INFLUENCE OF SOOT PARTICULATE MEDIUM IN RADIATION HEAT TRANSFER USING GRAY GAS MODEL

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Abstract. *The design accuracy involving combustion processes indicate energy savings and lower pollutants emission. Being the radiation heat transfer dominant, the thermal model requires a very accurate modelling for gases, taking into account all the spectral properties. On the other hand, the particulate medium (soot) present in the emissions shows spectral properties with subtle variations and easy determinations. Thus, most simplistic spectral models solve the modeling of soot. This paper presents a radiative heat transfer solution in a one-dimensional slab formed by a participating medium composed by CO_2, H_2O and soot. It is considered the Line-by-Line solution and Gray Gas (GG) model to solve the participating medium. The contribution of this work is to demonstrate the soot spectral dominance properties in high concentrations and the possibility to use simple spectral models in combustion problems where we have the situation of particulate medium dominance. In addition, are proposed correlations for the GG model based on HITEMP 2010 database.*

Keywords: *Radiation heat transfer, Participating Medium, Gray Gas, Soot.*

1. INTRODUCTION

A deep understanding of the heat transfer is essential to propose the optimization of the system design for thermal efficiency and pollution control. Mathematical models involving combustion process have been extensively studied in the last thirty years, but still with important simplifications. Different operating parameters influence the combustion and heat transfer processes, and this makes the modeling very difficult. The radiation heat transfer was probably the last energy mode of heat transfer studied by the scientific community, mainly by the nature and the complexity of the formulation. In most general form, the equations include differential and integral systems, so exact solution of the problem is not feasible in most of the real engineering systems. With presence of gases and soot, a complete modeling process represents a significant mathematic effort. Many combustion processes generate gases such as carbon dioxide and water vapor, whose radiative properties show a very complex dependence on the wavelength, where the difficulty is related to determining this radiative properties of the medium, which depends on the participating species, the thermodynamic state and the wavelength.

The approach of thermal radiation in combustion processes is found in Klason *et al.* (2008), which applies some spectral methods of solution, such as GG (Gray Gas) and SLW (Spectral Line Weighted-Sum-of-Gray-Gases), compared with experimental data. This paper shows that a good determination of chemical reactions depends on a good determination of the temperature field, however, nothing is discussed about the radiant properties of the participating media, and nothing is concluded about the presence of soot. Results considering the concentration of soot are presented by Bressloff (1997), using the WSGG model, and shows that with the increase of soot the WSGG solution approaches the TP (Total Property) solution. Similarly, Borjini *et. al.* (2007) using the WSGG (Weithted Sum of Gray Gases) model, compares different concentrations of soot in a 3D geometry, using different temperature profiles. Demarco *et. al.* (2011) also uses a medium composed of CO_2, H_2O and soot, and using different methods of spectral modeling (SNB, FSK, SLW and WSGG) compares the maximum and average errors for different concentrations of soot. However, no one of the authors compare the results using Line-by-Line (LBL) solutions, which represent the exact one. Using the LBL solution, Mossi *et al.* (2011) compares results of the mixture H_2O, CO_2 and soot using GG, WSGG and CW (Cumulative Wavenumber) models, but uses the database HITEMP 2008 and their relationships to the GG and WSGG spectral models come from a different database, which also adds a mistake, demonstrated by Chu *et al.* (2011). Situations involving combustion of liquids, such as kerosene (Byun and Seung, 2007), and solids, such as coal (Marakis et. al., 2000; Eriksson and Golriz, 2005), have significant presence of particulate. Many studies try to compare different spectral models for these situations, but there is no agreement about the best model to use.

