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INFLUENCE OF PARTICLE SIZE IN A PULVERIZED COAL COMBUSTION PROCESS OF A REAL 160 MW POWER PLANT'S BOILER

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Abstract. *This article presents the results of numerical simulations of a combustion chamber that uses benefited coal type CE3100 as fuel. To perform the simulations was used the geometry of a steam generator of a full-scale thermal power plant of 160 MW situated in Rio Grande do Sul state, Brazil. Three approaches were undertaken to compare the influence of the particle size in relation to the Ash, Char, chemical species mass fraction and the temperature fields in the combustion process. In the first case, it was considered the particle size range of 50-80 µm, around 55 µm; in the second case, the ranging was of 80-100 µm, around 65 µm; and in the last case, of 100-120 µm, around 75 µm. In all cases there was an Eulerian modeling of the conservation equations of mass, momentum, energy and chemical species, as well as the k-ω turbulence model in process. The heat transfer by radiation for the gas phase was modeled by Discrete Transfer Radiation Model – DTRM, and the absorption spectrum of the flue gases was modeled by WSGG - Weigthed-Sum-of-Gray-Gases, adopting the latest weighted mean factors obtained from the literature. Was connected to this a Lagrangian modeling for predict the transport, devolatization and oxidation of pulverized coal particles, where the solid phase being patterned with black body. For solving differential equations, the commercial software Ansys CFX V15.0 was used. The main results showing that the size of the coal particles has some influence in coal combustion process, acting directly on the temperature, CO and O_2 mass fraction fields in to the boiler.*

Keywords*: Pulverized coal, Combustion, Particle Size, WSGG, CFD.*

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 still will be used for a longtime. In coal burn, the particle size is an important parameter to be considered. Since it changes the process dynamics and the combustion results, the coal is submitted to a discontinuous milling process. The discontinuous grinding in ball mills is a process of particle size reduction normally used in this kind of Power Plant. The ball mills are machines that consists of a hollow cylinder of metal, with a horizontal shaft on which is imposed a rotational movement. Inside the grinding bodies roll together with the material to be ground. The grinding action occurs by shock, crushing, cutting and friction materials that are mixed with these grinding media (Higuera, 2009). During this process, shock and friction between balls, wall and raw material, cause an erosive effect on the coal particles. This milling occurs at low temperature and attack angles of 30º and 60º.

There are not many studies in the literature that investigate the influence of particle size on the combustion processes in steam generators, especially regarding of numerical simulation. However, several authors have been using CFD codes for boiler's arrangements studies, pulverized coal boilers with front burners, low NOx burners (Kurose et al., 2004), variations in operating conditions, such as moisture content and size of coal particle (Bosoaga et al., 2006; Abbas et al., 1993; Kumar and Sahour, 2007). Choi and Kim (2009), using the FLUENT code in a study similar to this work, simulated a pulverized coal burner, with tangential burn, 500MW boiler. In the same line, Asotani et al. (2008), also using a code FLUENT, studied the behavior of cloud ignition of pulverized coal in a 40MW boiler. Park et al. (2010), using a CFD code, has analyzed a furnace in Youngheung - South Korea. In Crnomarkovic et al. (2013), models of WSGG - Weigthed-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 pulverized coal, with tangential burners, furnace using the zonal method solution of radiant heat transfer. Silva et al. (2010) and Dondoni et al. (2013), also using a commercial CFD code, CFX (Ansys Inc., 2004), studied the behavior of pulverized coal combustion in the same boiler studied in this work, in order to validate the model, simulate the operation and identify possible factors of inefficiency, respectively. Following the same line of research, the present work has the main objective of evaluate and compare, through numerical simulations, the influence of coal particle size in a suspended burning coal combustion process in a full-scale steam generator. Analyzing and comparing temperature fields, Ash, Char and H_2O mass fractions on selected particle streams. The firing parameters will be addressed to the following three different ranges of particle size distribution: average size of 55 μm for a range of 50 – 80 μm; average size of 65 μm for a range of 80 – 100 μm; and average size of 75 μm for a range of 100 – 120 μm. These variations were compared with the variation in particle size for a case of actual operation,

where the particle size distribution was obtained by laboratory analysis, which indicates that most of the particles has size between 50 μm to 200 μm to an average particle size of 55 μm. The statistical model of Rosin-Rammler (Brown, 1995), available in CFX, is adopted to predict the random behavior of these particles injection coal for the tracks to be investigated. In this work, it will be focused on firing parameters for the three above checking and will be compared the temperature, CO and O_2 fields for both cases.

