

APPLICATION OF THE WEIGHTED-SUM-OF-GRAY-GASES MODEL IN MEDIA BOUNDED BY NON-GRAY WALLS

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Abstract. *In several engineering applications, such as in combustion problems, the study of the heat transfer by thermal radiation is a very complex task due to the presence of soot, particulates and participating gases. The strongly irregular spectral dependence of the absorption coefficient with the wavenumber, especially at elevated temperatures, makes it necessary to adopt spectral models to determine the radiative quantities. One competitive method, which presents low computational requirement and good accuracy, is the weighted-sum-of-gray-gases (WSGG) model. This method solves the spectral integration of the radiative transfer equation (RTE) by replacing it by a few bands with uniform absorption coefficients, where each one represents a gray gas. In this paper, the WSGG model is applied to a one-dimensional medium slab bounded by perfectly diffuse, non-gray walls. The medium is a homogeneous mixture of carbon dioxide and water vapour, whose radiative properties are taken from HITEMP2010 database. The discrete ordinates method (DOM) is employed to solve the angular integration of the RTE. The wall emission and absorption is characterized by a combination of bands, in which each region of the spectrum presents a specific value of emissivity and absorptivity. The problem is solved as a weighted-sum-of-gray-surfaces, in which, at the end of the calculations, it performs a summation over the contributions of each region. It is made a comparison between the results obtained by the WSGG model and the line-by-line (LBL) benchmark solution to evaluate of the accuracy of the proposed method.*

Keywords: *Radiative heat transfer, weighted-sum-of-gray-gases model, line-by-line solution, non-gray walls*

1. INTRODUCTION

Numerical modeling of combustion processes involves solving a very complex problem due to not only the presence of participating gases, but also the formation of particles soot. The study of the combustion gases requires a good understanding about the reaction mechanisms of chemical kinetics and the heat transfer by thermal radiation, which in itself is a challenging task. At elevated temperatures, radiation is generally the dominant mode of heat exchange, so it is fundamental to know to describe accurately the variables that govern these problems, such as the strongly irregular spectral dependence of the absorption coefficient with the wavenumber and the gaseous species.

Since the behavior of the radiative properties of the participating gases is complex, such as the absorption coefficient that is represented by thousands of spectral lines that vary rapidly with the wavenumber, a reliable alternative is to employ the weighted-sum-of-gray-gases (WSGG) model, to perform the integration of the radiative transfer equation (RTE). Proposed by Hottel and Sarofim (1967), the method replaces, with accuracy and low computational cost, the spectral integration by a few number of bands with uniform absorption coefficient, where each one symbolizes a gray gas. However, the implementation of the WSGG model requires a determination of the weighting absorption coefficients for each gray gas, whose can be calculated through of spectral databases, such as HITRAN (High Resolution Transmission Absorption Database) or HITEMP (High Temperature Molecular Spectroscopic Database). From the exponential wide-band model, Smith et al., 1982, obtained weighting absorption coefficients for carbon dioxide and water vapour. Maurente et al., 2007, made comparisons between the standard WSGG and the ALBDF (absorption-line blackbody distribution function) gas model, in a cylindrical chamber containing methane and fuel oil. Galarça et al., 2008, presented new absorption coefficients and temperature dependent weighted functions for three gray gases. From HITEMP2010 database, Dorigon et al., 2013, and Zienniczak et al., 2013, obtained absorption coefficients updated for a mixture composed by carbon dioxide and water vapour for a parallel flat medium bounded by black walls. Cassol et al., 2014, performed a similar study for the same problem, but including soot.

Most papers in the literature related to spectral modeling considers black walls because the calculations become faster, so that there are few studies that make use of gray or non-gray surfaces. Applying the efficient cumulative wavenumber (CW) model, Solovjov et al., 2013, investigated the radiative transfer in gaseous media bounded by non-gray walls. Fonseca et al., 2015, employ the WSGG model to a medium with gray surfaces and for a mixture formed by H₂O and CO₂. So, this paper presents the WSGG model applied to a one-dimensional system, which is composed by a flat plate parallel medium, in which the walls are non-gray, for a gaseous mixture composed by carbon dioxide and water vapour, in homogeneous and isothermal and non-isothermal conditions at 1.0 atm, using data from HITEMP2010 database. The emissivities of the surfaces are given by two bands, determined for certain wavenumbers, and is considered pressure ratio equal to 2 (more specifically, in this analysis, $p_{\text{H}_2\text{O}} = 0.2$ atm and $p_{\text{CO}_2} = 0.1$ atm), which are typical products in combustion of methane. Thus, the present work makes an advance to study the application of the weighted-sum-of-gray-gases model employed to non-gray walls. The RTE is resolved by the discrete ordinates method

(DOM) and the performance of the WSGG model is compared to integration of the benchmark line-by-line (LBL) solution.

