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A STUDY OF THE EMITTANCE BEHAVIOUR OF A CO₂-H₂O MIXTURE FOR
DIFFERENT SPECTRAL BANDS, PRESSURES, TEMPERATURES AND MOLAR
FRACTIONS

by

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EPIGRAPH

*Finally,
from so little sleeping
and so much reading,
his brain dried up
and he went completely
out of his mind.*

Miguel de Cervantes

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A STUDY OF THE EMITTANCE BEHAVIOUR OF A CO₂-H₂O MIXTURE
FOR DIFFERENT SPECTRAL BANDS, PRESSURES, TEMPERATURES
AND MOLAR FRACTIONS

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Resumo. Visando ampliar o conhecimento sobre o comportamento dos gases participantes na radiação térmica, este estudo tem como objetivo gerar e analisar a emitância de uma mistura de CO₂ e H₂O para cinco diferentes bandas do espectro eletromagnético (variando de 0 a 1.000 cm⁻¹, 1.000 a 2.600 cm⁻¹, 2.600 a 4.400 cm⁻¹, 4.400 a 6.000 cm⁻¹, 6.000 a 25.000 cm⁻¹), comprimentos de caminho (0,001 a 30 m), pressões (1, 2, 5, 10, 20 e 40 atm), temperaturas (300 K a 2500 K, em incrementos de 100 K) e diferentes frações molares (0,1 e 0,2 para CO₂ e 0,0125; 0,05; 0,1; 0,15; 0,2; 0,3 e 0,5 para H₂O). Para gerar essas emitâncias, o perfil de Lorentz é utilizado para calcular o coeficiente de absorção transversal de cada um dos gases participantes para os estudos de caso dados, utilizando o HITEMP-2010 como base de dados para os cálculos. Então, a partir desses coeficientes gerados, é possível calcular as emitâncias para estes casos. Os resultados mostram que aumentar o comprimento do caminho, a pressão e a fração molar também aumenta a emitância. Além disso, as bandas espectrais mais significativas analisadas são a banda 1 (ligeiramente superior) e depois a banda 2 e, à medida que avançamos no espectro eletromagnético, os valores de emitância diminuem. Finalmente, o comportamento da emitância varia de caso para caso quando se estuda o impacto da temperatura.

Palavras-chave: radiação, emitância, gases participantes

Abstract. Aiming to expand knowledge about the behavior of gases participating in thermal radiation, this study has the goal of generate and analyze the emittance of a mixture of CO₂ and H₂O for five different bands of the electromagnetic spectrum (ranging from 0 to 1,000 cm⁻¹, 1,000 to 2,600 cm⁻¹, 2,600 to 4,400 cm⁻¹, 4,400 to 6,000 cm⁻¹, 6,000 to 25,000 cm⁻¹), path lengths (0.001 to 30 m), pressures (1, 2, 5, 10, 20 and 40 atm), temperatures (300 K to 2500 K, in increments of 100 K), and different molar fractions (0.1 and 0.2 for CO₂ and 0.0125; 0.05; 0.1; 0.15; 0.2; 0.3 and 0.5 for H₂O). To generate these emittances, the Lorentz profile is used to calculate the transverse absorption coefficient of each of the participating gases for the given case studies, using HITEMP-2010 as the database for the calculations. Then, using these generated coefficients, it is possible to calculate the emittances for these cases. The results show that increasing the path length, pressure and molar fraction increases the emittance as well. Furthermore, the most significant spectral bands analyzed are bands 1 (slightly superior) and then band 2, and as we advance into the electromagnetic spectrum, the emittance values decrease. Finally, the emittance behavior varies from case to case when studying the impact of the temperature.

Keywords: radiation, emittance, participating gases

NOMENCLATURE

Symbols

C_1	First Planck's constants	$[W \mu m^4 / m^2 \text{ sr}]$
C_2	Second Planck's constants	$[\mu m K]$
C_η	Absorption cross-section	$[cm^2 / molecule]$
E_k	Energy of the lower state	$[J]$
$I_{\eta b}$	Blackbody radiation intensity	$[W / m^2 \mu m]$
I_η	Spectral intensity	$[W / m^2 \mu m]$
N	Molar density	$[molecule / cm^2 m]$
N_A	Avogadro's number	$[mol^{-1}]$
p	Pressure	$[atm]$
p_c	Partial pressure	$[atm]$
p_a	Partial pressure of the absorbing species	$[atm]$
Q	Total internal partition sums	$[J]$
R_u	Universal gas constant	$[J / mol^{-1} K^{-1}]$
S_k	Integrated line intensity	$[cm^{-1} / molecule \text{ cm}^{-2}]$
S	Path	$[m]$
T	Temperature	$[K]$
T_{ref}	Reference temperature	$[K]$
Y	Mole fraction	

Greek symbols

η	Wavenumber	$[cm^{-1}]$
η_k	Wavenumber	$[cm^{-1}]$
η_c	Temperature dependence coefficient	$[K]$
$\kappa_{p\eta,a}$	Pressure absorption coefficient	$[atm^{-1} m^{-1}]$
κ_η	Absorption coefficient	$[atm^{-1} m^{-1}]$
σ	Stefan-Boltzmann constant	$[W / m^2 K^4]$
$\gamma_{self,k}$	Line self-broadening	$[m]$
$\gamma_{air,k}$	Broadening caused by air	$[m]$
γ_k	Line half width	$[m]$

