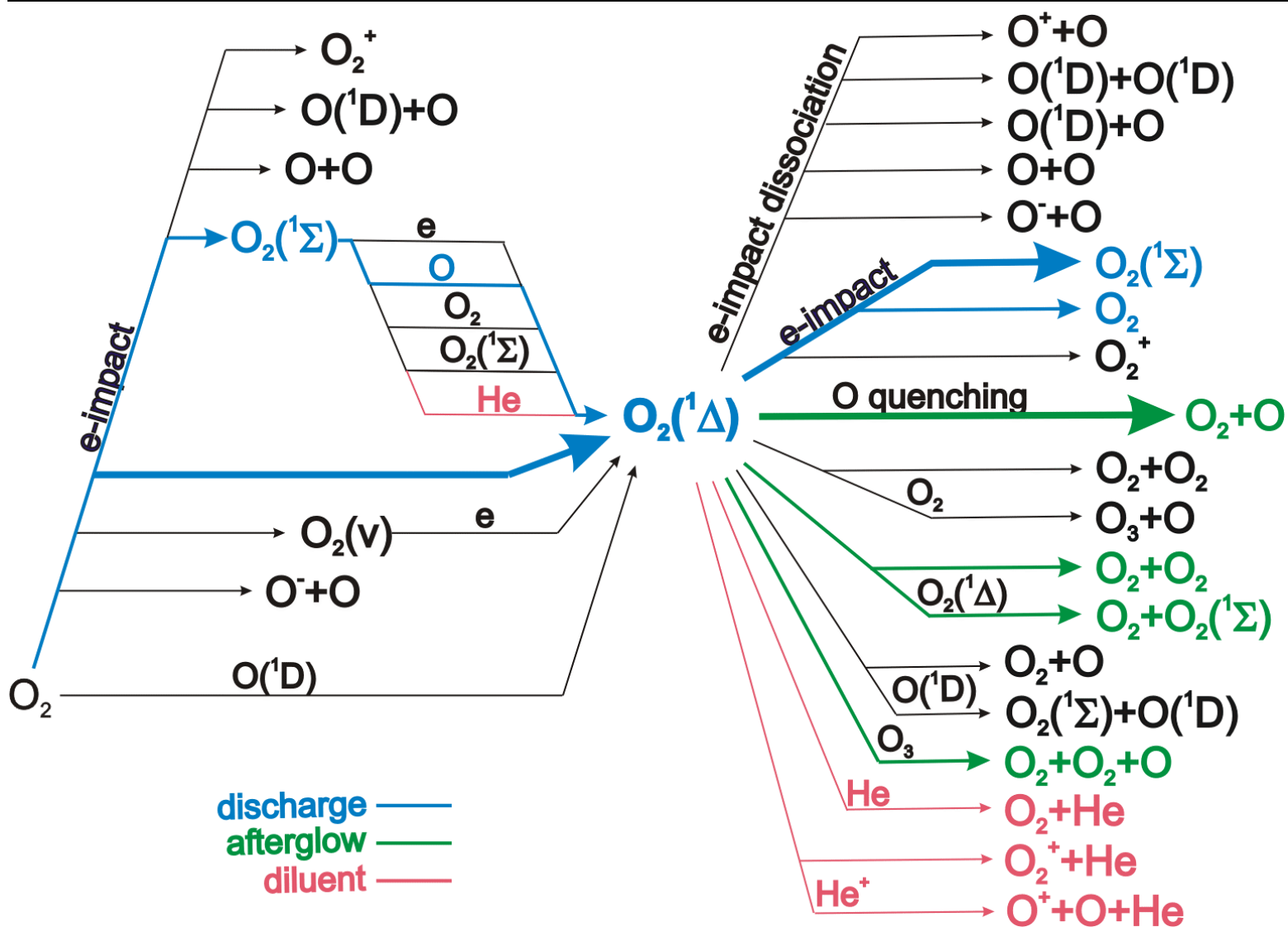


- O₂ is unique among common diatomic molecules as having low lying electronic states.
- O₂(¹Δ) [0.98 eV] and O₂(¹Σ) [1.6 eV] are readily accessible in the Frank-Condon corridor.

• J. S. Morrill, et al, www.nist.gov

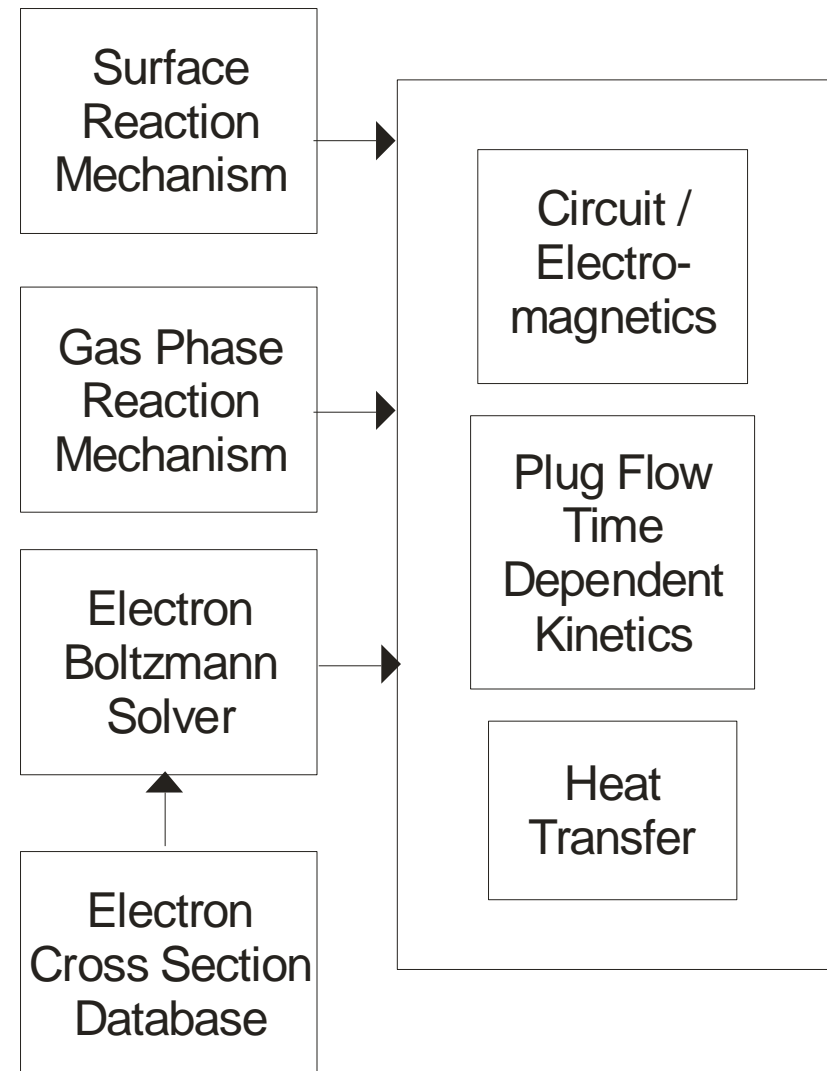
University of Illinois
Optical and Discharge Physics

