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RADIATIVE TRANSFER PREDICTION IN PARTICIPATING MEDIUM BOUNDED WITH NONGRAY WALLS USING THE SLW MODEL

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Abstract. *This study presents the application of the spectral line-based weighted-sum-of-gray-gases (SLW) model for the radiative transfer calculation in a participating medium bounded by two infinite, parallel and nongray walls. The proposed methodology presents a simplified approach to calculate the irradiation of the medium without the determination of the radiation intensity field at each wavenumber. The radiative transfer equation (RTE) is modeled in a one-dimensional domain in which there is a non-isothermal homogeneous or non-homogeneous gaseous mixture of water vapor and carbon dioxide. The results are compared with the line-by-line (LBL) benchmark solution in order to quantify the magnitude of the error when using the spectral model to describe the solution behavior. The results show that the applied methodology provides satisfactory agreements with respect to LBL solution. In addition, the importance of considering nongray walls, instead of gray, for an accurate computation of the radiative heat transfer is shown.*

Keywords: *radiative transfer, SLW model, line-by-line solution, nongray walls*

1. INTRODUCTION

At high temperatures, thermal radiation can significantly affect the heat transfer characteristics of a participating gas, such as in combustion systems and atmosphere processes. However, the prediction of the radiative heat transfer is yet a challenging task due to the strong spectral variation of the radiative properties, as the absorption coefficient of the medium (Denison and Webb, 1995d). Several studies show that the line-by-line (LBL) integration can provide a solution with high level of accuracy for this kind of problem (Cassol *et al.*, 2014). However, due to the many thousands of absorption lines present in gases spectra, LBL calculations are computationally expensive (Denison and Webb, 1995a), which often makes the solution impracticable. Thus, to overcome this issue, some global gas models have been developed that can perform the radiative transfer calculations with a satisfactory level of accuracy. One of them is the spectral line-based weighted-sum-of-gray-gases (SLW) model, proposed by Denison and Webb (1993). Problems employing the SLW approach have been solved mostly for black surfaces and a small quantity for gray surfaces (Denison and Webb, 1993, 1995c,b,d; Solovjov and Webb, 2000, 2001, 2008; Solovjov *et al.*, 2011a,b; Pearson *et al.*, 2013; Çayan and Selçuk, 2007). On the other hand, only a limited number of works deal with nongray walls using the spectral models as the SLW model (Denison and Webb, 1995d), the SLW model and k-distribution hybrid (Denison and Webb, 1994), the weighted-sum-of-gray-gases (WSGG) model (Fonseca *et al.*, 2018b,a) and the cumulative wavenumber (CW) method (Solovjov *et al.*, 2013). However, the modeling of the radiative transfer in combustion systems requires the treatment of surfaces whose radiative properties have strong spectral dependence, so that the nongray walls may have a significant influence on radiative transfer (Solovjov *et al.*, 2013). Moreover, there are several applications in engineering in which nongray boundaries play an important role in the radiative process, as, for instance, in the analysis of gas furnaces for controlled heating of materials undergoing thermal processing (Fonseca *et al.*, 2018b).

Thereby, this work proposes a method to make the prediction of the radiative transfer by means of the application of the SLW model in a 1D-domain. This problem is characterized by a non-isothermal homogeneous and non-homogeneous medium composed of a gaseous mixture of water vapor and carbon dioxide confined between two infinite, parallel and nongray walls. The total pressure of the system is 1 atm and the ratio between the partial pressure of the participating species is equal to 2 (p_{H_2O}/p_{CO_2} = 2). Results are compared with the line-by-line integration, in order to quantify the proportion of the deviation when solving the problem with the SLW model and the proposed methodology. Moreover, the importance of considering nongray walls, instead of gray, for an accurate computation of the radiative heat transfer is shown.

