ANALYSIS OF THE EFFECT OF HIGH PRESSURE LEVELS ON THE RADIATIVE HEAT TRANSFER OF PARTICIPATING GASES

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Abstract. *Thermal radiation is the dominant heat transfer mechanism in high pressure combustion processes such as oxy-fuel combustion. The solution of radiation in participating media is complex due to the integro-differential governing equation and the highly irregular spectral behavior of the absorption coefficient. Thus the radiative transfer equation (RTE) is usually solved using spectral models to determine the radiative quantities. The weighted-sum-of-gray-gases (WSGG) model replaces the spectral integration of the RTE by bands of uniform absorption coefficients, and has recently received considerable attention mainly because of its simplicity and overall great performance. However, this model is based on the assumption that the emittance of the participating gas is only a function of the temperature and the pressure path-length. This paper checks the validity of this assumption by studying the effect of different pressure values on the emittance of a participating gas composed by water vapor and carbon dioxide while keeping the pressure path-length constant. For the emittance calculation the RTE is solved by the line-by-line (LBL) method using the HITEMP2010 spectral emissivity database for the spectral integration. The results showed that the emittance varies significantly as the total pressure increases, implying that a WSGG model developed for a certain total pressure should not be applied in cases involving other total pressures to avoid further deviations.*

Keywords*: Radiative heat transfer, weighted-sum-of-gray-gases model, line-by-line, emittance, high pressures.*

1. INTRODUCTION

Thermal radiation is the dominant mode of heat exchange at elevated temperatures processes such as combustion. Combustion processes also generate participating gases as products which can emit, absorb or scatter radiation and the radiative heat transfer energy balance of the media results in the radiative transfer equation (RTE). The solution of the radiation problem requires the spatial and spatial integration of the RTE which is an integro-differential and some of its variables (mainly the absorption coefficient) have a strongly irregular spectral dependence.

In order to simplify this irregular spectral dependence and, consequently, the spectral integration several spectral models were developed. The weighted-sum-of-gray-gases (WSGG) model, proposed by Hottel and Sarofim (1967), is an example of spectral model which simplifies the spectral integration. The method replaces the highly irregular behavior of the absorption coefficient of a participating gas by a few equivalent gray gases with uniform absorption coefficient divided by bands. Each gray gas has a weighting absorption coefficient which is determined by a data fitting on the total emittance calculated through spectral emissivity databases such as HITEMP (High Temperature Molecular Spectroscopic Database). Dorigon et al., 2013, obtained absorption coefficients for a mixture composed by carbon dioxide and water vapor at atmospheric total pressure based on HITEMP2010 for a wide range of pressure path-lengths and temperatures. It concluded that despite the simplicity of the model it provides good results when compared to the benchmark solutions.

High pressure combustion processes such as oxy-fuel combustion are getting more popular because of better combustion performance and lower greenhouse gas emissions; some recent works attempt to apply the WSGG method for high pressures. Bordbar et al., 2014, developed a spectral database and absorption coefficients for oxy-fired combustion conditions for a wide range of temperature, pressure path-length, and molar ratios based on HITEMP2010. These WSGG coefficients developed by Bordbar were used by Chu et al, 2016, to solve an oxy-fuel combustion problem for total pressures ranging from 1.0 to 30 atm and found out that the WSGG had the lowest accuracy especially between 1.0 and 10 atm. However, it was not taken into account that the reference pressure for the WSGG coefficients was 1.0 atm. Kez et al., 2016, also solved an oxy-fuel combustion problem at 20 atm using the WSGG model from Bordbar et al., 2014, and had significant deviations, concluding that the WSGG model should not be applied for oxy-fuel combustion. Other high pressure combustion studies were made by Alberti et al., 2015, which re-created Hottel's emissivity charts for carbon dioxide from 0.1 to 40 bar, and by Pearson et al., 2014, which studied the effect of total pressure on the absorption spectrum from 0.1 to 50 atm, both using HITEMP2010.

Based on these recent studies, this study seeks to analyze the effect of high pressure values on the absorption spectrum and emittance behavior for carbon dioxide and water vapor. Since the WSGG model coefficients are fitted from the emittance values, this analysis studies the applicability of the WSGG for high pressure combustion.

