

APPLICATION OF THE WSGG MODEL TO DETERMINE THE INFLUENCE OF SOOT PARTICLES ON RADIATION IN THE COMBUSTION PROCESS OF A 320MW POWER PLANT BOILER

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Abstract. *In this paper, the WSGG (Weighted Sum of Gray Gases) model is applied to determine the influence of soot particles on radiation in the combustion process of a 320MW power plant boiler, using Computational Fluid Dynamics (CFD). Through a mathematical formulation, involving the conservation equations, devolatilisation models, the EBU Arrhenius model, NO_x formation mechanisms, soot particle model, the Discrete Transfer Radiation Model and a special radiation model, combining the WSGG with soot particles, four different cases are analysed. The results generated by the simulations show that there are perceptible differences in the outlet temperature between the cases, specially in the first one (Case GG – Gray Gas) compared to the others (Case A – WSGG; Case B – WSGG including soot model; and Case C – the most complete case, which integrates the soot particles coefficients in the global WSGG model). However, the values of the wall heat flux and the wall radiative heat flux are similar for the first and the fourth cases. Finally, the simulations indicate that if the WSGG model is used without considering soot particles, errors can be generated in the results, while that the GG model can be used in several applications similar to the one reported in this paper, with acceptable compromising of results' accuracy.*

Keywords: *WSGG, Soot, Pulverized Coal, CFD, Combustion.*

1. INTRODUCTION

Regarding global demand for energy, coal is one of the most important fuels, and its main application is the combustion in power plants for electricity generation. It is well known that global coal reserves already exceed the reserves of natural gas and oil, so that coal will still be used for a longtime, and study ways to improve the process is necessary. Several authors have been using CFD codes to study boiler's arrangements, pulverized coal boilers, and different types of burners such as low NO_x burners (Kurose et al., 2004). Others studied variations in operating conditions, such as moisture content and size of coal particle (Bosoaga et al., 2006; Al-Abbas et al., 1993). Choi and Kim (2009), using a FLUENT code in a study similar to this paper, simulated a pulverized coal burner, with tangential burn, of a 500MW boiler. In the same line, Asotani et al. (2008), also using a FLUENT code, studied the behavior of cloud ignition of pulverized coal in a 40MW boiler. Silva et al. (2010), using a commercial CFD code, studied the behavior of pulverized coal combustion in the same boiler studied in this paper, in order to validate the model, simulate the operation and identify possible factors of inefficiency. In a study made by Crnomarkovic et al. (2013), models of WSGG - Weighted-Sum-of-Gray-Gases were applied to the radioactive properties of the gas phase and were compared with the results in numerical investigation of a furnace of pulverized coal with tangential burners, using the zonal method solution of radiant heat transfer.

Many authors, who used WSGG model, adopted for soot-gas mixtures the same coefficients of the pure gas phase, although this practice could input significant errors, since the soot and gas coefficients have different dependences (Felske and Charalampopoulos, 1982). Among all parameters, which have influence in the combustion modeling, this paper seeks to analyze the WSGG model applied to a real boiler of a 320MW power plant, considering and comparing the influence of high levels of soot particles, present in the pulverized coal combustion. It was adopted the coefficient calculation proposed by Makhviladze et al. (1999).

2. MATHEMATICAL FORMULATION

The model adopted in this paper considers that the coal particle is composed of raw coal, ash and moisture. First occurs the drying reaction, then the devolatilization in two stages (Ubhayakar, 1976), yielding methane and carbon monoxide as an approximation, as shown in Fig. 1.

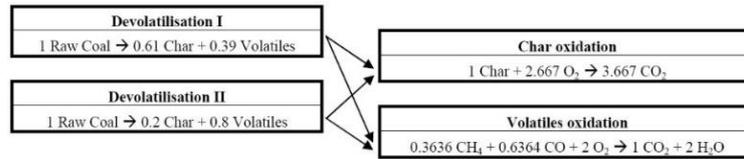


Figure 1. Basic chemical reactions of the raw coal (Ubhayakar, 1976).