ν_k	Energy difference between the initial and the final state	[J]
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Abbreviations and acronyms

HITEMP2010	High-Temperature Molecular Spectroscopic Database
LRT	Laboratory of Thermal Radiation
RTE	Radiative Transfer Equation
UFRGS	Federal University of Rio Grande do Sul
WSGG	Weighted-Sum-of-Gray-Gases

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1. INTRODUCTION

The event of radiation in a participating medium is a phenomenon that occurs in multiple scenarios, both in natural occurrences and also in industrial processes. This form of radiation has been extensively studied in theory. However, in numerical studies, if it is considered all the possible effects, it becomes a computational challenge followed by a substantial high resource demand due to all the calculations needed. So, in order to reduce computational cost and consequently the time required, it becomes necessary to introduce simplifications to the models. One of the main difficulties encountered is caused by the phenomenon of line broadening in participating gases. This happens when the gases along the photon path interact with it, inducing perturbations in the energy status of the molecules, resulting in the photon being absorbed in different wavenumbers.

In previous studies of Etges et al (2022) and Etges et al (2022), the behavior of the emittance of a CO₂-H₂O mixture was examined for different pressures (1, 2, 5, 10, 20, 40 atm), temperatures (from 300 to 2,500 K) and molar fractions (a combination of 0.1 and 0.2 for CO₂ and 0.2 for H₂O) across the electromagnetic spectrum (0 to 25,000 cm⁻¹). It was found that the increase of pressure also increased the emittance. In contrast, for an increase of temperature, the emittance started to decrease.

Selhorst (2020) studied and generated new WSGG coefficients through the emittance generation. In his work, he considered the molar fractions of 0.0125, 0.025, 0.05, 0.1, 0.125, 0.15, 0.2, 0.25, 0.3, 0.4, 0.5 for H₂O.

Fonseca et al (2021) studied and generated new WSGG coefficients for five different spectral bands, ranging from 0 to 1,000 cm⁻¹, 1,000 to 2,600 cm⁻¹, 2,600 to 4,400 cm⁻¹, 4,400 to 6,000 cm⁻¹, 6,000 to 25,000 cm⁻¹.

The goal of this research is to expand the previous study (Etges et al, 2022) of generating the emittance data of a combination of CO₂ and H₂O to a broader range of molar fractions, using as reference some values used in Selhorst (2020), and for different spectral bands, using as reference the bands used in Fonseca et al (2021), in order to better understand it and also to seek optimizations where it is possible. The emittances that are derived in the present study can be later explored in future studies as, for example, to develop new global gas models correlations, in particular for the WSGG (Weighted-Sum-of-Gray-Gases model) coefficients (Dorigon et al, 2013).

2. THEORETICAL FOUNDATION

In this section, the theoretical foundation is presented. It is categorized according to the specific variable under discussion.

2.1. Radiative transfer equation

The main equation that describes the variation of the radiative intensity in a participating medium is the radiative transfer equation (RTE). For a non-scattering medium, such as one that does not have ash or other particles to disperse the radiation rays, the RTE is given by Equation 1, where the first term on the right side of the equation represents the portion of radiation that is absorbed by the medium and the second term represents the portion that is emitted by the medium.

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

where I_η and $I_{\eta b}$ are the spectral intensity and the blackbody radiation intensity at the local position, respectively, and κ_η is the local absorption coefficient for a participating gas.

2.2. Blackbody radiation intensity

The blackbody radiation intensity can be found by the Planck's distribution, given in Eq. 2. It represents the rate of which radiation is emitted by an area for a given wavenumber for a blackbody.

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

where C_1 and C_2 are, respectively, the first and the second Planck's constants, and η is the wavenumber.

2.3. Absorption coefficient

The equation to calculate the absorption coefficient is given by Eq. 3.

$$\kappa_\eta = NYC_\eta \quad (3)$$

where N is the gas molar density, Y is the mole fraction of the gas and the C_η is the absorption cross-section.

2.4. Gas molar density

The gas molar density can be determined as shown in Eq. 4.

$$N = \frac{p N_A}{R_u T} \quad (4)$$

where p is the pressure, N_A is the avogadro number, R_u is the universal gas constant and T is the temperature.

2.5. Absorption cross-section

The equation to find the absorption cross-section, using the Lorentz spectral line model profile (Modest, 2003), is shown in Eq. 5.

$$C_\eta = \sum_{k=1}^k \frac{S_k}{\pi} \frac{\gamma_k}{\gamma_k^2 + (\eta - \eta_k)^2} \quad (5)$$

where S_k is the integrated line intensity, γ_k is the line half width and η_k is the wavenumber.

It is interesting to notice that changing the temperature or the pressure cause distinct reactions in the absorption cross-section of the CO₂ and H₂O. For example, increasing the pressure generally causes the erratic oscillations to be smoothen, as can be seen in Figure 1. Furthermore, increasing the temperature generally elevates the value of the absorption cross-section for the H₂O, as shown in the first image of Fig. 2.

