

RADIATIVE HEAT TRANSFER MODELING WITH HITEMP 2010 DATABASE USING CW AND SLW METHODS

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***Abstract.** The HITEMP 2010 spectral database is employed to obtain the necessary parameters for the prediction of radiative transfer in nonisothermal and homogeneous media. It is considered a one dimensional slab filled with 10 % of carbon dioxide and 20 % of water vapour. The spectral integration is performed with SLW and CW models and compared with line by line benchmark solution. It is observed that, for the thermal conditions and species concentrations considered, the SLW model is more suitable to predict the radiative heat source, which is one of the main parameters in the computation of radiation in the participating media.*

***Keywords:** radiative transfer, spectral integration, HITEMP database*

1. INTRODUCTION

Radiative transfer is the main process of heat transfer in applications at high temperature like gases in combustion. In these cases, poor prediction of radiation can miscalculate the heat transfer rates. However, an approach for gases is still a difficult task due to the highly irregular dependence of radiative properties with the wavelength. The line-by-line (LBL) integration, known as benchmark solution, is the most accurate method, in which the Radiative Transfer equation (RTE) is integrated over the detailed molecular spectrum. Nevertheless, this model is computationally expensive because the spectra of gases present several thousands of absorption lines. In recent years, many models have been developed to overcome these drawbacks.

The Weighted-Sum-of-Gray-Gases (WSGG) model, developed by Hottel and Sarofim (1967) in the context of the zonal method, has been broadly applied to solve spectral integration in radiation heat transfer. In this method a non-gray gas is replaced by a number of gray gases, for which the heat transfer rates are calculated independently. The total heat flux is found by adding the fluxes of each gray gas after multiplication with certain weight factors. Smith et al. (1982) obtained coefficients for the total emissivity and absorptivity in the WSGG model. The method may be applied to arbitrary geometries and arbitrary solutions methods of RTE, such as P-N approximations and discrete ordinates method (Modest, 1991). However, the WSGG model is limited to non-scattering media confined within a black-walled enclosure (Modest, 1991).

Denison and Webb (1993) introduced the Spectral Line Weighted-Sum-of-Gray-Gases (SLW) model as an extension of the classical WSGG approach where the weights are determined with the absorption-line distribution function, which is calculated directly from the high resolution molecular spectrum of gases. The SLW model has been extended for various applications: nonisothermal and nonhomogeneous media (Denison and Webb, 1995a), gas mixtures (Denison and Webb, 1995b; Solovjov and Webb, 2000) and gas mixtures with soot (Solovjov and Webb, 2001). The Spectral integration of the RTE with SLW model has a disadvantage. It produces Leibnitz terms (Denison and Webb, 1993; Solovjov and Webb, 2010) in non-isothermal media. The WSGG and SLW models are well-suited for the spectral integration in combination with arbitrary methods of solution on the RTE, but require additional approximation in the case of gas mixtures and non-uniform media (Goutiere et al., 2000).

Solovjov and Webb (2002) presented the Cumulative Wavenumber (CW) model as a new approach to spectral integration. This model employs a novel gas absorption distribution function which contains compressed information about the molecular spectra of gases. The spectral integration of RTE in CW model is performed over fixed intervals; therefore it does not produce Leibnitz terms (Solovjov and Webb, 2010). Solovjov and Webb (2005) presented enhancements to the CW model to consider gas mixtures with soot. Galarça et al. (2011) proposed a modification of the CW method to improve the estimation of the radiative heat flux, with the requirement that the energy balance be satisfied. This aspect, in general, the model cannot be ensured.

The parameters used in spectral models can be obtained from databases such as HITRAN (Rothman et al., 2009) and HITEMP, high-temperature molecular spectroscopic database, (Rothman et al., 2010). The HITRAN database was assembled for a gas temperature of 296 K. The lack of so-called hot lines, which are more significant at elevated temperatures, make HITRAN deficient when applied to problems where the gases are at sufficiently high temperature. For water vapor and carbon dioxide at high temperatures, the most appropriate database is the HITEMP, which is obtained for temperature equal to 1000 K.

