Zero Dimensional Plasma Chemistry Modeling of a Controlled Avalanche Electric Discharge for Oxygen Singlet Delta Production

Workshop on Discharge Pumped Oxygen-Iodine Lasers
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Overview of He/Ar/O_2 Plasma Chemistry Modeling

I review the modeling of the plasma chemistry of a controlled avalanche discharge in a mixture of He, Ar, & O_2. The modeling was performed with a 0-D, time dependent plasma chemistry code containing routines for solving the non-Maxwell-Boltzmann electron energy distribution.

Outline

1. Electron collision processes and cross sections
2. Validation of *cross section sets* via swarm analysis
3. Electron energy flow
4. Code capabilities
5. Test calculations on He/ Ar/ O_2 gas mixture

He/Ar/O_2 Plasma Chemistry Model – Electron Kinetics

The non-Maxwell-Boltzmann electron energy distribution is determined mostly by

(1) Electron momentum transfer to He, Ar, & O_2
(2) $e + O_2\ (v=0) \rightarrow e + O_2\ (v>0)$
(3) $e + O_2\,(X) \rightarrow e + \{O_2\ (a^1\Delta), O_2\,(B^1\Sigma), O+O\}$
(4) $e + Ar \rightarrow e + Ar^*$

Electron collision processes most important in driving the plasma chemistry are

(1) $e + \{Ar, O_2\} \rightarrow 2\ e + \{Ar^+, O_2^{\ +}\}$
(2) $e + O_2\,(X) \Leftrightarrow e + O_2\ (a^1\Delta)$
(3) $e + O_2\ (a^1\Delta) \rightarrow O + O^-$
(4) $e + O_2\,(X) \rightarrow O + O$

Electron Collision Cross Sections

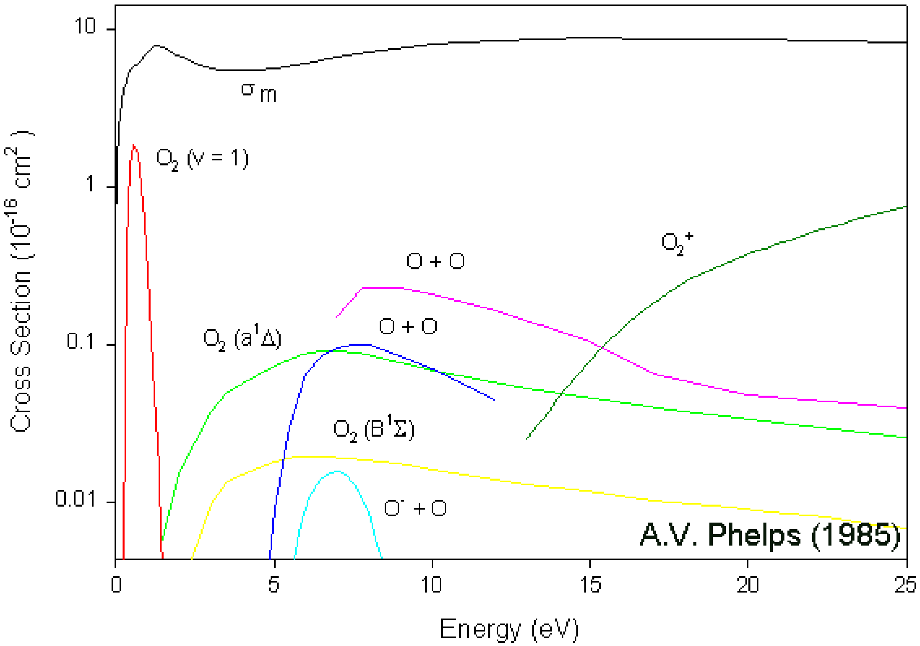
Helium: momentum transfer, 2^3S_1 & 2^1S_0 metastable excitation, He* excitation, He+

Argon: momentum transfer, 4^3P_2 & 4^3P_0 metastable excitation, Ar* excitation, Ar^+

Oxygen: momentum transfer, $O_2(v)$, $O+O^-$, $O_2(a^1\Delta)$, $O_2(B^1\Sigma)$, O+O, O_2^+

