RADIATION HEAT TRANSFER IN COAL COMBUSTION PROCUCTS

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Abstract. *This paper presents a radiative heat transfer solution in a one-dimensional slab formed by a participating medium considering coal combustion products. The coal combustion products include ash, soot and participating gases such as* CO_2 *and* H_2O*, which at high temperature can have a strong influence on the heat transfer through emission, absorption, and scattering of radiation. The radiative transfer equation is solved by the discrete ordinates method. The walls are considered gray emitters and absorbers. It is considered the weighted-sum-of-gray-gases (WSGG) model and correlations based on the Rayleigh scattering theory to solve the system. The major contribution of this work is to demonstrate the importance of considering the absorption and scattering of the various products in the combustion process, where these mechanisms of energy transport are often neglected.*

Keywords: *Radiation heat transfer, Absorption, Emission, Scattering, Participating Medium.*

1. INTRODUCTION

Several processes of power generation use coal. Examples include fluidized bed and reactors with the combustion of pulverized or gasified coal. 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. For example, a fluidized bed combustor has operating temperatures in the range of about 1100 K, particulate size of 1.0 to 3.0 mm and a complex motion of particles (Smoot and Smith, 1985). In methane combustion the temperature reaches up to 2000 K and the complete combustion of the products generate only CO_2 and H_2O (Bidi *et al.*, 2008). Pulverized coal combustion leads to temperatures around 1500 K, and forms absorption gases (CO_2 and H_2O) and particles such as fly ash and soot (Reinaldo, 2004). Works relating heat transfer in fluidized bed were developed by Zhou *et al.* (2009 and 2010), who examined the thermal characteristics of the fluidized beds in different conditions. In the study, it was considered the heat transfer by convection and conduction between the particles and thermal radiation. To determine the thermal radiation, it was considered the Stefan-Boltzmann law and the medium was not considered participant. Marakis *et al.* (2000) presented a medium consisting of coal, char and fly ash, and, using the zonal method, obtained good results for the wall heat flux in a cylindrical coal-fired.

It is important to known that heat transfer coefficients increase with increasing temperature and this fact has been attributed to increased thermal conductivity of gases and mainly to the increase of heat transfer by radiation, which is neglected at low temperatures, but in cases of combustion, the radiation heat transfer can account for most of the total heat transfer. 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. Some of the common simplifications include the consideration of the medium as non-participating or acting as gray, that is, with the radiative properties independent of the wavelength.

The presence of two phases in the mixtures is very common in thermal engineering, for example, the heat exchange between gas and particles in pulverized coal combustion engines, solid rocket fuel, etc. In two phase combustion, containing gas and particulate (fly ash and soot), the radiation phenomenon is not yet fully established, since the phenomenon is dependent on the particle density, size distribution, temperature and pressure, which cannot be determined with precision in such complex systems. Another difficulty is related to determining the radiative properties of the medium, which depends on the participating species, the thermodynamic state and the wavelength. The various particles found in combustion processes can be classified as carbonaceous (soot), and non-carbonaceous (fly ash); the absorption or scattering values can be found in Modest (1993) and in some studies for particular kinds of coal, as in Menguç *et al.* (1994) and Im and Ahluwalia (1990).

With presence of various gases, soot and other particles, a complete modeling process represents a significant mathematic effort. By difficulties in manipulate the spectral dependence of radiation, several authors adopt the gray gas model. Many combustion processes generate gases such as carbon dioxide and water vapor, whose radiative properties show a very complex dependence on the wavelength, so the gray gas model is not a good approximation. The weighted-sum-of-gray-gases (WSGG) model represent the real gas by a few gray gases, usually three gases, and can lead to much better results that the gray gas model. Some studies indicate an approximate error of about 5-10% when comparing the WSGG model and line-by-line (LBL) benchmark integration. An example of application of the WSGG model in a medium containing soot and fly ash can be found in Bressloff (1999) and Yu *et al.* (2000). In another work, showing only the influence of the concentration and properties of particles, Hua *et al.* (2005) used a three-dimensional model and showed the properties of coal, sand, ash and limestone in the combustion and Eriksson and Golriz (2005) used correlations for a fluidized bed. Hua *et al.* (2005) studied the influence of particle properties (diameter, composition and optical properties) in the heat transfer by radiation, and confirmed the influence on heat transfer between the bed and walls.

