

OBJECTIVE FUNCTION FOR NUMERICAL MEAN ABSORPTION BANDS OPTIMIZATION

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Abstract. Mean absorption coefficients (MACs) offer great potential for fast numerical calculation of radiation heat transfer. They are based on replacing complex absorption coefficient spectrum by a handful of frequency bands with a single, temperature dependent value assigned to each band. Accuracy of radiation transfer calculation thus depends on the accurate interpretation of the mean value inside each frequency band as well as on the proper band distribution. Yet finding optimal band distribution is not an easy task often requiring numerical optimization process. This contribution focuses on the parameters of such optimization process, namely selection of an objective function and its effect on the optimal band distribution. It demonstrates, that improper objective functions can produce physically unreasonable artifacts in the calculation of radiation heat transfer. Optimal formulation of the objective function is proposed in this contribution.

Keywords: mean absorption coefficients, numerical optimization, radiation transfer.

1. Introduction

It is a well known fact, that the temperature inside switching arc plasma can reach tens of thousands of Kelvins. At such high temperature levels, radiation transfer plays a very important role in the total energy balance of the arc. An accurate description of the radiation energy transfer is therefore crucial for any numerical simulation of the switching arc.

Only two radiation quantities are necessary to describe radiation energy transfer in the most cases. The first quantity is the divergence of radiation flux. It describes the energy sink or gain inside the plasma volume and must be incorporated into the plasma energy balance equation [1]. This quantity is therefore important for accurate simulation of a thermal plasma volume. The second quantity is tied to the radiation energy transfer at the outer boundary. Escaping radiation can induce plasma composition changes due to outer walls ablation and different material emission into the plasma volume. The amount of radiation reaching the outer walls is best quantified by the radiation flux quantity.

Fast and accurate evaluation of both radiation quantities is thus required for any reasonable numerical simulation of thermal plasma. Unfortunately, the accurate calculations are very computationally demanding due to a very complex nature of the radiation spectrum. Several approximate solutions were developed through the history, including Net Emission Coefficients (NEC) [2] and Mean Absorption Coefficients (MAC) [3]. The MACs show great promise in simplification of radiation transfer calculations, but require careful handling in order to maintain acceptable accuracy [4]. One possible way for achieving reasonable accuracy is using the numerical optimization of the

frequency bands distribution [5] or even the mean value inside each band itself [6].

The numerical optimization process relies on the so called objective function, i.e. a function, that is searched by a numerical optimization process for the position of minima. In theory, this objective function can be based on any radiation quantity such as radiation flux or divergence of radiation flux. However, due to the complex nature of the radiation transfer inside plasma it is very hard to predict, whether the outcome of the optimization process is independent of the objective function definition or whether different definitions produce unique results. We try to answer this question by a series of tests presented in this contribution.

2. Model

We wanted to keep the radiation model itself as simple as possible. Therefore, we considered infinitely long cylindrical domain with radius of $R = 1$ cm filled with air plasma at the uniform pressure of 1 bar. A fixed predefined temperature profile is imposed on the calculation domain (see Figure 1) to emulate the plasma column inside the domain. The temperature profile is described by the analytical function

$$T(r) = T_{\max} - (T_{\max} - T_{\min}) \frac{1 - e^{-n(\frac{r}{R})^3}}{1 - e^{-n}}, \quad (1)$$

which allows a large variety of different shapes. The following parameters were selected in this particular case to approximately represent a free burning arc: $T_{\min} = 300$ K, $T_{\max} = 25$ kK, $n = 7$.

The divergence of radiation flux as well as the radiation flux itself were evaluated in 50 points along the

