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.

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

\[
I(^2P_{1/2}) \rightarrow I(^2P_{3/2}) + h\nu \quad (1.315\mu m)
\]

- 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.
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.

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

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

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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.
BASE CASE: ElectriCOIL EXPERIMENT

Conditions
- He:O₂ = 4:1
- Velocity: 4 m/s
- Pressure: 6 Torr
- Power: 0.7 W/cc
- ~30 cm discharge
COMPARISON TO EXPERIMENTS

• Comparison of GlobalKin predictions to the ElectriCOIL experiment at UIUC: He:O₂ flow ratio = 4:1

- Ref: D. Carroll and W. Solomon, CU-Aerospace, 2003
A parameterization of velocity, pressure, power, and mixture was completed to determine scaling laws for $\text{O}_2(^1\Delta)$ yield.

A scaling law is proposed giving yield ($\beta$) as a function of specific energy deposition (in eV per inlet $\text{O}_2$ molecule):

$$\beta = \frac{[\text{O}_2(^1\Delta)]}{[\text{O}_2] + [\text{O}_2(^1\Delta)] + 0.5[\text{O}] + 1.5[\text{O}_3]} \Rightarrow \beta = f\left(\frac{\text{eV}}{\text{O}_2,\text{inlet}}\right)$$

Parameter ranges:

- Velocity: 500 – 5000 cm/s
- Pressure: 1 – 20 Torr
- Power: 0.1 – 1.5 W/cc
- Mixture: 3 – 100% $\text{O}_2$ in He
- Length: 20 cm

These ranges give specific energies of 0 – 250 eV.

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**O$_2$(1$\Delta$) YIELD VS. SPECIFIC ENERGY DEPOSITION**

- Parameterization results show that O$_2$(1$\Delta$) yield obeys the scaling law to 1$^{\text{st}}$ order:
  \[
  \beta = f\left( \frac{\text{eV}}{O_2,\text{inlet}} \right)
  \]

- 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).
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.

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

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

- Scaling laws apply to mixtures with diluents:

\[ \beta = f \left( \frac{eV}{O_2,\text{inlet}} \right) \]

Conditions:
- \( V_{\text{inlet}} = 2500 \text{ cm/s} \)
- Power = 21 W/cc
- \( P_{O_2} = 4.2 \text{ Torr} \)
- \( L_{\text{disch}} \) determined by energy dep.
SECONaRY EFFECTS: PRESSURE

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

- Scaling law applies at constant pressure:

\[ \beta = f \left( \frac{eV}{O_2,\text{inlet}} \right) \]

Conditions:
- \( V_{\text{inlet}} = 500 \text{ cm/s} \)
- Power = 1 W/cc/Torr O\(_2\)
- \( P_{O_2} = 10\% \text{ of total} \)
- \( L_{\text{disch}} \) 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:
- \( V_{\text{inlet}} = 2500 \, \text{cm/s} \)
- \( P_{O_2} = 3 \, \text{Torr} \)
- \( L_{\text{disch}} \) 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, $\sim 0.3$ W/cc/Torr $O_2$. 
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