A global model study of oxygen discharges – formation and annihilation of the singlet molecular metastables and influence of the electron energy distribution function and wall material

D. A. Toneli[1], R. S. Pessoa[1,2], M. Roberto[1] and J. T. Gudmundsson[3,4]

[1]Technological Institute of Aeronautics, São José dos Campos 12228-900, Brazil

[2] Paraíba Valley University, São José dos Campos 12244-000, Brazil

[3] Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

[4] KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden

Abstract

A volume average global model has been used to study an oxygen discharge. Considering a great number of reactions, it was identified that the $b^1\Sigma_g^+$ state could be present in amounts higher than the $a^1\Delta_g$ state. We explore the role of the EEDF and the chamber wall material in determining the plasma parameters in an oxygen discharge, in particular the formation and annihilation of the singlet molecular metastables.

Introduction

The metastable species $O_2(a^1\Delta_g)$ and $O_2(b^1\Sigma_g^+)$ are known to play a significant role in oxygen discharges. Although the $O_2(b^1\Sigma_g^+)$ density has been reported as being present in plasmas in lower amounts than the $O_2(a^1\Delta_g)$ density, previous global model studies showed that the $O_2(b^1\Sigma_g^+)$ is an important contributor to the loss of O^- through detachment.

Experimental findings indicate that the EEDF in inductively coupled discharges can be approximated by a Maxwellian distribution at low pressures. As the pressure increases, it becomes depleted of high-energy electrons. In capacitively coupled discharge the EEDF is commonly observed to be bi-Maxwellian.

Description of the model

In brief, the volume average global model consists of a set of equations that include balance particle equations, energy balance equation, and the charge neutrality requirement. Solving this system of equations, one can obtain the density of species, electron temperature, sheath potential, and other important parameters. The rate coefficients are calculated through

$$k(T_{\rm eff}) = (2e/m_{\rm e})^{1/2}\int_0^\infty \sigma(\varepsilon)\varepsilon^{1/2}f(\varepsilon)d\varepsilon \qquad (1)$$

so they depend on the cross section and the EEDF. The reaction set used and a detailed description of the model can be found in Toneli et al. [1].

For this study the reactor was assumed to be a cylindrical chamber of stainless steel or anodized aluminum with R = 15 cm and L = 30 cm. The gas temperature is assumed to be 600 K, the power 500 W, and the flow rate 50 sccm.

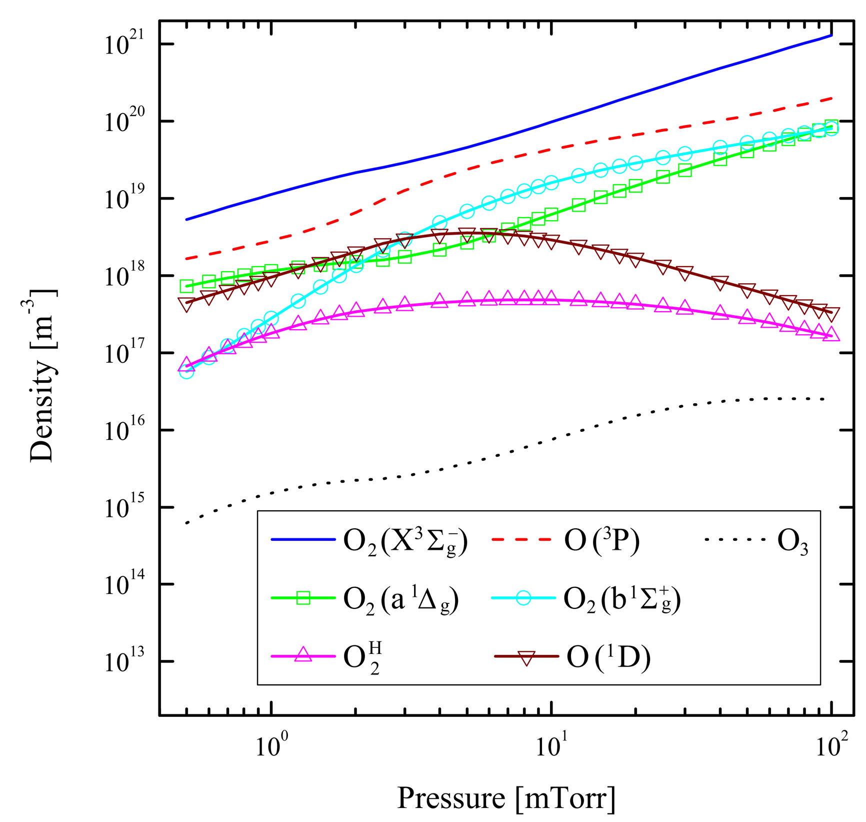

Figure 1: Mean density of neutral species as a function of pressure for a cylindrical stainless steel chamber with R=30 cm and L=30 cm and $P_{\rm abs}$=500W [1].