This paper presents the solution of the radiative heat transfer in a participating medium that is composed of two gases, CO_2 and H_2O, as well as soot. The medium is contained between two infinite parallel plates, and so the physical geometry is one-dimensional. The objective is to investigate the soot concentration importance to modeling the participating medium. While the soot has spectral properties with linear variation, the gases have a complex variation of their spectral properties. It is known that for gas modeling a detailed method is required. However, for the soot a simple model is capable to solve the problem. This fact indicate that using a simple spectral model, like Gray Gas model, is possible to obtain satisfactory results in situations with high soot concentration. The solution of the system of equations will be accomplished with the discrete ordinates method (DOM). For the spectral solution, it will be used the GG model for the gases and soot. Three temperature profile functions are used and various soot concentrations are tested to show the influence in the radiation heat transfer.

2. MATHEMATICAL MODELING

The discrete ordinates method is based on a discrete representation of the directional dependence of the radiation intensity. It is an extension of the method of two fluxes, in which the directional solid angles are divided into more than two hemispheres. The solution to the transport problem is found by solving the radiative transfer equation (RTE) for a set of discrete directions with a total solid angle of 4π.

2.1. General Relations

To demonstrate the method employed in this paper, it is first necessary to present the general equation of the radiative heat transfer. The equation of radiative transfer for a medium with absorption, emission and scattering intensities, over a path *S* in the direction of *dω*, is:

$$\frac{dI}{dS} = \kappa(S) I_b(S) - [\kappa(S) + \sigma(S)] I(S,\omega) + \frac{\sigma(S)}{4\pi}\int_0^{4\pi} I(S,\omega_i)\,\Phi(S,\omega,\omega_i)\cdot d\omega_i \tag{1}$$

where I is the radiation intensity and κ the absorption coefficient, σ the scattering coefficient and Φ the phase function.

To obtain the intensity along a direction *S*, the boundary condition must be specified. The boundary condition expresses the radiation intensity that leaves the surface of the wall, and corresponds to the sum of the intensities that are emitted and reflected, where the reflected intensities are written as a function of incident intensity. For a gray and diffuse surface, originating from $S = 0$, it takes the following form:

$$I_S(S=0) = \varepsilon_w I_{b,w} \tag{2}$$

where ε is the emissivity, I_b refers to the blackbody intensity and the subscript w refers to the wall.

The solution is given by first order equations and requires only one boundary condition (for the emitted intensity). With the discrete ordinates method, the equations are solved for a series of n directions, and the integrals solved by this method are solved with a numerical quadrature, given by:

$$\int_{4\pi} I(S)\ d\omega = \sum_{i=1}^{n} w_i\ I_i(S) \tag{3}$$

where w is the weight associated with the quadrature in the *S* direction. The equations are approximated by a series of n equations, and the accuracy of the integral solution is given by the number of directions. As can be seen, the Eq. 1 have an integral in the last term, referring to the scattering mechanism, and can be solved using an approximation of the angular quantities by a sum of weights.

The equation for the medium with absorption and emission, without scattering, takes the following form:

$$\mu\frac{dI_\eta}{dS} = \kappa_\eta I_{b,\eta} - \kappa_\eta I_\eta \tag{4}$$

where μ is the directional cosine and the subscript η refers the wavenumber. For the boundary condition, one finds:

$$I_\eta(S=0) = \varepsilon_{w,\eta} I_{b,w,\eta} \tag{5}$$

In the studied case, the scattering term (present in the general thermal radiation equation) is not considered, since soot is a very small particle and its scattering is of minor significance in comparison to its absorption and emission (Modest, 2003). In the same way, the gaseous species in the mixture do not scatter radiation. Normally, the intensities for the blackbody are separated from each particle, because the particle temperatures are not in the flame one. In cases having very small soot particle these temperatures are equal and the equation can be simplified. In the DOM method, the equation system are solved for a set of directions $0 < \mu < 1$ and $0 < \mu < -1$, which will lead to a system of equations for the positive and negative directions.

Considering the finite difference method, it leads to a system of equations given by:

$$I_\eta^+ = \frac{\Delta x \ \kappa_\eta \ I_{b,\eta} + \mu \ I_{x-1,\eta}}{\mu + \Delta x \ \kappa_\eta} \tag{6}$$

$$I_\eta^- = \frac{\Delta x \ \kappa_\eta \ I_{b,\eta} + \mu \ I_{x+1,\eta}}{\mu + \Delta x \ \kappa_\eta} \tag{7}$$

It is important to note that for the LBL solution the Eqs. (6) and (7) must be solved integrating for each wavenumber, while for the GG solution is made by the average absorption coefficients.