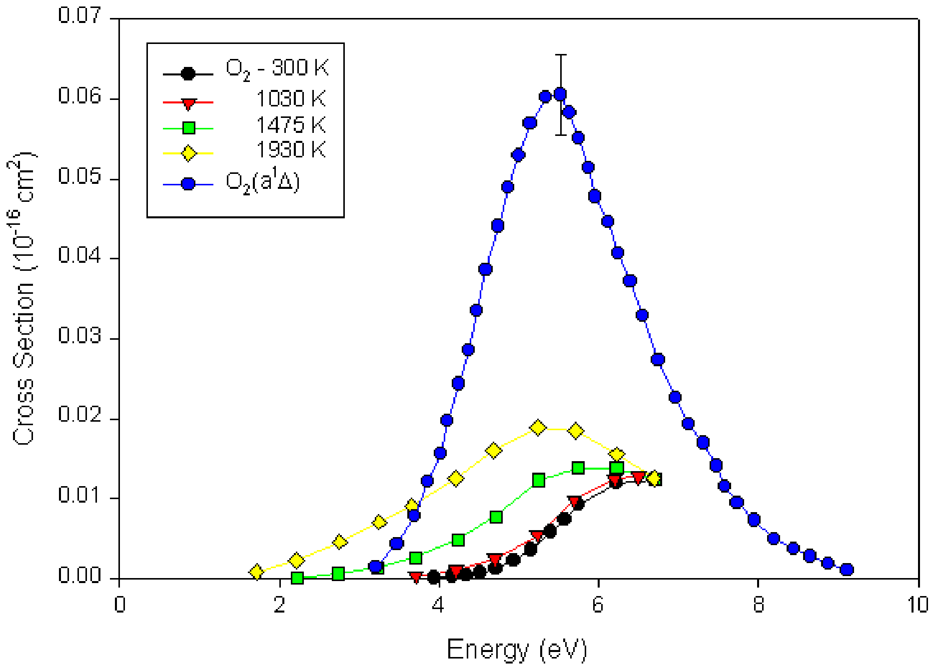
Molecular Oxygen Cross Sections

- O_2 cross section consistent with electron transport data
- Metastable excitation and dissociation dominate at modest electron energies.



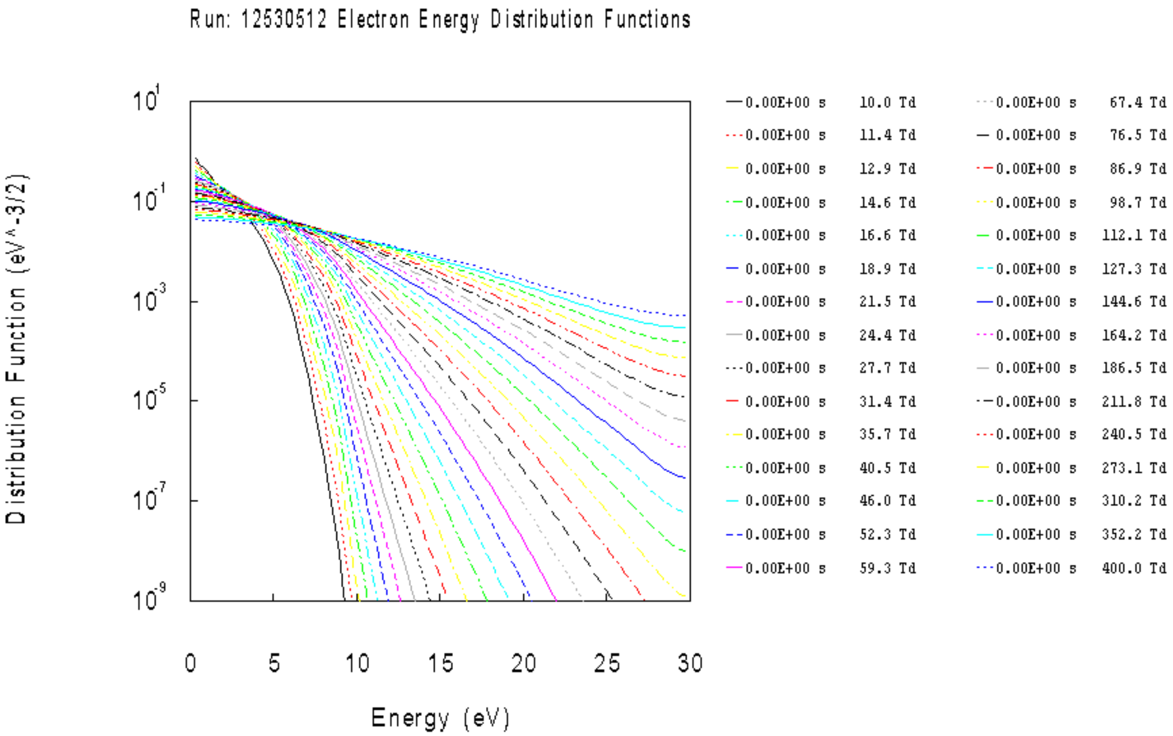
Dissociative Attachment of Vibrationally Excited O_2

