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.

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 ${\bf Keywords:} \ {\rm mean} \ {\rm absorption} \ {\rm coefficients}, \ {\rm numerical} \ {\rm optimization}, \ {\rm radiation} \ {\rm transfer}.$

1 **1. Introduction**

It is a well known fact, that the temperature inside ³⁷
switching arc plasma can reach tens of thousands of ³⁸
Kelvins. At such high temperature levels, radiation ³⁹
transfer plays a very important role in the total energy ⁴⁰
balance of the arc. An accurate description of the ⁴¹
radiation energy transfer is therefore crucial for any ⁴²

⁸ numerical simulation of the switching arc.

Only two radiation quantities are necessary to de-⁴⁴ q 45 scribe radiation energy transfer in the most cases. The 10 46 first quantity is the divergence of radiation flux. It 11 47 describes the energy sink or gain inside the plasma 12 48 volume and must be incorporated into the plasma en-13 49 ergy balance equation [1]. This quantity is therefore 14 50 important for accurate simulation of a thermal plasma 15 volume. The second quantity is tied to the radiation 16 energy transfer at the outer boundary. Escaping radi-51 17 ation can induce plasma composition changes due to 18 outer walls ablation and different material emission 19 into the plasma volume. The amount of radiation 20 reaching the outer walls is best quantified by the ra-21 diation flux quantity. 22

Fast and accurate evaluation of both radiation quan-23 tities is thus required for any reasonable numerical 24 simulation of thermal plasma. Unfortunately, the accu-25 rate calculations are very computationally demanding 26 due to a very complex nature of the radiation spec-27 trum. Several approximate solutions were developed 28 through the history, including Net Emission Coeffi-29 cients (NEC) [2] and Mean Absorption Coefficients 52 30 (MAC) [3]. The MACs show great promise in simplifi- 53 31 cation of radiation transfer calculations, but require 54 32 careful handling in order to maintain acceptable ac- 55 33 curacy [4]. One possible way for achieving reasonable 56 34 accuracy is using the numerical optimization of the 57 35

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

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

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

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.

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

In the subsequent step we used a numerical opti-69 mization procedure [8] to calculate the optimal band 70 distribution for three-band Planck mean absorption 71 coefficients. The process is similar to the one de-72 scribed in [5]. We used line limiting factor proposed 73 by Nordborg [9] with characteristic plasma length set 74 to 1.5 cm to mitigate the known overestimation of 75 atomic lines by Planck mean absorption coefficient. 76 By employing only three frequency bands we were 77 able to characterize the final band distribution by just 78 83 two parameters ν_1 and ν_2 , which define the bound-79 aries between the bands. The outer boundaries are $_{85}$ 80 fixed at 10^{12} Hz and 10^{16} Hz for lower and higher limit $_{86}$ 81 respectively. 82

88 We defined an universal numerical optimization 89 objective function to test the effect of several different 90 radiation quantities on the mean absorption band distribution. The objective function is written as

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

$$+\sqrt{\sum_{i=1}^{100}C_{i}^{2}\left(G_{i}-G_{i,\mathrm{sp}}\right)^{2}},$$
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¹⁰¹

where the summation is carried over all the 50 spatial 103 points in which the spectral properties were resolved 104



Figure 2. Absorption coefficient of air at 25 kK.

and G_i is the incident radiation defined as

$$G_i = \int_{0}^{\infty} \int_{4\pi}^{\infty} I(r_i, \nu) \mathrm{d}\Omega \,\mathrm{d}\nu \tag{3}$$

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

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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 ¹³⁷
tested objective functions to perform quite similarly, ¹³⁸
but the results show quite different picture. ¹³⁹

¹⁰⁸ 3.1. Divergence of radiation flux

142 The objective function is represented only by diver-109 143 gence of radiation flux in case of $A_i = 1/\nabla \cdot \mathbf{F}_{\text{sp,max}}, \frac{1}{144}$ 110 $B_i = 0$ and $C_i = 0$. With this definition the focus is 111 145 mainly on the areas where the divergence of radiation 112 flux exhibits high absolute value. The areas on the 113 147 outskirts of the cylinder as well as the position of the $_{_{148}}$ 114 transition between emitting and absorbing regions are $\frac{149}{149}$ 115 considered with lesser significance, thus some degree $\frac{1}{150}$ 116 of deviation can be expected. 117 151