2. MATHEMATICAL FORMULATION

Considered that the combustion takes place at finite rates of chemical reactions in which the devolatization of coal occurs in two stages (Ubhayakar, 1976), yielding methane and carbon monoxide as an approximation, as shown in Fig. 1. For the oxidation of gas-phase, was used the model of global chemical reactions "Methane Air WD2" (Westbrook and Dryer, 1981), burning the methane in the first stage, forming carbon monoxide and water vapor as a product. In the second stage of this global reaction, the carbon monoxide, adding to the carbon monoxide resulting of devolatization of coal, reacts with oxygen to form dioxide of carbon, completing de mechanism. The rates of chemical reaction were provided by the combined EddyBreakup – Arrhenius model (Kuo, 2005; Turns, 2000). The formation of NO in combustion process considers Thermal, Prompt and Fuel mechanisms, and the combined Eddy-Breakup – Arrhenius model were again used.

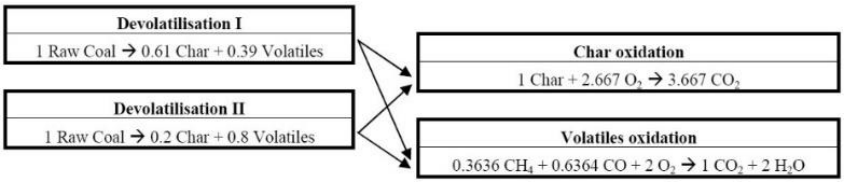

Figure 1 - Scheme basic chemical reactions of the raw coal (Ubhayakar, 1976).

A particle of coal consists of raw coal, *Co*, composed of char, *Char*, volatiles, moisture and *ash*. Therefore, after having occurred devolatization and drying, the particle becomes composed of char and ash, as shown in Fig. 2.

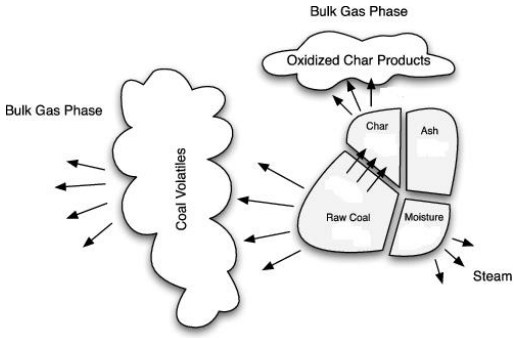

Figure 2 - Illustration of coal particle during devolatization.

On devolatization of coal, it was assumed that 98% of the nitrogen in the fuel is converted instantaneously to HCN, and the complement is not oxidized. The NOx formation is a complicate process. This work considers three main formation paths. The first is the Thermal NO and, due to the very high activation energy of reaction 1 (Eq. (1)), about 319 kJ/kmol, it is the predominant source of NOx in gas flames only at temperatures above 1800 K. The formation of NO comes from free radicals of two species, which are abundant at high temperatures, the O and N. The process develops in two steps, also known as Zeldovich mechanism. According 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 bellow can be assumed, and the main reactions described as follow:

$$O^{(16)} + {N_2}^{(28)} \leftrightarrow NO^{(30)} + N^{(14)} \quad (1)$$

$$N^{(14)} + {O_2}^{(32)} \leftrightarrow NO^{(30)} + ON^{(30)} \quad (2)$$

$${N_2}^{(28)} + {O_2}^{(32)} \leftrightarrow 2NO^{(60)} \quad (3)$$

Fenimore (1970) discovered that at temperatures lower than 1800 K, hydrocarbon flames presents high levels of NO that could not be formed by thermal mechanism. This faster mechanism of NO formation was termed as prompt NO. There are many reactions to be consider. However the predominant reaction is presented below, and has a activation energy about 75 to 92 kJ/kmol, which is much lower than thermal's activation energy for reaction.

$$CH + N_2 \leftrightarrow HCN + N \quad (4)$$

$$HCN + O_2 \leftrightarrow NO + \cdots \quad (5)$$

De Soete (1974) proposed a single reaction rate to this reaction, through Eq. (6) where W_{NO} is the molar mass and W, the mean molar mass of the mixture.

