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PROPOSITION OF A NEW METHODOLOGY FOR GENERATING THE COEFFICIENTS OF THE WEIGHTED-SUM-OF-GRAY-GASES MODEL IN MIXTURES OF PARTICIPATING GASES

William Ávila Hellwig

Department of Mechanical Engineering, Federal University of Rio Grande do Sul, Porto Alegre, Brazil
william.hellwig@ufrgs.br

Roberta Juliana Collet da Fonseca

Department of Mechanical Engineering, Federal University of Rio Grande do Sul, Porto Alegre, Brazil
roberta.fonseca@ufrgs.br

Fatmir Asllanaj

CNRS, LEMTA, Université de Lorraine, F-54000 Nancy, France
fatmir.asllanaj@univ-lorraine.fr

Francis Henrique Ramos França

Department of Mechanical Engineering, Federal University of Rio Grande do Sul, Porto Alegre, Brazil
frfranca@mecanica.ufrgs.br

Abstract. *In combustion problems, which occur at elevated temperatures due to the chemical reactions and the presence of soot and participating gases, thermal radiation tends to be the main mechanism of heat transfer. Thus, correctly describing the radiative heat transfer involved in the burning of fossil fuels is of fundamental importance for accurate simulation of combustion systems towards improved thermal efficiency and reduction of pollutant emission. However, the accurate calculation of thermal radiation requires the solution of the Radiative Transfer Equation (RTE), in which it is necessary to account for the hundreds of thousands of spectral lines that compose the absorption coefficient of the gases. Although the line-by-line (LBL) integration is the most accurate among the known methods, in most practical applications its use is unfeasible due to the high computational cost required. As an alternative to overcome this difficulty, the development of the global spectral models, such as the Weighted-Sum-of-Gray-Gases (WSGG), has received much attention in the radiation field. So, in this framework, the present study proposes a new methodology for the generation of the coefficients of the WSGG model for mixtures of water vapor and carbon dioxide – two typical products of the combustion of methane in air. This new approach aims to improve the solution of the standard WSGG model by implementing new considerations on the computation of the coefficients, in which the function that determines the weighting factors is composed of terms associated with positive and negative exponents. These new coefficients will be applied for computing the radiative heat flux and radiative heat source and compared with results provided by the LBL benchmark solution. It is expected that these correlations improve the accuracy of the solution and demonstrate a satisfactory agreement with the LBL integration, in addition to being a competitive method in comparison with the existing modern models.*

Keywords: *thermal radiation, participating gases, weighted-sum-of-gray-gases model, line-by-line integration.*

1. INTRODUCTION

In combustion problems, which occur at elevated temperatures due to the chemical reactions and the presence of soot and participating gases, thermal radiation tends to be the main mechanism of heat transfer. Some other important examples of radiative transfer in participating media are glass manufacturing, fibrous insulating layers, nuclear explosions, hypersonic shock layers, plasma generators for nuclear fusion, irradiation of biological systems, and heat transfer in porous materials (Howell, 2016). The process of emitting and absorbing radiative energy raises or lowers the energy of the molecule associated with the vibrational and rotational movements. These energy levels are quantized and lead to hundreds of thousands of the called spectral lines (Modest, 2013).

The accurate calculation of the thermal radiation requires the solution of the radiative transfer equation (RTE), in which it is necessary to account for the many thousands of spectral lines that compose the absorption coefficient of the gases. The spatial variation in radiative properties as absorption, emission and scattering can occur in every location within the medium at different levels that depend on the concentration of the species and on their temperature. Due to the inherently complex mathematics that describes the phenomena, significant effort has been being made to the development and enhancement of numerical methods for those calculations. Moreover, improvements in computer performance have also collaborated to the advancement in studies in this field.

There are a wide variety of methods used to calculate the thermal radiation in participating media. The spectral part of the problem can be precisely calculated through line-by-line (LBL) integration (Taine, 1983) through the use of data from high-resolution spectroscopic databases, such as HITEMP (Rothman et al., 2010) and HITRAN (Rothman et al., 2013). Recent developments of the WSGG model presented new coefficients for gas mixtures (Dorigon et al., 2013; Coelho and França, 2018) for constant partial pressure ratios. As an alternative to the constant partial pressure ratio coefficients, studies of (Cassol et al., 2014; Consalvi et al., 2019) present WSGG coefficients for individual species in order to account properly for inhomogeneous gas mixtures. In a recent work (Johansson et al., 2011; Bordbar et al., 2014) proposed new WSGG formulation and coefficients for variable partial pressure ratios. The purpose of the present study is to introduce new coefficients for gas mixture under constant partial pressure ratios with the aim of achieve better accuracy results when applying the WSGG model. The results of the WSGG model with the newly obtained coefficients are compared with LBL benchmark results for 1D test cases, showing that the new coefficients, in spite of its simplicity, can provide satisfactory accuracy.

