Pressure dependence of line-by-line calculation of argon plasma net emission coefficient

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Abstract: In order to fill the lack of detailed pressure dependent net emission coefficient data in literature a detailed line-by-line method was implemented to compute the net emission coefficient of Ar plasmas at temperatures ranging from 300 K to 30000 K and pressure ranging from 50 kPa to 500 kPa for optically thin and partially auto-absorbed (optically thick) plasmas. The model is suitable for performing calculation of the net emission coefficient at different plasma thicknesses, by considering the absorption over a large wavelength spectrum. Fractional contributions of different species and of emission mechanisms to the volumetric emission coefficient were determined and the influence of pressure on absorption is discussed.

Keywords: plasma radiative emission, net emission coefficient, Argon plasma

1. Introduction

Argon plasmas are widely used in many industrial and research applications, such as plasma arc cutting and welding, spray-coating, nano-particles synthesis and waste treatment. Radiative processes often represent an important component in energy transport, and the calculation of the radiative flux is necessary in advanced modeling of thermal plasma systems.

Radiation transport in plasma modeling can be addressed in details by means of e.g. Discrete Ordinate or P1 expansion methods. However these methods are computationally expensive and need the knowledge of the absorption coefficients which are functions of wavelength, temperature and plasma gas composition. For these reasons, the net emission coefficient (nec) approach is commonly used in plasma modeling literature [1-3]: in this method, total emission per unit volume is reduced by the amount of radiation that is absorbed in a plasma sphere with specified radius, which is usually estimated using the computational mesh size or a characteristic dimension of the plasma torch. Having detailed plasma properties describing the radiative emission is valuable to those interested in obtaining temperature profiles or computing heat fluxes. The knowledge of the dominating radiation mechanisms and species and of the spectral emission coefficient over a large spectrum span at different pressures and temperatures is needed for these purposes. Published results could not supply the complete set of data necessary to pursue these tasks and, in particular, a systematic study of the influence of plasma pressure on the radiative emission of optically thick plasma is lacking.

In view of the above, a line-by-line method was developed in the present work to compute the net emission coefficient of Ar plasmas in the temperature range 300 K - 30000 K and pressure range 50 kPa - 500 kPa, for optically thin and partially auto-absorbed plasmas.

2. Radiative emission calculation

A detailed line-by-line method was adopted to determine the radiant energy transport, performing a calculation of the emission coefficient on a wavelength basis before integrating over the selected spectrum range.

The primary assumptions of the nec calculation are that the plasma is homogeneous, isothermal and in local thermodynamic equilibrium. The first step for the calculation of the spectral emission coefficient is the computation of plasma species composition at pressures and temperatures of interest. Composition was in particular determined by solving the Saha-Eggert mass law equation and taking into account Dalton's law for ideal gas, macroscopic charge neutrality and conservation of heavy species mass [4]. The temperature range was fixed between 300 K and 30000 K, with pressure varying from 50 kPa to 500 kPa. Fundamental data for energy levels e_i, statistical weight g_i, transition probabilities A_{ul} and lines, atomic configurations and oscillator strengths, were taken integrating the NIST [5] and Kurucz [6] databases. A total of 7065 emission lines was considered for the Ar neutral (Ar I), first and second Ar ions (A II and Ar III respectively) as shown in Table 1.

Table 1. Lines considered for each specie in the computation of Ar net emission coefficient.

Ar (Ar I)	Ar^+ (Ar II)	Ar^{2+} (Ar III)	Total
2412	4573	80	7065

Spectral emission coefficient was then calculated considering line and continuum emission. The spectral emission coefficient ε_λ represents the radiation emitted (radiative power) at wavelength λ, for unit volume and unit solid angle. It comprises three contributions, according to the different emission mechanism [7]: line emission coefficient (*bound-bound* transitions), continuum emission coefficient due to radiative recombination (*free-bound* transitions) and continuum emission coefficient due to braking radiation or *bremsstrahlung* (*free-free* transitions).

As concerning line emission, Doppler, resonance and Stark broadening effects were considered for each absorbed line to compute its perturbed profile [7, 8]. For continuum emission, spectral emission due radiative recombination and *bremsstrahlung* was calculated according to the expression introduced by Cabannes and Chapelle [9] in the form proposed by Wilbers et al. [10]. Only electrons interactions with ions were considered for continuum emission, while free-bound radiative attachment and braking radiation due to interaction with neutrals were neglected. For each ion, the Biberman factors (accounting for non-classical as well as non-hydrogenic behavior of the ion [8]) for free-bound and *bremsstrahlung* continuum were taken from Hofsaess [11, 12]. Crude linear interpolation was used to determine Bibernam factors for missing temperatures and wavelengths, while the influence of pressure was considered as negligible.

