

EVALUATION OF THE NUMBER OF GRAY GASES IN THE WSGG MODEL

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Abstract. Predictions of radiative heat transfer in participating medium have been a challenge due to the strong spectral variation of the absorption coefficient. 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. In this model, the nongray gas is replaced by a number of gray gases, for which the heat transfer rates is calculated independently. The parameters for the WSGG model are obtained by the best fit of the total emittance data. In this work, new correlations are obtained for the WSGG model to the mixture of H_2O and CO_2 based on the HITEMP 2010 database. 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 model for non-isothermal, homogeneous and non-homogeneous conditions. The results show good agreement with the line-by-line (LBL) benchmark solution, for all cases.

Keywords: absorption coefficient, HITEMP 2010, WSGG model, LBL benchmark solution.

1. INTRODUCTION

The radiative heat transfer is an important phenomenon in engineering applications mainly in power generation, furnaces, steam generators and material processing. However the radiation is a very complex phenomenon due to the strong spectral dependence of the absorption coefficient.

Hottel and Sarofim (1967) proposed the weighted-sum-of-gray-gases (WSGG) model which consider 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 from fitting experimental data. In this way, Smith et al. (1982) obtained weighting functions and absorption coefficients of gray gases and water vapor for fitting data generated from the exponential wide-band model, to three gray gases. Galarça et al. (2008) also present new absorption coefficients, for three gray gases, and temperature dependent weighting functions using the WSGG model. Maurente et al., 2008, presented a comparison between the standard WSGG with the advanced gas model ALBDF- absorption-line blackbody distribution function, model that can be applied for homogenous and non-homogeneous gas mixtures. The work involved radiation heat transfer in a cylindrical chamber using combustion of methane and fuel oil. For the two gas models, the radiative exchanges are computed with the Monte Carlo method. In a recent work, 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 LBL solution. For all cases, the new oxy-fuel correlations provided the best agreement in comparison with the LBL (line-byline) integration. A similar work was implemented by Dorigon et al., 2012, which proposes new coefficients for the WSGG, also using the HITEMP 2010 database, for a gas mixture of water vapor and carbon dioxide for two different partial pressure ratios $p_{\text{H2O}} / p_{\text{CO2}}$ equal 1.0 and 2.0, it was compared the results of coefficients for four gray gases with the LBL benchmark solution showing good agreement between the methods for the different cases proposed.

This study presents new correlations for three, four and five gray gases applied to the solution of radiation heat transfer in non-isothermal homogeneous and non-homogeneous gas mixtures. The correlations were fitted from tabulated values of total emittance. The obtained correlations are valid for gaseous mixtures of $p_{\rm H2O} = 0.2$ atm (water vapor) and $p_{\rm CO2} = 0.1$ atm (carbon dioxide) and air, representing products of stoichiometric combustion methane, the nitrogen is considered inert therefore it is not used to obtain the correlations as well as the oxygen because it is a complete combustion. The correlations are valid for temperatures from 400K to 2500K and pressure-path length product from 0.0001 to 10 atm.m. The solution will be compared with benchmark LBL solutions to access the accuracy

of the model for a few illustrative cases. The main goal of the present study is to determine the number of gray gases that are enough for the WSGG model to become independent of the number of gray gases.

2. THE ABSORPTION COEFFICIENT

According to Siegel and Howell (2002), the Lorentz profile can be used in the determination of the absorption crosssection. It is given by:

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

where C_{η} is the absorption cross-section, in units cm²/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:

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n p_s \gamma_{self,i} + (1 - p_s) \gamma_{air,i}$$
(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⁻¹atm⁻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 269 K in its 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 is used:

$$S_{i}(T) = S_{i}(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\exp(-C_{2}E_{i}/T)}{\exp(-C_{2}E_{i}/T_{ref})} \frac{\left[1 - \exp(-C_{2}\nu_{i}/T)\right]}{\left[1 - \exp(-C_{2}\nu_{i}/T_{ref})\right]}$$
(3)

where Q is the total internal partition sums, dimensionless, v_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:

$$\kappa_{\eta} = NC_{\eta} \tag{4}$$

where N is is the Loschmidt number, in units of molecule/(cm³atm), and κ_{η} is the coefficient absorption, in cm⁻¹,

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

In order to obtain the absorption coefficient κ_{η} for the mixture, per unit of pressure in cm⁻¹atm⁻¹, the following equation is used:

$$\kappa_{\eta,mix} = \frac{\kappa_{\eta,\text{CO2}} + \kappa_{\eta,\text{H2O}}}{p} \tag{6}$$

where $p = p_{CO2} + p_{H2O}$, p_{CO2} and p_{H2O} are the partial pressure of H₂O and CO₂, respectively, $\kappa_{\eta,CO2}$ and $\kappa_{\eta,H2O}$ are the coefficient absorption, cm⁻¹, for the chemical species.

