

## CFD ANALYSIS OF THE COAL COMBUSTION IN A BOILER OF A THERMAL POWER PLANT USING DIFERENTS KINDS OF THE MANUFACTURED COALS

Cristiano Vitorino da Silva, [cristiano@uricer.edu.br](mailto:cristiano@uricer.edu.br)

Luis Carlos Lazzari, [luislazzari@yahoo.com.br](mailto:luislazzari@yahoo.com.br)

Aline Ziemniczak, [aline.zz@hotmail.com](mailto:aline.zz@hotmail.com)

Arthur Bortolin Beskow, [arthur@uricer.edu.br](mailto:arthur@uricer.edu.br)

Univ. Regional Integrada do Alto Uruguai e das Missões – URI. Av. Sete de Setembro, 1621, 99700-000, Erechim, RS – Brasil.

Maria Luiza Sperb Indrusiak, [sperbindrusiak@via-rs.net](mailto:sperbindrusiak@via-rs.net)

Univ. do Vale do Rio dos Sinos – UNISINOS. Av. Unisinos, n. 950, CEP 93022-000, São Leopoldo – RS – Brasil.

Paulo Smith Schneider, [pss@mecanica.ufrgs.br](mailto:pss@mecanica.ufrgs.br)

Univ. Federal do Rio Gande do Sul – UFRGS. Rua Sarmento Leite, n.425, CEP 90050-170, Porto Alegre – RS – Brasil.

**Abstract.** *The state of the art in computational fluid dynamics and the availability of commercial codes encourage numerical studies of combustion processes. In the present work the commercial software CFX © Ansys Europe Ltd. has been used to study the combustion of pulverized coal into the boiler of a thermal power plant. The objective of this work is to obtain new information for process optimization. Different kinds of manufactured coals were numerically tested in a thermal power plant installed at the southeast region of Brazil. The simulations were made using the actual burning conditions of the boiler. Results include the residence time of the fuel into the combustion chamber, temperature fields, flow fluid mechanics, heat transfer and pollutant formation, as well as the CO and NO<sub>x</sub> concentrations, aiming to determinate the best conditions to burn the investigated coals. The numerical investigation of the phenomena involved on the coal combustion processes are used to complete the experimental information obtained in operational tests. Considering the characteristics of different kinds of manufactured coals used, with this study is possible to achieve the most efficient boiler operation parameters, with decreasing costs of electricity production and reduction of environmentally harmful emissions. It was verified that the different kinds of manufactured coals demand different operation conditions, and the kind of manufactured coal used on the combustion process has a significant effect on the pollutant formation, minly in relation with ash concentration.*

**Keywords:** *Computational fluid dynamic, thermal power plant, Brazilian coal combustion.*

### 1. INTRODUCTION

In recent years, the interest on performance optimization of large utility boilers has become very relevant, aiming at extending their lifetime, increase the thermal efficiency and reduce the pollutant emissions, particularly the NO<sub>x</sub> emissions. However, the efficient and clean utilization of this fuel is a major problem in combustion processes. In Brazil, which are used mainly for electricity production in large utility boilers, the coal reserves are enough to meet the next 1,109 years demand, considering the consumption levels of 2006 (EIA/U.S. Department of Energy, 2009).

An efficient operation of combustion chambers of these boilers depends on the proper knowledge of the oxidation reactions and heat transfer between the combustion products and the chamber walls and heat exchangers, which requires a detailed analysis of the governing mechanisms. Many combustion modeling methodologies are now available, but only a few are able to deal with the process in its entirety. Eaton et al. (1999) present a revision of combustion models. The models are generally based on the fundamental conservation equations of mass, energy, chemical species and momentum, while the closure problem is solved by turbulence models such as the  $k-\varepsilon$  (Launder and Sharma, 1974), combustion models like Arrhenius (Kuo, 1996; Turns, 2000), Magnussen - EBU - “Eddy Breakup” (Magnussen and Hjertager, 1976), radiative transfer models based on the Radiative Transfer Equation - RTE (Carvalho et al., 1991) and models to devolatilisation and combustion of solid and liquid fuels. Li et al. (2003) numerically investigated the combustion process using only a two-fluid model (instead of the Eulerian gas - Lagrangian particle models) for simulating tree-dimensional turbulent reactive flows and coal combustion. To improve the simulation of the flow field and NO<sub>x</sub> formation, a modified  $k-\varepsilon-k_p$  two-phase turbulence model and a second-order-moment (SOM) reactive rate model were proposed. The results indicate that a pulverized coal concentrator installed in the primary air tube of the burner has a strong effect on the coal combustion and NO<sub>x</sub> formation.

In a numerical investigation, Kurose et al. (2004) employed a tree-dimensional simulation to the pulverized coal combustion field in a furnace equipped whit a low-NO<sub>x</sub> burner, called CI- $\alpha$ , to investigate in details the combustion processes. The validities of available NO<sub>x</sub> formation and reduction models were investigated too. The results show that a recirculation flow is formed in high-gas-temperature region near the CI- $\alpha$  burner outlet, and this lengthens the residence time of coal particles in this high-gas-temperature region, promotes the evolution of volatile matter and the

process of char reaction, and produces an extremely low-O<sub>2</sub> region for effective NO reduction. Zhang et al. (2005) presented a numerical investigation on the coal combustion process using an algebraic unified second-order moment (AUSM) turbulence-chemistry model to calculate the effect of particle temperature fluctuation on char combustion. The AUSM model was used to simulate gas-particles flows in coal combustion including sub-models as the  $k-\varepsilon-k_p$  two-phase turbulence model, the EBU-Arrhenius volatile and CO combustion model, and the six-flux radiation model. The simulation results indicate that the AUSM char combustion model presented good result, since the later totally eliminates the influence of particle temperature fluctuation on char combustion rate.

