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Generation of new correlations for the weighted-sum-of-gray-gases model for carbon monoxide

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Abstract. *The weighted-sum-of-gray-gases (WSGG) model has been extensively applied to perform the spectral integration of the radiative transfer equation in combustion problems, as an alternative to the highly computational demand of the line-by-line (LBL) integration. In the WSGG model, the nongray gas is replaced by a number of gray gases, for which the heat transfer rates are independently calculated. The parameters for the WSGG model are obtained by fitting total emittance data. In this work, new correlations are obtained for the WSGG model for monoxide carbon (CO) molecules based on the HITEMP 2010 database. The interest in studying the CO molecule is based on some combustion processes where the monoxide of oxygen is found in a significant amount, as biomass gasification technology. The path-length ranges are from 0.0001 atm.m to 10 atm.m, while the temperature varies between 400 K and 2500 K. The WSGG correlations are generated for four gray gases. A one-dimensional medium is solved with the WSGG model for non-isothermal, homogeneous and non-homogeneous conditions. The results show that the obtained WSGG correlations provide accurate results for CO compared with the LBL solution, as it has been observed for* H_2O *and* CO_2 *molecules.*

Keywords: *absorption coefficient, HITEMP 2010, WSGG model, LBL benchmark solution, CO molecule*

1. INTRODUCTION

Studies involving processes of heat transfer by radiation are very important in several scientific and industrial applications. However, the thermal radiation presents challenges for a complete understanding of the phenomenon and the main variables governing the process. As a consequence, it requires a modeling that accurately solves the phenomenon of heat transfer by radiation, in order to improve the operation of combustion systems, allowing for a reduction in fuel consumption and consequently the reduction of greenhouse gas emissions in the atmosphere.

Hottel and Sarofim (1967) proposed the weighted-sum-of-gray-gases (WSGG) model, which considers a few bands with uniform absorption coefficients, each band corresponding to a gray gas. The weighting coefficients correspond to the fractions of the blackbody energy in the spectrum regions where the gray gases are located. In general, these coefficients are obtained by fitting experimental data. In this way, Smith et al. (1982) obtained weighting functions and absorption coefficients of gray gases and water vapor by fitting data generated from the exponential wide-band model, and considering three gray gases. Galarça et al. (2008) also presented new absorption coefficients, for three gray gases based on data generated from the SLW model. Kangwanpongpan et al., 2012, obtained new correlations for the WSGG model using the HITEMP 2010 database to predict the radiative transfer in oxy-fuel gases. Results for the radiative source term obtained with the new correlations were compared with the benchmark line-by-line (LBL) solution. For all test cases, the new oxy-fuel correlations provided the best agreement in comparison with the LBL integration. A similar work was implemented by Dorigon et al., 2012, which proposed new coefficients for the WSGG, also using the HITEMP 2010 database, for a gas mixture of water vapor and carbon dioxide for partial pressure ratios equal to 1.0 and 2.0. Results of the model were compared with the LBL benchmark solution showing good agreement between the methods for different test cases.

Cassol et al., 2014, presented an application of the WSGG model to solve radiative heat transfer in mixtures with arbitrary concentrations of the participating species and for several types of chemical species, however the work considered that the medium was only composed of H_2O, CO_2 and soot. The method is based on first establishing independent correlations for each species, tests cases are presented to assess the accuracy of the method proposed and the original WSGG by comparisons with the LBL.

This study presents new WSGG correlations for the solution of radiation heat transfer in non-isothermal, non-homogeneous medium, for the carbon monoxide (CO). The CO molecule was chosen because there are several processes in literature in which CO is the main product, for instance, in some gasification process. Gasification is a term that is often used to describe thermochemical processes that take place between a solid fuel and a gaseous reacting media, such as air, oxygen or steam, in order to produce a combustible gas that might contain CO and hydrogen (H_2) (Kivisaari et al. 2002).

The correlations are fitted from tabulated values of total emittance, to temperatures from 400K to 2500K, and pressure-path length products from 0.0001 to 10 atm m. The solutions are compared with benchmark LBL solutions to access the accuracy of the model for a few illustrative cases. The literature does not present WSGG correlations based on the up-to-date HITEMP2010.

