# SIMULATION OF $O_2(^1\Delta)$ YIELDS IN MIXTURES OF $O_2$ AND INERT GASES IN LOW PRESSURE PLASMAS*

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# AGENDA

- Introduction
    - Conventional COILs
    - Electric discharge COILs

- Description of model
    - GlobalKin
    - Reaction mechanism

- Results
    - Yield scaling with energy deposition
    - Effect of He diluent
    - Effect of pressure
    - Effect of power

- Conclusion

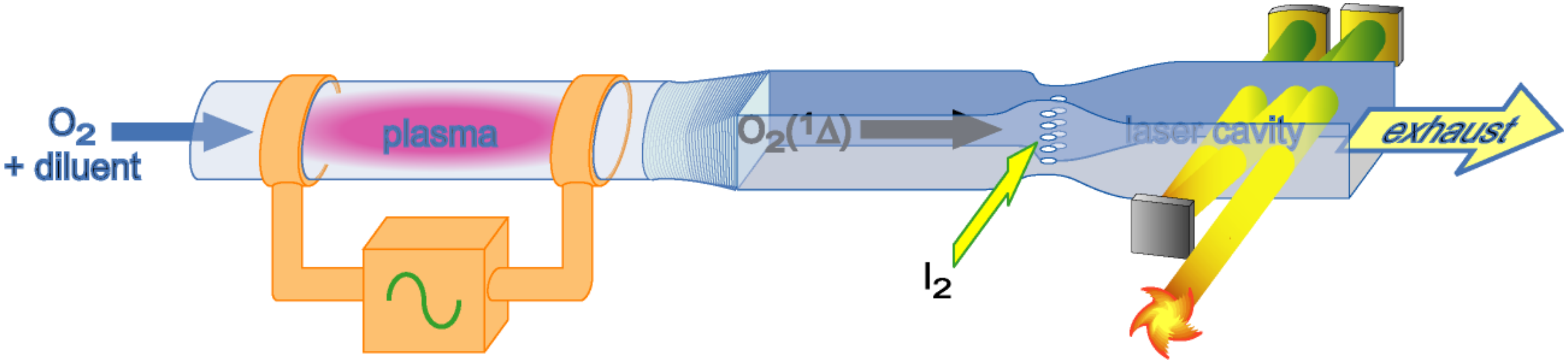
# OXYGEN-IODINE LASERS

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

$$O_2(^1\Delta) + I(^2P_{3/2}) \leftrightarrow O_2(^3\Sigma) + I(^2P_{1/2})$$

$$I(^2P_{1/2}) \rightarrow I(^2P_{3/2}) + h\nu \qquad (1.315\mu m)$$

- 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.



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# ELECTRIC DISCHARGE COILS

- **Advantages of Electrical $O_2(^1\Delta)$ Generation**
  - **Low system mass – all gas phase reactions, no liquid storage**
  - **Safe chemistry – no hazardous chemical generators**
  - **Simple design – no liquid recycling/disposal systems**

**.... and Disadvantages**

  - **Yield is low – reported yields are 10 – 30%, and laser gain has not been demonstrated.**
  - **Discharge heating – laser gain kinetics favor low temperatures, but discharge heats gas.**

$$\text{Yield} = \frac{[O_2(^1\Delta)]}{[O_2] + [O_2(^1\Delta)] + 0.5[O] + 1.5[O_3]}$$

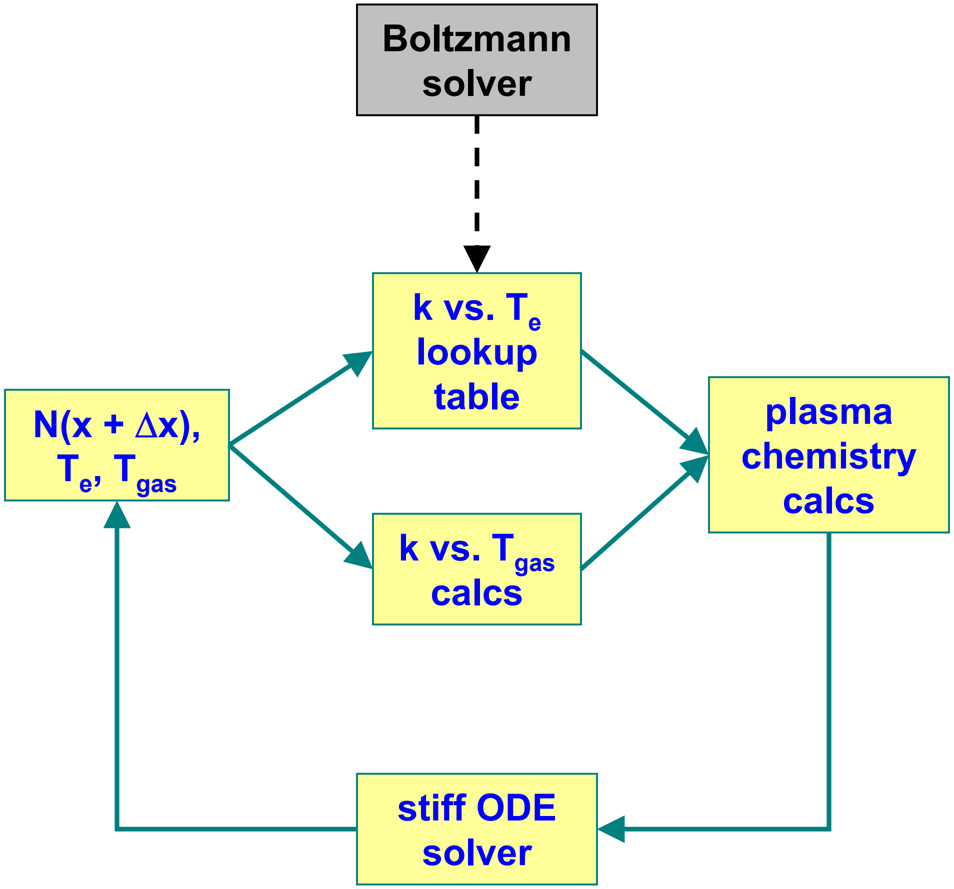
- **Modeling and experiments are investigating methods for high $O_2(^1\Delta)$ yield and laser gain.**