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

The Arrhenius coefficients depends on the fuel. De Soete (1974) proposed the values presented below:

$$A_{prompt} = 6{,}4.10^6 \left[\frac{1}{s}\right] \quad (7)$$

$$Ta_{prompt} = 36510\ [K] \quad (8)$$

The last path of NO formation occurs under fuel rich conditions. In this case there's no enough oxygen to oxidize all fuel, and the fuel excess lead to reduction of NO. For CH_4 and coal the stoichiometric reaction is:

$$NO + \frac{1}{4}CH_4 \rightarrow \frac{1}{2}N_2 + \frac{1}{4}CO_2 + \frac{1}{2}H_2O \quad (9)$$

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

$$R_{return} = 2{,}72.10^6[s^{-1}].\frac{W}{\rho}.[NO].[Fuel].exp^{((-9460[K])/T)} \quad (10)$$

An Eulerian modeling of conservation equations of mass, momentum, energy and chemical species as well as the turbulence and heat transfer by radiation to the gas-phase, was adopted. For coal transportation and ash particles a Lagrangian modeling coupled with gas-phase was used. Follow it was shown the mainly transport conservation equations of this combustion model as well as complementary models adopted.

2.1 Mass and species conservation

For a multicomponent fluid, scalar transport equations are solved for velocity, pressure, temperature and other quantities of the fluid. The bulk motion of the fluid is modeled using single velocity, pressure, temperature and turbulence fields. 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

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

where μ_t is the turbulent viscosity and Sc_t is the turbulent Schmidt number, $\overline{S}_i$ is the source term for component i which includes the effects of chemical reactions, D_i is the kinetic diffusivity, $\overline{\rho}$ are average density, x is the spatial coordinate, $\tilde{U}_j$ is the vector of velocity and the mass fraction of component i was defined as $\tilde{Y}_i = \tilde{\rho}_i / \overline{\rho}$. Note that the sum of component mass fractions over all components is equal to one.

2.2 Momentum conservation

For the fluid flow the momentum conservation equations are given by:

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

where $\mu_{eff} = \mu + \mu_t$ and 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 $p^* = \bar{p} - (2/3)k$ is the modified pressure, C_μ is an empirical constant of the turbulence model and equal to 0.09, $\bar{p}$ is the time-averaged pressure of the gaseous mixture, and δ_{ij} is the Krönecker delta function. $\overline{S}_U$ is the source term, introduced to model the buoyancy and drag force due to the transportation particles, and other mathematical terms due to turbulence models. The Boussinesq model was used to represent the buoyancy force due to density variations. The k-ϖ model was used to provide the turbulence on the flow Wilcox (1988).

2.3 Energy conservation

Considering the transport of energy due to diffusion of each chemical species, the energy equation can be written as

$$\frac{\partial}{\partial x_j}\left(\overline{\rho}\tilde{U}_j\tilde{h}\right)=\frac{\partial}{\partial x_j}\left(\kappa\frac{\partial\tilde{T}}{\partial x_j}+\sum_i^{Nc}\tilde{h}_i\left(\rho D_i+\frac{\mu_t}{Sc_t}\right)\frac{\partial\tilde{Y}_i}{\partial x_j}+c_p\frac{\mu_t}{Pr_t}\frac{\partial\tilde{T}}{\partial x_j}\right)+\overline{S}_{rad}+\overline{S}_{rea}+\overline{S}_T \tag{13}$$