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 118 at frequencies $\nu_1 = 2.7591 \cdot 10^{15} \text{ Hz}$ and $\nu_2 = 3.5528 \cdot 10^{15} \text{ Hz}$ 119 10^{15} Hz with corresponding profiles of radiation flux 120 and divergence of radiation flux are shown in Figure 3. 121 One can clearly see, that the divergence of radiation 122 flux is relatively well approximated. Only the position 123 of transition from emitting region to the absorbing one 124 is slightly shifted and the absorption is underestimated 125 by approximately 20%. However, this inaccuracy is 126 large enough to cause the difference by the factor of 2 127 in the radiation flux at the domain boundary. 128

129 **3.2. Radiation flux**

164 One obvious way to improve the radiation flux accu-130 racy is to use the radiation flux itself as the accuracy 131 166 evaluating quantity. This can be achieved in our test 132 objective function by defining the variables $A_i = 0$, $\frac{10}{168}$ 133 $B_i = 1/F_{\rm sp,max}$ and $C_i = 0$. This objective function 134 169 emphasize the area with high values of the flux around 135 170 $r = 0.4 \,\mathrm{cm}$ with lesser focus on the central areas. 136 171



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

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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- 227 182 ent room for improvement is an inclusion of multiple 228 183 radiation quantities into the objective function. This 229 184 can be easily achieved with our definition of the ob- 230 185 jective function by properly modifying the variables 231 186 A_i, B_i and C_i . 232 187

For this particular test, we decided to focus on 233 188 the most impactful quantities only. Therefore we ${}_{\rm 234}$ 189 used the following definition: $A_i = 1/\nabla \cdot \mathbf{F}_{\text{sp.max}}, ^{235}$ 190 $B_i = 1/F_{\text{sp.max}}$ and $C_i = 0$, which ensures, that both 236 191 radiation flux and divergence of radiation flux are 237 192 equally weighted in the objective function. It might 193 be advantageous to focus on one of the quantity in $^{\rm 238}$

194 the real scenario, but for this test the equal balance ²³⁹ 195 is more desired. 240 196



Figure 6. Divergence of radiation flux (left) and ra-249 diation flux (right) profiles evaluated by the objective function based upon weighted linear combination of 251 radiation flux and divergence of radiation flux.

The linear combination distribution function re- $^{\rm 254}$ 197 sults in frequency band distribution similar to the ²⁵⁵ 198 first test case based purely on the divergence of ra- $^{\rm 256}$ 199 diation flux. The band boundaries are located at ²⁵⁷ 200 258 $\nu_1 = 2.9146 \cdot 10^{15} \,\text{Hz}$ and $\nu_2 = 3.5528 \cdot 10^{15} \,\text{Hz}$ with 201 the corresponding approximate profiles shown in Fig-202 ure 6. The approximate divergence of radiation flux ²⁶⁰ 203 still exhibits some arbitrary absorption areas, but the $\frac{1}{262}$ 204 discrepancy is far smaller than in the case of pure $\frac{1}{263}$ 205 radiation flux objective function. Unfortunately, this 206 does not lead to the significant improvement in the $_{265}$ 207 radiation flux at the domain boundary. Rather the ra- $_{266}$ 208 diation flux is improved in the area around r = 0.7 cm. ₂₆₇ 209 The linear objective function therefore seems to be $_{268}$ 210 useful in the case when the domain is relatively small $_{269}$ 211 and the outer walls are close to the plasma boundary. 270 212

4. Conclusions 213

In this contribution we tested several different ob- $^{\rm 273}$ 214 jective functions for numerical optimization of mean $^{\rm 274}$ 215 275 absorption coefficients frequency band distributions. 216 The obtained results clearly indicate the importance $_{277}$ 217 of proper formulation of the objective function. The 218 278 optimized mean absorption coefficients can establish $_{279}$ 219 an artificial absorption area without careful handling $_{\scriptscriptstyle 280}$ 220 of the objective function. On the other hand, the im- $_{\scriptscriptstyle 281}$ 221 pact of the objective function formulation is minimal 282 222 in the central parts of the plasma column. 223 283

We propose the objective function based upon diver- 284 224 gence of radiation flux to be used for numerical opti-285 225 mization, since the radiation source term is important ²⁸⁶ 226

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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