After the drying and devolatilization processes, the oxidation of gas-phase is modeled by global chemical reactions “Methane Air WD2” (Westbrook and Dryer, 1981). In the first stage, the methane is burned, forming carbon monoxide and water vapor as products. In the second stage of global reaction, the carbon monoxide, together with the carbon monoxide resulting from the coal devolatilization, reacts with oxygen to form carbon dioxide, completing the mechanism. The process scheme is shown in Fig.2.

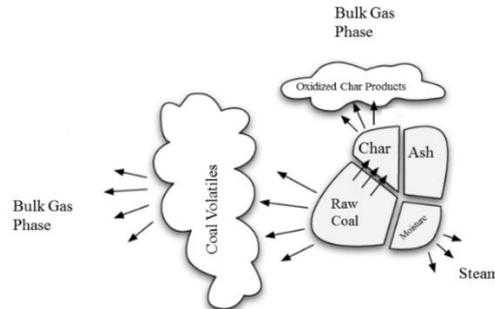
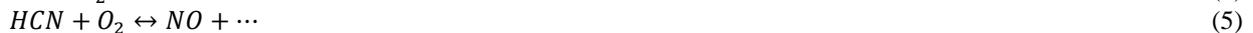


Figure 2. Coal particle devolatilization.

The chemical reactions rates were provided by the combined Eddy Break Up – Arrhenius model (Kuo, 2005; Turns, 2000). It was assumed that 98% of the nitrogen in the fuel is converted instantaneously to HCN, and the complement is not oxidized. For the NO_x formation, this paper considers three main formation paths. The first is the Thermal NO and, due to the very high activation energy of the reaction described in Eq. (1), about 319 kJ/kmol, it is the predominant source of NO_x in gas flames, and occurs only at temperatures above 1800 K. The process develops in two steps, also known as Zeldovich’s mechanism. According to Kuo (2005), this mechanism has a chain nature and because of its slow rate of NO formation compared with the fuel oxidation reactions, it can be decoupled from the fuel oxidation process. Therefore, the simplification is presented below.



Fenimore (1970) discovered that at temperatures lower than 1800 K, hydrocarbon flames present high levels of NO that could not be formed by thermal mechanism. This second mechanism was termed as prompt NO, and its predominant reactions are presented below. The activation energy lies about 75 to 92 kJ/kmol (for Eq. 4), which is much lower than thermal’s activation energy for the reaction presented in Eq. (1).



De Soete (1974) proposed a single reaction through Eq. (6), where W_{NO} is the molar mass and W is the mean molar mass of the mixture. The Arrhenius coefficients depends on the fuel, so the author proposed the values given by Eqs. (7) and (8).

$$S_{NO,prompt} = W_{NO} \cdot k_{prompt} [O_2]^{\frac{1}{2}} \cdot [N_2] \cdot [Fuel] \cdot \left(\frac{W}{\rho}\right)^{3/2} \quad (6)$$

$$A_{prompt} = 6,4 \cdot 10^6 \left[\frac{1}{s}\right] \quad (7)$$

$$T_{A,prompt} = 36510 [K] \quad (8)$$

The third path of NO formation occurs under fuel rich conditions. In this case, there is no enough oxygen to oxidize all the fuel, so the excess of the last one leads to a reduction of NO. For CH₄ and coal, the stoichiometric reaction is:



According to Ansys Inc (2004), the reaction rate will be fuel dependent. For coal volatiles and methane, the reaction rate is:

$$R_{return} = 2,72 \cdot 10^6 [s^{-1}] \cdot \frac{W}{\rho} \cdot [NO] \cdot [Fuel] \cdot \exp\left(\frac{-9460[K]}{T}\right) \quad (10)$$