2. SPECTRAL MODELLING

Radiation transfer with absorption, emission and scattering is a phenomenon that occurs in the three phases of matter: solid, liquids, and gases. When a photon (electromagnetic wave) interacts with a gas, it can be absorbed, which increases the energy level of the molecule, or scattered by the gas, which modifies the photon's travel direction. A gas molecule can also have its energy level decreased by emission of a photon. The radiation in participating media is the product of the quantized energy transitions in the vibration and rotational modes of the molecules compounding the mixture gas and the properties of absorption, emission and scattering have a large dependence on the wavelength. The energy level of a molecule or an atom is not precisely calculated according to Heisenberg's uncertainty principle and its uncertainty shows up as broadening effects of the spectral lines. The broadening by collision is usually the main contributor for the broadening effect of spectral lines under engineering problems in the infrared radiation spectrum. Thus, other mechanisms can be neglected (Howell, 2016). The specific energy levels in addition with the spectral broadening effect causes the sharp aspect of the properties as functions of frequency in the form of a large number of spectral lines. These strong variations are a remarkable challenge in modeling thermal radiation phenomena.

The efforts arising from the development of numerical methods provide correlations of these properties that can be used with great accuracy, avoiding the complex detailed calculations that result in high computational costs. The solution of radiation transfer in participating media requires the integration of the radiative transfer equation (RTE) over all the spectrum. For participating gases, it is a difficulty goal due to the highly complex dependence described earlier. For this study, the analyses were done under the assumption of local thermodynamic equilibrium (LTE), in which the states of energy depend only on pressure and temperature (Howell, 2016).

A single spectral line in the spectrum is characterized by its strength and its line width according to the broadening mechanism to be used. The generation of spectral lines comes from the combination of the very spectral lines as result from the transitions between the vibrational and rotational energy states. Its locations, strengths and widths are obtained from modern databases such as HITRAN and HITEMP, which allow the computation of the resulting absorption coefficient. The spectral lines in the present study are described by Lorentz profile, in which collisions among molecules in the media are the main cause of the broadening effect as represented by equation (Rothman et al. 2013) for the absorption cross-section:

$$C_{\eta}(p, T, Y) = \sum_{k=1}^K \frac{S_k(T)}{\pi} \frac{\gamma_k}{\gamma_k^2 + (\eta - \eta_k)^2} \quad (1)$$

where S_k is the integrated line intensity of line k , γ_k is the line half-width and η_k is the wavenumber of the line location. The line half-width γ_k is given by (Rothman et. al 2013):

$$\gamma_k(p, T, Y) = \left(\frac{T_{ref}}{T} \right)^{n_c} p_c \gamma_{self,k} + (p - p_c) \gamma_{air} \quad (2)$$

where γ_{air} is effect by air, $\gamma_{self,k}$ is the line self-broadening, p_c is the partial pressure of specie c , T_{ref} is the reference temperature of 296 K and n_c is the temperature dependence coefficient. The integrated line intensity for a temperature T

is given by:

$$S_k = S_k(T_{ref}) \frac{Q(T_{ref}) \exp(-C_2 E_k / T)}{Q(T) \exp(-C_2 E_k / T_{ref})} \frac{[1 - \exp(-C_2 \nu_k / T)]}{[1 - \exp(-C_2 \nu_k / T_{ref})]} \quad (3)$$

in which Q is the internal partitions sums, ν_k is the energy difference between the initial and final state, E_k is the energy of lower state, and C_2 is the second Planck's constant of magnitude 1.43877 cm K. All the previous parameters were obtained from the HITEMP 2010 database in order to generate the absorption cross-section given by Eq. (1). With the absorption cross-section, the absorption coefficient κ_η is obtained according to the equation:

$$\kappa_\eta(p, T, Y) = N(p, T) Y C_\eta(p, T, Y) \quad (4)$$

where N is the gas molar density, Y the gas mole fraction, and C_η the absorption cross-section. The gas molar density is given by:

$$N(p, T) = \frac{p N_A}{R_u T} \quad (5)$$

in which R_u is the universal gas constant, N_A is Avogadro's number and p is the total pressure.

As the present study considers the medium a mixture of water vapor and carbon dioxide, the absorption coefficient mixture is determined by summation of the absorption coefficients of each gas:

$$\kappa_\eta = \kappa_{\eta, CO_2} + \kappa_{\eta, H_2O} \quad (6)$$

The definition of the pressure absorption coefficient is:

$$\kappa_{p\eta, a} = \frac{\kappa_\eta}{p_a} \quad (7)$$

where p_a is partial pressure of the absorbing specie:

$$p_a = p_{H_2O} + p_{CO_2} \quad (8)$$

Thus, the pressure absorption coefficient $\kappa_{p\eta, a}$ can be written as:

$$\kappa_{p\eta, a} = \frac{p_{CO_2} \kappa_{p\eta, CO_2} + p_{H_2O} \kappa_{p\eta, H_2O}}{p_a} \quad (9)$$

The spectral absorption cross-sections were obtained considering molar fractions of $Y_{H_2O} = 0.2$ for water vapor and $Y_{CO_2} = 0.1$ for carbon dioxide. The total pressure was established at 1 atm. The temperature range was discretized in 100 K steps from 400 K to 2500 K. All other parameters as wavenumber ranges and number of elements used to the generation of the spectral lines was evaluated in (Dorigon, 2013).