# GLOBAL PLASMA MODEL

- GlobalKin is a spatially homogeneous and time-dependent discharge model, adapted to simulate time-independent plug flow in 1-D.

- Electric field is obtained from circuit model or electro-magnetics-power balance.

- Boltzmann solver periodically updates e-impact rate coefficients



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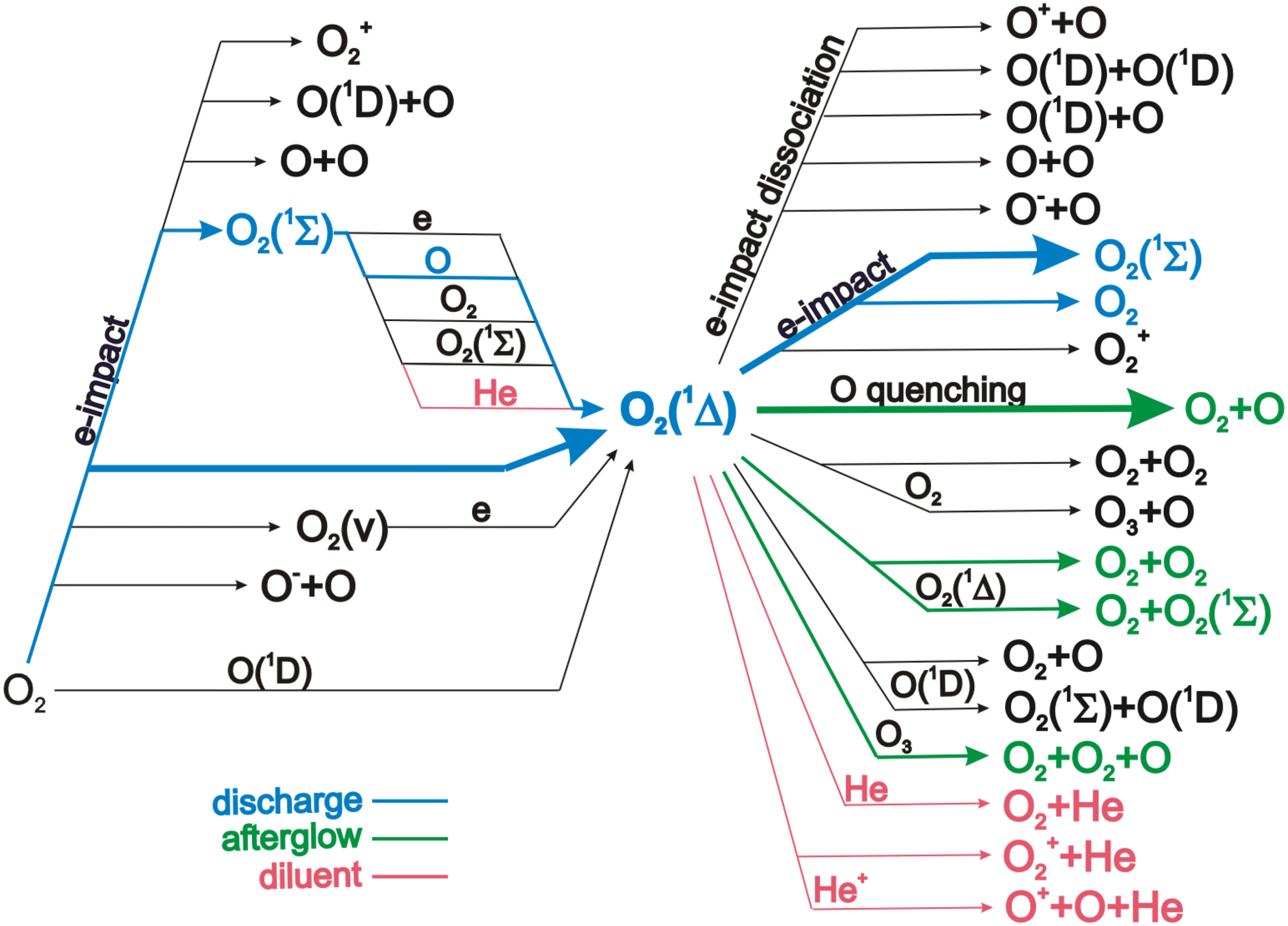
# REACTION MECHANISM