2. METHODOLOGY

The SLW is a model based on the absorption-line blackbody distribution function, that is defined as the fraction of the blackbody energy in the portions of the spectrum where the high-resolution spectral absorption cross-section of the gas $C_{abs,\eta}$ is less than the prescribed value C_{abs}. The scope of this model is to replace the spectral integration over the wavenumber with an integration over the spectral absorption cross-section. The distribution function is expressed as (Denison and Webb, 1995c):

$$F_s(C_{abs}, T_b, T_g, P_T, Y_s) = \frac{1}{\sigma T_b^4} \sum_i \int_{\Delta \eta_i} E_{\eta,b}(\eta, T_b) d\eta \tag{1}$$

where σ is the Stefan-Boltzmann constant and $E_{\eta,b}$ is the Planck's function evaluated at the wavenumber η and at the blackbody temperature T_b. The subscript i refers to the i^{th} spectral segment, and the summation is performed over all segments covering the entire spectrum. The spectral intervals $\Delta\eta_i$ are dependent on the absorption cross-section C_{abs}, the gas temperature T_g, the total pressure P_T, and the species concentration Y_s. Thus, the fraction of blackbody energy, a_j, for a given source temperature in the spectral regions where the absorption cross-section is between $C_{abs,j}$ and $C_{abs,j+1}$ is computed as the difference of the distribution function evaluated at the two absorption cross-sections:

$$a_j = F_s(C_{abs,j+1}, T_b, T_g, P_T, Y_s) - F_s(C_{abs,j}, T_b, T_g, P_T, Y_s) \tag{2}$$

Although the definition of the coefficient a_j in the SLW model is different than those the WSGG model, the radiative transfer equation (RTE) has the same form in both methods. So, in the absence of scattering, the RTE for the SLW model is written as (Denison and Webb, 1995c):

$$\frac{dI_j}{ds} = -\kappa_j I_j + \kappa_j a_j I_b \tag{3}$$

In the above equation, I_j and κ_j are the radiative intensity and the absorption coefficient of the medium, respectively, associated with the j^{th} gray gas, and $I_b = \sigma T^4/\pi$ is the blackbody intensity, which is given by the Planck's distribution law. Considering Figure 1, Eq. (3) can be written for the positive and negative directions, according to the discrete ordinates method (DOM), as:

$$\mu_l \frac{dI_{j,l}^+}{ds} = -\kappa_j I_{j,l}^+ + \kappa_j a_j I_b \tag{4}$$

$$-\mu_l \frac{dI_{j,l}^-}{ds} = -\kappa_j I_{j,l}^- + \kappa_j a_j I_b \tag{5}$$

In these equations, μ_l is the cosine in the l direction, $I_{j,l}^+$ and $I_{j,l}^-$ are the positive and negative intensities, respectively. Assuming nongray walls, the boundary condition for Eq. (3) is given by (Fonseca *et al.*, 2018a):

$$I_{w,j} = \varepsilon a_j(T_w) I_b(T_w) + \frac{(1-\alpha)}{\pi} G_j \tag{6}$$

where $G_j = \int_0^\infty G_{j,\eta} d\eta$ is the total hemispherical irradiation of the gray gas j, ε is the total hemispherical emissivity of the walls and α is the total hemispherical absorptivity stated, respectively, as:

$$\varepsilon = \frac{1}{I_b(T_w)} \int_0^\infty \varepsilon_\eta I_{\eta,b}(T_w) d\eta \tag{7}$$

$$\alpha = \frac{1}{G_j} \int_0^\infty \alpha_\eta G_{j,\eta} d\eta \tag{8}$$

in which $I_{\eta,b}$ is the blackbody spectral radiative intensity.

If the walls are black ($\varepsilon = \alpha = 1$) with known temperatures (T_w), the boundary condition is $I_{w,j} = a_j I_b$. To calculate ε in Eq. (7), it is only required the knowledge of T_w and the variation of the emissivity (ε_η) of the boundary with the radiation wavenumber. On the other hand, the determination of α from Eq. (8) is more complex, once it involves the correct evaluation of the total hemispherical irradiation G_j, and, as a consequence, entails the need to solve the entire radiation intensity field at each wavenumber (Fonseca *et al.*, 2018a). This procedure, however, spends so much computational time and, thus, is not a good option for engineering applications.