2.1 The Radiative Transfer Equation and WSGG model

There are four main groups of models developed to handle the spectral behavior of radiative energy transfer: line-by-line calculations, narrow band calculations, wide band calculations and global models. The LBL model, developed by (Hartmann et al., 1984), provides high accuracy results when compared with other spectral models. The reason is RTE is evaluated at each individual wavenumber where the absorption coefficient is known. In contrast, such results require a high computational cost. In order to overcome this difficulty, other models have been developed with the aim of reducing the spectral information weight on the calculations. Despite its computational cost, the LBL model is applied as a benchmark solution for spectral models.

The present study evaluates the Weighted-Sum-of-Gray-Gases (WSGG). The global model was developed by (Hottel and Sarofim, 1967), which established that the participating medium is a compound of a finite number of gray gases at fixed portions j in the spectrum, not necessarily contiguous, plus transparent windows to simulate the properties of the non-gray gas. In addition, the WSGG states that each pressure absorption coefficient p, j is independent of the temperature T and partial pressure p_a of the gases mixture. From this approximation, the dependence of the absorption coefficient on the wavenumber and the thermodynamic state are detached. The gases weighting is determined according to the fraction of radiative energy in the spectral interval where each gas is located. Correlations were proposed by (Smith et. al, 1982), for the absorption and weighting coefficients for water vapor and carbon dioxide molecules. Is demonstrated (Modest, 2013) the WSGG model could be coupled with any other model for the radiative transfer equation solution. The WSGG is one of the most used models and is largely applied in commercial softwares since its solution is compatible to engineering simulations in matter of time and accuracy.

The spectral RTE for one dimensional non-scattering medium bounded by black walls satisfies (Howell, 2016):

$$\frac{dI_\eta(x)}{dx} = -\kappa_\eta(x)I_\eta(x) + \kappa_\eta(x)I_{b\eta} \quad (10)$$

where $I_\eta(x)$ and $I_{b\eta}$ are the spectral radiative intensity and the blackbody spectral radiative intensity at position x on a given path.

The solution of RTE requires the knowledge of the spectral distribution of the absorption coefficient κ_η . When applying the WSGG model into the radiative transfer equation, the erratic spectrum of the absorption coefficient is replaced by a defined number of gray-gases J , with constant pressure absorption $\kappa_{p,j}$. The modified Eq. (10) is then given by:

$$\frac{dI_j(x)}{dx} = -\kappa_{p,j}p_a(x)I_j(x) + \kappa_{p,j}p_a(x)a_j(T)I_b(T) \quad (11)$$

in which I_b is the total blackbody radiative intensity and T the local temperature in position x . The $a_j(T)$ coefficients represent the fraction of the total blackbody emission in the j spectrum portion of the j -th gas. In order to compute the WSGG model, the fraction blackbody and the pressure absorption coefficients need to be determined. This is achieved by fitting functions to the data of total emittance calculated by LBL method in a certain path in the medium with specified temperature and molar composition. The total emittance is defined as:

$$\epsilon(T, p_a S) = \frac{\int_{\eta=0}^{\infty} I_{\eta b}(T)[1 - \exp(-\kappa_{p\eta,a} p_a S)] d\eta}{\sigma T^4 / \pi} \quad (12)$$

where $I_{\eta b}$ is the Planck's distribution given by:

$$I_{\eta b}(\eta, T) = \frac{2C_1 \eta^3}{\exp(C_2 \eta / T) - 1} \quad (13)$$

in which C_1 is the first Planck's constant. Under the assumptions of the WSGG model, the total emittance is expressed by:

$$\epsilon(T, p_a S) = \sum_{j=i}^J a_j(T)[1 - \exp(-\kappa_{p,j} p_a S)] \quad (14)$$

where the dependent coefficients are represented by polynomial functions of the temperature as:

$$a_j(T) = \sum_{k=0}^K b_{j,k} T^k \quad (15)$$

On Eq. (15), $b_{j,k}$ are the polynomial coefficients of k th order for the j th gray gas. The a_j coefficients corresponding to the transparent window are evaluated as $a_0 = 1 - \sum_{j=1}^J a_j(T)$.

3. METHODOLOGY

The WSGG model coefficients were determined through fitting applying the Levenberg-Marquardt method with emittance values calculated through LBL integration. The Levenberg-Marquardt minimizes the sum of the squares of the errors between the data points and the parameterized function as the objective function. The total emittance was calculated by LBL integration of Eq. (12) in the spectral range of $0 < \eta < 25000 \text{ cm}^{-1}$ using data generated through the HITEMP2010 database for a mixture of water vapor and carbon dioxide under the same conditions of the generation of the spectral lines, i.e, $p_{H_2O}/p_{CO_2} = 2$, as a typical stoichiometric balance of the combustion of methane remaining nitrogen as transparent gas. The spectrum for the spectral lines was divided in 375000 intervals resulting in a spectral resolution of 0.067 cm^{-1} . Previous studies have shown that this resolution is refined enough for accurate computation of the total emittance. The path lengths were varied from 0.001 to 30 m, in which 43 values were used, and are sufficient for most practical engineering applications. Temperature ranges from 400 to 2500 K, resulting in 22 temperature values, and a total pressure value of 1 atm was used.

