

APPLICATION OF THE WEIGHTED-SUM-OF-GRAY-GASES MODEL IN ENCLOSURES WITH GRAY SURFACES

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Abstract. Thermal radiation is the main heat transfer mode in combustion problems due to high temperatures. However, it has been a challenge to make predictions about these processes due to the complex spectral dependence of the absorption coefficient. Alternatively, it might use spectral models to obtain accurate results but requiring low computational effort, as the weighted-sum-of-gray-gases (WSGG), which is employed to perform the spectral integration of the radiative transfer equation (RTE). This method consists of dividing the spectrum into regions where the absorption coefficient can be considered constant and each band is represented by one gray gas. In this work, the WSGG model is applied to a flat plate parallel medium, in which surfaces are gray, with a mixture of carbon dioxide and water vapor based on the HITEMP 2010 database, in homogeneous and isothermal and non-isothermal conditions. The application of gas model is invariably demonstrated for black surfaces, for which the intensities at the boundaries are known, so the present study makes an advance to show its application to gray surfaces. A comparison between the results obtained by the WSGG model and the line-by-line (LBL) solution shows that the method is a good option to account the emissivity effect when the boundaries are not black.

Keywords: Radiative transfer, WSGG model, LBL integration, gray surfaces

1. INTRODUCTION

Works involving heat transfer by thermal radiation are highly relevant for engineering applications, such as furnaces and combustion chambers. However, the understanding of radiative phenomena has been challenging due to the complexity of the variables that govern the process, for instance, the irregular dependence of the absorption coefficient with respect to wavenumber, temperature and participating species.

Particularly in combustion processes, radiation is generally the dominant heat transfer mechanism due to high temperatures. In these systems, calculating of the radiation emitted and absorbed by participating gases, such as carbon dioxide and water vapor, it is an arduous task. So, alternatively, it might be applied the weighted-sum-of-gray-gases (WSGG) model, proposed by Hottel and Sarofim (1967), to solve the spectral integration of the radiative transfer equation (RTE). This method, besides replacing the spectral integration by a few bands with uniform absorption coefficients, where each one represents a gray gas, makes possible to estimate the real radiative characteristics of participating gases with low computational time. The weighting coefficients express to the fractions of the blackbody energy in the spectral region in which the gray gases are situated, which are obtained, generally, from fitting experimental data. Smith *et al.*, 1982, determined weighting absorption coefficients of gray gases and water vapor from the exponential wide-band model. Maurente *et al.*, 2007, compared the standard WSGG with the gas model ALBDF (absorption-line blackbody distribution function), studying the radiative transfer in a cylindrical chamber with methane and fuel oil. Using three gray gases, Galarça *et al.*, 2008, proposed new absorption coefficients and temperature dependent weighting functions employing the WSGG model. In recent studies, Dorigon *et al.*, 2013, and Ziemniczak *et al.*, 2013, proposed new coefficients for the WSGG for a mixture of CO₂ and H₂O, both for a parallel flat medium bounded by black walls. A similar analysis was implemented by Cassol *et al.*, 2014, discussing the WSGG model for media composed by concentrations of the same mixture, but including soot.

This paper presents the WSGG model applied to a one-dimensional system, which is formed by a flat plate parallel medium, in which surfaces are gray, for a mixture composed by carbon dioxide and water vapor, in homogeneous and isothermal and non-isothermal conditions at 1.0 atm, making use of HITEMP 2010 database. The emissivities of the surfaces ranging from 0.5 to 1.0 and is considered pressure ratio equal to 2 ($p_{H_2O} = 0.2$ atm and $p_{CO_2} = 0.1$ atm), which are typical products in combustion of methane. According to Modest, 2003, the WSGG model can be also applied when the boundaries are gray, and not only for black walls, although the most papers in literature apply black surfaces due to the computational effort is lower. So this work brings a contribution to discuss the WSGG model employed to gray

surfaces. The radiative transfer equation is solved by the discrete ordinates method and the accuracy 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 equation and the WSGG model

According to Siegel and Howel (2002), the radiative heat transfer, in participating and nonscattering media, is governed by the radiative transfer equation (RTE), which quantifies the spectral radiation intensity over a path in the medium.

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

Where κ_{η} is the absorption coefficient corresponding to wavenumber η and $I_{\eta}(s)$ and $I_{\eta b}(s)$ indicate the spectral intensity and the blackbody spectral intensity, respectively, at position s . Moreover, as Eq. (1) considers a mixture formed by carbon dioxide and water vapor, in the present work, the absorption coefficient is given by the sum of the absorption coefficient of each species.

