Numerical optimization of Mean Absorption Coefficient in Air using Planck Modified Mean Function

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Abstract. The Divergence of Radiative Flux (DRF) is the term present in the energy balance of the plasma that describes the radiative behavior of the arc. This property is obtained by the resolution of the Radiative Transfer Equation (RTE). Because of its complexity, many approximate methods are developed to reduce the computational time. This paper will describe the approximate methods already used in numerical simulation: Net Emission Coefficient (NEC) and Mean Absorption Coefficient (MAC). This last property requires having a good definition of spectral ranges and mean functions to have a physical representation of radiative losses. In this paper, the spectral ranges will be defined from the continuum of the absorption coefficient and Planck Modified Mean Function (PMMF) will be used to calculate MACs. This mean function requires a good definition of the characteristic absorption length $R$.

In this paper, we will develop an optimization methodology that allows finding the best $R$ in order to have an accurate DRF using MACs. To quantify the accuracy of these approximate methods, a 1D resolution of RTE will be performed in the case of Air plasma at $P=1$bar in Local Thermodynamic Equilibrium (LTE). The exact DRF solution will be considered as a reference when compared with the DRF of approximate methods.

1-Introduction

The accurate prediction of the radiative properties is essential for the development of new electrical devices. These properties are represented in the energy balance of the plasma by the Divergence of Radiative Flux (DRF). To obtain the DRF, a resolution of the Radiative Transfer Equation (RTE) is necessary. Unfortunately, this equation is complex to solve and has a high computational time due to numerous variables (temperature, pressure, wavelength and geometry). The complexity of the absorption spectrum makes the resolution of RTE very challenging and very demanding in terms of computational time. This is why many approximate methods have been developed in order to reduce either the computing time or the memory sizes.

The first approximate method is the Net Emission Coefficient (NEC) [1,2]. It is a geometric approximation that allows a good prediction of the radiation losses in the hottest regions of plasma. The NEC represents the net emission coming from the center of an isothermal sphere with a radius of $R_p$ per
volume unit per solid angle unit. This property is simple to introduce in a numerical method. For a
defined plasma composition, the NEC depends on the temperature, pressure and the radius Rp.
The second approximation is the Mean Absorpti on Coefficient (MAC). It relies on a spectral
simplification. This property is characterized to decrease an error on the radiative transfer in the medium
and cold regions of the plasma. However, for a high accuracy of this method, a good definition of the
spectral limits and mean functions are necessary. Many studies have been developed in this field.
Concerning the choice of the spectral ranges, there is no unique approach. Kloc highlighted the global
work done for the spectral range definition [3].
In his study, he developed a numerical optimization methodology to find the spectral distribution with a
parametric study on the effective mean value inside each spectral interval. In the present work, the
definition of the spectral range is based on the continuum spectra of the absorption coefficients [4].
Concerning the mean functions, classic, Planck, Planck Modified (PMMF) and Rosseland functions are
generally used in the literature. Here, we will focus our study on the PMMF. This mean function requires
a definition of a characteristic absorption length, R, which plays an important role in presence of intense
atomic and molecular lines [5]. The goal of this study is to give the values of R that permit to calculate
MACs using PMMF and obtain an accurate DRF.
A detailed description of these approximate methods will be developed for the case of Air plasma at
P=1bar. To have an estimation about the accuracy of these methods, a 1D resolution the RTE for given
temperature profiles will be presented. Also a comparison of the exact DRF and DRF using NEC, MACs
(PMMF) and MACs (PMMF) with optimization algorithm will be described.

