



encit 2020



18th Brazilian Congress of Thermal Sciences and Engineering
November 16–20, 2020 (Online)

ENC-2020-0269

A WIDE-BAND FORMULATION BASED ON THE GRAY GAS MODEL APPLIED TO NON-ISOTHERMAL AND HOMOGENEOUS WATER VAPOR MEDIA

Roberta Juliana Collet da Fonseca

Guilherme Crivelli Fraga

Francis Henrique Ramos Franca

Department of Mechanical Engineering, Federal University of Rio Grande do Sul, 425 Sarmiento Leite St., Porto Alegre, Brazil

roberta.fonseca@ufrgs.br

guilhermecfraga@ufrgs.br

frfranca@mecanica.ufrgs.br

Abstract. Modeling thermal radiation in participating gases is a complex task due to the highly irregular behavior of the absorption coefficient with the wavenumber, principally at elevated temperatures. In this framework, simple spectral models, such as the gray gas (GG) model, have received much attention for presenting an alternative to the spectral integration of the radiative transfer equation (RTE) with low computational effort. This paper proposes a methodology that aims to improve the GG model by dividing the spectrum into a set of intervals for which individual absorption coefficients are determined. The RTE is solved for each spectral interval separately using the GG approach and the total quantities are obtained by the summation of the contributions in each one of these segments. The obtainment of each set of coefficients is based on curve adjustments of the Planck-mean absorption coefficients from data extracted from the HITEMP2010 database. To test the methodology, absorption coefficients for water vapor are determined for each selected band. The accuracy of the resulting model is assessed for radiative transfer calculations in a one-dimensional homogeneous, non-isothermal medium slab bounded by black walls. Results are compared with those obtained employing other GG coefficients of the literature and the LBL solution.

Keywords: thermal radiation, Planck-mean absorption coefficient, gray gas model, line-by-line integration, spectral intervals

1. INTRODUCTION

The radiative heat transfer plays an important role in high temperatures applications, such as in combustion chambers and steam generation. In these combustion systems, the thermal radiation tends to be the dominant heat transfer due to the presence of soot and participating gases, and correctly describing the radiative properties of a gas in these scenarios is an arduous task, since the strong spectral dependence on the variables involved makes it difficult to obtain accurate results.

The determination of the radiative properties of a participating medium is a particularly challenging task, since, besides depending on the local temperature, species concentrations and pressure, they also can vary greatly with the radiation wavenumber. The spectral part of the problem can be accurately calculated through line-by-line (LBL) integration (Taine, 1983) by means of data from high-resolution spectroscopic databases, such as HITEMP (Rothman *et al.*, 2010) and HITRAN (Rothman *et al.*, 2013), taking into account the emission and absorption characteristics of each spectral line. Nevertheless, due to the large amount of lines that compose the radiation spectrum, this methodology requires a high computational effort, which can make this solution impracticable. As an alternative, global spectral models have been developed over the years, as a way to circumvent these difficulties.

One of the simplest spectral models is the gray gas (GG) model, in which the absorption coefficient of the medium is assumed to be independent of the radiation wavenumber. Despite its simplicity, the GG model has been applied in recent combustion studies (Crnomarkovic *et al.*, 2013; Fraga *et al.*, 2017, 2019a,b) and it is known for presenting good results in media where the concentration of soot is elevated (Mossi *et al.*, 2012; Cassol *et al.*, 2015). Among some of the global models, there are the weighted-sum-of-gray-gases (WSGG) model (Hottel and Sarofim, 1967), which replaces the spectrum of radiation by a few number of gray gases with uniform absorption coefficients and transparent windows, and the spectral line-based WSGG (SLW) model (Denison and Webb, 1993), in which the absorption-line blackbody distribution functions (ALBDF) are used to calculate weighting factors of the gray gases, which usually gives to this method a higher level of accuracy compared to the first one.

In the present paper, the radiative transfer calculation of a participating gas confined in a one-dimensional system

bounded by black walls is investigated. The wavenumber spectrum is divided into a set of regions and the GG model is applied to each one of these segments to determine the Planck-mean absorption coefficients. The chemical species under study is pure water vapor with a uniform molar concentration. This is the first time that such methodology has been applied and tested, as far as the authors know. The results found with the proposed model are compared with other correlations of the literature and the LBL benchmark solution.

2. RADIATION MODELING

The radiative transfer equation (RTE) represents an energy balance that accounts the variation intensity considering the absorption, emission and scattering contributions along a path s . Neglecting the scattering effects, the RTE is calculated as (Modest, 2013; Howell *et al.*, 2016)

$$\frac{dI_\eta}{ds} = -\kappa_\eta I_\eta + \kappa_\eta I_{b\eta}, \quad (1)$$

where η is the wavenumber, I_η is the spectral radiation intensity, s is the spatial coordinate along the path of radiation, κ_η is the spectral absorption coefficient of the medium and $I_{b\eta}$ is the blackbody spectral radiation intensity.

2.1 The standard gray gas model

The global solution of the RTE requires the spatial and spectral integrations of Eq. (1). The spectral part of the radiative transfer problem studied in this paper is resolved with the GG model. In this method, the radiative properties — more specifically, the absorption coefficient of the medium — are assumed independent of the wavenumber. Therefore, the spectral dependence of the RTE can be eliminated, so that Eq. (1) can be rewritten as:

$$\frac{dI}{ds} = -\kappa I + \kappa I_b, \quad (2)$$

in which κ is the absorption coefficient of the participating medium, $I = \int_0^\infty I_\eta d\eta$ is the total radiative intensity and $I_b = \int_0^\infty I_{b\eta} d\eta$ is the total blackbody radiative intensity.