Vibrational and metastable excitation enhance dissociative attachment cross section



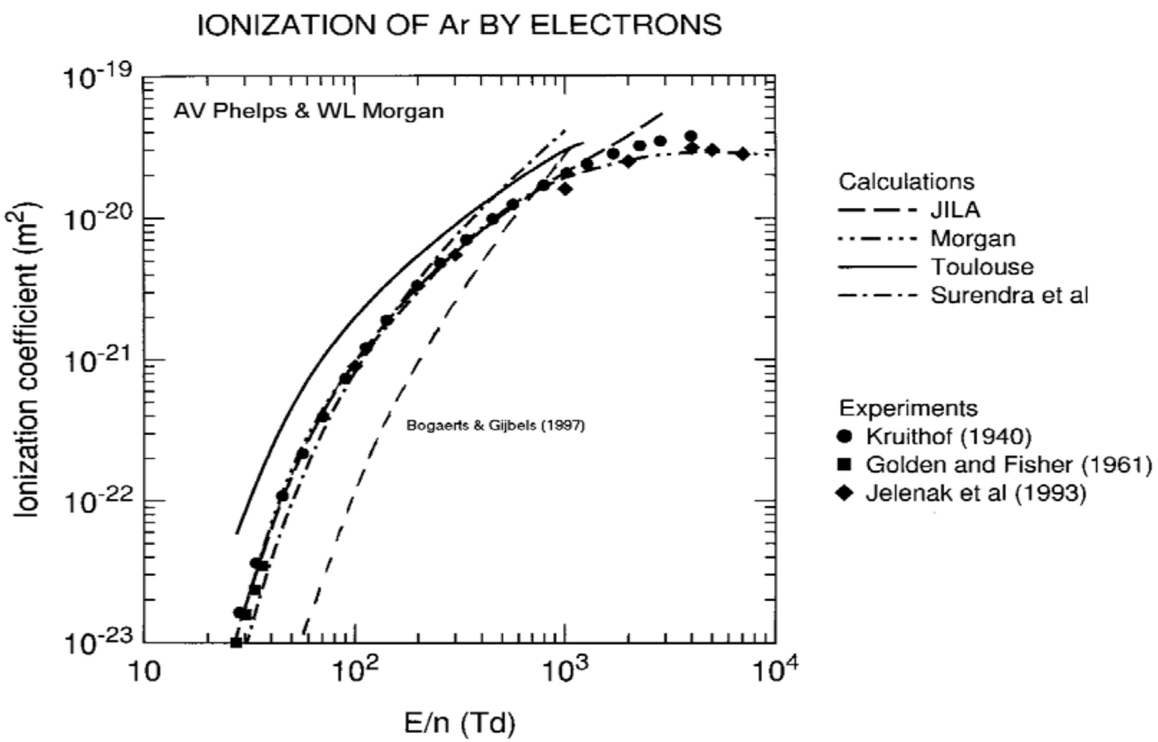
Non-Thermal Electron Energy Distributions Are the Rule

f(ε, E/N) for 25% Ar, 25% He, 50% O_2 @ 10 Torr & 300 K
10 Td ≤ E/N ≤ 400 Td



Swarm Analyzed Cross Section Set: Argon

Comparison of calculated and measured ionization coefficients for several Ar cross section sets