With the intensities determined, the directional integration can be performed. The radiation flux, in W/m^2, in a medium or a surface is given by:

$$q''_{R,\eta,l}(S) = 2\pi \ w_l \ \mu_l \left\lfloor I_{\eta,l}^+(S) - I_{\eta,l}^-(S) \right\rfloor \tag{8}$$

The volumetric radiative heat source, or the divergence of radiation flux, in W/m^3, can also be determined:

$$\dot{q}_{R,\eta,l}(S) = 2\pi \ \kappa_\eta \ w_l \left\lfloor I_{\eta,l}^+(S) + I_{\eta,l}^-(S) \right\rfloor - 4\pi \ \kappa_\eta \ I_{\eta,b}(S) \tag{9}$$

where the intensities for Eqs. (11) and (12) must have all direction additions:

$$q''_R(S) = \sum_l \int_\eta q''_{R,\eta,l}(S) \tag{10}$$

$$\dot{q}_R(S) = \sum_l \int_\eta \dot{q}_{R,\eta,l}(S) \tag{11}$$

3. RADIATIVE PROPERTIES

The medium analyzed is composed of a gas mixture (CO_2 and H_2O) as well as soot. Different databases can be used to obtain the gases properties, such as HITRAN, HITEMP or CDSC. In this work the gases has the spectral properties established with the HITEMP 2010 database, according Rothman *et. al.* (2010). As known, the absorption coefficient of gases has a strong variation along the wavenumber, and the properties change with the thermodynamic state. Different databases have considerable variation in the properties, which makes it important to use the same database for all the simulations, to avoid errors due to database and getting the real property of the spectral model.

According to Siegel and Howell (2002), for engineering applications, the absorption coefficient of the gases can be obtained using the Lorentz collision profile, given by:

$$\kappa = NC_\eta = N \sum_i \frac{S_i}{\pi} \frac{\gamma_i}{(\eta - \eta_i)^2 + \gamma_i^2} \tag{12}$$

where N is the molar density, 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, that is defined by:

$$\gamma_i = \left(\frac{T_{ref}}{T}\right)^n Y_S \gamma_{self,i} + \left(\frac{T_{ref}}{T}\right)^{0,5} (1 - Y_S) \gamma_{air,i} \tag{13}$$

where Y_s is the molar fraction, T is the temperature, γ_{self} is the self-broadening, γ_{air} is the air broadening half-width.

On the other hand, the absorption coefficient for the soot varies linearly with the wavenumber. According to Hottel and Sarofim (1967), it is obtained by the following relation:

$$\kappa_\eta = C \ f_v \ \eta \tag{14}$$

where f_v is the volumetric fraction and C is a constant which was assigned a value 7.0. Siegel and Howell (2002) proposed different values for different fuels: 6.3 for oil flames, 4.9 for propane, 4.0 for acetylene, and 3.7–7.5 for coal flames.

Since the soot particles are very small, they can be considered as having the flame temperature, and then emit thermal radiation in a continuous spectrum of the infrared region. Some experiments show that the emission of soot is higher than the emission of gases from combustion. In order to determine the radiative properties of a cloud of soot, it is necessary to know its concentration and distribution.

3.1. Line-by-Line Solution

The line-by-Line solves the equation radiant transport in all wavenumbers in which the absorption coefficient is given by the spectrum in different parts of the geometry, considering the local thermodynamic state of gas. Thus, the equation to be solved for each direction *S* is:

$$\frac{\partial I_\eta}{\partial S} = \kappa_\eta I_{b,\eta} - \kappa_\eta I_\eta \tag{15}$$

3.2. Gray Gas Model

In the gray gas model, it is considered that the absorption coefficient κ (m^{-1}) is independent of the wavenumber, is determined as an average term of issuance:

$$\kappa = \frac{\int_\eta \kappa_\eta I_{b,\eta} d\eta}{\int_\eta I_b d\eta} \tag{16}$$

Some correlations are proposed based on the HITEMP 2010 for the gas and the soot properties (Eq. 14), using the Eq. 16. These correlations can be applied directly taking care only with the partial pressure of the components. The Table 1 shows the values.

