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**DEVELOPMENT OF A NEW METHODOLOGY TO ESTIMATE THE
EMITTANCE OF COMBUSTION PRODUCTS USING SPECTRAL DATA**

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Abstract. *Combustion gases emit and absorb radiation in a wide range of temperatures; however, they do not do so continuously regarding the wavelength. The main references in literature contain charts for the emittance of carbon dioxide, water vapor and their mixtures that were produced more than fifty years ago. Using new spectral data from HITEMP-2010 and inserting them in a code in Fortran language, this work updates the charts available in literature. The values calculated of emittance differ in up to 10% for carbon dioxide and 25% for water vapor when compared to those presented by Hottel in 1954. It was concluded that the simplification proposed by Hottel of a variable “pressure path length” does not provide a good approximation for values of partial pressure lower than 0.2 atm. Therefore, a new methodology is presented in this work, capable of providing acceptable error levels for a wide range of lengths and partial pressures typically encountered in combustion products.*

Keywords: *Thermal radiation, Combustion gases, emittance, HITEMP-2010*

1. INTRODUCTION

The radiation heat transfer process in participating media (which absorbs, emits and scatters radiant energy) is a subject of great importance within the field of thermal engineering, but it has its share of complexity. For example, in order to calculate radiative exchanges in a furnace filled with flue gas it is essential to know the radiative properties of the species that compose such gas. This, however, can be challenging, since radiation in gases is not regularly distributed regarding the wavelength, but rather in specified intervals, called bands. Moreover, radiation in participating media is not a surface phenomenon, but instead a volumetric phenomenon, so possible changes in the temperature and species concentration of the gases throughout a three-dimensional space must also be accounted for.

A method for simplifying the spectral and directional effects of radiation exchange between a gas and a surface was developed by Hottel *et al.*, 1954. The methodology consists of determining the radiation emanated by a hemispherical gaseous mass by using the correlation of available data for temperature, partial and total pressures and the radius of the hemisphere and, then, extending the results for other geometries through the correlation of a characteristic length. It was also introduced a new variable, the pressure path length, which is the product of the partial pressure and the distance travelled by the radiative intensity. Therefore, the number of acting variables necessary to determine the emittance was reduced. It was then developed charts that presented multiple curves of emittance as a function of temperature, for a total pressure of 1 atm and different values of pressure path length. These results were obtained for water vapor and carbon dioxide, each one in a mixture with other non-participating gases. Furthermore, the results were also extended for mixtures of both species with other non-participating gases, and factors were introduced to correct the pressure for values besides the atmospheric pressure. Up to this day, Hottel’s work is one of the main references for calculation of emittance, and is referenced in many textbooks and thermal engineering manuals. Figure 1 illustrates the results obtained by Hottel for water vapor, while Fig. 2 presents the results for carbon dioxide.