The present 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 particulates, such as composed of fly ash and soot. The medium is contained between two infinite parallel plates, and so the physical geometry is one-dimensional. The objective is to investigate the interaction between the components and verify their influence in different configurations. 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 WSGG method for the gases and gray particles. A parabolic temperature function is used and various particles concentrations are tested to show the medium 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. The integrals over the solid angle are approximated by a numerical quadrature scheme.

2.1. General Relations

To demonstrate the method, 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, over a path *S* in the direction of *dω*, as shown Figure 1, is:

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

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

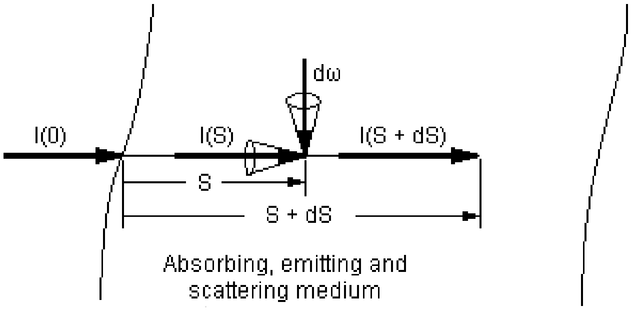


Figure 1 – Geometry for derivation of equation of radiative heat transfer.

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:

$$I_S(S=0) = \varepsilon_p \cdot I_{b,p} + \frac{1-\varepsilon_p}{\pi}\int_0^{2\pi} I_{s'}\cdot d\omega \tag{2}$$

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

The solution is given by first order equations and requires only one boundary condition (for the emitted intensity). If the scattering is present, the problem must be solved iteratively. With the discrete ordinates method, the equations are solved for a series of *n* directions, and the integrals solved by this method are transformed into a numerical quadrature, given by:

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

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 above equations 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 takes the following form:

$$\mu\frac{dI}{dS} = a_\lambda \cdot I_b - \left[a_\lambda + \sigma_\lambda\right]\cdot I + \frac{\sigma_\lambda}{4\pi}\sum_n w_n \cdot I_n \cdot \Phi_{mn} \tag{4}$$

where μ is the directional cosine, I_n refers to the incoming intensity, the subscripts m and n correspond to the outgoing and incoming radiation intensity, for each angular direction and each solid angle. For an isotropic scattering the phase function term (Φ_{mn}) is equal 1.0, so would not be considered. The above equations are valid for a gray or non gray-medium with scattering. For the boundary condition, one finds:

$$I(S=0) = \varepsilon_p I_{b,p} + \frac{1-\varepsilon_p}{\pi}\sum_n \mu_n w_n I_n \tag{5}$$

Considering that the medium is composed of particles absorbing, emitting and scattering, with a mixture of gases, the radiative transfer equation can be written as:

$$\mu\frac{dI}{dS} = \left(a_g \cdot I_{b,g} + a_a \cdot I_{b,a} + a_s \cdot I_{b,s}\right) - \left(a_g + a_a + a_s + \sigma_a\right)\cdot I + \frac{\sigma_a}{4\pi}\sum_n w_n \cdot I_n \tag{6}$$

where the subscripts g, a and s refer to gas, fly ash and soot, respectively. The scattering term is not considered for soot, since soot is a very small particle and its scattering is of minor significance in comparison to its absorption and emission (Modest, 1993). 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 the flame temperature. In cases such as 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. Figure 2 shows the positive and negative directions in the DOM method.