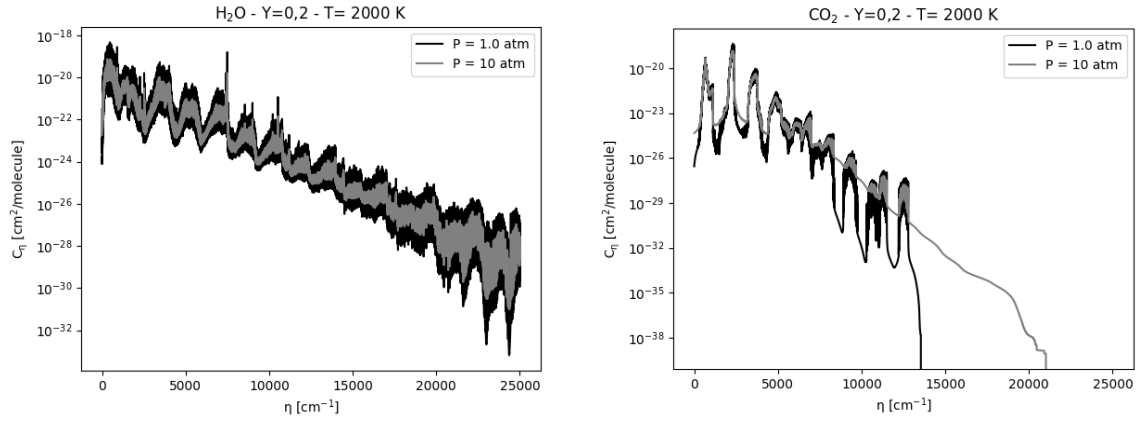


Figure 1 – The impact of increasing the pressure for H₂O on the left and for CO₂ on the right.

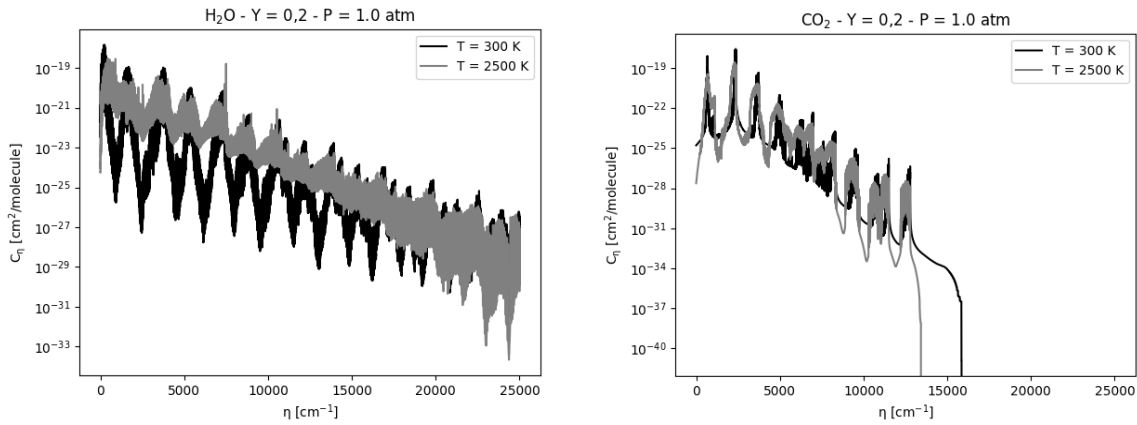


Figure 2 – The impact of increasing the temperature for H₂O on the left and for CO₂ on the right.

2.6. Integrated line intensity

The integrated line intensity is given by the following Eq. 6.

$$S_k = S_k(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\exp(-C_2 E_k/T)}{\exp(-C_2 E_k/T_{ref})} \frac{[1 - \exp(-C_2 \nu_k/T)]}{[1 - \exp(-C_2 \nu_k/T_{ref})]} \quad (6)$$

where Q is the total internal partition sums, E_k is the energy of the lower state and ν_k is the energy difference between the initial and the final state.

2.7. Line half width

The line half width can be described as Eq. 7.

$$\gamma_k = \left(\frac{T_{ref}}{T}\right)^{\eta_c} p_c \gamma_{self,k} + (p - p_c) \gamma_{air,k} \quad (7)$$

where T_{ref} is the reference temperature (296 K), η_c is the temperature dependence coefficient, p_c is the partial pressure of the species c , $\gamma_{self,k}$ is the line self-broadening and $\gamma_{air,k}$ is the broadening caused by air.

2.8. Emittance

The objective of this paper is to analyze the emittance of different scenarios. The emittance is the ratio of the total emitted radiation in a chosen path that is not absorbed by a participating medium, over the radiation emitted by a black body at the same temperature. The equation of the emittance is shown on Eq. 8.

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

where $\kappa_{p\eta,a}$ is the pressure absorption coefficient, p_a is the partial pressure of the absorbing species, S is the path and σ is the Stefan-Boltzmann constant.