2.1 Mass and species conservation

The first equation solved is the mass and species conservation. Assuming a multicomponent fluid, the equation is solved for velocity, pressure, temperature and other quantities of the fluid. The influence of the multiple components is felt only through property variation by virtue of differing properties for the various components. Each component has its own equation for conservation of mass. After Favre-averaging, the species conservation equation can be expressed, in tensor notation, as:

$$\frac{\partial(\bar{\rho}\bar{U}_j\bar{Y}_i)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\rho D_i + \frac{\mu_t}{Sc_t} \right) \frac{\partial \bar{Y}_i}{\partial x_j} \right) + \bar{S}_i \quad (11)$$

where $\bar{U}_j = \sum (\tilde{\rho}_i \tilde{U}_{ij}) / \bar{\rho}$ is the mass-averaged velocity field [m/s], $\tilde{\rho}_i$ is the specific mass [kg/m³]; the \bar{U}_j term represents the velocity vector and \tilde{U}_{ij} is the ij component's mass-averaged velocity. The relative mass flux is given by $\rho_i(\tilde{U}_{ij} - \bar{U}_j)$. The mass fraction of the i component is defined as $\bar{Y}_i = \tilde{\rho}_i / \bar{\rho}$, and the sum of all component mass fractions is equal to one.

2.2 Momentum conservation

The second equation to solve is the momentum conservation of the fluid, which is given by:

$$\frac{\partial(\bar{\rho}\bar{U}_i\bar{U}_j)}{\partial x_j} = -\frac{\partial p^*}{\partial x_j} \delta_{ij} + \frac{\partial(\mu_{eff} \frac{\partial \bar{U}_i}{\partial x_j})}{\partial x_j} + \frac{\partial \bar{u}}{\partial x_i \partial x_j} + \bar{S}_U \quad (12)$$

where $\mu_{eff} = \mu + \mu_t$; the term μ is the mixture dynamic viscosity and μ_t is the turbulent viscosity, defined as $\mu_t = C_\mu \rho k^2 / \varepsilon$. The term p^* is the modified pressure, C_μ is an empirical constant of the turbulence model, which is equal to 0.09. The variable \bar{p} is the time-averaged pressure of the gaseous mixture, and δ_{ij} is the Krönecker's delta function; \bar{S}_U is the source term. The Boussinesq model was used to represent the buoyancy force due to density variations, and the $k-\omega$ model was adopted to provide the turbulence in the flow (Wilcox, 1988).

2.3 Energy conservation

Considering the transport of energy due to diffusion of each chemical species, the energy equation is the third one that needs to be solved. This equation can be written as:

$$\frac{\partial(\bar{\rho}\bar{U}_j\bar{h})}{\partial x_j} = \frac{\partial}{\partial x_j} \left(k_{con} \frac{\partial \bar{T}}{\partial x_j} + \sum_i^{Nc} \tilde{h}_i \left(\rho D_i + \frac{\mu_t}{Sc_t} \right) \frac{\partial \bar{Y}_i}{\partial x_j} + C_p \frac{\mu_t}{Pr_t} \frac{\partial \bar{T}}{\partial x_j} \right) + \bar{S}_{rad} + \bar{S}_{rea} + \bar{S}_T \quad (13)$$

where \bar{T} , \bar{h} and C_p are the average temperature, enthalpy and specific heat of the mixture. The term \bar{Y}_i is the averaged mass fraction of the i -th chemical species, k_{con} is the thermal conductivity of the mixture, Pr_t is the turbulent Prandtl number; \bar{S}_{rad} , \bar{S}_{rea} and \bar{S}_T represent the sources of thermal energy due to the radiative transfer, the chemical reactions and energy sink. The term \bar{S}_{rea} can be written as:

$$\bar{S}_{rea} = \sum_\alpha \left[\frac{h_i^0}{MM_i} + \int_{\bar{T}_{ref,i}}^{\bar{T}} C_{p,i} d\bar{T} \right] \bar{R}_i \quad (14)$$

where h_i^0 and $\bar{T}_{ref,i}$ are the formation enthalpy and the reference temperature of the i -th chemical species. To complete the model, the density of the mixture can be obtained from the ideal gas state equation (Kuo, 2005; Turns, 2000), $\bar{\rho} = p \bar{MM} (\bar{R}\bar{T})^{-1}$, where p is the combustion chamber operational pressure, which is here set equal to 1 atm, and \bar{MM} is the mixture molecular mass. The mentioned equations are valid only in the turbulent core, where $\mu_t \gg \mu$. Close to the wall, the conventional logarithmic law of the wall is used (Nikuradse, 1933).