e-impact

$O_2^+$

$O(^1D)+O$

$O+O$

$O_2(^1\Sigma)$

e

O

$O_2$

$O_2(^1\Sigma)$

He

$O_2(v)$

e

$O^-+O$

$O_2$

$O(^1D)$

$O_2(^1\Delta)$

e-impact dissociation

$O^++O$

$O(^1D)+O(^1D)$

$O(^1D)+O$

$O+O$

$O^-+O$

e-impact

$O_2(^1\Sigma)$

$O_2$

$O_2^+$

O quenching

$O_2+O$

$O_2$

$O_2+O_2$

$O_3+O$

$O_2(^1\Delta)$

$O_2+O_2$

$O_2+O_2(^1\Sigma)$

$O(^1D)$

$O_2+O$

$O_2(^1\Sigma)+O(^1D)$

$O_3$

$O_2+O_2+O$

He

$O_2+He$

$He^+$

$O_2^++He$

$O^++O+He$

discharge

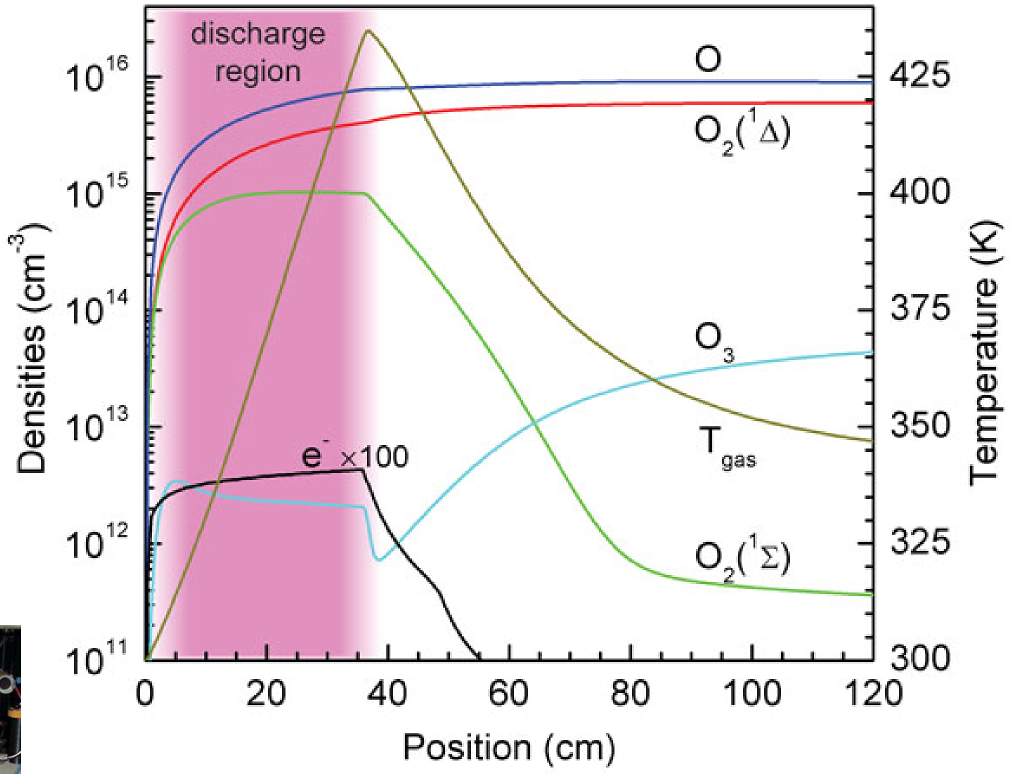
afterglow

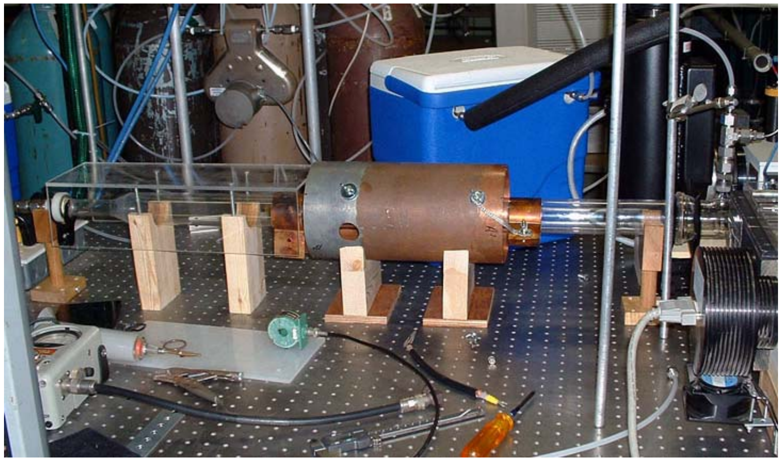
diluent

# BASE CASE:  ElectriCOIL EXPERIMENT

**Conditions**

- $He:O_2$ = 4:1
- Velocity:  4 m/s
- Pressure:  6 Torr
- Power:  0.7 W/cc
- ~30 cm discharge