2. PHYSICAL AND MATHEMATICAL MODELING

2.1 The radiative transfer equation and the weighted-sum-of-gray-gases-model

Neglecting scattering, the radiative transfer equation (RTE) accounts for the variation in the radiative intensity due to the mechanisms of absorption and emission in the medium, according to (Siegel and Howell, 2002):

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

in which κ_{η} corresponds to the absorption coefficient associated with the wavenumber η , in m^{-1} , and I_{η} and $I_{\eta b}$ represent the spectral intensity and the blackbody radiation intensity, respectively, at position x , both in $\text{W}/(\text{m}^2 \text{ cm}^{-1})$. Furthermore, in the present study, Eq. (1) considers a gaseous mixture composed by carbon dioxide and water vapour, the spectral absorption coefficient is given by the summation of the absorption coefficient of each chemical species.

Spectral modeling has played an important role in the radiative exchanges in participating media. The simplest method is the gray gas (GG) model, in which it assumes that the absorption coefficient is uniform over the spectrum and independent of the temperature and of the partial pressure of the participating species. However, the GG model presents a small reliability in the computation of radiation heat transfer, once, although it provides goods results for the local emission in the gas, fails in the determination of local absorption.

One competitive method is the weighted-sum-of-gray-gases (WSGG) model, in which the integration of the entire spectrum is replaced by a few gray gases plus the transparent windows. Dividing the spectrum into regions where the absorption coefficient is constant, each band, in this model, represents one gray gas. So, it is necessary to determine not only the absorption coefficients for each gray gas, but also the temperature dependent coefficients, which can be obtained from fitting data of total emittances of participating species that constitute the medium. The establishment of spectral databases, like HITRAN and HITEMP, allows the calculation of these parameters due to the existence of information with thousands of spectral lines with dependence of wavenumber. The HITEMP database is more indicated for combustion gases, because the data are obtained for temperatures around 1000 K, which means that extrapolations to elevated temperatures with this database are most suitable than HITRAN, which are obtained at 296 K. The most updated version is the HITEMP2010, which has been demonstrated most accurate results in comparison with the other available databases (Dorigon et al., 2013). According to Cassol et al., 2014, the central point of the WSGG model is to generate correlations for each gray gas, which are superposed to compose the correlations of the gaseous mixture. Originally, the WSGG model was proposed for situations where the medium is isothermal and homogeneous. However, it has been verified that these problems can be solved satisfactorily by using this method when the ratio between the partial pressures of species is constant or presents small variation (Dorigon et al., 2013).

Making use of the WSGG model and, therefore, integrating the RTE over the spectral regions where the absorption coefficient associated with the wavenumber η , κ_{η} , is replaced by absorption coefficient based on the pressure associated to each gray gas, $\kappa_{p,j}$, Eq. (1) becomes:

$$\frac{dI_j(x)}{dx} = -\kappa_{p,j}p_a(x)I_j(x) + \kappa_{p,j}p_a(x)a_j(T)I_b(T) \quad (2)$$

where the partial pressure of the absorbing-emitting species, $p_a(x)$, temperature dependent coefficient, $a_j(T)$, and total blackbody intensity, $I_b(T)$, are evaluated at local conditions. Another interpretation of the $a_j(T)$ is that this parameter describes a weighting factor to quantify the blackbody radiation fraction emitted at the local temperature, in position x , in the wavenumber interval represented by the gray gas j . The total radiation intensity can be determined by the summation of the partial intensities, I_j , in $\text{W}/(\text{m}^2 \text{ sr})$, to each gray gas, calculated from the integration of the RTE in the spectrum region related to gas j , according to the following equation:

$$I(x) = \sum_{j=1}^J I_j(x) \quad (3)$$

The total blackbody intensity is given by Planck's distribution law, as is presented in the expression below:

$$F_{0 \rightarrow \lambda T} = \int_0^{\lambda T} \frac{E_{\lambda T}(T)}{\sigma T^5} d(\lambda T) = \frac{15}{\pi^4} \sum_{n=1}^{\infty} \left[\frac{e^{-n\beta}}{n} \left(\beta^3 + \frac{3\beta^2}{n} + \frac{6\beta}{n^2} + \frac{6}{n^3} \right) \right] \quad (7)$$