2.4 The E-A (Eddy Break Up – Arrhenius) chemical reactions model

This paper assumes finite rate reactions and a steady state turbulent process to volatiles combustion. In addition, it was considered that the combined pre-mixed and non-premixed oxidation occurs in two global chemical reaction steps, and involving only ten species: O₂, CH₄, H₂, H₂O, Tar, HCN, HCO, NO_x, CO₂ and CO. The Tar composition considered was C_{3.878}H_{6.426}O_{3.561}. The formation and destruction rates are obtained through the combined Arrhenius-Magnussen model (Magnussen and Hjertager, 1976), called EBU-Arrhenius (Eaton et al., 1999). This model assumes high Reynolds and Damkohler numbers, and uses the Finite Rate Chemistry model and the Eddy Dissipation model. The EBU-Arrhenius assumes the lower result from these two models.

2.5 Soot model

According to Kuo (2005), the soot is solid carbonic particles that arises from combustion processes of liquid and solid fuels. The particle sizes can vary from 0.005 to 0.2 μm . The soot formation model used in this paper was proposed by Magnussen and Hjertager (1976). The model considers that the soot is formed from the fuel's gas phase, in two stages. The first is the nuclei formation, and can be described by Eq. (15), and the second stage represents the particle formation from the nuclei, which is given by the Eq. (16).

$$\frac{\partial(\bar{\rho}\bar{X}_N)}{\partial t} + \frac{\partial(\bar{\rho}\bar{u}_j\bar{X}_N)}{\partial x_j} = \left\{ \left(\bar{\mu} + \frac{\mu_t}{Pr_t} \right) \frac{\partial\bar{X}_N}{\partial x_j} \right\} + \tilde{S}_{nuclei,f} + \tilde{S}_{nuclei,c} \quad (15)$$

$$\frac{\partial(\bar{\rho}\bar{Y}_S)}{\partial t} + \frac{\partial(\bar{\rho}\bar{u}_j\bar{Y}_S)}{\partial x_j} = \left\{ \left(\bar{\mu} + \frac{\mu_t}{Pr_t} \right) \frac{\partial\bar{Y}_S}{\partial x_j} \right\} + \tilde{S}_{soot,f} + \tilde{S}_{soot,c} \quad (16)$$

The complete model can be divided in three different steps. First, comes the nuclei and soot particles formation, according to Tesner et al. (1971). This step can be expressed by the equation:

$$R_{n,f} = n_0 + (f - g) \cdot n - g_0 \cdot n \cdot N \quad (17)$$

where n_0 is the spontaneous nuclei formation rate, given in parts/m³.s. The term n describes the nuclei concentration, while f and g are, respectively, the linear ramification coefficient and the linear termination coefficient. The g_0 term is the termination coefficient of soot particles, and N represents the soot particle concentration. The n_0 term can be simplified to:

$$n_0 = a_0 \cdot c_f \cdot \exp\left(-\frac{E}{\Re T}\right) \quad (18)$$

In Eq. (18), a_0 is a constant equal to 1.16×10^{31} , c_f is the fuel mass concentration, E is the activation energy. \Re represents the universal gas constant and T is the absolute temperature.

The second step describes the nuclei and soot particles oxidation. The reaction rate can be written as:

$$R_{s,c} = A \cdot \bar{C}_s \cdot \left(\frac{\varepsilon}{k} \right) \quad (19)$$

The Eq. (19) is used in regions where the soot concentration is low, compared with the O₂ level. At the places where there is not enough oxygen, the soot particles should compete with the other species in the combustion process. Finally, in the third step, the model considers the turbulence effect over the reaction rates. The rates are determined using the (EDC) - Eddy Dissipation Concept, proposed by Magnussen and Hjertager (1976).