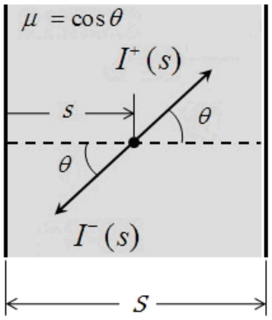


Figure 2 - Physical computation domain of the radiation intensities in the forward and backward directions.

Considering the relations given by the WSGG method, it leads to a system of equations given by:

$$I_p^+ = \frac{\Delta S \cdot \left(\kappa_g \cdot a_{g,i} + \kappa_a \cdot a_a + \kappa_s \cdot a_s\right)\cdot I_b + \mu \cdot I_{p-1} + \Delta S \cdot \frac{\sigma_a}{2}\sum_n w_n \cdot I_n}{\mu + \Delta S \cdot \left(a_{g,i} + a_a + a_s + \sigma_a\right)} \tag{7}$$

$$I_p^- = \frac{\Delta S \cdot \left(\kappa_g \cdot a_{g,i} + \kappa_a \cdot a_a + \kappa_s \cdot a_s\right) \cdot I_b + \mu \cdot I_{p+1} + \Delta S \cdot \frac{\sigma_a}{2} \sum_n w_n \cdot I_n}{\mu + \Delta S \cdot \left(a_{g,i} + a_a + a_s + \sigma_a\right)} \tag{8}$$

where I_p refers to intensity location, and I_n refers to incoming intensities. The coefficients κ (Eq. 9) and $\alpha_{g,i}$ refers to the WSGG method, which will be presented in the next section (Table 1).

$$k_i(T) = b_{i,1}T(i)^0 + b_{i,2}T(i)^1 + b_{i,3}T(i)^2 + b_{i,4}T(i)^3 \tag{9}$$

In this paper, it is found that the weighting factors for particles have the same functional form as for the gaseous species, corresponding to the local temperature and partial pressure. Consequently, if the gas and particles are in thermal equilibrium, it leads to:

$$k_g(T) = k_a(T) = k_s(T) \tag{10}$$

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:

$$q_l'' = 2\pi w_l \mu_l \left[I^+ - I^-\right] \tag{11}$$

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

$$\dot{q}_l = 2\pi a w_l \left[I^+ + I^-\right] - 4\pi a w_l I_b \tag{12}$$

Where the intensities for Eq. 11 and 12 must have all direction additions.

3. RADIATIVE PROPERTIES

The medium analyzed is composed of a gas mixture (CO_2 and H_2O) as well as fly ash and soot. The gaseous medium has the spectral properties established with the weighted-sum-of-gray-gases (WSGG) model. The concept of the WSGG model was first presented by Hottel and Sarofim (1967), where it was proposed in the framework of the zonal method. Later, Modest (1993) proved its applicability to other methods such as discrete ordinates method (DOM). In this method (WSGG), the full absorption coefficients are replaced by a number of gray gases. The total radiative flux is then found by a sum of all partial radiative flux multiplied by temperature dependent weighting factors. The absorption values for each spectral band and its corresponding weighting values can be found in the work of Galarça *et al.* (2008), which updated of the correlations proposed by Smith *et al.* (1982) with the use of more recent gas data. The used parameters are showed in Table 1.

Table 1. Emissivity coefficients for a mixture P_w/P_c=2 (Galarça *et al.*, 2008).

i	$a_{g,I}$ (1/atm·m)	$b_{i,1}\times10^1$	$b_{i,2}\times10^4$ (K^{-1})	$b_{i,3}\times10^7$ (K^{-2})	$b_{i,4}\times10^{11}$ (K^{-3})
1	0.517	2.801	3.244	-1.299	0.712
2	9.559	2.003	1.869	-2.394	5.454
3	161.988	1.240	-1.086	0.283	-0.114

To establish the properties of the particles, it is important to know that when an electromagnetic wave interacts with a medium containing particles, the radiation intensity can be altered by absorption and scattering. Considering the scattering to be the same for each particle, which are assumed to be of spherical shape, the scattering can be defined by two dimensionless parameters: the complex index of radiation, m, and the size parameter, x:

$$m = n - i \cdot k \tag{13}$$

$$x = \frac{2 \cdot \pi \cdot d}{\lambda} \tag{14}$$

where d is the diameter and λ is the wavelength.