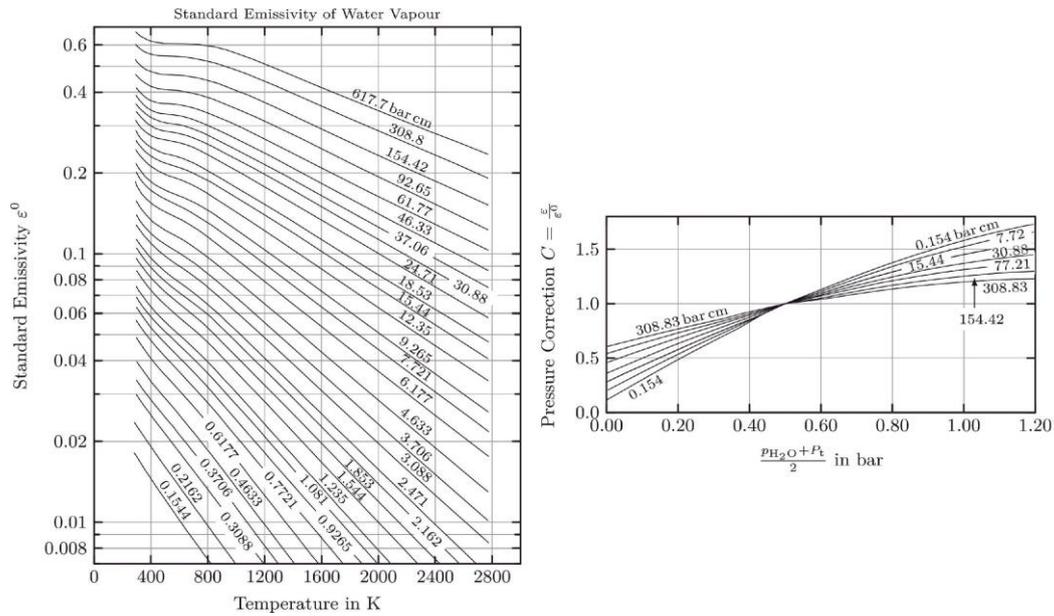


Figure 1. Standard emittance of water vapor as function of temperature and pressure path length and the correction factor for partial pressures different than 0 atm. Adapted from Alberti *et al.* (2016).

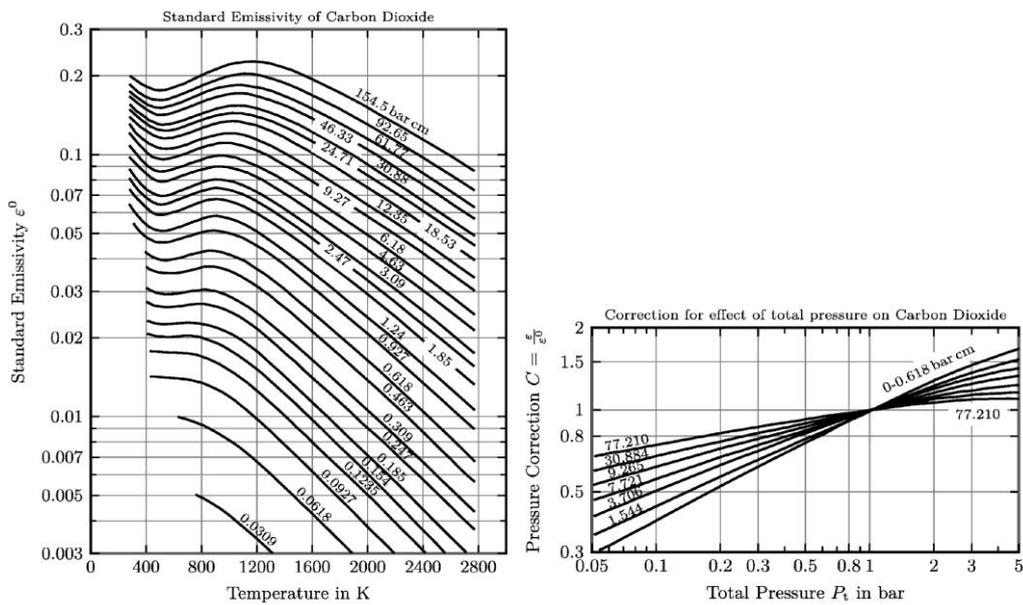


Figure 2. Standard emittance of carbon dioxide as function of temperature and pressure path length and the correction factor for total pressures different than 1 atm. Adapted from Alberti *et al.* (2015).

Although the work performed by Hottel was pioneering, there were important developments regarding detailed spectral data for combustion gases since its publication. One of these updates is the HITEMP, a spectral database for high temperature applications that presents data for combustion gases such as H₂O, CO₂, CO, and OH. The latest iteration, HITEMP-2010 (Rothman *et al.*, 2010), had important updates, expanding the number of transition lines and the covered spectrum, as well as the extension for temperatures up to 4000 K.

Besides Hottel, other researchers have tried to develop similar methodologies for simplifying the solution of the radiative transfer problem in participating media. For instance, Alberti *et al.*, 2016, produced updated charts for carbon dioxide and water vapor using the spectral database from HITEMP-2010, expanding the pressures for up to 40 atm. However, these charts introduced a higher level of complexity for the estimation of the emittance, which results in higher difficulty for fast and practical applications.