This paper considers a gas mixture comprised of some combustion gases (water vapor and carbon dioxide) that are confined between two black walls in a one dimensional system. The main goal is to verify some spectral models that were developed to compute the radiative heat transfer provided by several temperature profiles. The SLW and CW solutions are used to the calculation of radiative heat flux and radiative dissipation source. The results are compared with the LBL benchmark. All solutions are conducted with the latest version of the HITEMP spectral database.

2. THE RADIATIVE TRANSFER EQUATION

The radiation field in absorbing, emitting and non-scattering media is given by the radiative transfer equation (RTE), which can be expressed as:

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

where I_η is the spectral intensity of radiation along the path s , κ_η is the spectral absorption coefficient and $I_{b\eta}$ is the Planck spectral distribution of blackbody intensity. In the right-hand side of the above equation, the first and second terms correspond, respectively, to the increase and decrease of the spectral radiation intensity due to absorption and emission in the medium.

The spectral absorption coefficient of participating gases κ_η is known by its strongly irregular variation with the wavenumber and can be obtained with the Lorentz collision profile (Siegel and Howell, 2002; Modest, 2003) given by:

$$\kappa_\eta = NC_\eta = N \sum_i \frac{S_i}{\pi} \frac{\gamma_i}{(\eta - \eta_i)^2 + \gamma_i^2} \quad (2)$$

where η is the wavenumber, N is the molar density of the absorbing species, C_η is the gas absorption cross-section, S_i is the integrated intensity of line i , η_i is the line location, and γ_i is the half-width.

3. SPECTRAL MODELS

3.1 The Spectral Line Weighted-sum-of-gray-gases Model (SLW)

In the Spectral Line Weighted-sum-of-gray-gases model, developed by Denison and Webb (1993), the integration over wavelength (or wavenumber) in the classical line-by-line spectral solution is replaced by integration over absorption cross-section for a finite number of discrete absorption cross-sections (Solovjov et al., 2011). The transport equation for the radiation in a medium without scattering, Eq. (1), becomes:

$$\frac{dI_j}{ds} = -\kappa_j I_j + a_j \kappa_j I_b \quad \text{for } j = 1, 2, \dots, n \quad (3)$$

where n is the number of gray gases in the model, I_j is the intensity of gray gas j and a_j is the gray gas weight. The absorption coefficient of each gray gas κ_j is determined by the two adjacent cross-sections C_{j-1} and C_j :

$$\kappa_j = N \sqrt{C_{j-1} C_j} \quad (4)$$

where N is the gas molar density.

The absorption line blackbody (ALB) distribution function, which is applied to compute the weights in the SLW model, is defined as the fraction of the total blackbody energy, for the gas mixture at temperature T , corresponding to wavenumber for which the absorption cross-section C_η is less than the specified value C . The ALB distribution function can be expressed as (Denison and Webb, 1993):

$$F(C) = \frac{\int_{\{\eta: C_\eta < C\}} E_{b\eta}(T) d\eta}{\sigma T^4} \quad (5)$$

where σ and $E_{b\eta}$ are, respectively, the Stefan-Boltzmann constant and the spectral blackbody emissive power.

The gray gas weight a_j is calculated by the difference of two ALB distribution functions in two adjacent cross-sections $F(C_j)$ and $F(C_{j-1})$.

$$a_j = F(C_j) - F(C_{j-1}) \quad (6)$$

After solving Eq. (3) for each gray gas j , the total intensity of radiation I is obtained by the summation over all gray gases:

$$I = \int_0^\infty I_\eta d\eta = \sum_{j=1}^n I_j \quad (7)$$

For mixtures, in theory, one need to calculate the ALB distribution functions $F(C)$ for any composition of the mixture at any temperature. This is impractical due to the high resolution molecular spectra of the mixture. Instead, one can use the multiplication approach, which is based on the assumption that the absorption cross-sections of different species included in the mixture are statistically independent (Solovjov and Webb, 2000). According to the multiplication approach, the ALB distribution function of the composite absorption cross-section $F_{C_\eta}(C)$ is obtained by the product of the distribution functions of each individual contribution:

$$F_{C_\eta}(C) = F_{Y_1 C_{1,\eta}}(C) F_{Y_2 C_{2,\eta}}(C) \cdots F_{Y_m C_{m,\eta}}(C) \quad (8)$$

where m is the number of species in gas mixture. The ALB distribution function for arbitrary mole fraction Y_m can be calculated through the ALB distribution function of the each gas:

$$F_{Y_m C_{m,\eta}}(C) = F_{C_{m,\eta}}(C/Y_m) \quad (9)$$

When Eq. (9) is applied to Eq. (8), a relation to the ALB distribution function for mixture of gases can be obtained:

$$F_{C_\eta}(C) = F_{C_{1,\eta}}(C/Y_1) F_{C_{2,\eta}}(C/Y_2) \cdots F_{C_{m,\eta}}(C/Y_m) \quad (10)$$