Equation (13) sets the properties of the coal particle, where it indicate a real part, *n*, which varies little in the infrared and is relatively heavy for certain kinds of coal (anthracite, bituminous and lignite), while the absorption index, *k*, can vary strongly across the spectrum and for each kind of coal. Equation (14) sets the size of the particle: when x<<1 the particles are small; when x>> 1 the particles are considered large.

3.1. Soot and Fly Ash Radiation Properties

Soot particles are produced in rich burning fuel or parts of the rich fuel flame. Soot particles are small and spherical, having an approximate size ranging from 0.005 µm to 0.08 µm, having a size of 0.3 µm in extreme cases. Soot particles can appear in clouds with a concentration in the flame in the range of 10^{-4} to 10^{-6} %.

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, shape and distribution, as well as its optical properties, which depend on the chemical composition and porosity of the particles.

If soot particles are so small that one (size parameter) can apply Rayleigh theories, then the absorption coefficient is equal to the extinction coefficient and it will neglect scattering. The coefficients can be obtained from the relation:

$$a_s = \frac{3.72 \cdot f_v \cdot C_o \cdot T}{C_2} \tag{15}$$

in which:

$$C_o = \frac{36\pi \cdot n \cdot k}{\left(n^2 - k^2 + 2\right)^2 + 4 \cdot n^2 \cdot k^2} \tag{16}$$

where C_2=0.014388 m·K, which is the second function of Planck constant, n=1.85 and k=0.22. The function is an average of Rosseland and Planck functions (Modest, 1993). It is important to know that the equation can be applied only in very small particles of soot, and the extinction coefficient increases for larger particles.

For large particles (x>>1), the efficiency factor of absorption can be considered equal to the emissivity coefficient and the scattering efficiency factor equal to the coefficient of reflectivity. Under these conditions, one finds:

$$a_a = \frac{3 \cdot f_v \cdot Q_{abs}}{2 \cdot d_p} \tag{17}$$

$$\sigma_a = \frac{3 \cdot f_v \cdot Q_{sca}}{2 \cdot d_p} \tag{18}$$

where f_v is the fraction volumetric, Q_{abs} and Q_{sca} are the absorption and scattering efficiency, respectively, d_p is the particle diameter, that in the case of fly ash correspond a range 0.1 up to 100 µm, and, in the present work, it will set 50 µm. The emissivity corresponds to 0.8 and the reflectivity to 0.2 for a fly ash particle.

4. RESULTS AND DISCUSSION

For the solution of the system of equations, the geometry will be the same for all cases, that is, two flat plates with an emissivity of 0.8 and separated by a distance of 1.0 m. The gases concentrations, fly ash 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.

An initial verification of the solution is made by a comparison with results presented in Yu *et al.* (2000). In this problem, the medium is composed of a mixture of 40% H_2O and 20% CO_2 (as with the other cases, the remaining is composed of inert species, such as nitrogen or oxygen), the walls temperatures are 400 K (X=0) and 1500 K (X=1m), the medium temperature is equal to 1250 K, and the soot has a volumetric fraction of 1×10^{-6}. The soot properties are the same as those presented in Section 3.1. The result is presented in Figure 3. As seen, there is a satisfactory comparison between the results generated through LBL integration (Yu *et al.*, 2000) and the WSGG solution of the present work. It can be observed some discrepancy close to the walls, however the much smaller computational time required by the WSGG model makes the proposed solution a viable alternative for engineering calculation of radiative heat transfer in medium containing soot, and is used for the next results in this paper.