2.9. Line broadening

The phenomenon of line broadening in participating gases is when the molecules of the gases that are in the way of the photons interact with them. The line broadening happens when the energy status of the molecules is perturbed due to some factors and it can absorb photons in different wavenumbers. The types of broadening are: natural broadening, where it is intrinsic to the uncertainty motion and energy of the molecules and it is usually small comparing to the others and can often be neglected; Doppler broadening, where it is related to the motion of the atoms and it is important only for high temperatures such as higher than 2,500 K; Stark broadening, which can be important when there are electric fields; and collision broadening, due to the collisions between the molecules.

In the context of the present study, the main factor is the collision because of the chosen range of pressures and temperatures (Howell et al, 2016).

3. METHODOLOGY

The objective of this study is to generate and analyze the behavior of the emittance of a CO₂ and H₂O mixture for different scenarios, varying the spectral band studied (ranging from 0 to 1,000 cm⁻¹, 1,000 to 2,600 cm⁻¹, 2,600 to 4,400 cm⁻¹, 4,400 to 6,000 cm⁻¹, 6,000 to 25,000 cm⁻¹), path lengths (0.001 to 30 m), total pressures (1, 2, 5, 10, 20 and 40 atm), temperatures (300 K to 2500 K, in increments of 100 K), and different molar fractions (0.1 and 0.2 for CO₂ and 0.0125; 0.05; 0.1; 0.15; 0.2; 0.3 and 0.5 for H₂O), as shown on Table 1.

Table 1 – Parameters used

Parameter	Range
Spectral bands [cm ⁻¹]	0 to 1,000, 1,000 to 2,600, 2,600 to 4,400, 4,400 to 6,000, 6,000 to 25,000
Path lengths [m]	0.001 to 30
Total pressures [atm]	1, 2, 5, 10, 20 and 40
Temperatures [K]	300 to 2,500
Molar fractions (CO ₂)	0.1 and 0.2
Molar fractions (H ₂ O)	0.0125; 0.05; 0.1; 0.15; 0.2; 0.3 and 0.5

To calculate the emittance, it is necessary to have the absorption cross-section of the data required. Consequently, the preliminary step to obtain the emittances is to calculate these coefficients under their defined conditions, once they depended on temperature, total pressure and molar fraction of the species. In order to do so, it was used a Fortran code developed by the study group of the Laboratory of Thermal Radiation (LRT) at UFRGS. This code uses the data from high-temperature molecular spectroscopic database HITEMP2010 (Rothman et al., 2010) to obtain the following parameters: the total internal partition sums (Q), the energy difference between the initial and the final state (ν_k), the energy of the lower state (E_k), the integrated line intensity (S_k), the temperature dependence coefficient (η_c), the line self-broadening ($\gamma_{self,k}$), the broadening caused by air ($\gamma_{air,k}$) and the wavenumber (η_k). With these parameters it is possible to calculate the absorption cross-sections. To calculate the absorption cross-sections over the above specified characteristics, it was used the Lorentz profile. It is important to notice that the use of this profile is not recommended for applications under sub-atmospheric pressures or for temperatures over 2500 K. If the conditions surpass these limitations, it is recommended the use of Voigt's profile to correct the deviations from the other modes of broadening (Modest, 2003).

The spectral range chosen to evaluate the absorption cross-section spans from 0 to 25,000 cm^{-1} . In this study, it was used a variable discretization. For a pressure of 1 atm a total of 375,000 points were used to discretize the spectrum. Then, as pressure increases, the discretization was reduced accordingly to the inverse proportionality of the pressure, with 187,500 points for 2 atm, 75,000 points for 5 atm, and so forth. The cutoffs used in the calculations using the Lorentz profile were based on the line half-width, with 30,000 γ_k for CO_2 and 3,000 γ_k for H_2O (Coelho et al, 2021). Once the absorption cross-sections results were ready, the next step was to calculate the emittances through another Fortran code also developed by the LRT.

4. RESULTS

In this section, the results are presented. They are categorized according to the investigated attributes under consideration.

4.1. Path

Evaluating solely the influence of the path length on the emittance calculated, it is possible to observe, from Fig 3, that with the increase of the path, the emittance also increases, as expected, since the Eq. 8 shows us that the emittance is proportional to the path length. This behavior happens for all the cases studied, independently from the temperature, pressure, spectral band or molar fraction used.

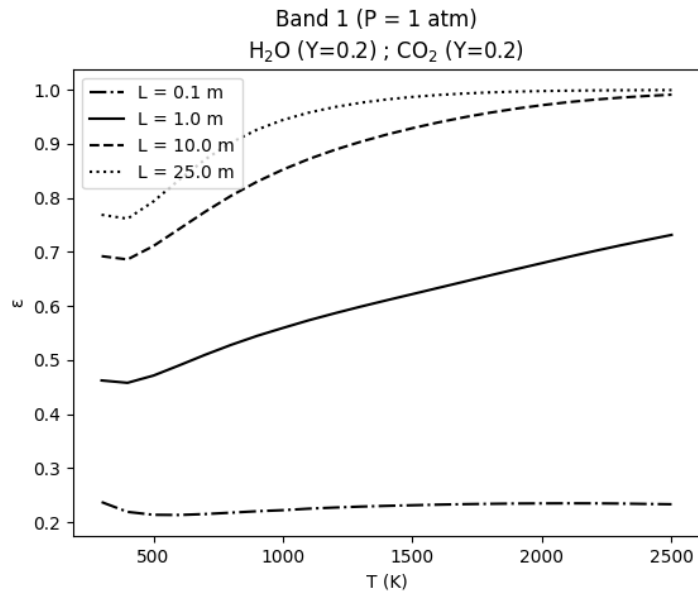


Figure 3 – The impact on the emittance changing the path length for a H₂O (0.2) - CO₂ (0.2) mixture, 1 atm, band 1.