Swarm Analysis and Cross Section Consistency

In swarm analysis electron collision cross sections are adjusted so that the cross section set yields electron transport coefficients that agree with measurements:

Cross Section Set **Swarm Coefficients**

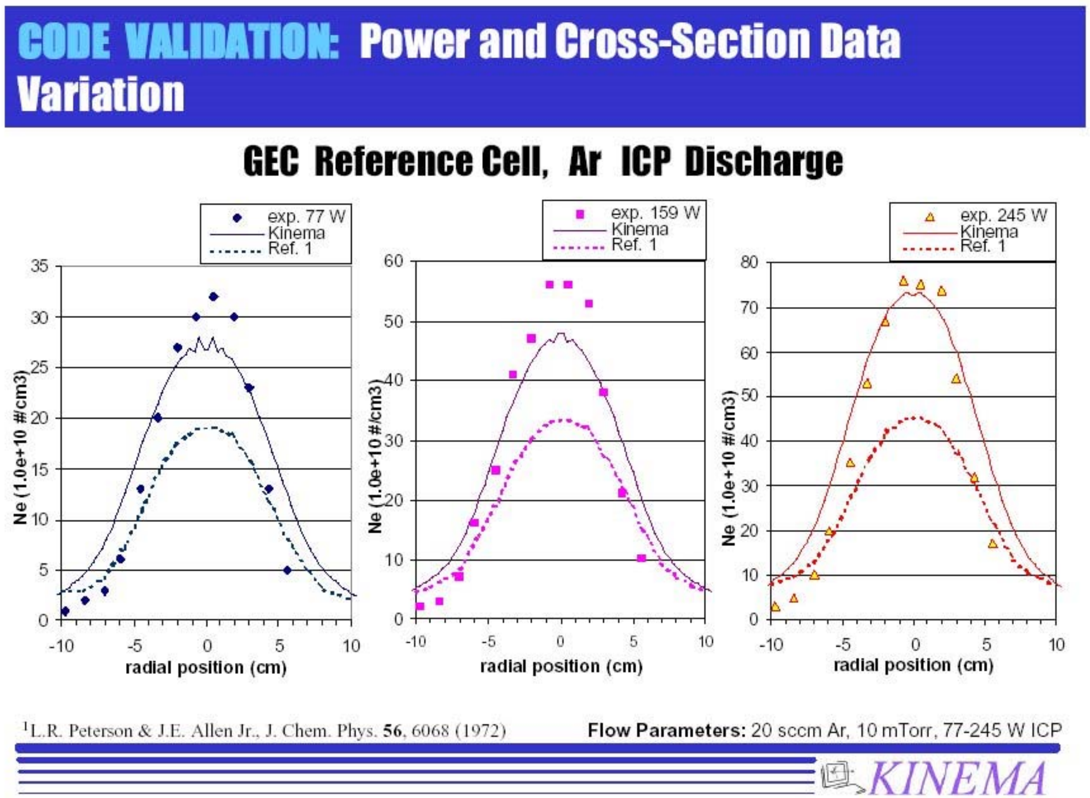
$$\{\sigma_m, \sigma_v, \sigma_e, \sigma_i, \sigma_a\} \Rightarrow f(\varepsilon, E/N) \Rightarrow \{V_d, D/\mu, \alpha, \eta\}$$

Plasma conductivity $\sigma_{pl} \propto V_d N_e/(E/N)$

Electron density $N_e \propto (\alpha\text{-}\eta)$ – (recombination loss + diffusion loss)