2-Divergence of Radiative Flux
In this section, we solved the RTE (1) in 1D taking into account all the wavelengths in the absorption
spectra (4.10⁶ wavelengths).
\[ \vec{s}\cdot \nabla L_\lambda(\vec{r},\vec{s}) = K'(\lambda)(L^0_\lambda(T) - L_\lambda(T)) \]
where \( L_\lambda \) represents the spectral flux (in \( \text{W.m}^{-3}\cdot\text{sr}^{-1} \)) and \( L^0_\lambda(T) \) represents the Planck function at the
temperature \( T \).
The absorption coefficients were obtained considering the atomic continuum (Radiative recombination,
attachment and Bremsstrahlung), the molecular continuum (photo-ionization, photo-dissociation, photo-
attachment), the atomic lines and their broadenings and the molecular lines of air plasma at \( P=1\text{bar} \) [6].
A line by line method [6] was used to take into consideration the overlapping of the lines.
We can solve the equation (1) analytically in 1D considering a temperature profile. The solution is the
sum of the general solution and the particular solution:
\[ L_\lambda(x) = L_\lambda(0) \exp(-\tau^') + \int_0^x L^0_\lambda(\xi) K'(\lambda, \xi) \exp(-\tau^\prime) d\xi \]
(2)
With optical thicknesses \( \tau^' = \int_0^x K'(\lambda, \xi) d\xi \) and \( \tau^\prime = \int_0^x K'(\lambda, \eta) d\eta \),
where \( L_\lambda(0) \) is the spectral flux coming from \( x=0 \) and \( L_\lambda(x) \) is the spectral flux coming from outside and
absorbed at \( x \).
In the equation (2), the first term represents the attenuation of the radiation coming from outside and the
second term is the fraction emitted at \( \xi \) and absorbed by the plasma in a distance of \( (x-\xi) \).

Figure 1. Schematic representation of the 1D mesh
Considering the plasma as a succession of isothermal elements of temperature $T_i$ (cf. figure 1) where $i$ represents the index of the nodal and $\Delta x = (x_i - x_{i-1})$ is the thickness of the mesh, the spectral flux becomes:

$$L_2(i) = L_1(i - 1) \exp(-K'(\lambda, T_i) \Delta x) + I_0^\lambda (T_i) (1 - \exp(-K'(\lambda, T_i) \Delta x))$$

The calculations were performed for three different profiles represented in figure 2.

To solve the RTE in 1D, after a study of the independence of the number of cells $i$, we chose to calculate the flux within 50 points (from the left to the right). We calculated the DRF, taking into account the two directions of propagation in all the solid angle.

The results of the DRF are presented in figure 3 for the three temperature profiles.

Figure 2. Temperature profiles used for the resolution of RTE

Figure 3. 1D resolution of RTE for the three temperature profiles

Figure 3 shows that value of DRF reaches its maximal in the axis in the central regions. Near the edges, the absorption is predominating. Three peaks in the absorption part are observed for all three temperature profiles. The first peak corresponds to the absorption of atoms (atomic lines and continuum) at $T=12000K$, the second peak represents the absorption of the molecular lines at $T=10000K$ and the third peak describes the absorption of the molecular continuum at $T=4000K$.

These results are taken as reference for the comparison of approximate methods (NECs, MACs (PMMF), MACs (PMMF)-Optimized). In the following sections, this resolution of RTE is referred as “exact DRF”.

3- Net Emission Coefficient

The NEC is a geometrical simplification that consists in considering plasma as an isothermal homogeneous sphere of radius $R_p$. It describes the divergence of flux for these particular hypotheses.

The NEC was calculated as follows:

$$\varepsilon_N(T, R_p) = \int_0^\infty L_2^\lambda (T) \kappa'(\lambda, T) e^{-\kappa'(\lambda, T) R_p} d\lambda$$

where $\kappa'(\lambda, T)$ is the monochromatic absorption coefficient corrected by the stimulated emission (in m$^{-1}$), $T$ is the local temperature, $L_2^\lambda (T)$ is the Planck function (in W.m$^{-3}$.sr$^{-1}$) and $R_p$ is the radius (in m).

Thanks to the line by line calculation of the absorption spectra, we calculated the NEC for different $R_p$. The figure 4 shows the influence of the radius $R_p$ on the net emission coefficient for air plasma at $P=1$ bar. We calculated the NEC for different $R_p (0, 1, 5$ and $10$mm).
To see the accuracy of this method, we plotted the DRF using NEC with different common Rp used in the literature for the three temperature profiles (see figures 5, 6 and 7).

The formula of the DRF using NEC was obtained as follows:

\[ \nabla F_{\text{NEC}} = 4\pi \varepsilon_N, \]

where \( \nabla F_{\text{NEC}} \) is the DRF using NEC (in W.m\(^{-3}\)) and \( \varepsilon_N \) is the NEC (in W.m\(^{-3}\).sr\(^{-1}\)).