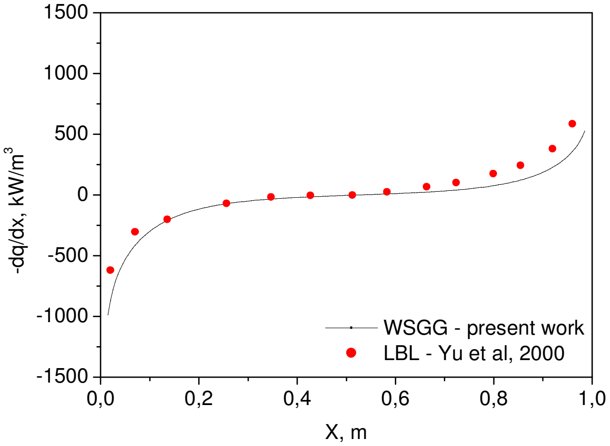
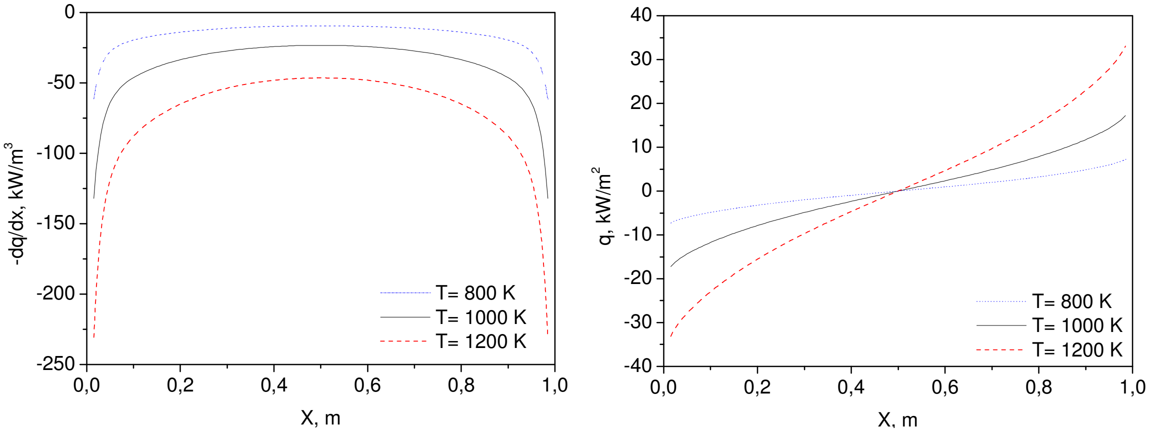


Figure 3. Comparison between LBL solution and the WSGG model. $T_{x=0}$=400K, $T_{x=1}$=1500K, T_m=1250K.

A further test of convergence can be demonstrated by analyzing a case with a medium composed of a mixture 20% H_2O, 10% CO_2 (70% of inert medium) and both walls at a temperature of 400 K, with a uniform medium temperature taking the values of 800, 1000 and 1200 K. The results can be seen in Figure 4, which demonstrates the increase in the divergence of the radiative heat flux (or the volumetric radiative heat source) and the radiative heat flux with the increase in the medium temperature.



(a)

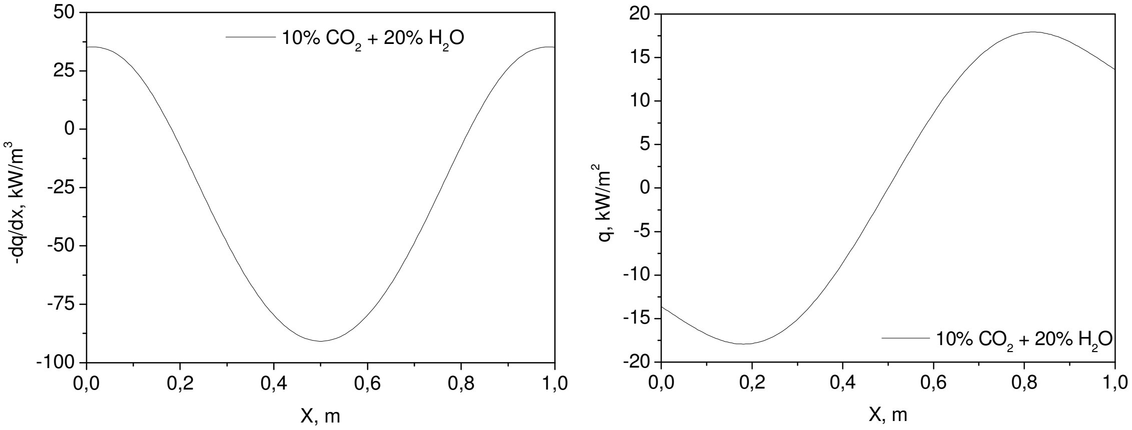
(b)