Integrating the spectral emission coefficient over the selected wavelength spectrum (0.03 – 25 μm), for every temperature and every pressure of interest, volumetric emission coefficient (i.e. nec for a optically thin plasma, R=0) was estimated at different pressures and temperatures. Once the emission spectrum of the optically thin Ar plasma, comprising broadened lines, was computed, the spectral absorption coefficient K_λ was determined as the ratio between the spectral emission coefficient and blackbody function according to Kirchhoff's law [13]. Nec at different plasma thickness R (or line-of-sight L) was finally calculated. Species and emission mechanisms fractional contribution to the net emission coefficient of Ar plasmas were determined at different temperatures and pressures.

3. Results

3.1 Atmospheric pressure

The absolute and fractional contribution of different species to line emission at atmospheric pressure is reported in Fig. 1. At low temperatures the main contributor to line emission is the Ar neutral (Ar I). Line emission of the first ion (Ar II) starts to be preponderant from about 17000 K, whereas the contribution second ion (Ar III) starts to be significant only over 25000 K although the main contribution at 30000 K is still given by Ar II.

Fig. 2 shows the absolute contribution of different species to for continuum emission, highlighting in both free-bound and free-free emission cases that the second ion has a greater effect over Ar I starting from about 24000 K. The radiative recombination gives the main contribution to the total continuum emission, representing about 87% of the total continuum radiation at 15000 K. The *bremsstrahlung* contribution increases with temperature up to 32% of the total continuum radiation at 30000 K.

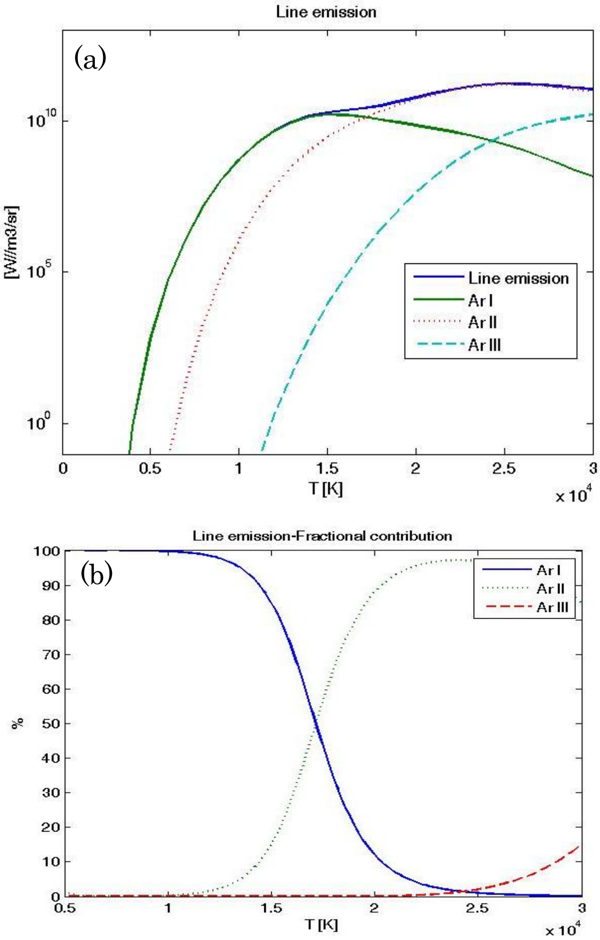

Fig. 1. Absolute (a) and fractional (b) contribution of different species to Ar plasma line emission at 100 kPa.

The main contribution to total emission is given by far by line emission, always higher than 90% of total emission. In particular, at temperatures ranging from 5000 K to 30000 K continuum emission due to free-bound transitions does not contribute more than 3% to the total volumetric emission. The contribution of *bremsstrahlung* to the total emission is almost negligible.

The effect of plasma thickness (1 and 10 mm) on the nec at atmospheric pressure is shown in Fig. 3. The nec decreases as the path length increases due to increased absorption, which is already relevant at 1 mm.