The establishment of the spectral models has been important to the radiation modeling in participating media. The most elementary method is the gray gas (GG) model, in which the absorption coefficient is considered uniform over the spectrum, being independent of the temperature and of the partial pressure of the participating species. Despite of simplicity, this model presents low reliability, because it fails in the determination of local absorption, although provides a good approximation of the local emission.

Another alternative is the weighted-sum-of-gray-gases (WSGG) model, which replaces the integration of the entire spectrum by a few number of gray gases plus transparent windows. Thereby, the spectrum is divided into regions in which it assumes that the absorption coefficient is constant and each band is represented by one gray gas. Therefore, the WSGG model requires the determination of absorption coefficients of the gray gases and the temperature dependence coefficients, which, generally, are obtained from fitting data of total emittances for each species that composes the medium. Currently, it is possible in due to the development of spectral databases, for example, HITRAN and HITEMP, which present thousands of spectral lines with dependence of wavenumber. For combustion studies, is more appropriate to use the HITEMP database, because the data are obtained for temperatures around 1000 K and 1500 K, which means that extrapolations to higher temperatures with this database are most adequate than HITRAN, which is obtained at the reference temperature of 296 K. Lastly, the essence of the WSGG model is to generate correlations for each participating species, which are superposed to compose the correlations of the gaseous mixture (Cassol *et al.*, 2014).

Originally, the WSGG model was proposed for situations where the medium is isothermal and homogeneous. However, have 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). Applying the WSGG model to Eq. (1), the total radiation intensity can be determined by the summation of the partial intensities, I_i , in W/m² sr, to each gray gas, calculated from the integration of the RTE in the spectrum region related to gas i :

$$I(s) = \sum_{i=1}^I I_i(s) \quad (2)$$

So, the RTE can be rewritten in the form of the Eq. (3):

$$\frac{dI_i(s)}{ds} = -\kappa_{p,i} p_a(s) I_i(s) + \kappa_{p,i} p_a(s) a_i(s) I_b(s) \quad (3)$$

where the quantities partial pressure of the absorbing-emitting species, $p_a(s)$, temperature dependent coefficient, $a_i(s)$ and total blackbody intensity, $I_b(s)$, are evaluated at local conditions. The total blackbody intensity is given by Planck's distribution law, as shown in Eq. (4):

$$I_b = \frac{\sigma T^4}{\pi} \quad (4)$$

in which σ is the Stefan-Boltzmann constant, equal to 5.6708×10^{-8} W/m² K⁴, and the T is the temperature, in K, at position s .

2.2 The gray surfaces

In order to obtain a global solution, Eq. (1) might be solved by any spatial and spectral integration method. In this study, was used the discrete ordinate method, which allows the transformation of the RTE into a set of simultaneous partial differential equations, which can be solved through a numerical method, such as the finite volume method. The basis of this method is the discretization of the directional variation of the radiation intensity (or the spectral radiation intensity) in a finite number of solids angles. More specifically, the transport problem is solved for a set of discrete directions covering the total solid angle range of 4π sr around each point. Therefore, the method is, fundamentally, a finite differencing of the directional dependence of the equations that govern the problem.

This paper proposes to solve a flat plate parallel medium, in which surfaces are gray, with a mixture of carbon dioxide and water vapor based on the HITEMP 2010 database, as shown in Fig. 1(a). One important point is that the WSGG model, according to literature, presents reliable results for black boundaries, but there are few studies in which the walls do not have emissivities equals to 1.0. Therefore, the main goal in this article is to evaluate the effect of emissivity for gray walls, employing the weighted-sum-of-gray-gases and analyzing the reliability of the model.