where $\tilde{T}$, $\tilde{h}$ and c_p are the average temperature, enthalpy and specific heat of the mixture. $\tilde{Y}_i$ are the specific heat and the average mass fraction of the *i*-th chemical species, κ is the thermal conductivity of the mixture, Pr_t is the turbulent Prandtl number, and $\overline{S}_{rad}$, $\overline{S}_{rea}$ and $\overline{S}_T$ represent the sources of thermal energy due to the radiative transfer, the chemical reactions and sink our source of energy. The term $\overline{S}_{rea}$ can be written as:

$$\overline{S}_{rea}=\sum_i\left[\frac{h_i^0}{\overline{MM}_i}+\int_{\tilde{T}_{ref,i}}^{\tilde{T}}c_{p,i}d\tilde{T}\right]\overline{R_i} \tag{14}$$

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

To consider thermal radiation exchanges inside the combustion chamber, the Discrete Transfer Radiation Model (DTRM) (Carvalho et al., 1991) was employed, considering that the scattering is isotropic. The effect of the non-gray gaseous mixture was considered by original WSGG model by Hottel and Sarofim (1967), using the coefficients obtained by Dorigon (2013). The WSGG model coefficients employed in this work were those for partial pressures of 0.1 atm, 0.2 atm and 0.7 atm for CO_2, H_2O and N_2, respectively, being those values commonly considered for methane-air combustion and while the N_2 is considered transparent to radiation, as usual in combustion of fuel gas. The radiative properties required for an entrained particle phase are the absorption coefficients and scattering phase function, which depend on the particle concentration, size distribution, as well as effective complex refractive indices. However, optical properties of coal are not well characterized (Asotani et al., 2008). Generally, as a starting point to arrive at a tractable method for calculating radiative properties, the particles were assumed as spherical and homogeneous. At this work, the heat transfer from gas mixture to particle considers that the particles are opaque bodies with emissivity equal to one (blackbodies), and the Hanz-Marshall correlation was used to model the heat transfer coupling between the gas mixture flow and the particles (Ansys Inc., 2004). In fact, heat transfer to the walls in coal combustion process is mainly due to radiation and the convective heat transfer has only a minor contribution (Xu et al., 2000).

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

The reduced chemical reactions model employed in this work 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 nine species: O_2, CH_4, H_2, H_2O, *Tar* ($C_{3.878}H_{6.426}O_{3.561}$), HCN, HCO, NOx, CO_2 e CO. A conservation equation is required for each species but nitrogen. Thus, one has the conservation equation for the *i*-th chemical species, given by Eq. (11), where the source term, S_i, considers the average volumetric rate of formation or destruction of the *i*-th chemical species at all chemical reactions. This term is computed from the summation of the volumetric rates of formation or destruction in all the k-th reaction where the *i*-th species is present, $\overline{R_{i,k}}$. Thus, $\overline{R_i}=\sum_k\overline{R_{i,k}}$. The rate of formation or destruction, $\overline{R_{i,k}}$, was obtained by a combined Arrhenius-Magnussen model (Magnussen and Mjertager, 1977), the EBU-Arrhenius (Eaton et al., 1999).

2.5 The coal devolatization model

The devolatization of the coal was modeled using the generic Arrhenius reactions capability in two steps (Ubhayakar et al., 1976) in which two reactions with different rate parameters and volatiles yields compete to pyrolysis the raw coal. The first reaction dominates at lower particle temperatures and has a yield Y_1 lower than the yield Y_2 of the second reaction which dominates at higher temperatures. As a result, the final yields of volatiles will depend on the temperature history of the particle, and will increase with temperature, lying somewhere between Y_1 and Y_2. In this model, the mass fraction of the raw coal is specified as the mass fraction of volatiles (here methane and carbon monoxide, see Fig. 1) since all this material could be converted to volatiles. At time t, it was assumed that a coal particle consist of mass of raw coal (C_O), of mass of residual char (C_{ch}), after devolatization has occurred, and of mass of ash (A). The rate constants k_1 and k_2 of two reactions determine the rate of conversion of the raw coal:

$$\frac{dC_O}{dt} = -(k_1 + k_2)C_O \tag{15}$$

the rate of volatiles production and the rate of char formation is, respectively, given by

$$\frac{dV}{dt} = (Y_1 k_1 + Y_2 k_2)C_O \tag{16}$$

$$\frac{dC_{ch}}{dt} = ((1-Y_1)k_1 + (1-Y_2)k_2)C_O \tag{17}$$

2.6 The field char oxidation model

The oxygen diffusion rate is given by $k_d(p_g - p_S)$, where p_g is the partial pressure of oxygen in the furnace gases far from particle boundary layer and p_S is the oxygen pressure at the particle surface. The value of k_d is given by $k_d = D_{ref} R_p^{-1}\left(T_p - \tilde{T}_g(2T_{ref})^{-1}\right)^{\alpha} p_A/p$, where R_p is the particle radius, T_p is the particle temperature, $\tilde{T}_g$ is the far-field gas temperature, p_A is atmospheric pressure, D_{ref} is the dynamic diffusivity, and α is the exponent with value 0.75. The char oxidation rate per unit area of particle surface is given by $k_c p_s$. The chemical rate coefficient is given by, $k_c = A_c \exp(-T_c/T_p)$, where the parameters A_c and T_c depends on the type of coal. The overall char reaction rate of a particle is given by $\left(k_d^{-1} + k_c^{-1}\right)^{-1} C_{O_2} 4\pi R_p^2 \bar{p}/p_A$, and is controlled by the smallest of the two rates, k_d and k_c.

3. DESCRIPTION OF THE BOILER AND BOUNDARY CONDITIONS

The boiler studied is part of a power generation plant that use 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 of the chamber. The Fig. 3-a and Fig. 3-b show the general arrangement of burners and heat exchangers of the boiler. They are aligned with the diagonal angular displacement with a horizontal line in order to generate a vortex in flow. As boundary conditions are the same as the work of Silva et al. (2010) for the data of the boiler design, which were provided by the staff operating the Power Plant.

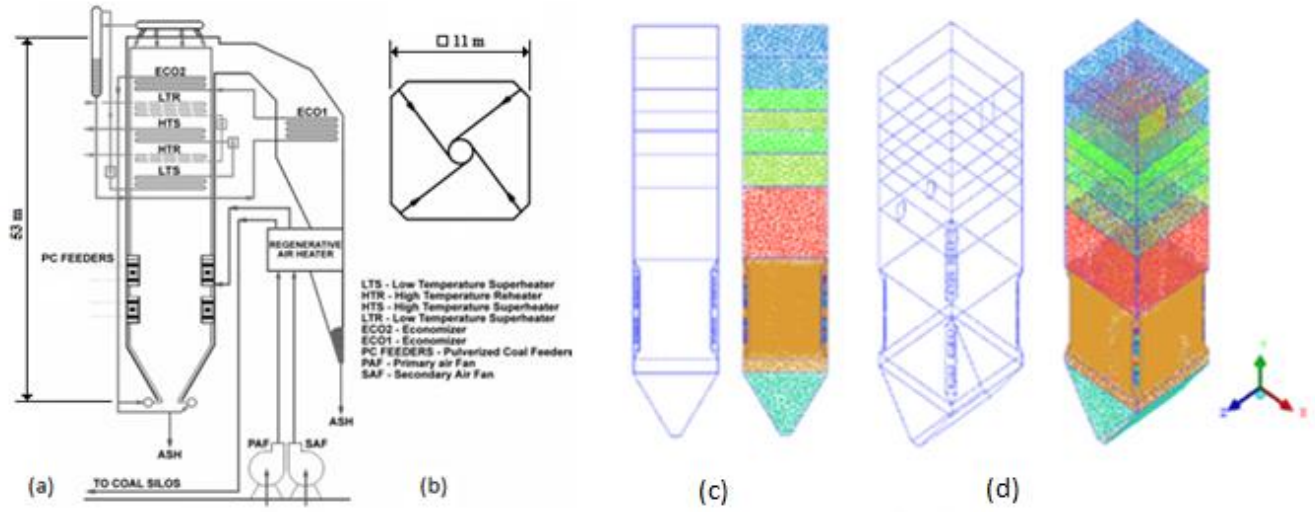

Figure 3. (a) General arrangement of the boiler components; (b) Horizontal cross section (Silva et al., 2010); geometry and mesh used in modeling: (c) Front view; (d) Perspective view (Silva et al., 2010).