3.2 The Cumulative Wavenumber Model (CW)

The Cumulative Wavenumber model (Solovjov and Webb, 2002) employs a distribution function w , which contains compressed information about the molecular spectra of gases. For any fixed value of absorption cross-section C and wavenumber η , the cumulative wavenumber function $w(C, \eta)$ can be defined by the following equation:

$$w(C, \eta) = \int_0^\eta H(C - C_\eta) d\eta \quad (11)$$

where $H(C - C_\eta)$ is the Heaviside step-function.

The cumulative wavenumber grows linearly with the wavenumber for those values of η where C_η is less than the value C , and remains constant elsewhere. Therefore, the differentiation of Eq. (11) with respect to η yields:

$$\frac{\partial w(C, \eta)}{\partial \eta} = \begin{cases} 1 & \text{for } C > C_\eta \\ 0 & \text{for } C < C_\eta \end{cases} \quad (12)$$

Equation (12) allows one to replace the integration with respect to the independent variable η over the spectral region defined by molecular absorption spectrum by integration with respect to the cumulative wavenumber.

$$\int_{\eta: C > C_\eta} d\eta = \int_0^\infty \frac{\partial w(C, \eta)}{\partial \eta} d\eta = \int_0^\infty dw(C, \eta) \quad (13)$$

In CW model, the full range of absorption cross-section is subdivided into gray gases by the supplemental cross-sections C_j ($j = 1, \dots, n$; n is the number of gray gases). The union of all spectral intervals for which the absorption cross-section lies between supplemental absorption cross-sections (C_j and C_{j-1}) H_j is stated as:

$$H_j = \{\eta: C_{j-1} \leq C_\eta \leq C_j, j = 1, 2, \dots, K, n\} \quad (14)$$

The CW model also makes a subdivision of the wavenumber region according to:

$$\Delta_i = [\eta_{i-1}, \eta_i], \quad i = 1, 2, \dots, K \quad (15)$$

where Δ_i represents a subinterval in the wavenumber.

The intersection of spectral subdivisions H_j and Δ_i define the fractional gray gas wavenumber D_{ij} . The union of all fractional gray gas wavenumbers gives the entire wavenumber space. Although Δ_i remains fixed for any location in the medium considered, H_j and D_{ij} are allowed to float with location depending on the local thermodynamic state of the gas.

The difference between cumulative wavenumber at two adjacent supplemental cross-sections for each fractional gray gas is represented by the product of two functions, one of which depends on the location s and the other on wavenumber η :

$$w(C_{j,s}, \eta) - w(C_{j-1,s}, \eta) = u_{ij}(s)v_{ij}(\eta) \quad \text{para } \eta \in \Delta_i \quad (16)$$

where $v_{ij}(\eta)$ is defined by Eq. (16) at some reference point s^* where the reference values of temperature $T(s^*)$ and species concentrations $Y(s^*)$ are known. One can arbitrarily assign for this location a value $u_{ij}(s^*) \equiv 1$. Therefore, for an arbitrary point s , the function $u_{ij}(s)$ can be calculated by:

$$u_{ij}(s) = \frac{\Delta w(C_{j,s}, \eta)}{v_{ij}(\eta)} = \frac{w(C_{j,s}, \eta) - w(C_{j-1,s}, \eta)}{w(C_{j,s^*}, \eta) - w(C_{j-1,s^*}, \eta)} \quad (17)$$

The integration of spectral intensity of radiation I_η over the fractional gray gas D_{ij} using the concept of cumulative wavenumber described by Eq. (13) yields:

$$\int_{D_{ij}} I_\eta d\eta = u_{ij}(s) \int_{\Delta_i} I_\eta d[v_{ij}(\eta)] = u_{ij}(s) J_{ij}(s) \quad (18)$$

where $J_{ij}(s)$ is viewed as a fractional gray gas intensity and $u_{ij}(s)$ can be interpreted as a local correction factor to the reference fractional gray gas intensity.