It is interesting to notice, however, that the emittance varies differently across the variation of temperature when increasing or decreasing the path length, and it is not a simple displacement equally distributed. Furthermore, this behavior also varies depending on the spectral band analyzed, as shown on Fig 4. For longer paths, the emittance seems to be more sensible to the variation of the temperature, as for shorter paths, less sensible.

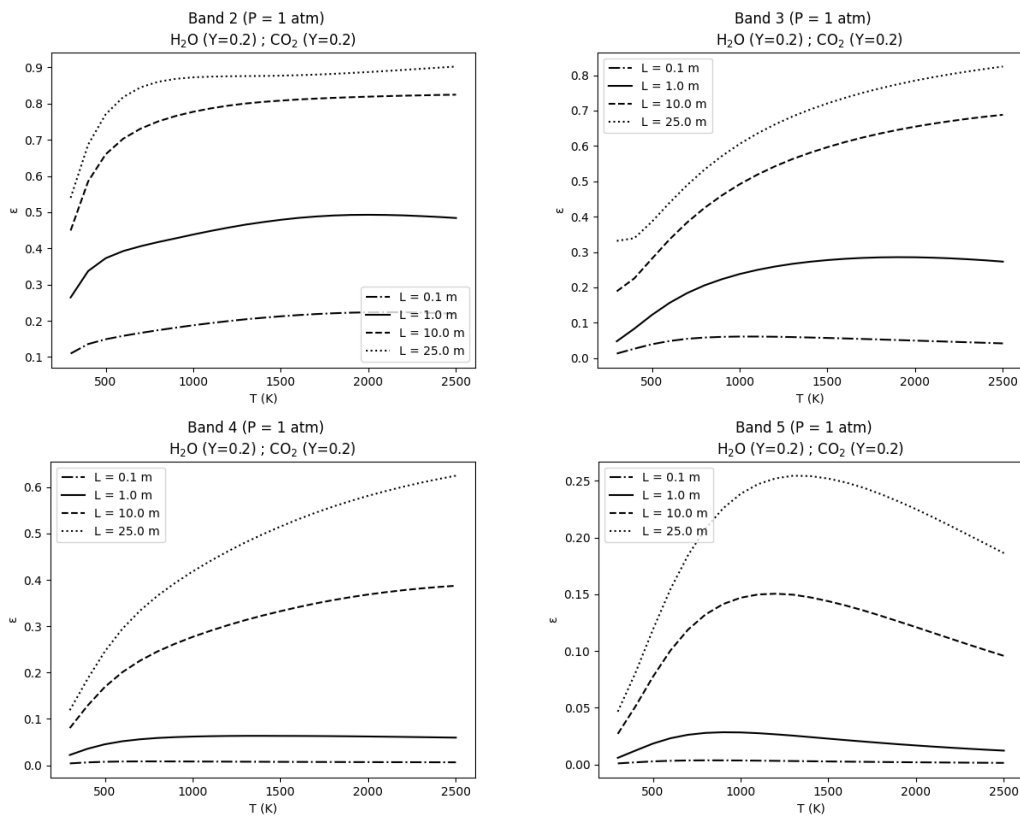


Figure 4 – The impact on the emittance changing the path length for a H₂O (0.2) - CO₂ (0.2) mixture, 1 atm, bands 2, 3, 4 and 5.

4.2. Spectral band

Evaluating solely the influence of the spectral band on the emittance calculated, it is possible to observe, from Fig 5, that each spectral band has its own behavior of the emittance. Also, the emittance values are the greatest at the first band analyzed, and its value decreases as the spectral bands advances further on the electromagnetic spectrum. This behavior happens for all the cases studied.