2.6 Radiative transfer equation

The radiation intensity can be expressed as:

$$\frac{dI_v(r,s)}{ds} = -(K_{av} + K_{sv}) \cdot I_v(r,s) + K_{av}I_b(v,T) + \frac{K_{sv}}{4\pi} \int_{4\pi} dI_v(r,s')\Phi(s,s')d\Omega' + \dot{S} \quad (20)$$

where v is the frequency, and r and s are the position and direction vectors, respectively. The S term represents the radiation path; K_{av} is the media absorption coefficient, and K_{sv} is the scattering coefficient. The black body emission is given by I_b , and I_v represents the spectral radiation intensity. The solid angle and the phase-function for the scattering is given by Ω and Φ , respectively. There is also a source term, written as \dot{S} . In this paper it was adopted an isotropic scattering, since pulverized coal generates high levels of particles.

Among several methods to solve radiative equations, it was employed the Discrete Transfer Radiation Model (DTRM) (Carvalho et al., 1991). According to Filkoski (2010), this method presents coherent results and demands a relatively low computational effort, despite its limitations. This paper uses the DTRM model with 16 rays.

Generally, as a starting point to arrive at a tractable method for calculating radiative properties, the particles were assumed as spherical and homogeneous. In this paper, the heat transfer, from gas mixture to particle, considers that the particles are opaque bodies with emissivity equal to one (black bodies), and the Hanz-Marshall correlation was used to model the heat transfer coupling between the gas mixture flow and the particles (Ansys Inc., 2004).

2.7 WSGG - weighted-sum-of-gray-gases

The effect of the non-gray gaseous mixture was considered by original WSGG model proposed by Hottel and Sarofim (1967), which compares experimental data with equations, using the following correlation:

$$\varepsilon(pS) = \sum_{i=0}^{N_G} a_j(T)(1 - e^{-K_j p S}) \quad (21)$$

In the Eq. (21), K_j represents the absorption coefficient, a_j is the weighting coefficient of the j -th gray gas. The gray gases numbers are defined as N_G ; K_j is the absorption coefficient of the j -th gas. The WSGG model allows to write the absorption coefficients in the polynomial form, as follows:

$$a_j(T) = \sum_{k=0}^k b_{j,k} T^{k-1} \quad (22)$$

Several researchers proposed coefficients for the WSGG model in the last years. Dorigon et al. (2013) proposed new coefficients, adjusting the emittance curves by the LBL – Line-by-Line Integration method, using the HITEMP 2010 database (Rothman et al., 2010). The authors used 4 gray gases, and the coefficients proposed are shown in Tab.1:

Table 1. Coefficients for WSGG model (Dorigon et al., 2013).

j	$K_{g,j}$ [$m^{-1}atm^{-1}$]	$b_{g,j,1} \times 10^1$	$b_{g,j,2} \times 10^1$ [K^{-1}]	$b_{g,j,3} \times 10^7$ [K^{-2}]	$b_{g,j,4} \times 10^{11}$ [K^{-3}]	$b_{g,j,5} \times 10^{14}$ [K^{-4}]
1	0.192	0.5617	7.8440	-8.5630	4.2460	-7.4400
2	1.719	1.4260	1.7950	-0.1077	-0.6972	1.7740
3	11.370	1.3620	2.5740	-3.7110	1.5750	-2.2670
4	111.016	1.2220	-0.2327	-0.7492	0.4275	-0.6608

2.8 WSGG – soot

Many studies have proposed different coefficients for WSGG model in gas-soot mixtures. Some authors used for the soot, the same coefficients of the gas phase, although this practice could input significant errors, since the soot and gas coefficients have different dependences (Felske and Charalampopoulos, 1982). This paper models the gas-soot mixture coefficients using the method proposed by Makhviladze et al. (1999), which combines both coefficients. The total number of gases is given by $N_{total} = (N_g + 1) \times N_s$, where N_g is the number of gases generated by the classic WSGG model, and N_s is the number of soot gases. The number 1 represents the radiation transparent window. In pure gas mixtures, these windows do not affect radiation, but in soot-gas mixtures, the emission and absorption in this spectral region should be considered (Centeno, 2016). Therefore, in this paper there are ten gases for the WSGG. The final absorption coefficients are given by Eq. (23), while the Eq. (24) expresses the final weighting coefficients.

$$k_{n,m} = k_{g,m} + k_{s,m} \quad (23)$$

$$a_{n,m} = a_{g,m} \times a_{s,m} \quad (24)$$

Cassol et al. (2014) proposed coefficients for soot that were adopted in this paper. They are presented in Tab. 2.