2. THE WEIGHTED-SUM-OF-GRAY-GASES (WSGG) MODEL

In the WSGG model, the medium is assumed to be composed of a few partial gray gases (usually three) and transparent windows. The absorption coefficient can be considered constant. This model was proposed by Hottel and Sarofin (1967). Figure 1 shows a representation of the model, in which the medium is represented by a number of partial gray gases with absorption coefficient $k_{p,i}$, and transparent windows.

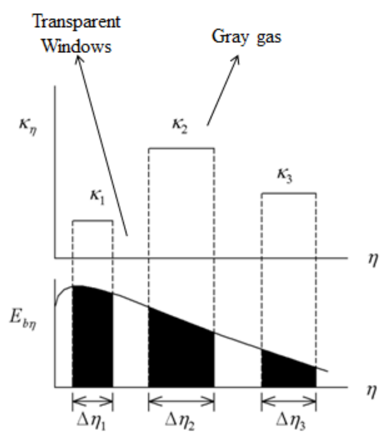


Figure 1. Representation of a medium composed of three gray gases.

2.1 WSGG absorption coefficient

Siegel and Howell (2002) proposed that the Lorentz profile, based on line broadening due to collision, can be used in the determination of the spectral absorption cross-section:

$$C_\eta = \sum_i \frac{S_i}{\pi} \frac{\gamma_i}{\gamma_i^2 + (\eta - \eta_i)^2} \tag{1}$$

where C_η is the absorption cross-section, in units cm^2 / molecule, S_i is the integrated line intensity cm / molecule, η_i is the line location, in cm^{-1} , and γ_i is the half-width, in cm^{-1}, and T is the medium temperature in K. The half-width is calculated by:

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n p_s \gamma_{self,i} + (1 - p_s)\gamma_{air,i} \tag{2}$$

where p_s is the partial pressure, in atm, T is the temperature, T_{ref} is the reference temperature (296 K), γ_{self} is the line self-broadening, γ_{air} is the broadening caused by the air, both in cm $^{-1}$atm^{-1} and n is the temperature dependence coefficient. The parameters n, γ_{self} and γ_{air} are provided by the HITEMP database (Rothman *et al*., 2010).

The integrated line intensity S_i in the HITEMP 2010 is obtained at the temperature of 1000 K, but is converted in a temperature of 296 K in its final compilation. When using the HITEMP2010, it is needed to convert S_i in the desired temperature. According to Rothman *et al*., 2010, the equation below should be used:

$$S_i(T) = S_i(T_{ref})\frac{Q(T_{ref})}{Q(T)}\frac{\exp(-C_2 E_i / T)}{\exp(-C_2 E_i / T_{ref})}\frac{[1-\exp(-C_2 \nu_i / T)]}{[1-\exp(-C_2 \nu_i / T_{ref})]} \tag{3}$$

where Q is the total internal partition sums, dimensionless, ν_i is the energy difference between the initial end final state in cm $^{-1}$, E_i is the energy of the lower state, also in cm $^{-1}$ and C_2 is the is the second Planck's constant, equal to 0.0143877 m.K.

To obtain the absorption coefficient, it is used the following equation:

$$\kappa_\eta = N C_\eta \tag{4}$$

where N is is the Loschmidt number, in units of molecule/(cm^{3}atm),and κ_η is the coefficient absorption,in cm^{-1},

$$N = 2.479 \times 10^{19}\left(\frac{296}{T}\right) \tag{5}$$

In order to obtain the absorption coefficient per unit of pressure, $\kappa_{p,\eta}$, in cm^{-1}atm^{-1}, the following equation is used:

$$\kappa_{p,\eta} = \frac{\kappa_\eta}{p} \tag{6}$$

With the values of κ_η obtained, it is possible determine the total emittance, by a specific temperature and pressure path-length. According to Siegel and Howell (2002), it is given by the following equation:

$$\varepsilon(s) = \pi \frac{\int_0^\infty I_{b,\eta}\{1-\exp[\kappa_{p,\eta,mix} pL]\} d\eta}{\sigma T^4} \tag{7}$$

where pL is the pressure path-length in units of atm.m, given by the product of partial pressure of the mixture by the path length, and $I_{b,\eta}$ is the radiation intensity emitted by a black body, in W/(m^{2}cm^{-1}) , which is given by Planck´s distribution:

$$I_{b,\eta} = \frac{2 C_1 \eta^3}{e^{C_2 \eta / T} - 1} \tag{8}$$

where C_1 is the first Planck's constant, equal to $0.59552137 \times 10^{-16}$ W.m^2/sr.

One fundamental assumption of the WSGG model is that each pressure absorption coefficient $\kappa_{p,i}$ is assumed to be independent of the temperature T as well as of the partial pressure path-length ps of the participating species. Making the integration on Eq. (7) over the spectrum with the WSGG model, the total emittance becomes (Smith et al, 1982):

$$\varepsilon(s) = \sum_{i=0}^{n} a_i(T)[1-\exp(\kappa_{p,i} pL)] \tag{9}$$

where a_i is the weighting factor for the *i-th* gray gas. Base on the assumptions of the model, the coefficient a_i corresponds to the fraction of the blackbody energy that is emitted in the region of the spectrum where the absorption coefficient is correspondent to the respective gray gas. Therefore, a_i depends solely on the temperature, and is represented by a polynomial function, given by the following equation:

$$a_i(T) = \sum_{j=1}^{n} b_{i,j} T^{j-1} \qquad (10)$$

where $b_{i,j}$ is the polynomial coefficients of (j − 1) order for the *i-th* gray gas. To determine the WSGG model coefficients, the Levenberg-Marquardt method was used to fit the emittance values that were calculated from the line-by-line integration, using the spectral lines obtained through HITEMP 2010 database. In order to obtain the values of $\kappa_{p,i}$, Eq. (1) is summed for the entire set of temperatures, considering that $\kappa_{p,i}$ are independent of the temperature:

$$\sum_{T=400\text{ K}}^{2500\text{ K}} \varepsilon(ps) = \sum_{i=1}^{n} \left\{ \sum_{T=400\text{ K}}^{2500\text{ K}} a_i(T)\left[1-\exp(\kappa_{p,i}\, pL)\right] \right\} \qquad (11)$$

It is necessary to use several values of pL in order to use the Levenberg-Marquardt method to determine the sum of ε. In this work, it was applied twenty five values for pL, ranging from 0,0001 to 10 atm m. After obtaining the $\kappa_{p,i}$ values, the b_j coefficients were obtained to compute coefficients a_i according to Eq. (2).

Figs. 2 compare the total emittances obtained with the coefficients of Tables 1 those obtained from the LBL integration for temperatures between 400 K and 2500 K, and for four pressure path-lengths: 10, 1.0, 0.1 and 0.01 atm m. As seen, the WSGG model correlations make a satisfactory fitting of the total emittance data for the entire range of temperatures and pressure path-lengths.

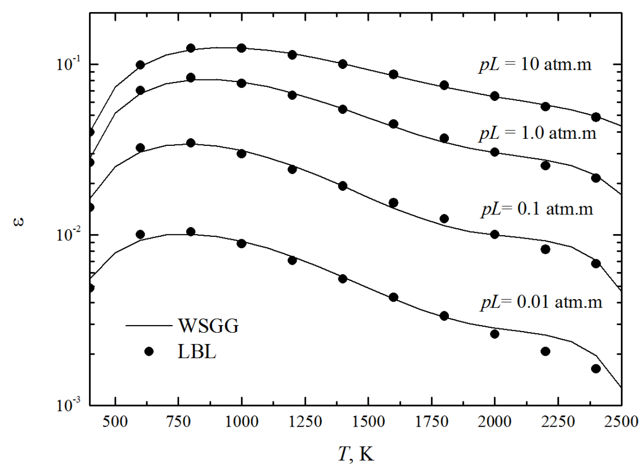


Figure 2. Comparison of the total emittances of CO computed from WSGG model and from LBL integration.