For combustion calculations, the use of mean absorption coefficients that are averaged over some or all of the radiation spectrum (Howell *et al.*, 2016) is convenient. Absorption coefficients can be determined in many ways; between them, a useful alternative is to employ the Planck-mean absorption coefficient (Modest, 2013)

$$\kappa = \frac{\int_\eta \kappa_\eta I_{b\eta} d\eta}{\int_\eta I_{b\eta} d\eta}, \quad (3)$$

where the absorption coefficient is determined by an emission-based average along the spectrum. Kaminski *et al.*, 1995, Zhang and Modest, 2002, and Wakatsuki *et al.*, 2008, determined Planck-mean absorption coefficients for gaseous species such as water vapor and carbon dioxide from the HITRAN and HITEMP databases. Although this formulation is simple compared to other spectral models due to its assumption for calculating the absorption coefficient, the GG model is widely used in combustion studies involving soot and participating gases (Liu *et al.*, 1998; Crnomarkovic *et al.*, 2013; Cassol *et al.*, 2015; Fraga *et al.*, 2019a).

Equation (3) is a useful approach, because it expresses the absorption coefficient as a function of temperature and gas concentration. Cassol *et al.*, 2015, provided one of the most up-to-date correlations for κ obtained through the HITEMP2010 database for H₂O, CO₂ and soot. Its values are computed by the following correlation

$$\kappa = p_a \sum_{i=0}^5 C_i T^i, \quad (4)$$

in which p_a is the partial pressure of the gas, T is the local temperature and C_i are the coefficients of this correlation, whose values are given in Table 1.

Assuming a 1D-medium slab bounded by two black walls and an arbitrary direction l , the boundary conditions in the framework of the discrete ordinates method (DOM) for Eq. (2) are expressed as $I_{l,x=0}^+ = I_{b,x=0}$ and $I_{l,x=L}^- = I_{b,x=L}$, where $I_l^+(x)$ and $I_l^-(x)$ are the intensities in the forward and backward directions, respectively, and $x = 0$ and $x = L$ represent the left and right boundaries of the domain. After solving the positive and negative intensities, the total radiative heat flux, q_r ,

Table 1. Absorption coefficients for H₂O for the GG model proposed by Cassol *et al.*, 2015, Eq. (4).

	Magnitude
$C_0(\text{m}^{-1} \text{atm}^{-1})$	7.5702×10^1
$C_1(\text{m}^{-1} \text{atm}^{-1} \text{K}^{-1})$	-1.9716×10^{-1}
$C_2(\text{m}^{-1} \text{atm}^{-1} \text{K}^{-2})$	2.1998×10^{-4}
$C_3(\text{m}^{-1} \text{atm}^{-1} \text{K}^{-3})$	-1.2492×10^{-7}
$C_4(\text{m}^{-1} \text{atm}^{-1} \text{K}^{-4})$	3.5385×10^{-11}
$C_5(\text{m}^{-1} \text{atm}^{-1} \text{K}^{-5})$	-3.9663×10^{-15}

and the total radiative heat source, S_r , again for the DOM, are given by the equations below:

$$q_r(x) = \sum_{l=1}^{n_d} 2\pi\mu_l\omega_l[I_l^+(x) - I_l^-(x)] \quad (5)$$

$$S_r(x) = \sum_{l=1}^{n_d} 2\pi\omega_l\kappa(x)[I_l^+(x) + I_l^-(x)] - 4\pi\kappa(x)I_b(x), \quad (6)$$

where μ_l and ω_l are, respectively, the cosine and the quadrature weight for direction l , and n_d is the number of directions employed in the angular integration of the RTE.

2.2 The proposed gray gas model

A new approach is proposed for the GG model in the present paper. This approach seeks to improve the standard GG model through refinement the method by the division of the radiation spectrum into several spectral intervals $\Delta\eta_j$. For each of these regions, the GG model is applied, so that the total result will be given by the summation of the contributions from each of the segments.

In this framework, the RTE, the boundary conditions and the radiative heat source equations have to be modified. Since the spectrum is divided into $\Delta\eta_j$ spectral intervals, the GG model is applied to each of these regions by accounting for the fraction of blackbody energy emitted in each band. Thus, for a band j , Eq. (2) becomes:

$$\frac{dI_j}{ds} = -\kappa_j I_j + \kappa_j f_j I_{b,j}, \quad (7)$$

in which f_j is the fraction of the blackbody energy emitted in the spectral interval $\Delta\eta_j$ and that is given by

$$f_j = \frac{\int_{\Delta\eta_j} I_{b\eta} d\eta}{I_b}, \quad (8)$$

which can be computed from Planck's distribution (Modest, 2013; Howell *et al.*, 2016).