Table 2. Coefficients for soot in WSGG model (Cassol et al., 2014).

j	$K_{g,j}$ [$m^{-1}atm^{-1}$]	$b_{g,j,1} \times 10^1$	$b_{g,j,2} \times 10^1$ [K^{-1}]	$b_{g,j,3} \times 10^7$ [K^{-2}]	$b_{g,j,4} \times 10^{11}$ [K^{-3}]	$b_{g,j,5} \times 10^{14}$ [K^{-4}]
1	22,313.49	0.95552	-1.431	9.871	-3.390	4.555
2	466,624.8	0.08010	1.290	-7.874	2.322	-3.084

3. BOILER DESCRIPTION AND BOUNDARY CONDITIONS

The boiler studied is part of a power generation plant, located in Candiota-RS, Brazil. It uses pulverized coal as fuel, and operates in a subcritical vapor cycle. The combustion chamber, with tangential burning, is rectangular with four burners in each corner. The Fig. 3-a and Fig. 3-b show the general arrangement of the burners and the heat exchangers of the boiler. They are aligned with the diagonal angular displacement with a horizontal line in order to generate a vortex in the flow. The boundary conditions used in this paper follow the employed ones by Silva et al. (2010).

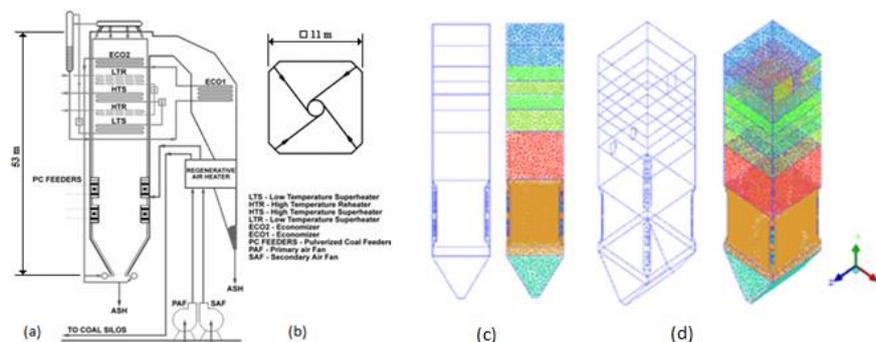


Figure 3. (a) General arrangement of the boiler components; (b) Horizontal cross section (Silva et al., 2010); Geometry and mesh used: (c) Front view; (d) Isometric view (Silva et al., 2010).

4. NUMERICAL METHOD

Property fields in the boiler (speed, temperature, pressure, concentration, etc.) were numerically determined using the commercial software Ansys CFX v.15, which is based on the finite volume method (Patankar, 1980). The power law was selected to assess the flow on control's volume surface and the function up-wind was prescribed for the interpolation scheme. The pressure-velocity coupling was solved by the SIMPLE algorithm (Patankar, 1980). As the conservation equations are nonlinear, relaxation factors were used for all conservation equations and additional models.

The mesh designed has about 3.1×10^6 elements of different sizes, and the density function was used in the regions close to the burners. In order to prove the mesh independence, tests were made to determine the best relation between refinement and computational effort. Figure 4 shows the trend of the results' stabilization, indicating that more refined meshes would not bring different results. Instead, the computational effort would rise up significantly.