The purpose of the present study is to recreate the charts developed initially by Hottel, using the spectral database HITEMP-2010 to achieve better accuracy when using the charts. It is also an objective to verify the proposed approach regarding the variable “pressure path length” when applied to typical values of combustion products. In case of confirming

the limitations of this approach, it will be presented a new methodology for estimating the emittance while maintaining a good compromise between simplicity and accuracy for fast, practical engineering applications

2. CALCULATING THE EMITTANCE OF PARTICIPATING MEDIA

The calculation of the emittance of participating media is made by means of the determination of the spectral absorbance, and as long as Kirchoff's Law is valid, the spectral emittance is equal to the spectral absorbance. Considering a monochromatic beam with intensity $I_{\eta,0}$ propagating in a homogeneous media, its intensity is reduced due to absorption. Within an infinitesimal width dx , such reduction is:

$$dI_{\eta}(x) = -\kappa_{\eta} \cdot I_{\eta,0}(x) dx \quad (1)$$

where κ_{η} stands for the absorption coefficient at a certain wavelength η . Separating and integrating over the whole path S , while considering the absorption coefficient to be independent of x :

$$\int_{I_{\eta,0}}^{I_{\eta,S}} \frac{dI_{\eta}(x)}{I_{\eta}(x)} = -\kappa_{\eta} \int_0^S dx \quad (2)$$

The solution of this integration yields:

$$\frac{I_{\eta,S}}{I_{\eta,0}} = e^{-\kappa_{\eta} S} \quad (3)$$

This exponential decay is known as Beer's Law (Incropera *et al.*, 2007), and represents the spectral transmittance of the media. It is useful to determine the spectral absorbance and, as consequence, the spectral emittance:

$$\varepsilon_{\eta} = \alpha_{\eta} = 1 - \tau_{\eta} = 1 - e^{-\kappa_{\eta} S} \quad (4)$$

This modeling is presented in the literature in full depth (Incropera *et al.*, 2007). However this result is for the media, it stands necessary to expand this result for an absorbing gas "a" that is mixed with other gases "r", non-participating, in an isothermal (with value of T), homogeneous media along the path S . With P_t as total pressure, p_a as the partial pressure of the absorbing gas and p_r as the partial pressure of the remaining "r" gases, the equation is:

$$\varepsilon_{\eta,a}(\eta, T, P_t, p_a, p_r, p_o, S) = 1 - e^{(-\kappa_{p\eta,a} p_a S)} \quad (5)$$

where $\kappa_{p\eta,a}$ is the spectral pressure absorption coefficient of the gas "a" at a certain wavelength η . Through the Eq. (5), one can notice the appearance of the pressure path length variable $p_a S$, which stands as a measure of the number of particles in the trajectory of the irradiating beam. The formulation for the spectral pressure absorption coefficient is:

$$\kappa_{\eta,a} = \kappa_{p\eta,a} p_a \quad (6)$$

Increments in the molar fraction are also increments in the partial pressure of the gas; this implies an increase in the ratio between emitting gases and non-participating ones. It was proposed the concept of a "standard emittance" (Hottel *et al.*, 1954, *apud* Alberti *et al.*, 2016), in which the pressure of the gas is null for simplification in its standalone effect, but not in the pressure path length. This implies disregarding the effect of self-scattering, the collision of the same species. In other words, it only considers the scattering due to collisions of the species "a" with others species "r". However, since the spectral data from HITEMP-2010 can account for self-broadening effects, this simplification is no longer required, and integrating in the whole spectrum becomes:

$$\varepsilon_a(T, p_r, p_a, S) = \frac{\int_{\eta=0}^{\infty} I_{\eta b}(\eta, T) \cdot \varepsilon_{\eta,a}(\eta, T, P_t = 1 \text{ atm}, p_a, p_r, p_o, S) d\eta}{\sigma T^4 / \pi} \quad (7)$$

in which σ is the Stefan-Boltzmann constant. Then, applying the Eq. (5) in the Eq. (7), yields:

$$\varepsilon_a(T, p_a, S) = \frac{\int_{\eta=0}^{\infty} I_{\eta b}(\eta, T) \cdot 1 - e^{(-\kappa_{p\eta,a} p_a S) d\eta}{\sigma T^4 / \pi} \quad (8)$$

where $I_{\eta b}$ is the spectral intensity of radiation of the black body which is given by Planck's distribution:

$$I_{\eta b}(\eta, T) = \frac{2C_1\eta^3}{e^{(C_2\eta/T)} - 1} \quad (9)$$

in which C_1 is the first Planck's constant, equal to $0.59552137 \times 10^{-12}$ Wcm²/sr and C_2 is the second Planck's constant, equal to 0.0143877 mK.