So, according to the discrete ordinates method, the spectral intensities in the forward and backward directions, $I_{i,l}^+(s)$ and $I_{i,l}^-(s)$, are calculated from Eqs. (5) and (6), respectively:

$$\mu_l \frac{dI_{i,l}^+(s)}{ds} = -\kappa_{p,i} p_a(s) I_{i,l}^+(s) + \kappa_{p,i} p_a(s) a_i(s) I_b(s) \quad (5)$$

$$-\mu_l \frac{dI_{i,l}^-(s)}{ds} = -\kappa_{p,i} p_a(s) I_{i,l}^-(s) + \kappa_{p,i} p_a(s) a_i(s) I_b(s) \quad (6)$$

Where μ_l indicates the cosine in the l direction and $a_i(T)$ is the weighting factor for the i -th gray gas, which depends only on temperature and is given by polynomial function, as shown in Eq. (7).

$$a_i(T) = \sum_{j=0}^J b_{i,j} T^j \quad (7)$$

The terms $b_{i,j}$ are the polynomial coefficients of j -th order for the i -th gray gas. To ensure energy conservation, the transparent window is calculated as $a_0(T) = 1 - \sum_{i=1}^I a_i(T)$. Assuming that the medium has gray surfaces and emissivities, ε , the boundary conditions for Eqs. (5) and (6) are, respectively:

$$I_{i,l}^+(s=0) = \frac{\varepsilon a_i \sigma T^4(s=0)}{\pi} + \frac{1-\varepsilon}{\pi} \int I_{i,l}^-(s=0) \cos \theta_l dw \quad (8)$$

$$I_{i,l}^-(s=S) = \frac{\varepsilon a_i \sigma T^4(s=S)}{\pi} + \frac{1-\varepsilon}{\pi} \int I_{i,l}^+(s=S) \cos \theta_l dw \quad (9)$$

Where θ_l represents the angle between the incoming direction and the surface normal, w is the solid angle and $s=0$ and $s=S$ indicate the domain boundaries to the left and to the right, respectively, as shown in the representation of the Fig 1(a).

Moreover, the solution of Eqs. (5) and (6) allows to determine the net radiative heat flux, q_R'' , in W/m^2 , and volumetric source, $\dot{q}_R$, in W/m^3 , respectively, in each point along the path. It is important to observe that $\dot{q}_R(s) = -dq_R''(s)/ds$.

$$q_R''(s) = \sum_{i=0}^I \sum_{l=1}^L 2\pi \mu_l \omega_l \left[I_{i,l}^+(s) - I_{i,l}^-(s) \right] \quad (10)$$

$$\dot{q}_R(s) = \sum_{i=1}^I \sum_{l=1}^L 2\pi \omega_l \kappa_{p,i} p_a(s) \left\{ \left[I_{i,l}^+(s) - I_{i,l}^-(s) \right] - 2a_i(s) I_b(s) \right\} \quad (11)$$

In which ω_l , in Eqs. (10) and (11), is the quadrature weight for l direction from the discrete ordinates method.

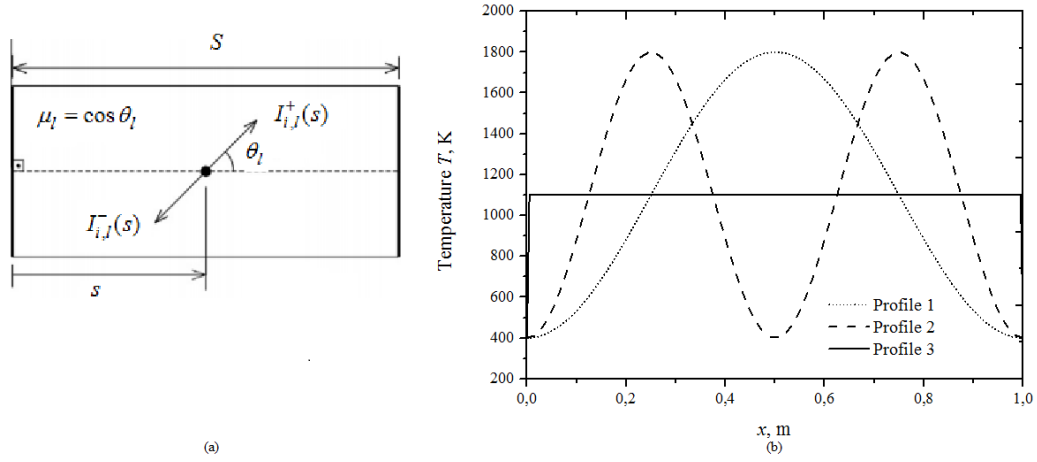


Figure 1. (a) Schematic representation of the one-dimensional domain; (b) Temperature profiles given in Eqs. (12)-(14).