Typical value for the number of gray gases j to be used in Eq. (15) is 4 (four), since the increase in the number of gray gases does not improve the accuracy of the model (Dorigon, 2013). In order to evaluate the increments on the model accuracy, new polynomial functions for the fraction of the blackbody emittance coefficients were proposed. After the fitting with the new objective functions, the values for heat flux and heat source for an one dimensional non-scattering medium bounded by black walls were compared with LBL benchmark results. The proposed functions to evaluate the dependent coefficients on Eq. (15) are shown in Table 1:

Table 1: Formulations of the weighting factors.

Function name	Function equation
Linear	$a_j(T) = b_{j,0} + b_{j,1}T$
Tn0	$a_j(T) = b_{j,0} + b_{j,1}T + b_{j,2}T^2 + b_{j,3}T^3 + b_{j,4}T^4$
Tn1	$a_j(T) = b_{j,-1}T^{-1} + b_{j,0} + b_{j,1}T + b_{j,2}T^2 + b_{j,3}T^3 + b_{j,4}T^4$
Tn2	$a_j(T) = b_{j,-2}T^{-2} + b_{j,-1}T^{-1} + b_{j,0} + b_{j,1}T + b_{j,2}T^2 + b_{j,3}T^3 + b_{j,4}T^4$
Tn3	$a_j(T) = b_{j,-3}T^{-3} + b_{j,-2}T^{-2} + b_{j,-1}T^{-1} + b_{j,0} + b_{j,1}T + b_{j,2}T^2 + b_{j,3}T^3 + b_{j,4}T^4$

Table 2: kappa coefficients.

Gray-gas j	A_j	$\kappa_{p,j}$ (atm m) ⁻¹
1	1.09437	85.8398
2	2.53871	9.08292
3	4.49901	1.49905
4	7.69784	0.18832

The coefficients of $\kappa_{p,j}$ and $b_{j,k}$ for each path length was determined in two different steps. For each path length, the total emittances were summed for each temperature value as:

$$A_j = \sum_{m=1}^{M=22} a_j(T_m) \quad (16)$$

where T_m are the 22 values of temperature varying from 400 to 2500 K. The emittance is then written as:

$$\epsilon = \sum_{j=1}^{J=4} A_j [1 - \exp(-\kappa_{p,j} p_a S)] \quad (17)$$

First, the A_j and $\kappa_{p,j}$ were evaluated. The results are presented on Table 2.

Then, the fractions of blackbody $a_j(T)$ were obtained fitting Eq. (16) for each gray-gas j at each temperature value m on the equation:

$$\epsilon = \sum_{j=1}^{J=4} \left[\sum_{m=1}^{M=22} a_j(T) [1 - \exp(-\kappa_{p,j} p_a S)] \right] \quad (18)$$

The unknown $b_{j,k}$ coefficients are then obtained through the fitting of polynomial functions presented in Table 1. The WSGG model coefficients generated in this study for the mixture of H_2O and CO_2 at total pressure of 1 atm, temperature of the medium ranging from 400 to 2500 K, path lengths from 0.01 to 30 m and mole ratio of $Y_{H_2O}/Y_{CO_2} = 2$ are shown in Table 3.

A practical evaluation can be made by analyzing the total emittance predicted from the WSGG modeling with one calculated through the LBL integration. Though this comparison does not allow a complete view of the performance of the WSGG model with each set of coefficients, as the assumptions of WSGG itself are a limiting factor, it still can be used as a simple visual result for the fitting. The fitting result for the path lengths of $S = 0.1$ and 30 m is shown in Fig. 1.

In order to obtain a formal validation of the model, data of heat flux and heat source generated by the WSGG model is compared with LBL solution.

Both WSGG and LBL solutions for the radiative heat flux and volumetric source are calculated for the one dimensional non-scattering medium bounded by two infinite parallel black walls. The distance between the walls is $L = 1$ m. The participating medium is a mixture of CO_2 and H_2O , with uniform mole fractions $Y_{CO_2} = 0.1$ and $Y_{H_2O} = 0.2$. Two scenarios are considered. In case 1, the temperature distribution in the medium varies according to:

$$T(s) = 400 + 1400 \sin^2(\pi s) \quad (19)$$

In case 2, the temperature follows:

$$T(s) = 800 + 920 \sin(2\pi s) \quad \text{if } s \leq 0.25 \quad (20)$$

$$T(s) = 400 + 1400 \{1 - \sin^{3/2}[2\pi/3(s - 0.25)]\} \quad \text{if } s > 0.25 \quad (21)$$

where $T(S)$ is in Kelvin K. The temperature distributions profiles can be seen in Fig. 2.

Table 3: Formulations for the fraction of total blackbody emission coefficients.

