25th ABCM International Congress of Mechanical Engineering
October 20-25, 2019, Uberlândia, MG, Brazil

COB-2019-0146
A STUDY OF THE ABSORPTION CROSS-SECTION WITH THE PRESSURE AND CO_2 GASES CONCENTRATION IN RADIATIVE TRANSFER CALCULATIONS.

Gabriel de Lima Bernardino
André Maurente
Laboratório de Sistemas Térmicos I, Departamento de Engenharia Mecânica, Universidade Federal do Rio Grande do Norte, Campus Universitário, Lagoa Nova, Natal, RN, 59090-970, Brazil
gabriellima050695@gmail.com, amaurente@gmail.com

Abstract. *Spectrally dependent properties are important in radiative heat transfer in participating media. Absorption cross-section is a spectral property that is related with the emission and absorption of radiation by molecular gases. Solution of the radiative heat transfer depends on the absorption coefficient and consequently depends on the absorption cross-section. A study about how the absorption cross-section varies with pressure and with the CO_2 concentration will be presented. Nonuniform and uniform media will be considered in simulations for a layer of one-dimensional media. This analysis seeks to verify how much the absorption cross-section is sensitive to the CO_2 concentration in order to use it how a constant in radiative heat transfer calculations for CO_2 nonuniform gases. The results present that the absorption cross-section obtained at 1 atm and 25 % of CO_2 can be used as constant with relation to concentration and pressure for nonuniform media at 3 atm with good accuracy.*

Keywords: *Absorption cross-section, spectral properties, pressure, concentration, radiative transfer equation*

1. INTRODUCTION

Spectrally dependent properties are very important in radiative heat transfer studies in that the medium is radiatively participating. Between such properties, the spectral absorption coefficient is a property which is connected to absorption and emission of radiation in molecules gases.

Absorption coefficient is proportional to molecular number density (Modest, 2013), but its obtainment also depends a property called absorption cross-section. Such property is influenced by temperature, pressure and molecular gas concentration in medium. Line parameters required to obtain these properties are obtained from databases as HITEMP (Rothman et al., 2010) and HITRAN (Gordon et al., 2017).

Exact line-by-line solution requires large computational time, since its integration considers absorption coefficient line-by-line of the spectrum. When used in non-uniform media, the amount of spectral absorption cross-section data is generally large since it depends on the thermodynamic state of the medium. In order to minimize computational time, these data can be pre-calculated considering various temperature, pressure and chemical species concentration conditions. Consequently, such databases required in line-by-line integration are generally large, thus requiring large computational resources.

Considering the high computational cost, spectral models were implemented in order to maintain high accuracy in the results with reduced computational time. These methods include weighted-sum-of-gray gases (WSGG) (Hottel and Sarofim, 1967), full-spectrum k-distribution (FSK) (Zhang and Modest, 2002; Singh and Modest, 2005), spectral-line-based-weighted-sum-of-gray gases (SLW) (Denison and webb, 1993a; Solovjov et al., 2011), cumulative wavenumber (CW) (Solovjov and Webb, 2002; Galarça et al., 2011), absorption distribution function (ADF) (Rivière et al., 1996; Pierrot et al., 1999) and spectral line moment-based (SLMB) (Andre and Vaillon, 2008).

Bernardino and Maurente (2017) carried out a study of how the absorption cross-section varies with the CO_2 concentration. This analysis consists in verify whether the absorption cross-section is sensitive to the concentration of the chemical species to the point of being able to use an absorption cross-section as a constant in the radiative transfer calculations in nonuniform gases composed CO_2 and inert species. The study was performed for isothermal medium at a temperature of 500 K, 1500 K and 2500 K, as well as an analysis for non-isothermal medium with temperature profile provided by Solovjov and Webb (2010). The medium considered was homogeneous to 5 %, 50 %, 75 % and 100 % of CO_2.

The analysis showed that accurate results to radiative heat transfer may be obtained for different concentrations of CO_2 by approaching the absorption cross-section obtained for 25 % of CO_2 (Bernardino and Maurente, 2017). Based on

this analysis, databases consisting of pre-calculated absorption cross-sections will be smaller when compared to those that do not make use of the approximation since the data will be obtained varying temperature and pressure with constant concentration.

In this work, an analysis of how the absorption cross-section varies with CO_2 concentration and with pressure will be performed. The method line-by-line will be employed for integration of Radiative Transfer Equation (RTE). Here, the spectral radiative properties are calculated using the HITEMP2010 (Rothman et al., 2010) database.

2. CALCULATION AND ANALYSIS PROCEDURE

Some media composed by gases such as CO_2, H_2O and air do not scatter radiation significatively. Thus, in this work the scattering is not considered. The radiative transfer equation for absorbing/emitting medium is given by Eq. 1 (Modest, 2013).

$$\frac{dI_\eta}{ds} = \kappa_\eta I_{b,\eta} - \kappa_\eta I_\eta \tag{1}$$

Where $I_{b,\eta}$ is spectral intensity of black body given by function of Planck, I_η is the spectral intensity of radiation, ds is the differential element of path traveled by radiation beam and κ_η is the spectral absorption coefficient.