3. APPLICATION WITH THE HITEMP-2010

In order to solve Eq. (7), it is first required to obtain the spectral pressure absorption coefficient, which depends on variables contained within the HITEMP-2010. For this purpose, this study used a code in Fortran language, developed by the LRT-UFRGS, for the calculation of spectral pressure absorption coefficient. The code works by solving the Lorentz profile for the broadening of the spectral lines as described in literature (Dorigon *et al.*, 2013):

$$C_{\eta}(\eta) = \sum_{k=1}^K \frac{S_k(T)}{\pi} \frac{\gamma_k}{\gamma_k^2 + (\eta - \eta_k)^2} \quad (10)$$

in which C_{η} is the absorption cross-section, S_k is the integrated intensity of line k , η_k is the line location, γ_k is the line half-width and K is the total number of lines that form the spectrum. The half-width can be computed (Rothman *et al.*, 2010) as:

$$\gamma_k = \left(\frac{T_{ref}}{T}\right)^{n_c} p_a \gamma_{self,k} + (P_t - p_a) \gamma_{air,k} \quad (11)$$

where $\gamma_{self,k}$ and $\gamma_{air,k}$ are respectively the line self-broadening and the broadening caused by air, T_{ref} is the reference temperature, equal to 296 K, and n_c is the temperature dependence coefficient. The integrated line intensity is calculated at the temperature of 1000 K and then converted to its reference temperature. For a given temperature T , the integrated line intensity is given (Rothman *et al.*, 2010):

$$S_k(T) = S_k(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{e^{(-C_2 E_k/T)}}{e^{(-C_2 E_k/T_{ref})}} \frac{[1 - e^{(-C_2 \nu_k/T)}]}{[1 - e^{(-C_2 \nu_k/T_{ref})}]} \quad (12)$$

in which Q is the total internal partition sums, ν_k is the energy difference between the initial and final state, given as a vacuum wave-number and E_k is the energy of lower state. The parameters: η_k , $\gamma_{self,k}$, $\gamma_{air,k}$, n_c , $S_k(T_{ref})$, Q , ν_k and E_k are all provided by the HITEMP-2010 database.

The absorption cross-section can be related to the spectral pressure absorption coefficient:

$$\kappa_{p\eta} = A \left(\frac{T_{ref}}{T}\right) C_{\eta} \quad (13)$$

where A is equal to 2.479×10^{19} molecules/(cm³atm). Therefore, the code solves the Eq. (9) for a specified partial pressure and for each wave number, across the entire spectrum and for different values of temperatures. A second in-house code was developed in order to calculate the emittance over the whole spectrum, using the line-by-line (LBL) method. It solves the Eq. (8) discret over the spectrum for several values of temperature and path length.

4. COMPARISON WITH LITERATURE

As it is possible to have the same values of pressure path length with different partial pressures (by compensating in the length), it was developed an extensive database of different partial pressures for both water vapor and carbon dioxide to evaluate the simplification proposed by Hottel *et al.* (1954) in various situations. In total, there were produced 22 results for the emittance for each species from a partial pressure of 0.0125 atm to 1 atm. For each partial pressure value, the emittance was calculated for a pressure path length from 0.001 atm·m to 10 atm·m, and, for each pressure path length, for temperatures ranging from 300 K to 2500 K.

The results were then exported to a spreadsheet, organized and compiled in a single file for each species. Then, it was possible to compare the results with those presented by Hottel. Figure 3 presents a comparison for water vapor of the results obtained in this work with those acquired using the methodology proposed in the literature, and also presents the difference in percentage. An arbitrary value of pressure path length of 1.0 atm.m was selected and it was calculated using three different values of partial pressure (compensating with the path length).