Function	j	$\beta_{j,0}$	$\beta_{j,1}$ (K ⁻¹)	$\beta_{j,2}$ (K ⁻²)	$\beta_{j,3}$ (K ⁻³)	$\beta_{j,4}$ (K ⁻⁴)	$\beta_{j,-1}$ (K)	$\beta_{j,-2}$ (K ²)	$\beta_{j,-3}$ (K ³)
Linear	1	0.1	-5.5e-05	-	-	-	-	-	-
	2	0.2	-7.8e-05	-	-	-	-	-	-
	3	0.2	-4.6e-05	-	-	-	-	-	-
	4	0.2	6.2e-05	-	-	-	-	-	-
Tn0	1	0.14	-3.8e-05	-6.2e-08	3.5e-11	-5.1e-15	-	-	-
	2	0.16	1.3e-04	-2.3e-07	9.5e-11	-1.3e-14	-	-	-
	3	0.11	2.3e-04	-8.3e-08	-3.2e-11	1.1e-14	-	-	-
	4	0.04	8.1e-04	-8.8e-07	4.3e-10	-7.5e-14	-	-	-
Tn1	1	-0.1	4.1e-04	-4.3e-07	1.7e-10	-2.5e-14	46.4	-	-
	2	0.4	-3.7e-04	1.9e-07	-6.8e-11	1.0e-14	-53.6	-	-
	3	0.08	2.9e-04	-1.3e-07	-1.2e-11	8.5e-15	6.5	-	-
	4	1.2	-1.4e-03	9.6e-07	-2.7e-10	2.6e-14	-232.1	-	-
Tn2	1	0.75	-6.5e-04	2.4e-07	-3.9e-11	1.7e-15	-291.3	50752.7	-
	2	-4.6e-03	1.8e-04	-1.5e-07	4.5e-11	-4.0e-15	123.1	-26538.4	-
	3	-1.5	2.3e-03	-1.4e-06	3.9e-10	-4.2e-14	643.8	-95731.1	-
	4	4.8	-5.8e-03	3.8e-06	-1.2e-09	1.4e-13	-1653.3	213501	-
Tn3	1	1.74	-1.5e-03	7.2e-07	-1.7e-10	1.5e-14	-885.4	236542	-2.3e+07
	2	-2.18	2.2e-03	-1.2e-06	3.3e-10	-3.5e-14	1438.2	-437853	5.1e+07
	3	-1.83	2.6e-03	-1.5e-06	4.4e-10	-4.7e-14	827.7	-153234	7.2e+06
	4	-0.5	-8.6e-04	1.2e-06	-4.8e-10	6.2e-14	1625.6	-812040	1.3e+08

The radiative heat flux q_R'' and volumetric source S_R is evaluated by the integration of Eq. (10) applying the discrete ordinates method. According to this method, the spectral intensities in the backward and forward directions $I_{j,m}^-(x)$ and $I_{j,m}^+(x)$ are computed from the solution of equations below:

$$\mu_m \frac{dI_{j,m}^+(x)}{dx} = -\kappa_{p,j} p_a(x) dI_{j,m}^+(x) + \kappa_{p,j} p_a(x) a_j(x) I_b(x) \quad (22)$$

$$-\mu_m \frac{dI_{j,m}^-(x)}{dx} = -\kappa_{p,j} p_a(x) dI_{j,m}^-(x) + \kappa_{p,j} p_a(x) a_i(x) I_b(x) \quad (23)$$

in which μ_m is the cosine in direction m . Equations (22) and (23) are applied as boundary conditions to the problem considering black walls with known temperatures. Then, $I_{j,m,x=0}^+ = a_j(T_{x=0}) I_{b,x=0}$ and $I_{j,m,x=S}^- = a_j(T_{x=S}) I_{b,x=S}$. For the transparent window ($j = 0$), the partial radiative intensity is constant along the path.

The radiative heat flux q_R'' and volumetric source S_R are expressed by equations:

$$q_R''(x) = \sum_{j=0}^J \sum_{m=1}^M 2\pi \mu_m w_m [I_{j,m}^+(x) - I_{j,m}^-(x)] \quad (24)$$

$$S_R(x) = \sum_{j=1}^J \sum_{m=1}^M 2\pi w_m \kappa_{p,j} p_a(x) \{ [I_{j,m}^+(x) + I_{j,m}^-(x)] - 2a_j(x) I_b(x) \} \quad (25)$$

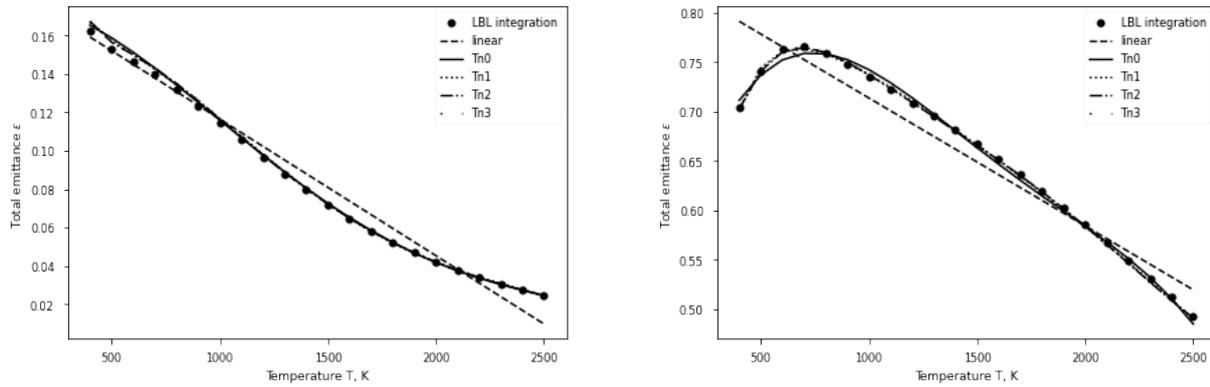
where w_m is the quadrature weight for m direction.

