

NEW COEFFICIENTS OF THE WEIGHTED-SUM-OF-GRAY-GASES MODEL USING HITEMP 2010 DATABASE

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Abstract. In this work, new coefficients for the WSGG model are proposed based on the up to date HITEMP 2010 database. The coefficients are determined for gas mixtures of water and carbon dioxide. The coefficients are obtained for partial pressure ratios p_{H_2O}/p_{CO_2} of 1.0 and 2.0, simulating combustion products of fuel oil and methane. The path-length ranges from 0,001 atm-m to 10 atm-m, while the temperature varies between 400 K and 2500 K. This study also makes a comparison of the total emittance values obtained from the model with benchmark line-by-line (LBL) results, showing an excellent agreement. With the obtained coefficients, one-dimensional radiant heat transfer problems are solved in order to compare the solution obtained by the WSGG model with the solution obtained by the LBL integration. In the comparisons, different temperature profiles, temperature gradients and species concentrations are used. In all cases it is possible to verify the good agreement of the WSGG and LBL results.

Keywords: Radiation heat transfer, Participating Medium, Weighted-Sum-of-Gray-Gases.

1. INTRODUCTION

The radiative heat transfer occupy an important place in thermal engineering applications, such as furnaces, steam generators and material processing. The measurement of radiation heat transfer in combustion gases is a complex task due to the highly irregular variations of the absorption coefficient with the wavenumber. A method used to determine de radiation heat transfer is the line-by-line method (LBL), which provides the exact solution, but requires large computational effort. Thus, gas models are needed to make possible the solution of engineering problems. Hottel and Sarofin (1967) proposed the weighted-sum-of-gray-gases (WSGG) which consider the emittance of the medium represented by the sum of some gray gases. The coefficients used in this model were proposed by Smith et al. (1982). These coefficients are outdated, since new database are available and updated frequently. Galarça et al. (2008) proposed new coefficients using the HITEMP 2008 (High Temperature Molecular Spectroscopy Database) in order to turn the WSGG model results more reliable. HITEMP 2010 was presented by Rothman *et. al.* (2010), showing significant modifications in the database and spectral behavior of the substances, if compared whit the previous edition.

This paper proposes new coefficients for WSGG model for a participating media composed of two gases, H₂O and CO₂, using the HITEMP 2010. The coefficients are obtained for the same proportion mixture presented by Smith et al. (1982), considering a path-length form 0,001 to 10 atm-m, but a ranging temperature from 400 K to 2500 K. The coefficients are tested, comparing the WSGG results, calculated according Denison and Webb (1991) with the LBL solution, calculated according Chu et al. (2011). The results are obtained for different profiles temperatures and different uniform concentrations. The medium is contained between two infinite parallel plates, and so the physical geometry is one-dimensional. The solution of the system of equations will be accomplished with the discrete ordinates method.

2. RADIATIVE GASES PROPIERTIES

2.1. Determination of the total emittance

The medium that was considered to obtain the coefficients for WSGG model is composed of a gas mixture of CO₂ and H₂O. The database used is HITEMP 2010, as presented in Rothman *et. al.* (2010). The database can be downloaded in <http://www.cfa.harvard.edu/HITRAN/>.

According to Siegel and Howell (2002), the Lorentz profile can be used in the determination of the absorption cross-section. It is given by:

$$C_{\eta}(\eta) = \sum \frac{S_i(T)}{\pi} \frac{\gamma_i}{\gamma_i^2 + (\eta - \eta_i)^2} \quad (1)$$

where C_η is the absorption cross-section, S_i is the integrated line intensity, η_i is the line location, and γ_i is the half-width. The half-width that is defined by:

$$\gamma_i = \left(\frac{T_{ref}}{T} \right)^n p_s \gamma_{self,i} + (1 - p_s) \gamma_{air,i} \quad (2)$$

where p_s is the partial pressure, T is the temperature, T_{ref} is the reference temperature (296 K), γ_{self} is the self-broadening, γ_{air} is the broadening caused by the air and n is the dependence coefficient by the temperature.