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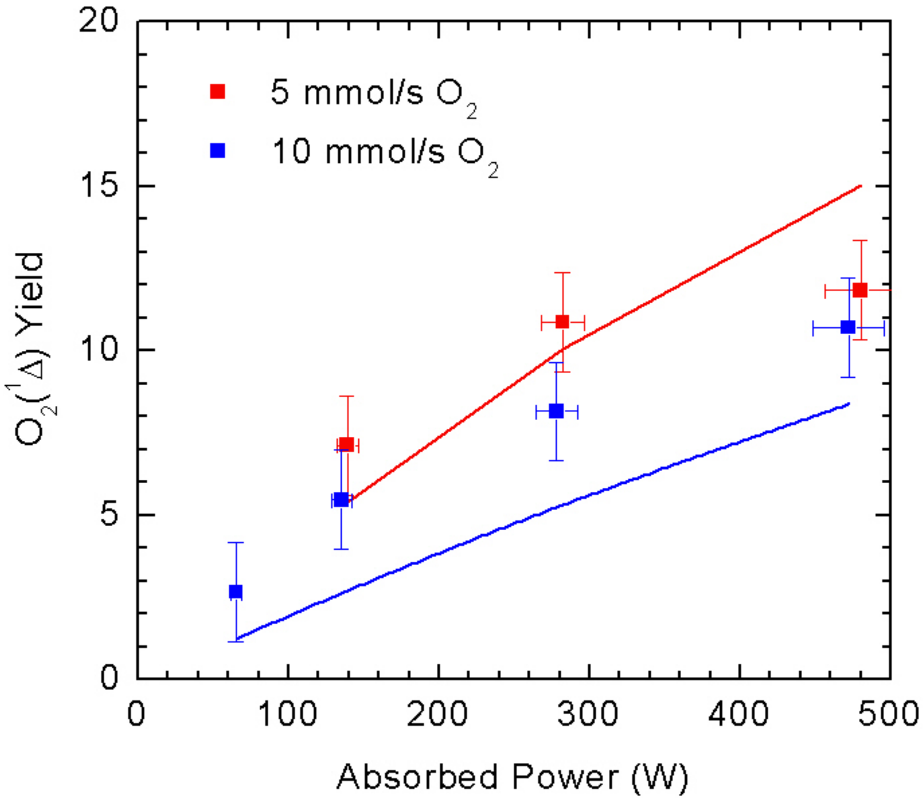
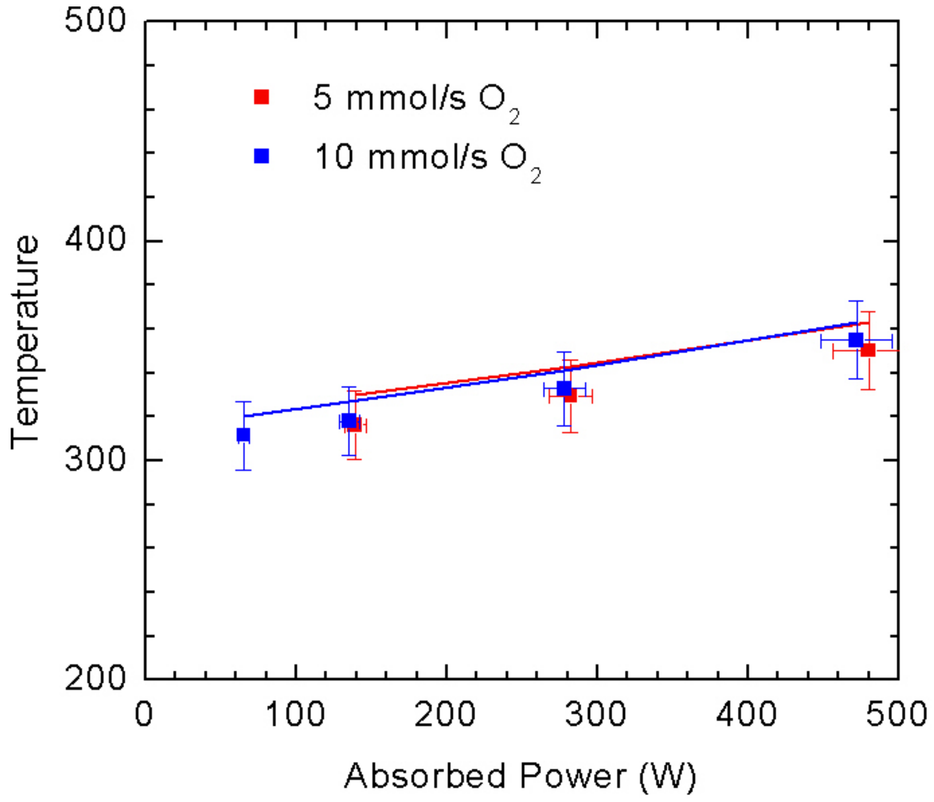
# COMPARISON TO EXPERIMENTS