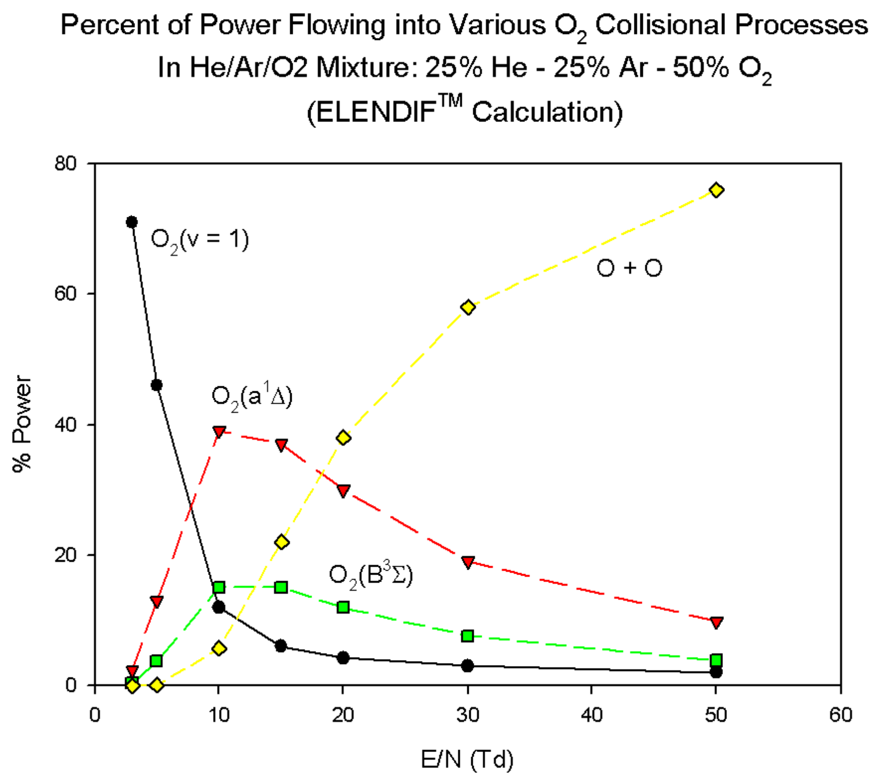
The Cross Section Set Makes a Difference

Ar cross section set that is consistent with swarm data yields better modeling results than set that is not consistent with measured transport coefficients



Partition of Power
Is A Strong Function of E/N

At moderate values of E/N most power flows into O_2 metastable excitation and dissociation



The KINEMA 0-D Plasma Modeling Code

KINEMA is a 0-D, fully time dependent plasma chemistry and chemical kinetics rate equation modeling code.

- No limit on number of atomic or molecular species or chemical reactions
- Reactions read in symbolic form
- Handles neutral, ionic & electron collisional, radiation, and diffusion processes
- Line broadening and escape factor model for radiation
- Uses ELENDIF for computing transport and rate coefficients for non-Maxwell-Boltzmann electrons
- Can treat time dependent external sources such as electron or photon beams

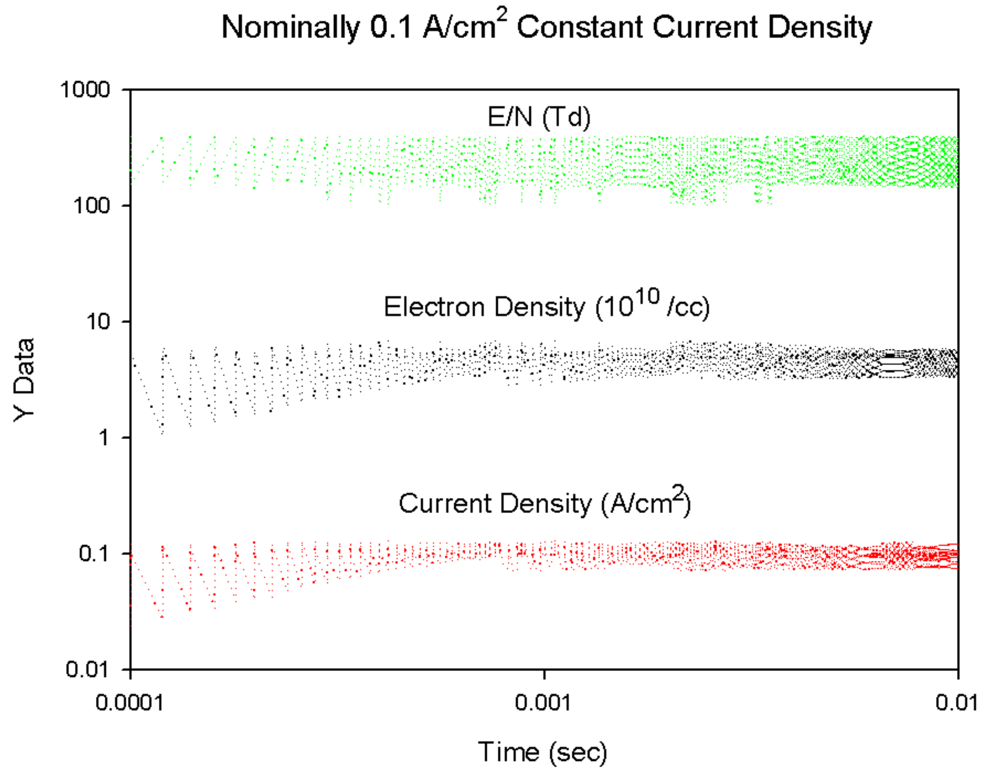
The ELENDIF Code for Solving Boltzmann's Equation

