Influence of the molecular lines on the radiative transfer: application to atmospheric air thermal plasmas and coplanar geometries

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This paper deals with the radiative transfer of atmospheric air thermal plasmas in coplanar configuration (1D), considering different temperature profiles with different lengths (5mm, 2cm, 5cm) and different maximum temperatures (6kK, 8kK, 15kK, 20kK). The radiative transfer equation (RTE) is solved according to a given direction perpendicular to the isothermal planar surfaces. The radiative flux and its divergence are studied. The objectives of this work are not to predict the radiation fluxes but to highlight the role of the radiative mechanisms in the transport energy, especially the contribution of the molecular lines which are usually neglected. The results show that the molecular lines can be important in emission and absorption for maximum temperatures lower than 6kK. For higher temperatures, the emission is mainly due to atomic species but molecular species are still responsible for the absorption in the surrounding regions.

1. Introduction

Several industrial processes use thermal plasmas containing air plasmas such as low voltage circuit breakers, (LVCB), plasma torches, or plasma reactors used for combustion for instance. The energy transported by radiation is obtained by solving the Radiative Transfer Equation (RTE). The solution can be used either in numerical modelling to estimate the radiative losses through the divergence of the radiative flux, or in experimental studies to characterize the plasma. This work studies the radiative transfer in atmospheric air plasma and for a one dimensional coplanar configuration. The RTE is solved along a given direction perpendicular to the isothermal planar surfaces. The aim of this study is not to predict the radiative flux or its divergence but to highlight the role of the radiative mechanisms in the energy transport, especially the contribution of the molecular lines which is usually neglected even for applications at high current.

2. Elaboration of the radiative spectra

To solve the RTE, it is necessary to elaborate a spectroscopic database allowing us to determine the radiative spectra for lots of plasmas applications, in a large temperature range (300-30.000K) and a large pressure range (1-100 bar). For this study, we considered air plasmas at atmospheric pressure. The radiation was obtained by taking into account both atomic and molecular radiation contributions from 33nm to 10^5nm: molecular continuum (O_2, N_2, NO, O_3, NO_2, N_2O, NO_3, N_2O_5), atomic continuum (O, O^+, O^{2+}, O^{3+}, N, N^+, N^{2+}, N^{3+}, O^-), diatomic molecular lines (O_2, N_2, NO, N_2^+) and atomic lines (6217 for oxygen and 8313 for nitrogen). Two examples are given in Figures 1 and 2.

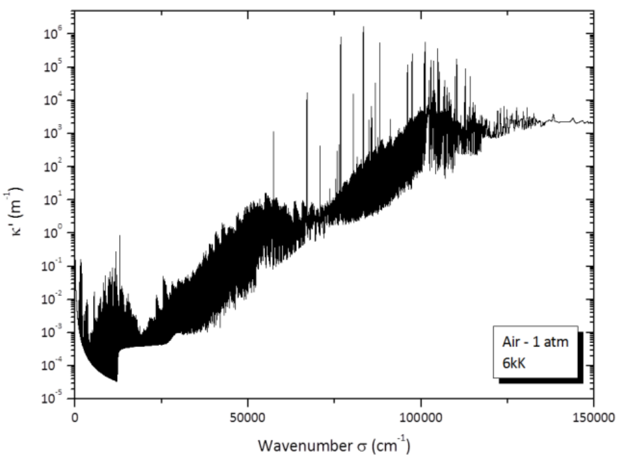

Fig.1 : Spectral absorption coefficient of air thermal plasma at 6kK and atmospheric pressure.