2. METHODOLOGY

2.1 The radiative transfer equation and spectral modeling

The energy balance for the radiative heat transfer in a participating media results in the RTE, which neglecting the scattering effect, is given by

$$\frac{dI_\eta(x)}{dx} = -\kappa_\eta(x) I_\eta(x) + \kappa_\eta(x) I_{\eta b}(x) \tag{1}$$

in which κ_η is the absorption coefficient, in m^{-1}, and I_η and $I_{\eta b}$ represent the spectral intensity and the blackbody radiation intensity in W/(m² cm^{-1}).

The absorption coefficient κ_η is calculated from

$$\kappa_\eta = NYC_\eta \tag{2}$$

where Y is the mole fraction, N is the gas molar density in molecule/(cm² m), and C_η is the absorption cross-section in cm²/molecule. The absorption cross-section, in the majority of engineering applications, is given by the Lorentz profile, which considers collisions between molecules the main reason for the broadening of the spectral lines (Siegel and Howell, 2002) and is calculated from

$$C_\eta(\eta) = \sum_{k=1}^{K} \frac{S_k(T)}{\pi} \frac{\gamma_k}{(\gamma_k{}^2 + (\eta - \eta_k)^2)} \tag{3}$$

in which S_k is the integrated intensity of line k, η_k is the line location, and γ_k is the line half-width. The line half-width γ_k can be calculated from

$$\gamma_k = \left(\frac{T_{ref}}{T}\right)^{\eta_c} p_c \gamma_{self,k} + (p - p_c)\gamma_{air,k} \tag{4}$$

where $\gamma_{self,k}$ is the line self-broadening and $\gamma_{air,k}$ is the broadening caused by air, p_c and p are the partial pressure and the total pressure, T_{ref} is the reference temperature equal to 296 K, and η_c is the temperature dependence coefficient.

The integrated line intensity S_k is given by

$$S_k(T) = S_k(T_{ref}) \frac{Q(T_{ref})}{Q(TO} \frac{\exp(-C_2 E_k / T)}{\exp(-C_2 E_k / T_{ref})} \frac{\left[1 - \exp(-C_2 \nu_k / T)\right]}{\left[1 - \exp(-C_2 \nu_k / T_{ref})\right]} \tag{5}$$

in which Q is the total internal partition sums, ν_k is the energy difference between the initial and final state as a vacuum wavenumber, E_k is the energy of the lower state, and C_2 is the second Planck's constant. The following parameters from Eqs. (3), (4), and (5) are provided in the HITEMP 2010 database: Q, ν_k, E_k, $S_k(T_{ref})$, η_c, $\gamma_{self,k}$, $\gamma_{air,k}$ *and* η_k.

In this study the absorption cross-section spectral distribution is obtained from Eqs. (1)-(5) along with the HITEMP 2010 database for molar fraction Y=0.1 for carbon dioxide and Y=0.2 for water vapor (which are typical methane combustion molar fractions), temperatures ranging from 400 K to 2500 K, and total pressure values of 1, 2, 5, 10, 20, and 40 atm. The results from these charts are the effect of the total pressure on the absorption cross-section which can be compared with those obtained by Pearson et al., 2014.

2.2 The WSGG model

The WSGG model divides the spectrum into regions where the absorption coefficient is constant which represents a gray gas. Integrating the RTE over the spectral regions where the absorption coefficient κ_η is replaced by the absorption coefficient based on the pressure associated to each gray gas, $\kappa_{p,j}$, Eq. (1) becomes

$$\frac{dI_j(x)}{dx} = -\kappa_{p,j} p_a(x) I_j(x) + \kappa_{p,j} p_a(x) a_j(T) I_b(T) \tag{6}$$

where p_a is the partial pressure, a_j is the temperature dependent coefficient, $I_b(T)$ is the total blackbody intensity.