The integrated line intensity S_i in the HITEMP 2010 is obtained at the temperature of 1000 K, but is converted in a temperature of 269 K in its compilation to let it uniform with others databases. When using the HITEMP 2010, it is needed to convert S_i in the desired temperature. According to Rothman *et al.* (2010), the equation below is used:

$$S_i(T) = S_i(T_{ref}) \frac{Q(T_{ref})}{Q(T)} \frac{\exp(-C_2 E_\eta / T) [1 - \exp(-C_2 \nu_i / T)]}{\exp(-C_2 E_\eta / T_{ref}) [1 - \exp(-C_2 \nu_i / T_{ref})]} \quad (3)$$

where Q is the total internal partition sums, ν_i is the energy difference between the initial and final state, E_i is the energy of the lower state and C_2 is the second Planck's constant, equal to 0.0143877 m·K.

The values of C_η must be calculated for several temperatures in order to obtain the properties of the H₂O and CO₂ in combustion conditions. To obtain the absorption coefficient per unit of pressure, it is used the following equation:

$$\kappa_\eta = N C_\eta \quad (4)$$

where κ_η is the coefficient absorption per unit of pressure, in m⁻¹·atm⁻¹, N is the Loschmidt number. It is defined by:

$$N = 2,479 \cdot 10^{19} \left(\frac{296}{T} \right) \quad (5)$$

In order to obtain the absorption coefficient k_η for the mixture, the following equation is used:

$$k_{\eta,mix} = \frac{p_{CO_2} \kappa_{\eta,CO_2} + p_{H_2O} \kappa_{\eta,H_2O}}{p_{CO_2} + p_{H_2O}} \quad (6)$$

where p_{H_2O} and p_{CO_2} are the partial pressure of H₂O and CO₂, respectively, κ_{H_2O} and κ_{CO_2} is the coefficient absorption per unit of pressure for the substances.

With the values of $\kappa_{\eta,mix}$ obtained, it is possible to determine the total emittance, by a specific temperature and pressure path-length. According to Siegel and Howell (2002), it is given by the following equation:

$$\varepsilon(pL) = \pi^0 \frac{\int_0^\infty i_{\eta,b}(\eta) \{1 - \exp[-\kappa_{\eta,mix}(p_{CO_2} + p_{H_2O})L]\} d\eta}{\sigma T^4} \quad (7)$$

where $(p_{CO_2} + p_{H_2O})L$ is the pressure path-length, given by the product of partial pressure of the mixture by the path length, and $i_{\eta,b}$ is the radiation intensity emitted by a black body, which is given by:

$$i_{\eta,b} = \frac{2C_1 \eta^3}{e^{C_2 \eta / T} - 1} \quad (8)$$

where C_1 is the first Planck's constant, equal to 0.59552137 × 10⁻¹⁶ W·m²/sr.

2.2. The coefficients of the WSGG model

The WSGG model was proposed by Hottel and Sarofin (1967). The model represents the participating medium with some gray gases where the absorption coefficient can be considered constant. Thus, it is possible to greatly simplify the integrating in the spectral properties. The emittance in the WSGG models is given by the following relation (Smith et al, 1982):

$$\varepsilon(pL) = \sum_{i=1}^I a_i(T)(1 - \exp(-k_i p_{mix} L)) \quad (9)$$

where $a_i(T)$ is the emittance weighting factor for the i -th gray gas, k_i is the absorption coefficient per unit of pressure, $(\text{atm}\cdot\text{m})^{-1}$, and p_{mix} is the sum of the partial pressure of the all gases participating on the medium. The coefficient $a_i(T)$ depends only on temperature, and is represented by the polynomial function, given by the following equation:

$$a_i(T) = \sum_{j=1}^J b_{i,j} T^{j-1} \quad (10)$$

where $b_{i,j}$ is the polynomial coefficients of $(j-1)$ order for the i -th gray gas.