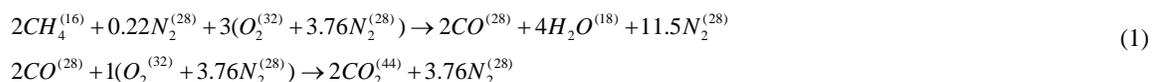
Bosoaga et al. (2006) presented a study developing a CFD model for the combustion of low-grade lignite and to characterize the combustion process in the test furnace, including the influence of the geometry of burner and furnace. A number of computations were made in order to predict the effect of coal particle size, the moisture content of lignite, and the influence of combustion temperature and operation of the support methane flame on the furnace performance and emissions. It was found that the increase of moisture tends to reduce NO<sub>x</sub>, and the methane support flame greatly increases NO<sub>x</sub>. In another work, Backreedy et al. (2006) presented a numerical and experimental investigation of the coal combustion process to predict the combustion process of pulverized coal in a 1 MW test furnace. The furnace contains a triple-staged low-NO<sub>x</sub> swirl burner. A number of simulations were made using several coal types in order to calculate NO<sub>x</sub> and the unburned carbon-in-ash, the later being a sensitive test for the accuracy of the char combustion model. The NO<sub>x</sub> modelling incorporates fuel-NO, thermal, and prompt mechanisms to predict the NO formation on the combustion processes.

Kumar and Sahur (2007) studied the effect of the tilt angle of the burners in a tangentially fired 210 MWe boiler, using commercial code FLUENT. They showed the influence of the tilt angle in the residence time of the coal particles and consequently in the temperature profiles along the boiler. Follow in the same line, Asotani et al. (2008), also using the code FLUENT, studied the ignition behavior of pulverized coal clouds in a 40 MW commercial tangentially fired boiler. The results for unburned carbon in ash and for outlet temperature were validated respectively by the operating data and by the design parameter. A qualitative comparison between the results for temperature and ignition behavior in the vicinity of the burners was made, using the images of a high temperature resistant video camera system. At the similar work Choi and Kim (2009), also using the code FLUENT, investigated numerically the characteristics of flow, combustion and NO<sub>x</sub> emissions in a 500 MWe tangentially fired pulverized-coal boiler. They showed that the relation among temperature, O<sub>2</sub> mass fraction and CO<sub>2</sub> mass fraction has been clearly demonstrated based on the calculated distributions, and the predicted results have show that the NO<sub>x</sub> formation in the boiler highly depend on the combustion process as well as the temperature and species concentration. Recently, Silva et al. (2010) studied, using the commercial code CFX (Ansys Inc., 2004), a behavior of pulverized coal combustion in a 160 MWe commercial tangentially fired boiler erected in the core of the Brazilian coal reserves region, with the objective of simulating the operation conditions and identifying inefficiency factors. The results of simulations indicates that this software is perfectly capable to solve this kind of problem and it is possible obtain good agreement between the experimental and simulations data, to become an important tools to predict different situations of boiler operation and even so to be used for design of this equipment.

In the present work the commercial CFD code CFX © Ansys Europe Ltd. was used to study the pulverized-coal combustion process in a 15 MWe thermal power plant, with the objective of simulating the boiler operation conditions using two different kinds of benefited coal, one available in Brazil, the CE3100, and other available in USA, that has a higher energetic value and lower quantities of ash, both for use in generating electricity in thermal power plants, aim to identify possible operation problems and try to obtain data about the pollutants formations, temperature and concentrations fields for each benefited coal used, indicating the best option of the benefited coal to be used. The same thermal power will be used for all cases for comparisons questions.

## 2. MATHEMATICAL FORMULATION

A steady-state combustion of raw coal in air for a boiler combustion chamber is considered in order to determine the temperature, chemical species concentrations and the velocity fields for multi-component-flow (gas mixture and raw coal particles), as well as to study the influence of the operational parameters, such as heterogeneous condition for fuel and air flow in the chamber, on the combustion process and NO<sub>x</sub> formation. The complete chemical reaction of the raw coal used at this work, including two devolatilisation processes, is modeled according to the basic scheme showed in Fig. 1. As basic assumptions, it is considered that the mass fractions of volatiles are 0.3636 of methane and 0.6364 of carbon monoxide, and that the combustion processes of these volatiles occur at finite rates. The methane oxidation is modeled by two global steps, given by:

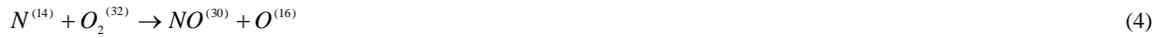


where the carbon monoxide oxidation is modeled by the second reaction above.

The hydrogen oxidation is modeled by:



The formation of  $NO_x$  is modeled by Zeldovich mechanisms using two different paths, the thermal-NO and the prompt-NO, where the first, that is predominant at temperatures above 1800 K, is given by tree-step chemical reaction mechanisms:



In sub or near stoichiometric conditions, a third reaction is also used



where the chemical reaction rates are predicted by combined Eddy Breakup - Arrhenius model.

The prompt-NO is formed at temperatures lower than 1800 K, where radicals can react rapidly with molecular nitrogen to form HCN, which may be oxidized to NO under flame conditions. The complete mechanism is not straightforward. However, De Soete proposed a single reaction rate to describe the NO source by Fennimore mechanism, which is used at this work, and the combined Eddy Breakup - Arrhenius model are used for predict this chemical reaction rate. At this way, the HCN oxidation to form NO is modeled by:



The HCN oxidation to consume the NO is



The HCO oxidation is modeled by



And, to the reburn of NO by the  $CH_4$  fuel gas:



Scalar transport equations are solved for velocity, pressure, temperature and chemical species. The bulk motion of the fluid is modeled using single velocity, pressure, temperature, chemical species and turbulence fields (CFX Inc., 2004).