REACTION MECHANISM



DESCRIPTION OF GLOBAL_KIN

- **Global model with a user defined gas and surface reaction mechanism.**
- **Boltzmann's equation solved for electron distribution (linked to cross section database).**
- **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.**

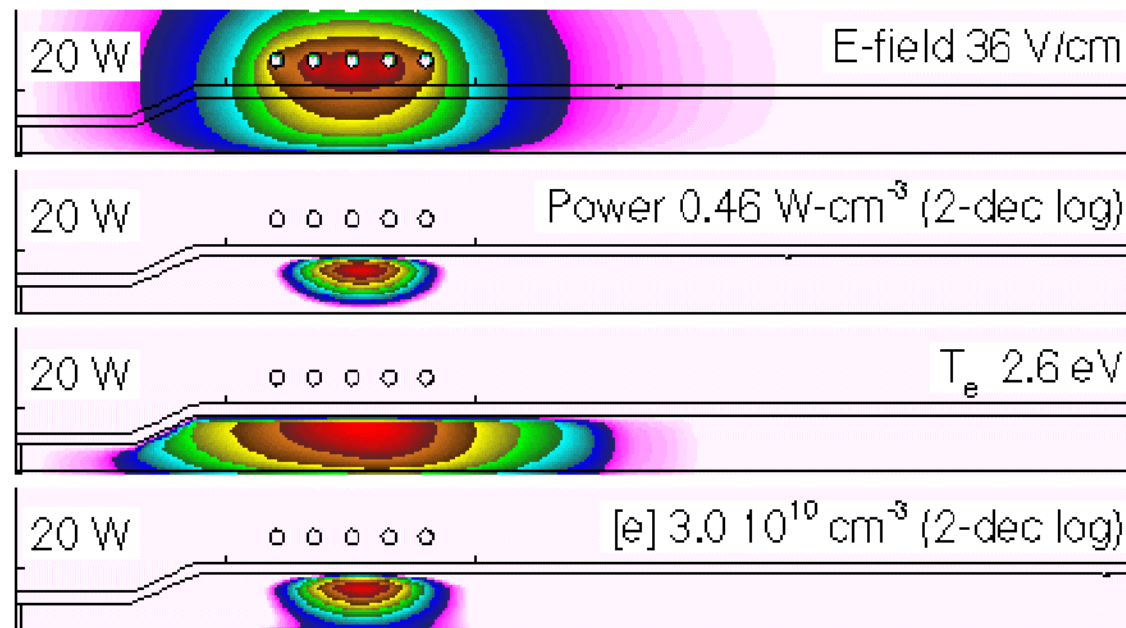


nonPDPSIM: 2-DIMENSIONAL PLASMA DYNAMICS

- **nonPDPSIM was developed to investigate plasma hydrodynamics at moderate to high pressures in complex geometries.**
 - **2-d rectilinear or cylindrical unstructured mesh**
 - **Implicit drift-diffusion for charged**
 - **Poisson's equation with volume and surface charge, and material conduction.**
 - **Circuit model**
 - **Electron energy equation coupled with Boltzmann solution for electron transport coefficients**
 - **Optically thick radiation transport with photoionization**
 - **Secondary electron emission by impact, thermally enhanced electric field emission, photoemission**
 - **Surface chemistry.**
 - **Monte Carlo Simulation for secondary electrons**
 - **Navier-Stokes for neutrals with individual diffusion speeds**

ELECTRICAL AND ELECTRON PARAMETERS

- Thermal conduction and diffusion produces warm electrons upstream. Electron density peaks near maximum in T_e as attachment distance is short.



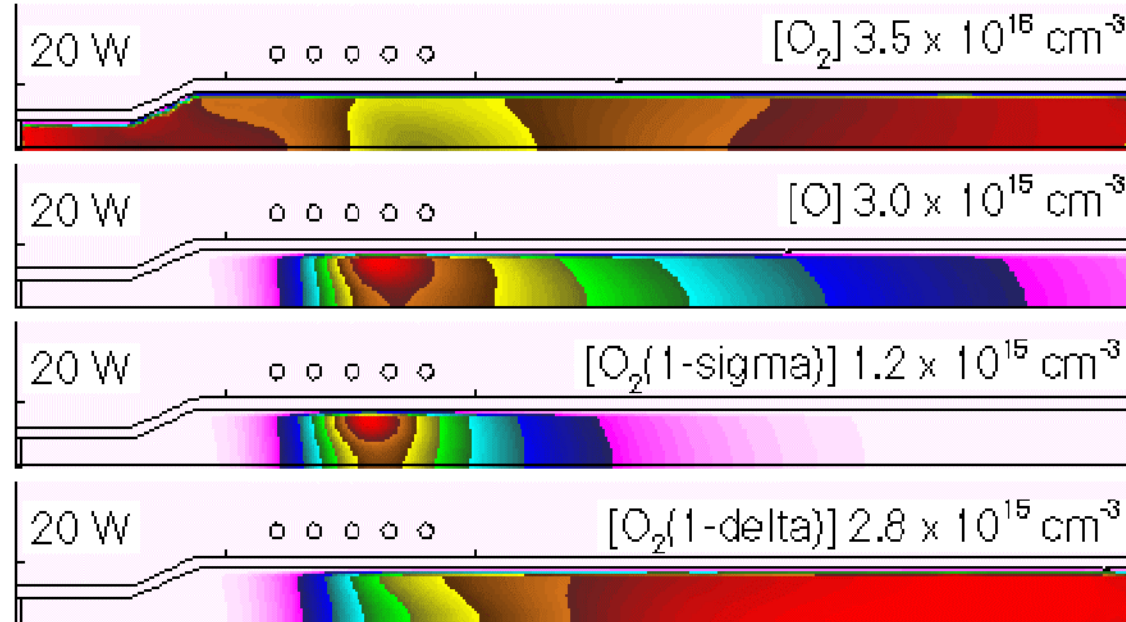
- 3 Torr, He/O₂=0.7/0.3, 6000 sccm, 20 W

MIN  MAX

University of Illinois
Optical and Discharge Physics

OXYGEN ATOMIC AND MOLECULAR DENSITIES

- $O_2(^1\Sigma)$ and O densities are maximum near peak power deposition.
- $O_2(^1\Delta)$ increases downstream as $O_2(^1\Sigma)$ is quenched and transfer occurs from $O(^1D)$. Yield here is 8%.
- O_2 is depleted by dissociation and gas heating.