ELENDIF solves for the time dependent energy distribution function f(ε, t) for electrons in a plasma.

- Inelastic & superelastic collisions, attachment & recombination, ionization including secondary electrons
- Electron-electron collisions, electron-ion collisions
- Photon-electron processes
- An external electron source
- Diffusion
- AC & DC electric fields; pulsed or continuous

Example of Constant Current Density Plasma Chemistry Calculation

KINEMA code adjusts E/N to keep current density $j = -eN_eV_d(E/N)$ approximately constant



Modeling A Pulsed Discharge in He/Ar/O_2

Parameters:

25% He, 25% Ar, 50% O_2 @ 10 Torr, 300 K

$R_{Ballast}$ = 500 Ω

30 nsec pulses spaced 20 μsec apart

V_{max} = 4200 V & V_{min} = 100 V across 5 cm gap

$(E/N)_{max}$ = 240 Td

Approximate Breakdown E/N:

O_2	121 Td
He	40 Td
Ar	11 Td

He/Ar/O_2 Plasma Chemistry Model – Kinetics of Atomic & Molecular Species

Key Reactions With Pulse On:

$$O_2 + e \Leftrightarrow O_2\,(a^1\Delta) + e$$

$$O_2\,(a^1\Delta) + e \rightarrow \begin{cases} O_2^+ + 2e \\ O + O^- \\ 2O + e \end{cases}$$

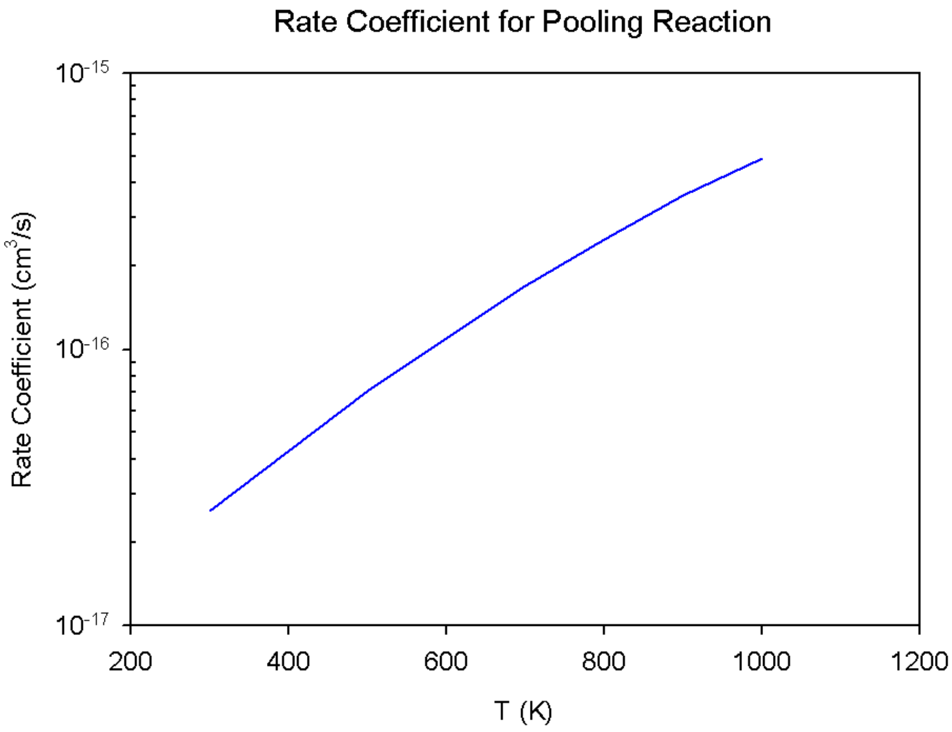
$$O- + O_2\,(a^1\Delta) \rightarrow O_3 + e$$