The WSGG coefficients are obtained by fitting the WSGG total emittance to the total emittance obtained by the line-by-line (LBL) method, which is given by

$$\varepsilon(T, p_a S) = \frac{\int_{\eta=0}^{\infty} I_{\eta b}(\eta, T)[1 - \exp(-\kappa_{p\eta,a} p_a S)] d\eta}{\sigma T^4 / \pi} \tag{7}$$

where $p_a S$ is the pressure path-length, and $I_{\eta b}$ is the blackbody intensity given by Planck's distribution. Applying Eq. (7) in the WSGG spectrum

$$\varepsilon(T, p_a S) = \sum_{j=1}^{J} a_j(T)[1 - \exp(-\kappa_{p,j} p_a S)] \tag{8}$$

The coefficient $a_j(T)$ is the weighting factor for the j-th gray gas which is frequently fitted as a polynomial function of temperature as

$$a_j(T) = \sum_{k=0}^{K} b_{j,k} T^k \tag{9}$$

In this work the total emittances are calculated using Eq (7) along with the absorption cross-section database generated using HITEMP 2010 for the temperature range from 400 K to 2500 K and for the pressure path-lengths of 10, 1, 0.1 and 0.01 atm m. Since the emittance is only a function of temperature, pressure path-length, and the absorption cross-section data, fixing the temperature and the pressure path-length will isolate the effect of the total pressure on the total emittance. If the emittance for a certain temperature and pressure path-length changes significantly between two total pressure values, then the WSGG coefficients obtained for one of these values cannot be used for the other value without causing significant deviations.

3. RESULTS AND DISCUSSION

3.1 Effect of the total pressure on the absorption cross-section

The absorption cross-section data as a function of wavenumber at 1500 K and total pressures of 1, 10, and 40 atm is shown in Fig. 1 for CO_2 and in Fig. 2 for H_2O. Both graphs present the full spectrum behavior of the absorption cross-section which is shown to smooth the data variation when the total pressure is increase from 1 to 40 atm, similar to the results of Pearson et al., 2014. Also, some bands of the CO_2 spectrum present higher values of the absorption cross-section as the pressure increases.

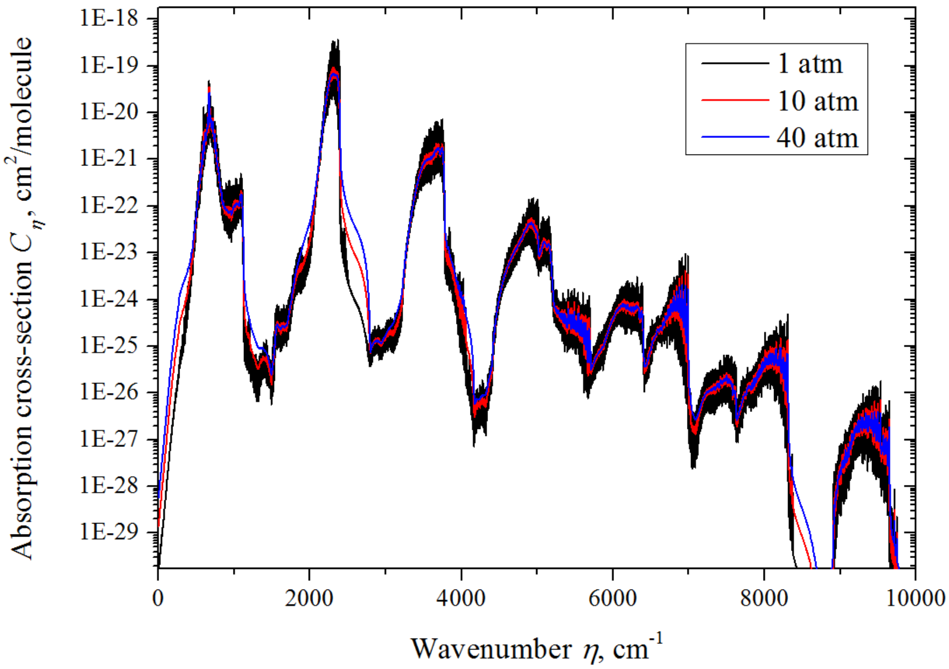


Figure 1. Absorption cross-section as a function of wavenumber for CO_2 at 1500 K and total pressures of 1, 10, and 40 atm.