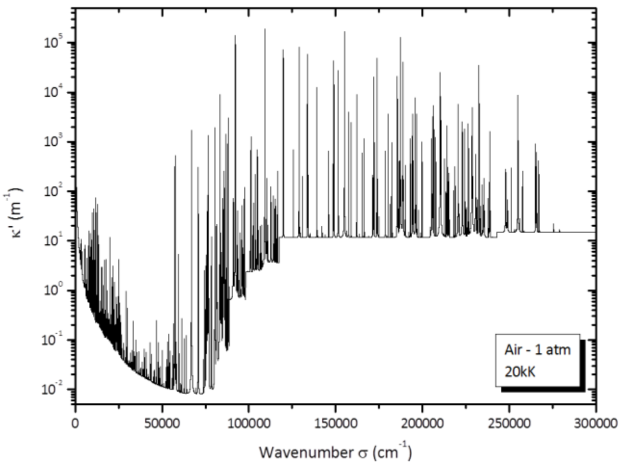

Fig.2 : Spectral absorption coefficient of air thermal plasma at 20kK and atmospheric pressure.

All the absorption and emission spectra were calculated with a number of wavelengths between 1.10^6 at 30.000K and 7.10^6 at 300K, in order to well describe the radiative mechanisms by keeping a correct time calculation. For the different temperatures, they were compared to the software SPECAIR [1], LIFBASE [2] and the HTGR works of the EM2C laboratory [3-5].

3. Resolution of the ETR equation

In this study, the RTE is solved by neglecting the diffusion, and by assuming a refractive index equal to 1:

$$\vec{s}\cdot\vec{\nabla}L_\lambda = \kappa'_\lambda B_\lambda - \kappa'_\lambda L_\lambda \qquad (1)$$

In order to characterise a large number of industrial applications, we considered 3 axisymmetric temperature profiles (see Figure 2), with 3 different radial distances (5mm, 2cm and 5cm), minimum temperature of 300K on the edges and different maximum temperatures on the axis (6kK, 8kK, 15kK and 20kK). The equation (1) is solved for a given direction divided in several cells which have different lengths corresponding to isothermal regions (step of 100K in order to consider correctly the temperature gradients in the plasma). According to these assumptions, we realised a parametric study of the radiative fluxes and their divergences with the profile width and the maximum temperature in the axis. We also divided the spectrum into 8 spectral intervals (IRC, IRB, IRA, Vis-Red, Vis-Blue, UVA, UVB, UVC, far UVC) in order to evaluate their contribution in emission and in absorption.

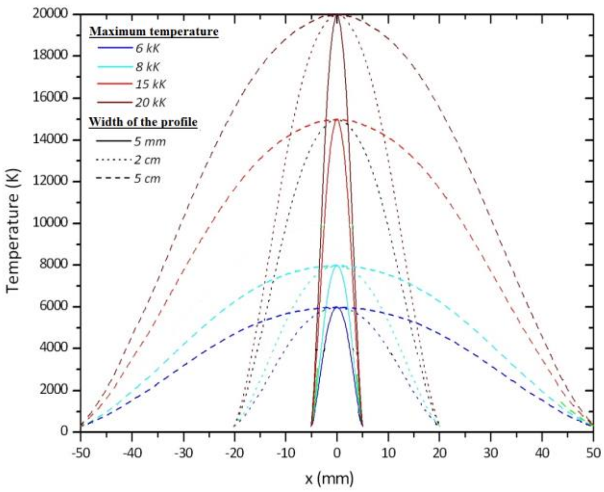

Fig.3 : Temperature profiles used to solve the RTE equation.

In these conditions, the solution can be written:

$$L_\lambda(x_i) = L_\lambda(x_{i-1})\cdot e^{-\kappa'_\lambda(T_i)\cdot(x_i-x_{i-1})} + B_\lambda(T_i)\cdot\left(1-e^{-\kappa'_{\lambda,}(T_i)\cdot(x_i-x_{i-1})}\right) \qquad (2)$$

with T_i and (x_i-x_{i-1}) the temperature and the thickness of the cell, $\kappa_\lambda(T_i)$ and $B_\lambda(T_i)$ the spectral absorption coefficient and the intensity of the black body at the temperature T_i, respectively. Due to the symmetry of our configuration, the divergence is obtained by taking into account the two directions of the radiation propagation, leading to a symmetric profile for the divergence: from x=0 to $x=r_m$, r_m being the maximum length of the temperature profile T(x).