2.2 WSGG coefficients for CO

The coefficients were obtained for CO for partial pressures of $p_{CO} = 1.0$ atm, which represent typical pressure scales in combustion processes. The results were obtained for a total pressure of 1.0 atm, gas temperatures ranging from 400 K to 2500 K and pressure-path length products from 0.0001 to 10 atm m. Table 1 present the coefficients for CO

Table 1. WSGG coefficients for CO.

n	$\kappa_{p,i}$ (atm m)$^{-1}$	$b_{i,1}$	$b_{i,2}$ (K^{-1})	$b_{i,3}$ (K^{-2})	$b_{i,4}$ (K^{-3})	$b_{i,5}$ (K^{-4})
1	0.146	-0.1574	9.6692	-2.1476	-1.5298	4.6650
2	1.121	-1.2526	46.1210	-42.7286	15.8466	-21.0145
3	5.686	-0.6889	34.7105	-40.3923	18.0998	-28.1649
4	72.102	-0.2227	12.5098	-14.0355	6.0398	-9.0911

3. RESULTS AND DISCUSSION

For this study, it is considered two flat plates with black walls (emissivity of 1.0) separated by a distance of 1.0 m. The discrete ordinates method was applied to 30 directions, using a Gauss-Legendre quadrature. To evaluate the accuracy of the WSGG models against benchmark LBL solutions for non-isothermal media, the following temperature and molar concentration profiles are considered:

- Case 1

$$T(x) = 400 + 1400 \mathrm{sen}^2(\pi x / L) \quad (12)$$

$$Y(x) = Y_{max} \mathrm{sen}^2(\pi x / L) \quad (13)$$

- Case 2

$$T(x) = 400 + 1400 \mathrm{sen}^2(2\pi x / L) \quad (14)$$

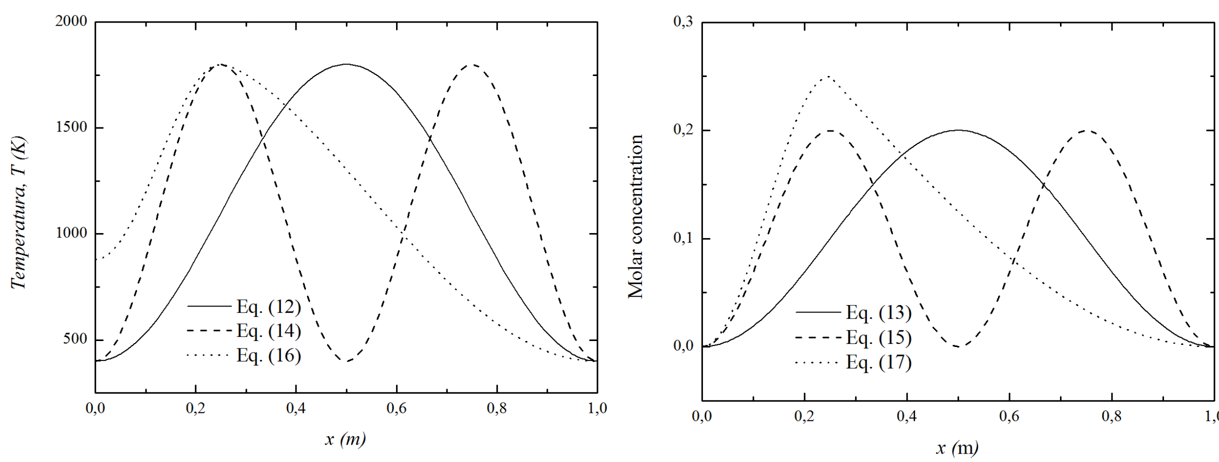
$$Y(x) = Y_{max} \mathrm{sen}^2(2\pi x / L) \quad (15)$$

