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# A STUDY OF THE ABSORPTION CROSS-SECTION WITH THE H<sub>2</sub>O GASES CONCENTRATION IN RADIATIVE TRANSFER CALCULATIONS.

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**Abstract.** Problems of radiative heat transfer involving gases at high temperatures, such as combustion, emit and absorb large amounts of radiation. Absorption cross-section is a property that is involved with the emission and absorption of energy by these molecular gases. The study to be presented has a medium composed H<sub>2</sub>O. This study consists of verifying how the absorption cross-section varies with H<sub>2</sub>O concentration. The analysis is performed through radiative heat transfer and divergence of the radiative heat transfer calculations for isothermal and non-isothermal media. Test cases are for homogeneous media with 5 %, 50 %, 75 % and 100 % H<sub>2</sub>O concentration. The results present that the absorption cross-section is not very sensitive to the concentration, so that a fixed molar fraction can be used to obtain it in line-by-line radiative heat transfer calculations for H<sub>2</sub>O gases.

**Keywords:** Absorption cross-section, spectral radiative properties, concentration, radiative heat transfer, H<sub>2</sub>O

## 1. INTRODUCTION

The last few decades have seen much progress in the understanding of molecular gas radiation, in particular the radiation from water vapor and carbon dioxide, which is of great importance in the combustion of hydrocarbon fuels, and which also dominates atmospheric radiation its thermodynamic implications on Earth's atmosphere (Modest, 2013).

In many engineering applications the interaction of thermal radiation with an absorbing, emitting and/or medium must be accounted, that is, the medium is radiatively participating. In combustion problems, for example, the gases generated at high temperatures emit large amounts of thermal radiation.

The study performed involves medium composed of H<sub>2</sub>O. Some media composed of CO<sub>2</sub>, H<sub>2</sub>O and air does not scatter radiation significantly. Therefore, scattering effect is not considered. Since every molecule is, of course, a very small particle, the scattering of photons by molecules is always negligible for heat transfer applications (Modest, 2013).

This analysis must be carried out in such a way that spectral variation of radiative properties (variation in relation to wavenumber, frequency or wavelength) must be accounted. All the properties may vary strongly with wavelength, adding another dimension to the governing equation (Modest, 2013). The strong spectral variation of the radiative absorption coefficient (spectral properties that is related to emission and absorption of radiation) leads to great mathematical complexity in radiative transfer calculations in absorbing/emitting molecular gases (Modest and Zhang, 2002a). Line parameters available by database such as HITEMP (Rothman et al., 2010) and HITRAN (Gordon et al., 2017) are used to calculate the absorption coefficient.

Line-by-line method is utilized for the spectral integration. Because of strongly varying values of the absorption coefficient, the spectral radiative transfer problem must be solved for several hundred thousand wavenumbers, followed by integration over the spectrum. While such calculations may be the most accurate to date, they require vast amounts of computer resources (Modest, 2013).

Some methods were implemented alternately to line-by-line method aiming at a faster calculation with good accuracy. The Weighted-Sum-of-Gray Gases (WSGG) (Hottel and Sarofim, 1967), spectral-line-based-weighted-sum-of-gray gases (SLW) (Denison and Webb, 1993a; Denison and Webb, 1995), cumulative wavenumber (Solovjov and Webb, 2002; Galarça et al., 2011), full-spectrum k-distribution (FSK) (Modest and Zhang, 2002b; Zhang and Modest, 2003) and absorption distribution function (ADF) (Pierrot et al., 1999a; Pierrot et al., 1999b) are some examples.

Since spectral properties such as the absorption cross-section must be calculated for performing the line-by-line calculation of radiative transfer, such amount of data may be large when made for non-uniform media. One way to minimize calculation time is to obtain the absorption cross-sections for a constant molar fraction of the chemical species. Bernardino and Maurente (2017) performed an analysis about how the absorption cross-section varies with the CO<sub>2</sub> concentration. In this work is carried out a similar analysis for media composed by H<sub>2</sub>O, aiming to achieve satisfactory results according to the obtained in the analysis performed by Bernardino and Maurente (2017). Thus, a study of how

sensitive the absorption cross-section is with respect to the H<sub>2</sub>O concentration is presented. In this work, absorption cross-section is obtained from HITEMP2010 database (Rothman et al., 2010).

## 2. CALCULATION AND ANALYSIS PROCEDURE

The complete Radiative Transfer Equation (RTE) for an absorbing-emitting medium is given by Eq. (1) (Modest, 2013).