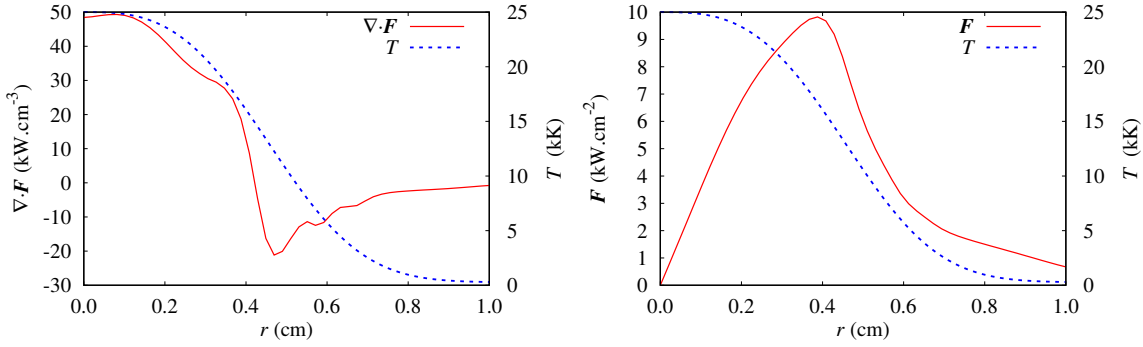


Figure 1. Divergence of radiation flux (left) and radiation flux (right) along the radius of infinitely long cylindrical domain with fixed temperature profile.

58 cylinder radius (see Figure 1) using a model and material
 59 data taken from [7]. Both profiles were calculated
 60 using a full spectral resolution of absorption coefficient
 61 (an example of absorption coefficient spectrum
 62 is in Figure 2) and are referred to as *spectral* solutions
 63 through the text or *sp* subscript in equations. The
 64 spectral solution serves two purposes. Firstly, it is
 65 used to evaluate the accuracy of the approximate solution
 66 described in the following paragraph and secondly
 67 it is used for definition of the numerical optimization
 68 objective function.

69 In the subsequent step we used a numerical optimization
 70 procedure [8] to calculate the optimal band distribution
 71 for three-band Planck mean absorption coefficients. The
 72 process is similar to the one described in [5]. We used
 73 line limiting factor proposed by Nordborg [9] with
 74 characteristic plasma length set to 1.5 cm to mitigate
 75 the known overestimation of atomic lines by Planck
 76 mean absorption coefficient. By employing only three
 77 frequency bands we were able to characterize the final
 78 band distribution by just two parameters ν_1 and ν_2 ,
 79 which define the boundaries between the bands. The
 80 outer boundaries are fixed at 10^{12} Hz and 10^{16} Hz
 81 for lower and higher limit respectively.
 82

We defined an universal numerical optimization
 objective function to test the effect of several different
 radiation quantities on the mean absorption band
 distribution. The objective function is written as

$$\Delta f(\nu_1, \nu_2) = \sqrt{\sum_{i=1}^{50} A_i^2 (\nabla \cdot \mathbf{F}_i - \nabla \cdot \mathbf{F}_{i,sp})^2} + \sqrt{\sum_{i=1}^{50} B_i^2 (\mathbf{F}_i - \mathbf{F}_{i,sp})^2} + \sqrt{\sum_{i=1}^{50} C_i^2 (G_i - G_{i,sp})^2}, \quad (2)$$

where the summation is carried over all the 50 spatial
 points in which the spectral properties were resolved

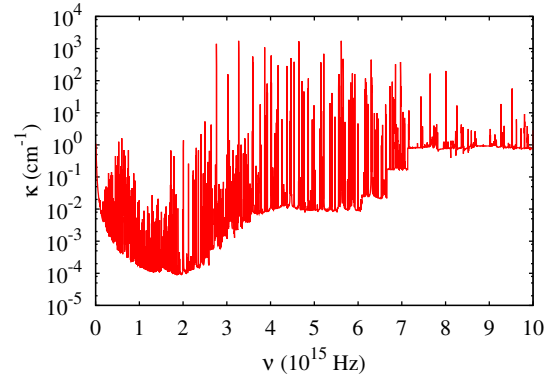


Figure 2. Absorption coefficient of air at 25 kK.

and G_i is the incident radiation defined as

$$G_i = \int_0^\infty \int_{4\pi} I(r_i, \nu) d\Omega d\nu \quad (3)$$

with $I(r_i, \nu)$ representing radiation intensity at point
 r_i and frequency ν . The variables A_i , B_i and C_i
 are used to modify the objective function according to
 our needs. In total we calculated eight series of numerical
 optimization procedure, each series containing minimum of
 3 optimization attempts to verify the convergence
 repeatability. Finally, we evaluated the accuracy of
 radiation flux and divergence of radiation flux calculated
 with the optimized three-band mean absorption model by
 comparing the profiles with the spectral solution.