Key Reactions With Pulse Off:

$$O^- + O_2\,(a^1\Delta) \rightarrow O_3 + e$$
$$O^- + O \rightarrow O_2 + e$$
$$O_2\,(a^1\Delta) + e \rightarrow O + O^-$$

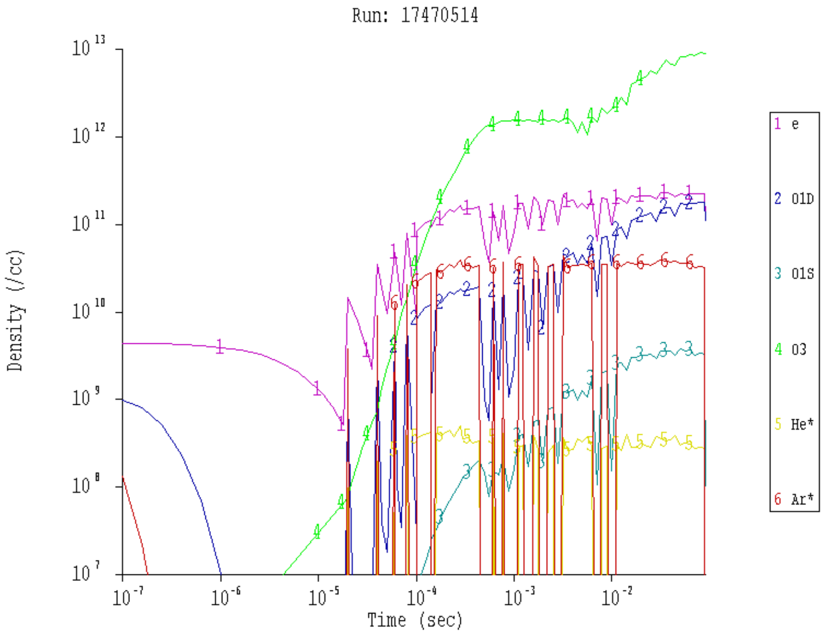
The O_2 ($a^1\Delta$) Pooling Reaction

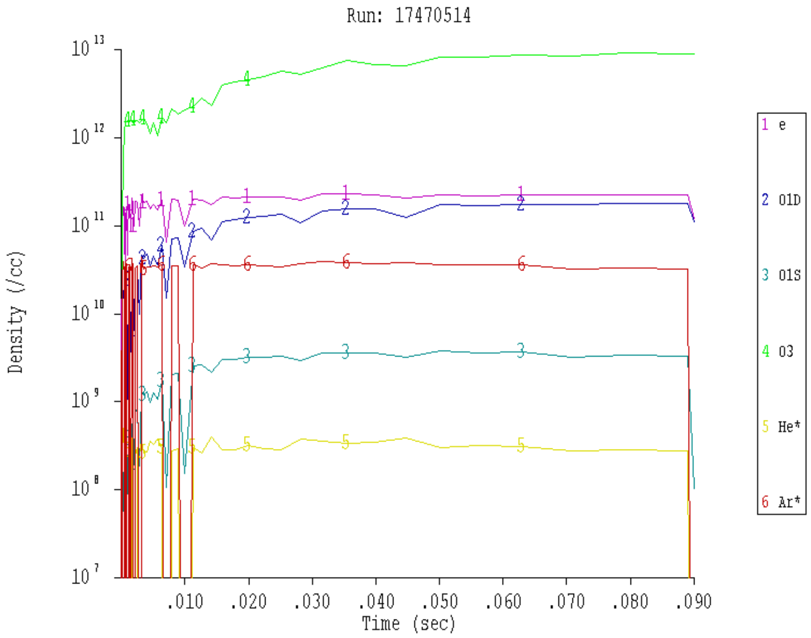
$$2\ O_2(a^1\Delta) \rightarrow O_2(X^1\Sigma) + O_2(B^3\Sigma)$$
$$k = 2.5\times10^{-18}(T/300)^{3.8} \exp(700/T)$$