In order to determine the WSGG model coefficients, the Levenberg-Marquardt method was used to fit the emittance values that were calculated from the line-by-line integration of Eq. (7) using the spectral lines obtained through HITEMP 2010 database, which can be considered exact but for minor errors that arise in the numerical integration that are involved in the process. In order to obtain the k_i values, apply the sum of two hands on the Eq. (9) for all considered temperatures, leading to Eq. (11) below. For that, is considered that the k_i values are independent of temperature (Galarça et al., 2008).

$$\sum_{T=400K}^{2500K} \varepsilon(pL) = \sum_{i=1}^4 \left\{ \left[\sum_{T=400K}^{2500K} a_i(T) \right] (1 - e^{-k_i pL}) \right\} \quad (11)$$

In order to apply the Levenberg-Marquardt method, it is necessary determine the sum of $\varepsilon(pL)$ for several pL values. In this work, twenty four values were used, ranging from 0,001 to 10 atm·m. The values of sum of $\varepsilon(pL)$ as functions of pL is informed to the software, as well as the right hand of the Eq. (11).

After obtaining the k_i values, it is determined the $a_i(T)$ coefficients. For that, it is informed to the software, for a specific temperature, the values of $\varepsilon(pL)$ as functions of pL . It is informed also the right hand of the Eq. (9), with the k_i determined values, in order to fit the values. This procedure is carried for all temperatures. After determining the $a_i(T)$ values for all temperatures, a fourth order polynomial function is used to fit the $a_i(T)$ values as a function of T , for each i gray gas, thus obtaining the $b_{i,j}$ coefficients of Eq. (10).

3. RESULTS AND DISCUSSION

The correlations presented here are valid for gaseous mixtures that are generated in the stoichiometric combustion of two typical hydrocarbon fuels: methane and fuel oil. The products of the combustion of fuel oil are formed of $p_{H_2O} = 0.1$ atm and $p_{CO_2} = 0.1$ atm. The products of the methane combustion contain $p_{H_2O} = 0.2$ atm and $p_{CO_2} = 0.1$ atm. The results were obtained for a total pressure of 1.0 atm, gas temperatures ranging from 400 K to 2500 K and pressure-path length products from 0.001 to 10 atm·m. The coefficients of the WSGG correlations are presented in the Table 1 for $p_{H_2O}/p_{CO_2} = 1.0$ and in the Table 2 for $p_{H_2O}/p_{CO_2} = 2.0$.

Table 1 – Coefficients for WSGG for $p_{H_2O}/p_{CO_2} = 1.0$.

i	$k_i (\text{atm}\cdot\text{m})^{-1}$	$b_{i,1}$	$b_{i,2} (\text{K}^{-1})$	$b_{i,3} (\text{K}^{-2})$	$b_{i,4} (\text{K}^{-3})$	$b_{i,5} (\text{K}^{-4})$
1	0.187	7.197E-02	8.724E-04	-9.690E-07	4.651E-10	-7.917E-14
2	1.723	1.107E-01	3.397E-04	-2.467E-07	4.647E-11	-1.039E-15
3	12.484	2.091E-01	-6.423E-05	-3.200E-08	1.718E-11	-2.105E-15
4	144.938	7.092E-02	6.586E-05	-1.278E-07	5.577E-11	-7.709E-15

Table 2 – Coefficients for WSGG for $p_{H_2O}/p_{CO_2} = 2.0$.

i	$k_i (\text{atm}\cdot\text{m})^{-1}$	$b_{i,1}$	$b_{i,2} (\text{K}^{-1})$	$b_{i,3} (\text{K}^{-2})$	$b_{i,4} (\text{K}^{-3})$	$b_{i,5} (\text{K}^{-4})$
1	0.192	5.617E-02	7.844E-04	-8.563E-07	4.246E-10	-7.440E-14
2	1.719	1.426E-01	1.795E-04	-1.077E-08	-6.971E-11	1.774E-14
3	11.370	1.362E-01	2.574E-04	-3.711E-07	1.575E-10	-2.267E-14
4	111.016	1.222E-01	-2.327E-05	-7.492E-08	4.275E-11	-6.608E-15

Figure 1 shows the comparison between the exact emittance values, that is, computed from LBL integration, with the values obtained by the WSGG model. Once can observe the excellent agreement between the values.