4. NUMERICAL METHOD

Property fields in the boiler (speed, temperature, pressure, concentration, etc.) were numerically determined using the commercial software Ansys CFX 15, which was based on the finite volume method (Patankar, 1980). The *power law* was selected to assess the flows on the surface of the control volume and 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. Figures 3-c and 3-d shows the geometry and the generated mesh in front view and in perspective. The mesh used is about 1.5×10^6 elements of different sizes, using mesh refinement in the reactive regions near the burners.

5. RESULTS AND DISCUSSION

The simulation results are presented on the following. Figure 4 shows the temperature field of a transverse vertical plane inside the boiler. It is possible to verify temperatures rising from 477 K to 1965 K. The highest temperature is registered in the combustion chamber. The most significant energy loss occurs when the gas goes thru the tube bank's region of the heat exchangers, on boiler's top (energy sinks).The Temperature fields and heat exchange behavior are very similar in all cases. The temperatures differences can be better observed in Tab. 1, where becomes clear that smaller particle sizes generate higher temperatures.

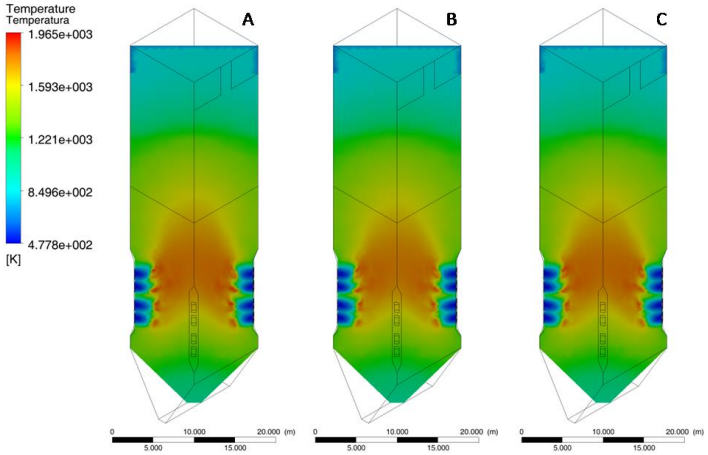

Figure 4 - Temperature fields: (A) particle size of 55 μm; (B) particle size of 65 μm; (C) particle size of 75 μm.

The *ash* and *Char* mass fraction are showed, thru several particle tracks, on Fig. 5.