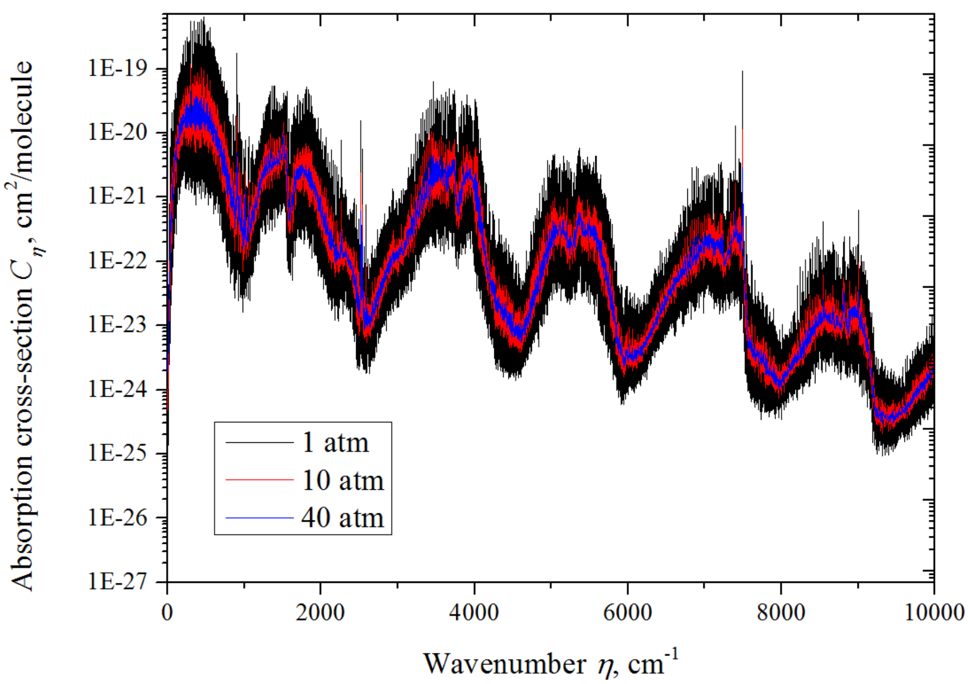
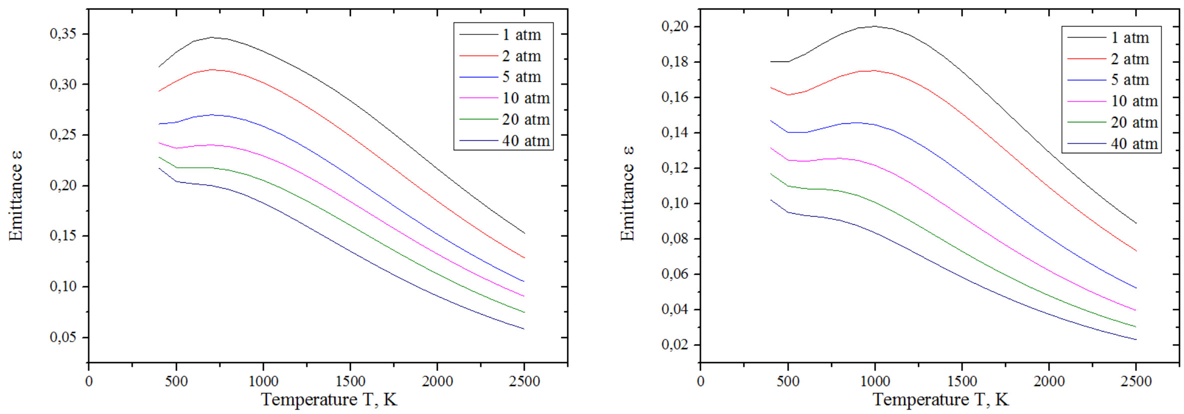


Figure 2. Absorption cross-section as a function of wavenumber for H_2O at 1500 K and total pressures of 1, 10, and 40 atm.