4. Results and discussions

In Figure 4, we plotted the radiative flux and its divergence for the temperature profile T_{max}=20kK on the axis. The divergence of the radiative flux is also compared to the values deduced from the method of the Net Emission Coefficient (eq.1) (with a plasma size R_P taken equal or the closest to the studied configuration) in order to evaluate the validity of this last method often used in the numerical model. We also studied the influence of the molecular radiation in the plasma by comparing the values obtained with and without the contribution of the molecular lines.

Globally, we can observe in figure 4 that:

- the width of the temperature profile has no real influence on the radiative transfer. The radiative flux increases with the width of the plasma showing the volume impact of the central hot region (dominated by the atomic radiation) compared to the impact of the surface flux escaping towards the surrounding regions;

- the central region is strongly emissive. The divergence of the radiative flux is positive and corresponds to the emission of the atomic lines, most particularly to the neutral resonance lines of oxygen and nitrogen which strongly emit in UVA and UVL regions. This divergence decreases when the width of the temperature profile increases, showing the strong self-absorption of the atomic lines in this region (mainly the resonance lines in UVC and UVL regions). This behaviour according to the size of the plasma is similar to the exponential term of the Net Emission Coefficient which represents the self-absorption along the distance R_p:

$$\varepsilon_n(T,R_p) = \int B_\lambda \kappa'_\lambda \cdot \exp\left(-\kappa'_\lambda R_p\right)\cdot d\lambda \qquad (3)$$

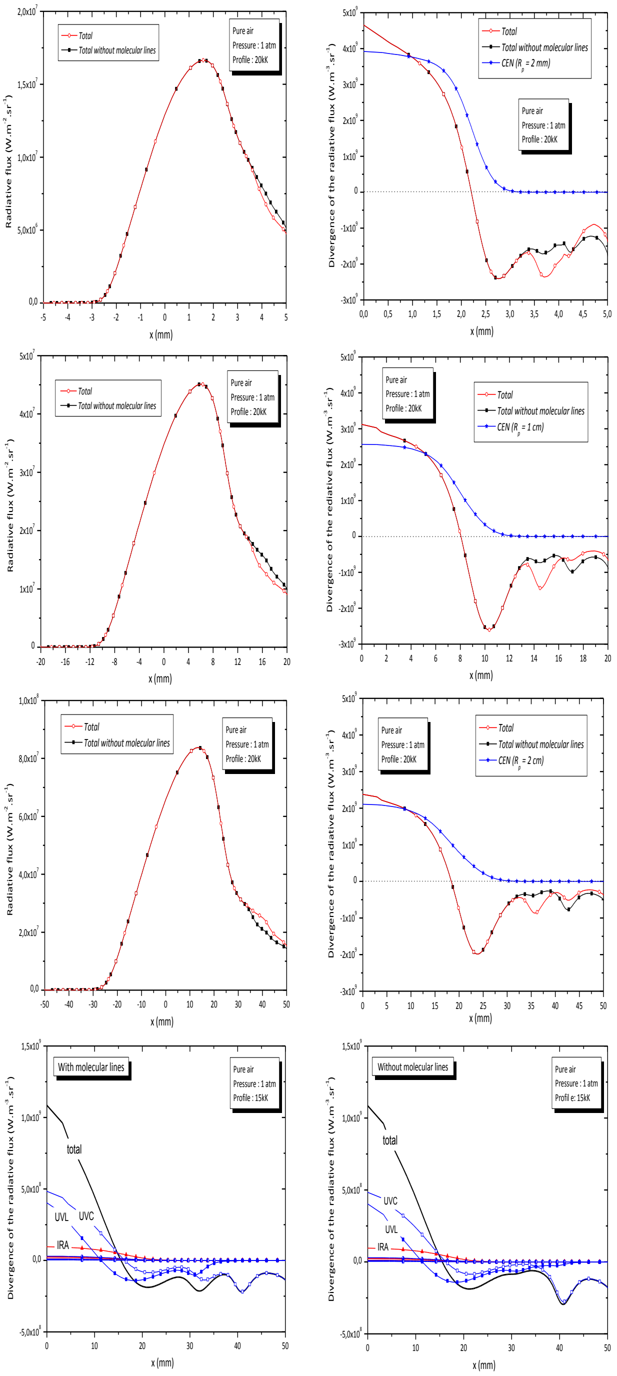

Fig.4: Influence of the temperature profile (width) on the radiative transfer for an atmospheric air plasma. Contribution of the spectral intervals.