With the values of $\kappa_{\eta,mix}$ 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:

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$$\varepsilon(s) = \pi \frac{\int_{0}^{\infty} I_{b,\eta} \{1 - \exp[\kappa_{\eta, mix} ps]\} d\eta}{\sigma T^{4}}$$
(7)

where *ps* 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/(cm.sr), which is given by Planck's distribution:

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

where C_1 is the first Planck's constant, equal to $0.59552137 \times 10^{-12}$ W.cm²/sr.

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

The WSGG model represents the participating medium by some gray gases where the absorption coefficient can be considered constant; this model was proposed by Hottel and Sarofin (1967). Another fundamental assumption of the WSGG model is that each pressure absorption coefficient $\kappa_{p,i}$ is assumed to be independent of the temperature *T* and

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):

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

where a_i is the weighting factor for the *i*-th gray gas. The coefficient a_i depends only on temperature, and is represented by polynomial function, given by the following equation:

$$a_i(T) = \sum_{j=1}^n b_{i,j} T^{j-1}$$
(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 lineby-line integration of Eq. (7), using the spectral lines obtained through HITEMP 2010 database. In order to obtain the $\kappa_{p,i}$ the sum for all considered temperatures. For that, is considered that the $\kappa_{p,i}$ values are independent of temperature is applieds in the Eq. (9).

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

It is necessary to use several values of ps in order to use the Levenberg-Marquardt method to determine the sum of ε . In this work was applied twenty five values for ps, ranging from 0,0001 to 10 atm m.

After obtaining the $\kappa_{p,i}$ values, it is necessary to determine the a_i coefficients. For that, it is getting for a specific temperature, the values of ε as functions of *ps*. It is getting also the right hand of the Eq. (9) with the $\kappa_{p,i}$ determined values, in order to fit the values. This procedure is carried for all temperatures. After determining the a_i values for all temperatures, a polynomial function as same order than the number of gray gases wanted is used to fit the a_i values as a function of *T*, for each *i* gray gas, thus obtaining the $b_{i,j}$ coefficients of Eq. (10). This process has to be repeated for each different number of gases.

4. RESULTS AND DISCUSSION

The coefficients were obtained for gas mixtures that are formed in the combustion of methane ate 1.0 atm, so the partial pressures of their products are $p_{CO2} = 0.1$ atm and $p_{H2O} = 0.2$ atm. 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. Tables 1, 2 and 3 presents the coefficients for three, four and five fray gases, respectively.

n	$\kappa_{p,i} \text{ (atm m)}^{-1}$	$b_{i,1}$	$b_{i,2}(K^{-1})$	$b_{i,3}({ m K}^{-2})$	$b_{i,4}({\rm K}^{-3})$
1	0.237	2.256E-01	1.629E-04	-3.114E-08	-1.699E-12
2	2.611	1.429E-01	3.509E-04	-2.495E-07	4.184E-11
3	36.409	2.743E-01	-9.669E-05	-4.743E-08	1.858E-11

Table 1. WSGG coefficients for three gray gases, n=3, $p_{H2O}/p_{CO2}=2$.

Table 2.	WSGG	coefficients	for t	four	gray	gases,	<i>n</i> =4,	рн20/1	<i>co2</i> =2.
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n	$\kappa_{p,i}$ (atm m) ⁻¹	$b_{i,1}$	$b_{i,2}\left(\mathbf{K}^{-1}\right)$	$b_{i,3} (\mathrm{K}^{-2})$	$b_{i,4} (\mathrm{K}^{-3})$	$b_{i,5} (\mathrm{K}^{-4})$
1	0.183	5.305E-02	7.903E-04	-8.783E-07	4.393E-10	-7.715E-14
2	1.533	1.296E-01	1.717E-04	1.027E-08	-7.952E-11	1.923E-14
3	9.339	1.440E-01	2.648E-04	-3.741E-07	1.565E-10	-2.237E-14
4	100.340	1.298E-01	-1.203E-05	-9.266E-08	5.020E-11	-7.629E-15

Table 3. WSGG coefficients for five gray gases, n=5, $p_{H2O}/p_{CO2}=2$.