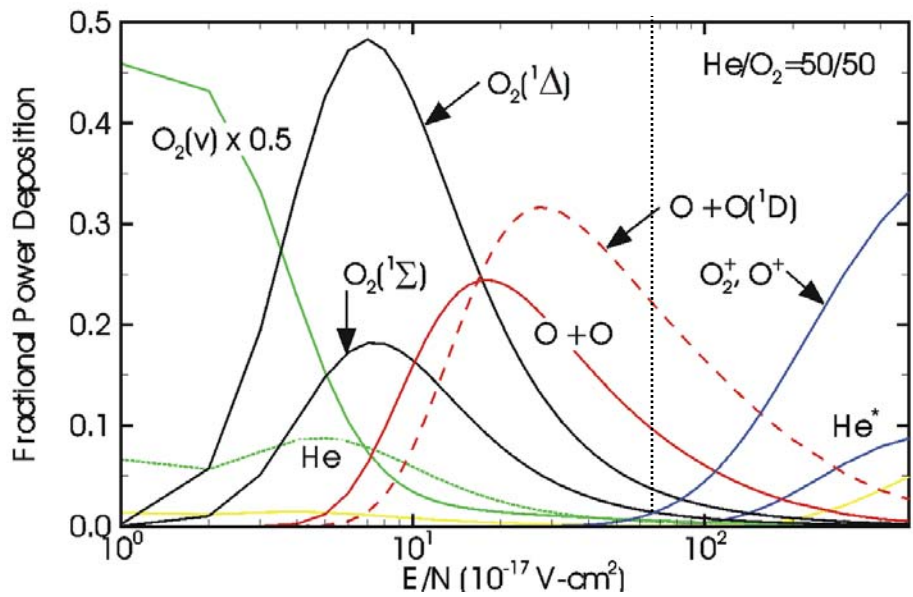
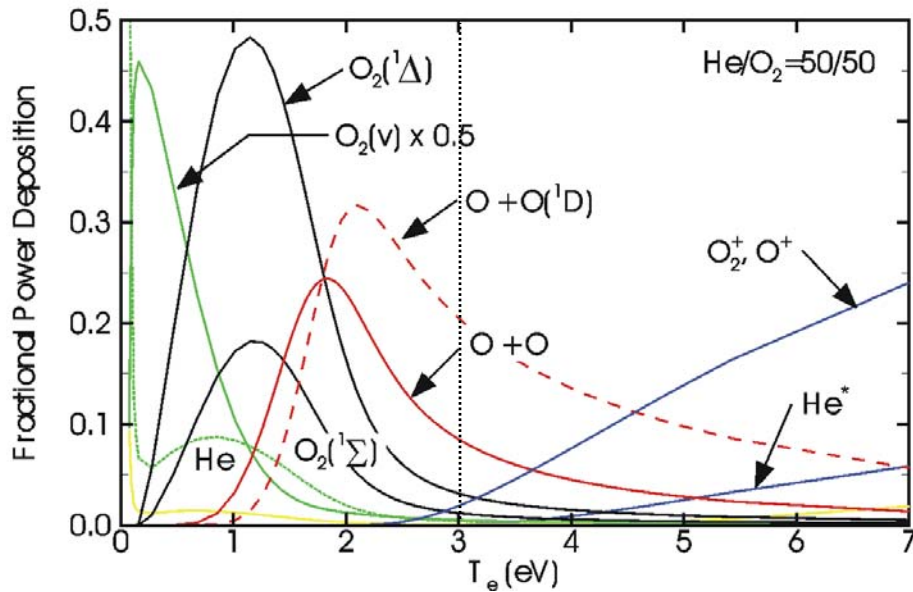


- 3 Torr, He/ O_2 =0.7/0.3, 6000 sccm, 20 W

MIN  MAX

University of Illinois
Optical and Discharge Physics

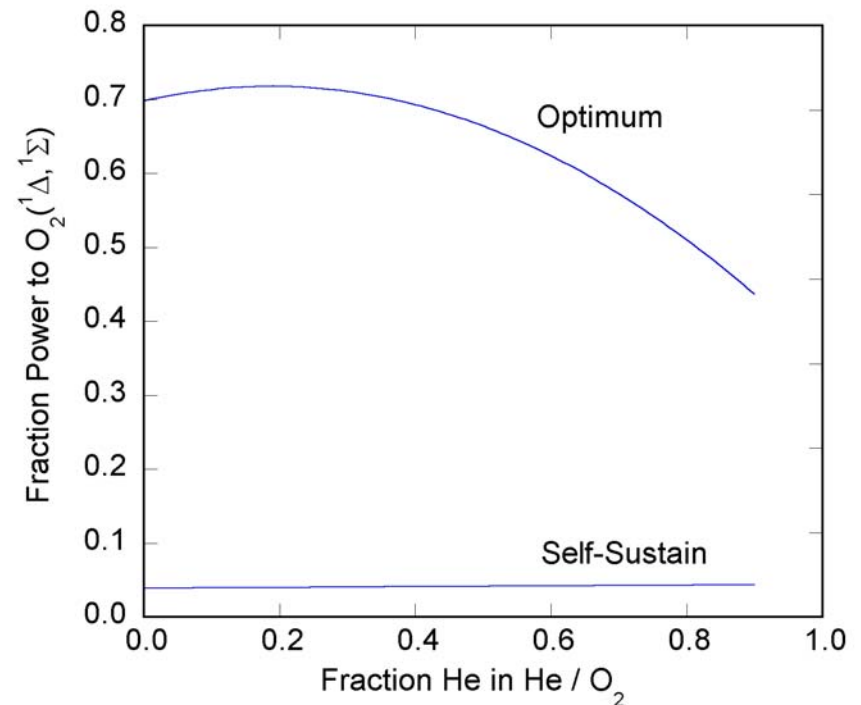
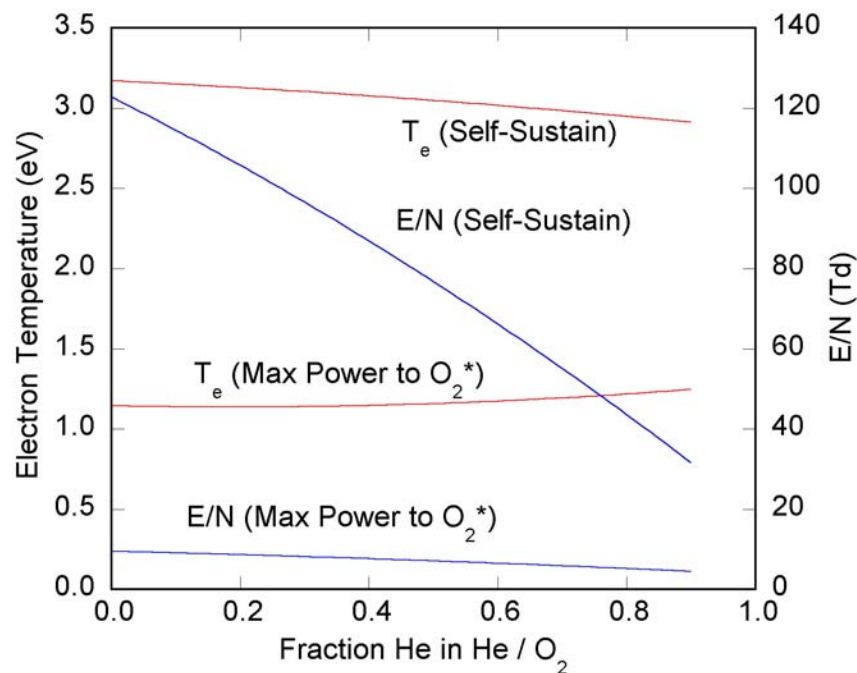
FRACTIONAL POWER DEPOSITION