3. Results

Even though the numerical optimization procedure can
 operate with any arbitrary value of a objective function,
 it is often advantageous to limit the objective function
 to the interval between 0 and 1. To do so, the definition
 of objective function often rely on the maximum value
 of the appropriate quantity. In such case, this maximum
 value is denoted by additional subscript *max* in the text.

Four distinct objective functions were tested in total
 with each test being described in more details in the

following subsections. Generally, we expected all the tested objective functions to perform quite similarly, but the results show quite different picture.

3.1. Divergence of radiation flux

The objective function is represented only by divergence of radiation flux in case of $A_i = 1/\nabla \cdot \mathbf{F}_{\text{sp,max}}$, $B_i = 0$ and $C_i = 0$. With this definition the focus is mainly on the areas where the divergence of radiation flux exhibits high absolute value. The areas on the outskirts of the cylinder as well as the position of the transition between emitting and absorbing regions are considered with lesser significance, thus some degree of deviation can be expected.

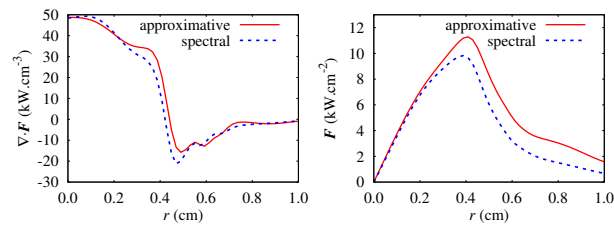


Figure 3. Divergence of radiation flux (left) and radiation flux (right) profiles evaluated by the objective function based upon divergence of radiation flux only.

The calculated optimal band boundaries were found at frequencies $\nu_1 = 2.7591 \cdot 10^{15}$ Hz and $\nu_2 = 3.5528 \cdot 10^{15}$ Hz with corresponding profiles of radiation flux and divergence of radiation flux are shown in Figure 3. One can clearly see, that the divergence of radiation flux is relatively well approximated. Only the position of transition from emitting region to the absorbing one is slightly shifted and the absorption is underestimated by approximately 20%. However, this inaccuracy is large enough to cause the difference by the factor of 2 in the radiation flux at the domain boundary.

3.2. Radiation flux

One obvious way to improve the radiation flux accuracy is to use the radiation flux itself as the accuracy evaluating quantity. This can be achieved in our test objective function by defining the variables $A_i = 0$, $B_i = 1/F_{\text{sp,max}}$ and $C_i = 0$. This objective function emphasize the area with high values of the flux around $r = 0.4$ cm with lesser focus on the central areas.

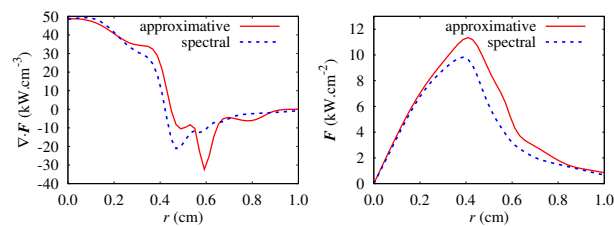


Figure 4. Divergence of radiation flux (left) and radiation flux (right) profiles evaluated by the objective function based upon radiation flux only.

The optimal band distribution differs significantly from the previous test case. The band boundaries are now located at $\nu_1 = 2.3965 \cdot 10^{15}$ Hz and $\nu_2 = 3.0232 \cdot 10^{15}$ Hz. The impact of the changed band boundaries is visible in Figure 4, where the radiation flux profile is quite improved and matches the spectral profile much closer. Especially the value at the domain boundary is resolved quite accurately with the error less than 20%. Unfortunately this improvement was not achieved by improving the divergence of radiation flux profile. An arbitrary absorption area is created around $r = 0.6$ cm which is responsible for the improvements in the radiation flux profile. Consequently, using these band boundaries would lead to the incorrect evaluation of the energy balance inside plasma.

3.3. Incident radiation

Incident radiation represent another tempting option for objective function. Unlike the previous quantities, incident radiation profile never reaches zero value making its impact more uniform across the calculation domain. In our test objective function we can achieve the pure incident radiation evaluation by setting variables $A_i = 0$, $B_i = 0$ and $C_i = 1/G_{\text{sp,max}}$. Maximum of incident radiation $G_{\text{sp,max}}$ is located at the cylindrical domain axis.