Equation (2) show the relation to obtain absorption coefficient (Howell et al., 2016; Modest, 2013).

$$\kappa_\eta = \mathrm{C}_\eta D \tag{2}$$

Where D is the density number and C_η is the spectral absorption cross-section. Density number is provided by Eq. (3) and, for most combustion problems, absorption cross-section is given by Eq. (4) (Denison and Webb, 1993b).

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

$$\mathrm{C}_\eta = \sum_i \frac{S_i}{\pi}\ \frac{\gamma_i}{(\eta - \eta_i)^2 + \gamma_i^2} \tag{4}$$

Where P is the pressure, Y is the molar fraction of molecular gas, T is the temperature, S_i is the line intensity, η_i is the line number and γ_i is the half width for each transition given by Eq. (5).

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

Where n is the coefficient of temperature dependence, T_{ref} is the reference temperature of database, $\gamma_{self,i}$ is the half width due to the collision broadening between the species molecules and $\gamma_{air,i}$ is the half width due to the collision broadening of species molecules with air molecules. Quantities exposed in the Eq. (4) and in the Eq. (5) are obtained based in HITEMP2010 (Rothman et al., 2010) database.

With the absorption coefficient calculated, it is possible to perform the integration of RTE. Method line-by-line is the used in this work. Total intensity is obtained based on the integration of spectral intensity over the entire spectrum, as shown by Eq. (6).

$$I = \int_0^\infty I_\eta d\eta \tag{6}$$

In this work, the simulations are carried out for a layer of one-dimensional medium. The heat flux is provided by Eq. (7).

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

Where Ω is the solid angle.

Analysis of variation of the absorption cross-section with the pressure and with CO_2 concentration will be based in simulations of radiative heat transfer consisting of calculations of the heat flux and the divergence of the heat flux for a given profile of temperature, pressure and CO_2 concentration.

Observing the Eq. (4) and the Eq. (5), it is possible to note absorption cross-section is influenced by pressure of the medium and by chemical species concentration. Research seeks to analyze whether absorption cross-section for CO_2 molecular gases is sensitive to changes on concentration and on pressure imposed on Eq. (5) (half width for each

transition). Analysis is based on the radiative transfer simulations, verifying if results are significantly affected by such changes.

It is necessary to define standard values for performing of approximation of the absorption cross-section both by pressure and concentration. Such values will be of Y_p equal at 25 % for CO_2 concentration and of P_p equal at 1 atm for pressure.

When the analysis is applied to a determined medium with a profile of temperature T_m, CO_2 concentration Y_m and pressure P_m, the approximation will consist to perform simulation of the heat flux and of its divergence based in an absorption cross-section approximated obtained with the same temperature T_m of the medium, however with the concentration and pressure equals to Y_p and P_p, respectively.

With the approximated simulations obtained, simulations of the real heat transfer shall be carried out. Analysis consists to investigate how much the approximated results of the radiative transfer differ of the reals through the error calculation. Errors for the heat flux and for the divergence of the heat flux are given by Eq. (8) and by Eq. (9), respectively.

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

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

Where q is the radiative heat flux and d is the divergence of the radiative heat flux. The denominator of both the relations are the highest value, because divisions by zero or by very low values invalidate the analysis.

3. RESULTS AND DISCUSSION

Absorption coefficient for temperature of 1500 K, concentration of 50 % of CO_2 and pressure of 3 atm, without and with approximation (real and approximated spectrum, respectively) are shown in Fig. 1.