- **Comparison of GlobalKin predictions to the ElectriCOIL experiment at UIUC: He:$O_2$ flow ratio = 4:1**





- **Ref: D. Carroll and W. Solomon, CU-Aerospace, 2003**

# PROPOSED SCALING LAW

- **A parameterization of velocity, pressure, power, and mixture was completed to determine scaling laws for $O_2(^1\Delta)$ yield.**

- **A scaling law is proposed giving yield ($\beta$) as a function of specific energy depostion (in eV per inlet $O_2$ molecule):**

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

**Parameter ranges**

- **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**

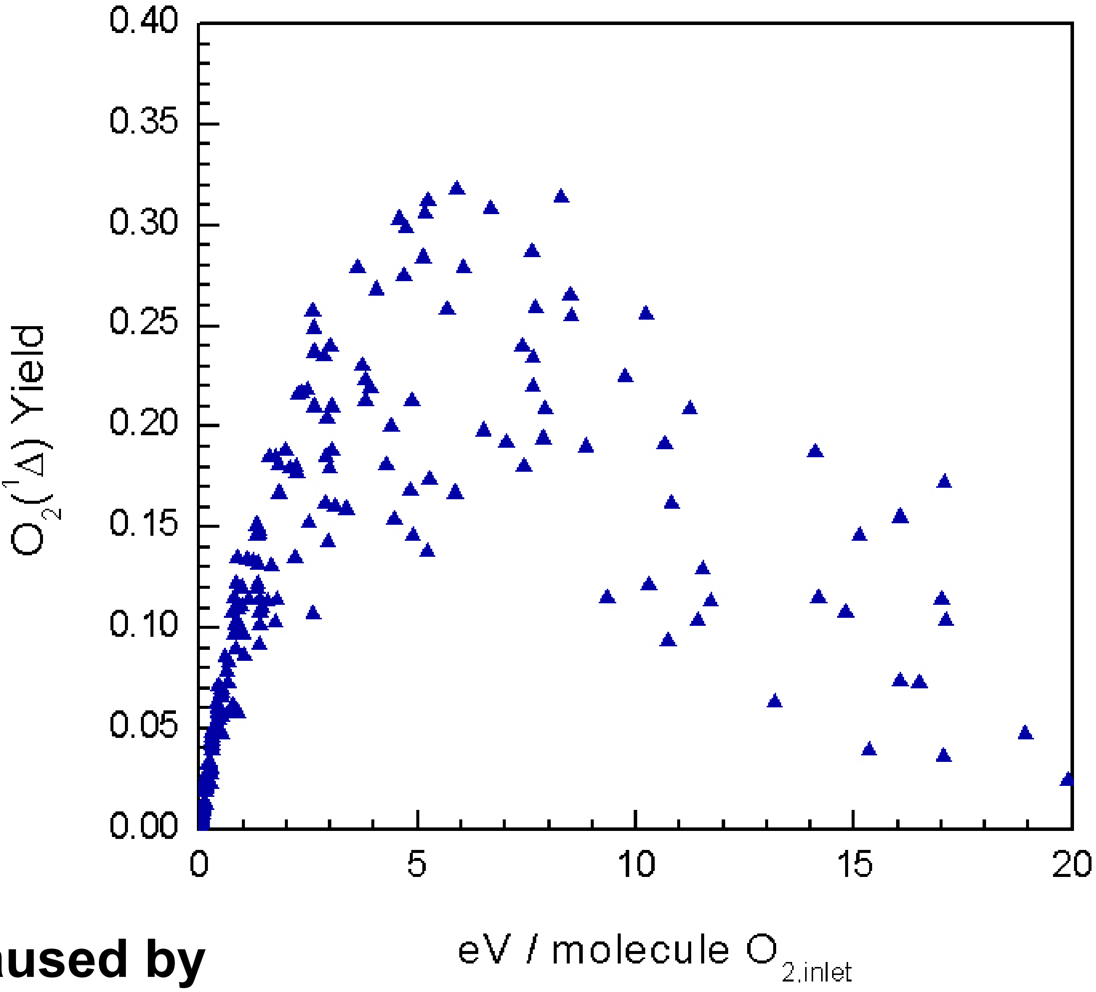
**These ranges give specific energies of 0 – 250 eV**

# $O_2(^1\Delta)$ YIELD VS. SPECIFIC ENERGY DEPOSITION

- **Parameterization results show that $O_2(^1\Delta)$ yield obeys the scaling law to 1st order:**

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

- **$O_2(^1\Delta)$ yield decreases after 5 – 8 eV as dissociation into O atoms dominates chemistry.**



- **Scatter at high yield is caused by secondary effects (mixture, pressure, power).**