3. RESULTS AND DISCUSSION

3.1 The WSGG coefficients

From the HITEMP 2010 database, Dorigon *et al.*, 2013, obtained correlations for WSGG model for gaseous mixture formed in the combustion of methane at 1.0 atm. Consequently, the partial pressures of products are $p_{\text{CO}_2} = 0.1$ atm and $p_{\text{H}_2\text{O}} = 0.2$ atm. These correlations 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. The WSGG coefficients shown in Tab. 1 are 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 can become independent of the number of gray gases; specifically, for the case analyzed, four gray gases are sufficient.

Table 1. WSGG coefficients for four gray gases, $i = 4$, $p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 2$ (Dorigon *et al.*, 2013).

i	$\kappa_{p,i} \text{ (atm m)}^{-1}$	$b_{i,0}$	$b_{i,1} \text{ (K}^{-1}\text{)}$	$b_{i,2} \text{ (K}^{-2}\text{)}$	$b_{i,3} \text{ (K}^{-3}\text{)}$	$b_{i,4} \text{ (K}^{-4}\text{)}$
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

3.2 Comparison between WSGG model and LBL solution

In this paper, it is considered a few isothermal, non-isothermal and homogeneous cases in order to evaluate the accuracy of the WSGG model against the benchmark line-by-line (LBL) solution for a domain formed by a flat parallel medium, which surfaces are gray and the emissivities are different to 1.0 (situation corresponding to black surfaces), separated by a distance of 1.0 m, as shown in Fig 1(a). Using a Gauss-Legendre quadrature, the discrete ordinates method was applied to 30 directions. The temperature profiles are proposed in Eqs. (12)-(14), which will be referred, posteriorly, as Profile 1, Profile 2 and Profile 3, respectively.

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

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

$$T(x) = \begin{cases} 400 \text{ K, if } x = 0 \text{ and } x = 1.0 \\ 1100 \text{ K, } \forall x \neq 0 \text{ and } \forall x \neq 1.0 \end{cases} \quad (14)$$

The maximum temperature in Eq. (12), 1800 K, occurs in the middle of the domain and the minimum value of temperature is 400 K. Eq. (13) presents a symmetrical profile, in which the minimum temperature is 400 K and the maximum value reaches 1800 K in two positions: $x = 0.25$ m and $x = 0.75$ m. Eq. (14) shows a uniform medium, in which the walls temperature is 400 K and the medium temperature is 1100 K, which corresponds exactly to the average temperature of the domain in previous profiles. Figure 1(b) demonstrates these behaviors.

In order to evaluate the deviations between the WSGG model and the LBL solution, the following equations were used to estimate the maximum and average errors for the radiative heat flux and the volumetric source, δ and ζ , respectively. The reason to show the variations of the heat flux and the source term is that these quantities are of great importance for engineering analysis. Further, the notation $\delta_{\max}$ and δ_{avg} will be employed to designate the maximum and average errors for radiative heat flux, respectively, and $\zeta_{\max}$ and ζ_{avg} to the maximum and average errors for source term, respectively.

$$\delta = \frac{\left| q_{R,WSGG}'' - q_{R,LBL}'' \right|}{\max \left| q_{R,LBL}'' \right|} \times 100\% \quad (15)$$

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

As the scope of this paper is to analyze the emissivity effect on the calculation of the radiative heat flux and the volumetric source, the next figures present results for a few number of illustrative situations in which the emissivity assumes values of 0.5, 0.8 and 1.0 (corresponds to the case of black surfaces). Previous studies show that the results obtained by LBL and WSGG methods present good agreement, so that the result was computed for black walls in order to compare it with the estimation for gray surfaces. The cases analyzed are for isothermal and non-isothermal medium and homogeneous concentrations for temperature profiles presented previously and for four gray gases.

Figures 2(a)-2(f) show the radiative heat flux and the source term for the temperature profile described in Eq. (12) for emissivities ranging from 0.5 to 1.0, making comparisons between WSGG and LBL solutions. In Figs. 2(a)-2(c), 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 opposite direction, $x > 0.5$ m. For the other hand, the source term, in Figs. 2(d)-2(f), has the maximum absolute value in the average distance, $x = 0.5$ m, in which the temperature is maximum, i.e., 1800 K. In this case, the negative sign for the source term indicates energy loss due to radiation. As is to be expected, both the heat flux and the source term is noticed that, as the emissivity decreases, occurs a reduction in the intensity of both quantities, since we are moving away from the ideal case, i.e., when $\epsilon = 1.0$ (black surfaces). For instance, when $\epsilon = 0.8$, is expected that q_R'' be reduced by 20% compared to the values obtained for black boundaries due to the reflection which occurs due to the wall is gray. Analogously, for $\epsilon = 0.5$, the amount should decrease to half the value when the emissivity is equal to 1.0. Figures 2(a)-2(f) show a good agreement between WSGG model and LBL solution for all cases examined.