Analogously to Eq. (7), the boundary conditions also have to be modified in order to include the term that accounts the fraction of blackbody energy that emanates from each spectral interval $\Delta\eta_j$: $I_{l,x=0}^+ = f_{j,x=0} I_{b,x=0}$ and $I_{l,x=L}^- = f_{j,x=L} I_{b,x=L}$. After solving these intensities, Eqs. (5) and (6) become:

$$q_r(x) = \sum_{l=1}^{n_d} \sum_{j=1}^{n_b} 2\pi\mu_l\omega_l[I_{l,j}^+(x) - I_{l,j}^-(x)] \quad (9)$$

$$S_r(x) = \sum_{l=1}^{n_d} \sum_{j=1}^{n_b} 2\pi\omega_l\kappa_j(x)[I_{l,j}^+(x) + I_{l,j}^-(x)] - 4\pi\kappa_j(x)f_j I_{b,j}(x), \quad (10)$$

in which n_b is the number of intervals in which the spectrum is divided. One can observe that, in the case of Eq. (9), the inclusion of the term f_j is not necessary, since the total blackbody intensity does not appear in the standard expression of q_r , so that Eq. (9) is analogous to Eq. (5), except that a summation is made over all the intervals in which the spectrum is partitioned. However, for the radiative heat source, it is required to multiply I_b by the fraction of blackbody energy emitted in each spectral interval.

2.3 Solution methodology

The results discussed in this study are presented in terms of the radiative heat flux and the radiative heat source, through comparisons between the proposed methodology and correlations for the GG model available in the literature with the LBL benchmark solution. The problem under study is the heat transfer by thermal radiation in a 1D medium system consisting of two infinite parallel black plates separated by a distance of $L = 1$ m, containing a participating medium between them, as is shown in Fig. 1. The region between the plates is filled by a homogeneous concentration of pure H_2O , with molar fraction equal to $Y = 0.2$ and with a total pressure $p = 1$ atm. The RTE is solved using the discrete ordinates method (Howell *et al.*, 2016) for 8 ordinates and adopting the set of weights and directional cosines proposed in Lathrop and Carlson, 1964, with the computational domain discretized in 200 equal-sized cells. Separate analyses showed that further refinements of the spatial and angular discretizations did not significantly affect the results.

To evaluate the proposed methodology, two temperature profiles are tested, according to the following equations:

$$T(\hat{x}) = 400 + 1400 \sin^2(2\pi\hat{x}) \quad (11)$$

$$T(\hat{x}) = \begin{cases} 880 + 920 \sin^2(2\pi\hat{x}), & \text{if } \hat{x} \leq 0.25 \\ 400 + 1400 \left\{ 1 - \sin^{3/2}[2\pi/3(\hat{x} - 0.25)] \right\}, & \text{if } \hat{x} > 0.25 \end{cases} \quad (12)$$

in which $\hat{x} = x/L$ is the dimensionless distance from the left plate. Equation (11) (referred to Profile 1) represents a profile with double symmetry, with the medium temperature having an average of 1100 K and reaching the maximum value of 1800 K in $\hat{x} = 0.25$ and $\hat{x} = 0.75$; the temperatures of the two walls are 400 K. In Eq. (12) (referred to Profile 2), the temperature in the medium rises from 880 K at the left wall ($\hat{x} = 0$) to a maximum value of 1800 K at $\hat{x} = 0.25$, then decreases to 400 K at the right wall ($\hat{x} = 1$), and the average temperature of the medium is also 1100 K, as in the previous case. The left-hand side of Fig. 2 presents the behavior of these temperature profiles.

Since the proposed method consists of dividing the entire spectrum into a series of intervals, the calculation of the absorption coefficient for each band is required. For this reason, a modification in Eq. (3) is necessary, since the fraction of blackbody energy emitted in each spectral interval has to be determined. Thus, the value of κ for a band j is given by:

$$\kappa_j = \frac{\int_{\Delta\eta_j} \kappa_\eta I_{b\eta} d\eta}{f_j I_{b,j}}, \quad (13)$$

where f_j is the fraction of blackbody emission from the spectral interval $\Delta\eta_j$ and is computed by Eq. (8). The right-side of Fig. 2 shows the absorption coefficient of a participating gas for the LBL and GG approaches within a single interval $\Delta\eta_j$. According to this figure, one can easily see the difference between the solutions: while the absorption coefficient of the gas obtained with the LBL integration presents thousands of spectral lines in a small range of wavenumber, the GG model assumes a single value for κ in this same segment of the spectrum. This simplicity of the GG model in the treatment of the absorption coefficient of the gas justifies the attention given to this method in the solution of radiative problems in participating media.

To evaluate the performance of the present methodology, the results obtained in the next section are compared with those found through the correlation of Eq. (4) proposed by Cassol *et al.*, 2015, presented in Table 1. For this study, the absorption spectra required to solve the LBL integration are generated from the HITEMP2010 database for a wavenumber range $0 \text{ cm}^{-1} < \eta < 10\,000 \text{ cm}^{-1}$, with the radiation spectrum divided into 150 000 elements and a spectral resolution of 0.067 cm^{-1} . The spectral data are obtained for temperatures between 400 K and 2500 K, with steps of 100 K, resulting in 22 temperatures in the range adopted; for calculations outside this temperature range, a linear interpolation is applied, which is consistent with the literature (André and Vaillon, 2010).

3. RESULTS AND DISCUSSION

The values of the Planck-mean absorption coefficients for each spectral interval are obtained through an in-house Fortran code, which calculates the magnitudes of κ from HITEMP2010 database. The division of the spectrum is based on the

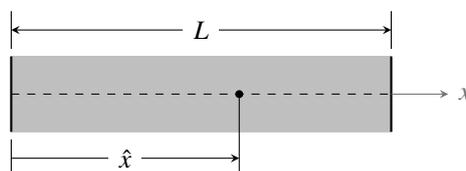


Figure 1. Geometric representation of the one-dimensional problem.