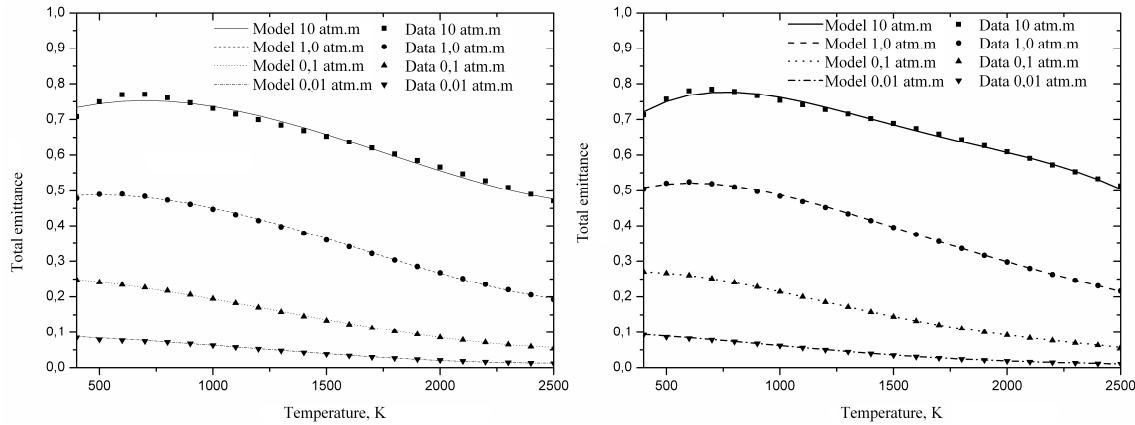


Figure 1 – Comparison of the total emittances computed with the LBL integration (data values) and the WSGG model for different pressure-paths lengths and temperatures. (a) $p_{H_2O}/p_{CO_2} = 1.0$. (b) $p_{H_2O}/p_{CO_2} = 2.0$.

3.1. WSGG and LBL results comparison

An important issue related to the model WSGG is the hypothesis that the absorption coefficient per unit of pressure, k_i , is independent of temperature, which is clearly a simplification. In fact, all the WSGG model dependence on temperature is fitted with the polynomial coefficients, which represent the energy fraction of the blackbody spectrum in the regions corresponding to each gray gas. One must also take into account that the coefficients of the model were determined for isothermal medium. Thus, it is necessary to analyze how the model compares with the benchmark LBL solution in non-isothermal medium, a study which does not appear clearly in the literature.

The geometry proposed is two flat plates with an emissivity of 1.0 (black walls) and separated by a distance of 1.0 m. The physical mesh between the two black surfaces was divided into 200 equal-sized elements. The discrete ordinates method was applied to 30 directions, using a Gauss-Legendre quadrature. The concentration of the gases is considered uniform and the temperature profile is proposed in the following equations:

$$T(x) = 2000 - 1600 \left(\frac{2x}{L} - 1 \right)^2 \quad (12)$$

$$T(x) = 1600 - 800 \left(\frac{2x}{L} - 1 \right)^2 \quad (13)$$

$$T(x) = 1400 - 400 \left(\frac{2x}{L} - 1 \right)^2 \quad (14)$$

The ranging of temperatures in Eq. (12), (13) and (14) are $\Delta T = 1600$ K, $\Delta T = 800$ K and $\Delta T = 400$ K, respectively. The results are presented in Figs. 2(a) and 2(b), for $p_{H_2O}/p_{CO_2} = 1.0$ and 2.0, respectively.