Table 1. Absorption coefficients for use in gray gas model

Specie	Absorption coefficients, in cm^{-1} atm^{-1}		
CO_2 and H_2O	$\kappa = c_0 + c_1 T + c_2 T^2 + c_3 T^3 + c_4 T^4 + c_5 T^5$		
	c_i	CO_2	H_2O
	c_0	-7.36885×10^{-1}	7.73541×10^{-1}
	c_1	4.77678×10^{-3}	-2.05946×10^{-3}
	c_2	-7.57382×10^{-6}	2.36822×10^{-6}
	c_3	5.29649×10^{-9}	-1.39663×10^{-9}
	c_4	-1.75069×10^{-12}	$4.13422.\times10^{-12}$
	c_5	2.23907×10^{-16}	-4.86695×10^{-17}
Soot	$\kappa = C\, f_v\left(c_0 + c_1 T + c_2 T^2\right)$		
	c_i	Soot	
	c_0	-245.85633	
	c_1	3.31161	
	c_2	-3.78198×10^{-4}	

Valid only for temperatures between 400 and 2400 K.

For both models (LBL and GG) is proposed a solution based on the sum of the partial absorption for each gas, or particulate. In LBL solution this occurs for each wavenumber, or in the case of GG correlations, for each κ coefficient. In the end, the total absorption will be given according to the equation:

$$\kappa_\eta = Y_{CO_2} \cdot \kappa_{\eta,CO_2} + Y_{H_2O} \cdot \kappa_{\eta,H_2O} + Y_{soot} \cdot \kappa_{\eta,soot} \tag{17}$$

or

$$\kappa = Y_{CO_2} \cdot \kappa_{CO_2} + Y_{H_2O} \cdot \kappa_{H_2O} + Y_{soot} \cdot \kappa_{soot} \tag{18}$$

where *Y* is the specie concentration.

4. RESULTS AND DISCUSSION

In the present work, the geometry will be the same for all cases, that is, two flat plates with an emissivity of 1.0 (black walls) and separated by a distance of 1.0 m. The gases concentrations and soot will be uniform between the slabs. This approximation is reasonable when studying, for example, the heat transfer in the exhaust of combustion chambers, in which the medium components are fairly well mixed. 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. To study non-isothermal medium, it will be considered three different temperature profiles, given by Eq. 19, 21 and 20, where the temperature varies of 400 K up to 1800 K. The purpose is to reproduce a range of temperatures, which normally happens in combustion processes.