- Significant power can be channeled into excitation of $O_2(^1\Delta)$ and $O_2(^1\Sigma)$.
- Optimum conditions are $T_e = 1-1.2$ eV, $E/N = 8-10$ Td.
- The challenge is operating at those values.
- Self sustaining (based on attachment) for $He/O_2 = 50/50 = 3$ eV, 80 Td. Higher with diffusion losses.

DISCHARGE PARAMETERS: SELF-SUSTAIN vs OPTIMUM

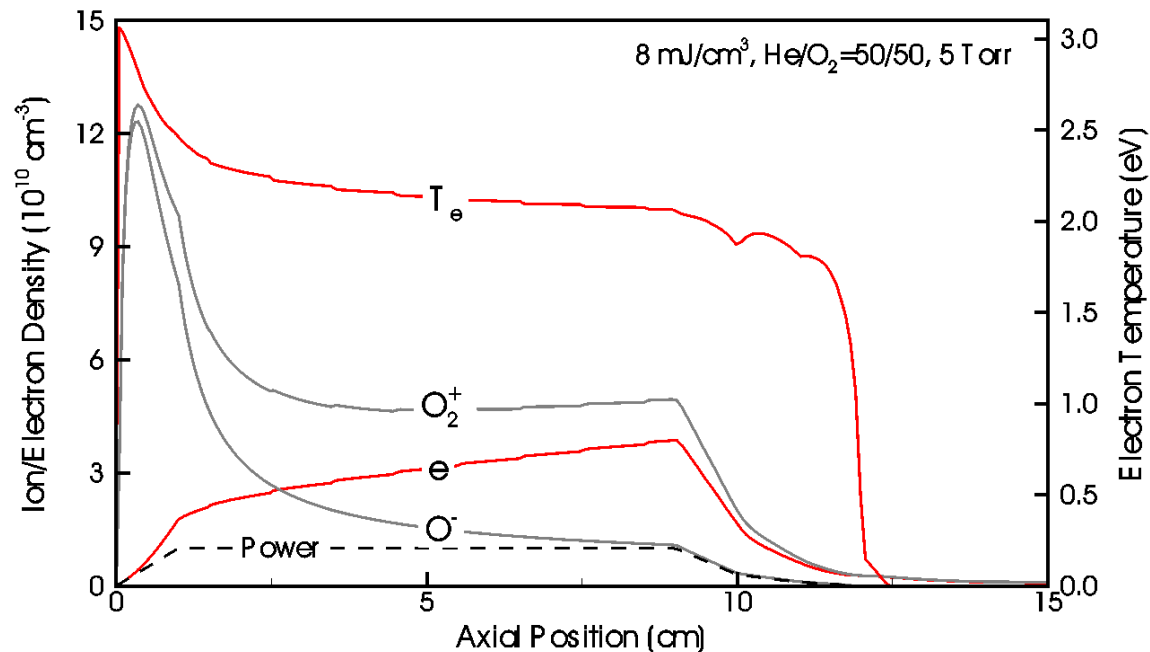
- Self sustaining based on balance between ionization and attachment for ground state feedstock gases.
- Optimum conditions based on maximum power dissipated in $O_2(^1\Delta, ^1\Sigma)$ excitation.
- Dilution does not achieve significant improvements.



University of Illinois
Optical and Discharge Physics

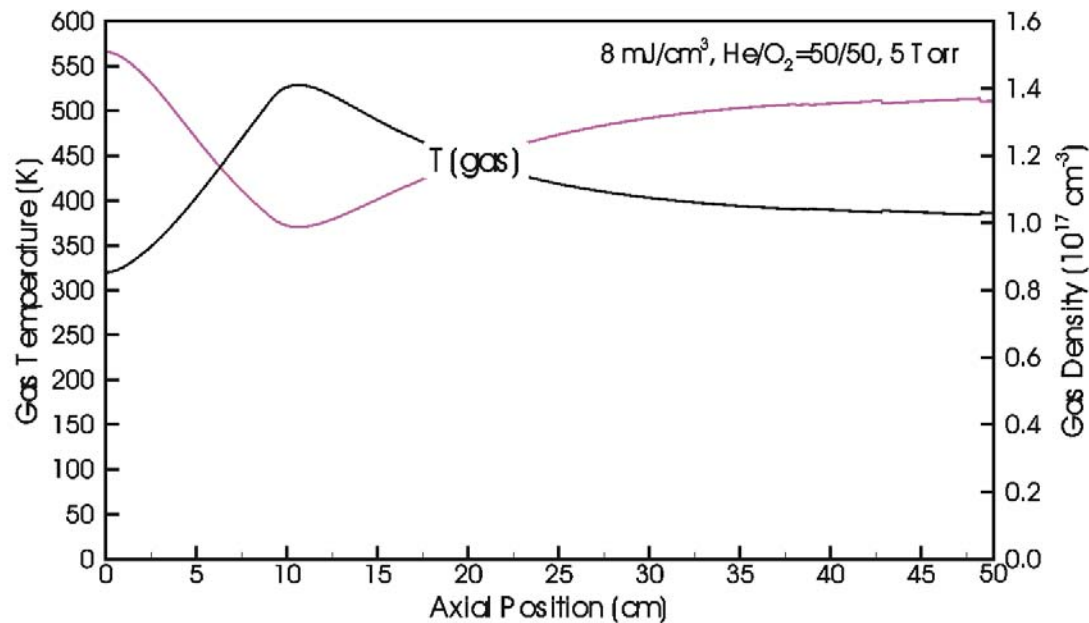
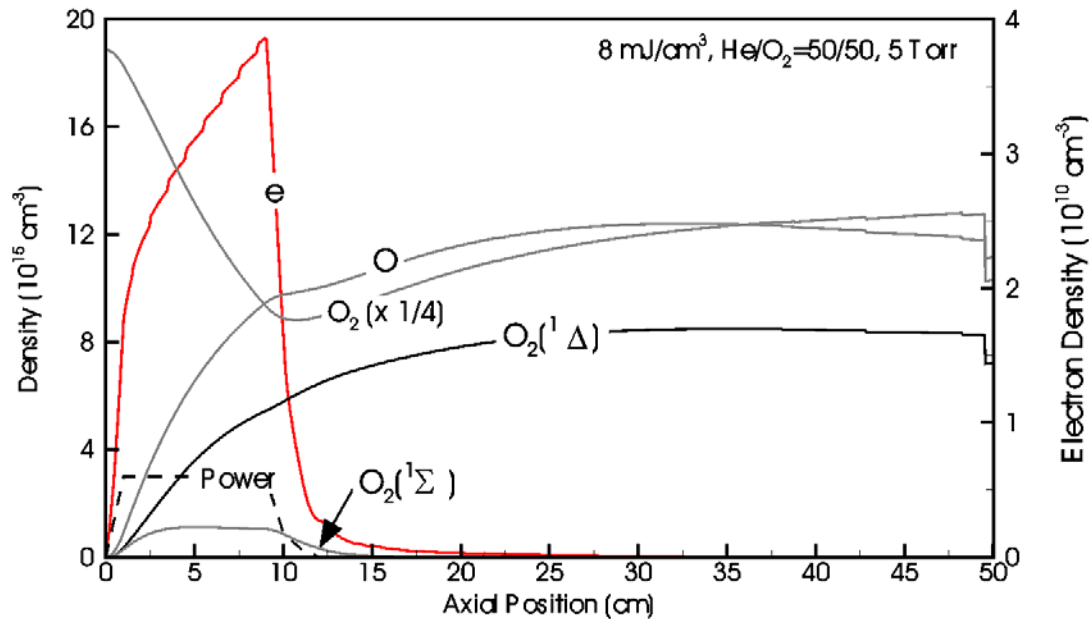
TYPICAL PLASMA PROPERTIES: He/O₂ = 50/50, 5 Torr