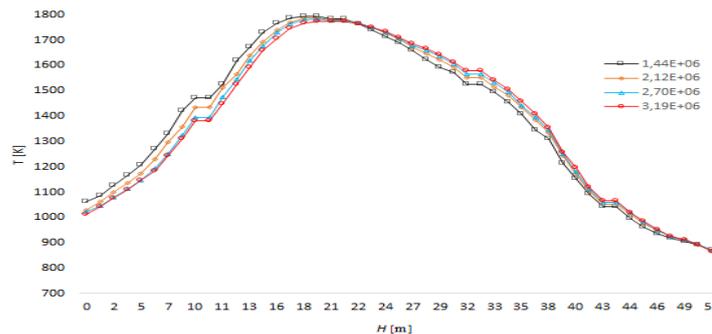


Figure 4. Mesh independence test.

5. RESULTS AND DISCUSSIONS

The first comparison made was between the spectral models and they relation with the soot-gas mixtures. Since the Gray Gas (GG) is one of the simplest models and gives acceptable approximations (Crnomarkovic, 2013), it was considered as reference. Table 3 presents some parameters in the boiler's gas outlet. Case (A) is a WSGG model, with weighting H_2O and CO_2 partial pressures; case (B) is the same of case (A), with the soot model from Magnussen and Hjertager (1976), but not considering soot particles in the WSGG model. Case (C), which is the most complete case, integrates the soot particles coefficients in global WSGG model.

Table 3. Parameters in the boiler's gas outlet.

Parameter	Gray Gas	Case A	Case B	Case C
Y_{soot} [kg/kg]	0.00128933	--	0.00141038	0.00137665
Y_{CO} [kg/kg]	1.89E-06	9.36E-07	9.36E-07	8.97E-07
Y_{CO_2} [kg/kg]	0.217487	0.217521	0.217518	0.219178
Y_{HCN} [kg/kg]	3.84E-06	1.52E-06	1.52E-06	1.95E-06
Y_{NO} [kg/kg]	4.64E-06	3.58E-06	3.58E-06	6.72E-06
Temperature [K]	821	902.541	902.53	872

The temperature fields are shown in Fig. 5 (a), while the temperature in several points over a centered vertical line is presented in Fig. 5(b). Figure 6(a) and Fig. 6(b) present the comparison of the cases for the radiation intensity.

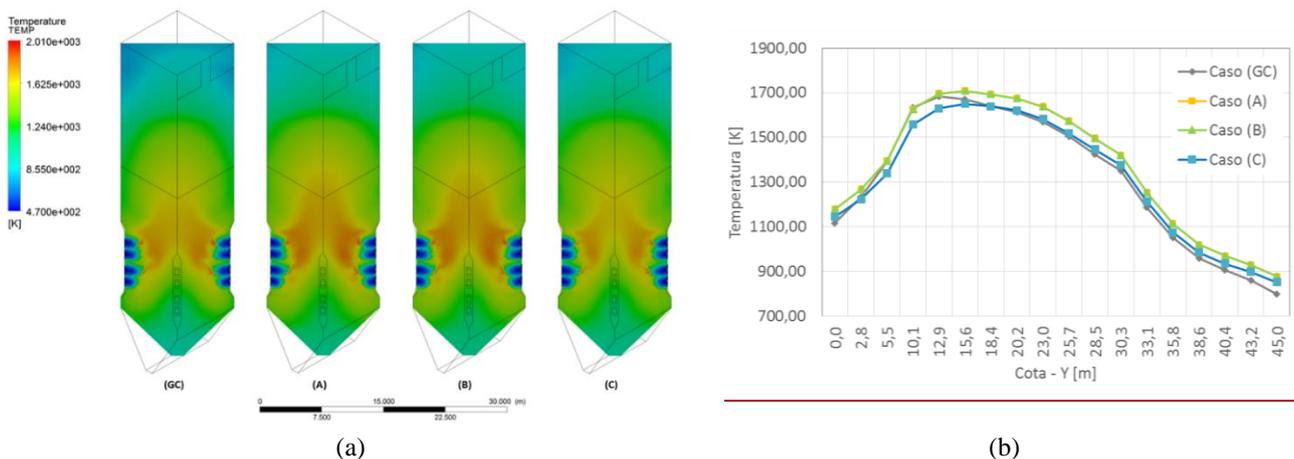


Figure 5. (a) Temperature fields in the boiler cross-section; (b) Temperature in a centered vertical line