So, the present work proposes the extension to the SLW model of the approach developed in Fonseca *et al.* (2018a). In this methodology, is shown an alternative way to calculate the total hemispherical absorptivity in Eq. (8) that consists in defining a reference medium temperature T_{ref} that satisfy the relation $G_\eta \approx I_{\eta b}(T_{ref})$. Thus, Equation (8) can be rewritten as:

$$\alpha = \frac{1}{I_b(T_{ref})} \int_0^\infty \alpha_\eta I_{\eta b}(T_{ref}) d\eta \tag{9}$$

where, assuming a diffusely emitting and reflecting surface, yields $\alpha_\eta = \varepsilon_\eta$. Hence, the total hemispherical absorptivity in Eq. (9) may be obtained solely from the temperature T_{ref} and the spectral distribution of the emissivity of the boundary. This approach allows to associate the corresponding spectral variations of the emissivity of the boundaries with the spectral variations of the absorptivity of the medium.

After solving Eqs. (4) and (5) for each gray gas and for all directions, the net radiative heat flux, $q_R^{"}$, and the volumetric radiative heat source, S_R, can be determined, respectively, by:

$$q_R^{"}(x) = \sum_{j=0}^{n_g} \sum_{l=1}^{n_d} 2\pi \mu_l \omega_l \left[I_{j,l}^{+}(x) - I_{j,l}^{-}(x) \right] \tag{10}$$

$$S_R(x) = \sum_{j=1}^{n_g} \sum_{l=1}^{n_d} 2\pi \omega_l \kappa_j \left\{ \left[I_{j,l}^{+}(x) + I_{j,l}^{-}(x) \right] - 2a_j(x) I_b(x) \right\} \tag{11}$$

from which can be derived that $S_R = -dq_R^{"}/dx$. In previous equations, n_d and n_g are, respectively, the number of the discrete directions of the DOM and the number of gray gases.

In this work, the solution methodology is performed for a one-dimensional geometry shown in Fig. 1, consisting of two parallel plates separated by the distance of 1 m, between which there is a mixture of carbon dioxide and water vapor. The domain between the plates was divided into 200 equal-sized elements and the DOM was applied to 8 and 30 directions, respectively, for the SLW solution and the LBL integration using the Gauss-Legendre quadrature.

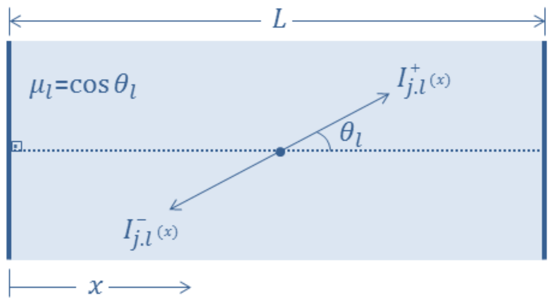

Figure 1. Scheme of the one-dimensional problem analyzed.

3. RESULTS AND DISCUSSION

In the present study, the methodology employed is similar to that proposed by Fonseca *et al.* (2018b), for the weighted-sum-of-gray-gases model, but applied to the SLW model. The method is applied to a one-dimensional medium slab bounded by two infinite, parallel and nongray walls, in which the distance that separates these plates is 1.0 m. It is considered a gaseous mixture composed of water vapor and carbon dioxide, where the total pressure of the system is 1 atm and the ratio between the partial pressure of the participating species is equal to 2 ($p_{H_2O}/p_{CO_2} = 2$). The domain was discretized in 200 uniformly-sized cells and the RTE was solved with the discrete ordinates method considering 8 and 30 directions, respectively, for the SLW solution and the LBL integration. Previous studies show that 8 directions are sufficient to obtain satisfactory results in comparison with the benchmark solution.

In order to evaluate the proposed methodology for the SLW model in relation to the LBL solution applied to nongray surfaces, were considered the same test cases presented in Fonseca *et al.* (2018b). Analogously to the above-mentioned paper, it was chosen to calculate the total hemispherical absorptivity α of the participating medium at the reference temperature T_{ref} = 1100 K, that corresponds to the domain-average temperature of the investigated temperature profile in this work. Results are presented in terms of the radiative heat flux ($q^{"}_R$) and the volumetric radiative heat source (S_R) applying the SLW model and compared against the LBL solution.