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

Where  $I_\eta$  is the spectral intensity of radiation,  $I_{b,\eta}$  is the black body spectral intensity, given by Planck function and  $ds$  is the differential element of path length of propagation of the radiation ray.  $\kappa_\eta$  is the spectral absorption coefficient, which is related to absorption cross-section ( $C_\eta$ ) by Eq. (2) (Howell et al., 2016; Modest, 2013).

$$\kappa_\eta = C_\eta D \quad (2)$$

Where  $D$  is the density number, given by Eq. (3). The spectral absorption cross-section may be calculated according to Eq. (4) for most combustion problems (Denison and Webb, 1993b).

$$D = 2,479 \times 10^{19} \left(\frac{296}{T}\right) PY \quad (3)$$

$$C_\eta = \sum_i \frac{S_i}{\pi} \frac{\gamma_i}{(\eta - \eta_i)^2 + \gamma_i^2} \quad (4)$$

In the relation of the density number,  $Y$  is the molar concentration of the species,  $P$  is the pressure and  $T$  is the temperature of the medium. In the equation of the absorption cross-section,  $S_i$  is the line intensity for each line of the database at a given wavenumber  $\eta_i$ .  $\gamma_i$  is the half width for each transition that may be calculated based on Eq. (5). For calculating Eq. (4), it is necessary to have all spectral parameters generated with aid of the HITEMP2010 database (Rothman et al., 2010).

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n [Y P \gamma_{self,i} + (1 - Y) P \gamma_{air,i}] \quad (5)$$

Where  $T_{ref}$  is the reference temperature of the database,  $n$  is the temperature dependence coefficient,  $\gamma_{self,i}$  is the half width due to the collision broadening between the molecule of the emitting/absorbing species and  $\gamma_{air,i}$  is the half width due to the collision broadening of the molecules of the emitting/absorbing species with the air molecules.

The total intensity is obtained through integration in all spectra, as shown by Eq. (6).

$$I = \int_0^\infty I_\eta d\eta \quad (6)$$

The heat flux to one-dimensional media layer, where all properties only vary along the direction  $x$ , is given by Eq. (7).

$$q_{r,x} = \int_0^{4\pi} I(\Omega) \cos(\theta) d\Omega \quad (7)$$

Where  $\Omega$  is the solid angle.

The analysis of the variation of the absorption cross-section with the H<sub>2</sub>O concentration will be performed on the basis in the calculation of heat flux and divergence of the heat flux for given medium. This medium may be uniform or nonuniform. Certain profiles of temperatures, pressure and species concentration will be considered to the study.

Through Eq. (4) and Eq. (5) is possible to note that absorption cross-section is influenced by species concentration. The study seeks to analysis whether absorption cross-section is affected, to the point of significantly altering, the results of the radiative heat transfer by changes in concentration imposed on the equation to obtain the half width (Eq. (5)).

First it is necessary to define a standardized value to the execution of approximation by H<sub>2</sub>O concentration. Such value will be of  $Y_p$  equal to 25 %.

Assuming this analysis will be applicated to a medium determined at temperature  $T_m$ , molar concentration of H<sub>2</sub>O  $Y_m$  and pressure  $P_m$ , the approximation will consist in to perform the simulation of the heat flux and divergence of the heat flux on basis in an approached absorption cross-section obtained with the same temperature  $T_m$  and pressure  $P_m$  of medium, but with the standard concentration equal to  $Y_p$ .

Performed the approached simulations, simulations to reals radiative heat transfer (no approximation) shall be performed. The analysis will consist on the comparison between real and approximate results. The errors will be calculated on basis in Eq. (8) and Eq. (9).

$$Error = \frac{q_{real} - q_{approximated}}{|highest(q_{real})|} \quad (8)$$

$$Error = \frac{d_{real} - d_{approximated}}{|highest(d_{real})|} \quad (9)$$

Where  $q$  is the heat flux and  $d$  is the divergence of the heat flux. The denominator is the highest value due to the fact that the division by zero or very small values to unfeasible the analysis.

### 3. RESULTS AND DISCUSSION

Absorption coefficient obtained for temperature of 1000 K, 5 % H<sub>2</sub>O molar concentration at pressure of 1 atm is shown in the Fig. 1.