In the above expression, $\beta = hc_0 / \lambda k_B T$, where h is the Planck's constant ($h = 6.626 \times 10^{-34}$ J s); c_0 indicates the speed of light ($c_0 = 2.998 \times 10^8$ m/s); and k_B represents the Boltzmann's constant ($k_B = 1.3806 \times 10^{-23}$ J/K); the wavelength λ in this equation is given in m (or in cm^{-1} when λ is replaced by the wavenumber η). The term $E_{\lambda T}$ is the Planck's spectral distribution of emissive power. Although the Eq. (7) is given by an infinite sum, Chang and Rhee (1984) showed that only four terms provide approximate results of exact solution.

2.3 The WSGG coefficients

Dorigon et al., 2013, generated correlations for WSGG model for a typical gas mixture resulting from the combustion of methane at 1.0 atm using the HITEMP2010 database. These coefficients are recommended for gas temperatures ranging from 400 K to 2500 K and pressure path-length products from 0.0001 atm m to 10 atm m. In the present work, the partial pressures of the products are 0.1 atm and 0.2 atm for the CO_2 and H_2O , respectively. The WSGG coefficients shown in Tab. 1 were obtained for equivalence ratio equal to 2 ($p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 2$) and for four gray gases. Ziemniczak et al., 2013, verified that the WSGG model could become independent of the number of gray gases; particularly, for the problem investigated, four gray gases are sufficient.

One important point of the WSGG model is that the coefficient $a_j(T)$ is the weighting factor for the j -th gray gas that depends only on temperature and can be determined by a polynomial function, as is presented below.

$$a_j(T) = \sum_{k=0}^K b_{j,k} T^k \quad (8)$$

The terms $b_{j,k}$ of Eq. (8) are the polynomial coefficients of k -th order for the j -th gray gas. The transparent window is determined as $a_0(T) = 1 - \sum_{j=1}^J a_j(T)$ to assure the energy conservation. Table 1 presents the correlations employed in the problem studied in this work.

Table 1. WSGG coefficients for four gray gases and double equivalence ratio; $j = 4$, $p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 2$ (Dorigon et al., 2013)

j	$\kappa_{p,j} (\text{atm m})^{-1}$	$b_{j,0}$	$b_{j,1} (\text{K}^{-1})$	$b_{j,2} (\text{K}^{-2})$	$b_{j,3} (\text{K}^{-3})$	$b_{j,4} (\text{K}^{-4})$
1	1.921E-01	5.617E-02	7.844E-04	-8.563E-07	4.246E-10	-7.440E-14
2	1.719E+00	1.426E-01	1.795E-04	-1.077E-08	-6.971E-11	1.774E-14
3	1.137E+01	1.362E-01	2.574E-04	-3.711E-07	1.575E-10	-2.267E-14
4	1.110E+02	1.222E-01	-2.327E-05	-7.492E-08	4.275E-11	-6.680E-15

For a medium that has non-gray walls and the emissivities described by a combination of bands, in which each region presents an emissivity ε_{η} , corresponding to the wavenumber interval η , the boundary conditions for Eqs. (5) and (6) are given, respectively, by:

$$I_{j,l}^+(x=0) = \frac{\varepsilon_{\eta} a_k a_j \sigma T^4(x=0)}{\pi} + \frac{1-\varepsilon_{\eta}}{\pi} \int I_{j,l}^-(x=0) \cos \theta_l dw \quad (9)$$

$$I_{j,l}^-(x=X) = \frac{\varepsilon_{\eta} a_k a_j \sigma T^4(x=X)}{\pi} + \frac{1-\varepsilon_{\eta}}{\pi} \int I_{j,l}^+(x=X) \cos \theta_l dw \quad (10)$$

where θ_l is the angle between the incoming direction and the surface normal, w indicates the solid angle and $x = 0$ and $x = X$ indicate the boundaries to the left and to the right of the domain, respectively, as shown in the representation of Fig 1.