The accuracy of the WSGG model with the different polynomial functions shown in Table 1 is compared with the LBL solution using the normalized deviations for the heat flux and volumetric source as:

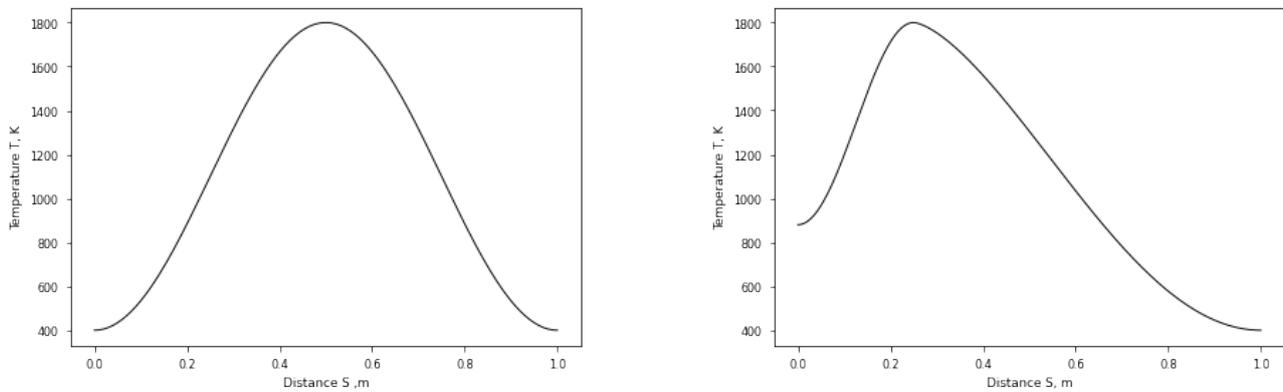
$$\chi(x) = \frac{|q_{R,WSGG}''(x) - q_{R,LBL}''(x)|}{\max |q_{R,LBL}''|} \times 100\% \quad (26)$$

$$\delta(x) = \frac{|S_{R,WSGG}''(x) - S_{R,LBL}''(x)|}{\max |S_{R,LBL}''|} \times 100\% \quad (27)$$

in which χ and δ are the local errors in the evaluation of the radiative heat flux and volumetric source, and $\max |q_{R,LBL}''|$ and $\max |S_{R,LBL}''|$ are the maximum absolute values computed.



(a) Path-length = 0.1 m (b) Path-length = 30 m
Figure 1: Total emittance comparison between WSGG fitting and LBL integration



(a) Case 1 (b) Case 2
Figure 2: Temperature for the medium. (a) Symmetrical distribution (b) Non-symmetrical distribution

4. RESULTS AND DISCUSSION

The WSGG model coefficients generated in this work for the mixture of H_2O and CO_2 are presented in Table 2 and Table 3 for total pressure of 1.0 atm. The coefficients are valid for temperatures ranging from 400 K to 2500 K, path-lengths from 0.01 m to 30 m and mole ratio $Y_{H_2O}/Y_{CO_2} = 2$. A comparison between the total emittance values obtained from these WSGG coefficients and the LBL solution is presented in Fig. 1.

Figures 3(a) and (b) show comparisons between the radiative heat flux calculated through WSGG models and LBL integration for case 1 and case 2 of temperature profiles. Figures 4(a) and (b) show the comparison of the volumetric source calculated from WSGG models and LBL integration for both temperature distributions conditions. Table 4 shows the deviations for both heat flux and volumetric source for all tested conditions considered in this study. The deviations distribution for heat flux and volumetric source are shown in Figs. 5 and 6 respectively. The formulation used to model the Tn3 function whose coefficients is shown in Table 3 produced the less accurate results for the heat flux for both symmetrical and non-symmetrical distribution temperature profiles, with an average error of 7.38% for the symmetrical case and 4.50% for the non-symmetrical distribution. As can be seen in Figs. 5 and 6, the correlation of Tn3 presented the highest local deviations which occurred next the walls for the heat flux, and in the center between the walls for the volumetric source. Analysing the volumetric source results, although the Tn3 modeling presented the highest local errors in both temperature distributions, the Tn0 function rendered the less accurate average deviations for both symmetrical and non-symmetrical profiles, with respective values of 3.88% and 3.21%. The function that produced the best fit for both heat flux and volumetric source, in all temperature distribution scenarios, was the Tn1 modeling. The best correlations occurred for the heat flux computations, with deviations around 1.4% of the benchmark LBL solution. For the volumetric source, the maximum average error was in the symmetrical temperature distribution with the value of 2.17%.