Figure 4. Different temperatures analysis for a mixing medium 20 %H_2O and 10% CO_2.
(a) Divergent flux. (b) Heat flux.

To study non-isothermal medium, it will be considered a parabolic temperature profile, given by Eq. 19, where the walls have a temperature of 400 K and the temperature in the medium achieves a maximum of 1200 K in the center. The purpose is to reproduce a range of temperatures, which normally happens in combustion processes.

$$T(x) = 1200 - 800(2x/L - 1)^2 \tag{19}$$

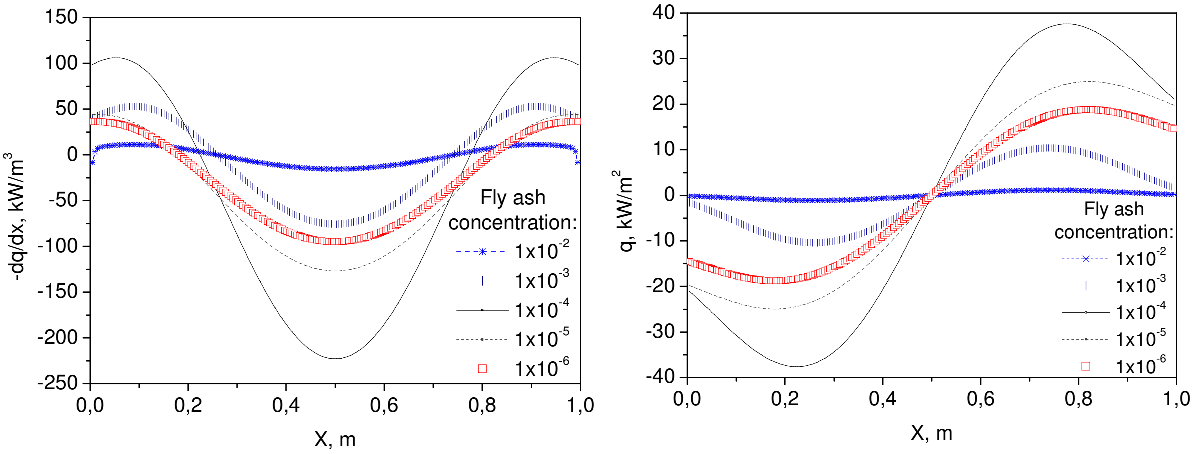
In a first analysis, it is analyzed the radiative heat flux and its divergence with parabolic temperature profile, using a gaseous medium composed of 20% H2O, 10% CO2 and inert gas. The results are shown in Figure 5. In the center, where the medium presents the maximum temperature, there is a loss of energy with a radiation exchange with the colder regions of the domain. This is indicated by the negative value of the divergence of the radiative heat flux (radiative heat source). As for the medium closer to the wall, the divergence of the radiative heat flux becomes positive, indicating that the energy received from the high temperature gas in the center is larger than the energy lost to the wall. These results will be interesting for comparison with other cases, when soot and fly ash are added to the medium, since the behaviors in Figure 5 will be modified.



(a) (b)

Figure 5. Parabolic temperature profile analysis for a mixing medium with 20% H_2O and 10% CO_2.
(a) Divergence of the radiative flux. (b) Radiative heat flux.