The spectral integration of Eq. (1) is similar to the derivation of Eq. (18). Hence, according to Eq. (13) leads to:

$$\frac{\partial J_{ij}}{\partial s} = -\kappa_j J_{ij} + \kappa_j J_{bij} \quad (19)$$

where κ_j is the gray gas absorption coefficient, determined from the supplemental absorption cross-section as:

$$\kappa_j = N \sqrt{C_j C_{j-1}} \quad (20)$$

and J_{bij} is the blackbody radiative energy source:

$$J_{bij}(s) = \int_{\Delta_i} I_{b\eta} [T(s), \eta] d[v_{ij}(\eta)] \quad (21)$$

The total intensity of radiation $I(s)$ is determined by the summation of all gray gas intensities weighted by the function $u_{ij}(s)$.

$$I(s) = \sum_{i,j} u_{ij}(s) J_{ij}(s) \quad (22)$$

If the mole fraction Y of the species in a gas mixture changes, the cumulative wavenumber, which is assumed to vary linearly with the mole fraction, is obtained straightforward form molecular spectrum.

$$w_{YC_\eta}(C, \eta) = w_{C_\eta}(C/Y, \eta) \quad (23)$$

where w_{C_η} and w_{YC_η} are the cumulative wavenumber of the absorption cross-sections C_η and YC_η , respectively, neglecting the effect of self-broadening.

The extension of CW model to gas mixtures can be done with the superposition approach, which assumes that spectral lines of absorption cross-sections of m different species are not overlapping, $C_\eta = Y_1C_1 + Y_2C_2 + \dots + Y_mC_m$, (Solovjov and Webb, 2002). Thus:

$$w_{C_\eta}(C, \eta) = (1 - m)\eta + \sum_{k=1}^m w_k(C/Y_k, \eta) \quad (24)$$

4. RESULTS

This work considers a homogeneous and nonisothermal plane-parallel slab filled with spatially uniform gaseous mixture – 10% CO₂ and 20% H₂O (the remainder is an inert gas such as nitrogen). From the ideal gas theory, the ratio between the partial pressure of each species to the total pressure is equivalent to its molar concentration, thus $Y_{CO_2} = 0.1$ and $Y_{H_2O} = 0.2$. The one dimensional media is bounded by black walls, which are 1.0 m apart. The spectral integrations with SLW, CW and LBL models were obtained with the same spectral database (HITEMP 2010). The RTE was solved with discrete ordinates method employing 200 grid points and 30 ordinates. The CW and SLW simulations employed 20 gray gases.

In this paper, three temperature distributions of the gas were modeled. In Eq. (25) and Eq. (26), the temperature is ranging from 400 K at the walls to 1800 K at the medium center. The Eq. (27) shows other distribution where the temperatures are 920 K and 400 K at the left and right walls, respectively. And the maximum temperature (1800 K) is reached in one quarter of the length L .

$$T(x) = 400 + 1400 \sin\left(\frac{\pi x}{L}\right)^2 \quad (25)$$

$$T(x) = 400 + 1400 \sin\left(\frac{2\pi x}{L}\right)^2 \quad (26)$$

$$T(x) = \begin{cases} 920 + 880 \sin\left(\frac{2\pi x}{L}\right)^2 & \text{if } x \leq L/4 \\ 1100 + 700 \cos\left|\frac{4x}{L} - 1\right| & \text{if } x > L/4 \end{cases} \quad (27)$$

where the position in the medium is defined by x , with the walls located at $x = 0$ and $x = L$.

The results will be displayed in terms of the radiative heat source, in units of W/m³, which is equal to the divergence of the radiative heat flux with opposite sign ($\dot{q}_R = -dq_R''/dx$). The divergence of the radiative heat flux states that physically the net loss of radiative energy from a control volume is equal to emitted energy minus absorbed irradiation.