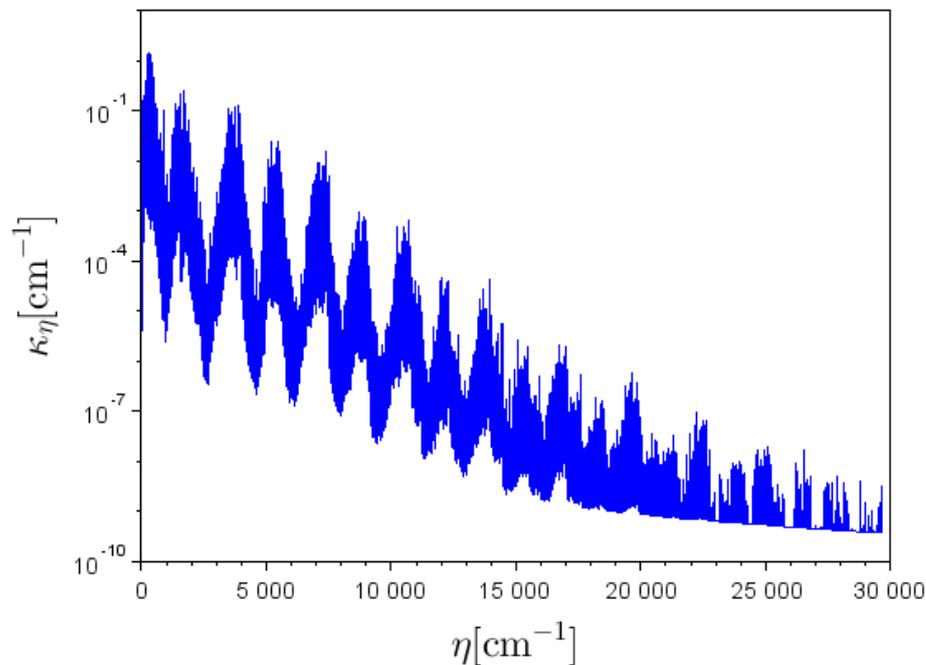


Figure 1. Absorption coefficient versus wavenumber at 1500 K, 5 % H<sub>2</sub>O molar concentration and 1 atm.

The calculation procedure was applied to isothermal and non-isothermal media. H<sub>2</sub>O concentration distribution was considered homogeneous at 1 atm pressure. Figures 2-4 show the results of the real heat flux and with the proposed approximation for isothermal media at 500 K, 1500 K and 2500 K at 1 atm and 5 %, 50 %, 75 %, 100 % H<sub>2</sub>O concentrations. The approximation errors are also presented. The length of the one-dimensional media layer  $L$  is equal to 1 m, in which the mixture of air and H<sub>2</sub>O is between black walls at the temperature of 300 K.

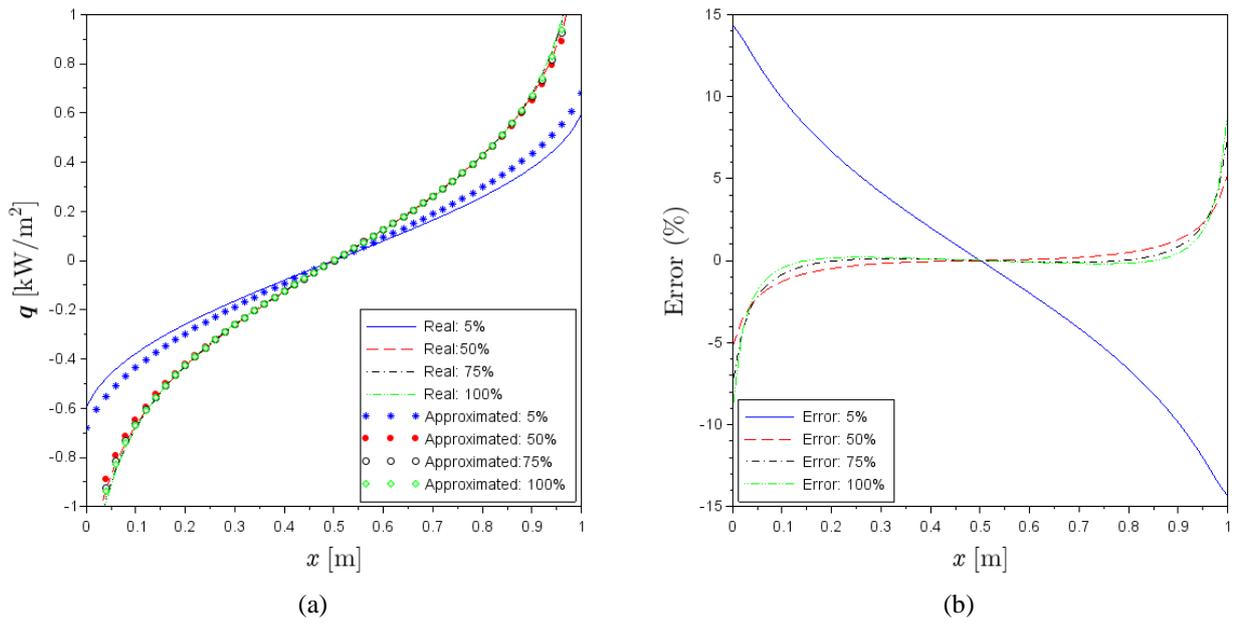


Figure 2. Heat flux (a) and error (b) for temperature of 500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