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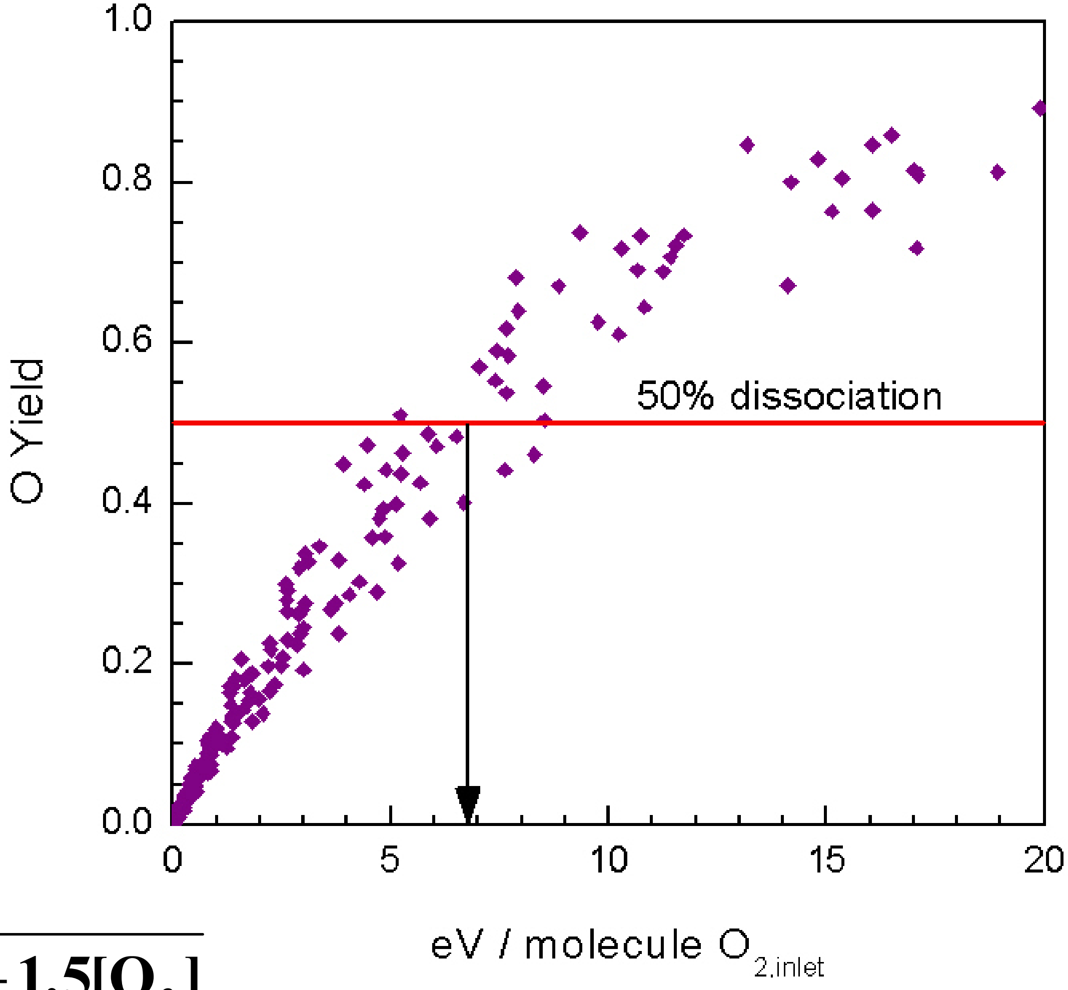
# O YIELD VS. SPECIFIC ENERGY DEPOSITION

- **Atomic O yield increases monotonically with specific energy input until near complete dissociation is achieved.**

- **50% dissociation occurs by 5 – 8 eV, when $O_2(^1\Delta)$ yield begins to decrease.**



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

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# SECONDARY EFFECTS: DILUENT