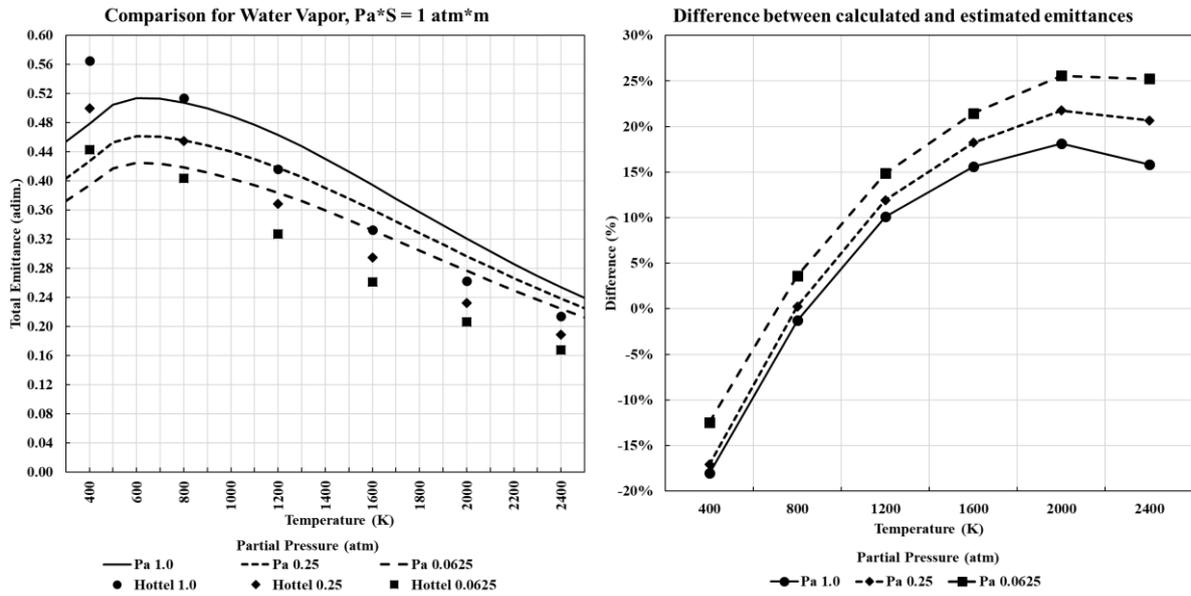


Figure 3. Comparison between the emittance of water vapor calculated with the use of the LBL method and that estimated by Hottel's charts.

The results presented in the figure provide two important conclusions. Firstly, the HITEMP-2010 indeed provides an important update in the values of emittance for water vapor, with a difference of 25% in 2000 K; secondly, the simplification of the pressure path length variable has limitations as the three curves presented have the same value of pressure path length but different partial pressures, and the differences between them can reach 10%.

The same comparison was extended for the carbon dioxide, and the results are presented in Fig. 4. In this case, it can be seen that, although there is a difference between the calculated and the measured values, there is no relevant difference regarding the change in partial pressure. Therefore, for the carbon dioxide, the simplification of the pressure path length provides a good method for calculation. It can also be noted that the HITEMP-2010 provided a relevant update in the values of emittance for carbon dioxides, as the differences with estimated data can reach 10% in higher temperatures.