## 2.1. Mass and species conservation

Each component has its own Reynolds-Averaged equation for mass conservation which, considering incompressible and stationary flow can be written in tensor notation as:

$$\frac{\partial \left( \tilde{\rho}_i \tilde{U}_j \right)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho}_i \left( \tilde{U}_{ij} - \tilde{U}_j \right) - \overline{\tilde{\rho}_i'' U_j''} \right) + S_i \quad (10)$$

where  $\tilde{U}_j = \sum \left( \tilde{\rho}_i \tilde{U}_{ij} \right) / \tilde{\rho}$ .  $\tilde{\rho}_i$  and  $\tilde{\rho}$  are the mass-average density of fluid component  $i$  in the mixture and average

density, respectively,  $x$  is the spatial coordinate,  $\tilde{U}$  is the vector of velocity and  $\tilde{U}_{ij}$  is the mass-averaged velocity of fluid component  $i$ . The term  $\tilde{\rho}_i \left( \tilde{U}_{ij} - \tilde{U}_j \right)$  represents the relative mass flow, and  $S_i$  is the source term for component  $i$

which includes the effects of chemical reactions. Note that if all the equations represented by Eq. (10) are added over all components, and the source term is set to zero, the result is the standard continuity equation.

The relative mass flow term accounts for differential motion of the individual components. At this work, this term is modeled for the relative motion of the mixture components and the primary effect is that of concentration gradient. Therefore,

$$\tilde{\rho}_i \left( \tilde{U}_{ij} - \tilde{U}_j \right) = \frac{\tilde{\rho} D_i}{\tilde{\rho}} \frac{\partial \tilde{\rho}_i}{\partial x_i} \quad (11)$$

where  $D_i$  is the kinetic diffusivity. The mass fraction of component  $i$  is defined as  $\tilde{Y}_i = \tilde{\rho}_i / \tilde{\rho}$ . Substituting this expressions into Eq. (9) and modeling the turbulent scalar flows using the eddy dissipation assumption it follows that

$$\frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{U}_j \tilde{Y}_i \right) = \frac{\partial}{\partial x_j} \left( \left( \bar{\rho} D_i + \frac{\mu_t}{Sc_i} \right) \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + \bar{S}_i \quad (12)$$

where  $\mu_t$  is the turbulent viscosity and  $Sc_i$  is the turbulent Schmidt number. 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:

$$\frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{U}_i \tilde{U}_j \right) = - \frac{\partial p^*}{\partial x_j} \delta + \frac{\partial}{\partial x_j} \left( \mu_{eff} \frac{\partial \tilde{U}_i}{\partial x_j} \right) + \frac{\partial \tilde{U}}{\partial x_j \partial x_i} + \bar{S}_U \quad (13)$$

where  $\mu_{eff} = \mu + \mu_t$  and  $\mu$  is the mixture dynamic viscosity and  $\mu_t$  is the turbulent viscosity, defined as  $\mu_t = C_\mu \bar{\rho} k^2 / \varepsilon$ . The term  $p^* = \bar{p} - (2/3)k$  is the modified pressure,  $C_\mu$  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  $\delta$  is the Kronecker delta function.  $\bar{S}_U$  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 is used to represent the buoyancy force due to density variations. The  $k-\omega$  model are used to provide the turbulence on the flow (Menter, 1994).

## 2.3. Energy conservation

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

$$\frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{U}_j \tilde{h} \right) = \frac{\partial}{\partial x_j} \left( \left( \frac{\kappa}{c_p} \right) \frac{\partial \tilde{h}}{\partial x_j} + \sum_i^{N_c} \bar{\rho} D_i \tilde{h}_i \frac{\partial \tilde{Y}_i}{\partial x_j} + \frac{\mu_t}{Pr_t} \frac{\partial \tilde{h}}{\partial x_j} \right) + \bar{S}_{rad} + \bar{S}_{rea} \quad (14)$$

where  $\tilde{h}$  and  $c_p$  are the average enthalpy and specific heat of the mixture. The latter is given by  $c_p = \sum_\alpha \tilde{Y}_\alpha c_{p,\alpha}$ , where  $c_{p,\alpha}$  and  $\tilde{Y}_\alpha$  are the specific heat and the average mass fraction of the  $\alpha$ -th chemical species,  $\kappa$  is the thermal conductivity of the mixture,  $Pr_t$  is the turbulent Prandtl number, and  $\bar{S}_{rad}$  and  $\bar{S}_{rea}$  represent the sources of thermal energy due to the radiative transfer and to the chemical reactions. The term  $\bar{S}_{rea}$  can be written as:

$$\bar{S}_{rea} = \sum_\alpha \left[ \frac{h_\alpha^0}{MM_\alpha} + \int_{\tilde{T}_{ref,\alpha}}^{\tilde{T}} c_{p,\alpha} d\tilde{T} \right] \bar{R}_\alpha \quad (15)$$

where  $\tilde{T}$  is the average temperature of the mixture,  $h_\alpha^0$  and  $\tilde{T}_{ref,\alpha}$  are the formation enthalpy and the reference temperature of the  $\alpha$ -th chemical species. To complete the model, the density of mixture can be obtained from the ideal gas state equation (Kuo, 1996; Turns, 2000),  $\bar{\rho} = p \overline{MM} \left( \bar{R} \tilde{T} \right)^{-1}$ , 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  $\mu_t \gg \mu$ . Close to the wall, the logarithmic law of the wall is used.

To consider thermal radiation exchanges inside the combustion chamber, the Discrete Transfer Radiation Model - DTRM is employed (Carvalho et al., 1991), considering that the scattering is isotropic. The effect of the wavelength dependence is not considered, and the gas absorption coefficient is considered uniform inside the combustion chamber and its value is  $0.5 \text{ m}^{-1}$ . 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, and effective complex refractive indices. However, optical properties of coal are not well characterized (Eaton et al., 1999). Generally, as a starting point to arrive at a tractable method for calculating radiative properties, the particles are assumed to be 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, and the Hanz-Marshall correlation is used to model the heat transfer coupling between the gas mixture flow and the particles (CFX Inc., 2004). In fact, heat transfer to the walls in a utility boiler is mainly due to radiation and the convective heat transfer has only a minor contribution (Xu et al., 2000). Conversely, heat transfer in the tube banks, which were simulated as porous media, was modeled by means of volumetric sink

coefficients representing the total amount of thermal energy transferred to working fluid inside the tubes of each bank. The pressure losses due to the tube banks were also modeled assigning quadratic directional loss coefficients to the porous media, computed from the tube bank geometry data (Knudsen et al., 1958).