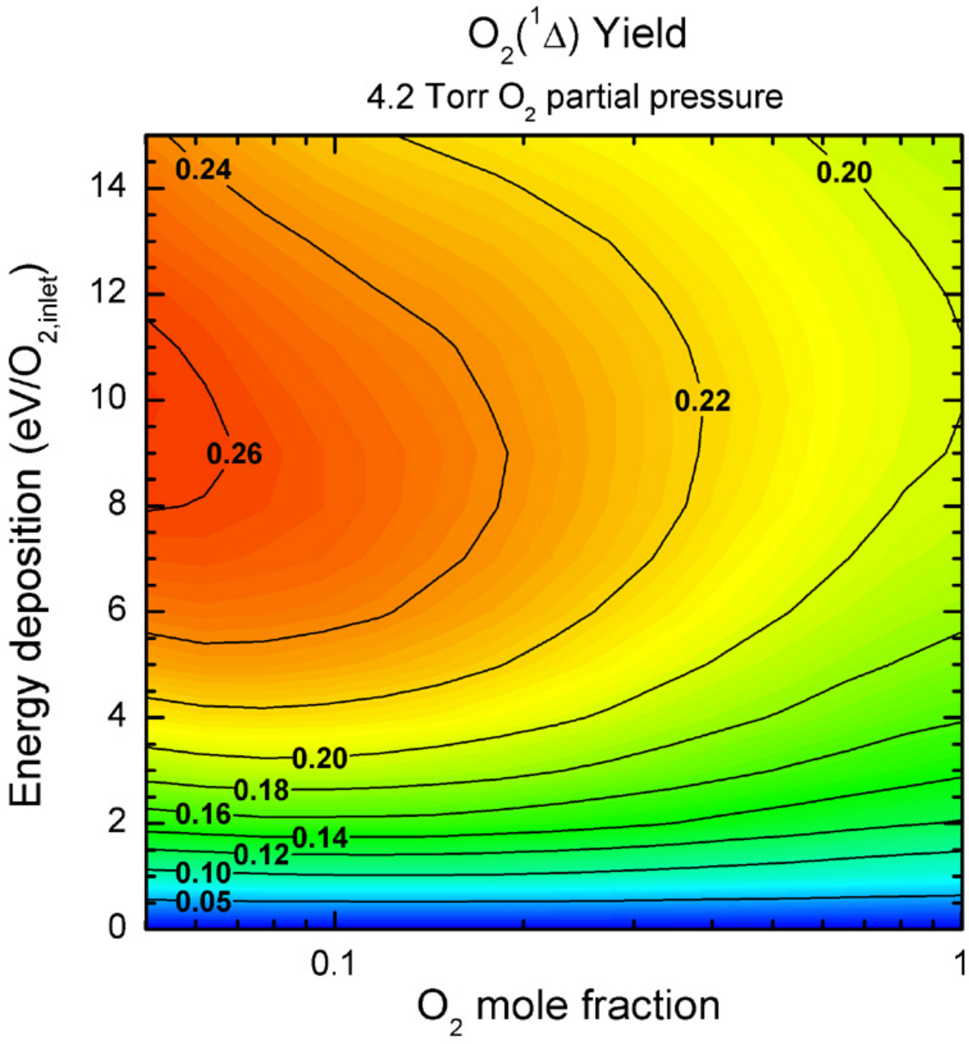
- **Addition of He increases yield at fixed specific energy deposition by reducing E/N.**

- **Scaling laws apply to mixtures with diluents:**

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

**Conditions:**

- $V_{inlet}$ = 2500 cm/s
- Power = 21 W/cc
- $P_{O2}$ = 4.2 Torr
- $L_{disch}$ determined by energy dep.



# SECONDARY EFFECTS: PRESSURE

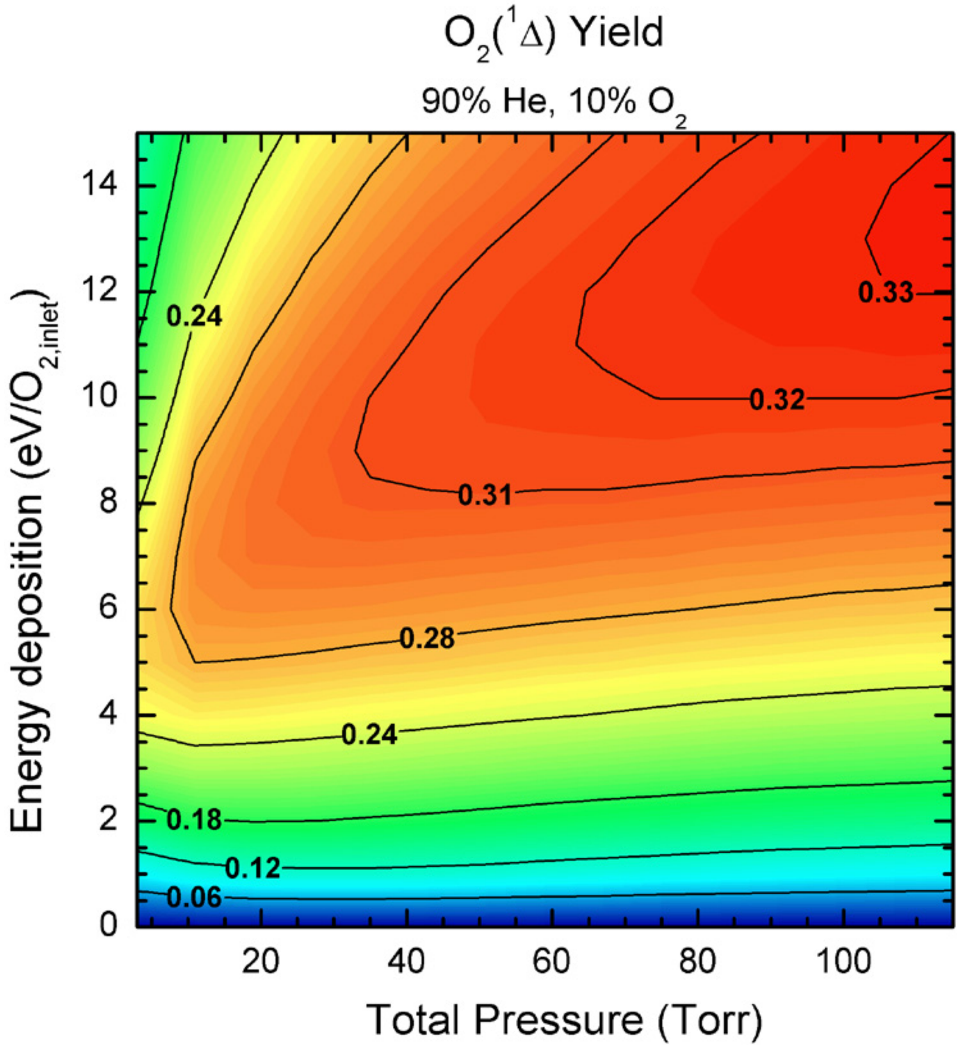
- **Increasing total pressure increases potential yield, esp. below 40 Torr.**