$$T(x) = 400 + 1400\, sen\,(\pi\, x / L)^2 \tag{19}$$

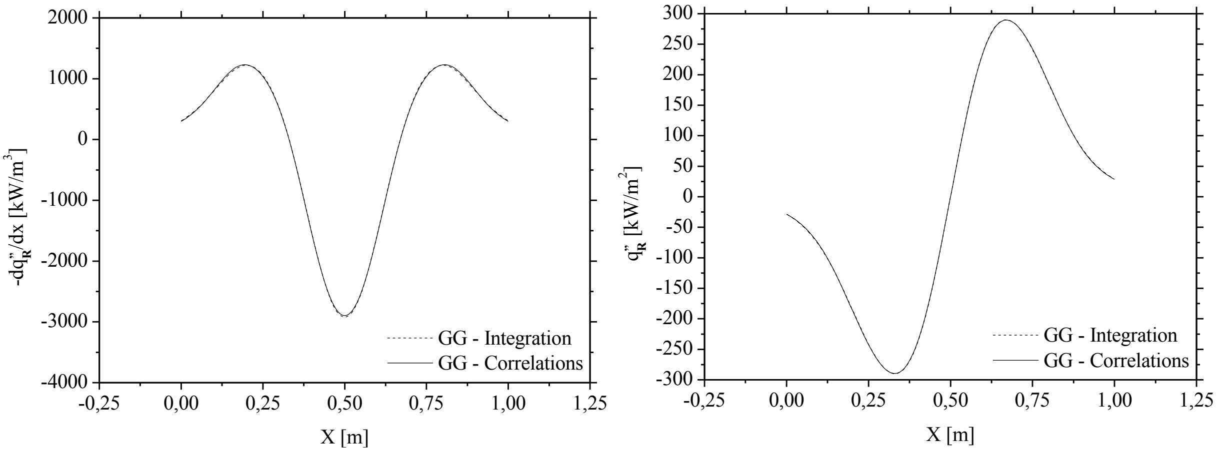
$$T(x) = 400 + 1400\, sen\,(2\pi\, x / L)^2 \tag{20}$$

$$T(x) = \begin{cases} 920 + 880\, sen\,(2\pi\, x / L)^2\,, & x \le L/4 \\ 1100 + 700\cos\left(\left|\dfrac{x}{L/4} - 1\right|\right), & x > L/4 \end{cases} \tag{21}$$

The average error is proposed by a integration in the values of the radiative heat source along the proposed geometry. The error of the source term is expressed for the entire domain: the difference from the LBL solution is integrated across the domain and compared with the integrated absolute value of the GG source term, according Eq. 21.

$$Error_{\text{average}} = \frac{1}{\int_0^S \left|\dot{q}_{R,LBL}\right| ds} \int_0^S \left|\left(\dot{q}_{R,LBL} - \dot{q}_{R,GG}\right)\right| ds \tag{22}$$

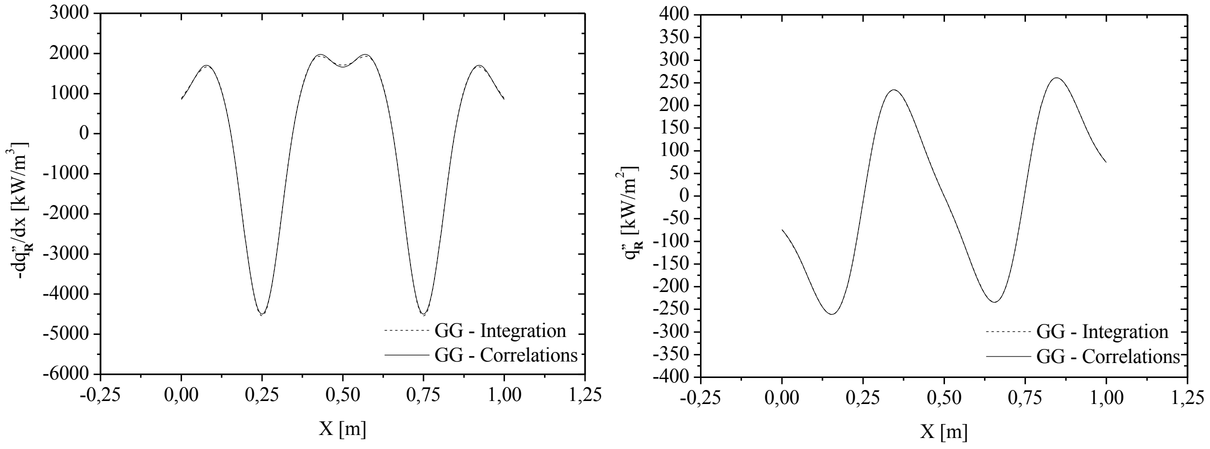
All the following simulations will consider the same concentrations of 20% H_2O, 10% CO_2 and 70% of inert medium to enable a comparative basis, gradually adding fractions of soot. For the analysis of soot is varying the volumetric fraction concentrations from 1×10^{-7} up to 1×10^{-5}. In a first analysis, is checked the proposed correlations presented in Table 1. These results are shown in Fig. 1 to 3, using the three proposed temperature profiles for medium composed by 20% H_2O, 10% CO_2 and soot volumetric fraction equal 1×10^{-6}.