- Plug flow model with inductively coupled plasma (nearly always a self-sustaining.)
- Initial high T_e to avalanche plasma favors dissociative attachment and formation of O⁻.
- Steady state T_e = 2.1 eV exceeds optimum to excite O₂(¹Δ, ¹Σ).



- He/O₂ = 50/50, 5 Torr, v₀ = 10 m/s, 1 W/cm³

University of Illinois
Optical and Discharge Physics



TYPICAL PLASMA PROPERTIES: He/O₂ = 50/50, 5 Torr

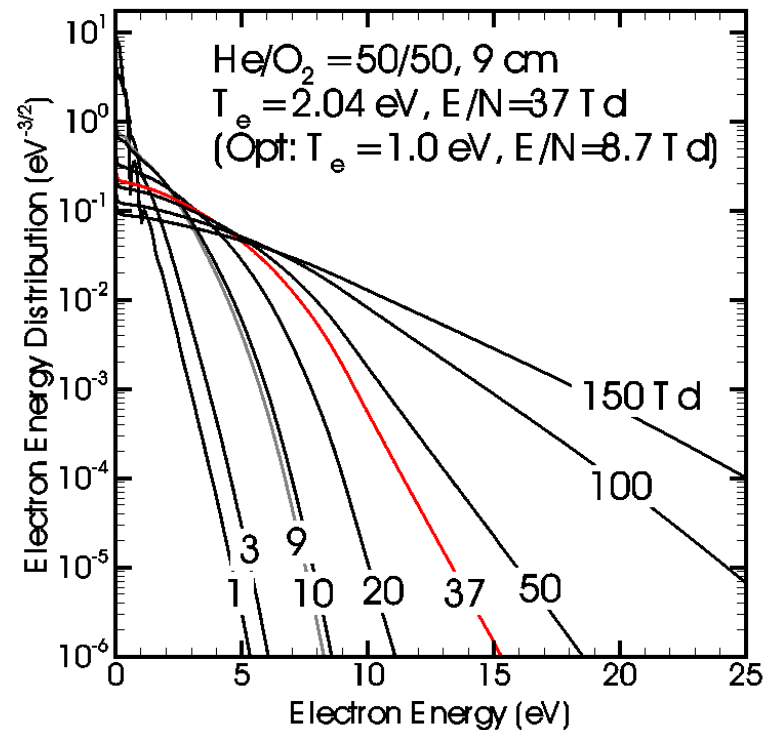
- O₂(¹Σ) is collisionally quenched to O₂(¹Δ) after the plasma zone. O₂(¹Δ) resists quenching when energy pooling is not important.
- O atom production nearly equals O₂(¹Δ).
- Gas heating is significant, due to V-T relaxation, Frank-Condon heating.

University of Illinois
Optical and Discharge Physics

• He/O₂ = 50/50, 5 Torr, v₀ = 10 m/s, 1 W/cm³
ECOIL_SCALE_ICOPS_0504_04

LIFE IS BETTER THAN ADVERTISED: WHAT SAVES YOU?

- Performance of self sustained discharges is better than advertised with more optimum production of $O_2(^1\Delta)$.
- Dissociation and excitation of O_2 results in:
 - Less attachment
 - More efficient ionization
 - Lower self-sustaining T_e
 - Higher fractional power into $O_2(^1\Delta, ^1\Sigma)$ provided dissociation is not large.
- For $He/O_2 = 50/50$, opt $T_e = 1.0$ eV. Self sustaining is
 - 3.1 eV ($x = 0$ cm)
 - 2.0 eV ($x = 9$ cm)



PROPOSED SCALING LAW

- A full factorial parameterization of velocity, pressure, power, and mixture was performed to determine scaling laws for $O_2(^1\Delta)$ yield.
- A scaling law is proposed giving yield (β) as a function of specific energy deposition (in eV per inlet O_2 molecule):

$$\beta = \frac{[O_2(^1\Delta)]}{[O_2] + [O_2(^1\Delta)] + 0.5[O] + 1.5[O_3]} \Rightarrow \beta = f\left(\frac{\text{eV}}{O_{2,\text{inlet}}}\right)$$

- Parameter ranges for ideal plug-flow system

- Velocity: 500 – 5000 cm/s
- Pressure: 1 – 20 Torr
- Power: 0.1 – 1.5 W/cc
- Mixture: 3 – 100% O_2 in He
- Length: 20 cm

