Discussion on using the approach of a Maxwellian electron energy distribution function from low to moderated pressures in a global kinetic model for pure O_2 discharges

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This paper presents a study on the influence of the Electron Energy Distribution Function (EEDF) on the calculated species densities in pure O_2 DC discharges, for pressures in the range 0.075 – 5 Torr. A time dependent global kinetic model is used, considering either a Maxwellian EEDF or one calculated by solving the electron Boltzmann equation. The study focus on the $O_2(a)$, $O_2(b)$, $O(^3P)$, O_3 and O^- species densities, together with their creation and destruction mechanisms. The results point out that the differences in these two distribution functions can have an important effect on the electron reaction rates and ensuing densities of some of the major species, which draws attention to the limits of validity of using a Maxwellian distribution, even at low pressure conditions.

1. Introduction

The Electron Energy Distribution Function (EEDF) in nonequilibrium discharges is usually strongly exponential, with a significant influence on the reaction rates of electron collision reactions and the electron transport parameters [1]. Accordingly, the analysis of its evolution with different parameters becomes especially important in plasma kinetics studies.

Several simple possibilities exist to describe this function, like the Maxwellian or Druyvesteyn distributions, based, respectively, on the assumption of a constant (*i.e.* independent of electron energy) collision frequency and cross section. A more precise approach is to obtain the EEDF from the solution of the electron Boltzmann equation. The use of a Maxwellian distribution function is common in the literature and constitutes a simple way of accounting for the behaviour of electrons. Moreover, it has been implemented successfully to investigate nonequilibrium low-pressure discharges with high ionisation degrees. For these reasons, it is widely used in global models. However, this approximation should be used with caution, as it has some evident limitations and the influence of inelastic collisions of electrons with heavy particles has to be precisely determined. Indeed, these processes can change the shape of the EEDF and cause important departures from a Maxwellian distribution, since drops of the EEDF at higher energies emerge.

Hereby we investigate the influence of the EEDF on plasma modelling results for the case of a pure O_2 DC discharge, by comparing the results obtained with a Maxwellian EEDF and with an EEDF computed form the solution of the electron Boltzmann kinetic equation, for different values of the operating pressure.

2. Description of the kinetic model

The O_2 kinetic model has been extensively described in previous papers [2,3]. The self-consistent LoKI (LisbOn KInetics) numerical code is used in this study [4]. It is based on a system of rate balance equations describing the formation and loss of the most important neutral and charged heavy species, namely $O_2(X, a, b)$ molecules, ground-state (O_3) and vibrationally excited (O_3^*) ozone, $O(^3P, ^1D)$ atoms, and O^+, O_2^+ and O^- ions. This system of equations is either coupled to the homogeneous electron Boltzmann equation solved in a two-term expansion in spherical harmonics, or else the electron impact rate coefficients are obtained from a Maxwallian EEDF. The input parameters to the model are the electron density and gas temperature, which are kept constant along this work ($[n_e] = 1.7\times10^{10}$ cm^{-3}, $T_g = 300$ K [2]), and pressure, $p = 0.075$, 0.25, 0.5, 1 and 5 Torr. The calculations are made considering a DC discharge in a tube with a radius of 1 cm. In the case of solving the Boltzmann equation, the self-consistent reduced electric field, E/N, is obtained from the requirement that the total electron creation rate must compensate its destruction rate, under the assumption of a quasi-neutral discharge. When assuming the Maxwellian distribution, the electron temperature, T_e, is

calculated as to verify the same requirement. Note that electron-electron collisions are not taken into account in the base calculations, due to the low ionization degrees involved, ≤ 7×10^{-6} (*cf.* section 3), much lower than the onset value of ~ 10^{-4}. Nevertheless, their influence is evaluated for the higher ionization degree considered.

3. Results and discussion

Table 1 summarizes the working conditions studied and the corresponding calculated electron temperatures, T_e. The Maxwellian temperatures are about 45 - 50 % lower than the ones calculated from the averaged kinetic electron energy. The ionization degree is rather low so that electron-electron collisions have a negligible role for the conditions under investigation.

Tab. 1: Parameters calculated from the kinetic model

***p* (Torr)**	**Ionisation degree**	**T_e from <u> (eV)**	**Maxwellian T_e (eV)**
0.075	7×10^{-6}	4.2	2.4
0.25	2×10^{-6}	3	1.7
0.5	1×10^{-6}	2.7	1.5
1	5×10^{-7}	2.5	1.3
5	1×10^{-7}	2.2	1

(<u> - averaged kinetic energy)

Figure 1 presents a comparison of the EEDFs calculated form the Boltzmann equation and with an imposed Maxwellian shape, for p = 0.075 and 1 Torr. For the lower pressure and large energy values, the Maxwellian can be a good approximation for the EEDF. However, the figure clearly demonstrates the existence of significant differences at small energies, below 8 eV. These differences may have an important influence on the simulation results, since the energy range around the interval of 1 - 12 eV is responsible for the energy distribution in elastic and inelastic processes of electrons in low temperature, non-equilibrium O_2 discharges. In addition, it can be seen that the inclusion of electron-electron collisions (dotted line in figure 1) in the kinetic scheme alters only slightly the calculated distribution function, as expected from the low ionization degree in these conditions.