#### 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 is considered that the combined pre-mixed and non-premixed oxidation occurs in two global chemical reaction steps, and involving only nine species: O<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>, H<sub>2</sub>O, CO<sub>2</sub>, CO, NO<sub>x</sub>, HCN and HCO. A conservation equation is required for each species but nitrogen. Thus, one has the conservation equation for the  $\alpha$ -th chemical species, given by Eq. (12), where the source term,  $S_i$ , considers the average volumetric rate of formation or destruction of the  $\alpha$ -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 equations where the  $\alpha$ -th species is present,  $\overline{R_{\alpha,k}}$ . Thus,  $\overline{R_{\alpha}} = \sum_k \overline{R_{\alpha,k}}$ . The rate of formation or destruction,  $\overline{R_{\alpha,k}}$ , was obtained from a combined Arrhenius-Magnussen model, the EBU-Arrhenius (Eaton et al., 1999). Such relations are appropriate for a wide range of applications, for instance, laminar or turbulent chemical reactions with or without pre-mixing. Such, the rate of formation or destruction of the chemical species is taken as the lowest one between the values obtained from each model. It follows that Silva et al. (2007) used this formulation in this work to simulate the combustion process of methane and air in a cylindrical chamber obtaining good results.

#### 2.5 The coal decomposition

Pulverized coal particles are treated at this work as non-interacting spheres with internal reactions and heat transfer and full coupling of mass, momentum and energy with the gaseous phase. The combustion of coal particles is a two stage process: the devolatilisation of raw coal particle followed by oxidation of residual char to leave incombustible ash. The devolatilisation was modeled with two competing reactions (see Fig. 1) in order to deal with the strong dependence on temperature and heating rate of the bituminous coal. The two equations have different rate parameters and volatile yields. The yield fractions for the lower temperature equation were obtained from proximate analysis and to the ones for the higher temperature equation were given the values suggested by Li et al. (2003). The model adopted for the char burn out computes the rate of the reaction taking into account the rate of diffusion of oxygen within the pores of the char particle and its partial pressure at the particle surface (Kanury, 1975). Particle size plays an important role in the char combustion process and is usually modeled by a statistical distribution like the one developed by Rosin-Rammler (Brown, 1995), with the parameters adjusted from pulverized coal analysis.

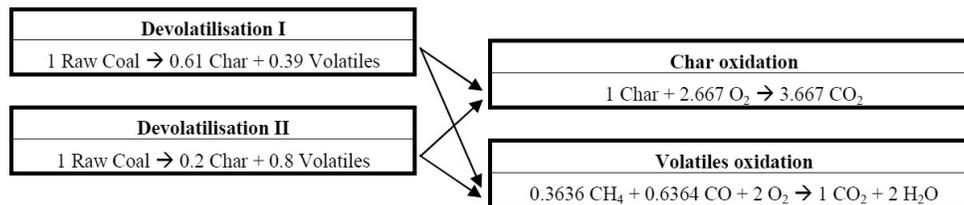


Figure 1. Basic scheme of the full chemical reactions of the raw coal.

##### 2.5.1 The coal devolatilisation model

The devolatilisation of the coal is 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 pyrolyse 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 is assumed that a coal particle consist of mass of raw coal ( $C_o$ ), mass of residual char ( $C_{ch}$ ) after devolatilisation has occurred, and mass of ash ( $A$ ). The rate constants  $k_1$  and  $k_2$  of two reactions determine the rate of conversion of the raw coal:

$$\frac{dC_o}{dt} = -(k_1 + k_2)C_o \quad (16)$$

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

$$\frac{dV}{dt} = (Y_1 k_1 + Y_2 k_2) C_o \quad (17)$$

$$\frac{dC_{ch}}{dt} = ((1 - Y_1) k_1 + (1 - Y_2) k_2) C_o \quad (18)$$

### 2.5.2 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  $k_d = D_{ref} R_p^{-1} \left( T_p - \bar{T}_g (2T_{ref})^{-1} \right)^\alpha \frac{P_A}{P}$ , where  $R_p$  is the particle radius,  $T_p$  is the particle temperature,  $\bar{T}_g$  is the far-field gas temperature,  $P_A$  is atmospheric pressure,  $D_{ref}$  is the dynamic diffusivity, and  $\alpha$  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  $(k_d^{-1} + k_c^{-1})^{-1} C_{O_2} 4\pi R_p^2 \frac{\bar{P}}{P_A}$ , and is controlled by the smallest of the two rates,  $k_d$  and  $k_c$ .

## 3. BOILER DESCRIPTION

The boiler under consideration is part of a pulverized coal (PC) power plant operating in a subcritical steam cycle. The frontal firing combustion chamber is rectangular in shape with two lines with four burners firing from each line, forming two large vortexes, one above and other below of jets produced in these burner lines. The evaporation process occurs mainly in the tubes covering the boiler walls. In the top of the boiler are the superheater tube banks. The second stage of the boiler comprises a large rectangular curved duct, the economizer tube bank and the regenerative air heater (Ljungström). From there the flue gases are directed through the electrostatic precipitator to the chimney. Figure 2-a shows the general disposition of the boiler heat exchangers.