3.1 Test case 1

In test case 1, the medium presents homogeneous molar concentration, with partial pressures of H_2O and CO_2 equal to 0.2 atm and 0.1 atm, respectively, and the temperature profile (given in K), depicted in Fig. 2(a), is described by the following equation:

$$T(x) = 400 + 1400\sin^2(2\pi x) \tag{12}$$

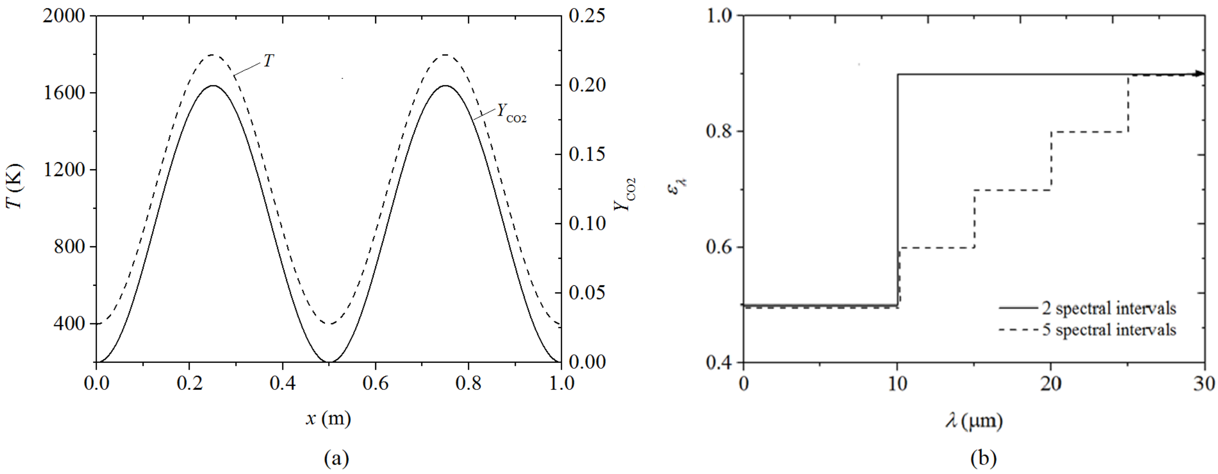

Figure 2. (a) Profiles of temperature and concentration of carbon dioxide; (b) Wall emissivities with two- and five-band stepwise variation.

For simplicity, the walls are considered identical and, therefore, have the same spectral distribution of emissivity ε_λ (presented in terms of the wavelength λ, instead of the wavenumber η, just for convenience in this study), however, the proposed methodology is not restricted to this situation. The emissivity profile for the test case 1 is represented by a stepwise function composed of two constant values, as illustrated in Fig. 2(b), such that: ε_λ = 0.5 for $\lambda \leq 10$ μm and ε_λ = 0.9 for $\lambda >$10 μm.

Considering the temperature profile presented in Eq. (12), the wall temperature is T_w = 400 K. So, applying the Eq. (7), the total hemispherical emissivity of the walls is equal to ε = 0.7076. As in this paper the surfaces are not assumed to be gray, the values of emissivity and absorptivity are not equivalent ($\varepsilon \neq \alpha$). Following the approach proposed by Fonseca *et al.* (2018b), the value of the total hemispherical absorptivity obtained through the Eq. (8) in the optimal reference medium temperature, which is approximately 1100 K for this study, is α = 0.5272. Moreover, also is interesting to evaluate the accuracy of the applied methodology by means of comparisons of the normalized deviations between the radiative heat fluxes and the radiative heat sources obtained with the SLW model and the LBL solution:

$$\delta = \left| \frac{q^{"}_{R,SLW} - q^{"}_{R,LBL}}{max(q^{"}_{R,LBL})} \right| \times 100\% \tag{13}$$

$$\zeta = \left| \frac{S_{R,SLW} - S_{R,LBL}}{max(S_{R,LBL})} \right| \times 100\% \tag{14}$$

in which δ and ζ are the local deviations of $q^{"}_R$ and S_R, respectively; $max(q^{"}_{R,LBL})$ and $max(S_{R,LBL})$ are the maximum absolute values of heat flux and radiative heat source, respectively. Further on, the normalized percentage differences will be presented in terms of the maximum and average deviations (denoted posteriorly by the subscripts max and avg, respectively).