He/Ar/O_2 Modeling Results: Electron and Atomic Excitation State Densities

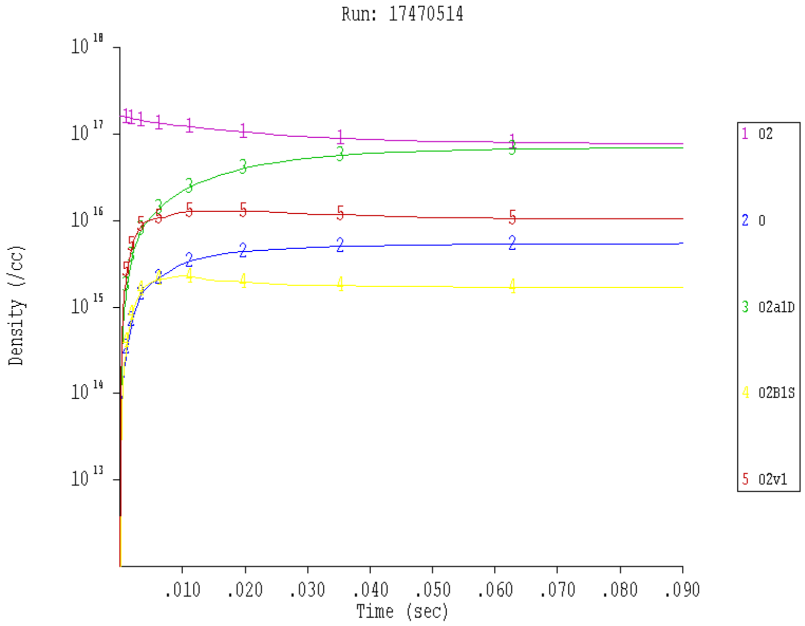
Densities on Log-Log & Semi-Log scale: steady state in about 10 msec

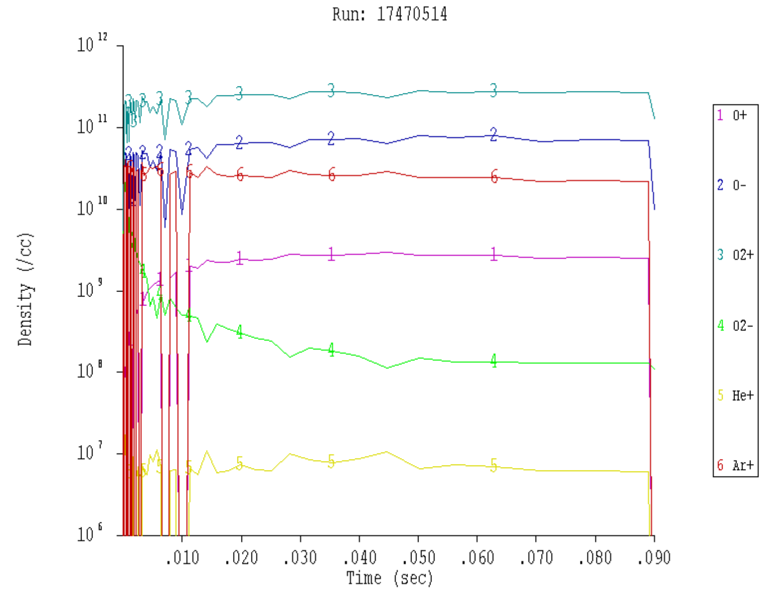




He/Ar/O_2 Modeling Results: O_2 Metastable States and Ion Densities

- [O_2 ($a^1\Delta$)] approaches [O_2(X)]
- [O^-] is about 20% [O_2^+]





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Summary

(1) 0-D calculations are quick to setup and perform
(2) They can be very helpful in distilling out the important physical and chemical processes among the myriad possible collisional processes
(3) In the absence of severe transport issues the 0-D modeling should provide reasonable results for the electron and heavy particle kinetics

Acknowledgement: I performed this work in collaboration with Dr. Alan Hill.