п	$\kappa_{p,i} \text{ (atm m)}^{-1}$	$b_{i,1}$	$b_{i,2}(\mathbf{K}^{-1})$	$b_{i,3}({ m K}^{-2})$	$b_{i,4}(\mathrm{K}^{-3})$	$b_{i,5}({ m K}^{-4})$	$b_{i,6}({ m K}^{-5})$
1	0.127	-3.381E-01	2.714E-03	-4.378E-06	3.255E-09	-1.109E-12	1.411E-16
2	0.752	1.479E-01	-2.608E-04	8.186E-07	-7.516E-10	2.802E-13	-3.771E-17
3	3.094	5.298E-02	5.607E-04	-8.839E-07	6.564E-10	-2.406E-13	3.366E-17
4	14.828	1.051E-01	2.180E-04	-2.962E-07	1.047E-10	-5.589E-15	-1.992E-18
5	124.977	1.257E-01	-9.273E-05	4.385E-08	-4.233E-11	2.229E-14	-3.816E-18

4.1 Comparasion between WSGG model and LBL integration

For this study, it is considered two flat plates with black walls (emissivity of 1.0) and 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 conditions the temperature profiles is proposed in equations below:

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

$$T(x) = \begin{cases} 880 \,\mathrm{K} + (920 \,\mathrm{K}) \sin^2(2\pi x) & \text{if } x \le 0.25 \\ 400 \,\mathrm{K} + (1400 \,\mathrm{K}) \left\{ 1 - \sin^{3/2} \left[\frac{2}{3} \pi (x - 0.25) \right] \right\} & \text{if } x > 0.25 \end{cases}$$
(13)

Equation (12) shows a symmetric profile, with temperatures ranging from 400 K at the walls to a maximum value of 1800 K at the midpoint between the two walls. The temperature profile in Eq. (13) is not symmetric, with the walls at the temperatures of 400K and 880K, but the maximum temperature in the medium is also 1800K.

Two profiles for the molar concentrations of CO₂ are considered:

$$Y_{\rm CO_2}(x) = 0.2\sin^2(2\pi x) \tag{14}$$

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$$Y_{\text{CO}_{2}}(x) = \begin{cases} 0.25\sin^{2}(2\pi x) & \text{if } x \le 0.25 \\ 0.25 \left\{ 1 - \sin\left[\frac{2}{3}\pi(x - 0.25)\right] \right\} & \text{if } x > 0.25 \end{cases}$$
(15)

In all cases, the average molar concentration of CO₂ is $\overline{Y}_{CO_2} = 0.1$. The partial pressure of the absorbing-emitting species can be obtained as $p(x) = [Y_{CO_2}(x) + Y_{H_2O}(x)]p$, where the ratio $Y_{H_2O}(x)/Y_{CO_2}(x)$ are kept equal 2 for proper use of the WSGG coefficients in Tabs.1, 2 and 3. Figures 1(a) and (b) show the temperature and the CO₂ molar concentration profiles according the Eq. (12) to (15).



Figure 1. (a) Temperature profiles; (b) CO₂ molar concentration profiles.

The deviations between the WSGG model and LBL benchmark solution are given by:

$$\delta = \frac{\left| q_{R,\text{WSGG}}^{''} - q_{R,\text{LBL}}^{''} \right|}{\max \left| q_{R,\text{LBL}}^{''} \right|} 100\%$$
(16)

$$\zeta = \frac{\left|\dot{q}_{R,\text{WSGG}} - \dot{q}_{R,\text{LBL}}\right|}{\max\left|\dot{q}_{R,\text{LBL}}\right|} 100\% \tag{17}$$

where δ is the radiative heat deviation flux and ζ is a radiative heat source deviation. The notations δ_{max} and δ_{avg} will be used for the maximum and average errors for radiative heat flux. For the radiative heat source, the notations ζ_{max} and ζ_{avg} will be used for the maximum and average errors.

Figures 2(a) and 2(b) present the radiative heat flux and source, corresponding to the temperature profile given by Eq. (12) for a profile with double symmetry. As can be seen in Fig. 2(a) the radiative heat flux maximum value is in the points x = 0.25 m and x = 0.75 m. This is because a radiative heat flux tends to be directed to the higher temperature. For radiative heat source seen in Fig. 2(b), the two points of symmetry x = 0.25 m and x = 0.75 m reaches their maximum, because again of the higher temperature on medium.

Figures 3(a) and 3(b) show the radiative heat flux and heat source, corresponding to the temperature and CO₂ molar concentration given by profiles in Eqs. (12) and (14), with a behavior that is similar to the previous case, except that the radiative heat flux is zero in the middle of domain, which did not occur for the homogeneous case in Fig. 2(a). The negative signal indicates the energy loss. In Table 4 it is possible to observe that the greatest error for the homogeneous case, Eq. (12), occurs for three gray gases: radiative heat flux error is $\delta_{max} = 6.67\%$ and radiative heat source $\zeta_{max} = 9.14\%$. While for the case non-homogeneous media, given by Eqs. (12) and (14) the radiative heat flux error is $\delta_{max} = 4.19\%$ and radiative heat source $\zeta_{max} = 8.77\%$, for the three gray gases model. The differences between the four and five gray gases are not so significant for both homogeneous and non-homogeneous cases, showing errors smaller than 5%.