- Case 3

$$T(x) = \begin{cases} 880 + 920 \mathrm{sen}^2(2\pi x / L) & \text{se } x/L \le 0.25 \\ 400 + 1400\left\{1 - \mathrm{sen}^{3/2}\left[\frac{2}{3}\pi(x/L - 0.25)\right]\right\} & \text{se } x/L > 0.25 \end{cases} \quad (16)$$

$$Y(x) = \begin{cases} Y_{max} \mathrm{sen}^2(2\pi x / L) & \text{se } x/L \le 0.25 \\ Y_{max}\left\{1 - \mathrm{sen}\left[\frac{2}{3}\pi(x/L - 0.25)\right]\right\} & \text{se } x/L > 0.25 \end{cases} \quad (17)$$

Equation (12) leads to a symmetric profile for the temperature, ranging from 400 K at the walls to a maximum value of 1400 K at the midpoint between the two walls. Equation (14) shows a symmetric profile, with temperatures ranging from 400 K at the walls to a maximum value of 1800 K at two points, that are x = 0.25m and x = 0.75m. The temperature profile in Eq. (16) is not symmetric, with the walls at the temperatures of 400K and 880K, but the maximum temperature in the medium is again 1800K, as can be seen in Fig. 3(a). CO concentration profiles are shown in Fig. 3(b).



(a) (b)

Figure 3. (a) Temperature profiles; (b) CO molar concentration profiles.

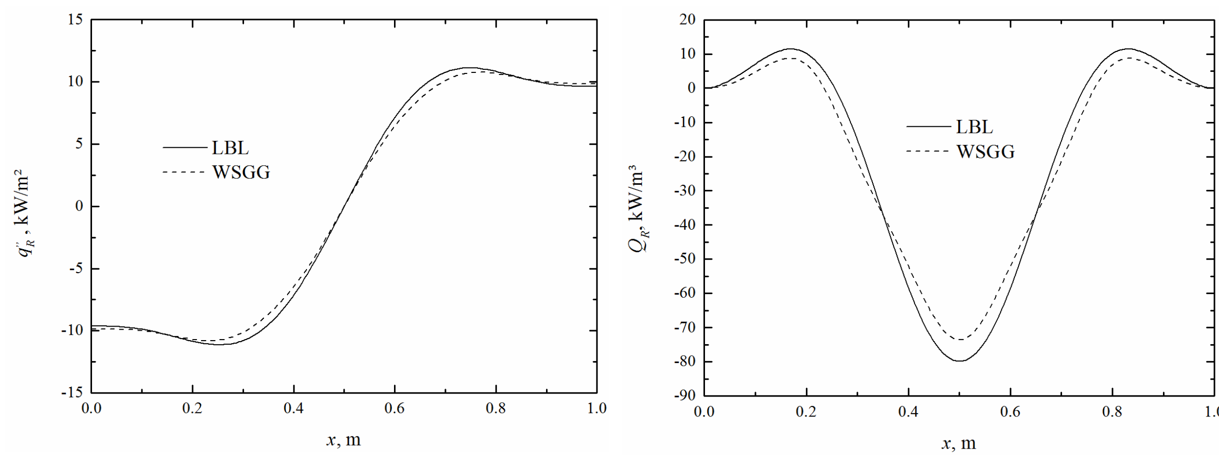
The deviation between the WSGG model and LBL benchmark solution, for radiative heat flux q_R'' and for radiative heat source $\dot{q}_R$ are computed by the following relations, respectively:

$$\delta = \frac{\left| q''_{R,\text{WSGG}} - q''_{R,\text{LBL}} \right|}{\max \left| q''_{R,\text{LBL}} \right|} \times 100\% \quad (18)$$

$$\zeta = \frac{\left| \dot{q}_{R,\text{WSGG}} - \dot{q}_{R,\text{LBL}} \right|}{\max \left| \dot{q}_{R,\text{LBL}} \right|} \times 100\% \quad (19)$$

where δ is the radiative heat deviation flux and ζ is a radiative heat source deviation. It will be used the notation δ_{max} and δ_{avg} to maximum error (%) and average error (%), respectively, for the radiative heat flux. As for the radiative heat source, ζ_{max} and ζ_{avg} will correspond to the maximum (%) and average errors (%).