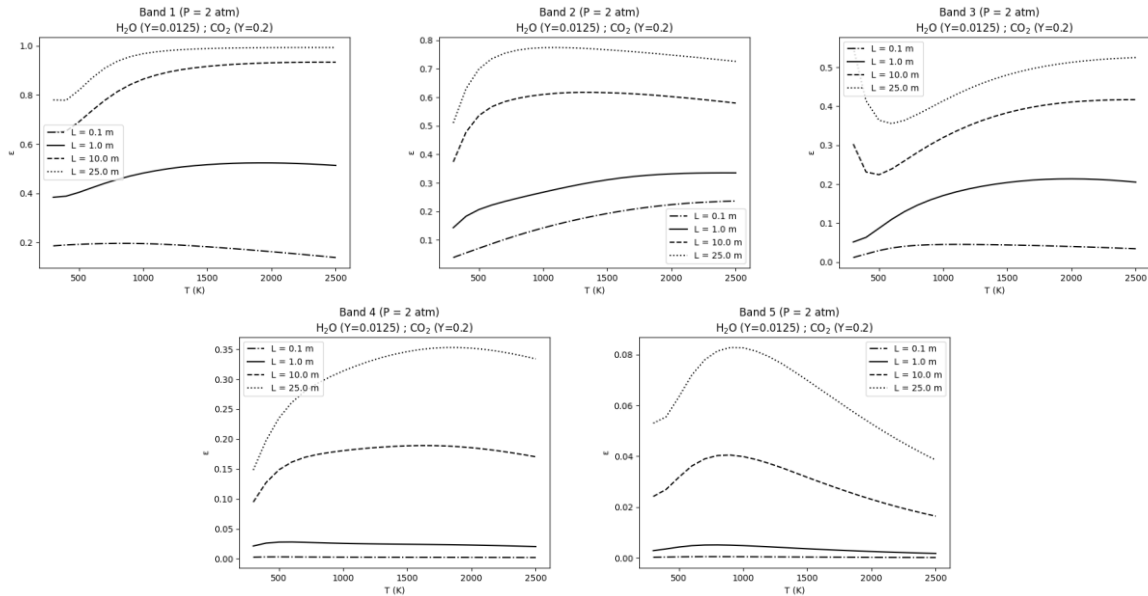


Figure 5 – The impact on the emittance changing the spectral band for a H₂O (0.0125) - CO₂ (0.2) mixture, 2 atm, bands 1, 2, 3, 4 and 5.

For pressures near the atmospheric value, the spectral band 5 is almost zero. However, if one looks at the results for a different case with a higher pressure, for example in Fig 6, this spectral band also becomes significant.

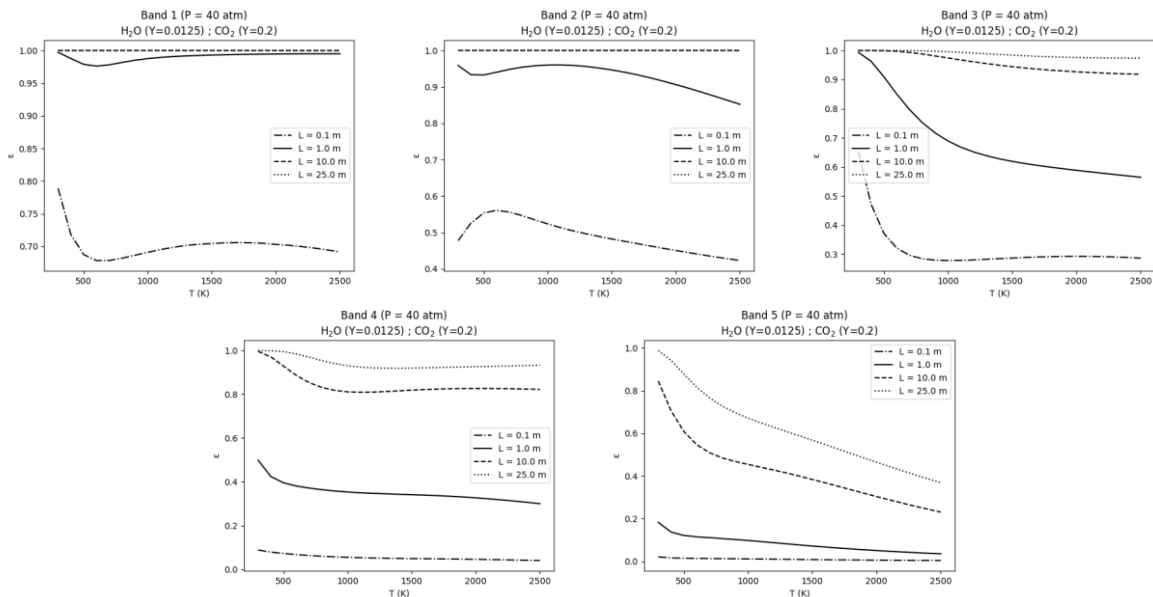


Figure 6 – The impact on the emittance changing the spectral band for a H₂O (0.0125) - CO₂ (0.2) mixture, 40 atm, bands 1, 2, 3, 4 and 5.

4.3. Pressure

Evaluating solely the influence of the pressure on the emittance calculated, it is possible to observe, from Fig 7, that with the increase of the pressure, the emittance also increases. This behavior happens for all the cases studied.

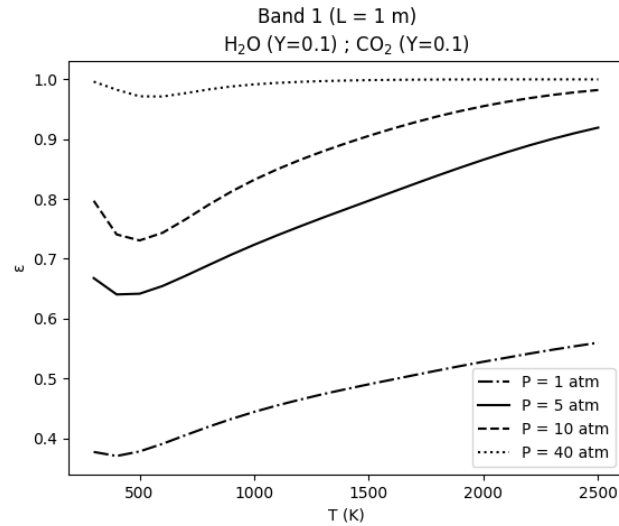


Figure 7 – The impact on the emittance changing the pressure for a H₂O (0.1) - CO₂ (0.1) mixture, 1 m, band 1.