Solving Eqs. (5) and (6) allows determining the net radiative heat flux, q_R'' , in units of W/m^2 , and radiative source term, \dot{q}_R , in units of W/m^3 , respectively, in each point along the path for each case studied in this paper. It is interesting to perceive that $\dot{q}_R(x) = -dq_R''(x)/dx$. The following equations allow calculating these two quantities, where l represents the number of directions of integration of the radiative transfer equation and ω_l is the quadrature weight for l direction from the discrete ordinate method.

$$\dot{q}_R''(x) = \sum_{j=1}^J \sum_{l=1}^L 2\pi\mu_l\omega_l \left[I_{j,l}^+(x) - I_{j,l}^-(x) \right] \quad (11)$$

$$\dot{q}_R(x) = \sum_{j=1}^J \sum_{l=1}^L 2\pi\omega_l\kappa_{p,j}p_a(x) \left\{ \left[I_{j,l}^+(x) + I_{j,l}^-(x) \right] - 2a_j(T)I_b(x) \right\} \quad (12)$$

3. RESULTS AND DISCUSSION

3.1 Emissivity distribution by bands

For the analyzed problem, were considered a combination of two bands for the emissivity profile of the walls. It makes the assumption that both surfaces have the same distribution of emissivity, so that the two regions of the spectrum shown in Fig. 2(a) have the same values. In this study, were chosen, arbitrarily, the emissivity values of $\varepsilon_{\eta,1} = 0.8$, for the first band ($0 \text{ cm}^{-1} < \eta < 6000 \text{ cm}^{-1}$), and $\varepsilon_{\eta,2} = 0.5$, for the second one (for $\eta > 6000 \text{ cm}^{-1}$).

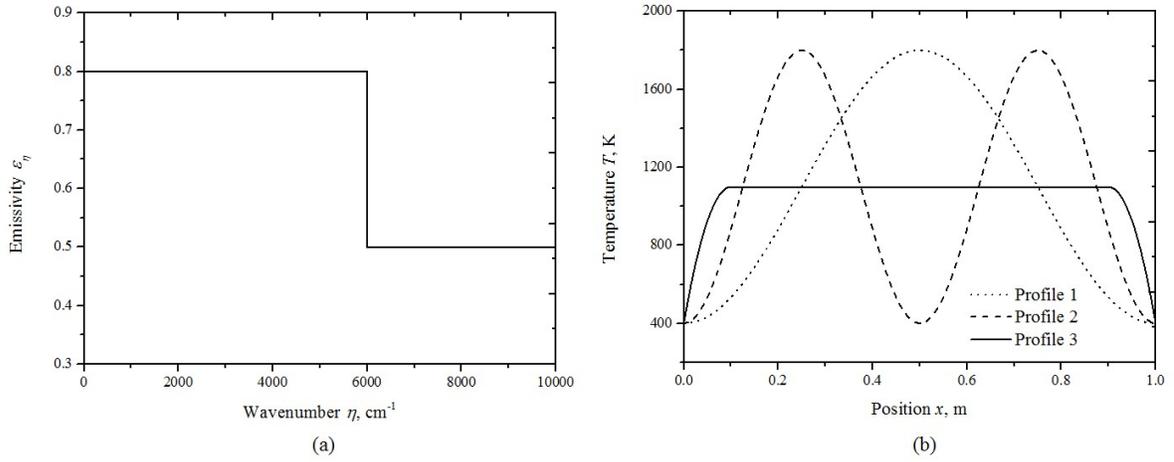


Figure 2. (a) Emissivity profile for describing the walls emission; (b) Temperature profiles given by Eqs. (13)–(15).