These ranges give
specific energies
of 0 – 250 eV

University of Illinois
Optical and Discharge Physics

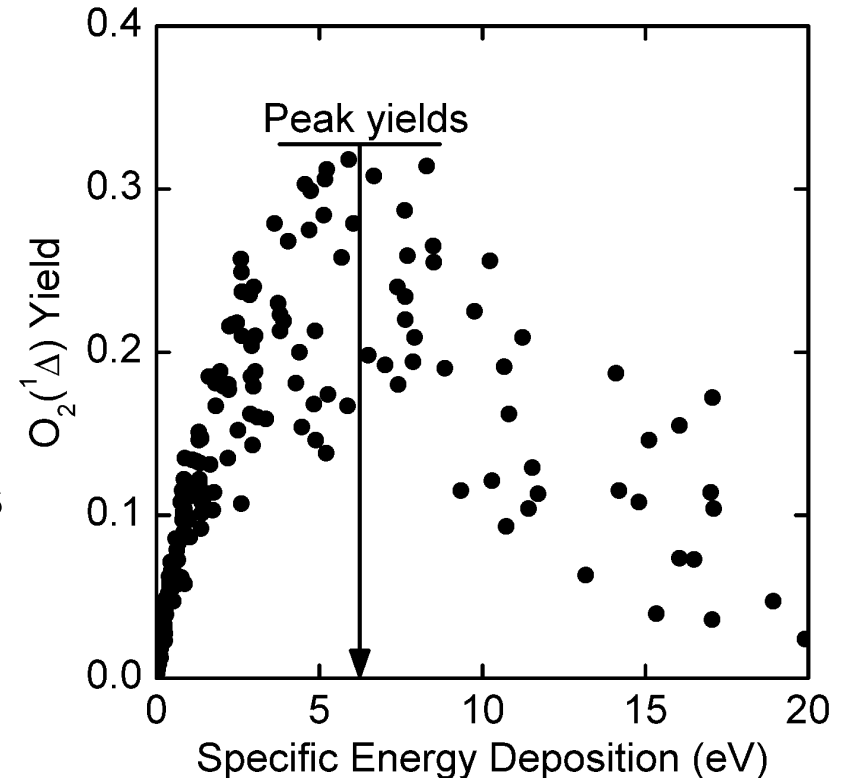
O₂(¹Δ) YIELD VS. SPECIFIC ENERGY DEPOSITION

- O₂(¹Δ) yield obeys energy deposition scaling law to 1st order:

$$\beta = f\left(\frac{\text{eV}}{\text{O}_{2,\text{inlet}}}\right)$$

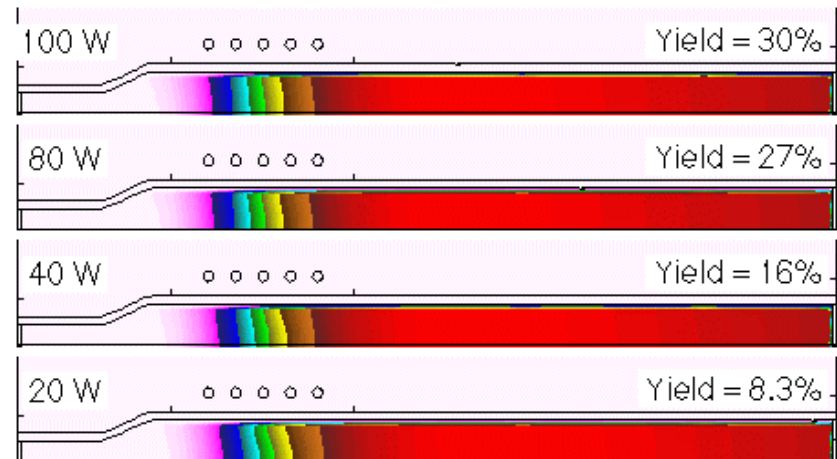
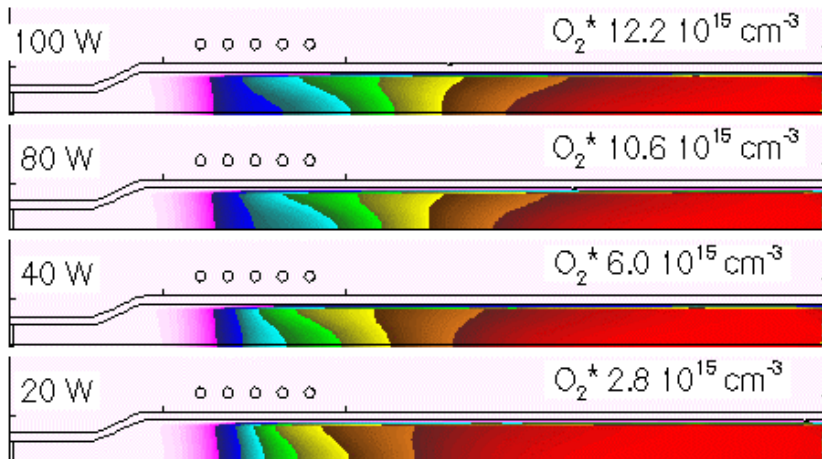
- O₂(¹Δ) yield increases with energy as inventory integrates.
- O₂(¹Δ) yield decreases > 5 – 8 eV as dissociation depletes ground state and O₂(¹Δ).
- Scatter is due to secondary effects (mixture, pressure, power).

$$\text{Yield} = \frac{[\text{O}_2(^1\Delta)]}{[\text{O}_2] + [\text{O}_2(^1\Delta)] + [\text{O}_2(^1\Sigma)] + 0.5[\text{O}] + 1.5[\text{O}_3]}$$



O₂(¹Δ) AND YIELD vs POWER

- Yield scales sub-linearly with power in a parameter space where energy scaling should be valid.
- Increasingly less uniform power deposition and local depletion of O₂ is likely the cause.