(a) (b)

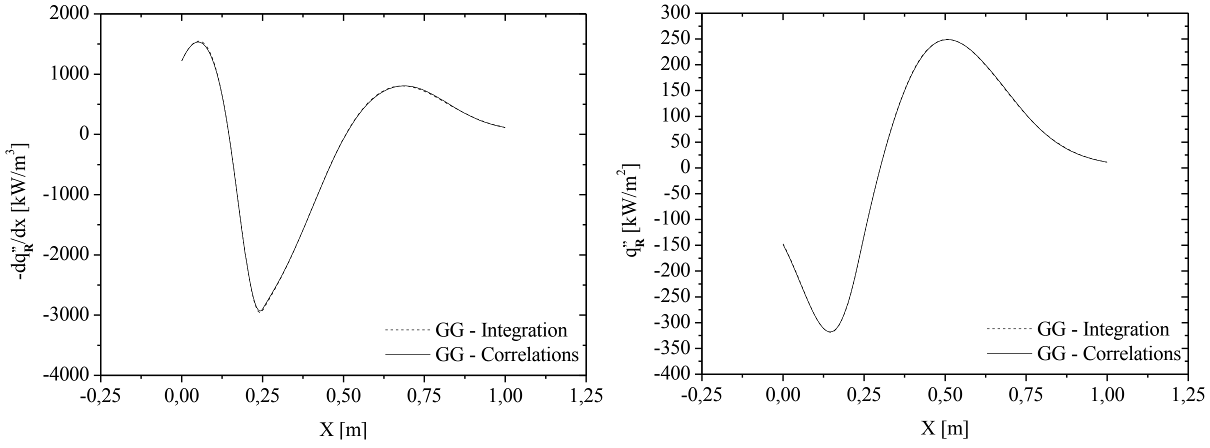
Figure 1 – Radiative volumetric heat source and radiative heat flux using Eq. (19) temperature profile for 20% H_2O, 10% CO_2 and 1×10^{-6} soot volumetric fraction. (a) Radiative volumetric heat source. (b) Radiative heat flux.

With satisfactory results, the proposed correlations can be used directly without the necessity of use a spectral integration for the gases or a wavenumber relationship, in the case of the soot. Despite the proposed correlations, all the results generate in the present work are implemented with the mathematical Eqs. (15) and (16), to obtain a better solution. The results obtained using Eq. (20) for the temperatures are shown in Figs. 4 to 6, varying the soot volumetric fraction. The presented results shown clearly the approximation of results using LBL and GG model solutions.



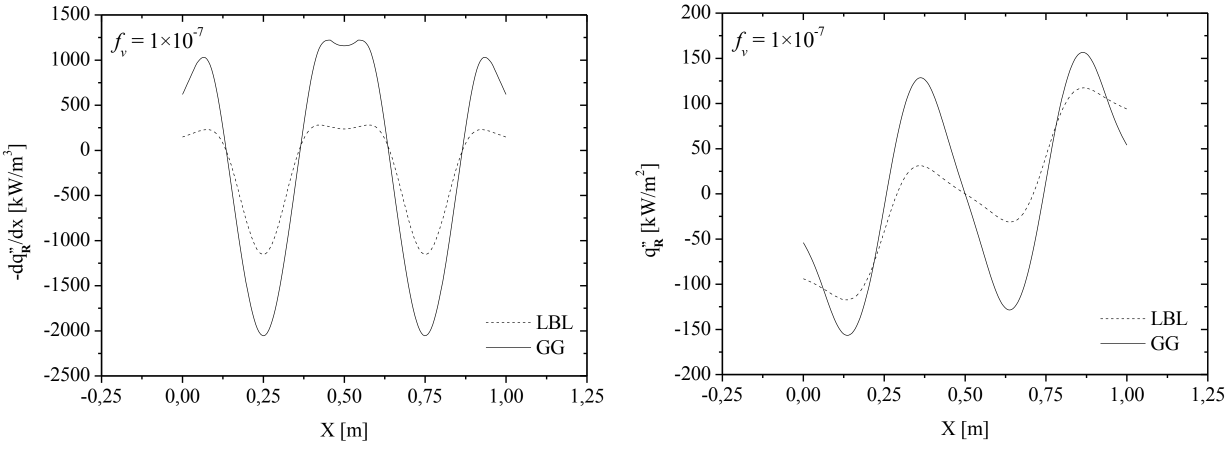
(a) (b)