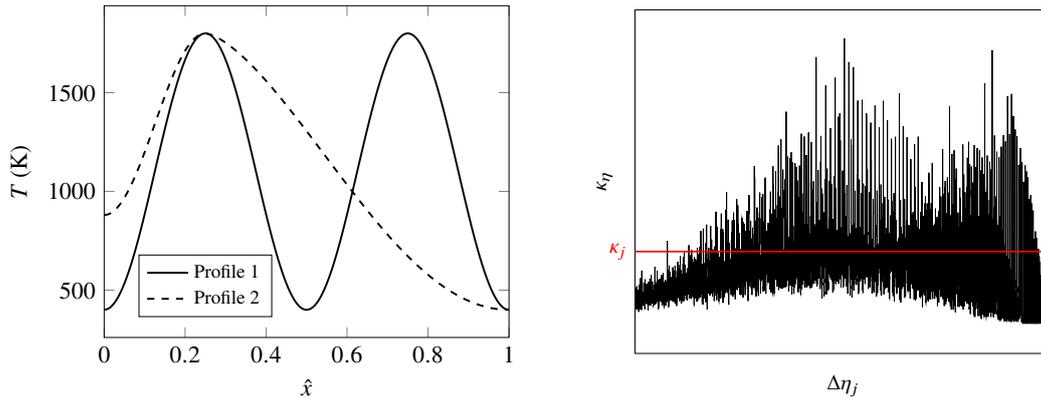


Figure 2. On the left: Temperature profiles given by Eqs. (11) and (12). On the right: Schematic representation of the absorption coefficient of a participating gas for an arbitrary interval $\Delta\eta_j$ — black lines: LBL solution; red line: GG model.

methodology of Marin and Buckius, 1998, who developed correlations for the study of wide-bands models using LBL data. In the aforementioned paper, the authors proposed five spectral intervals for water vapor, a criterion that is employed in the first part of this work. In a second phase, the proposed formulation is applied to ten spectral intervals and the behavior of the solution is evaluated. The results of both approaches are presented in the following sections.

3.1 The GG model applied to five spectral intervals

Based on the absorption spectra of the H_2O generated from the HITEMP2010, the fit of κ for each spectral interval in the range of 400 K to 2500 K is carried out on the software Statistical Package for the Social Sciences (SPSS) 18 (IBM, 2016) through non-linear adjustments. For an initial analysis, the parameters obtained are based on the correlation of Eq. (4), but for a fixed pressure partial of 0.2 atm, and the wavenumber spectrum is divided into five regions, following the criterion proposed in Marin and Buckius, 1998. Thus, for each band j , the absorption coefficient is calculated as

$$\kappa_j = \sum_{i=0}^5 C_i T^i. \quad (14)$$

The parameters of the above equation represent the curve adjustments for the five intervals in which the radiation spectrum was divided are presented in Table 2. According to Eq. (14), each spectral interval presents six parameters that have to be determined. Figure 3 shows the behavior of κ for each spectral interval investigated: the markers indicate the benchmark solution are the solid lines represent the GG model with the proposed methodology. In this figure, a good agreement between the both methods is observed for all spectral bands, which indicates that the fit of κ was done properly.

Using the parameters of Table 2 to determine the values of κ to the corresponding spectral intervals, the solutions of the radiative heat flux and the radiative heat source can be obtained through Eqs. (9) and (10). In this table, each spectral interval corresponds to one gray gas. The main advantage of the present methodology over other spectral models, such as the WSGG model, which employs a similar number of gray gases (usually three or four gases), is that the proposed approach may be useful in problems with mixtures of participating gases, since, unlike others global models, it is not necessary to account for the overlapping effects of the species when combining them. At this stage of the work, only pure H_2O was analyzed, but gas mixtures is a subject that will be explored in future studies.

Figure 4 shows the behaviors of q_r and S_r for Profile 1. In the figure, the LBL benchmark solution and the approaches

Table 2. Planck-mean absorption coefficients for H_2O obtained for $400 \text{ K} \leq T \leq 2500 \text{ K}$ with the present methodology for five spectral intervals.

	$0 \text{ cm}^{-1} < \eta$ $< 1000 \text{ cm}^{-1}$	$1000 \text{ cm}^{-1} < \eta$ $< 2600 \text{ cm}^{-1}$	$2600 \text{ cm}^{-1} < \eta$ $< 4400 \text{ cm}^{-1}$	$4400 \text{ cm}^{-1} < \eta$ $< 6000 \text{ cm}^{-1}$	$6000 \text{ cm}^{-1} < \eta$ $< 10\,000 \text{ cm}^{-1}$
$C_0(\text{m}^{-1})$	24.203	6.754	-1.083	-6.885×10^{-2}	-6.840×10^{-2}
$C_1(\text{m}^{-1} \text{ K}^{-1})$	-6.650×10^{-2}	-1.339×10^{-2}	6.680×10^{-3}	5.800×10^{-4}	3.735×10^{-4}
$C_2(\text{m}^{-1} \text{ K}^{-2})$	8.590×10^{-5}	1.237×10^{-5}	-9.367×10^{-6}	-8.319×10^{-7}	-4.941×10^{-7}
$C_3(\text{m}^{-1} \text{ K}^{-3})$	-5.501×10^{-8}	-5.985×10^{-9}	5.999×10^{-9}	5.477×10^{-10}	3.061×10^{-10}
$C_4(\text{m}^{-1} \text{ K}^{-4})$	1.717×10^{-11}	1.466×10^{-12}	-1.840×10^{-12}	-1.719×10^{-13}	-9.194×10^{-14}
$C_5(\text{m}^{-1} \text{ K}^{-5})$	-2.085×10^{-15}	-1.437×10^{-16}	2.188×10^{-16}	2.081×10^{-17}	1.077×10^{-17}