We have compared the DRF using NEC to the exact DRF. To find the ‘best Rp’ we have developed an optimization methodology that leads, in the hottest regions, to the smallest difference between the exact DRF and the DRF calculated from the NEC.

This methodology consists in finding the best Rp that permits to minimize the function \( F'_{\text{NEC}} \) defined in (6). We decided to use Nelder-Mead simplex algorithm [3]. This latter permits only to have a local minimum. To avoid this issue, many random initial Rp are tested until a convergence to a unique ‘best Rp’.

\[ F'_{\text{NEC}}(R_p) = \frac{|\nabla F_{\text{exact}}(x=0) - \nabla F_{\text{NEC-Rp}}(x=0)|}{\nabla F_{\text{exact}}(x=0)}, \]

\( \nabla F_{\text{exact}} \) is the exact DRF and \( \nabla F_{\text{NEC-Rp}} \) is the DRF calculated using NEC with Rp. These two quantities are calculated at X=0.
Figure 7. Comparison of the exact DRF and DRF using NEC for different $R_p$ (3rd temperature profile)

For the profile 1, after the optimization process we obtain $R_p=0.8$ mm. This value represents the radius for which the temperature is equal to 93% of the maximum temperature. We will note this percentage for the rest of the study as $P_R$. Concerning the second temperature profile, we can notice that $R_p=5.6$ mm ($P_R=88\%$) permits to have the nearest DRF using NEC to the exact DRF. For the third temperature profile, $R_p=18$ mm ($P_R=80\%$) is the best to have the closest DRF using NEC to the exact DRF.

Table 1 summarizes the values of $R_p$ and $P_R$ for the three temperature profiles:

| Profile | Best $R_p$ | $P_R$   |
|---------|-----------|---------|
| Profile 1-5 mm | 0.8 mm | 93%     |
| Profile 2-20 mm | 5.6 mm | 88%     |
| Profile 3-50 mm | 18 mm  | 80%     |

We can notice that NEC is a good approximation in central regions where the temperature is maximal when using $R_p$. These values of $R_p$ represent the radius for which the temperature is equal to 80–93% of the maximum temperature depending on the temperature profile. However, this method is not suitable to describe the absorption at low temperatures corresponding to the surrounding regions or the edge of the arc. This comparison confirms that this approximation gives a good overview of the radiative power emitted in the hottest regions of arc plasmas if $R_p$ is well defined.

4- Mean Absorption Coefficient

The NEC method gives an approximation of the radiation from the hot part of the plasma but underestimates the radiation absorption at low temperatures near the edge of the arc. Thus, an alternative radiative property is defined: MAC. The latter is a simplified spectral description based on the splitting of the spectrum into a restricted number of intervals. We have calculated the mean absorption coefficients with the mean functions used in the literature: classic mean function (7), Planck mean function (8), PMMF (9) and Rosseland mean function (10).

\[
\kappa(\lambda, T) = \frac{\int_{\lambda_1}^{\lambda_2} \kappa(\lambda, T) d\lambda}{\int_{\lambda_1}^{\lambda_2} d\lambda}, \quad (7)
\]

\[
\overline{\kappa}(\lambda_1, \lambda_2) = \frac{\int_{\lambda_1}^{\lambda_2} \kappa(\lambda, T) L_e(\lambda, T) d\lambda}{\int_{\lambda_1}^{\lambda_2} L_e(\lambda, T) d\lambda}, \quad (8)
\]
\[ \kappa'([\lambda_i, \lambda_j], T, R) = \frac{\int_{\lambda_i}^{\lambda_j} \kappa(\lambda, T) L_\lambda^0(T) \exp(-\kappa(\lambda, T) R) d\lambda}{\int_{\lambda_i}^{\lambda_j} L_\lambda^0(T) d\lambda}, \] (9)

\[ \kappa''([\lambda_i, \lambda_j], T) = \frac{\int_{\lambda_i}^{\lambda_j} dL_\lambda^0(T) d\lambda}{\int_{\lambda_i}^{\lambda_j} \kappa(\lambda, T) d\lambda}, \] (10)

where \( \kappa' \) represents the MAC (in m\(^{-1}\)) and \( \kappa'(\lambda, T) \) is the monochromatic absorption coefficient (in m\(^{-1}\)) for a wavelength \( \lambda \) and for a temperature \( T \). \([\lambda_i, \lambda_j]\) is the spectral range (in m). \( L_\lambda^0(T) \) is the Planck function (in \( \text{W.m}^{-3}\text{sr}^{-1} \)).