Figure 2 – Radiative volumetric heat source and radiative heat flux using Eq. (20) temperature profile for 20% H_2O, 10% CO_2 and 1×10^{-6} soot volumetric fraction. (a) Radiative volumetric heat source. (b) Radiative heat flux.



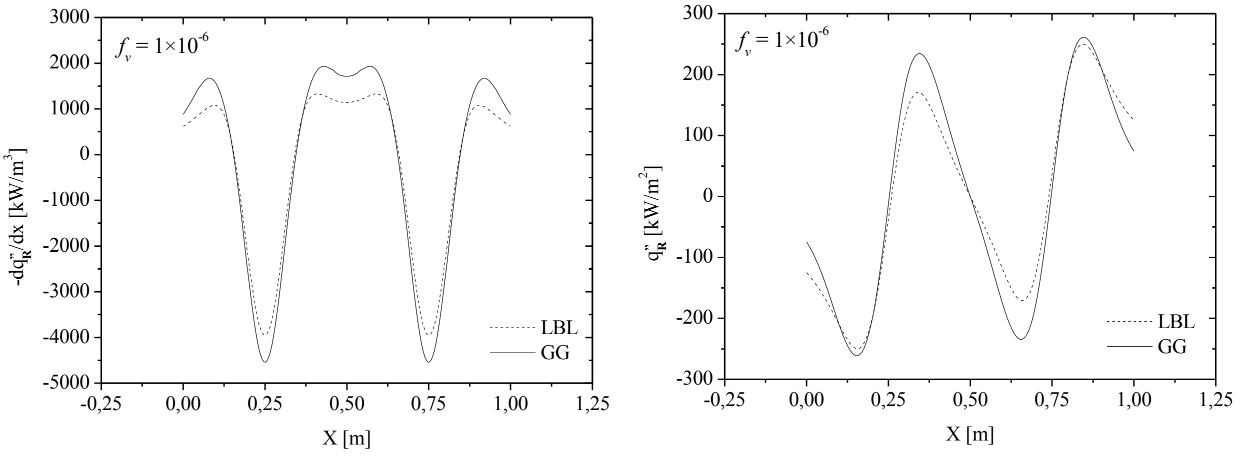
(a) (b)

Figure 3 – Radiative volumetric heat source and radiative heat flux using Eq. (21) temperature profile for 20% H_2O, 10% CO_2 and 1×10^{-6} soot volumetric fraction. (a) Radiative volumetric heat source. (b) Radiative heat flux.