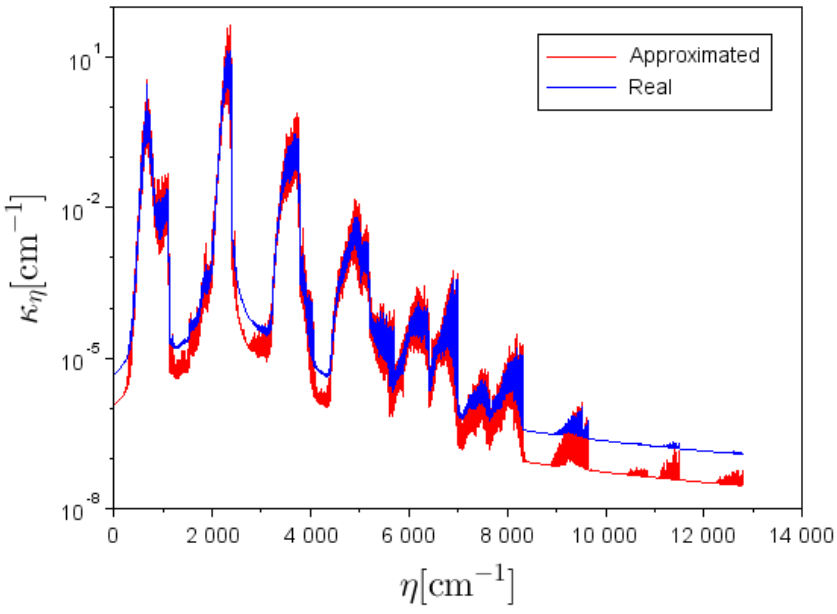


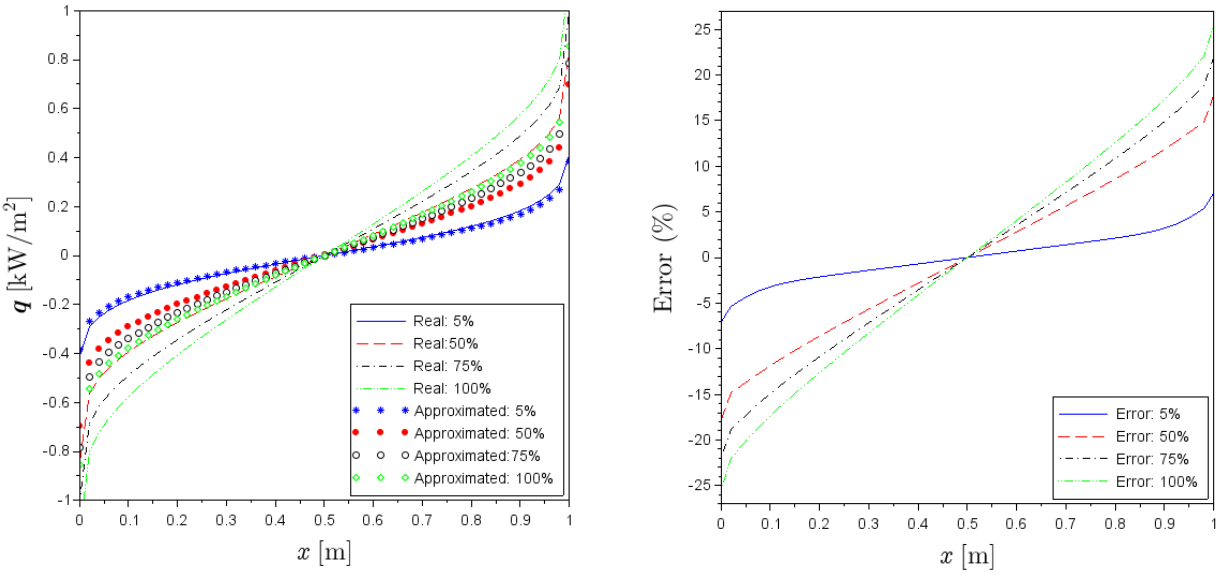
Figure 1. Real and approximated absorption coefficient versus wavenumber.

The results following the methodology presented in section 2 were obtained for the uniform and non-uniform media. The following are the results for each of the cases to be presented.

3.1 Uniform media

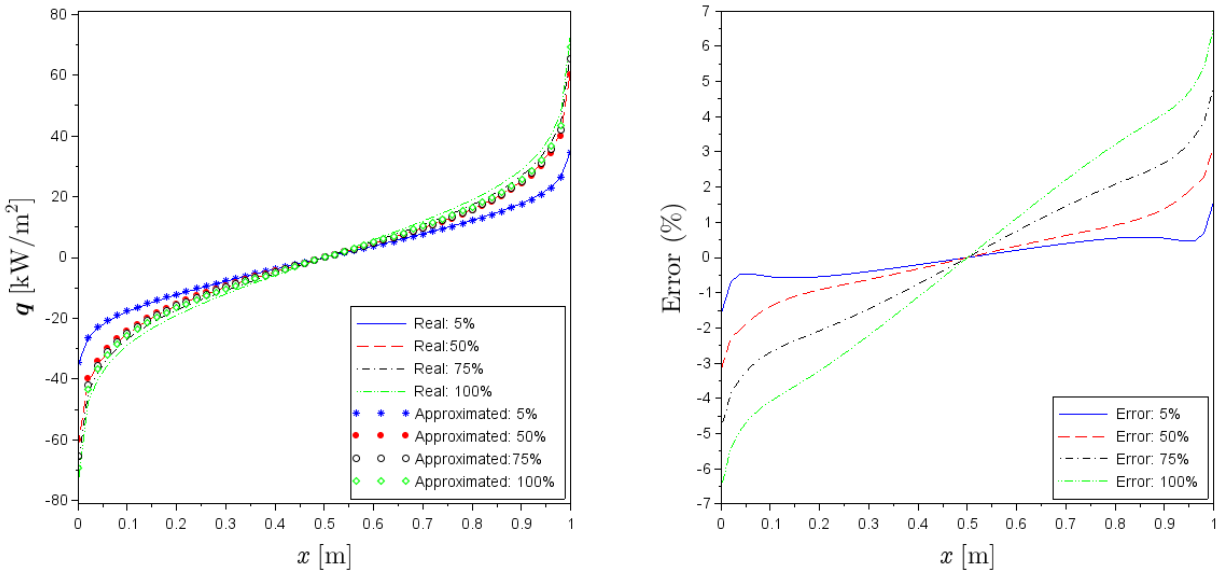
For uniform media, the proposed approximation was applied for 3 temperatures: 500 K, 1500 K and 2500 K. CO_2 concentration in the medium was 5 %, 25 %, 75 % and 100 % at a pressure of 3 atm. Simulations are performed for one-