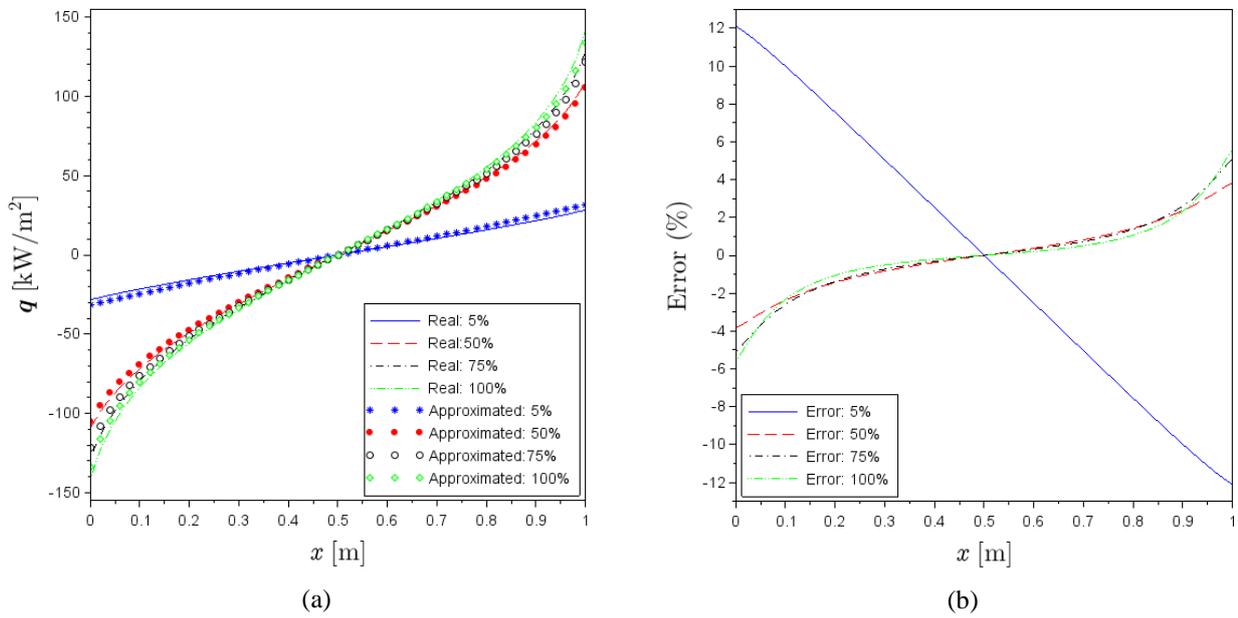


Figure 3. Heat flux (a) and error (b) for temperature of 1500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