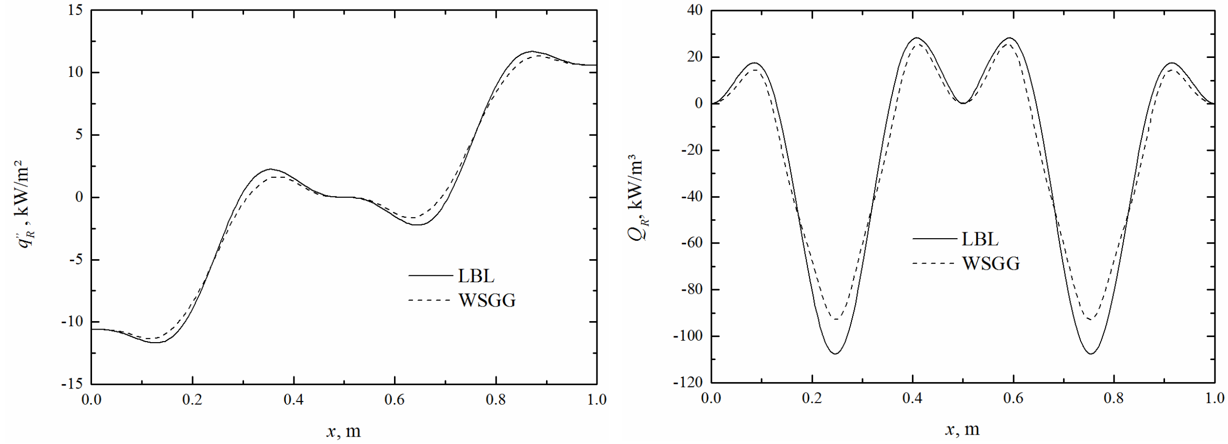
Figures 4(a) and 4(b) present the radiative heat flux and source, corresponding to the temperature profile given by Eq. (12) and Eq. (13) for a profile with symmetry. Figure 4(a) shows that the radiative heat flux was zero in the middle of the domain x=0.5m due the symmetry in the profile. As radiative heat flux tends to be directed to the higher temperature medium to the walls, the heat flux is negative for x < 0.5m and positive for x > 0.5m. However for the radiative heat source Fig. 4(b) the maximum value is located in the middle. This happens because it is where the medium temperature and concentrations of the participating species reaches their maxima; the negative signal indicates loss of energy due to radiation. Table 2 shows the radiative heat flux error is δ_{max} = 7.6% and radiative heat source ζ_{max} = 9.5%. These values show good agreement between the solutions WSGG with LBL.



(a) (b)

Figure 4. Comparison between the variation in the number of gases for WSGG with the LBL solutions: (a) radiative heat flux q''_R, and (b) radiative heat source $\dot{q}_R = -dq''_R / dx$, for temperature and CO_2 molar concentration profiles given by Eqs. (12) and (13).