Figures 3(a)-3(f) present the radiative heat flux and the volumetric source corresponding to Profile 2, Eq. (13), which has double symmetry. As can be seen in Figs. 3(a)-3(c), q_R'' is equal to zero 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. Figures 3(d)-3(f) demonstrate that the source term, in the symmetric points, $x = 0.25$ m and $x = 0.75$ m, reaches the maximum values, where the heat flux gradients are higher. Similarly to previous case, it is expected that the radiative heat flux decreases by 20% when $\epsilon = 0.8$ and, when $\epsilon = 0.5$, the amount should reduce to half the initial value. Figures 3(a)-3(f) show a reasonable conformity between both methods for all tests analyzed.

Figures 4(a)-4(f) show a uniform temperature profile, as presented in Eq. (14), in which the medium temperature is constant and both walls are in the same temperature, but with different value of the medium. It perceives a good agreement between the line-by-line and weighted-sum-of-gray-gases solutions for all the cases when it is analyzed the radiative heat flux. However, there is a divergence more relevant between the methods for the volumetric source, showing that the WSGG model presents low performance as the emissivity is reduced.

For the purpose to measure the deviations between WSGG and LBL methods, Tab. 2 makes a comparison of maximum and average errors for radiative heat flux and the volumetric source, δ and ζ , respectively, obtained by Eqs. (15) and (16), with the emissivities ranging from 0.5 to 1.0, for a gaseous mixture of H_2O and CO_2 , whose concentration is homogeneous and the equivalence ratio is equal to 2. Despite of the simplicity of the method, the WSGG model presented satisfactory results for symmetrical and regular temperature profiles, since the maximum values were around 8% and 3% for the maximum and average errors, respectively, for the radiative heat flux; the maximum error for the source term was less than 11% and beneath of 5% for the average error. For the isothermal medium, the deviations

found were less than 2% for the radiative heat flux and around 14% for the source term. The deviations of the Profile 3, specially for $\dot{q}_R$, indicate that WSGG model does not present such good results when applied to low emissivities and media that contain a discontinuity, since, in this case, there is a large temperature gradient between the boundaries and the medium.