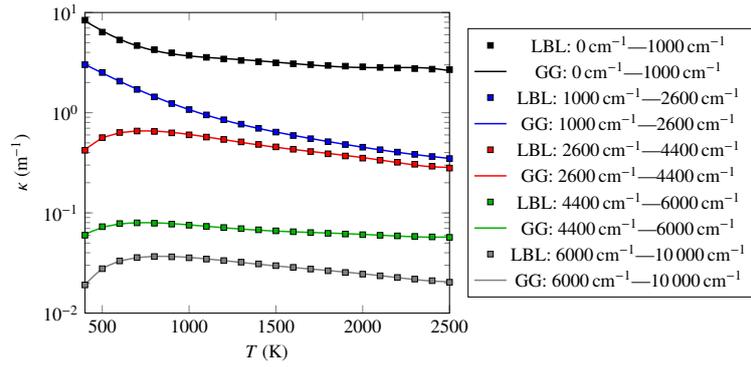


Figure 3. Comparison between the absorption coefficient computed by LBL and GG solutions with five spectral intervals.

with the GG model proposed by Cassol *et al.*, 2015, and with the present methodology are shown. To assess the performance of each approach, a normalized percentage deviation from the reference solution is defined as

$$\Delta\phi = \frac{|\phi_{\text{ref}} - \phi_{\text{app}}|}{\max(|\phi_{\text{ref}}|)}, \quad (15)$$

where ϕ is either the radiative heat flux or the radiative heat source, the subscripts “ref” and “app” are the reference and approximate solutions, respectively, and $\max(|\phi_{\text{ref}}|)$ is the maximum absolute local value of ϕ_{ref} in the domain. Table 3 shows the maximum and average normalized deviations (subscripts “max” and “avg”, respectively) for q_r and S_r computed with the different solutions presented in this paper regarding LBL integration. Although the GG solution with five bands has presented a better performance in relation to the LBL method when compared with the Cassol’s model, since the maximum deviation of S_r has fallen by almost a third, average errors are still around 30 %, which is not a good prediction of the result.

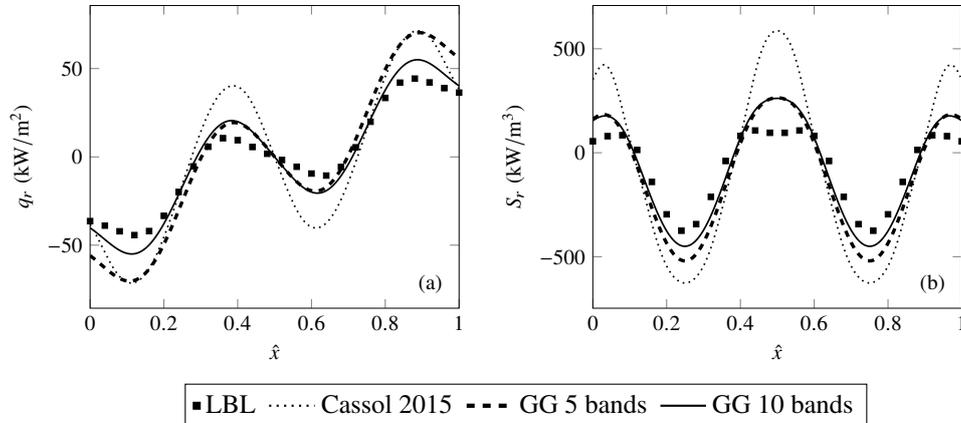


Figure 4. Radiative heat transfer for Profile 1: (a) radiative heat flux; (b) radiative heat source.

Table 3. Maximum and average normalized deviations of q_r and S_r predicted by the different GG approaches.

Profile	LBL x Cassol (%)				LBL x GG 5 bands (%)				LBL x GG 10 bands (%)			
	$(\Delta q_r)_{\text{max}}$	$(\Delta q_r)_{\text{avg}}$	$(\Delta S_r)_{\text{max}}$	$(\Delta S_r)_{\text{avg}}$	$(\Delta q_r)_{\text{max}}$	$(\Delta q_r)_{\text{avg}}$	$(\Delta S_r)_{\text{max}}$	$(\Delta S_r)_{\text{avg}}$	$(\Delta q_r)_{\text{max}}$	$(\Delta q_r)_{\text{avg}}$	$(\Delta S_r)_{\text{max}}$	$(\Delta S_r)_{\text{avg}}$
1	68.37	39.63	130.69	60.12	60.53	30.42	45.32	28.46	25.05	14.74	44.62	20.97
2	87.57	43.33	80.31	52.06	55.97	25.05	43.10	25.61	30.96	12.89	20.31	14.85

Figure 5 plots the results for the radiative heat flux and the radiative heat source for the asymmetric temperature profile, i.e., Eq. (12). Similar to what was observed with the previous case, in Profile 2 there is also a drop by a half in the maximum error for S_r between the formulation with five spectral intervals and that proposed by Cassol *et al.*, 2015; in addition, the average deviations are of the order of 25 % compared to the LBL solution. However, the magnitude of these errors is still not adequate to make the proposed model competitive with other spectral models in the literature, that lead to deviations from the benchmark solution below 5 % (see, e.g., Dorigon *et al.*, 2013).