The maximum error is calculated in the following equation:

$$Error = \frac{\left| (dq_r(x)/dx)_{LBL} - (dq_r(x)/dx)_{WSGG} \right|_{\max}}{\left| (dq_r(x)/dx)_{\max,LBL} \right|} \quad (15)$$

The maximum errors obtained for $p_{H_2O}/p_{CO_2} = 1.0$ were 7.85%, 3.04% and 2.67% for $\Delta T = 1600$ K, $\Delta T = 800$ K and $\Delta T = 400$ K, respectively. For $p_{H_2O}/p_{CO_2} = 2.0$, the maximum errors were 2.62%, 1.60%, 2.95% for $\Delta T = 1600$ K, $\Delta T = 800$ K and $\Delta T = 400$ K, respectively. It is possible to verify the good agreement in the results for WSGG and LBL solution, indicating that the assumption of constant values of k_i for each gray gas is reasonable for engineering applications, in which the problems usually involve uncertainties that can be much higher than the maximum deviations that were shown for the WSGG model.

The correlations obtained in this study consider that the combustion is stoichiometric. In order to compare the results for different concentrations from $p_{H_2O} = 0.1$ atm and $p_{CO_2} = 0.1$ atm for $p_{H_2O}/p_{CO_2} = 1.0$ and $p_{H_2O} = 0.2$ atm and $p_{CO_2} = 0.1$ atm for $p_{H_2O}/p_{CO_2} = 2.0$, results are presented for mixtures of $p_{H_2O} = 0.005$ atm and $p_{CO_2} = 0.05$ atm, $p_{H_2O} = 0.2$ atm

and $p_{CO_2} = 0.2$ atm, for $p_{H_2O}/p_{CO_2} = 1.0$, and $p_{H_2O} = 0.1$ atm and $p_{CO_2} = 0.05$ atm, $p_{H_2O} = 0.3$ atm e $p_{CO_2} = 0.15$ atm, for $p_{H_2O}/p_{CO_2} = 2.0$. The results are shown in Figs. 3 and 4.

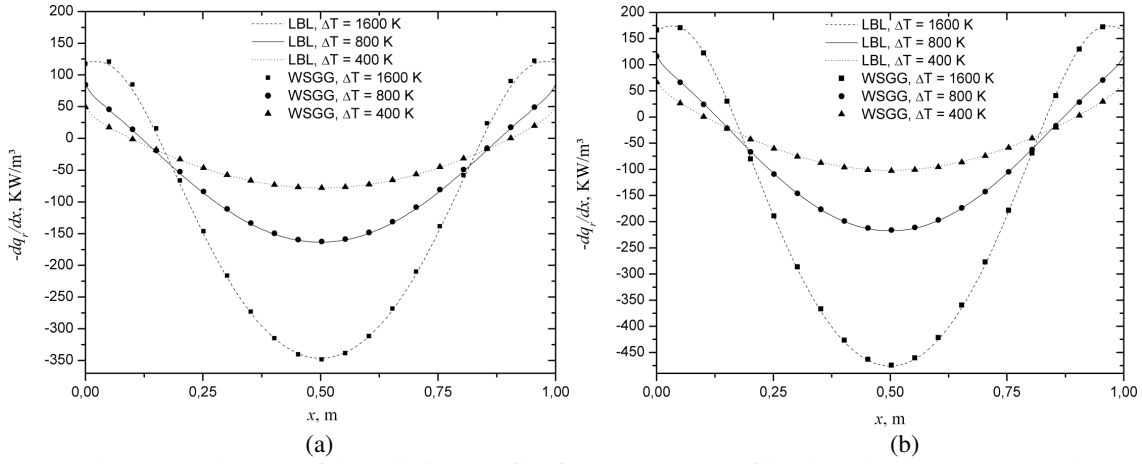


Figure 2 – Divergent of the radiative heat flux for temperature profiles given by Eqs. (12), (13) and (14). (a) $p_{H_2O}/p_{CO_2} = 1.0$. (b) $p_{H_2O}/p_{CO_2} = 2.0$.