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 and fly ash. The temperature distribution corresponds to Eq. (19). A first simulation is performed by adding only fly ash, and varying the volumetric fraction concentrations from 1×10^{-2} to 1×10^{-6}. The imposed concentration of fly ash is considerably large, but the purpose is to verify extreme situations of fly ash excess, such as in some cases where fly ash is injected to reduce the temperature in certain parts of the equipment. The results using fly ash can be seen in Figure 6. The objective is to analyze the influence of the absorption and scattering particles in the radiation heat transfer process.

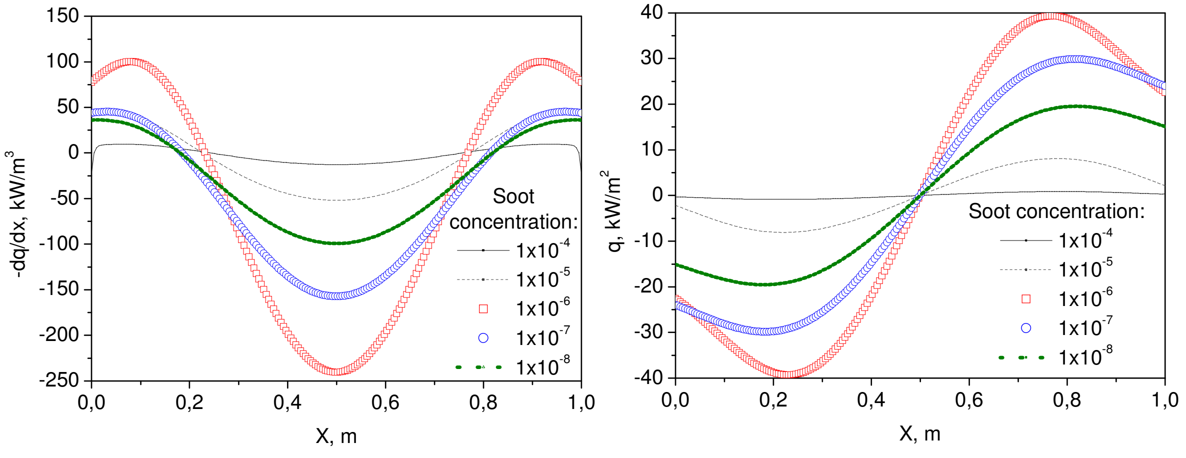


(a) (b)

Figure 6. Medium with a parabolic temperature profile. Fly ash with volumetric fraction ranging 1×10^{-2} up to 1×10^{-8}.
(a) Radiative volumetric heat source. (b) Radiative heat flux.

Comparing the solutions shown in Figure 6 with those in Figure 5, where the only participating species are water vapor and carbon dioxide, adding fly ash in the beginning leads to a considerable increase in the radiation heat transfer, since the particles have a much higher absorption coefficient. However, a further increase in the volumetric fraction of fly ash leads to a situation where scattering prevents the radiation to escape from the high temperature regions, decreasing the radiation heat transfer.

Next, it is considered a medium with soot. It is analyzed soot with volumetric fractions concentrations taking values of 1×10^{-4}, 1×10^{-5}, 1×10^{-6}, 1×10^{-7} and 1×10^{-8}. With a medium without scattering, the radiation heat transfer behaves like the previous case (Figure 6), increasing up to a certain concentration and then decreasing. The continuing increase in the concentration of the soot leads to a medium with a very high absorption coefficient or, alternatively, very high optical thickness. As such, it prevents the radiation energy from escaping from the center towards the wall.