In the literature, when the effect of self-broadening is neglected, one assumes that the absorption cross-section coefficient C varies linearly with the mole fraction Y . According to this assumption, if the absorption cross-section $C_\eta(Y_1)$ is known to the mole fraction $Y_1 = 1$, the absorption cross-section to the mole fraction $Y_2 = 0.1$ is given by $C_\eta(Y_2) = 0.1C_\eta(Y_1)$. When the mole fraction depends on the position, this approximation is very advantageous. However, it can lead to very large errors in the radiative heat transfer rates for the water vapor.

Two test cases are proposed to verify the linear approximation for the absorption cross-section. In the first one, is considered a medium with 20% of water vapor and an inert gas. In the second case, is considered a mixture with 10% of carbon dioxide and an inert gas. In the solutions with linear approximations, the absorption cross-sections coefficients for water vapor and carbon dioxide can be obtained by, respectively, $C_{\eta_{H_2O}}(Y = 0.2) = 0.2C_{\eta_{H_2O}}(Y = 1.0)$ and $C_{\eta_{CO_2}}(Y = 0.1) = 0.1C_{\eta_{CO_2}}(Y = 1.0)$. The absorption cross-sections coefficients for the solutions without linear approximations are obtained directly for $Y = 0.2$ and $Y = 0.1$. The Figure 1 shows the LBL solution to the radiative heat source when the gas temperature is given by Eq. (25). When the aforementioned approximation is employed for the water vapor, Fig. 1(a), there is an over prediction in the radiative heat source. The main reason for this behavior is the self-broadening (collisions between two molecules of absorbing species). This effect is quite substantial for the water vapor (since H₂O molecules are much smaller than air molecules). Nevertheless, for carbon dioxide, Fig. 1(b), the self-broadening is negligible (since the CO₂ molecules and air molecules have roughly the same size) (Modest, 2003).

Therefore, in this work, the absorption cross-section coefficient for carbon dioxide was obtained to $Y = 1.0$ and it was applied the linear approximation to obtain the absorption cross-section coefficient at $Y = 0.1$. However, for water vapor the absorption cross-section coefficient was obtained directly for $Y = 0.2$. The spectrum was generated for temperature ranging from 400 K to 2500 K with steps of 100 K.

The Figures 2 and 3 show the results for the temperature distributions given by Eq. (26) and Eq. (27), respectively. The Figures 2(a) and 3(a) show the solutions for the radiative heat flux. As expected, the SLW solutions present better agreement with the LBL benchmark than CW solution does. As discussed in Galarça et al. (2011), the CW model, in most cases, fails to predict the radiative heat flux. The Figures 2(b) and 3(b) show the solutions for the radiative heat source. Another time, the SLW solutions was better than CW ones.

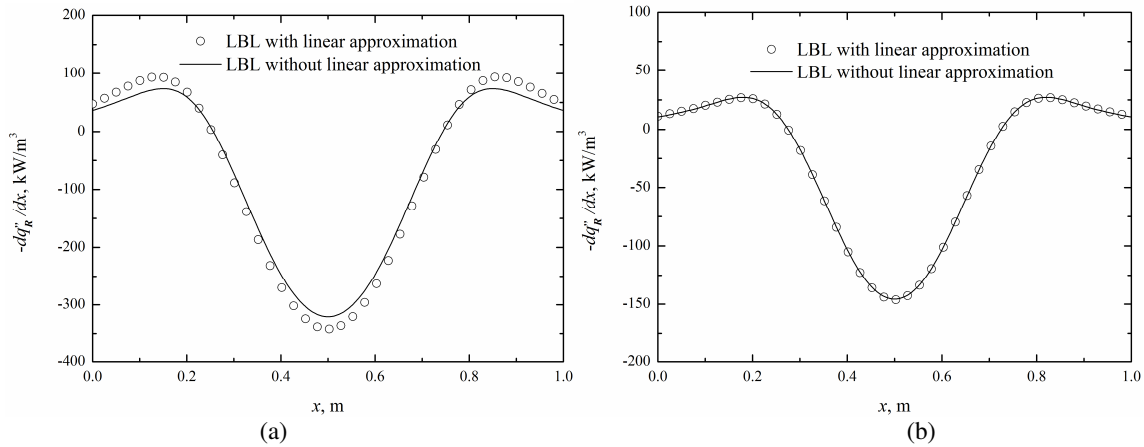


Figure 1. LBL solutions with and without linear approximation to absorption cross-section coefficient. (a) Mixture composition: 20 % of H₂O and an inert gas. (b) Mixture composition: 10 % of CO₂ and an inert gas. Temperature distribution given by Eq. (25).