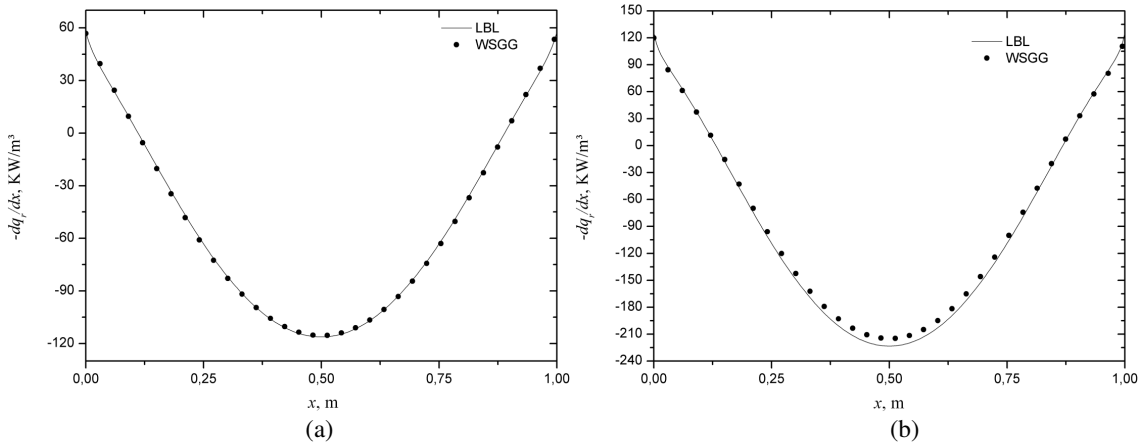


Figure 3 – Divergent radiative heat flux using Eq. (13) for $p_{H_2O}/p_{CO_2} = 1.0$. (a) $p_{H_2O} = 0.05$ atm and $p_{CO_2} = 0.05$ atm. (b) $p_{H_2O} = 0.2$ atm and $p_{CO_2} = 0.2$ atm.

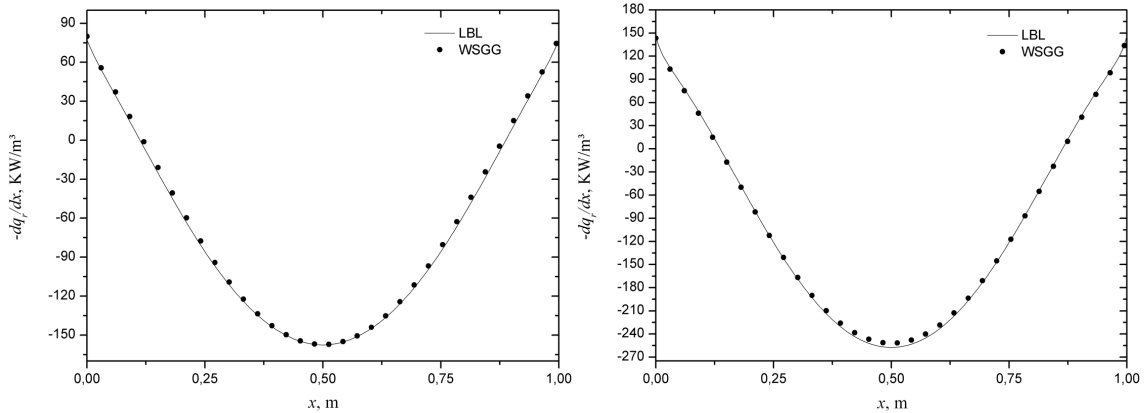


Figure 4 – Divergent radiative heat flux using Eq. (13) for $p_{H_2O}/p_{CO_2} = 2.0$. (a) $p_{H_2O} = 0.1$ atm and $p_{CO_2} = 0.05$ atm. (b) $p_{H_2O} = 0.3$ atm and $p_{CO_2} = 0.15$ atm.