- in the surrounding regions, the radiation flux increases of a factor 5 and the divergence of the flux decreases of a factor 2 when the width of the temperature profile increases of a factor 10. The radiation coming from the continuum (atomic and molecular) and from the atomic lines (issued from the central region) is then absorbed in the surrounding regions of the plasma (the divergence of the flux becomes negative). This region is then totally absorbent whatever the width of the temperature profile. Due to the low radiation of most of the lines compared to the radiation of the resonance lines in UV, the total radiation is weakly absorbed in the medium and constitutes a significant contribution of the flux to walls. The first peak corresponds to the absorption of the atomic radiation by the atomic species. Its amplitude is relatively constant for the three widths of profile. Figure 4 shows that this absorption is mainly due to the atomic continuum in far UV. The other peaks of the divergence of the flux correspond to the absorption of the molecular species (bands and continuum). Its amplitudes increase when the width of the profile decreases. It can be explained by the weak self-absorption of the atomic radiation in the central region of the plasma, compensated by an overabsorption of this radiation by the molecules in the surrounding regions. On the wall, the values of the divergence remain appreciably identical by considering or not the molecular lines in the calculations. It is due to the absorption of the molecular lines in the UV region (mainly NO and the VUV system of N_2). If we do not take into consideration the radiation of the molecular lines in our calculation, the absorption of the radiation coming from the central region is just delayed, the molecular continuum compensating for the few number of molecular lines with a stronger absorption (in UVC region in this case).

5. Conclusions

In this work, we calculated the emission and absorption spectra for atmospheric air plasmas. We solved the Radiative Transfer Equation (RTE) along a given direction, for a 1D coplanar configuration. The use of a simplified model highlighted that fact that the emission in the hottest region is mainly due to the atomic lines and that the molecular lines are mainly responsible for the absorption in the surrounding regions, if temperature profiles have a maximum temperature higher than 15kK. Consequently, to neglect the emission of the molecular lines is in good agreement with most of the studies devoted to high current electrical arcs. Indeed, the fact of neglecting the molecular lines in the calculation will be compensated with the strong absorption of the molecular continuum in the UV region and the surrounding regions of the plasma.

On the other hand, if the maximum temperature does not exceed 15kK, the contribution of the molecular lines on the radiative transfer cannot be neglected any more, justifying the necessity to implement a most complete databank including a large number of molecular systems. Indeed, the diatomic molecular system can have a significant contribution not only in absorption but also in emission.

For the two other temperature profiles (maximum temperatures of 6kK and 8kK on the axis), the results were not presented here but showed similar behaviours. Nevertheless, a fine analysis of the contribution shows that the emission in the central region of the plasma is quasi-exclusively due to the molecular mechanisms: molecular lines with 50% of the total emission for a maximum temperature of 8kK and 90% for 6kK; the emission is mainly due to the molecular systems N_2, NO and N_2^+ for 6kK and 8kK, the emission of the molecular continuum is negligible for 8kK but becomes significant for 6kK, (approximatively 10%). Concerning the absorption, the radiation coming from the central region is mainly absorbed by the molecular lines for 6kK and by these lines and the continuum (50%) for 8kK. This difference can be explained by a stronger radiation in the far UV for 8kK (strong radiation of the atomic species and VUV of N_2). The region where the absorption is the strongest is often localised close to x=30-35mm, corresponding to 2kK-5kK, and is due to the strong absorption of the radiation by the diatomic molecular systems of NO and O_2 (Schumann-Runge de O_2).

6. References

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