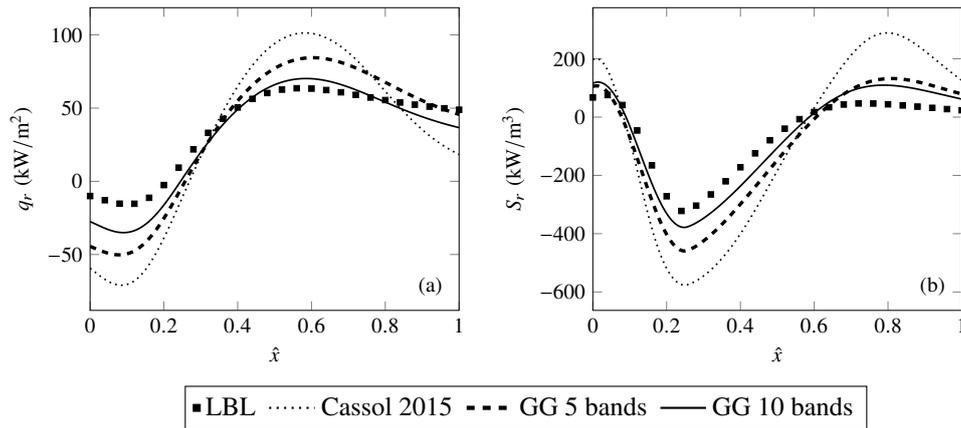


Figure 5. Radiative heat transfer for Profile 2: (a) radiative heat flux; (b) radiative heat source.

3.2 The GG model applied to ten spectral intervals

As an attempt to improve the result compared to the LBL integration, the radiation spectrum is divided again, but into ten regions — each one of them with 1000 cm^{-1} —, and Eq. (14) is applied to determine the Planck-mean absorption coefficients of the GG model proposed in this paper for each selected region. Table 4 shows the parameters that describe the fit of Eq. (14) for each spectral interval. By Fig. 6, one can observe a good accordance between the LBL solution and the GG model applied to ten bands in the calculation of κ for each spectral interval.

Table 4. Planck-mean absorption coefficients for H_2O obtained for $400 \text{ K} \leq T \leq 2500 \text{ K}$ with the present methodology for ten spectral intervals.

	$0 \text{ cm}^{-1} < \eta < 1000 \text{ cm}^{-1}$	$1000 \text{ cm}^{-1} < \eta < 2000 \text{ cm}^{-1}$	$2000 \text{ cm}^{-1} < \eta < 3000 \text{ cm}^{-1}$	$3000 \text{ cm}^{-1} < \eta < 4000 \text{ cm}^{-1}$	$4000 \text{ cm}^{-1} < \eta < 5000 \text{ cm}^{-1}$
$C_0(\text{m}^{-1})$	24.203	5.211	3.211×10^{-3}	5.851×10^{-2}	9.402×10^{-3}
$C_1(\text{m}^{-1} \text{ K}^{-1})$	-6.650×10^{-2}	-5.027×10^{-3}	1.485×10^{-4}	6.181×10^{-3}	2.433×10^{-5}
$C_2(\text{m}^{-1} \text{ K}^{-2})$	8.590×10^{-5}	8.902×10^{-7}	-1.984×10^{-7}	-1.027×10^{-5}	1.125×10^{-7}
$C_3(\text{m}^{-1} \text{ K}^{-3})$	-5.501×10^{-8}	1.285×10^{-9}	1.364×10^{-10}	7.088×10^{-9}	-1.330×10^{-10}
$C_4(\text{m}^{-1} \text{ K}^{-4})$	1.717×10^{-11}	-7.465×10^{-13}	-4.470×10^{-14}	-2.276×10^{-12}	5.412×10^{-14}
$C_5(\text{m}^{-1} \text{ K}^{-5})$	-2.085×10^{-15}	1.180×10^{-16}	5.641×10^{-18}	2.794×10^{-16}	-7.618×10^{-18}
	$5000 \text{ cm}^{-1} < \eta < 6000 \text{ cm}^{-1}$	$6000 \text{ cm}^{-1} < \eta < 7000 \text{ cm}^{-1}$	$7000 \text{ cm}^{-1} < \eta < 8000 \text{ cm}^{-1}$	$8000 \text{ cm}^{-1} < \eta < 9000 \text{ cm}^{-1}$	$9000 \text{ cm}^{-1} < \eta < 10000 \text{ cm}^{-1}$
$C_0(\text{m}^{-1})$	8.716×10^{-1}	-3.293×10^{-3}	1.098	-1.287×10^{-3}	6.229×10^{-4}
$C_1(\text{m}^{-1} \text{ K}^{-1})$	-1.914×10^{-3}	1.506×10^{-5}	-2.910×10^{-3}	2.409×10^{-5}	3.817×10^{-6}
$C_2(\text{m}^{-1} \text{ K}^{-2})$	2.094×10^{-6}	1.429×10^{-8}	3.431×10^{-6}	-3.630×10^{-8}	-6.114×10^{-9}
$C_3(\text{m}^{-1} \text{ K}^{-3})$	-1.209×10^{-9}	-1.600×10^{-11}	-2.051×10^{-9}	2.505×10^{-11}	4.090×10^{-12}
$C_4(\text{m}^{-1} \text{ K}^{-4})$	3.519×10^{-13}	6.006×10^{-15}	6.071×10^{-13}	-8.105×10^{-15}	-1.241×10^{-15}
$C_5(\text{m}^{-1} \text{ K}^{-5})$	-4.059×10^{-17}	-8.145×10^{-19}	-7.067×10^{-17}	9.991×10^{-19}	1.428×10^{-19}