3.2 Comparison between WSGG model and LBL solution

The application of the weighted-sum-of-grays-gases model to non-gray walls is investigated in this paper through of a set of simulations of non-isothermal and homogeneous cases in order to evaluate the performance of the method against the benchmark line-by-line (LBL) solution. The domain is a one-dimensional medium slab, which walls have an emissivity profile given by Fig. 2(a), space apart by a distance of 1.0 m, as shown in Fig. 1. The DOM was applied to 30 directions utilizing a Gauss-Legendre quadrature for solving the RTE. Three different temperature profiles are proposed, which will be referenced, posteriorly, as Profile 1, Profile 2 and Profile 3, respectively.

$$T(x) = 400 \text{ K} + (1400 \text{ K})\sin^2(\pi x) \quad (13)$$

$$T(x) = 400 \text{ K} + (1400 \text{ K})\sin^2(2\pi x) \quad (14)$$

$$T(x) = \begin{cases} 400 \text{ K}, & \text{for } x = 0 \text{ m and } x = 1.0 \text{ m} \\ \left(-7 \times 10^4 \frac{\text{K}}{\text{m}^2} \right) x^2 + \left(1,4 \times 10^4 \frac{\text{K}}{\text{m}} \right) x + 400 \text{ K}, & \text{for } 0 \text{ m} < x < 0.1 \text{ m} \\ \left(-7 \times 10^4 \frac{\text{K}}{\text{m}^2} \right) x^2 + \left(1,26 \times 10^5 \frac{\text{K}}{\text{m}} \right) x - 5,56 \times 10^4 \text{ K}, & \text{for } 0.9 \text{ m} < x < 1.0 \text{ m} \\ 1100 \text{ K}, & \text{for } 0.1 \text{ m} < x < 0.9 \text{ m} \end{cases} \quad (15)$$

Equation (13), which shows a simple symmetry profile, has a maximum temperature, 1800 K, in the middle of the domain, and a minimum value of temperature in 400 K, more specifically in both walls. Equation (14) presents a double symmetry profile, in which the minimum temperature is also 400 K and occurs at the boundaries and the middle of domain; the maximum value reaches 1800 K twice, occurring in the points $x = 0.25$ m and $x = 0.75$ m. Finally, Eq. (15) demonstrates a parabolic profile, in the intervals $0 < x < 0.1$ m and $0.9 < x < 1.0$ m; the wall temperatures are 400 K and the remaining domain temperature is 1100 K, which corresponds to the maximum value in this case. Figure 2(b) demonstrates these behaviors.

According to Modest, 2003, the WSGG model can be employed not only when the boundaries are black, although the most papers in literature apply this methodology to walls that behave as blackbodies, due to the computational effort is lower (Fonseca et al., 2015). The main goal of this article is to evaluate the WSGG performance, applied to non-gray walls, in comparison with the LBL solution.

To verify the discrepancy between the WSGG model and the LBL solution, were calculated the maximum and average deviations for the radiative heat flux and the radiative source term, symbolized by δ and ζ , respectively, as the equations below. For analysis of importance in engineering calculations, the heat flux and the source term are the quantities that have greater relevance, so it is interesting to evaluate the discrepancies between the methods. Further, the notation δ_{\max} and δ_{avg} will be employed to designate the maximum and average deviations for radiative heat flux, respectively, and ζ_{\max} and ζ_{avg} to the maximum and average deviations for source term, respectively. Table 2 shows the percentage differences between the two methods for the three temperature profiles and its results are commented hereafter.

$$\delta = \frac{\left| \dot{q}_{R,WSGG}'' - \dot{q}_{R,LBL}'' \right|}{\max \left| \dot{q}_{R,LBL}'' \right|} \times 100\% \quad (16)$$

$$\zeta = \frac{\left| \dot{q}_{R,WSGG} - \dot{q}_{R,LBL} \right|}{\max \left| \dot{q}_{R,LBL} \right|} \times 100\% \quad (17)$$

Figures 3(a) and 3(b) demonstrate the radiative heat flux and the radiative source term, respectively, for the temperature profile given by Eq. (13) for emissivity distribution presented in Fig. 2(a) making a comparison between WSGG and LBL solutions. In Fig. 3(a), the heat flux is equal to zero in the central region of the domain, that it was expected due to symmetry of the Profile 1. Since the radiative heat flux tends to be directioned from the higher to the lower temperatures to center, q_R'' is negative for $x < 0.5$ m and positive in the other half of the domain. On the other hand, the source term, in Fig. 3(b), has the maximum absolute value in the average distance, $x = 0.5$ m, in which the temperature is maximum, i.e., 1800 K. According to Tab. 2, it is perceived an agreement between WSGG model and LBL solution for Profile 1, since the maximum deviations for the radiative heat transfer and the source term is of the order of 5%, according to Tab. 2.