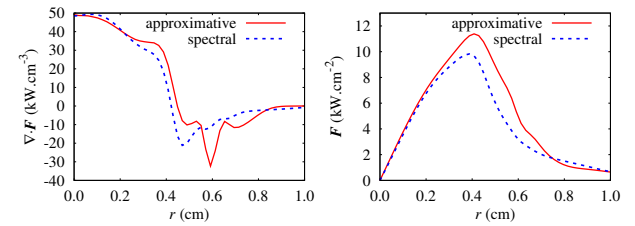


Figure 5. Divergence of radiation flux (left) and radiation flux (right) profiles evaluated by the objective function based upon incident radiation only.

Even though the incident radiation seems like good candidate for radiation objective function, its performance is inferior to the previous cases. The best band distribution band boundaries are located at $\nu_1 = 2.0123 \cdot 10^{15}$ Hz and $\nu_2 = 3.0404 \cdot 10^{15}$ Hz with corresponding divergence of radiation flux and radiation flux profiles captured in Figure 5. The results are quite similar to those obtained with objective function based upon radiation flux. Direct comparison reveals that the absorption part is even more overestimated in the case of incident radiation. This is clearly documented on the radiation flux profile where the approximate mean absorption coefficients solution reaches below the spectral solution in area close to the domain boundary.

3.4. Weighted linear combination

All the previous objective function were based on a single radiation quantity only. However, in many cases the results did not satisfy all the expectations. Each one improved the related quantity, usually at the cost

of decreased accuracy in other quantities. The appar-
 ent room for improvement is an inclusion of multiple
 radiation quantities into the objective function. This
 can be easily achieved with our definition of the ob-
 jective function by properly modifying the variables
 A_i , B_i and C_i .

For this particular test, we decided to focus on
 the most impactful quantities only. Therefore we
 used the following definition: $A_i = 1/\nabla \cdot \mathbf{F}_{\text{sp,max}}$,
 $B_i = 1/F_{\text{sp,max}}$ and $C_i = 0$, which ensures, that both
 radiation flux and divergence of radiation flux are
 equally weighted in the objective function. It might
 be advantageous to focus on one of the quantity in
 the real scenario, but for this test the equal balance
 is more desired.

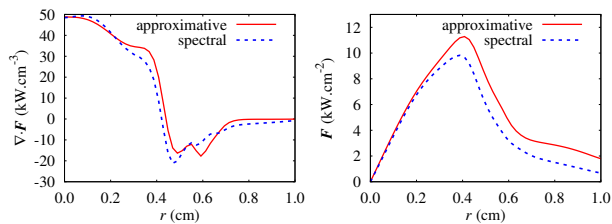


Figure 6. Divergence of radiation flux (left) and radiation flux (right) profiles evaluated by the objective function based upon weighted linear combination of radiation flux and divergence of radiation flux.

The linear combination distribution function results in frequency band distribution similar to the first test case based purely on the divergence of radiation flux. The band boundaries are located at $\nu_1 = 2.9146 \cdot 10^{15}$ Hz and $\nu_2 = 3.5528 \cdot 10^{15}$ Hz with the corresponding approximate profiles shown in Figure 6. The approximate divergence of radiation flux still exhibits some arbitrary absorption areas, but the discrepancy is far smaller than in the case of pure radiation flux objective function. Unfortunately, this does not lead to the significant improvement in the radiation flux at the domain boundary. Rather the radiation flux is improved in the area around $r = 0.7$ cm. The linear objective function therefore seems to be useful in the case when the domain is relatively small and the outer walls are close to the plasma boundary.

4. Conclusions

In this contribution we tested several different objective functions for numerical optimization of mean absorption coefficients frequency band distributions. The obtained results clearly indicate the importance of proper formulation of the objective function. The optimized mean absorption coefficients can establish an artificial absorption area without careful handling of the objective function. On the other hand, the impact of the objective function formulation is minimal in the central parts of the plasma column.

We propose the objective function based upon divergence of radiation flux to be used for numerical optimization, since the radiation source term is important

for the plasma energy balance equation. Although, linear combination of radiation flux and divergence of radiation flux can be useful for cases, where the correct evaluation of radiation energy transfer to the outer walls plays critical role or the outer walls are close to the plasma boundaries.

We would like to note, that our conclusion is based on the limited number of tests. Only one temperature profile with a single plasma composition was considered in the tests. More test are required for broader applicability assessment of our conclusions.

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