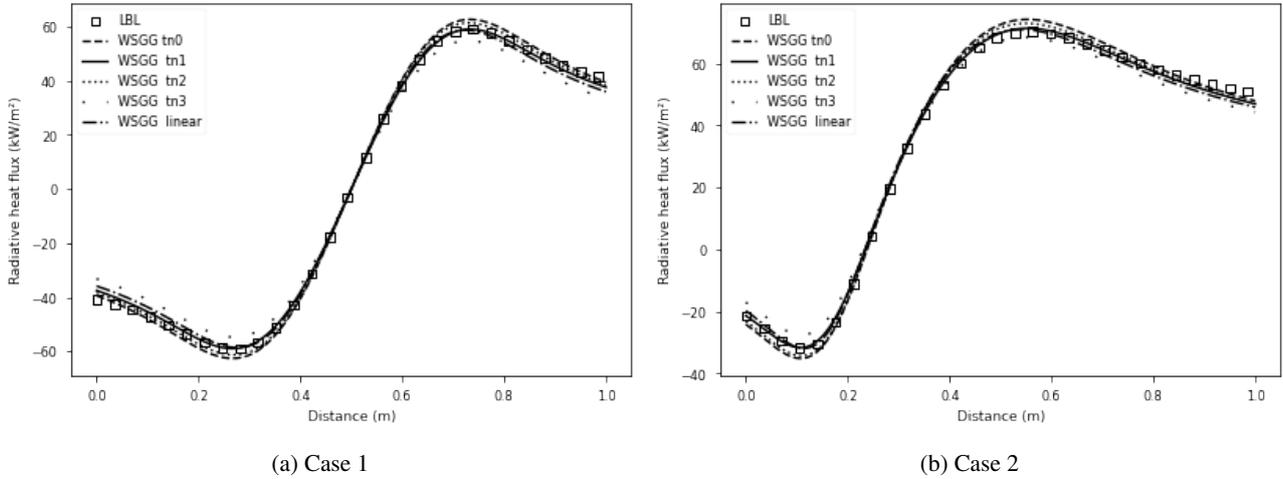


Figure 3: Heat flux q_R'' comparison between WSGG and LBL solutions. (a) radiative heat flux for symmetrical temperature distribution case (b) radiative heat flux for non symmetrical temperature distribution case

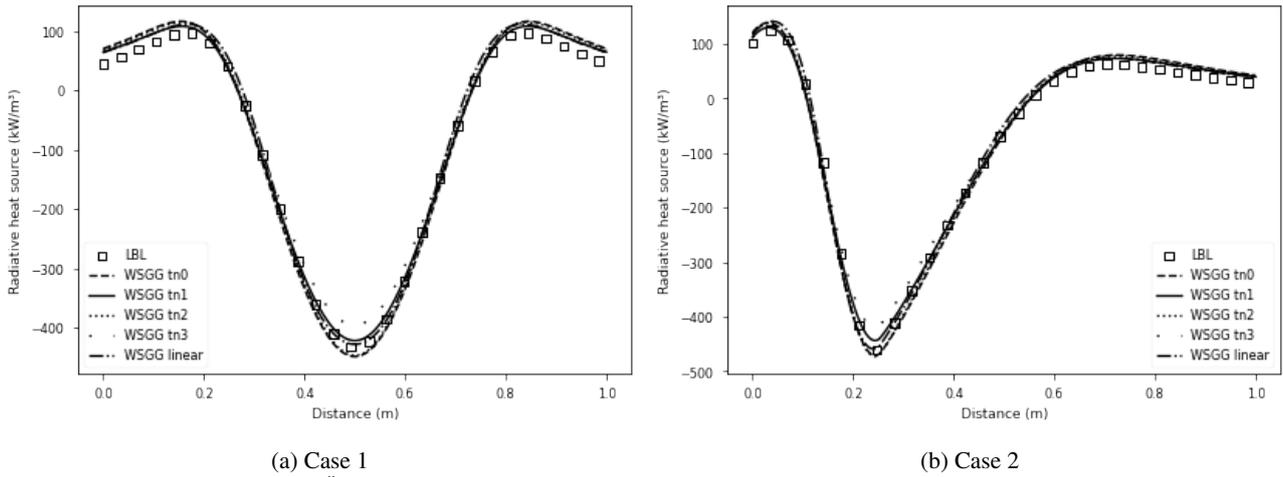
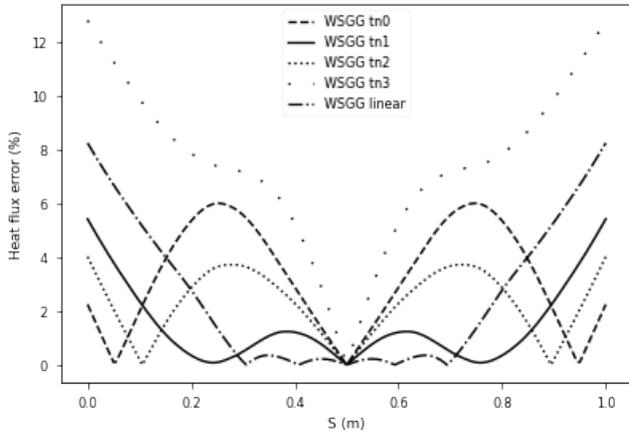