In all cases, the radiative heat source is positive in the medium regions close to the walls, indicating that the gain of radiation from the hot regions of the medium exceeded the loss of radiation to the surfaces. Figure 2(b) shows that the radiative heat source is positive at the half distance between the walls, therefore the gain of radiative energy is greater than the loss in this location. Figure 2(b) also depicts two “valleys” in the radiative heat source shape. In these regions, the radiative heat source is negative, hence, the loss of radiative energy exceeded the gain. In the Fig. 3(b), the radiative heat source reaches negative values in the neighborhood of $x = 0.25$ m, meaning that the loss exceeded the gain of radiative energy.

Additional comparison between the SLW and CW models can be made with the analysis of their errors with respect to the LBL benchmark, which are defined as:

$$\delta(\%) = \left| \frac{\dot{q}_{R,Model}'' - \dot{q}_{R,LBL}''}{\max(\dot{q}_{R,LBL}'')} \right| 100 \quad (28)$$

where δ , $\max(\dot{q}_{R,LBL}'')$ are the error in the radiative heat flux and the maximum absolute value of the radiative heat flux for the LBL solution, respectively.

$$\gamma(\%) = \left| \frac{\dot{q}_{R,Model} - \dot{q}_{R,LBL}}{\max(\dot{q}_{R,LBL})} \right| 100 \quad (29)$$

where γ and $\max(\dot{q}_{R,LBL})$ are the error in the radiative heat source and the maximum absolute value of the radiative heat source for the LBL solution, respectively.

The Table 1 summarizes the average and maximum errors, respectively, in the radiative heat flux δ_{avg} and δ_{max} ; and the average and maximum errors γ_{avg} and γ_{max} , respectively, in the radiative heat source for the SLW and CW solutions. For all cases discussed in this study, CW model leads to larger maximum error than SLW solution. One can observe that the maximum errors in the radiative heat source calculations for CW solutions are observed close to the regions where the maximum temperatures are reached in the medium.

While the maximum error in the radiative heat flux for CW solution is greater than 40%, in the SLW solution this value remains less than 24%. The major disagreement between SLW and LBL solutions occurs when the temperature is given by Eq. (27).

The CW and SLW models over predict the medium emission (radiative heat source with negative sign) next to $x = 0.25$ m e $x = 0.75$ m in the Fig. 2(b), however the maximum error for SLW solution is $\gamma_{\max} = 11.1\%$ while the maximum error for CW solution is $\gamma_{\max} = 32.2\%$. The SLW model also over estimates the absorption of the gas in the Fig. 2(b), close to $x = 0.5$ m. Finally, both models over predict the emission in the vicinity of $x = 0.25$ m in the Fig. 3(b). Another time, the maximum error for SLW solution ($\gamma_{\max} = 7.6\%$) is less than the CW solution error ($\gamma_{\max} = 16.3\%$).