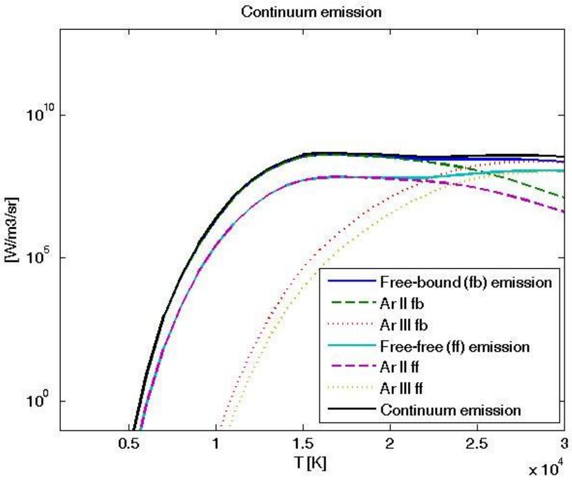

Fig. 2. Ar plasma continuum emission at 100 kPa with absolute contribution of different emission mechanisms and chemical species.

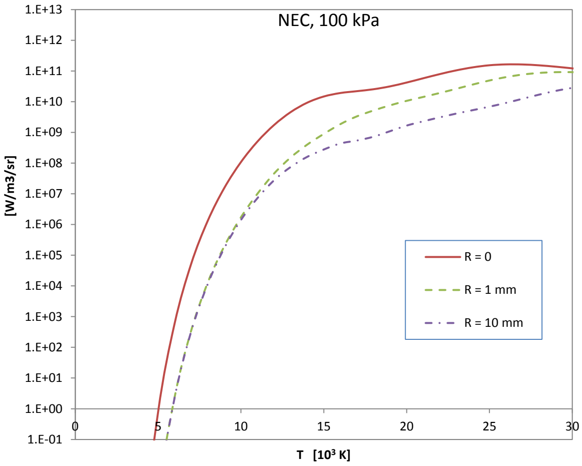

Fig. 3. Net emission coefficient for a Ar plasma at 100 kPa for different geometrical path lengths, wavelength range 0.03–25 µm.

3.2 Influence of plasma pressure

The effect of Ar plasma pressure on total radiative emission is shown in Fig 4 for optically thin plasmas. The higher particle densities implies, as expected, an increase in the emission coefficient. At 5000 K, the emission coefficient increases linearly with plasma pressure, as shown by the normalized emission coefficient with respect to 100 kPa case at different plasma temperatures (Fig. 5), while at 30000 K the nec increases more than linearly with plasma.

Continuum emission for optically thin plasma at different pressures is reported in Fig. 6. The continuum emission achieves a maximum between 15000 K and 17000 K depending on the plasma pressure. It should be noted that, over the pressure range explored, line emission is always the dominating mechanism and the main contributor is Ar I up to about 17000 K.

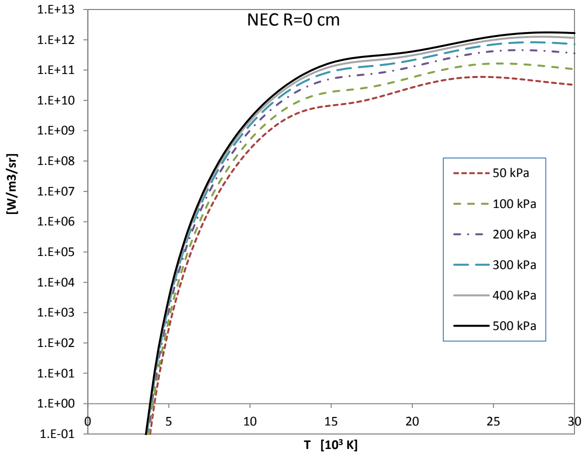

Fig. 4. Optically thin Ar plasma net emission coefficient at different plasma pressures (50-500 kPa).

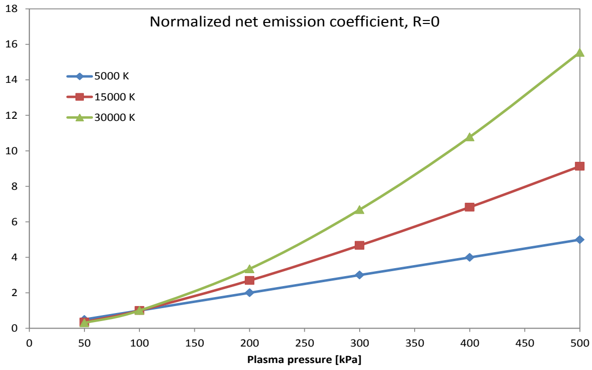

Fig. 5. Ar plasma normalized net emission coefficient (R=0) with respect to the 100 kPa case at different plasma temperatures as a function of plasma pressure.