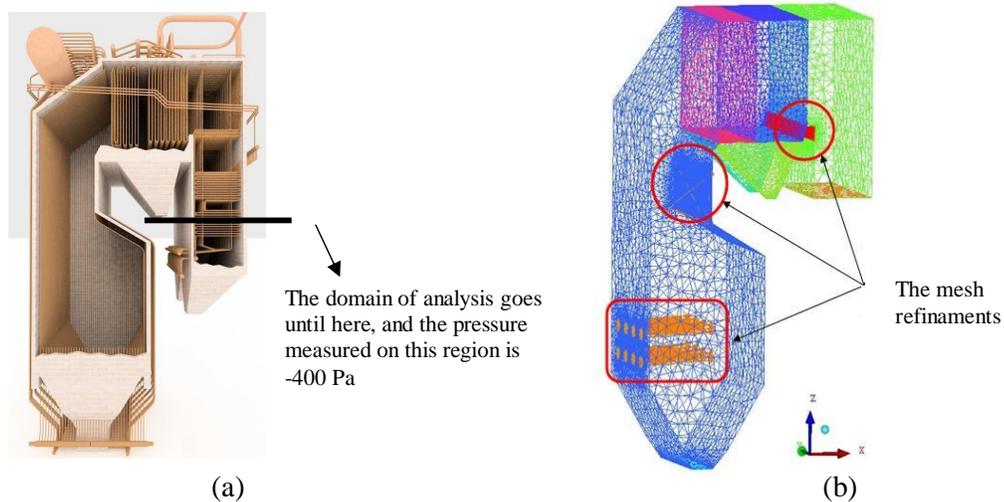


Figure 2 – (a) General disposition of the boiler components; (b) Mesh details: General view at the walls and refinements.

## 4. NUMERICAL METHOD

The flow fields inside the boiler (velocity, temperature, concentrations, etc.) were numerically determined with the commercial software Ansys CFX 10, based on the finite volume method (Patankar, 1980). The “power-law” scheme was selected for evaluating the fluxes at the control volume faces. The velocity-pressure coupling was solved by the SIMPLE algorithm (Patankar, 1980). Since the conservation equations are non-linear, relaxation factors were used.

## 5. MESH SETTINGS AND CONVERGENCE CRITERIA

The domain under consideration comprises the just the first stage of the boiler: the combustion chamber with the two lines of burners and the heat exchangers on the top of the boiler, considering too the rectangular curve until the

region entrance of economizer bank tubes. The entrance to the second stage was considered the outlet of the domain and a pressure of -400 Pa was used. The discretization was done using tetrahedral volumes, and the grid details are depicted in Fig. 2-b. Prismatic volumes were used at the walls in order to capture the boundary layer behavior. Due to computational limitations, the mesh size used has approximately  $2.8 \times 10^6$  elements, using mesh refinements into the chamber combustion, has shown at Fig. 2-b. The convergence criterion adopted was the RMS – Root Mean Square of the residual values, and the value adopted was  $1 \times 10^{-4}$  for all equations.

## 6. BOUNDARY CONDITIONS

The boundary conditions were obtained from the design data set and also from the daily operation data sheets. The operating conditions considered were the rated ones, for 15 MWe. The parameters of operations were considered for each benefited coal as follow, as well as the chemical composition of two benefited coals is show in Tab. 1. For booth cases was considered the same air excess and the same thermal charge.

### *Case I: Benefited coal CE3100 from Brazil*

Inlet: The inlet conditions are those for air and coal flows entering the domain from the burner nozzles. Total primary and secondary combustion air and pulverized coal mass flow rates were set as 4.5 kg/s, 10.71 kg/s and 6 kg/s respectively. Temperatures of primary air and coal, and secondary combustion air were set as 373 K and 550 K respectively. Pulverized coal size was modeled by a probabilistic distribution and limited between 50  $\mu\text{m}$  and 200  $\mu\text{m}$ .

### *Case II: Benefited coal of Kentucky from USA*

Inlet: The inlet conditions are those for air and coal flows entering the domain from the burner nozzles. Total primary and secondary combustion air and pulverized coal mass flow rates were set as 2.99 kg/s, 6.98 kg/s and 1.04 kg/s respectively. Temperatures of primary air and coal, and secondary combustion air were set as 373 K and 550 K respectively. Pulverized coal size was modeled by a probabilistic distribution and limited between 50  $\mu\text{m}$  and 200  $\mu\text{m}$ .

Table 1 – Chemical composition of two benefited coals.

Coal Chemical Species	Case I: Coal CE 3100		CaseII: Coal JENKIN-KENTUCKY	
	Dry Base	Wet Base	Dry Base	Wet Base
Char	33,21 %	27,74 %	79,20 %	66,16 %
Ash	54,78 %	<b>45,76 %</b>	3,00 %	<b>2,51 %</b>
Oxygen	7,92 %	6,62 %	10,00 %	8,36 %
Hydrogen	2,34 %	1,95 %	5,70 %	4,76 %
Sulfur	1,14 %	0,95 %	0,60 %	0,50 %
Nitrogen	0,61 %	0,51 %	1,50 %	1,25 %
Humidity	0,00 %	16,47 %	0,00 %	16,47 %

For the two cases the outlet boundary condition to the flue gas was set as the mean static pressure with a value equal to -400 Pa. The same way, the boiler walls that are covered with slanting tubes from the bottom until the top, the wall roughness and outlet temperature were set equal to 550K, which is the saturation temperature to the pressure of vapor into the boiler tubes. The wall emissivity was set 0.6 and all the others regions, as inlet and outlet regions, it were considered as blackbodies. The methodology employed in the present work has been tested and validated in Silva et al. (2010), presenting good agreement. In this work, the coal sulfur was considered inert on the combustion processes. Following the work, will be implemented a chemical reaction for this chemical species.