Figure 2 represents the evolution of the $O_2(a, b)$, $O(^3P)$, O_3 and O^- species densities with pressure, comparing the results obtained with a Maxwellian and a calculated EEDF. At 0.075 Torr the two distributions provide consistent results for the concentrations of $O_2(a, b)$ molecules and $O(^3P)$ atoms. This is not so much the case for O_3 molecules and O^- ions, where the error on the calculated densities assuming a Maxwellian against the values obtained from the computed EEDF exceed 140 and 110 %, respectively.

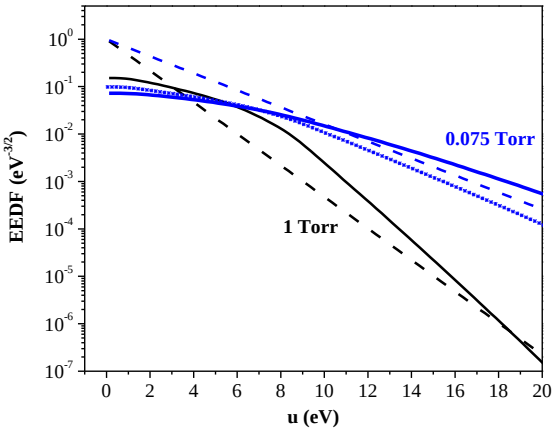

Fig. 1: Simulated EEDF at 0.075 and 1 Torr. The dashed lines correspond to a Maxwellian EEDF while the solid lines show the calculated one by solving the electron Boltzmann equation (without electron-electron collisions). The influence of electron-electron collisions is illustrated by the dotted line.

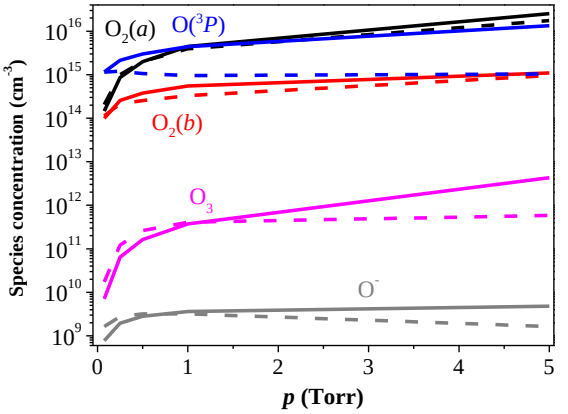

Fig. 2: Evolution of species concentration as function of pressure for a Maxwellian and calculated EEDF (dashed and solid lines, respectively).

The creation and loss rates were analysed for all the oxygen species studied. Figure 3 presents one representative process of creation and one of destruction of $O_2(a)$ metastables and $O(^3P)$ atoms, namely:

$$e + O_2(X, v=0) \rightarrow e + O_2(a) \quad \text{(R1)}$$

$$e + O_2(a) \rightarrow e + O_2(b) \quad \text{(R2)}$$

$$e + O_2(X, v=0) \rightarrow e + O + O \quad \text{(R3)}$$

$$O(^3P) + wall \rightarrow 1/2\ O_2(X,v=0) \quad \text{(R4)}$$

Despite the fact that the final concentrations for these two species (Fig. 2) have the tendency to approach at the lowest considered pressure towards a characteristic value, somehow validating the use

of a Maxwellian EEDF at low pressures, we cannot straightforwardly deduce the same trend for all the individual reaction rates. These evolutions point out to the necessity of using with care the assumption of a Maxwallian distribution for modelling O_2 discharges, even at low-pressures. In fact, for relatively low ionization degrees, such as the ones used here, the high reduced electric fields are not enough to sufficiently "Maxwellianize" the EEDF.

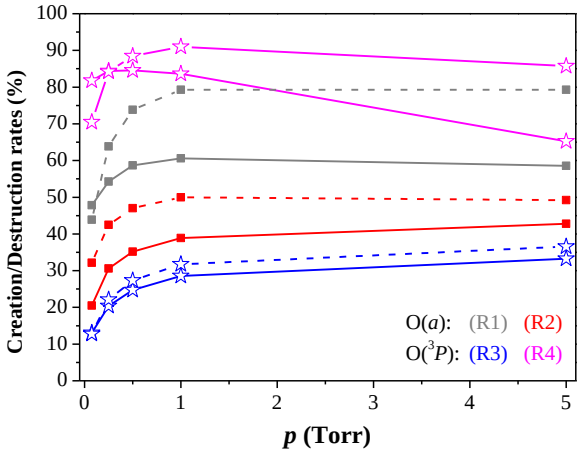

Fig. 3: Some important creation and destruction rates as function of pressure for $O_2(a)$ and $O(^3P)$ species denoted by ■ and ☆, respectively. The dashed lines correspond to the case of a Maxwellian EEDF while the solid lines to the case of the calculated one by solving the electron Boltzmann equation.

4. Conclusion

In this paper we have used Maxwellian and self-consistently calculated electron energy distribution functions in a global model for pure O_2 DC discharges, in the pressure range 0.075 – 5 Torr. It is shown that the consideration of a Maxwellian EEDF in the context of kinetic modelling studies can bring important differences in the resulting species densities, as well as in their creation and destruction rates, even at low pressure conditions, as long as the ionisation degree remains relatively small.

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5. References

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