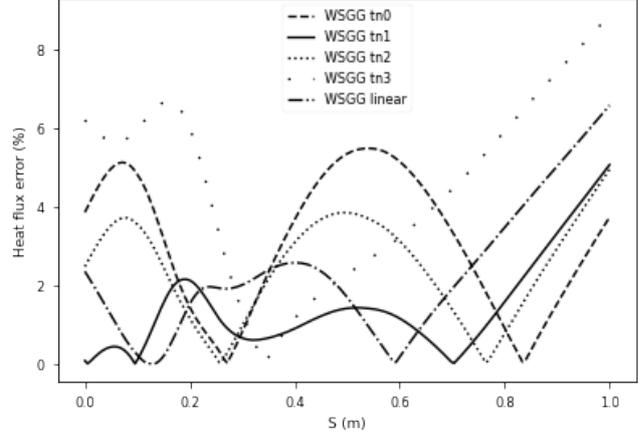
Figure 4: Volumetric source S_R'' comparison between WSGG and LBL solutions. (a) volumetric source for symmetrical temperature distribution case (b) volumetric source for non symmetrical temperature distribution case

Table 4: Radiative heat flux and volumetric source deviations for all tested scenarios

Temperature distribution	Function	q_R''		S_R''	
		$\chi_{max}(\%)$	$\chi_{avg}(\%)$	$\delta_{max}(\%)$	$\delta_{avg}(\%)$
Symmetrical	Linear	8.24	2.53	4.45	2.62
	Tn0	6.00	3.28	5.91	3.88
	Tn1	5.42	1.41	4.63	2.17
	Tn2	4.01	2.27	5.45	3.10
	Tn3	12.79	7.38	8.56	3.47
Non-symmetrical	Linear	6.58	2.29	4.88	2.22
	Tn0	5.48	3.08	6.40	3.21
	Tn1	5.07	1.43	5.06	1.88
	Tn2	4.95	2.44	4.40	2.67
	Tn3	8.88	4.50	8.63	2.64

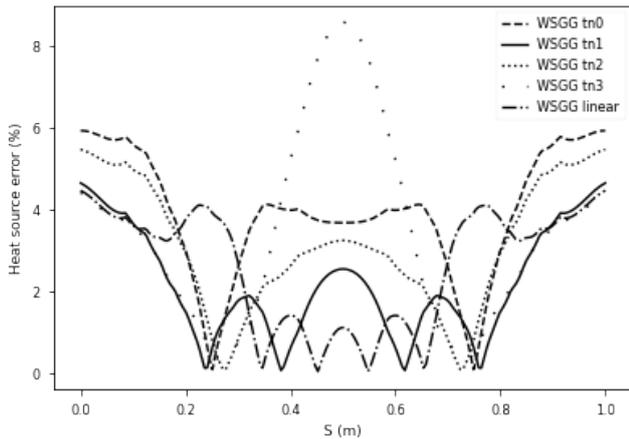


(a) Case 1

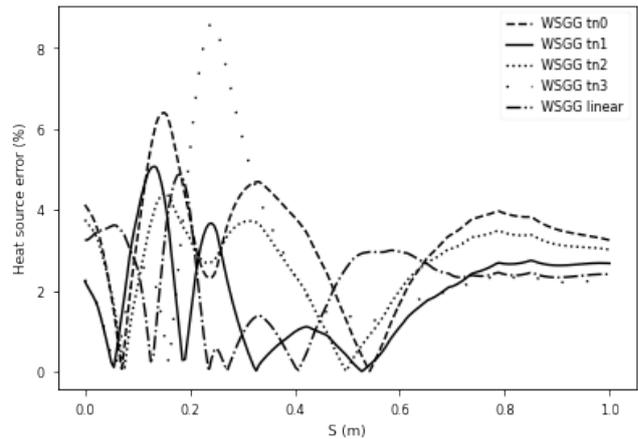


(b) Case 2

Figure 5: Local deviation heat flux q_R'' comparison between WSGG and LBL solutions. (a) local heat flux deviation for symmetrical temperature distribution case (b) local heat flux deviation for non symmetrical temperature distribution case



(a) Case 1



(b) Case 2

Figure 6: Local deviation volumetric source S_R'' comparison between WSGG and LBL solutions. (a) local volumetric source deviation for symmetrical temperature distribution case (b) local volumetric source deviation for non symmetrical temperature distribution case

5. CONCLUSION

This study has presented new WSGG correlations for mixture of H_2O and CO_2 through fitting emittance data obtained from HITEMP2010 database. The correlations were applied under partial pressure ratio of $p_{H_2O}/p_{CO_2} = 2$ and temperatures in the interval of 400 - 2500K. The correlations were tested for two different temperature distribution in the medium and values of heat flux and volumetric source were compared with benchmark LBL solutions. For the two test cases considered in this study, the functions having exponents of -1 and -2 for the absolute temperature (namely, Tn1 and Tn2 functions) proved to be more accurate than the standard WSGG polynomial functions, in which all exponents of the temperature terms are non-negative. Comparing the five sets of functions, the one having exponent of -1 (Tn1) led to the best results for most cases, always improving the accuracy of the WSGG model in comparison to the standard polynomial formulation. Thus, this simple modification, adding only one more term in the temperature coefficient, seems recommendable for future developments of correlations of the WSGG model. Additional studies considering different degree of the positive exponents with lower values and different scenarios of mole fractions, pressure ratios and temperature distribution must be analyzed in order to conclude that the results obtained indeed represent an improvement of the WSGG model.

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