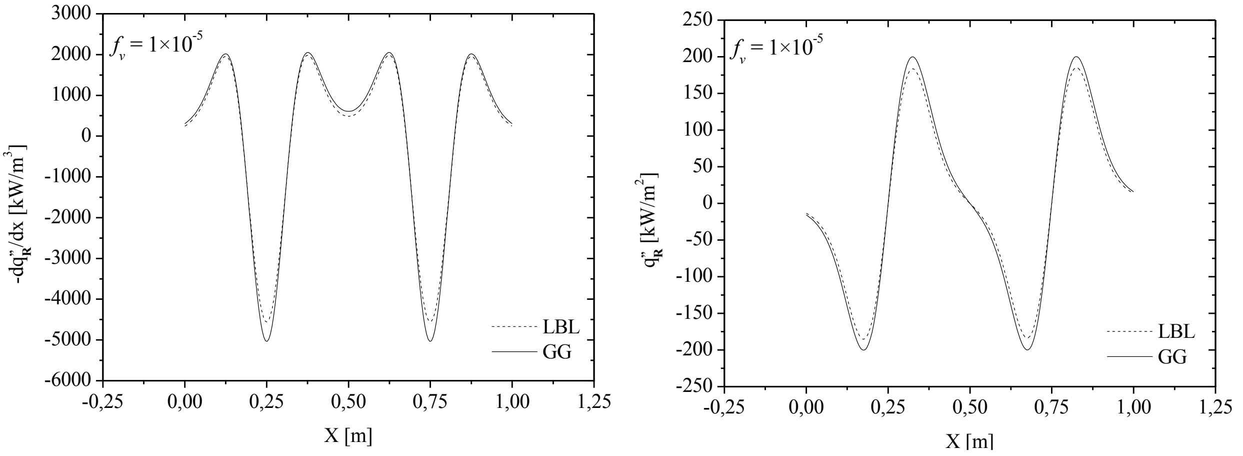
(a) (b)

Figure 4 – Radiative volumetric heat source and radiative heat flux using Eq. (20) temperature profile. (a) Radiative volumetric heat source. (b) Radiative heat flux.



(a) (b)

Figure 5 – Radiative volumetric heat source and radiative heat flux using Eq. (20) temperature profile. (a) Radiative volumetric heat source. (b) Radiative heat flux.



(a) (b)

Figure 6 – Radiative volumetric heat source and radiative heat flux using Eq. (20) temperature profile. (a) Radiative volumetric heat source. (b) Radiative heat flux.

Results are presented for the divergence of the radiative heat flux, in units of W/m^3, which is one of the main parameters in the computation of radiation in participating media. It corresponds to the net rate of energy that leaves each element of volume in the medium per unit of volume, and is equivalent to the radiative heat source, but with opposite sign: $dq''_R/dx = -\dot{q}_R$. When the divergence of the radiative heat flux is positive, it means that the element loses energy due to radiation. The divergence of the radiative heat flux is expected to be positive in the higher temperature regions of the medium and negative in the lower temperature regions of the medium.

In order to extend the comparisons, the results for all temperature profiles and average errors based on Eq. (22) are shown in Table 2. With Table 2 results we can check that as proposed for a medium composed only for gases the error is extremely high, however, the presence of particulates in an average concentration of 1×10^{-6} is already possible to use spectral models not so detailed, and from this concentration of particles, the GG model produces satisfactory results.

Table 2: Average error for the proposed cases, using radiative heat source values.

Soot	*Temperature profile*		
	Eq. 18	Eq. 19	Eq. 20
f_v	*Error (%)*	*Error (%)*	*Error (%)*
0	314,56	281,28	292,89
1×10^{-7}	142,64	152,72	122,38
1×10^{-6}	21,47	28,45	18,04
1×10^{-5}	6,16	8,12	7,81

5. CONCLUSIONS

This paper solved a radiation heat transfer problem between a medium composed of participating gases (water vapor and carbon dioxide) and soot. The spatial integration of the radiative transfer equation was accomplished with the use of the discrete ordinates method. For the participating medium, it was applied LBL solution and GG model. The simulations was proposed with different temperature profiles, and different concentrations of soot were tested. In addition, correlations were established for the implementation of GG. The proposed correlations showed good results when compared with the ratio based on spectral integration. The results presented show that the GG used to the gas spectral properties does not produce good results, with an average error over 300%. However, with the addition of soot occur a decreasing of the average error, which for high volume fractions of soot, the error decrease so much, leads to conclude that the GG results are satisfactory. This shows that the predominance of soot on the gas, with linear variation spectral properties, a simple spectral modeling model is enough. In addition, all temperature profiles presented show the same trend with a small variation in the average error, which shows that temperature variations have little influence on the model.

6. ACKNOWLEDGEMENTS

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