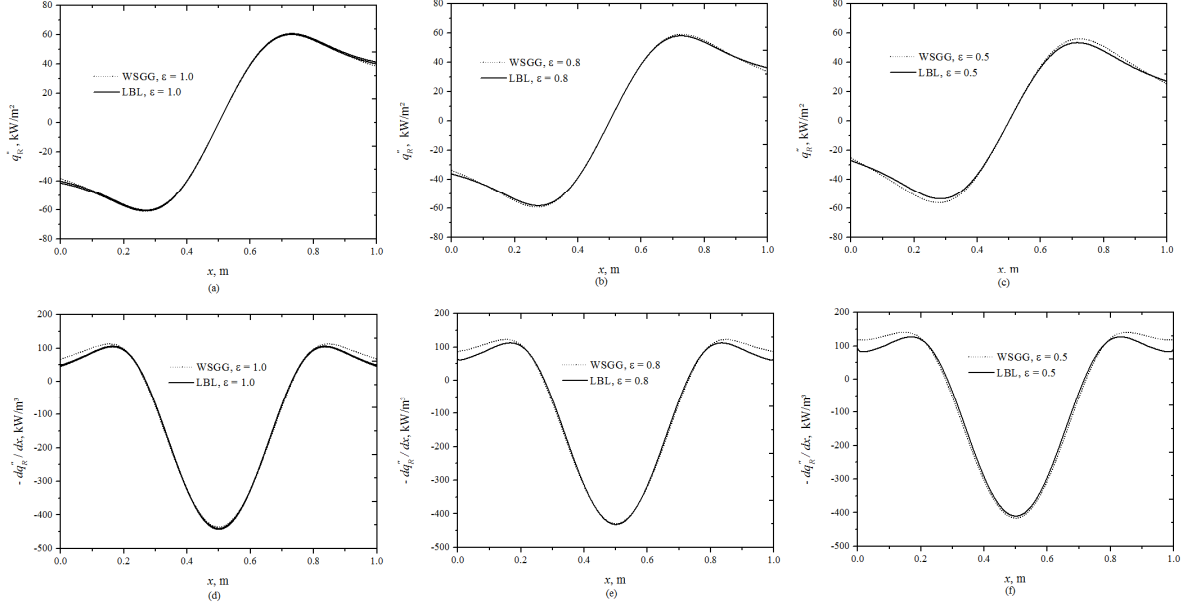


Figure 2. Comparison between the WSGG model and the LBL solution for different emissivities for the temperature profile given in Eq. (12): Radiative heat flux, q_R'' , for: (a) $\varepsilon = 1.0$; (b) $\varepsilon = 0.8$; (c) $\varepsilon = 0.5$; Volumetric source, $\dot{q}_R$, for: (d) $\varepsilon = 1.0$, (e) $\varepsilon = 0.8$; (f) $\varepsilon = 0.5$.

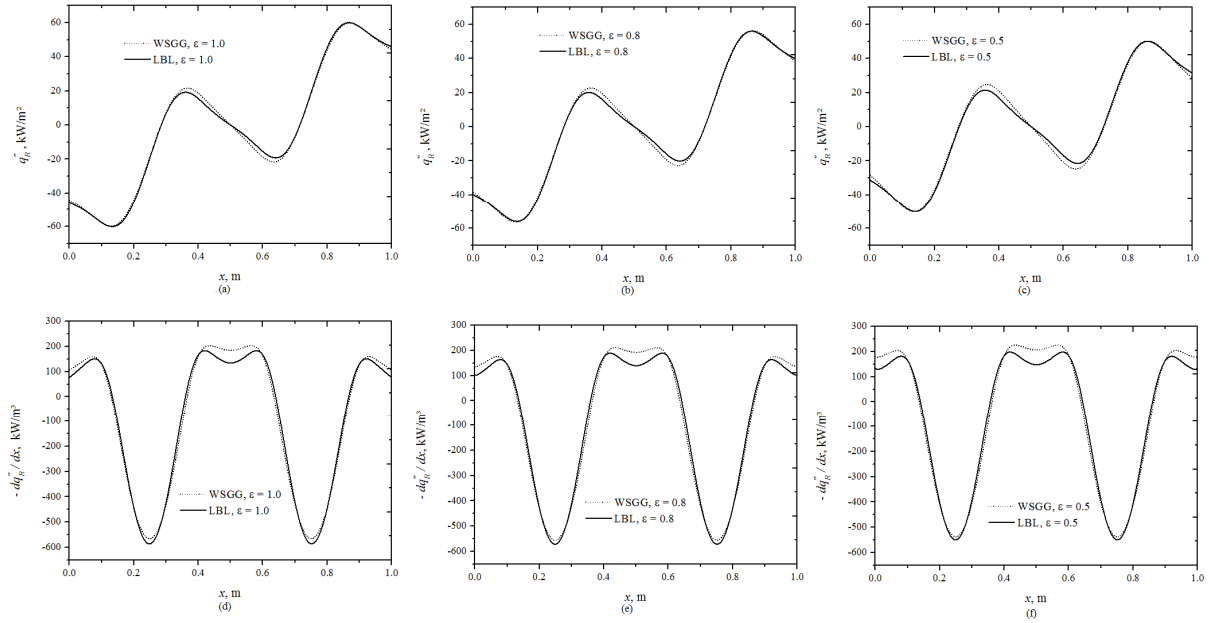


Figure 3. Comparison between the WSGG model and the LBL solution for different emissivities for the temperature profile given in Eq. (13): Radiative heat flux, q_R'' , for: (a) $\varepsilon = 1.0$; (b) $\varepsilon = 0.8$; (c) $\varepsilon = 0.5$; Volumetric source, $\dot{q}_R$, for: (d) $\varepsilon = 1.0$, (e) $\varepsilon = 0.8$; (f) $\varepsilon = 0.5$.