- Energy scaling says yield=40%

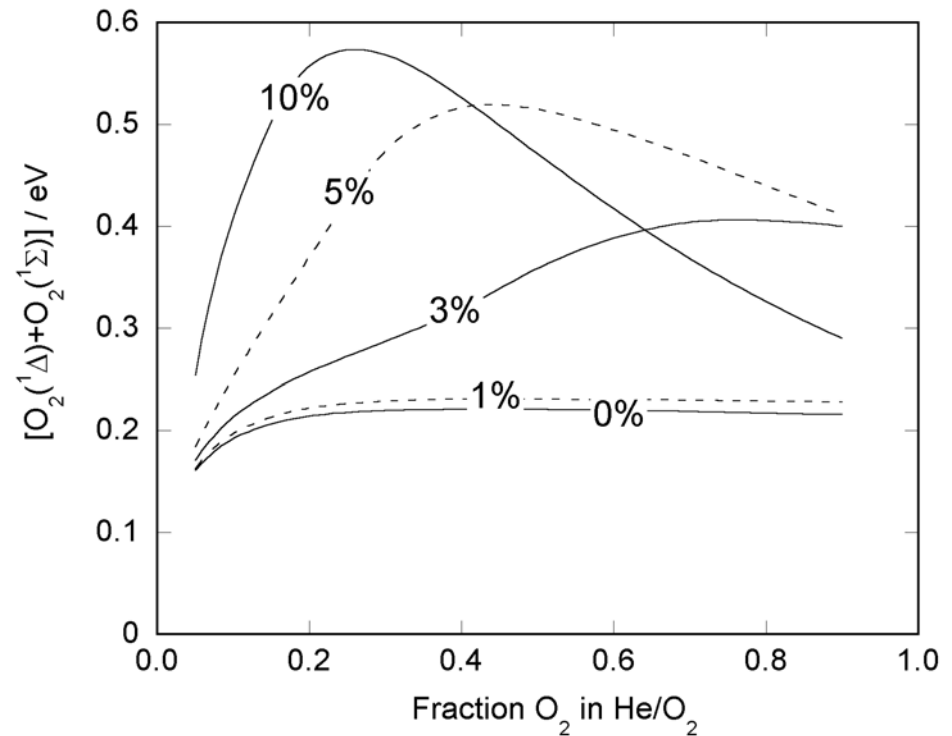
- 3 Torr, He/O₂=0.7/0.3, 6000 sccm

MIN  MAX

University of Illinois
Optical and Discharge Physics

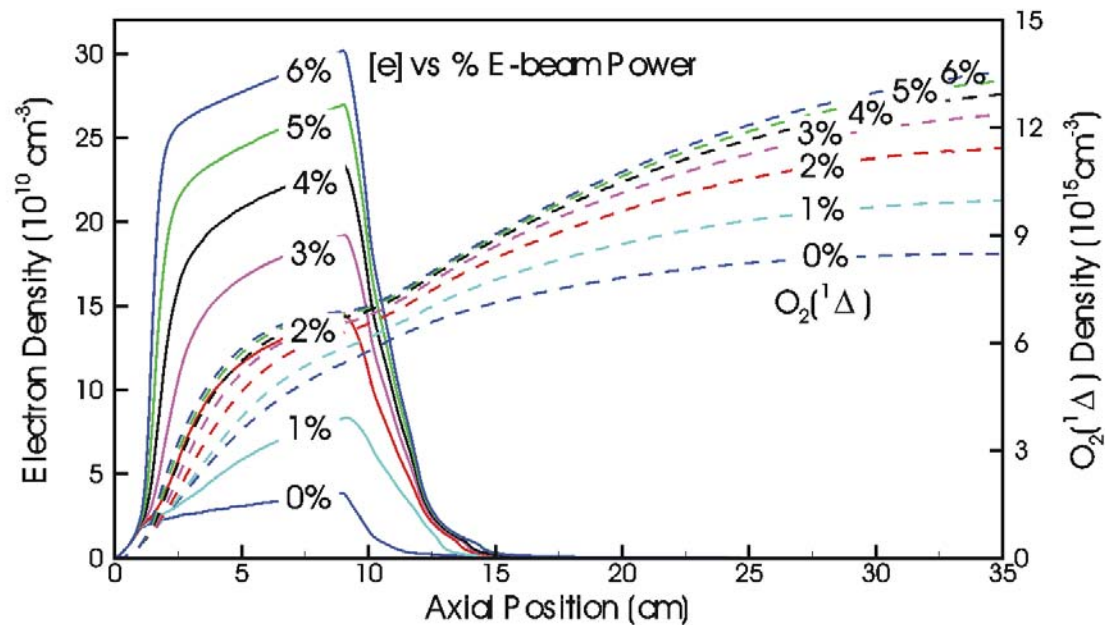
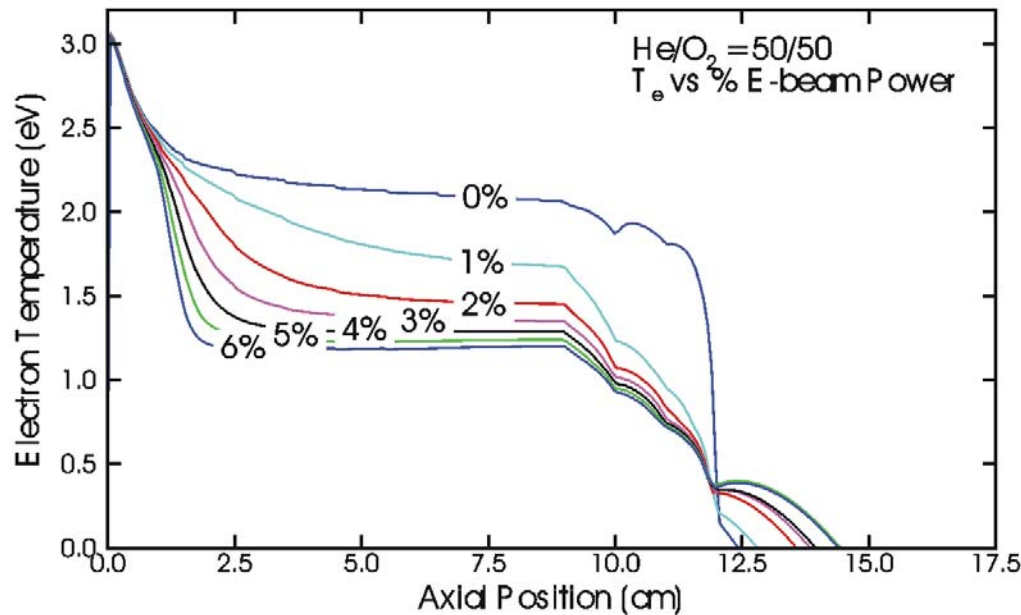
NON-SELF SUSTAINED DISCHARGES

- **Self sustained systems are limited by need to balance attachment and diffusion losses by ionization.**
- **This pushes system to larger T_e or E/N .**
- **Externally sustained system provides means to reduce T_e or E/N . to more optimum regime.**
- **Example: E-beam sustained plug flow system.**



- **Low-energy deposition yield (molecules/eV) vs Fraction of energy from E-beam (5 Torr).**