The maximum errors obtained for $p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 1.0$ were 2.93% in Fig. 3 (a), and 6.56% in Fig. 3 (b). For $p_{\text{H}_2\text{O}}/p_{\text{CO}_2} = 2.0$, the maximum errors were 5.45% in Fig. 4 (a), and 3.7% in Fig. 4 (b).

It is possible to verify a good agreement in the results, indicating that the correlations can be used in different concentrations of H_2O and CO_2 , but always keeping the relation $p_{\text{H}_2\text{O}}/p_{\text{CO}_2}$ shown in this work and respecting the maximum values of $p_{\text{H}_2\text{O}}$ and p_{CO_2} that are presented above.

5. CONCLUSIONS

This paper shows the correlations for WSGG obtained. It is solved a radiation heat transfer problem between a medium composed of participating gases, comparing the WSGG and LBL results. The spatial integration of the radiative transfer equation was accomplished with the use of the discrete ordinates method. The simulations were carried out for different temperature profiles, and different uniform concentrations of the absorbing species. The proposed correlations showed good results when compared with LBL in both cases.

6. ACKNOWLEDGEMENTS

The first author thanks CAPES due to its financial support by means of a Master Degree scholarship.

7. REFERENCES

- Chu, H., Liu, F. and Zhou, H., 2011, "Calculations of gas thermal radiation transfer in one-dimensional planar using LBL and SNB models." *International Journal of Heat and Mass Transfer*, vol. 54 pp. 4736-4745.
- Denison, M.K.; Webb, B.W., 1991, "The Weighted Sum of Gray Gas Model for Arbitrary Solution Methods in Radiative Transfer". *Journal of Heat Transfer*, vol. 113, pp. 650-657.
- Galarça, M.M.; Mossi, A.; França, F.H.R., 2011, "A modification of the cumulative wavenumber method to compute the radiative heat flux in non-uniform media". *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 112, pp. 384-393.
- Gamache, R.R.; Hawkins, R.L.; Rothman, L.S., 1990, "Total internal partition sums in the temperature range 70–3000 K". *Atmospheric linear molecules*, *Journal of Molecular Spectroscopy*, vol. 142, pp. 205-219.
- Hottel, H.C., Sarofim, A.F., 1967, "Radiative Transfer". McGraw-Hill, New York, United States of America, 520p.
- Levenberg, K., 1944, "A Method for the Solution of Certain Non-linear Problems in Least Squares". *Quarterly of Applied Mathematics*, vol. 2, pp. 164-168.
- Marquardt, D.W., 1963, "An Algorithm for the Least-Squares Estimation of Nonlinear Parameters". *SIAM Journal of Applied Mathematics*, vol. 11, pp. 431-441.
- Maurente, A., Vielmo, H.A., França, F.H.R., 2007, "A Monte Carlo implementation to solve radiation heat transfer in non-uniform media with spectrally dependent properties". *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 108, pp. 295-307.
- Modest, M.F., 2003, "Radiative Heat Transfer". Academic Press, San Diego, California, United States of America, 822p.
- Mossi, A., Galarça, M.M., Vielmo, H.A. and França, F.H.R., 2011, "The accuracy of the radiative heat transfer gas models in non-isothermal and non-homogeneous media with soot". *Proceedings of the 21th Congress of Mechanical Engineering*, Natal, RN.
- Rothman, L.S., Gordon, I.E., Barber, R.J., Dothe, H., Gamache, R.R., Goldman, A., Perevalov, V.I., Tashkun, S.A., Tennyson, J., 2010, "HITEMP, the high-temperature molecular spectroscopic database". *Journal of Quantitative Spectroscopy and Radiative Transfer*, vol. 111, pp. 2139-2150.
- Siegel, R. and Howell, J., 2002, "Thermal Radiation Heat transfer". Taylor and Francis, New York, United States of America, 868p.
- Smith, T.F., Shen, Z.F., Friedman, J.N., 1982, "Evaluation of Coefficients for the Weighted Sum of Gray Gases Model". *Journal of Heat Transfer*, vol. pp. 104-602-8.

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