Figures 3(a) and 3(b) show, respectively, the behaviors of the radiative heat flux and the radiative heat source for the test case 1 considering the LBL nongray solution and the SLW model evaluated at the reference medium temperatures T_{ref} = 400 K (equivalent to assuming the surfaces as gray, i. e., $\varepsilon = \alpha$) and T_{ref} = 1100 K (corresponding to the case with the domain-average temperature). According to Table 1, the maximum percentage differences between the LBL nongray and the SLW gray solution (SLW model applied to 400 K) are 17.5% and 14% for q''_R and S_R, respectively. Comparing the LBL solution and the SLW model to T_{ref} = 1100 K, the maximum deviations found were 9%, for the heat flux, and 11.5%, for the radiative heat source, which indicates a good improvement in the result in relation to the case assuming gray walls. It is important to observe that there was a considerable reduction in the discrepancies in both radiative heat flux and heat source, so that the average deviation for fell from 9% to less than 5%, for example. However, in Fonseca *et al.* (2018b), are reported maximum deviations of 10% for this test case, which suggests that, for a participating medium filled with a homogeneous mixture of water vapor and carbon dioxide, the SLW model tends to present a less satisfactory performance regarding to the LBL solution than with the WSGG model calculated at T_{ref} = 1100 K. Previous works show that the performance of the SLW model is better than that of the WSGG model when studying problems with pure species (for instance, H_2O or CO_2).

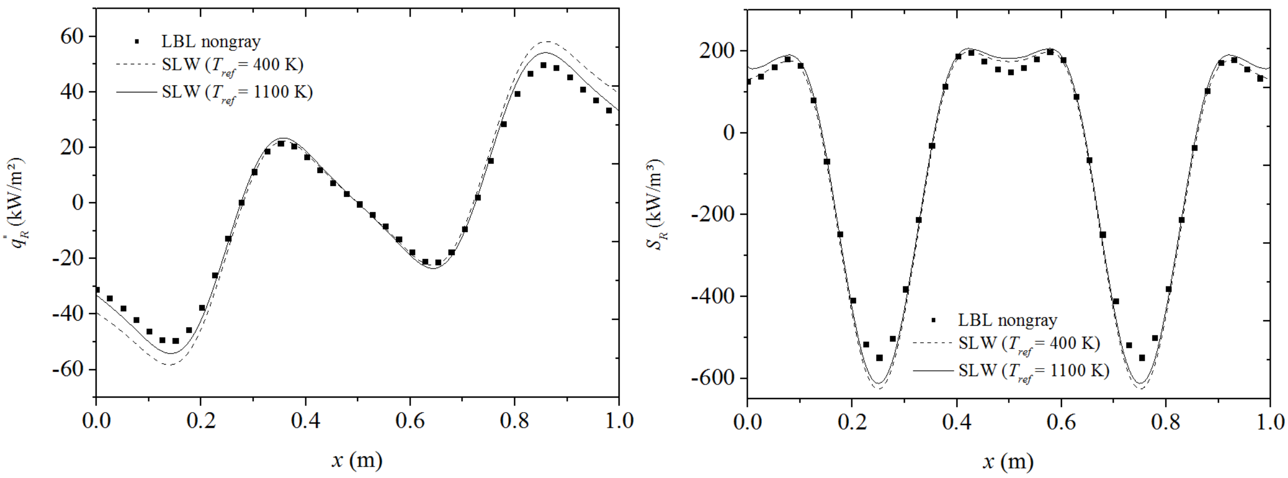

Figure 3. Radiative heat transfer results for the test case 1: (a) Radiative heat flux; (b) Radiative heat source.

Table 1. Maximum normalized deviations between the LBL nongray solution and the proposed SLW model for case 1.