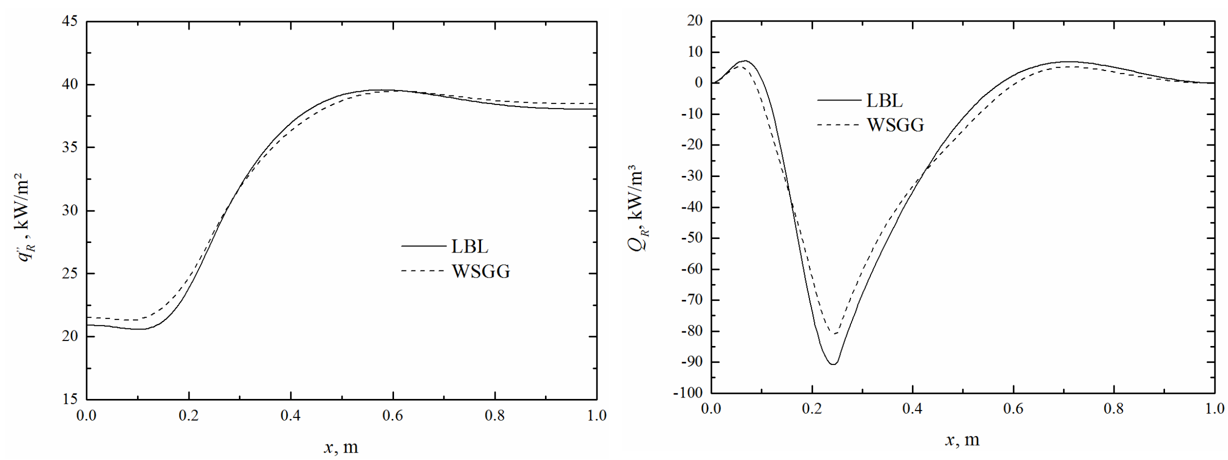
Figures 5(a) and 5(b) present the radiative heat flux and source, corresponding to the temperature profile given by Eq. (14) for a profile with double symmetry. As can be seen in Fig. 5(a) the radiative heat flux maximum value is in the points x = 0.25 m and x = 0.75 m, because a radiative heat flux tends to be directed to the higher temperature as well the heat source seen in Fig. 5(b), when the maxima happens at the points of symmetry (x = 0.25 m and x = 0.75 m). The predominance of negative signal indicates the energy loss occurs due to radiation. In Table 2 it is possible to observe that the greatest error happens for the radiative heat source equal 15.2% and radiative heat flux equal 8.3% in relation for LBL.



(a) (b)

Figure 5. Comparison between the variation in the number of gases for WSGG with the LBL solutions: (a) radiative heat flux q_R'', and (b) radiative heat source $\dot{q}_R = -dq_R''/dx$, for temperature and CO_2 molar concentration profiles given by Eqs. (14) and (15).

Figures 6(a) and 6(b) show the radiative heat flux and heat source, corresponding to the temperature and molar concentration obtained by the profiles given by Eqs. (16) and (17), which are not symmetric. For radiative heat flux Fig. 6(a) it can be seen the predominance of absorption with all the values are positive. In x = 0.85 m, the radiative heat source is close to zero, which is due to the low concentration of the absorbing-emitting species; this behavior can be viewed in Fig. 6 (b). The agreement between the WSGG and LBL model was again satisfactory with maximum errors: δ_{max} = 2.8% for radiative heat flux and ζ_{max} = 13.0% for heat source.



(a) (b)

Figure 6. Comparison between the variation in the number of gases for WSGG with the LBL solutions: (a) radiative heat flux q_R'', and (b) radiative heat source $\dot{q}_R = -dq_R''/dx$, for temperature and CO_2 molar concentration profiles given by Eqs. (16) and (17).

Table 2 presents the maximum and average errors, for each case for the WSGG model, in the computation of the radiative heat flux and the heat. It is possible to observe a higher error occurs for case 2 profile with double symmetry, in which the maximum error for the radiative heat source is ζ_{max} = 15.2%. However the agreement between the WSGG model and the LBL integration was notably satisfactory, with averages errors less than 6%.

Table 2. Maximum (δ_{max}) and average (δ_{avg}) errors of the WSGG solutions for the radiative heat flux, and the radiative heat source.

ERROR (%)	Radiative heat flux q''_R		Radiative heat source. $\dot{q}_R = -dq''_R / dx$	
	δ_{max}	δ_{avg}	ζ_{max}	ζ_{avg}
Figure 1	7.6	3.1	9.5	4.9
Figure 2	8.3	3.0	15.2	6.5
Figure 3	2.8	1.1	13.0	3.7

4. CONCLUSIONS

This paper shows new correlations for WSGG model for a CO specie obtained from the total emittance through the HITEMP2010 spectral database, considering pressure paths lengths between 0.0001 and 10 atm·m, and temperatures in the range of 400 to 2500K. It is presented results for different temperature profiles, and molar concentrations for non-homogenous. Comparing the results obtained by the WSGG model with the LBL benchmark solution, relatively small errors were found for all the cases proposed. In conclusion there was a consistent agreement between WSGG and LBL solutions, as it has been observed for other species, such as H_2O and CO_2.

5. ACKNOWLEDGEMENTS

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7. RESPONSIBILITY NOTICE