## 7. RESULTS

Here the simulation results were analyzed and compared for booth cases. The main available parameters were the temperature and mass fraction of some chemical species, as well as the trajectories of the coal particles into the outlet. As mentioned, two cases were evaluated. Figures 3 and 5 show the temperature field and the mass fraction field of CO and of O<sub>2</sub> for a vertical plane into the boiler. This plane is situated under one of burner lines. It is possible to verify in Fig. 3 that the ranges of temperature in this plane into the boiler are similar for booth cases, and are too physically coherent. As was applied the same thermal load for booth cases, and the USA coal has a higher energetic value, the mass flow of the fuel and the air are lower than for the Brazilian coal (here, CE3100), and, as a consequence, the inlet velocities are too lower for the USA coal, altering the inlet jets configurations. Such, for the USA coal the residence time of the raw coal particle on the flame zone is higher, being better to burner the coal particles, as show the Figs. 6 and 7, when you look the mass fraction of the char on the particle of coal. Observe that, for the CE3100 remains a large amount of carbon in the coal particles along the particles trajectories into the chamber, showing that the operation conditions adopted for this kind of coal is not so efficient.

Observe too in Fig. 4 that the CO, one devolatilisation product of the coal, for the CE3100 is more concentrated when it is close to the wall opposite entrance jets, indicating that the velocities really are not so appropriated for this coal, making one vary long flame, not appropriated for this kind of chamber. The same was observed to the CH<sub>4</sub> mass fraction, the other product of devolatilisation of coal. In Fig. 5 is possible to see a large difference between the cases. Although the thermal load be the same for two cases, air and coal mass flow are not, hence the conditions of the coal combustion are too not. The rates of chemical reactions are different for two cases. For the other planes there is the

same compartment, and the reactions indicated in Eq. (8) acts to consume the  $O_2$  remnant, and not consumed in the combustion of volatile on the flame zone.

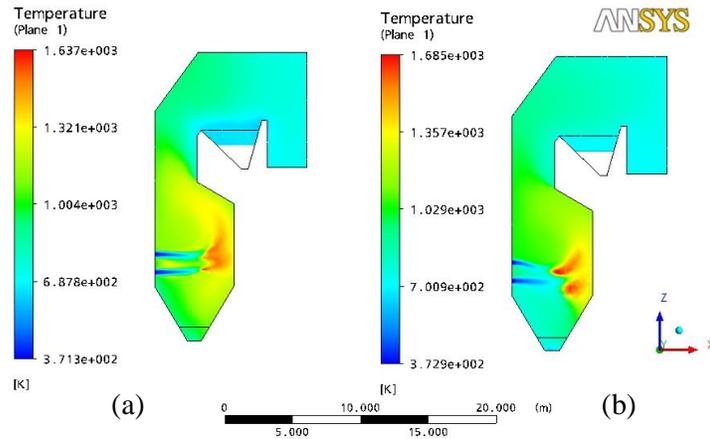


Figure 3 - Temperature field for a vertical plane into the boiler: (a) CE3100; (b) JENKIN-KENTUCKY.

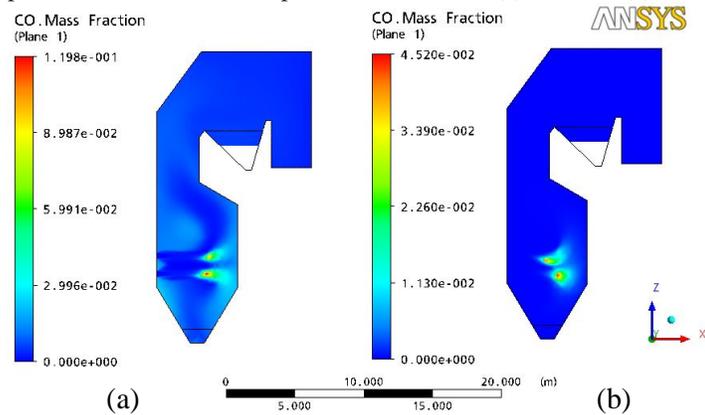


Figure 4 - CO mass fraction for a vertical plane into the boiler: (a) CE3100; (b) JENKIN-KENTUCKY.

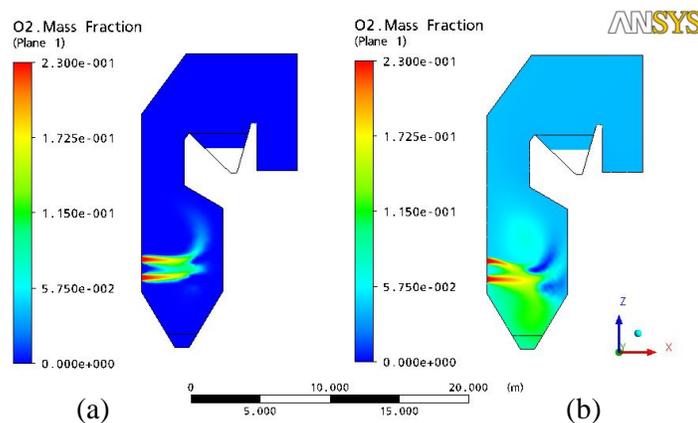


Figure 5 - Oxygen mass fraction for a vertical plane into the boiler: (a) CE3100; (b) JENKIN-KENTUCKY.

Figure 6 shows the trajectories lines for some particles of coal as a function of char, ash and raw coal to the particles of CE3100 coal, while the Fig. 7 shows the same case to the JENKIN-KENTUCKY coal. Evaluated the Figs. 6 and 7 you can see that there is a large difference between the booth cases, mainly for the coal ash mass fraction and the coal char mass fraction. For the CE3100 there is a large amount of particles that have not burned into the flame zone, indicated that there is large quantities of coal in flay ash, again indicated that this operation condition for the CE3100 is not the best, resulting in inefficiencies at combustion process. Thus, it is confirmed that the amount of ash in Brazilian

coal really becomes a big problem for operation of the boiler, indicating that prior treatment of coal to remove the ashes, really can be an alternative to improve the performance of this equipment for this type of coal, which in this case, was not built for operating with Brazilian coal.