dimensional layer of gas (mixture of air and CO_2) with length L = 1 m contained between two black walls at 300 K. The results for the heat flux and the error associated with approximation for layer temperatures of 500 K, 1500 K and 2500 K are presented from Fig. 2 to 4.



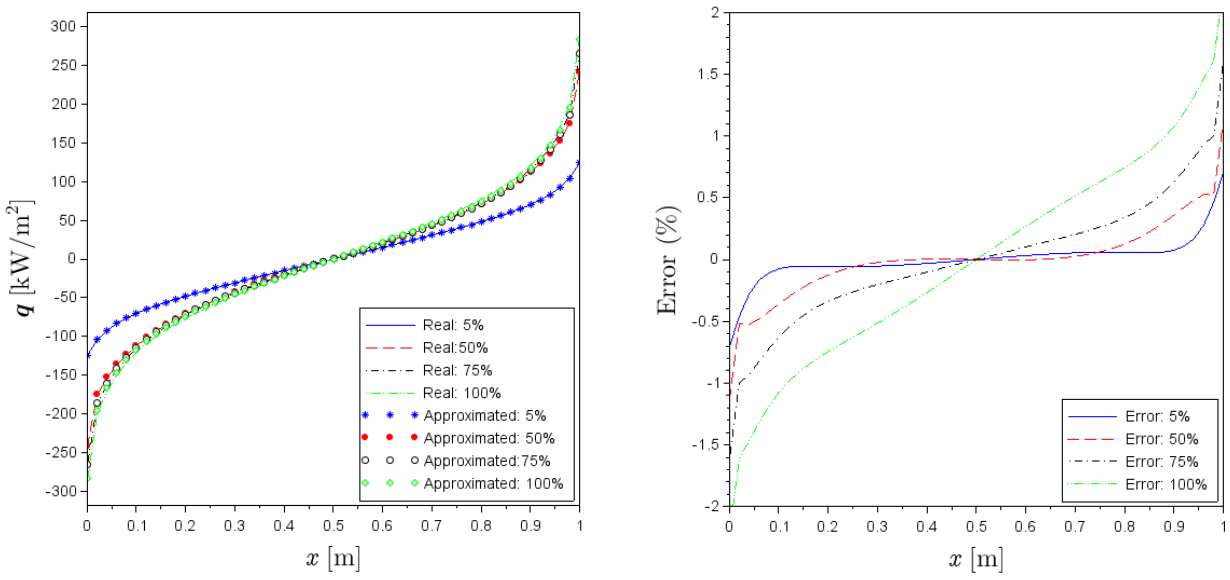
(a) (b)

Figure 2. Heat flux (a) and error (b) for temperature of 500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 3 atm.



(a) (b)