LBL nongray x SLW (T_{ref} = 400 K)				LBL nongray x SLW (T_{ref} = 1100 K)			
δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)
17.50	9.02	14.00	4.10	9.03	4.93	11.50	3.95

3.2 Test case 2

For test case 2, it is considered the same temperature profile used in case 1, Eq. (12), but the medium concentration, presented in Fig. 2(a), is described by:

$$Y_{CO_2} = 0.2\sin^2(2\pi x) \tag{15}$$

where Y_{CO_2} is the molar concentration for carbon dioxide. To keep the same ratio p_{H_2O}/p_{CO_2} = 2 of the previous test case, it is assumed that Y_{H_2O} = $2Y_{CO_2}$. The emissivity profile is given by a stepwise function with five constant values, as shown in Fig. 2(b), according to the spectral distribution of Table 2.

Figures 4(a) and 4(b) present the radiative heat flux and the radiative heat source obtained through the proposed methodology applied to the SLW model evaluated at T_{ref} = 400 K and T_{ref} = 1100 K against the nongray solutions. For this case, the emissivity, evaluated at the wall temperature (T_w = 400 K), is ε = 0.6011, and the absorptivity, calculated at the medium reference temperature (T_{ref} = 1100 K), is α = 0.5111. Analogously to case 1, the proposed methodology for 1100 K shows an improvement over the gray solution, when compared to the LBL integration, since the maximum deviations of 20.6% and 16.8% for q''_R and S_R decay to 11.6% and 13.5%, respectively, as shown in Table 3. Nevertheless, the highest percentage deviation between the T_{ref} = 1100 K and nongray solutions reported in the paper of Fonseca *et al.* (2018b), was less than 3% for the case with medium with variable molar concentration, in addition to an average deviation of not more than 2%. Again, as in the previous case, the WSGG model proved to be a better alternative than the SLW

Table 2. Spectral distribution of the emissivity for case 2.

ε_λ	λ
0.5	$\lambda \leq 10\mu m$
0.6	$10\mu m < \lambda \leq 15\mu m$
0.7	$15\mu m < \lambda \leq 20\mu m$
0.8	$20\mu m < \lambda \leq 25\mu m$
0.9	$\lambda > 25\mu m$

model to represent the results found by the LBL solution when the medium is composed of a mixture of H_2O and CO_2.

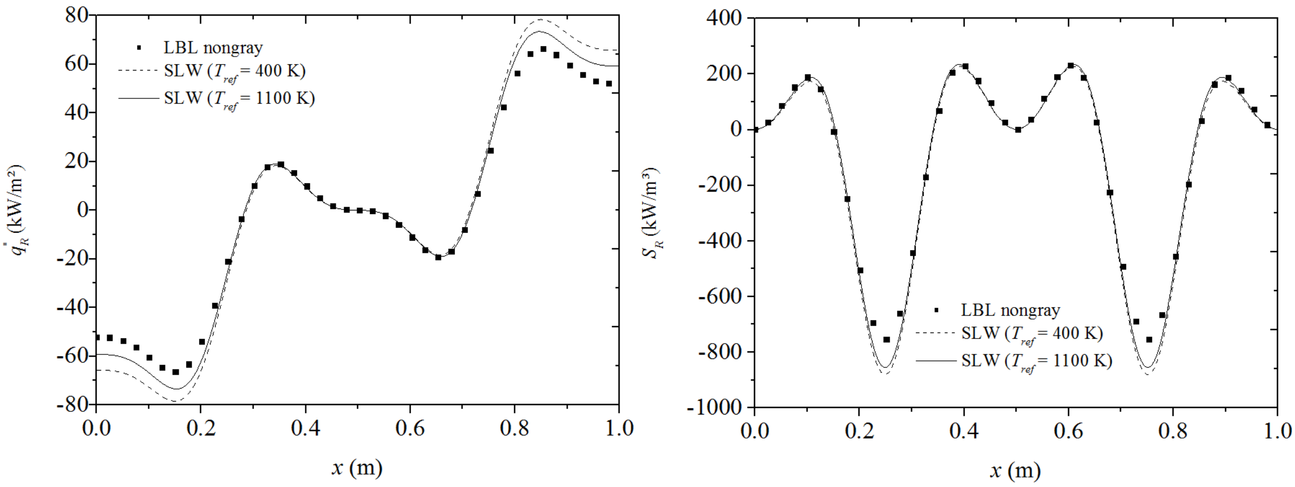

Figure 4. Radiative heat transfer results for test case 2: (a) Radiative heat flux; (b) Radiative heat source.