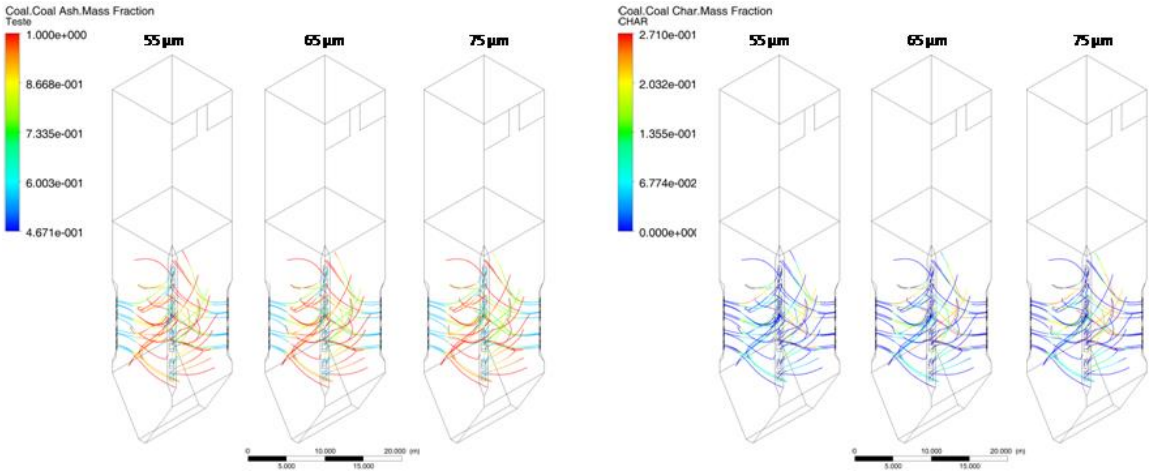

Figure 5 - *Ash* and *Char* mass fraction: particle track with sizes of 55 μm, 65 μm and 75 μm.

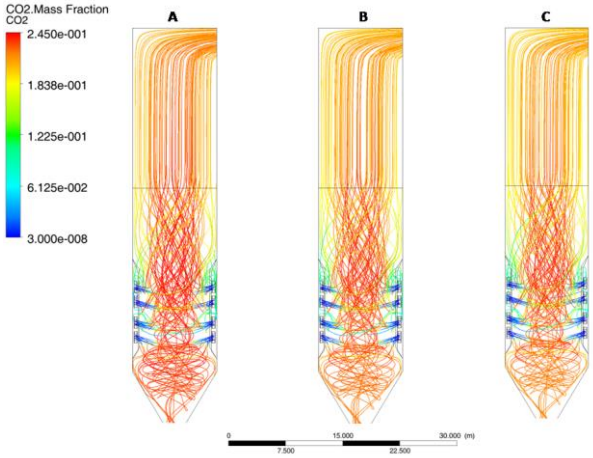

Figure 6 – CO_2 mass fraction: particle track with sizes: (A): 55 µm, (B): 65 µm, (C): 75 µm.

On Fig. 6 it is possible to observe the differences of CO_2 mass fractions between the three cases, where the higher levels were founded in the 55 μm particle size case. Even that some tracks presents small differences between the studied cases, they are better visualized in Tab.1.

Table 1- Mean properties in output region of the boiler.

Properties	**55 μm**	**65 μm**	**75 μm**
CH_4 [kg/kg]	1.55E-07	1.25E-07	1.11E-07
CO [kg/kg]	9.67E-07	7.81E-07	7.17E-07
CO_2 [kg/kg]	2.15E-01	2.12E-01	2.10E-01
H_2O [kg/kg]	9.21E-02	9.18E-02	9.15E-02
HCN [kg/kg]	2.24E-06	1.63E-06	1.23E-06
HCO [kg/kg]	4.50E-09	4.41E-09	4.53E-09
N_2 [kg/kg]	6.66E-01	6.67E-01	6.67E-01
NO_x [kg/kg]	3.45E-06	3.73E-06	3.90E-06
O_2 [kg/kg]	2.70E-02	2.92E-02	3.10E-02
Temperature [K]	883.65	879.18	876.13

The study results are in agree with those obtained in the work of Slezak (2010), who reported that the boiler efficiency varies with particle size. Analyzing the data from Tab.1 it is possible to conclude that the smallest particle size generate a more appropriate combustion process. In the 55μm case were registered higher proportion of CO and CO_2, which indicates higher devolatização and burning rates, showing that the particle's trajectory in the combustion chamber requires smaller residence times. The lower levels of O_2 also shows a more complete burning process. Regarding NO_x the use of smaller particle sizes, allows a significant decreasing of pollutant emission. However, though the smaller particle sizes showed better devolatization results, the CH_4, H_2O, HCN, and HCO readings may indicates that the combustion process could be improved. With a higher devolatization level, other combustion process's parameters could be adjusted to reach a complete burning with higher efficiency and lower emission levels.

6. CONCLUSION

With the results obtained from the simulations, it was observed that the particle size has some influence on coal combustion process, acting directly on the temperature field, O_2, CO and NO_x concentration. For the studied case, smaller particle sizes proves to be better for the combustion process in study, as expected. Since the residence time, the time that the particle remains under the flame zone, decrease, and the devolatization rates were higher, it is possible to conclude that the smaller particle sizes are more suitable for this power plant's boiler.

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