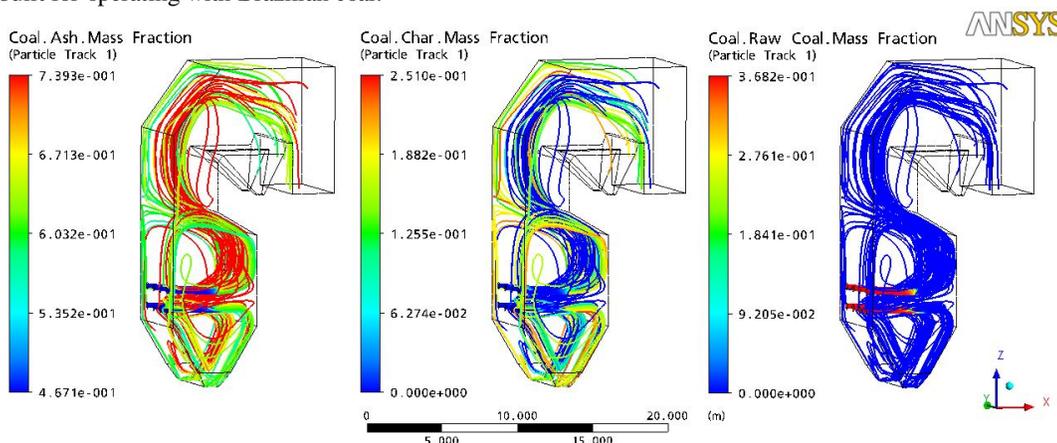


Figure 6 - Trajectories lines for some particles of coal as a function of char, ash and raw coal to CE3100.

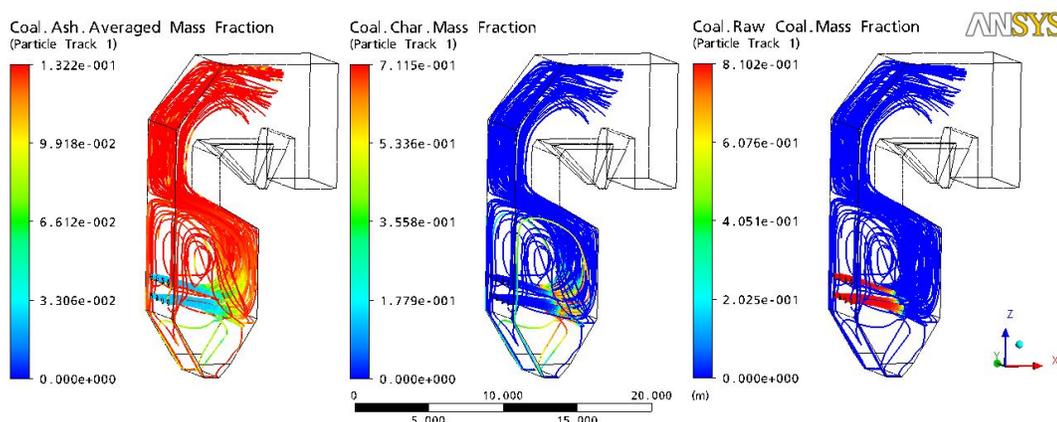


Figure 7 - Trajectories lines for some particles of coal as a function of char, ash and raw coal to JENKIN-KENTUCKY.

The Tab. 2 shows the average mass fraction of the chemical species in the outlet flue gases on the outlet region. Due to the larges concentration of nitrogen in USA coal (see Tab. 1), as the result, there is too a large quantities of NOx formation on the combustion process. Notice that the oxygen is almost completely consumed, for the conditions studied, for the CE3100. When observed globally the fractions of HCO, CH<sub>4</sub> and O<sub>2</sub> into the boiler, and remembering of Eq. (8), you can see that oxygen react with HCO to form H<sub>2</sub>O and CO<sub>2</sub>, and it is occurs mainly on the top steam generator and above of the inlet jets, under the flow recirculation region. As for USA coal, the velocities of the inlet jets are lower, the oxygen is consumed to oxidize the volatiles and the char under the flame zone, leaving a small quantity of this chemical species to react with the others elements in the upstream regions of the flow.

Table 2 – Average mass fraction of the chemical species at the outlet flue gases.

	Coal CE 3100		Coal JENKIN-KENTUCKY	
	Absolute value	Relative	Absolute value	Relative
Temperature	712.8 K	-	714.3 K	-
CO	0.0033 [kg/kg]	0.33 %	1.47x10 <sup>-9</sup> [kg/kg]	1.47 ppm
CO <sub>2</sub>	0.2571 [kg/kg]	25.7 %	0.2250 [kg/kg]	22.5 %
CH <sub>4</sub>	0.0016 [kg/kg]	0.15 %	2.40x10 <sup>-8</sup> [kg/kg]	0.024 ppm
H <sub>2</sub> O	0.0591 [kg/kg]	5.9 %	0.0380 [kg/kg]	3.8 %
N <sub>2</sub>	0.6804 [kg/kg]	68 %	0.7001 [kg/kg]	70 %
NOx	1.12x10 <sup>-9</sup> [kg/kg]	1.12x10 <sup>-3</sup> ppm	4.94x10 <sup>-6</sup> [kg/kg]	4.94 ppm
O <sub>2</sub>	~0 [kg/kg]	~0 %	0.0360 [kg/kg]	3.6 %
HCN	3.4x10 <sup>-4</sup> [kg/kg]	0.034 %	4x10 <sup>-4</sup> [kg/kg]	0.04 %
HCO	4.47x10 <sup>-9</sup> [kg/kg]	4.47x10 <sup>-3</sup> ppm	5.6x10 <sup>-12</sup> [kg/kg]	5.6x10 <sup>-4</sup> ppm
Total	1 [kg/kg]	100 %	1 [kg/kg]	100 %

## 8. CONCLUSIONS

Based on the study realized on this work, the main conclusion is that the boiler operation condition for the CE3100 is not the best, resulting in inefficiencies at combustion process, confirming that the amount of ash in Brazilian coal really becomes a problem to the boiler operation, indicating that a prior treatment of coal to remove the ashes really can be an alternative to improve the performance of this equipment for the use of this type of coal, which in this case, was not built for Brazilian coal.