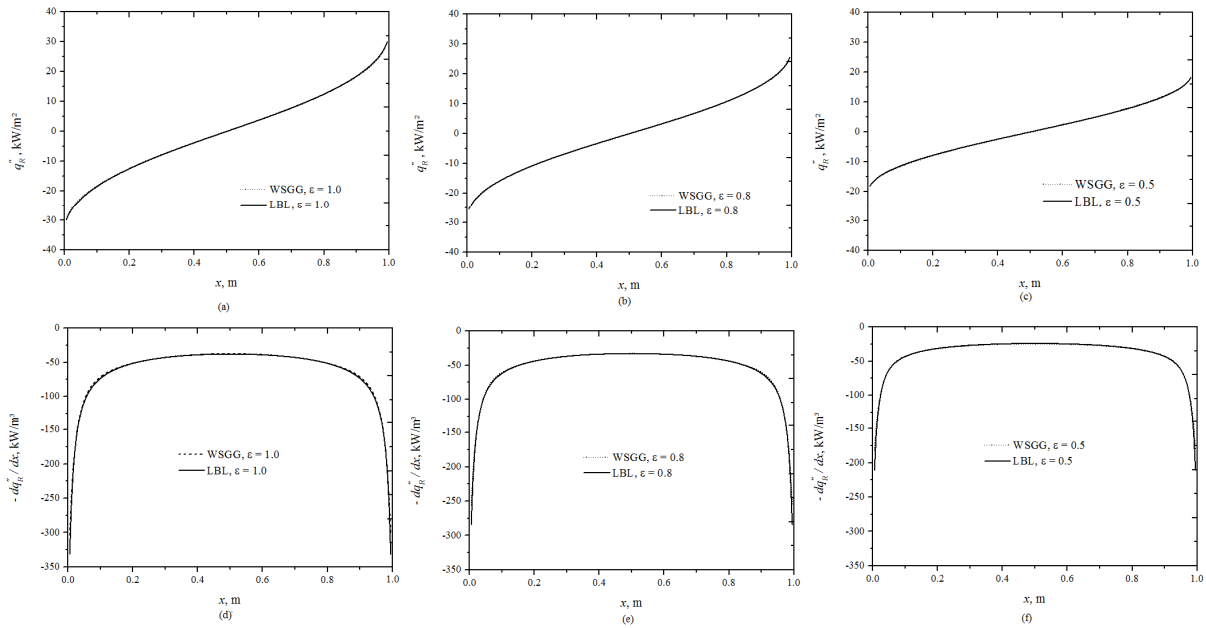


Figure 4. Comparison between the WSGG model and the LBL solution for different emissivities for the temperature profile given in Eq. (14): Radiative heat flux, q_R'' , for: (a) $\varepsilon = 1.0$; (b) $\varepsilon = 0.8$; (c) $\varepsilon = 0.5$; Volumetric source, $\dot{q}_R$, for: (d) $\varepsilon = 1.0$, (e) $\varepsilon = 0.8$; (f) $\varepsilon = 0.5$.

Table 2. Maximum and average deviations of the WSGG and LBL solutions for radiative heat flux and source term.

Emissivity	Radiative heat flux (q_R'')						Source term ($\dot{q}_R$)					
	$\varepsilon = 1.0$		$\varepsilon = 0.8$		$\varepsilon = 0.5$		$\varepsilon = 1.0$		$\varepsilon = 0.8$		$\varepsilon = 0.5$	
Deviation (%)	$\delta_{\max}$	δ_{avg}	$\delta_{\max}$	δ_{avg}	$\delta_{\max}$	δ_{avg}	$\zeta_{\max}$	ζ_{avg}	$\zeta_{\max}$	ζ_{avg}	$\zeta_{\max}$	ζ_{avg}
Profile 1	4.83	0.98	4.24	1.17	5.82	3.07	4.98	1.85	6.17	2.31	8.65	3.86
Profile 2	5.34	1.96	6.10	2.16	8.04	3.29	8.65	3.59	9.27	3.95	10.79	4.70
Profile 3	1.63	0.37	1.16	0.13	0.92	0.52	8.37	0.38	9.96	0.34	13.79	0.46

4. CONCLUSIONS

This work used the correlations for the WSGG coefficients obtained by Dorigon *et al.*, 2013, for analyzing the emissivity effect in the radiative heat transfer in a flat parallel medium, whose surfaces are gray, filled with a homogeneous concentration of a gaseous mixture of water vapor and carbon dioxide, in which isothermal and non-isothermal conditions. The pressure ratio is equal to 2 ($p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 2$) and were used four gray gases. It was verified that, when the emissivity is near to 1.0, the WSGG model provides satisfactory results when compared with LBL solution, since the deviation was around 10%. However, the discrepancy between the two methods becomes more significant when the emissivity is reduced to 0.5 and where there is a high temperature gradient, although the results are reasonable considering the simplicity of the model WSGG.

5. ACKNOWLEDGEMENTS

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