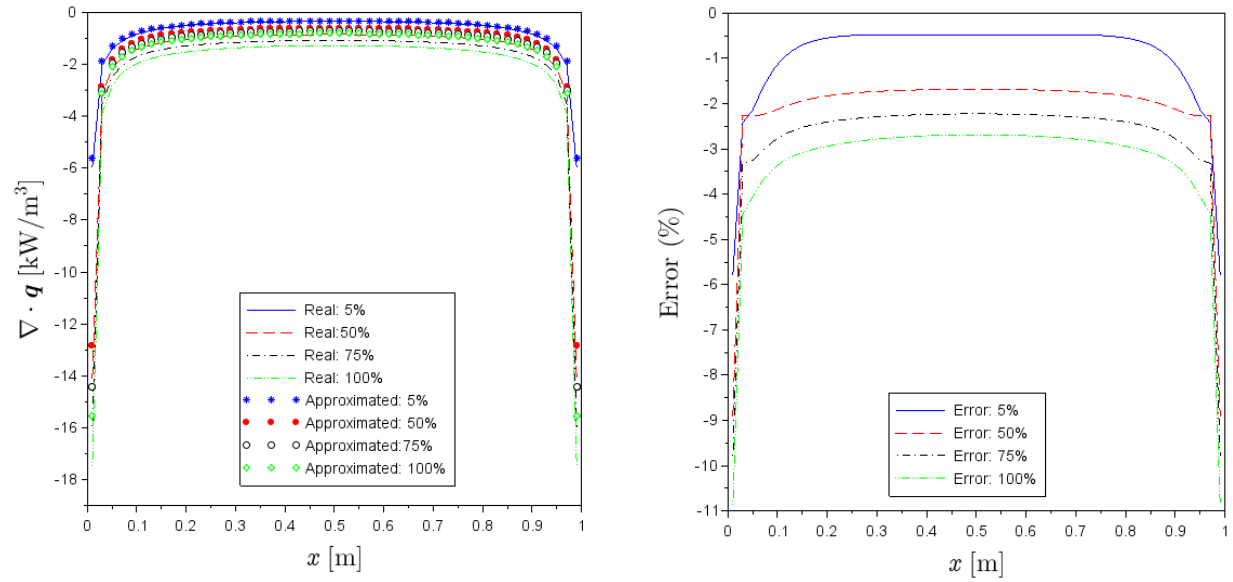
Figure 3. Heat flux (a) and error (b) for temperature of 1500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 3 atm.



(a) (b)

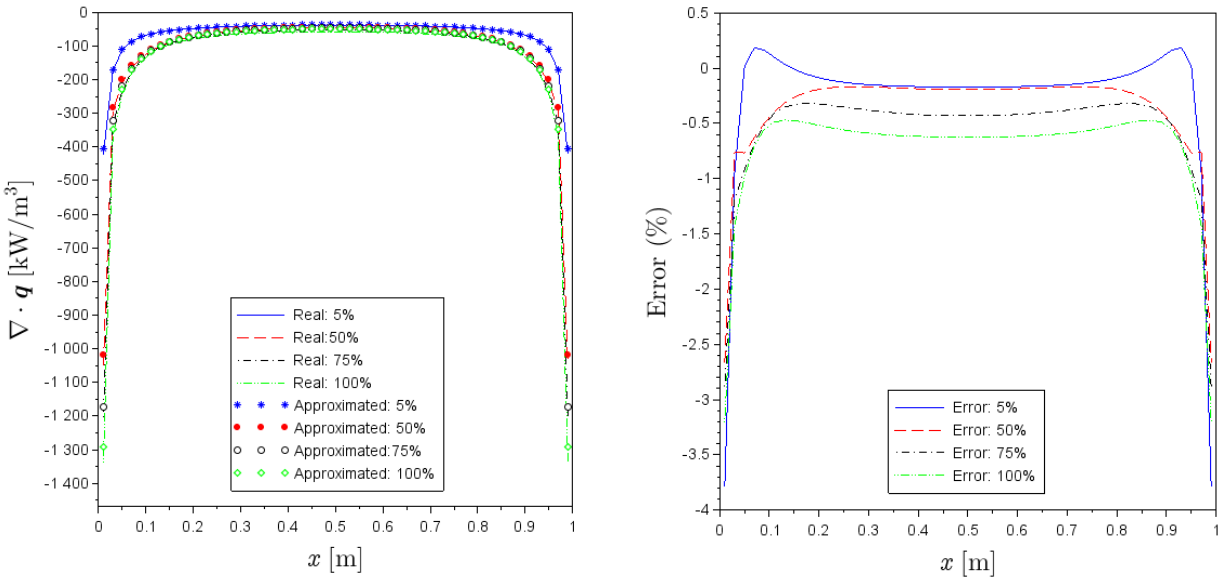
Figure 4. Heat flux (a) and error (b) for temperature of 2500 K and concentrations of 5 %, 50 %, 75 % and 100 % at 3 atm.

The results for the divergence of the heat flux and error associated with approximation for layer temperatures of 500 K, 100 K and 1500 K are presented from Fig. 5 to 7.