Figures 4(a) and 4(b) show the radiative heat flux and heat source, corresponding to the temperature profile given by Eq. (14). In this non-symmetric profile, a maximum value takes place in the position where the temperature of the

medium is higher. The maximum value is around x = 0.25 m, which is where both the temperature and concentrations of the participating species are at their maximum. For 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 also be observed for the non-homogeneous case shown in Fig 5 (b).



Figure 2. 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 profiles given by Eq. (12).



Figure 3. 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 CO₂ molar concentration profiles given by Eqs. (12) and (14).

Figure 5 considers the non-homogeneous case in which the temperature profile is given by Eq. (13), and the CO₂ molar concentration profile is given by Eq. (15). One observes that the maximum values obtained for radiative heat flux and source is higher than for the case seen in Figs. 4(a) and 4(b), which can be explained by variation of concentration the absorbing emitting species. The higher error obtained for the WSGG occurs for the non-homogeneous case with three gray gases, reaching the values of $\delta_{max} = 7.12\%$ for radiative heat flux and $\zeta_{max} = 9.42\%$ for heat source. The results with the highest accuracy occur for four gray gases with homogeneous concentration. In this case, $\delta_{max} = 3.38\%$ and $\zeta_{max} = 7.04\%$, as can be verified in Table 4.

Table 4 presents the maximum and average errors in the computation of the radiative heat flux and the heat source for the solutions with different number of gray gases in the WSGG model, considering the homogeneous and non-homogeneous cases. It is possible to observe that the highest error occurs for the case with three gray gases in all cases,

while the solutions the correlations for four and five gases are quite similar, indicating that the WSGG model becomes independent of the number of gray gases when using four or more gases. However, even for the three gray gases model, the agreement between the WSGG model and the LBL integration was notably satisfactory, with maximum local errors less than 10%.



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 profiles given by Eq. (13).



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 CO₂ molar concentration profiles given by Eqs. (13) and (15).

Table 4. Maximum (δ_{max}) and average (δ_{avg}) errors of the WSGG solutions for the radiative heat flux, and the radiative heat source.

HOMOGENEOUS												
	Radiative heat flux $q_{R}^{"}$							Radiative heat source. $\dot{q}_R = -dq_R'' / dx$				
	<i>n</i> = 3 <i>n</i> = 4				<i>n</i> =	= 5	<i>n</i> = 3		<i>n</i> = 4		<i>n</i> = 5	
ERROR (%)	δ_{max}	δ_{avg}	δ_{max}	δ_{avg}	δ_{max}	δ_{avg}	ζ_{max}	ζ_{avg}	ζ_{max}	ζ_{avg}	ζ_{max}	ζ_{avg}
Eq. (12)	6.67	2.71	3.88	1.85	4.55	1.83	9.14	4.48	7.04	3.54	8.09	3.65
Eq. (13)	5.61	1.80	3.66	1.77	3.65	1.77	7.43	1.88	4.74	1.74	4.87	1.75

NON-HOMOGENEOUS												
		Ra	diative h	eat flux	$q_R^{"}$		Radiative heat source. $\dot{q}_R = -d\dot{q}_R' / dx$					dx
	<i>n</i> = 3 <i>n</i> = 4 <i>n</i> = 5						<i>n</i> = 3 <i>n</i> = 4			n	= 5	
ERROR (%)	δ_{max}	δ_{avg}	δ_{max}	δ_{avg}	δ_{max}	δ_{avg}	ζ_{max}	ζ_{avg}	ζ_{max}	ζ_{avg}	ζ_{max}	ζ_{avg}
Eqs. (12),(14)	4.19	1.69	3.25	1.37	2.9	1.16	8.77	2.33	5.29	1.82	4.81	1.64
Eqs. (13),(15)	7.12	7.12 2.04 4.43 1.34 4.35 1.15 9.42 1.67 3.38 0.76 3.61 0.75										0.75

5. CONCLUSIONS

This paper show new correlations for WSGG model with different number of gases: three, four and five, for mixture of H₂O and CO₂, with partial pressure (or molar concentration) $p_{H2O}/p_{CO2} = 2$, obtained from the total emittance data generated 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. Results were presented for different temperature profiles, and molar concentrations non-homogenous and homogenous. Larger values of errors are found for the case with three gray gases. The results for the WSGG model based on four and five gray gases presented a notable similarity, indicating the WSGG model can become independent of the number of gray gases, in this particular case the model with four gray gases seems to be the optimum choice. However, even for the three gray gases, the agreement between the WSGG model and LBL integration was satisfactory in all cases proposed, with maximum errors less than 10%.

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