Figures 4 and 5 show that the increase in the number of regions in which the spectrum is segmented leads, in fact, to a result closer to the reference solution. However, Table 3 shows that, for the two temperature profiles studied, even after doubling the number of spectral intervals, the average deviations for q_r and S_r in relation to the LBL solution are still between 15 % and 20 %. By the behavior of the approaches, one can see that, although the proposed method has improved the result in relation to that obtained with the correlations of Cassol *et al.*, 2015, even the division of the spectrum into ten segments and the assignment of a gray gas to each of them has not led to a satisfactory agreement with the LBL benchmark solution. Therefore, analyses involving further refinements of the spectrum should be carried out, which may lead to more accurate results and close to the benchmark solution in future steps of this work. Moreover, other species or gas mixtures with non-homogeneous concentrations could also be studied. Additionally, a possible way to improve the performance of the methodology proposed in this paper would be to apply the present formulation to other spectral models, such as the WSGG model, and to evaluate the impact on the solution of the problem with the same conditions studied here.

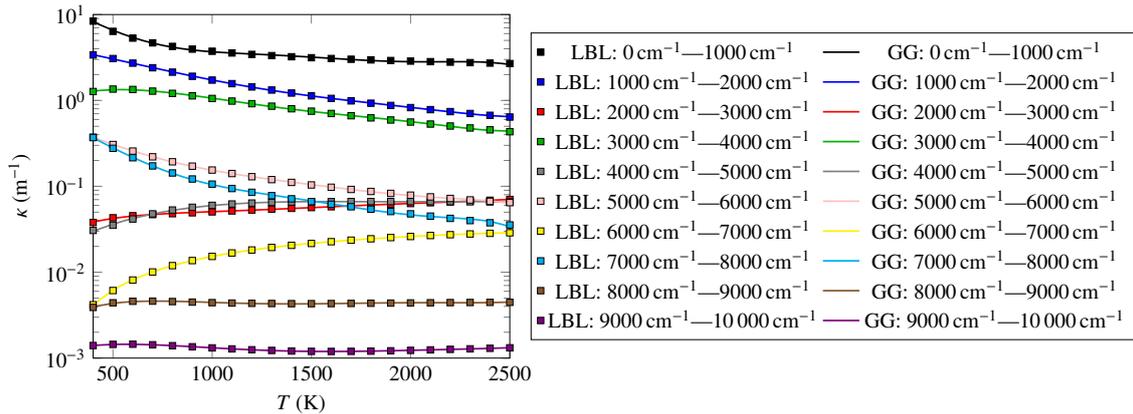


Figure 6. Comparison between the absorption coefficient computed by LBL and GG solutions with ten spectral intervals.

4. CONCLUSIONS

This study presented an analysis of a radiative transfer problem that consists of pure water vapor confined to a one-dimensional system bounded by black walls. A new formulation for the GG model was proposed, in which the radiation spectrum was divided into a set of segments following recommendations in the literature and one gray gas was assigned to each one of these intervals. The Planck-mean absorption coefficients of these spectral intervals were determined and the calculations of the radiative heat flux and radiative heat source were done. Although the curves that describe κ for each spectral band have presented a good accuracy in relation to the benchmark solution, the computation of q_r and S_r demonstrates average deviations of the order of 20 % regarding to the LBL integration. In this framework, the future perspectives for the present paper consist of dividing the spectrum in a non-uniform way so that in the regions in which the emission of radiation is greater there is a higher concentration of gray gases, and where there is less energy being emitted, there are less gray gases. Moreover, the present methodology could be applied to other spectral models in order to obtain evaluate a better agreement with the LBL solution.

5. ACKNOWLEDGMENTS

This work has been partially supported by the Brazilian Agency CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior). Authors RJCF and GCF thank CAPES and CNPq (Conselho Nacional de Desenvolvimento Tecnológico e Científico) for doctorate scholarships, respectively. Author FHRF thanks CNPq for research grant 302686/2017-7.