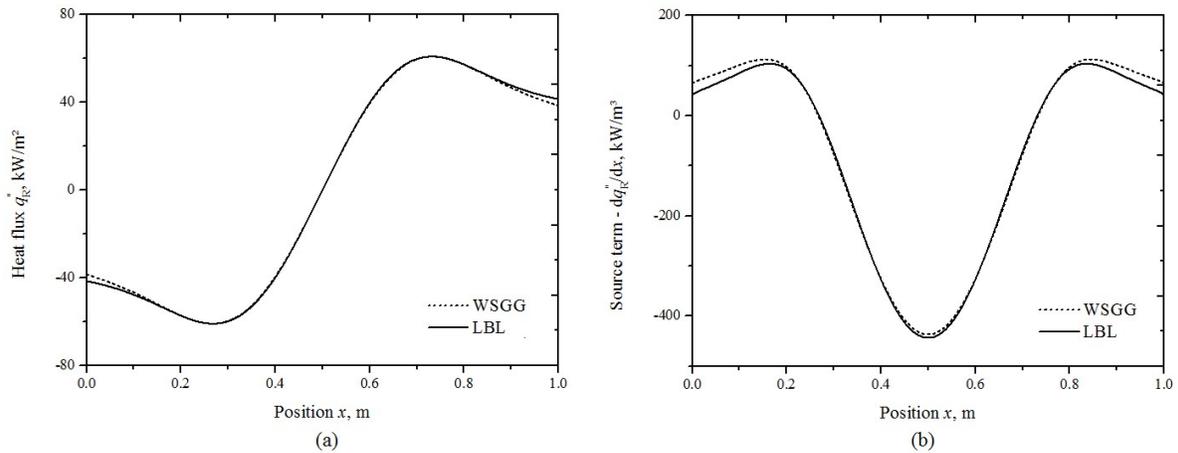


Figure 3. Comparison between the WSGG model and the LBL solution for the temperature profile given by Eq. (13):
(a) Radiative heat flux, q_R'' ; (b) Radiative source term, \dot{q}_R .

Figures 4(a) and 4(b) present q_R'' and \dot{q}_R for Profile 2, given by Eq. (14), which has double symmetry. The radiative heat flux is null in center of the domain, i.e., in $x = 0.5$ m, and in the positions in which are the higher temperatures, i.e., in $x = 0.25$ m and $x = 0.75$ m, due to the symmetry of the Profile 2; the source term, in the points, $x = 0.25$ m and $x = 0.75$ m, reaches the maximum absolute values, where the heat flux gradients are higher. Analogously to previous case, there is also a satisfactory accordance between the two methods, since the maximum deviation is around 9% and the average deviation is less than 4%, as is shown in Tab. 2.

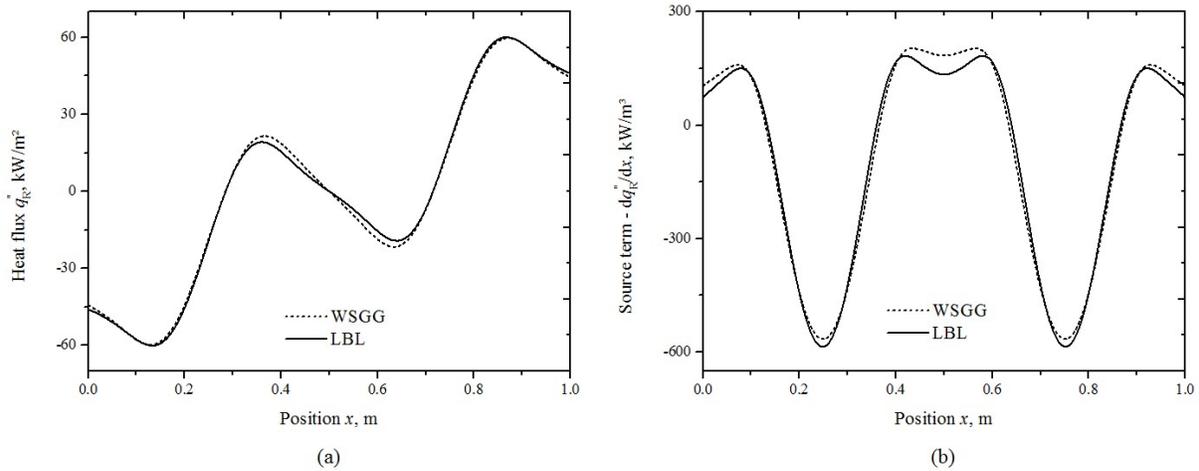


Figure 4. Comparison between the WSGG model and the LBL solution for the temperature profile given by Eq. (14):
 (a) Radiative heat flux, q_R'' ; (b) Radiative source term, \dot{q}_R .