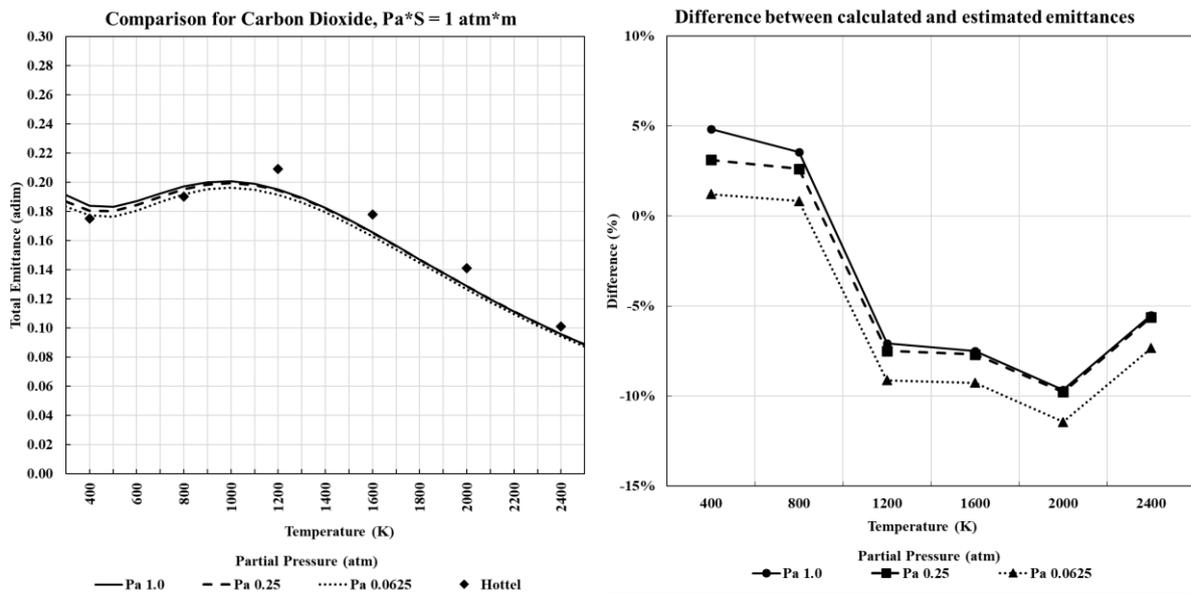


Figure 4. Comparison between the emittance of carbon dioxide calculated with the use of the LBL method and that estimated by Hottel's charts.

5. RESULTS AND PROPOSED METHODOLOGY

As part of the present study, the next step is focused on presenting a new methodology for fast and practical engineering applications. It should be noted that the LBL method provides a benchmark solution for the emittance; in this step, the objective is to create new charts based upon these new results that can fairly well present practical means to calculate values of emittance. This way, it was opted to analyze separately the effects of partial pressure and path length.

Since hydrocarbon fuels still represent the primary source of energy on a world basis, it was decided to focus the proposed methodology for values of partial pressure typical of the combustion of such fuels. In that manner, values of 0.0125 atm to up to 0.25 atm were listed in analysis, and since it was noted that the pressure path length simplification for carbon dioxide provides good results, this methodology was only applied for water vapor. Therefore, Fig. 5 presents the updated results for the carbon dioxide as a function of temperature and for different values of pressure path length.

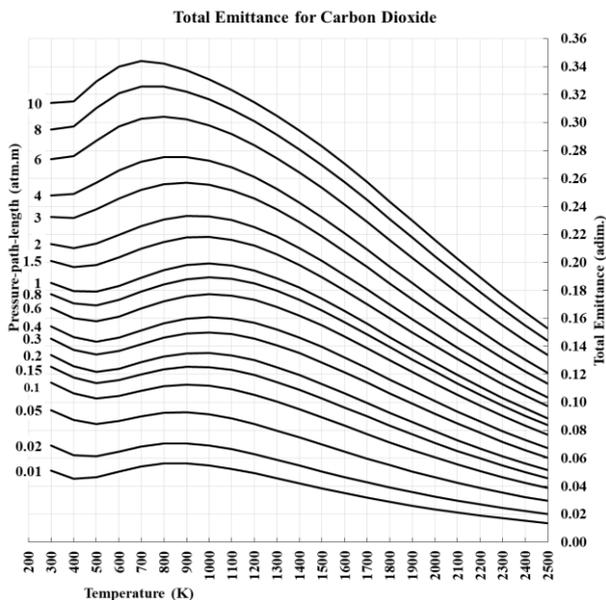


Figure 5. Total emittance for Carbon Dioxide, evaluated at a partial pressure of 0.1 atm.

For water vapor, it was opted for the methodology for fast, practical engineering solutions to be performed by using two coupled charts. One using these charts would first calculate emittance concerning the partial pressure of the gas and then multiply it by a correction factor considering the length of the furnace that is under analysis. However, in order to maintain a good accuracy regarding the values computed with the LBL method while providing a wide range of path length values, it was decided to divide the charts in two reference lengths, the first of 0.5 m, with a correction chart spanning from 0.05 to 2 meters, and the second with the reference of 12 m, with a correction chart spanning from 2 m to 30 m. These charts are depicted in Figs. 6 and 7, respectively.