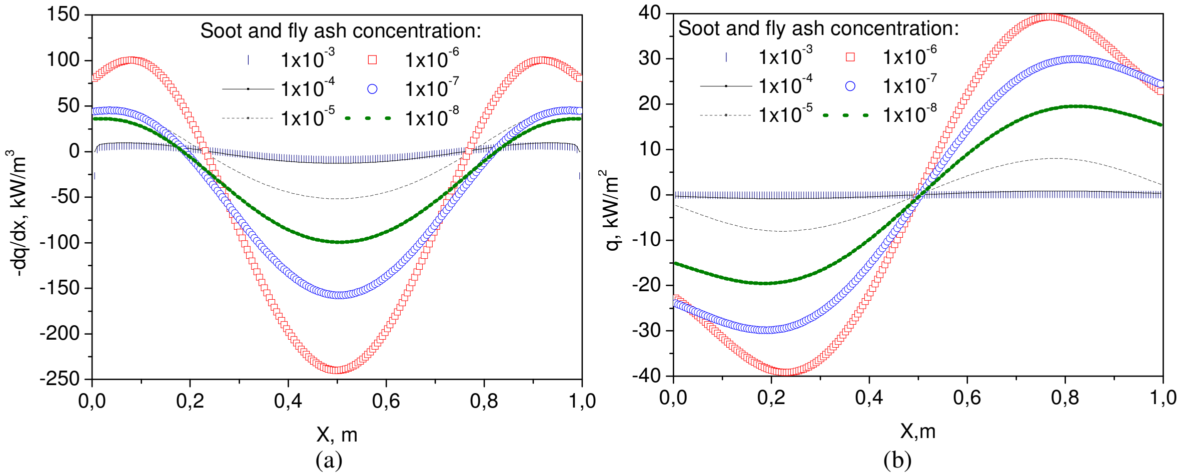


(a)

(b)

Figure 7. Medium with a parabolic temperature profile. Soot volumetric fraction variation 1×10^{-4} until 1×10^{-8}. (a) Radiative volumetric heat source. (b) Heat flux.

Finally, a medium consisting of a mixture of H_2O, CO_2, fly ash and soot is considered. The volumetric fractions concentrations of both soot and fly ash take the values of 1×10^{-3} to 1×10^{-8}. The different concentrations ranges used in both simulations were chosen because they were the ones that showed the most significant increases and decreases in the radiation intensity for each particular case. The results can be seen in Figure 8.



(a)

(b)

Figure 8. Medium with a parabolic temperature profile. Fly ash and soot with volumetric fraction 1×10^{-3} up to 1×10^{-8}. (a) Radiative volumetric heat source. (b) Heat flux.

Making a closer inspection in the heat transfer from the medium to the wall, the heat flux is of 12.5 kW/m^2 for a medium composed of only water vapor and carbon dioxide (Figure 5). On the other hand, with a volumetric fraction of 1×10^{-7} of soot and fly ash, the radiative heat flux on the wall raised to a value close to 25 kW/m^2, or twice as much, showing the importance of the particulate medium. However, for high concentrations of soot and ash, the divergence of the radiative heat flux approached to zero, indicating a clear that the technique to add particles in a medium to increase the heat transfer should search for a point of maximum.

5. CONCLUSIONS

This paper solved a radiation heat transfer problem between medium composed of participating gases (water vapor and carbon dioxide), fly ash and ash, as can be found in the combustion of coal particles, and two parallel plates. The spatial integration of the radiative transfer equation was accomplished with the use of the discrete ordinates method. As for the spectral integration, it was applied WSGG model for the participating gases and correlations proposed in literature for the fly ash and soot. The solution methodology was successfully verified with a comparison with another work in the literature. The example cases attempted to show the effect of increasing the concentration of the fly ash and soot in the radiation heat transfer. As seen, adding the particles can lead to a considerable increase in the heat transfer when compared to the case where the medium is composed of only water vapor and carbon dioxide, due to the increase in the absorption coefficient of the medium. However, a further increase in the concentration of the particles can lead to a situation where the radiation emitted in the high temperature regions of the medium cannot escape towards the wall due to scattering and absorption in the medium, and therefore decreasing the heat transfer. This indicates that the technique to add particles in the medium should search for an optimum point. For future works, it suggested to use more advanced spectral methods, such as CW (Cumulative Wavenumber) and SLW (Spectral Line Weighted Sum of Gray Gases), to obtain results of higher accuracy, and to consider two and three-dimensional effects.

6. ACKNOWLEDGEMENTS

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