Increasing the pressure has an analog effect on emittance as increasing the path length. It increases the emittance but not in an evenly distributed way, as shown on Fig 8.

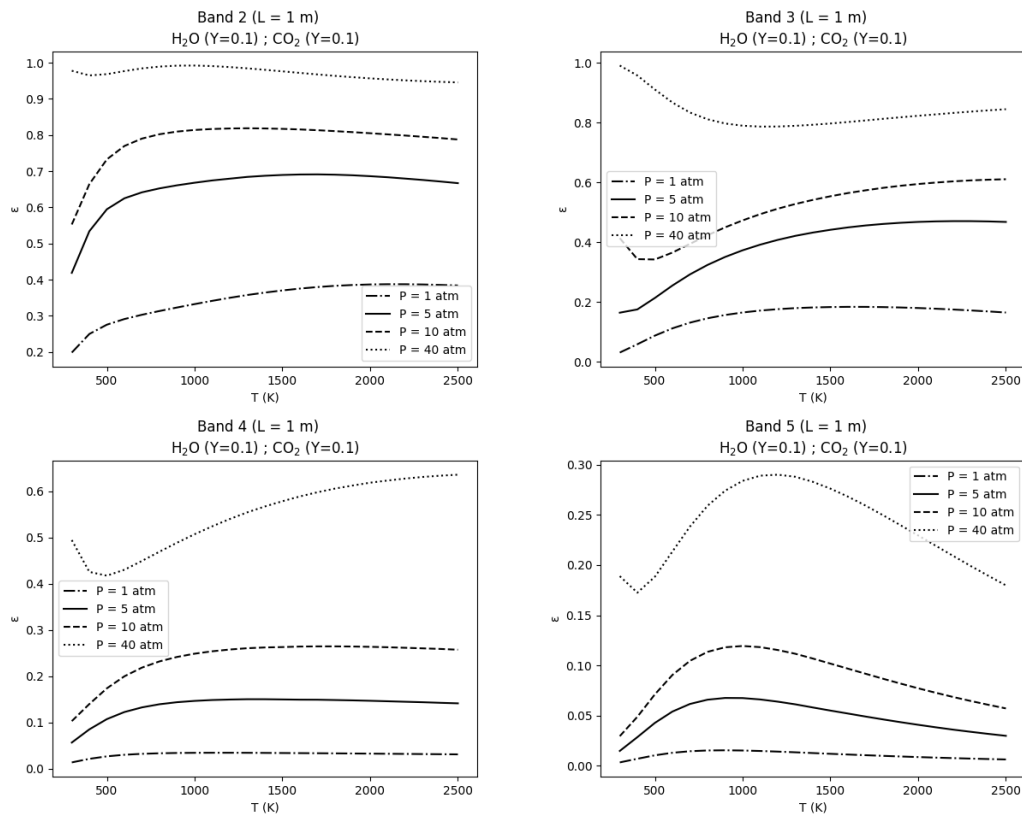


Figure 8 – The impact on the emittance changing the pressure for a H₂O (0.1) - CO₂ (0.1) mixture, 1 m, bands 2, 3, 4 and 5.

4.4. Temperature

Evaluating solely the influence of the temperature on the emittance calculated, it is possible to observe, from Fig 9, that with the increase of the temperature, depending on which spectral band is under investigation and also on which path length is used, the emittance has different behaviors.

For the first band, for longer paths, when increasing the temperature, the emittance initially decreases until, approximately, 500 K. From this temperature further, the emittance starts to slowly increase until it becomes almost constant.

For the second band, for longer paths, when increasing the temperature, the emittance initially increases until, approximately, 800 K. From this temperature further, the emittance starts to slowly decrease until it becomes almost constant.

For the third band, for longer paths, when increasing the temperature, the emittance initially decreases until, approximately, 600 K. From this temperature further, the emittance starts to slowly increase until it becomes almost constant. The behavior of this band is analog of the behavior observed on the first band, except it is more accentuated and the overall value of the emittance is lower.

For the fourth band, for longer paths, when increasing the temperature, the emittance initially increases until, depending on the path length chosen, reaches a temperature on which the emittance starts to slowly decrease until it becomes almost constant. Again, the behavior of this band is also analog of the behavior observed on the other band, this time the first band, except it is more accentuated and the overall value of the emittance is lower.

Finally, for the fifth band, for longer paths, when increasing the temperature, the emittance initially increases until, approximately, 900 K. From this temperature further, the emittance starts to decrease.