Results and discussion

Formation of $O_2(a^1\Delta_g)$ is mainly through:

$e+O_2(X^3\Sigma_g^-) \longrightarrow O_2(a^1\Delta_g)+e$ (dominant process)

$O(^1D)+O_2(X^3\Sigma_g^-) \longrightarrow O(^3P)+O_2(a^1\Delta_g)$

$O(^1D)+O_2(b^1\Sigma_g^+) \longrightarrow O(^3P)+O_2(a^1\Delta_g)$

Annihilation of $O_2(a^1\Delta_g)$ is mainly through:

$e+O_2(a^1\Delta_g) \longrightarrow O(^3P)+O(^1D)+e$

$e+O_2(a^1\Delta_g) \longrightarrow O(^3P)+O(^3P)+e$

$e+O_2(a^1\Delta_g) \longrightarrow O_2^++2e$

$e+O_2(a^1\Delta_g) \longrightarrow O_2(X^3\Sigma_g^-)+e$

Formation of $O_2(b^1\Sigma_g^+)$ is mainly through:

$O(^1D)+O_2(X^3\Sigma_g^-) \longrightarrow O(^3P)+O_2(b^1\Sigma_g^+)$ (dominant process)

Annihilation of $O_2(b^1\Sigma_g^+)$ is mainly through:

wall quenching

$e+O_2(b^1\Sigma_g^+) \longrightarrow O(^3P)+O(^1D)+e$

$e+O_2(b^1\Sigma_g^+) \longrightarrow O(^3P)+O(^3P)+e$

$e+O_2(b^1\Sigma_g^+) \longrightarrow O_2^++2e$

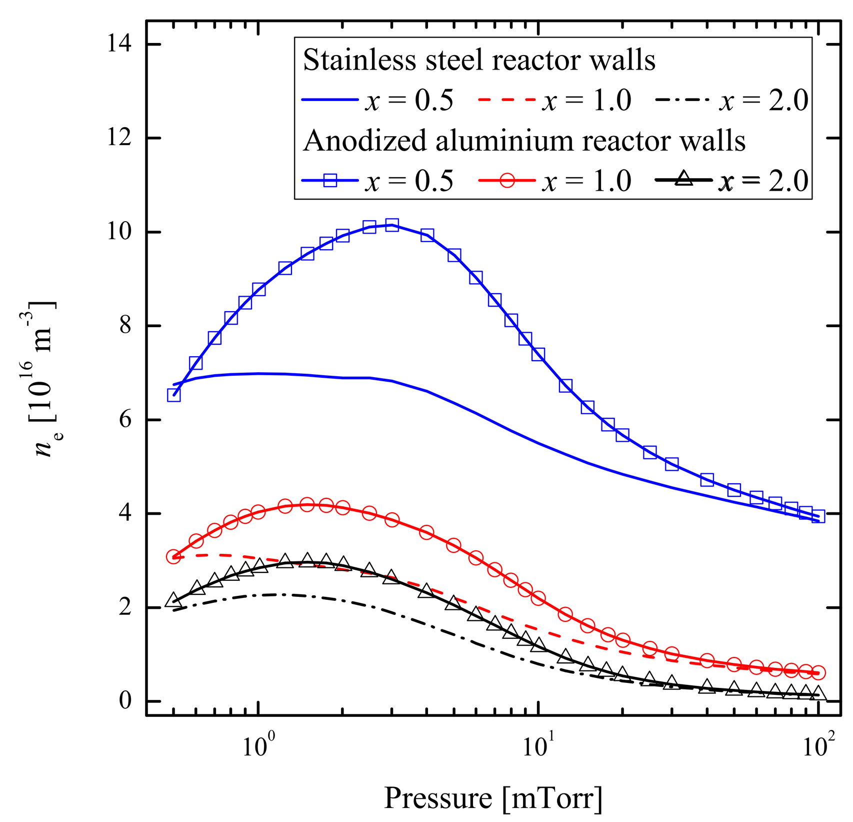

Figure 2: Mean electron density as a function of pressure for x = 0.5, x = 1.0 (Maxwellian EEDF), and x = 2.0 (Druyvesteyn EEDF) for cylindrical stainless steel chamber and cylindrical anodized aluminum chamber of radius R = 15 cm and length L = 30 cm, and absorbed power of 500 W [2].