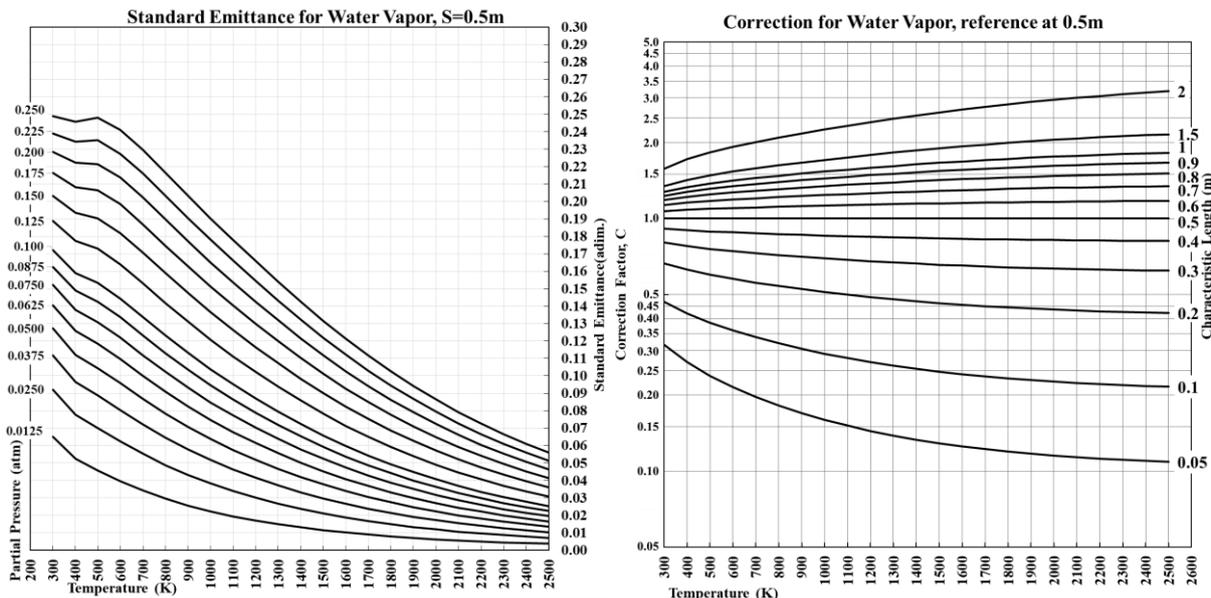


Figure 6. Chart for water vapor at a reference length of 0.5 m with the correction chart for different values of characteristic length.