PLUG-FLOW WITH E-BEAM POWER DEPOSITION



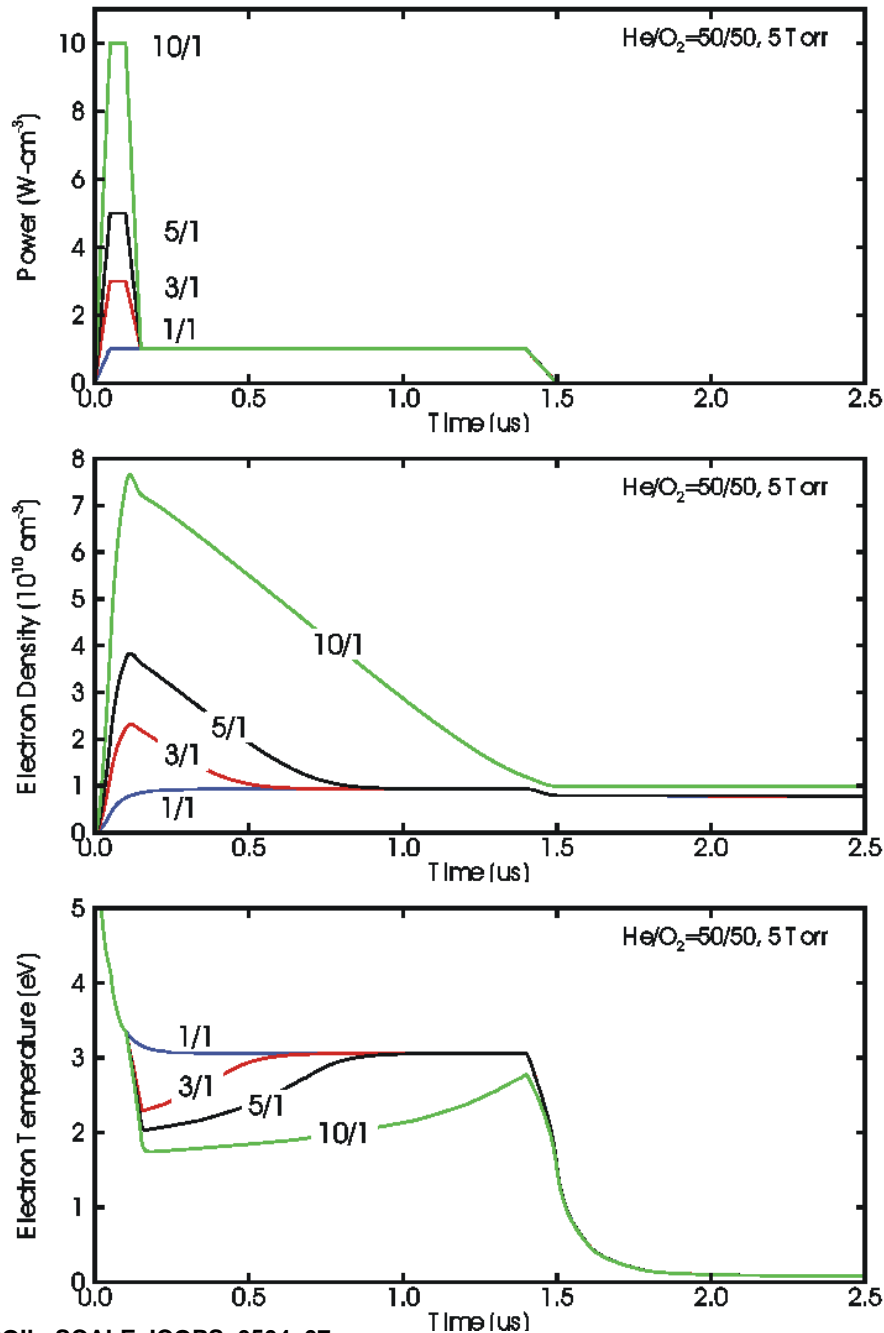
- He/O₂ = 50/50, 5 Torr, v₀ = 10 m/s

- Increasing fraction of e-beam power lowers T_e, saturating at 5-6%
- Reduction in T_e shifts operating point closer to optimum value, increasing yield from 15% to 26%; and reducing dissociation.

- 1 W/cm³

University of Illinois
Optical and Discharge Physics

SPIKER-SUSTAINER



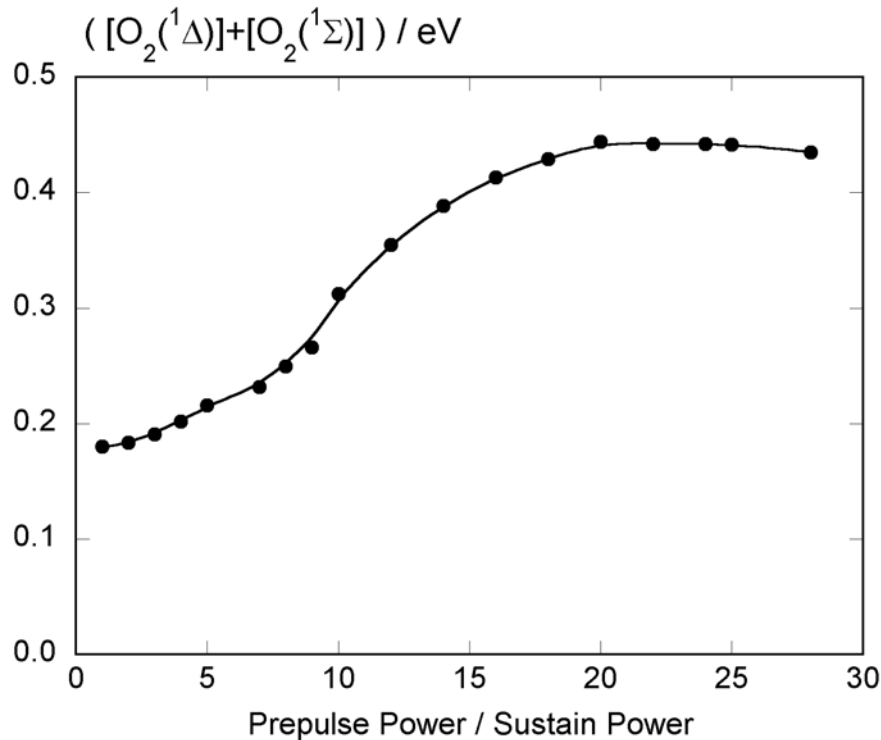
ECOIL_SCALE_ICOPS_0504_07

- Spiker-sustainer circuit provides in situ “external ionization”
- Short high voltage (power) pulse is followed by plateau of lower voltage (power).
- Excess ionization in “after-glow” following spiker allows sustainer to operate below self sustaining T_e (E/N).
- Excess ionization decays within 0.5-1.5 μ s, during which T_e is below self sustaining value.

- He/O₂ = 50/50, 5 Torr

University of Illinois
Optical and Discharge Physics

SPIKER-SUSTAINER: $O_2(1\Delta, 1\Sigma)$ PRODUCTION EFFICIENCY



- Lower T_e during sustain pulse better matches cross sections for excitation of $O_2(1\Delta, 1\Sigma)$.
- End result is a higher energy efficiency for $O_2(1\Delta, 1\Sigma)$ production.

- $He/O_2 = 50/50, 5$ Torr

CONCLUDING REMARKS

- $O_2(^1\Delta)$ production is largely an energy driven process. Yields scale as eV/molecule. Low efficiency systems can produce large yields.
- Yield will ultimately either be statistically limited (e.g., super-elastic relaxation) or limited by depletion of fuel (e.g., dissociation).
- Efficiency of yield is largely determined by lowering T_e (E/N) to better match cross sections for $O_2(^1\Delta, ^1\Sigma)$. Negative-glow like devices might be ideal.
- Secondary effect of T_e (E/N) engineering is reducing dissociation rates (less depletion of fuel).
- External sources and spiker-sustainers are both attractive, though utmost care must be taken in physical overlap of two regimes.