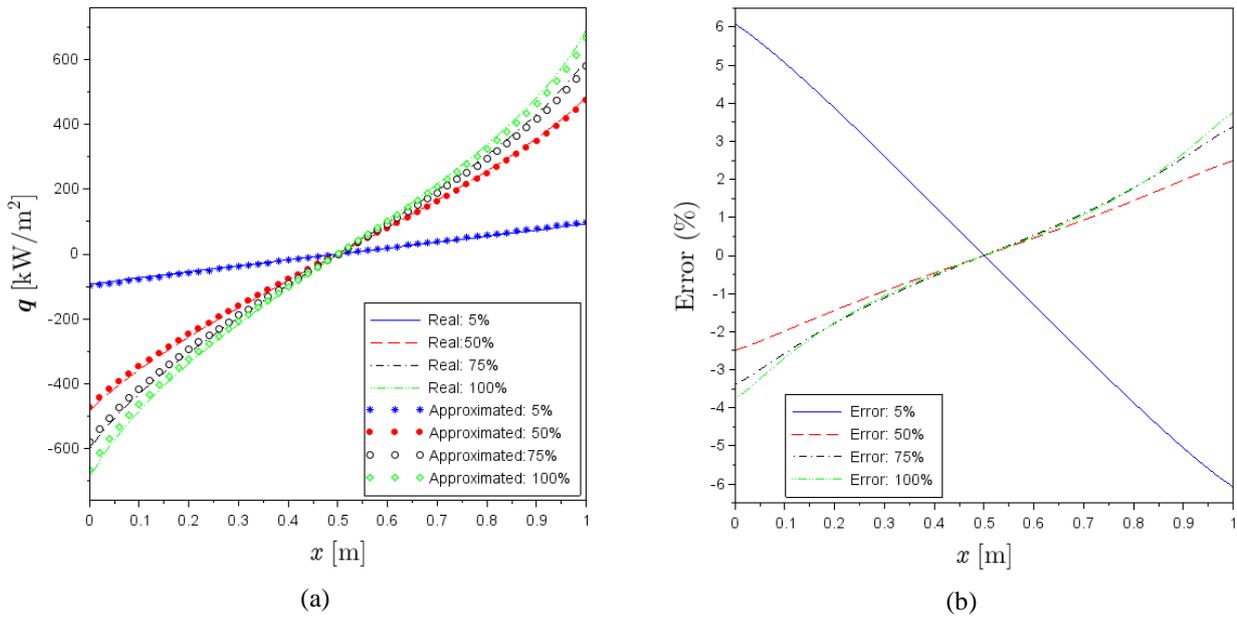


Figure 4. Heat flux (a) and error (b) for temperature of 2500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

Figures 5-7 present the real and approximated divergence of the heat flux for isothermal media at 500 K, 1500 K and 2500 K. Error of approximation is also presented.

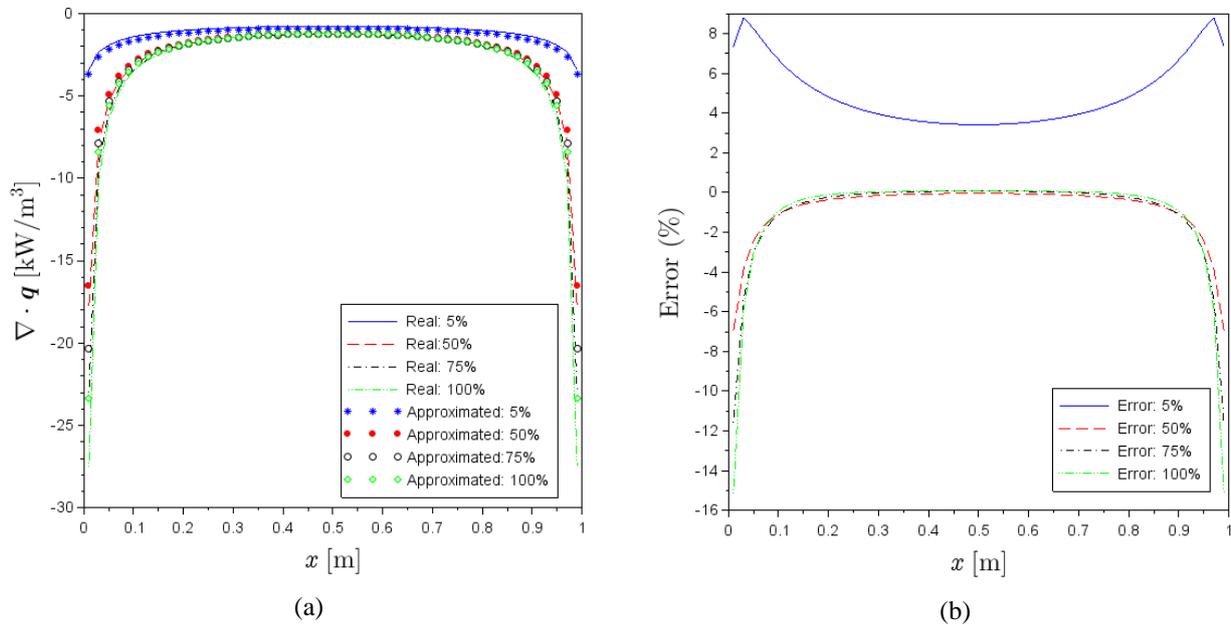


Figure 5. Divergence of the heat flux (a) and error (b) for temperature of 500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