In the figure 8, we have plotted the continuum spectra at different temperatures (12000, 15000 and 20000K). To calculate MACs, we defined the spectral ranges from the behavior of the continuum absorption coefficient. We chose to define 3 spectral ranges as done by Kloc et al. [3].

**Figure 8.** Continuum spectra for different temperature \( T=12000, 15000 \text{ and } 20000K \)

The Table 2 summarizes the spectral ranges used to calculate MACs.

| Band  | \([\lambda_i, \lambda_j]\)            |
|-------|--------------------------------------|
| 1     | \([30 \text{ nm}, 81.5 \text{ nm}]\) |
| 2     | \([81.5 \text{ nm}, 194.67 \text{ nm}]\) |
| 3     | \([194.67 \text{ nm}, 4500 \text{ nm}]\) |

**Table 2.** Spectral ranges used to calculate MACs

Figures 9-11 illustrate the MACs obtained for the different mean functions.

**Figure 9.** MACs calculated with classic mean function

**Figure 10.** MACs calculated with PMMF(1 mm)
To see the accuracy of the MACs, we calculated the DRF deduced from the MACs (PMMF) for different R. Figures 12-14 compare the results with the “exact DRF” for the three temperature profiles.

For the first temperature profile, we can notice that R=1 mm gives a good approximation of the DRF in the hottest region of the plasma. However, using this characteristic absorption length, the DRF in the edge of the arc is not well approximated. In the other hand, R=0.5 mm gives a relatively good description of the absorption for the low temperatures but it over-estimates the radiation losses in the hottest region of the plasma.
For the second temperature profile, R=5 mm gives a good approximation of the radiation losses in the hottest region of the plasma. R=1 mm, in turn, is suitable to describe the DRF in the edges of the plasma. For the third temperature profile, R=10 mm describes well the DRF at hottest regions of the plasma. However, R=0.5 mm gives a better description in the arc edges.

In general, for the three temperature profiles, there is no unique characteristic absorption length R that can describe the radiation losses in both central regions and at the edges of the arc. Consequently, the development of an optimization methodology is necessary to find the best R giving a good approximation of the DRF at both high and low temperature regions.

5-Optimization process

In this section, we present the optimization methodology as shown in figure 15. The characteristic absorption length R is the input parameter for the optimization process. R is defined for each spectral range (i.e. R= [R1 , R2 , R3] in our case). These three values are used to calculate the MACs with the PMMF (9) and the corresponding DRF. We chose to define the objective function (11) as a relative quantity describing the differences between the exact DRF and the DRF using MACs with PMMF for R= [R1, R2, R3] in each point of the plasma. The objective function is based on the DRF in different points of the plasma and is dedicated to applications where the radiative energy in the different areas of the plasma plays a significative role.

The formula for the objective function is:

$$ f(R) = \frac{1}{50} \sum_{i=1}^{50} \frac{|\Delta F_{\text{exact},i} - \Delta F_{\text{MAC},i}(R)|}{|\Delta F_{\text{exact},i}|} $$

where $\Delta F_{\text{exact},i}$ is the exact DRF calculated for the point i and $\Delta F_{\text{MAC},i}$ is the DRF calculated using MACs with PMMF, calculated at the point i. This mean function is calculated using the characteristic absorption length R.

The numerical optimization process is used to find the ‘best’ R= [R1, R2, R3] that allows to minimize the objective function. We decided to use Nelder-Mead simplex algorithm [3]. For the same reason than in the section 3, many random initial R are tested until a convergence to a unique ‘best R= [R1, R2, R3]’.