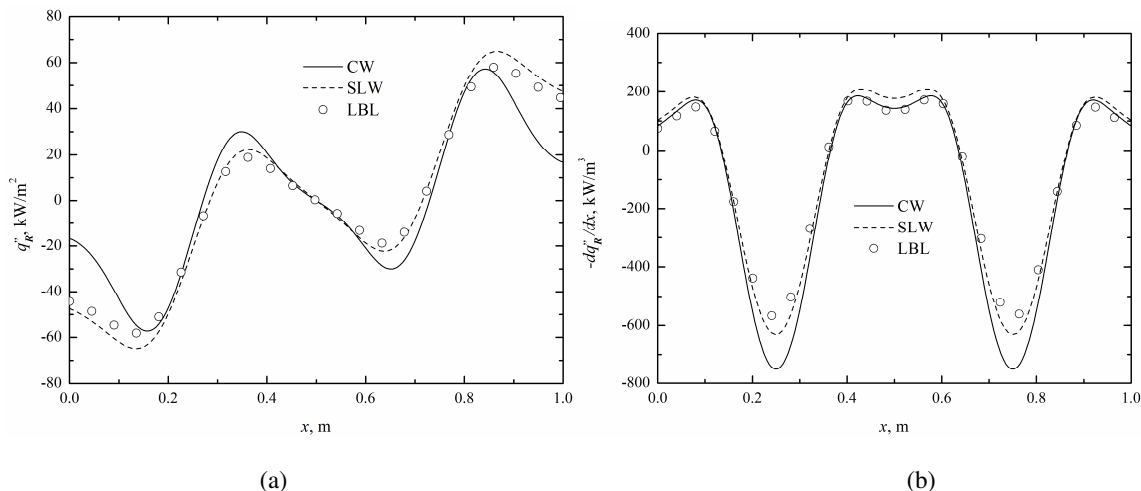


Figure 2. Radiative heat flux (a) and radiative heat source (b) for the temperature distribution given by Eq. (26).

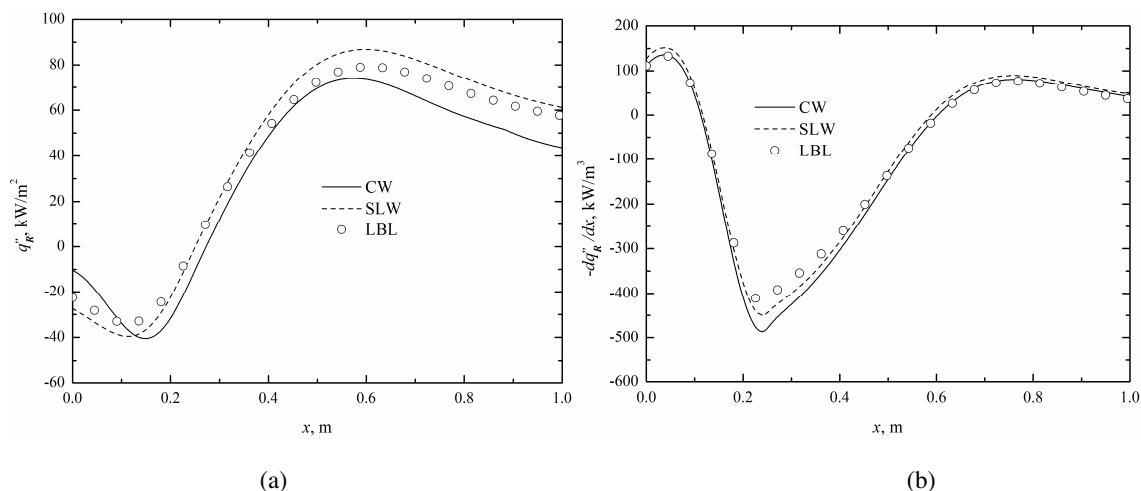


Figure 3. Radiative heat flux (a) and radiative heat source (b) for the temperature distribution given by Eq. (27).

Table 1. Average and maximum errors in SLW and CW solutions when compared with LBL (benchmark).

Temperature distribution	SLW				CW			
	δ_{avg} (%)	δ_{max} (%)	γ_{avg} (%)	γ_{max} (%)	δ_{avg} (%)	δ_{max} (%)	γ_{avg} (%)	γ_{max} (%)
Eq. (26)	6.4	11.8	5.7	11.1	15.0	47.5	10.1	32.2
Eq. (27)	15.8	23.7	3.7	7.6	24.6	40.3	4.4	16.3

5. CONCLUSIONS

This work considered a one dimensional slab filled with participating gas with homogeneous composition (carbon dioxide and water vapor). The spectral integration of the RTE was performed with two models (SLW and CW). The solutions, obtained with the same spectral database (HITEMP 2010), were compared with the LBL benchmark. The CW

results showed considerable deviation from the LBL solution, mainly for the radiative heat flux. The CW model presented better agreement with benchmark solution when applied for the radiative heat source calculation, nevertheless showed greater errors in the regions where the medium is hotter. For the thermal conditions and concentrations of the chemical species, the SLW model showed better agreement with the LBL solution. The results also illustrate that, for the same temperature profile, the SLW model can give good results for the radiative heat source and poor results for the radiative heat flux. These conclusions show that the spectral integration in participating media is still a challenge. To next steps, one can apply the CW and SLW solutions to non isothermal and non homogeneous media.

6. ACKNOWLEDGEMENTS

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