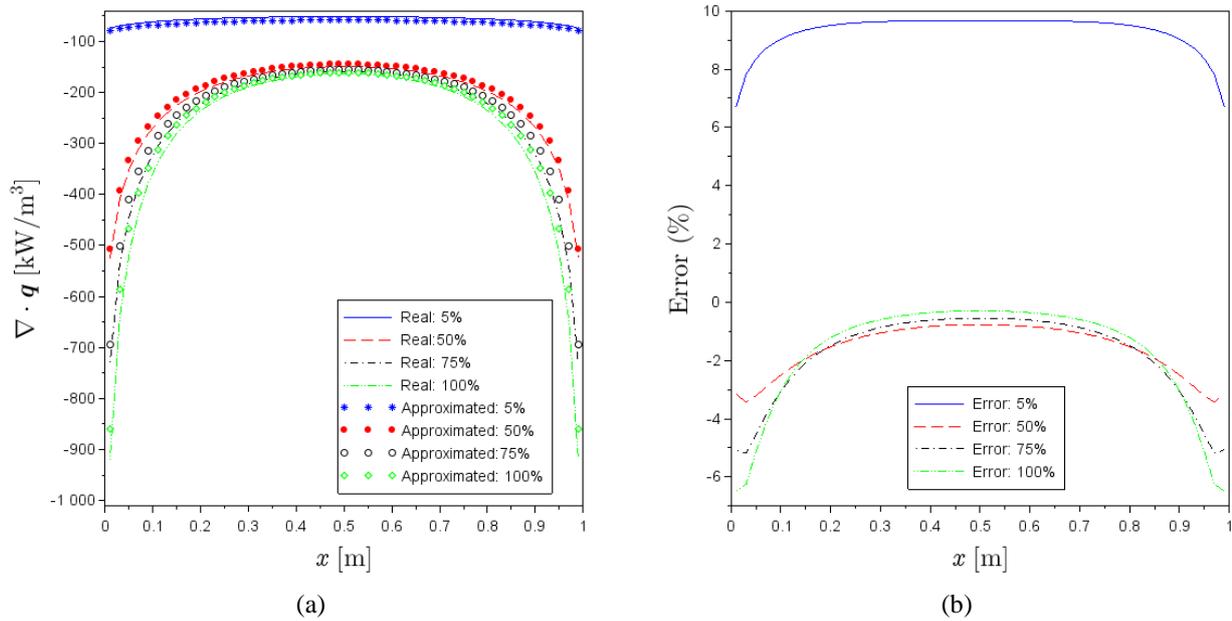


Figure 6. Divergence of the heat flux (a) and error (b) for temperature of 1500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

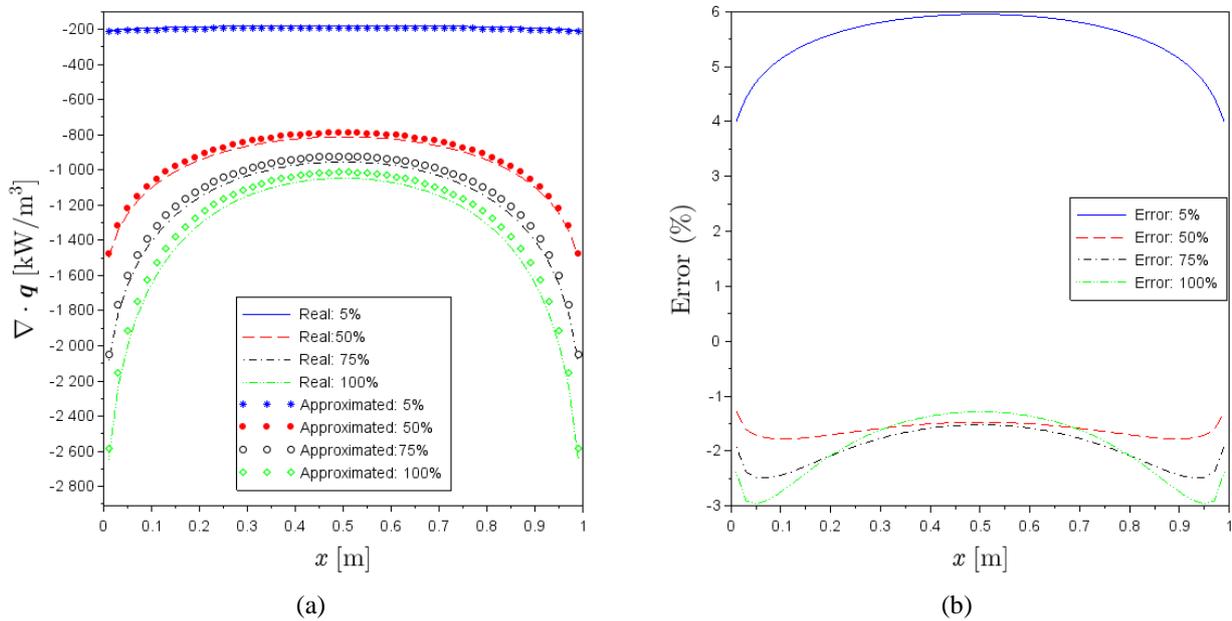


Figure 7. Divergence of the heat flux (a) and error (b) for temperature of 2500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 1 atm.

Analyzing the profiles obtained with the heat flux, it was verified that those with the approximation agree with the real ones. It is also verified the increase of the accuracy in the approximation with the temperature. That is, with respect to the heat flux, the absorption cross-section becomes less sensitive to the H<sub>2</sub>O concentration as the temperature increases. However, the accuracy of the results obtained here were less significant when compared with those obtained with the CO<sub>2</sub> isothermal gas layer one-dimensional (Bernardino and Maurente, 2017). The maximum error was about 15 % for the temperature of 500 K and concentration of 5 %. The biggest error for the temperature of 1500 K was about 12 % at 5 % concentration. For the 2500 K temperature, the maximum error was about 6 % for the 5 % concentration.