Table 3. Maximum normalized deviations between the LBL nongray solution and the proposed SLW model for case 2.

LBL nongray x SLW (T_{ref} = 400 K)				LBL nongray x SLW (T_{ref} = 1100 K)			
δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)
20.59	9.96	16.80	4.01	11.63	5.60	13.50	3.38

For the two test cases analyzed, the SLW model presented a performance lower than that reported by the paper that was the main reference on which the present study was based (Fonseca *et al.*, 2018b), which is, in fact, a topic that deserves a little attention, since, for being a method with a higher level of complexity, the most obvious expectation would be that the result would improve due to the greater precision of the method. However, the objective of this work was just to promote the application of the methodology proposed to other spectral gas models, without restricting it only to the WSGG model, so that a detailed study of the problem has not yet been done. For example, the continuity of the work could be used to investigate the utilization of other ways of determining the optimum temperature, rather than employing the simple arithmetic mean, for the calculation of the absorptivity of the medium and other temperature and molar concentration profiles.

3.3 Comparison between gray and black solutions

In view of the maximum deviations of the order of 13% shown in Tables 1 and 3, which illustrate the percentage differences between the LBL integration applied to nongray surfaces and the SLW model employed with the proposed methodology (T_{ref} = 1100 K) for the test cases 1 and 2, a possible interpretation would be that the formulation presented in this study is not adequate and that the discrepancies found are due to the simplifications used for the proposition of the method. However, Table 4 shows a more appropriate comparison with the standard maximum deviations between LBL and SLW solutions, both applied to gray walls (T_{ref} = 400 K) and between LBL and SLW solutions, both applied to black walls. According to this table, it is seen that the maximum deviations between both gray and black surfaces are the same magnitude as those found for the comparisons between nongray LBL and the proposed methodology, so that it can be concluded that the disagreements between the approaches are not simply due to problems in the development of the method.

Table 4. Maximum normalized deviations between the gray and black solutions for cases 1 and 2.

Test case	LBL gray x SLW gray				LBL black x SLW black			
	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)	δ_{max} (%)	δ_{avg} (%)	ζ_{max} (%)	ζ_{avg} (%)
1	8.21	4.45	10.94	3.61	6.84	3.56	9.91	3.21
2	11.53	5.65	13.59	3.37	10.95	4.85	14.56	3.93

4. CONCLUSIONS

In this paper, it was studied the radiative heat transfer in a 1D-medium slab filled by homogeneous and non-homogeneous mixtures composed of water vapor and carbon dioxide. This study presented an extension of the proposed approach by Fonseca *et al.* (2018b), applied to the SLW model. The methodology provides a simplified alternative for the line-by-line calculations of nongray boundaries by assuming that the total absorptivity of the walls may be determined considering that the spectral irradiation to the surfaces is equivalent to that of a blackbody at a reference temperature T_{ref}. It was verified an improvement in the results for T_{ref} = 1100 K and those obtained for gray surfaces (T_{ref} = 400 K) compared to the LBL solution calculated for nongray walls, since the maximum and average deviations between the approaches were reduced. However, the deviations reported in the work that employs the WSGG model (Fonseca *et al.*, 2018b) present a greater agreement with the LBL solution, which indicates that, when studying gaseous mixtures, the SLW model tends to show less success in the radiative heat flux and heat source calculations. Nevertheless, it is important to point out that the results presented in this work are only part of a preliminary study, in which the main objective was to extend the application of the methodology already applied to the WSGG model for the SLW model. Therefore, to ensure that the performance of the SLW model is, in fact, lower than that of the WSGG model, it would be necessary to investigate several other profiles of temperature, emissivity and concentration of H_2O and CO_2 in future works.

5. ACKNOWLEDGEMENTS

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