6. REFERENCES

- André, F. and Vaillon, R., 2010. "A nonuniform narrow band correlated- k approximation using the k -moment method". *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 111, No. 12-13, pp. 1900–1911.
- Cassol, F., Brittes, R., Centeno, F.R., da Silva, C.V. and França, F.H., 2015. "Evaluation of the gray gas model to compute radiative transfer in non-isothermal, non-homogeneous participating medium containing CO₂, H₂O and soot". *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, Vol. 37, No. 1, pp. 163–172.
- Crnomarkovic, N., Sijercic, M., Belosevic, S., Tucakovic, D. and Zivanovic, T., 2013. "Numerical investigation of processes in the lignite-fired furnace when simple gray gas and weighted sum of gray gases models are used". *International Journal of Heat and Mass Transfer*, Vol. 56, No. 1-2, pp. 197–205.
- Denison, M.K. and Webb, B.W., 1993. "A spectral line-based weighted-sum-of-gray-gases model for arbitrary RTE solvers". *Journal of Heat Transfer*, Vol. 115, No. 4, pp. 1004–1012.
- Dorigon, L.J., Duciak, G., Brittes, R., Cassol, F., Galarça, M. and França, F.H.R., 2013. "WSGG correlations based on HITEMP2010 for computation of thermal radiation in non-isothermal, non-homogeneous H₂O/CO₂ mixtures". *International Journal of Heat and Mass Transfer*, Vol. 64, pp. 863–873.
- Fraga, G., Centeno, F., Petry, A., Coelho, P. and França, F., 2019a. "On the individual importance of temperature and concentration fluctuations in the turbulence-radiation interaction in pool fires". *International Journal of Heat and Mass Transfer*, Vol. 136, pp. 1079–1089.
- Fraga, G., Zannoni, L., Centeno, F. and França, F., 2019b. "Evaluation of different gray gas formulations against line-by-line calculations in two- and three-dimensional configurations for participating media composed by CO₂, H₂O and soot". *Fire Safety Journal*, Vol. 108, p. 102843.
- Fraga, G.C., Centeno, F.R., Petry, A.P. and França, F.H.R., 2017. "Evaluation and optimization-based modification of a model for the mean radiative emission in a turbulent non-reactive flow". *International Journal of Heat and Mass*

Transfer, Vol. 114, pp. 664–674.

- Hottel, H.C. and Sarofim, A.F., 1967. *Radiative Transfer*. McGraw-Hill.
- Howell, J.R., Mengüç, M.P. and Siegel, R., 2016. *Thermal Radiation Heat Transfer*. CRC press, 6th edition.
- IBM, 2016. *IBM SPSS Modeler 18.0 User's Guide*. IBM Corporation.
- Kaminski, D., Fu, X. and Jensen, M., 1995. “Numerical and experimental analysis of combined convective and radiative heat transfer in laminar flow over a circular cylinder”. *International Journal of Heat and Mass Transfer*, Vol. 38, No. 17, pp. 3161–3169.
- Lathrop, K.D. and Carlson, B.G., 1964. “Discrete ordinates angular quadrature of the neutron transport equation”.
- Liu, F., Becker, H. and Bindar, Y., 1998. “A comparative study of radiative heat transfer modelling in gas-fired furnaces using the simple grey gas and the weighted-sum-of-grey-gases models”. *International Journal of Heat and Mass Transfer*, Vol. 41, No. 22, pp. 3357–3371.
- Marin, O. and Buckius, R., 1998. “A simplified wide band model of the cumulative distribution function for water vapor”. *International Journal of Heat and Mass Transfer*, Vol. 41, No. 19, pp. 2877–2892.
- Modest, M.F., 2013. *Radiative Heat Transfer*. Academic Press.
- Mossi, A., Galarça, M.M., Brittes, R., Vielmo, H.A. and França, F.H.R., 2012. “Comparison of spectral models in the computation of radiative heat transfer in participating media composed of gases and soot”. *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, Vol. 34, No. 2, pp. 112–119.
- Rothman, L.S., Gordon, I.E., Babikov, Y., Barde, A., Chris Benner, D., Bernath, P.F., Birk, M., Bizzocchi, L., Boudon, V., Brown, L.R., Campargue, A., Chance, K., Cohen, E.A., Coudert, L.H., Devi, V.M., Drouin, B.J., Fayt, A., Flaud, J.M., Gamache, R.R., Harrison, J.J., Hartmann, J.M., Hill, C., Hodges, J.T., Jacquemart, D., Jolly, A., Lamouroux, J., Le Roy, R.J., Li, G., Long, D.A., Lyulin, O.M., Mackie, C.J., Massie, S.T., Mikhailenko, S., Müller, H.S.P., Naumenko, O.V., Nikitin, A.V., Orphal, J., Perevalov, V., Perrin, A., Polovtseva, E.R., Richard, C., Smith, M.A.H., Starikova, E., Sung, K., Tashkun, S., Tennyson, J., Toon, G.C., Tyuterev, V.G. and Wagner, G., 2013. “The HITRAN2012 molecular spectroscopic database”. *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 130, pp. 4–50.
- Rothman, L., Gordon, I., Barber, R., Dothe, H., Gamache, R., Goldman, A., Perevalov, V., Tashkun, S. and Tennyson, J., 2010. “HITEMP, the high-temperature molecular spectroscopic database”. *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 111, No. 15, pp. 2139–2150.
- Taine, J., 1983. “A line-by-line calculation of low-resolution radiative properties of CO₂-CO-transparent nonisothermal gases mixtures up to 3000 K”. *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 30, No. 4, pp. 371–379.
- Wakatsuki, K., Jackson, G.S., Kim, J., Hamins, A., Nyden, M.R. and Fuss, S.P., 2008. “Determination of Planck mean absorption coefficients for hydrocarbon fuels”. *Combustion Science and Technology*, Vol. 180, No. 4, pp. 616–630.
- Zhang, H. and Modest, M.F., 2002. “Evaluation of the Planck-mean absorption coefficients from HITRAN and HITEMP databases”. *Journal of Quantitative Spectroscopy and Radiative Transfer*, Vol. 73, No. 5, pp. 649–653.

7. RESPONSIBILITY NOTICE

The authors are solely responsible for the printed material included in this paper.