Lastly, Figs. 5(a) and 5(b) show an isothermal medium, as described by Eq. (15), in which the medium temperature is uniform (1100 K), both walls are in the same temperature (400 K), but there is a parabolic profile in the domain sides. According to Tab. 2, it is possible observe that this profile presents the best results among the cases analyzed, since the deviations are around 1%, except for the maximum deviation of the source term, which is of the order of 8%. Possibly, the good concordance between the results obtained by the WSGG model and the LBL solution occurs in virtue of the continuity of temperature that there is along the domain.

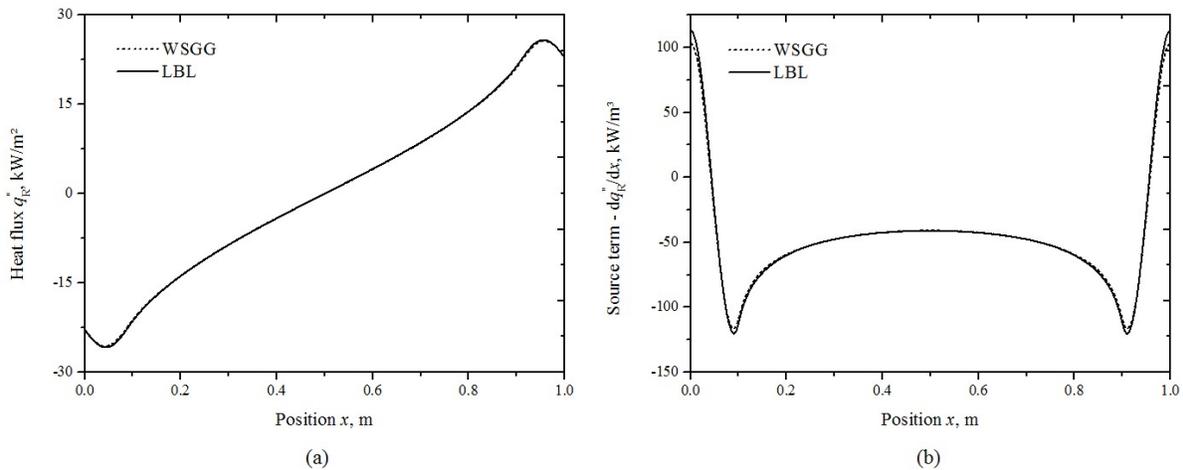


Figure 5. Comparison between the WSGG model and the LBL solution for the temperature profile given by Eq. (15):
 (a) Radiative heat flux, q_R'' ; (b) Radiative source term, \dot{q}_R .

Table 2. Deviations of the WSGG model and LBL solution for radiative heat flux and source term.

Deviation (%)	Heat flux (q_R'')		Source term (\dot{q}_R)	
	δ_{\max}	δ_{avg}	ζ_{\max}	ζ_{avg}
Profile 1	4.90	1.00	5.52	1.86
Profile 2	5.34	1.98	8.65	3.59
Profile 3	1.02	0.27	8.15	1.21

4. CONCLUSIONS

This paper studied the radiative heat transfer in a flat parallel medium, in which the walls are non-gray and the emissivity is given by a combination of two bands, composed by a mixture of participating gases, more specifically, water vapour and carbon dioxide, in isothermal and non-isothermal conditions and homogeneous concentration. The WSGG coefficients employed were obtained by Dorigon et al., 2013, for four gray gases and pressure ratio equal to 2.

In view of the simplicity of the WSGG model, it was observed that the method provides satisfactory results when compared with LBL solution, since the maximum deviations are less than 9%. Even so, this study makes a first attempt in applying the WSGG model to non-gray walls, since studies employing spectral models to problems in which the surfaces are not black are scarce in the literature. As next steps, it can be attempted to improve the method in the vicinity of the walls, where the errors trend to become more important, besides investigate some cases with non-homogeneous concentrations.

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