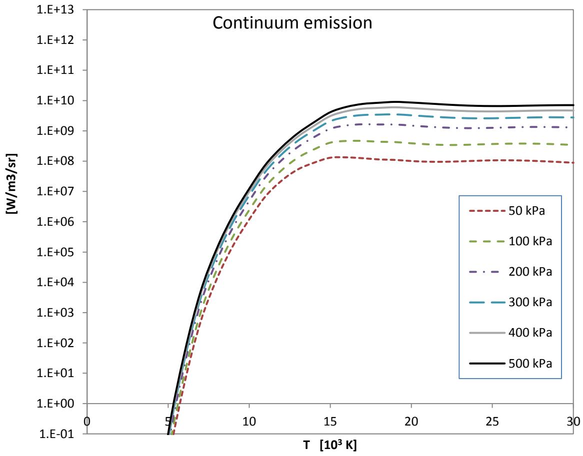

Fig. 6. Ar plasma continuum emission coefficient at different plasma pressures (50-500 kPa).

The effect of absorption in optically thick plasma nec is shown in Fig. 7 and 8 respectively for the 1 mm and 10 mm plasma radius case. The effect of plasma pressure on the net emission coefficient is generally reduced for optically thick plasma with respect to the optically thin case, especially at high temperature (over 10000 K). At 0 mm plasma radius, nec increases by a factor of 9 when passing from 100 to 500 kPa at 15000 K, while it increases only by a factor of 2.4 in the 1 mm plasma radius case. On one hand, the increased plasma pressures causes a stronger volumetric radiative emission, while on the other hand a more relevant absorption is induced by the increased plasma density, thus explaining the lower dependence of thick plasmas from plasma pressure.

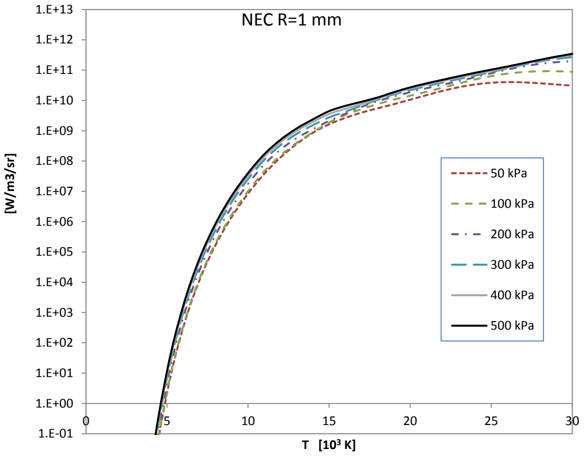

Fig. 7. 1 mm radius Ar plasma net emission coefficient at different plasma pressures (50-500 kPa).

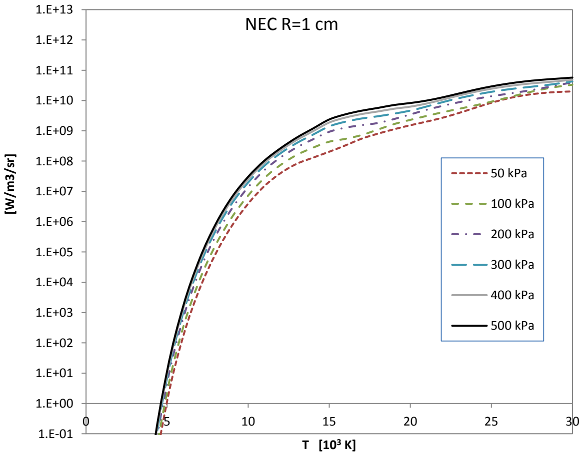

Fig. 8. 10 mm radius Ar plasma net emission coefficient at different plasma pressures (50-500 kPa).

4. Conclusions

In the present work the net emission coefficient of Ar plasmas in the temperature range 300 K - 30000 K and pressure range 50 kPa - 500 kPa was computed by a line-by-line method developed for optically thin and partially auto-absorbed plasmas.

The dominating radiative mechanism was found to be line emission over the entire temperature and pressure range. The main contributor is Ar I up to about 17000 K in the pressure range explored, while Ar II dominates up to 30000 K.

The net emission coefficient for optically thin plasma shows a nonlinear dependence from the pressure for temperatures higher than 10000 K. The effect of plasma pressure on the net emission coefficient is generally reduced for optically thick plasma at high temperatures (over 10000 K) with respect to the optically thin case due to increased absorption owing to the higher plasma density.

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