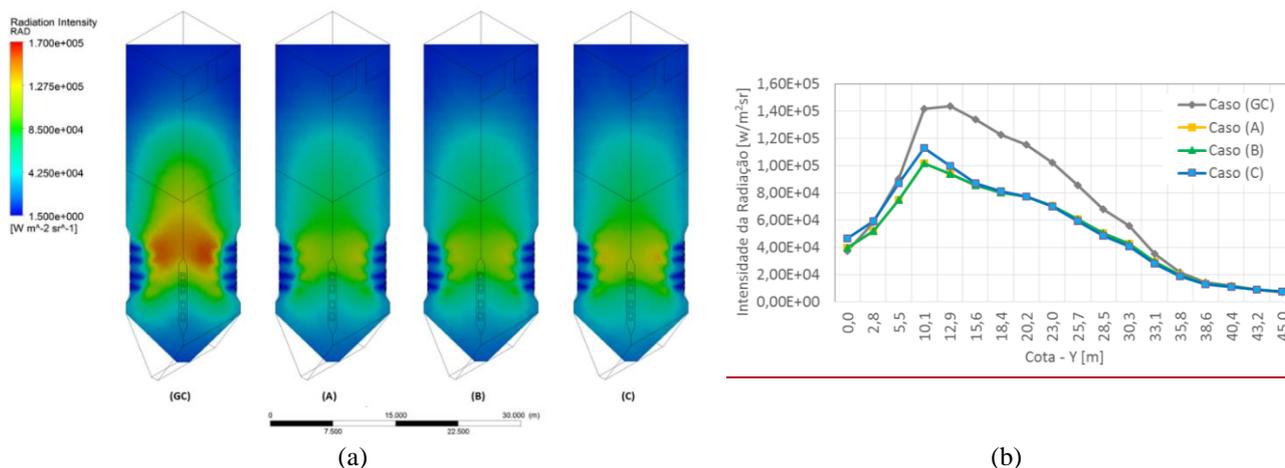


Figure 6. (a) Radiation intensity fields in the boiler cross-section; (b) Radiation intensity in a centered vertical line.

Concerning to the temperature field, the Gray Gas model (GG) practically agrees with case (C), the most complete case. The cases with WSGG model, not considering the influence of soot in radiation, seem to produce higher temperatures that may not represent reality. Figure 5(b) presents the temperature along a centered vertical line across the boiler. The differences noticed in the temperature profile between the cases are not significant. Considering the radiation, it is clear that the higher level is found in the combustion chamber, near the flame region, as presented in Fig. 6(a). Figure 6(b) shows that the GG model predicts radiation intensity levels much higher than WSGG. This difference was also reported by DeMarco et al. (2010), and shall be researched more specifically. Table 4 shows that, despite the radiation field appearance, the wall heat flux and wall radiative heat flux bring closer the GG model and the WSGG – Soot model.

Table 4. Parameters in the boiler combustion chamber.

Parameter	Gray Gas	Case A	Case B	Case C
Wall heat flux [$W m^{-2}$]	-151,823	-138,724	-138,722	-150,708
Wall radiative heat flux [$W m^{-2}$]	-145,475	-131,668	-131,665	-143,938

6. CONCLUSIONS

The present paper presents the differences and errors that could be generated by using the WSGG model, without the consideration of soot particles influence on radiation heat transfer. Specifically, the wall radiative heat flux demonstrates differences of 9.3% in cases (B) and (C), implying that soot has an important role in this application. Analyzing the simulations results, it can be concluded that soot particles cannot be undervalued in pulverized coal combustion applications. Since the soot concentration is relatively high, its effect on radiative heat transfer can imply in errors in the modeling. That is also important to highlight the satisfactory results obtained with the Gray Gas model. Despite to its simplicity, the approximations with more complex models, such as WSGG, allow to use the Gray Gas model in several applications, similar to this paper, without great precision loss.

7. ACKNOWLEDGEMENTS

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