This reduction in the absorption cross-section data variation is enough to imply that the emittance values should vary with the increase in total pressure since from Eqs. (2) and (7) the emittance is a function of the absorption cross-section.

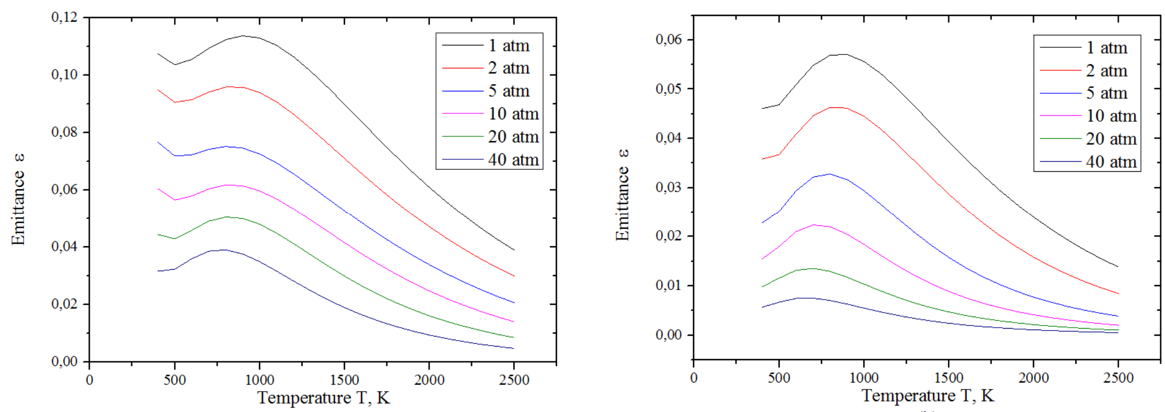
3.2 Effect of the total pressure on the emittance

The total emittance of CO_2 as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm was obtained for various pressure path-lengths. Figures 3(a), 3(b), 4(a), and 4(b) present these results for pressure path-lengths of 10, 1, 0.1, and 0.01 atm m, respectively.



(a) (b)

Figure 3. Emittance of CO_2 as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm and for (a) pressure path-length p_aS = 10 atm·m and (b) pressure path-length p_aS = 1 atm·m.



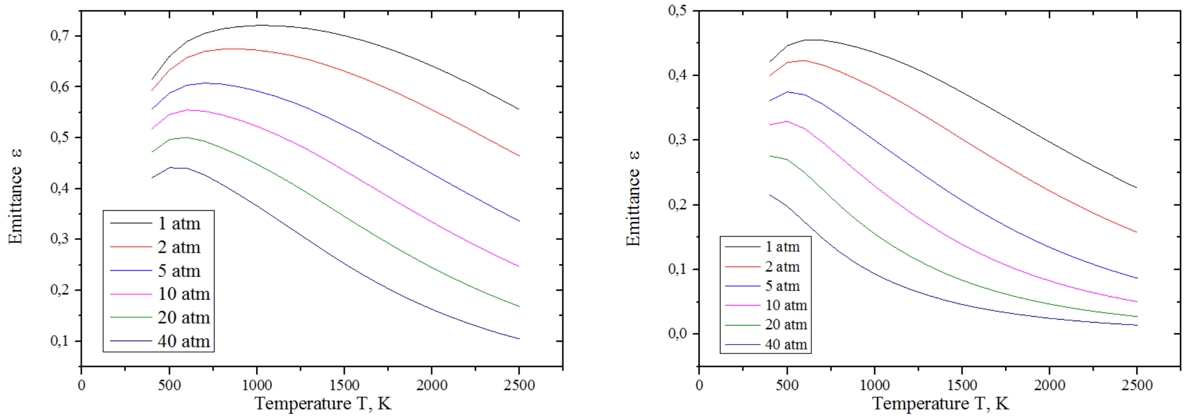
(a) (b)

Figure 4. Emittance of CO_2 as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm and for (a) pressure path-length p_aS = 0.1 atm·m and (b) pressure path-length p_aS = 0.01 atm·m.