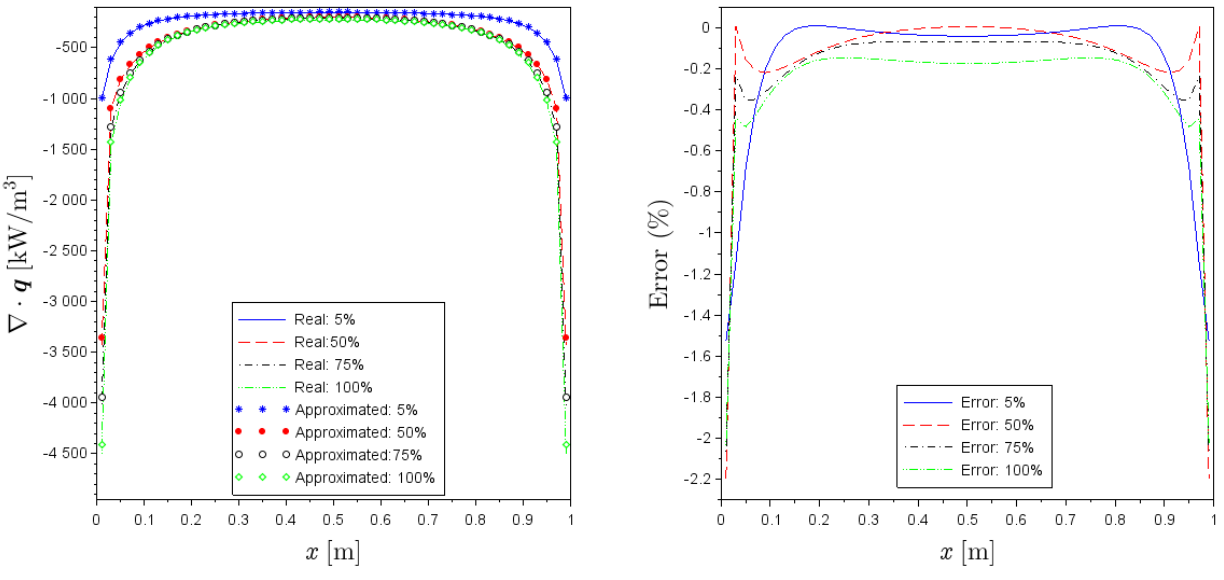
(a) (b)

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 3 atm.



(a) (b)

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 3 atm.



(a) (b)

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 3 atm.

Analyzing the figures referring to the heat flux and their respective approximation errors (Figs. 2-4), it is possible to observe that the simulations obtained with the approximation proposed in the absorption cross-section are according with the real ones. Observing all these results, the maximum error relative to the proposed approach occurred for the temperature of 500 K and 100% of CO2 at 3 atm, where the error was approximately 25% near the walls. With respect to the other molar fractions of CO_2, the lowest accuracy in the approximate results were obtained at a temperature of 500 K. For 5% CO_2 molar fraction, the error was below 7%. It is possible to note that the approach improves with increasing temperature. For temperature of 1500 K the maximum error was for 100 % CO_2 molar fraction, where the error was below

7 %. Then, for the temperature of 2500 K the results were the most accurate. Here, the maximum error was for 100 % CO_2 molar fraction being the value close to 2 %.

Similar to that observed with the heat flux, the profiles of the results obtained from the divergence of the heat flux with the approximation are according to ones without. That is, the approximations that present less accuracy are those related to the temperature of 500 K, where the biggest error is close to walls of the layer. For the 100 % CO_2 concentration, extreme case that presents less accuracy, the maximum error was about 11 % in modulus. For the central region of the layer under analysis, the error was below 3.5% in modulus. For all temperatures and concentrations, it was verified that the proposed approach presented better accuracy in the central region of the layer. The maximum error for temperature of 1500 K was for 5 % concentration, where the error found close to walls was about 3.8 % in modulus. For temperature of 2500 K, the maximum error was about 2.2 % close to walls for 50 % CO_2 concentration.