With respect to the results obtained with the divergence of the heat flux also it was verified that the profiles of the results acquired with the proposed approximation agree with the real ones. The maximum error was about 15 % for the temperature of 500 K and 100 % concentration. For the temperature of 1500 K, the maximum error was about 10 % for the 5 % concentration. For the temperature of 2500 K, the maximum error was about 6 % for the 5 % concentration. The increase in accuracy with temperature was also verified here.

A test case is also presented for non-isothermal media with temperature distribution given by Eq. (10) (Solovjov and Webb, 2010). H<sub>2</sub>O concentration distribution was considered homogeneous at 1 atm pressure. Figure 8 shows the results of the real divergence of the heat flux and with the proposed approximation for non-isothermal media at 1 atm and 5 %, 50 %, 75 %, 100 % H<sub>2</sub>O concentrations. The approximation errors are also presented. The length of the one-dimensional media layer  $L$  is equal to 0,2 m, in which the mixture of air and H<sub>2</sub>O is between black walls at the temperature of 1750 K on left and 750 K on right.

$$T_m = 1000 + 250 \cos(5\pi x) \tag{10}$$

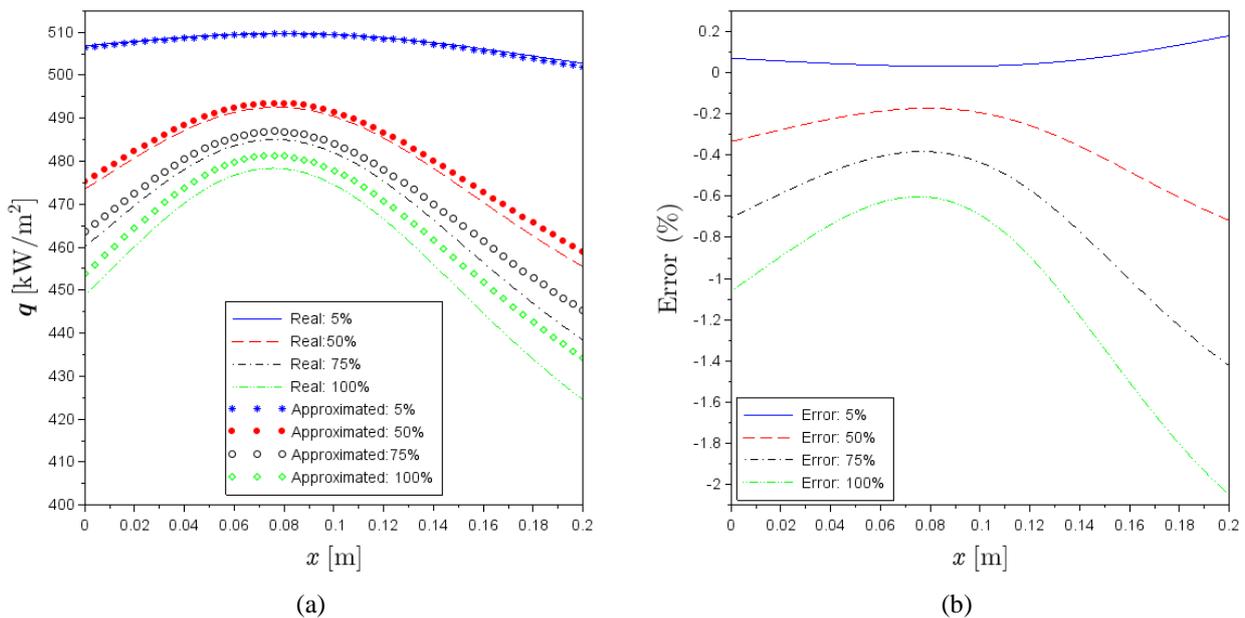


Figure 8. Heat flux (a) and error (b) for temperature distribution  $T_m = 1000 + 250 \cos(5\pi x)$  and concentrations of 5 %, 50 %, 75 % and 100 %.

Figure 9 presents the real and approximated divergence of the heat flux for non-isothermal media and error of approximation.