## 9. ACKNOWLEDGEMENTS

The authors thank for the support of MCT/CNPq – National Research Council (Brazil).

## 10. REFERENCES

- Ansyst Inc, 2004. "User's guide - CFX Solver Theory".
- Asotani, T., Yamashita, T., Tominaga, H., Uesugi, Y., Itaya, Y. and Mori, S., 2008. "Prediction of ignition behavior in a tangentially fired pulverized coal boiler using CFD". *Fuel*, Vol. 87, pp. 482-490.
- Backreedy, R. I., Fletcher, L. M., Ma, L., Pourkashanian, M. and Williams, A., 2006, "Modelling Pulverised Coal Combustion Using a Detailed Coal Combustion Model", *Combust. Sci. and Tech.*, Vol. 178, pp. 763-787.
- Bosoaga, A., Panoiu, N., Mihaescu, L., Backreedy, R. I., Ma, L., Pourkashanian, M. and Williams, A., 2006, "The combustion of pulverized low grade lignite", *Fuel*, Vol. 85, pp. 1591-1598.
- Brown, W. K., 1995, "Derivation of the Weibull distribution based on physical principles and its connection to the Rosin-Rammler and lognormal distributions", *Journal of Applied Physics*, Vol. 78, n. 4, pp. 2758-2763.
- Carvalho, M.G., Farias, T. and Fontes, P., 1991. "Predicting radiative heat transfer in absorbing, emitting, and scattering media using the discrete transfer method", *ASME HTD*, Vol. 160, pp.17-26.
- Choi, C.R. and Kim, C.N., 2009. "Numerical investigation on the flow, combustion and NOx emission characteristics in a 500 MWe tangentially fired pulverized-coal boiler", *Fuel*; Vol. 88, pp. 1720-1731.
- Eaton, A. M., Smoot, L. D., Hill, S. C. and Eatough, C. N., 1999, "Components, formulations, solutions, evaluations, and applications of comprehensive combustion models", *Prog. in Energy and Comb. Science*, Vol. 25, pp. 387-436.
- EIA/U.S. Department of Energy. International Energy Outlook 2009. Available in <[www.eia.doe.gov/oiaf/ieo/index.html](http://www.eia.doe.gov/oiaf/ieo/index.html)>. Downloaded in nov. 2009.
- Kanury, A. M., 1975, "Introduction to Combustion Phenomena", Gordon and Beach Science Publishers, New York.
- Knudsen, J. G., 1958, "Fluid Dynamics and Heat Transfer", Mc Graw Hill.
- Kumar, M. and Sahu, S.G., 2007. "Study on the effect of the Operating Condition on a Pulverized Coal-Fired Furnace Using Computational Fluid Dynamics Commercial Code". *Energy & Fuels*, Vol. 21, pp. 3189-3193.
- Kuo, K.K., 1996. "Principles of combustion", John Wiley & Sons, New York.
- Kurose, R., Makino, H. and Suzuki, A., 2004, "Numerical analysis of pulverized coal combustion characteristics using advanced low-NOx burner", *Fuel*, Vol. 83, pp. 693-703.
- Lauder, B.E. and Sharma, B.I., 1974. "Application of the energy-dissipation model of turbulence to the calculation of flow near a spinning disc", *Letters in Heat and Mass Transfer*, Vol. 19, pp. 519-524.
- Li, Z. Q., Wei, Y. and Jin, Y., 2003, "Numerical simulation of pulverized coal combustion and NO formation, Chemical Engineering Science", *Chemical Engineering Science*, Vol. 58, pp. 5161-5171.
- Magnussen B.F. and Hjertager B. H., 1976. "On mathematical models of turbulent combustion with special emphasis on soot formation and combustion". In: 16<sup>th</sup> Int. Symp. on Combustion. The Combustion Institute, pp. 719-729.
- Menter, F. R., 1994. "Two-Equation Eddy-Viscosity Turbulence Models for Engineering Applications". *AIAA Journal*, Vol. 32, n. 8, pp. 1598-1605.
- Patankar, S.V., 1980. "Numerical Heat Transfer and Fluid Flow". Hemisphere, Washington, DC.
- Silva, C. V., França, F. H. R. and Vielmo, H. A., 2007. "Analysis of the turbulent, non-premixed combustion of natural gas in a cylindrical chamber with and without thermal radiation". *Comb. Sci. and Tech.*, Vol. 179, pp. 1605-1630.
- Silva, C. V., Indrusiak, M. L. S. and Beskow, A., 2010. "CFD analysis of the pulverized coal combustion processes in a 160 MWe tangentially-fired-boiler of a thermal power plant". *Journal of the Braz. Soc. of Mech. Sci. & Eng.*, Vol. 2, pp. 50-55.
- Turns, S. T., 2000, "An introduction to combustion – Concepts and applications", 2<sup>nd</sup> edn, McGraw-Hill, New York.
- Ubhayakar, S. W., Stickler, D. B., Rosenberg Jr., C. W. and Gannon, R. E., 1976, "Rapid Devolatilization of Pulverized Coal in Hot Combustion Gases". *Symp. Int. on Combustion*, The Combustion Institute, Vol. 16, pp. 427-436.
- Xu, M., Azevedo, J.L.T. and Carvalho, M.G., 2000. "Modelling of the combustion process and NOx emission in a utility boiler". *Fuel*, Vol. 79, pp. 1611-1619.
- Zhang, Y., Wei, X., Zhou, L. and Sheng, H., 2005, "Simulation of coal combustion by AUSM turbulence-chemistry char combustion model and a full two-fluid model", *Fuel*, Vol. 84, pp. 1798-1804.

## 11. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.