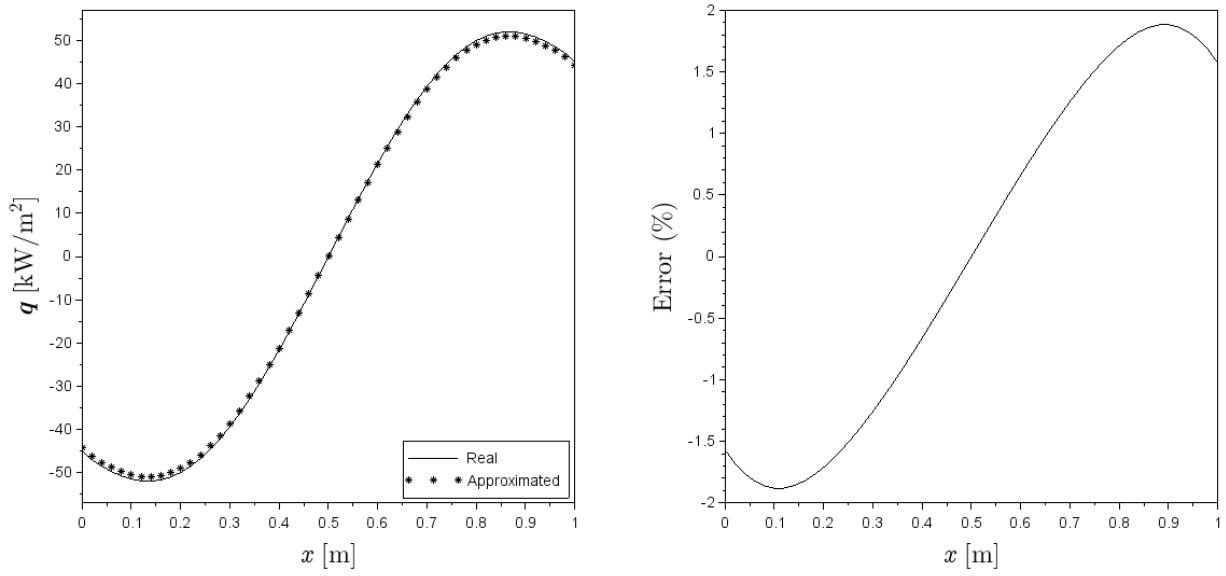
3.2 Non-uniform media

For non-uniform media, the proposed approximation was applied for one-dimensional layer of gas (mixture of air and CO_2) contained between two black walls at 300 K with profile temperature given by Eq. 10 and length L = 1 m. CO_2 concentration in the medium is given by Eq. 11 at pressure of 3 atm. The results for the heat flux and the error associated with approximation for presented case are shown from Fig. 8.

$$T_m = 950 + \frac{4000x(L-x)}{L^2} \tag{10}$$

$$Y_m = 0.15 + \frac{0.8x(L-x)}{L^2} \tag{11}$$

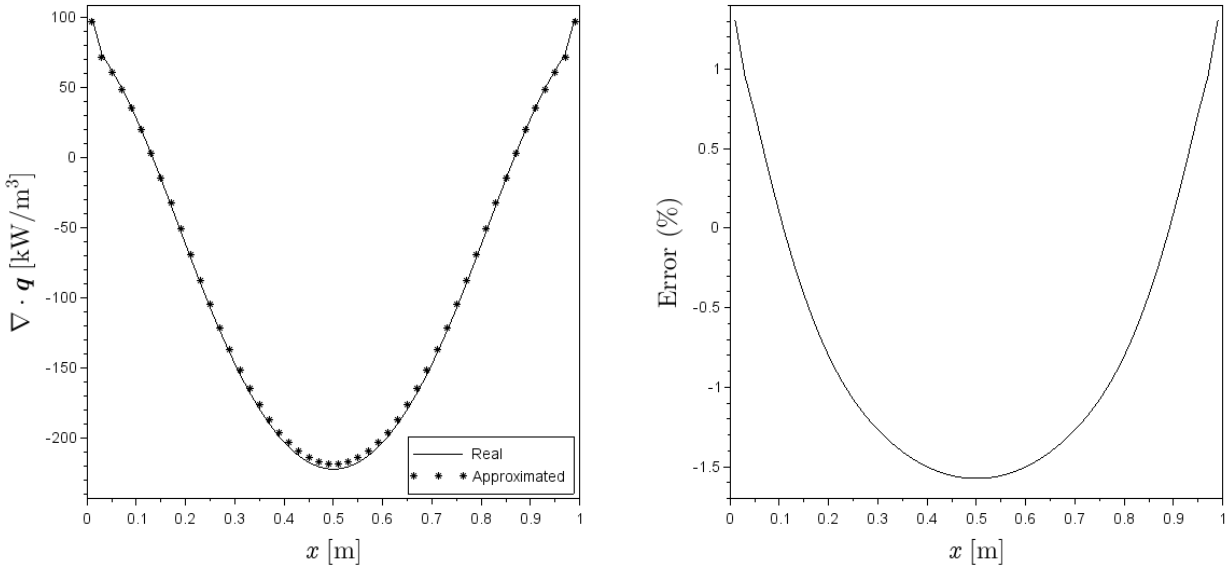
Where L =1 m is the length of layer.



(a) (b)

Figure 8. Heat flux (a) and error (b) for temperature distribution $T_m = 950 + 4000x(L-x)/L^2$ and concentrations distribution $Y_m = 0.15 + 0.8x(L-x)/L^2$ at 3 atm.

The results for the divergence of the heat flux and error associated with approximation are presented from Fig. 9.



(a) (b)

Figure 9. Divergence of the heat flux (a) and error (b) for temperature distribution $T_m = 950 + 4000x(L-x)/L^2$ and concentrations distribution $Y_m = 0.15 + 0.8x(L-x)/L^2$ at 3 atm.

By the analysis of the heat flux, the maximum error of the approximation was about 1.9 %. The maximum error obtained for the divergence of the heat flux was about 1.6 % in modulus. Here, the results obtained were more accurate when compared to those for uniform medium. Again, the approximate profiles of the heat flux and its divergence agree with the real ones.

4. CONCLUSION

Line-by-line calculation of radiative transfer requires a large computational resource when compared to the spectral models for the integration of the Radiative Transfer Equation (RTE). One way to streamline the calculation process using line-by-line is to assemble a pre-calculated absorption cross-section database. The study proposed to conduct a study of how the cross section of spectral absorption varies with CO_2 concentration and with pressure. So, if the absorption cross-section is not significantly sensitive to concentration and pressure, it can be obtained at a fixed concentration of 25 % and at a fixed pressure of 1 atm.