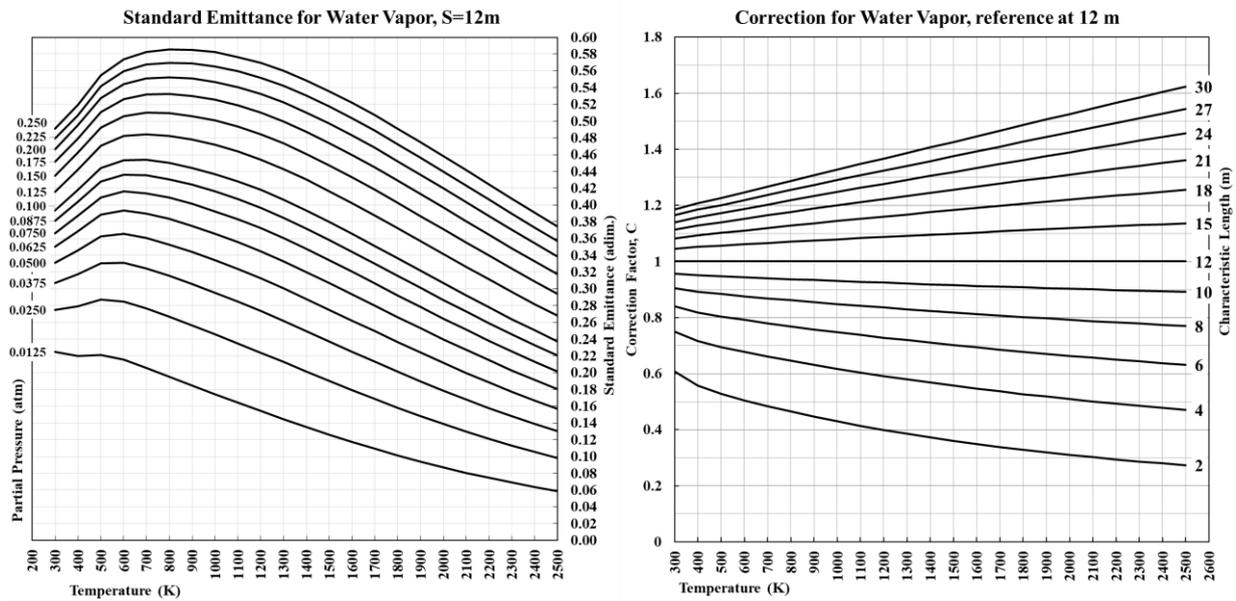


Figure 7. Chart for water vapor at a reference length of 12 m with the correction chart for different values of characteristic length.

The charts developed in this study can maintain a good accuracy the closer the project is to the reference values (0.05 atm and 0.5 m or 12 m). Values going further from this, especially in terms of length, can lead to differences of up to 30% regarding that calculated by the LBL method. Table 1 presents the errors for applying this new methodology regarding the different values of path length S . It can be noted that on average values, the proposed methodology presents a good approximation to the LBL results, maintaining itself on average at less than 7%. The increase in error comes from the extrapolation to lengths close to the limits of the correction charts.

Table 1. Average and maximum errors for the methodology proposed in estimating the emittance for H_2O .

Length (Ref. of 0.5 m)	Average Error	Maximum Error
$0.05 \text{ m} < S < 0.5 \text{ m}$	6.1 %	26.9 %
$0.5 \text{ m} < S < 2 \text{ m}$	3.5 %	18.6 %
$0.1 \text{ m} < S < 1.0 \text{ m}$	3.2 %	20.1 %
Length (Ref. of 12 m)	Average Error	Maximum Error
$2 \text{ m} < S < 12 \text{ m}$	6.8 %	28.3 %
$12 \text{ m} < S < 30 \text{ m}$	4.2 %	15.4 %
$6 \text{ m} < S < 24 \text{ m}$	3.0%	18.9 %

As a last comparison with the literature, it was calculated the values of emittance for a same pressure path length but with the upper and lower limits of emittance presented in Fig. 6 and Fig. 7. The results obtained with LBL were compared with the values calculated with the proposed methodology and with the estimated charts provided in Fig. 1. The comparison is presented in Fig. 8. It can be noted that the proposed methodology maintains the error more stable through changes in temperature.

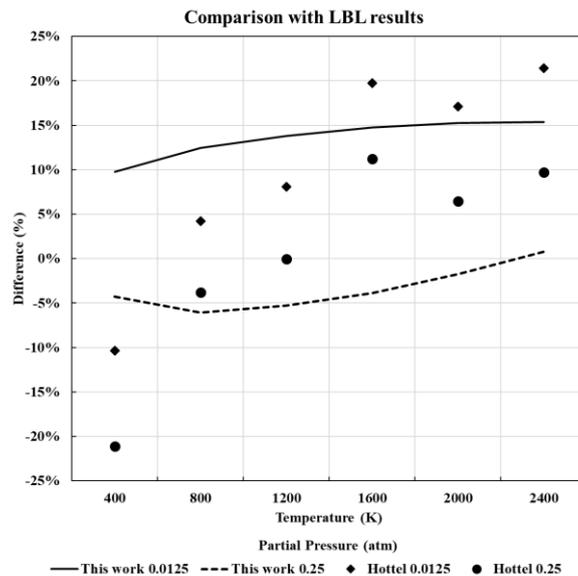


Figure 8. Comparison between proposed methodology and calculated values of emittance.

6. CONCLUSIONS

The emittance for carbon dioxide and water vapor were calculated using the spectral database HITEMP-2010. The updated values were compared with those available in literature and a difference of up to 25% was perceived. A new methodology for fast, practical engineering solutions was proposed using updated charts at reference of 0.5 m and 12 m together with correction charts for different characteristic lengths. This new methodology maintains average error under 7% and more stable results compared with the literature.

7. ACKNOWLEDGEMENTS

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