The best R is called $R_{\text{opt}}$. This optimization process is done for the three temperatures profiles shown in figure 2. Results are presented in figures 16-18.
Figure 16. Comparison of the exact DRF and DRF-MAC with R_{\text{optim}} using 3 intervals (1\textsuperscript{st} temperature profile)

Figure 17. Comparison of the exact DRF and DRF-MAC with R_{\text{optim}} using 3 intervals (2\textsuperscript{nd} temperature profile)

Figure 18. Comparison of the exact DRF and DRF-MAC with R_{\text{optim}} using 3 intervals (3\textsuperscript{rd} temperature profile)

We obtained R_{\text{optim}}= [0.0001, 0.0146, 0.0956 m], R_{\text{optim}}= [0.0002, 0.0217, 0.1000 m] and R_{\text{optim}}= [0.0007, 0.0302, 0.0942 m] for the first, second and third temperature profile respectively.

Table 3. Summary of the values of R_{\text{optim}} and the values F' for each temperature profile

| R_{\text{optim}} | F'(R_{\text{optim}}) |
|------------------|------------------|
| profile 1= [0.0001, 0.0146, 0.0956 m] | 0.27 |
| profile 2= [0.0002, 0.0217, 0.1000 m] | 0.2179 |
| profile 3= [0.0007, 0.0302, 0.0942 m] | 0.29762 |

It can be noticed that the DRF when using R_{\text{optim}} gives better results compared to the unique R in section 4 for the three temperature profiles. However, using Planck MACs with 3 spectral ranges leads to an underestimation of the absorption at the outskirt of the plasma column. The error of the objective function can be decreased by increasing the number of spectral ranges. Indeed, in figure 19 we can see that using R_{\text{optim}} for 6 spectral ranges leads to higher accuracy at the outskirt of the plasma column. In this case, the characteristic absorption length used is R_{\text{optim}}= [0.0004, 0.0011, 0.0532, 0.0986, 0.0062, 0.0980 m] for F'(R_{\text{optim}})=0.08.
The focus of the present study is to highlight the importance of having the best characteristic absorption length, $R$, for each spectral range. The table 4 shows the values of the objective functions when using a unique optimized $R$ (i.e. an optimized $R$ non-dependent on the spectral ranges) for 3 and 6 spectral ranges and for $R_{\text{optim}}= [R_1, R_2, R_3]$. This comparison is done for the second temperature profile.

| $R_{\text{optim}}$               | $F'(R_{\text{optim}})$ |
|-------------------------------|------------------------|
| $R_{\text{optim}}$= 3 spectral ranges=[0.0002, 0.0217, 0.1000 m] | 0.2179                 |
| $R_{\text{optim}}$= 3 spectral ranges=0.0092 m         | 0.56                   |
| $R_{\text{optim}}$= 6 spectral ranges=0.0028 m         | 0.47                   |

It can be noticed that with $R_{\text{optim}}= [R_1, R_2, R_3]$, we have a significant amelioration on the DRF using MAC compared to that using a unique $R_{\text{optim}}= [R, R, R]$. Moreover, having a depending $R$ for each spectral range gives better approximation for 3 spectral ranges than when using a unique optimized $R$ for 6 spectral ranges $R_{\text{optim}}= [R, R, R, R, R]$. From that, we can conclude that a good choice of the characteristic absorption length for each spectral range gives a better approximation of the DRF than when using a unique $R$.

We observe from the results in this section that when using an optimized characteristic absorption length for each spectral range in the case of 3 intervals, an error of 20-30% is observed. The latter is explained by the fact that the approximation using Planck MACs tends to underestimate the absorption at the outskirt of the plasma column. Increasing the number of intervals, while using different absorption length for each spectral range is decreasing this error up to 8% (for 6 spectral ranges).

6-Conclusion

This paper presents the comparison of a 1D exact resolution of RTE and the approximate methods (NEC and MACs) for 3 temperature profiles. An optimization methodology is developed to find the best characteristic absorption length in order to minimize the difference between the ‘exact DRF’ and DRF using MACs (PMMF). In this paper, we chose 3 spectral ranges defined from the continuum. The optimization process allows to find the best 3 characteristic absorption lengths for each spectral range. In comparison with the method of Kloc [3], this work focuses not on choosing optimized spectral ranges, but on defining optimized characteristic absorption length for each spectral range. This approach shows good results. In fact, using a characteristic absorption length for each spectral range gives lower error...
comparing with a unique characteristic absorption length. This error tends to decrease with an increase of the interval numbers. However, the biggest disadvantage of this methodology is the requirement to have already estimated temperature profile.

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