Test cases were for uniform and non-uniform media under a pressure of 3 atm. The results showed that the accuracy of the proposed approach increased with the temperature in uniform media. The proposed approximation obtained results for the divergence of the heat flux with optimum accuracy in the central region of the layers. The maximum errors of the approximation with respect to the heat flow was for the concentration of 100 %. Such a concentration is not usually found in real combustion problems, since the gases are often found unevenly distributed in the media.

The proposed approximation was applied in a test case for non-uniform media. The results obtained presented better accuracy when compared to the test cases for uniform media. The maximum error was about 1.9 % for the heat flux and 1.6 % for the divergence.

For all test cases, the results obtained with the proposed approximation agreed with those obtained without approximation. Thus, absorption cross-section obtained at 1 atm and 25 % of CO_2 can be used as constant with relation to concentration and pressure for nonuniform media at 3 atm with good accuracy.

5. ACKNOWLEDGEMENTS

This work was supported by CNPQ, under financing code 001.

6. REFERENCES

Andre, F. and Vaillon, R., 2008. “The spectral-line-moment-based (SLMB) modeling of the wide band and global black body-weighted transmission function and cumulative distribution function of the absorption coefficient in uniform media*”. J Quant Spectr Rad Transfer* 109: 2401–16.

Bernardino, G. and Maurente, A., 2017. "An investigation about the use of a constant absorption cross-section for radiative heat transfer computations in nonuniform CO_2 gases." *In Proceedings of the 24nd International Congress of Mechanical Engineering - COBEM 2017*. Curitiba, Brazil.

Denison, M.K. and Webb, B.W., 1993a. "A spectral line based weighted-sum-of-gray-gases model for arbitrary RTE solvers", J. *Heat Transfer* 115 (4). 1004–1012.

Denison, M.K. and Webb, B.W., 1993b. "An absorption-line blackbody distribution function for efficient calculation of gas radiative transfer". *J Quant Spectrosc Radiat Transfer* 50, 499-510.

Galarça, M.M., Mossi, A. and França, F.H.R., 2011. "A modification of the cumulative wavenumber method to compute the radiative heat flux in non-uniform media", *J. Quant. Spectrosc. Radiat. Transfer* 112 (3). 384–393.

Gordon, I.E. et al., 2017. "The HITRAN2016 molecular spectroscopic database", *J Quant Spectrosc Radiat Transfer* 203: 3-69.

Howell, J.R., Meng¨uc¸ M.P. and Siegel, R., 2016. *Thermal Radiation Heat Transfer*. 6th ed. Taylor & Francis Group, New York.

Hottel, H.C. and Sarofim, A.F., 1967. *Radiative Transfer*, McGraw-Hill, New York.

Modest, M.F., 2013. *Radiative Heat Transfer*. 3th ed. Academic Press, New York.

Modest, M.F. and Zhang, H., 2002. "The full-spectrum correlated-k distribution for thermal radiation from molecular gas–particulates mixtures", *J. Heat Transfer* 124 (1). 30–38.

Modest, M.F. and Singh, V., 2005. "Engineering correlations for full spectrum k-distribution of H2O from HITEMP spectroscopic databank", *J. Quant. Spectrosc. Radiat. Transfer* 93 (1–3). 263–271.

Pierrot, L., Soufiani, A. and Taine, J., 1999. "Accuracy of narrow-band and global models for radiative transfer in H2O, CO2, and H2O–CO2 mixtures at high temperature", *J. Quant. Spectrosc. Radiat. Transfer* 62 (5). 523–548.

Rivière, P., Soufiani, A., Perrin, M.Y., Riad, H. and Gleizes, A., 1996. "Air mixture radiative property modelling in the temperature range 10,000–40,000 K", *J. Quant. Spectrosc. Radiat. Transfer* 56 (1). 29–46.

Rothman, L.S. et al., 2010. "The high-temperature molecular spectroscopic database". *J Quant Spectrosc Radiat Transfer* 111, 2139-2150.

Solovjov, V.P. and Webb, B.W., 2002. "A local-spectrum correlated model for radiative transfer in non-uniform gas media", *J. Quant. Spectrosc. Radiat. Transfer* 73 (2–5). 361–373.

Solovjov, V.P. and Webb, B.W., 2010. "Application of CW local correction approach to SLW modeling of radiative transfer in non-isothermal gaseous media", *Journal of Quantitative Spectroscopy & Radiative Transfer* 111, 318–324.

Solovjov, V.P., Lemonnie, D. and Webb, B.W., 2011. "SLW-1 modeling of radiative heat transfer in nonisothermal nonhomogeneous gas mixtures with soot", *J. Heat Transfer* 133 (10). 102701(1–9).

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.