These results show that for a fixed path-length and temperature the emittance varies considerably as the pressure increases. Because the other parameters are fixed, this effect is due to solely the absorption coefficient variation with the total pressure and it seems to attenuate as the temperature and pressure increases.

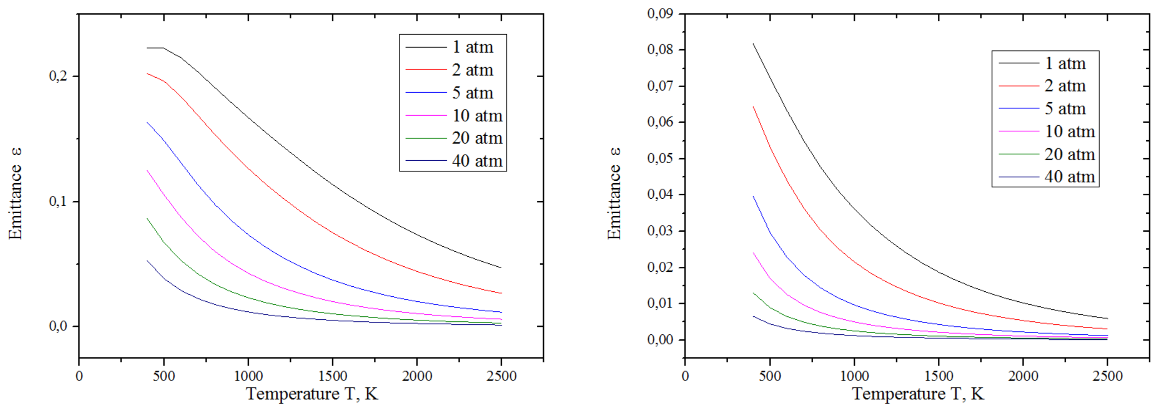
The same analysis was performed for the H_2O and its total emittance as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm is shown in Figs. 5(a), 5(b), 6(a), and 6(b) for pressure path-lengths of 10, 1, 0.1, and 0.01 atm m, respectively. In this case there is also a considerable variation on the emittance as the pressure increases. However, this variation seems to reduce near low temperatures in Fig. 5(a) and near high temperatures and high pressures in Figs. 5(b), 6(a), and 6(b).

Since the WSGG coefficients are fitted based on the emittance values, these variations indicate that using coefficients fitted for different total pressure values is not ideal and increases the error associated with the model. This conclusion shows that developing a WSGG model for high pressures is necessary. An alternative would be to fit new WSGG coefficients for each total pressure value and correlate them so that WSGG could be used for different pressure values from 1 to 40 atm.



(a) (b)

Figure 5. Emittance of H_2O as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm and for (a) pressure path-length p_aS = 10 atm·m and (b) pressure path-length p_aS = 1 atm·m.



(a) (b)

Figure 6. Emittance of H_2O as a function of temperature for total pressure of 1, 2, 5, 10, 20, and 40 atm and for (a) pressure path-length $p_aS = 0{,}1$ *atm m* and (b) pressure path-length $p_aS = 0{,}01$ *atm m*.

4. CONCLUSIONS

This paper analyzed the effect of high pressure values on the absorption cross-section spectral distribution and on the total emittance for water vapor and carbon dioxide with temperature ranging from 400 to 2500 K and total pressure values of 1, 2, 5, 10, 20, and 40 atm. The absorption cross-section analysis showed that as the pressure increases, the variation of the absorption cross-section along the wavenumber reduces significantly and this effect should have an impact on the radiative heat transfer as reported by Pearson et al., 2014.

Increasing the total pressure also had a significant impact on the emittance curves even though the temperature and pressure path-length remained constant. This emittance sensibility to total pressure variations implies that the WSGG model is not reliable when dealing with problems of higher pressure than that of when the coefficients were fitted. That would explain why some WSGG applications for higher pressures are resulting in significant deviations as stated by Chu et al., 2016, and Kez et al., 2016. Alternatives for using the WSGG model for high pressure combustion applications would be to either fit new coefficients for the high total pressure values or extend the WSGG for various different total pressure values and correlate these coefficients in order to enable the models application for a wide range of pressures.

5. ACKNOWLEDGEMENTS

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