- **Scaling law applies at constant pressure:**

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

**Conditions:**

- **$V_{inlet}$ = 500 cm/s**
- **Power = 1 W/cc/Torr $O_2$**
- **$P_{O2}$ = 10% of total**
- **$L_{disch}$ determined by energy dep.**



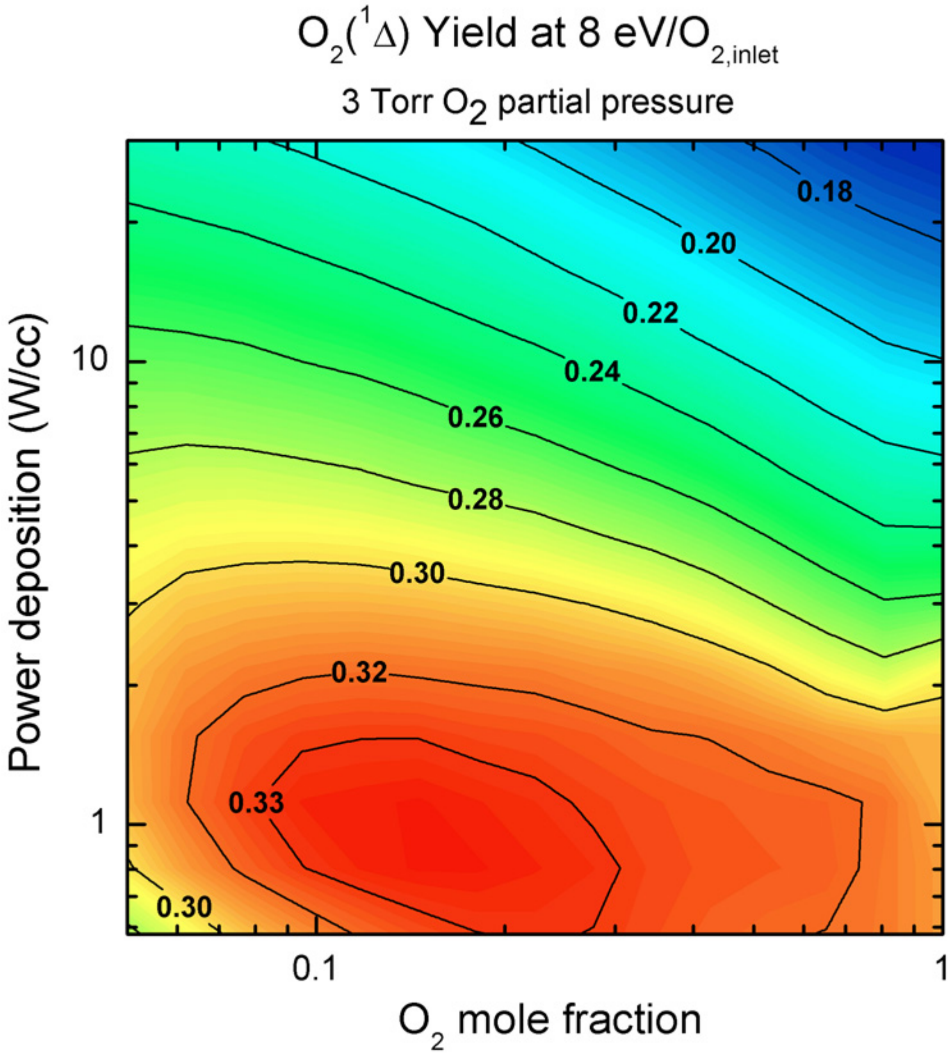
# SECONDARY EFFECTS: POWER DEPOSITION

- **Low power produces the highest yields, by allowing operation at a more favorable E/N.**

- **However, low power requires longer residence times, which may not be practical.**

**Conditions:**

- **$V_{inlet}$ = 2500 cm/s**
- **$P_{O2}$ = 3 Torr**
- **$L_{disch}$ determined by energy deposition.**



# CONCLUSIONS

- A global plasma chemistry model was adapted to simulate steady-state plug flow discharges.
- $O_2(^1\Delta)$ yield in rf discharges is primarily a function of specific energy deposition into oxygen species.
- He diluent increases the yield by reducing the operating E/N of the discharge.
- Increasing the pressure raises the yield, although more energy is required.
- The highest yields are likely achieved at low power deposition, ~ 0.3 W/cc/Torr $O_2$.

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