Figure 1 shows the mean density of neutral species calculated for a Maxwellian EEDF and stainless steel chamber. In the pressure range 2.5 to 80 mTorr, the $O_2(a^1\Delta_g)$ density is lower than the $O_2(b^1\Sigma_g^+)$ density.

Figure 2 shows the mean electron density as a function of pressure for Maxwellian and non-Maxwellian EEDFs and for stainless steel and anodized aluminum chambers. The decrease of the mean electron density as pressure increases is due mainly to the decrease of the mean density of O_2^+ since this is the dominant positive ion in the discharge and the mean electron density is calculated through the charge neutrality requirement. The mean electron density is lower for stainless steel reactor that presents a higher recombination coefficient for $O(^3P)$ at the walls.

Figure 3 shows the yield of atomic oxygen as a function of pressure. Differences in the oxygen atom densities for different EEDFs are important only for pressures below 10 mTorr. The low recombination coefficient of oxygen atom at anodized aluminum walls results in high yield of atomic oxygen.

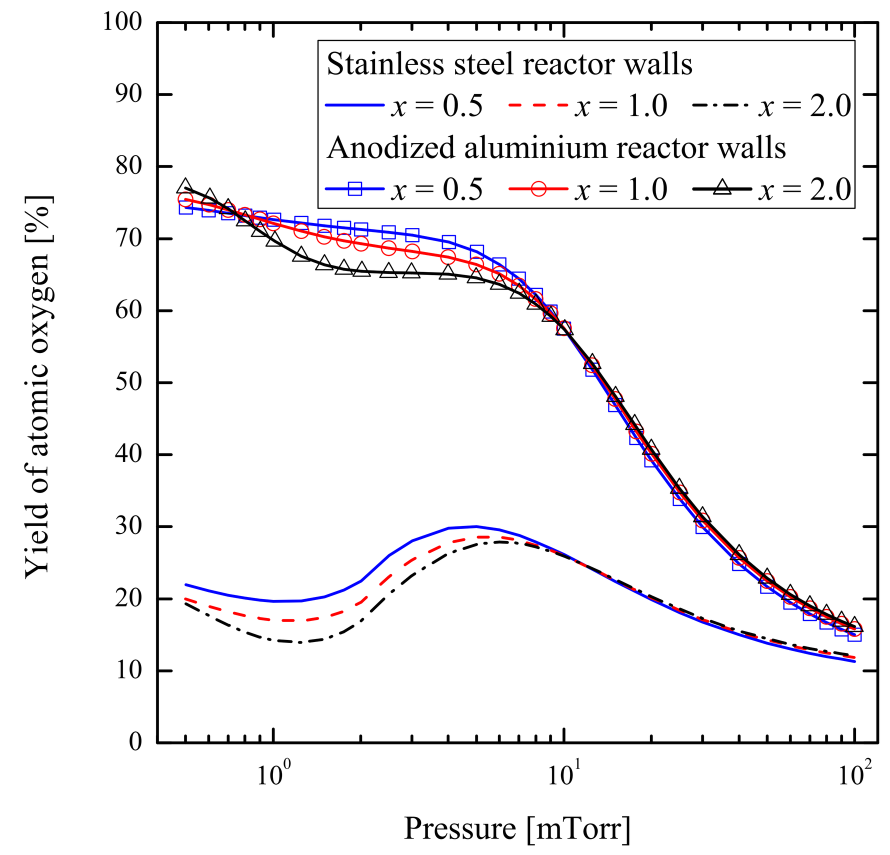

Figure 3: The yield of atomic oxygen as a function of pressure for x = 0.5, x = 1.0 (Maxwellian EEDF), and x = 2.0 (Druyvesteyn EEDF) for cylindrical stainless steel chamber and anodized aluminum chamber of radius R = 15 cm and length L = 30 cm, and absorbed power of 500 W [2].

Conclusions

- In the pressure range 2.5 to 80 mTorr assuming a Maxwellian EEDF, the $O_2(a^1\Delta_g)$ density is lower than the $O_2(b^1\Sigma_g^+)$ density.
- The mean electron density presents higher values for bi-Maxwellian EEDF as compared to Maxwellian and Druyvesteyn EEDFs.
- The yield of atomic oxygen is high at anodized aluminum reactor especially at low pressures.

References

[1] D. A. Toneli, R. S. Pessoa, M. Roberto, and J. T. Gudmundsson. *Journal of Physics D: Applied Physics*, 48(32):325202, 2015.

[2] D. A. Toneli, R. S. Pessoa, M. Roberto, and J. T. Gudmundsson. A volume averaged global model study of influence of the electron energy distribution on an oxygen discharge. *Journal of Physics D: Applied Physics*, submitted 2015.