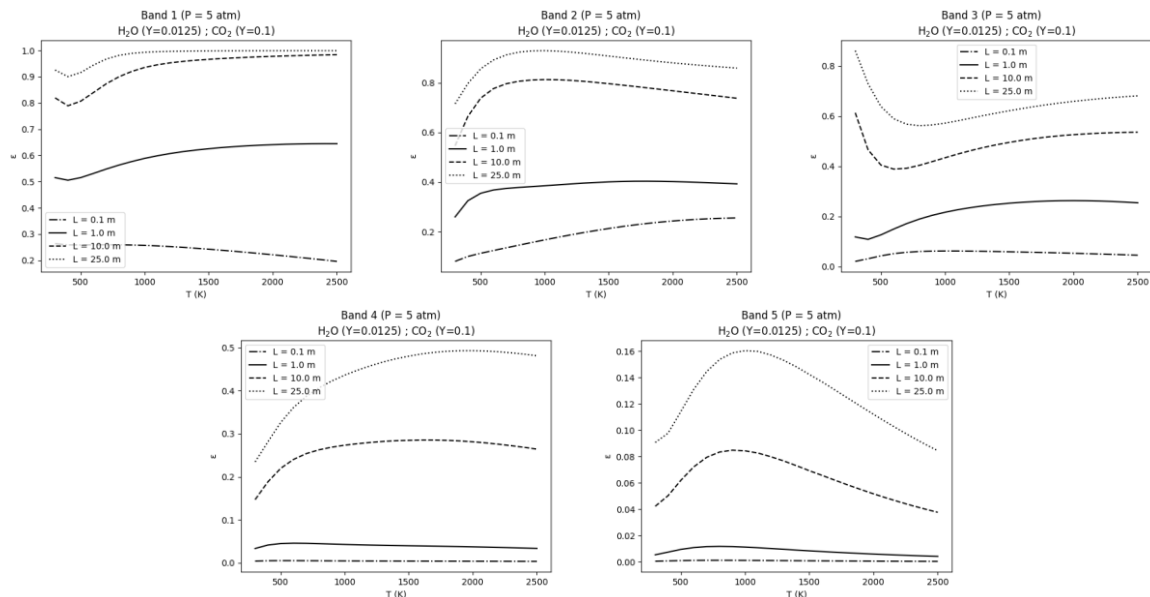


Figure 9 – The impact on the emittance changing the temperature for a H_2O (0.0125) - CO_2 (0.1) mixture, 5 atm, bands 1, 2, 3, 4 and 5.

4.5. Molar fraction

Evaluating solely the influence of the molar fraction on the emittance calculated, it is possible to observe, from Fig 10, that with the increase of the molar fraction, the emittance also increases. This behavior happens for all the cases studied.

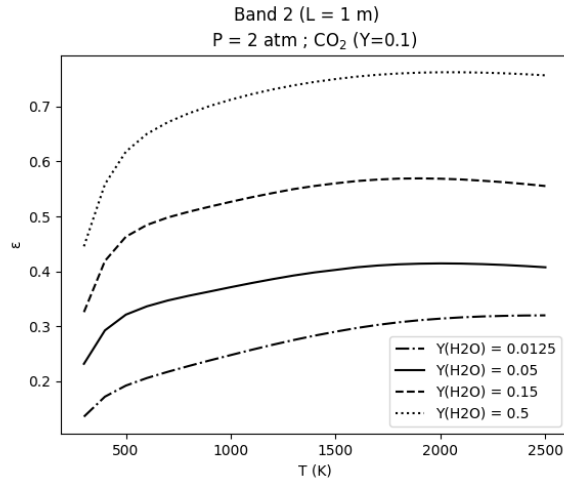


Figure 10 – The impact on the emittance changing the molar fraction for a H₂O - CO₂ mixture, 2 atm, 1 m, band 2.

5. CONCLUSIONS

Analyzing the results, one can denote some behaviors of the emittance for a H₂O-CO₂ mixture. First, it is possible to deduce an increase of the emittance when using longer paths than shorter. Likewise, increasing the total pressure has the same response, as well as the increase of the molar fraction of the chemical species.

Also, separating the electromagnetic spectrum in different bands makes the emittance to have different distribution according to the band chosen. For pressures near the atmospheric, the further bands in the electromagnetic spectrum have an emittance near zero. When increasing the pressure, though, these bands become important to notice.

Furthermore, the emittance behavior regarding the variation of the temperature varies according to the spectral band used. For the bands 1 and 3, the behavior is analog, the emittance initially decreases and then starts to slowly increase until it becomes almost constant. Likewise, for the bands 2 and 4, the emittance initially increases until, depending on the path length chosen, reaches a temperature on which the emittance starts to slowly decrease until it becomes almost constant. For the band 5, when increasing the temperature, the emittance initially increases until reaching a temperature on which it starts to decrease.

It is interesting to notice that, for higher pressures, the computational time necessary to generate the spectral lines for the absorption cross-section was lower than for lower pressures, as expected. This happens due to the different discretization used for different pressures. Also, the band emittance more time consuming to calculate was band 5, as expected as well, due to the larger range used in this band.

For further studies, it is possible to implement the Voigt's profile to explore more scenarios on which the Lorentz profile is not recommended. Also, it is possible to introduce new chemical species in the analysis, and compare its behavior with the mixture used in the present study. Moreover, it is possible to utilize the results here obtained and generate new WSGG coefficients.

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