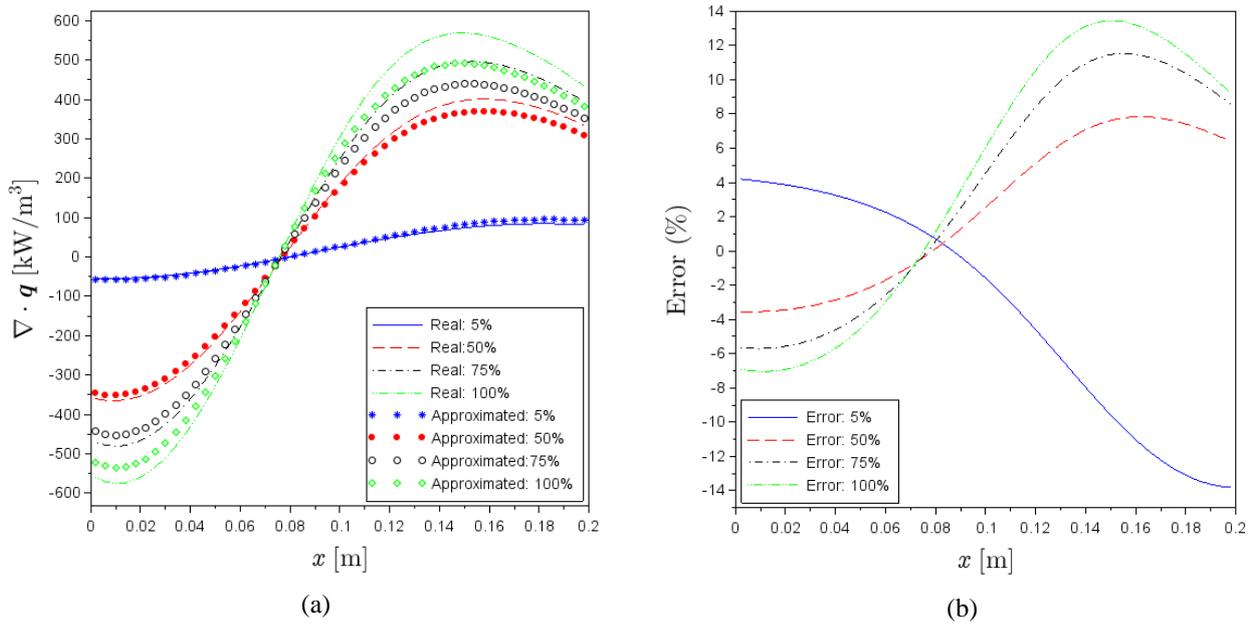


Figure 9. Divergence of the heat flux (a) and error (b) for temperature distribution  $T_m = 1000 + 250 \cos(5\pi x)$  and concentrations of 5 %, 50 %, 75 % and 100 %.

Verifying the results obtained for the test cases for non-isothermal media, it is observed the agreement of the approximate ones with the real ones. The maximum error for the heat flux was about 2 % for 100 % concentration while for the divergence it was about 14 % for the 5 % concentration, close to the wall, and 14 % for the 100 % concentration about  $x = 0,15$ . The effect of temperature on the accuracy of the applied method on the absorption cross-section in line-by-line calculation is verified in the results for non-isothermal media, since the error is lower for higher layer temperatures and increases in the regions where the temperature is smaller.

#### 4. CONCLUSION

An analysis of the absorption cross-section with a fixed molar fraction was performed by Bernardino and Maurente (2017) for isothermal and non-isothermal media consisting of a CO<sub>2</sub> layer one-dimensional. Here, the analysis was applied to a H<sub>2</sub>O layer one-dimensional.

Heat flux and divergence results were obtained, and errors related to the accuracy of the method were analyzed. In all the results it was verified that the profiles obtained with the approximation agree with the real ones. The biggest errors were for the lower temperatures, with the most accurate results linked to higher temperatures. Therefore, the absorption cross-section becomes less sensitive to the effect of the molar fraction as the temperature increases.

The maximum error for the heat flux in the isothermal H<sub>2</sub>O layer was about 15 % at the 500 K temperature and decreased to 6% at the 2500 K temperature, both at the 5 % concentration. The maximum error for the divergence of the heat flux in the isothermal H<sub>2</sub>O layer was about 15 % at the 500 K temperature and 100 % concentration. The maximum error for the 2500 K temperature was about 6 %. In most of the results obtained for isothermal media, the accuracy is less expressible near the walls. The maximum error for the non-isothermal H<sub>2</sub>O layer for the heat flux was about 2 % at 100 % concentration and for the divergence was about 14 % at 5 % concentration. Maximum error occurs in the region of the layer where temperatures are higher.

Thus, for the analyzed cases, the absorption cross-section obtained at a fixed molar fraction equal to 25 % promotes accurate results for line-by-line calculation of the radiative transfer, especially when the method is applied at high temperatures.

#### 5. ACKNOWLEDGEMENTS

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