

## CFD ANALYSIS OF THE COAL COMBUSTION IN A BOILER OF A THERMAL POWER PLANT USING THE OXYFUEL PROCESSES

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**Abstract.** *In the present work the commercial software CFX © Ansys Europe Ltd. has been used to study the pulverized coal combustion – PC - into the boiler of a thermal power plant using the oxyfuel process. The objective of this work is to obtain information for optimization of the process and to study the viability of conversion of the boiler of this power plant to oxyfuel combustion. A manufactured pulverized coal blend CE3100 was numerically tested in the model of a thermal power plant installed at the southeast region of Brazil. To simulate the oxyfuel processes, the usual oxidant, atmospheric air, was replaced for a mixture of oxygen and carbon dioxide, the last one coming from recirculation flue gas of the combustion process. The simulations were made using the actual burning conditions of the boiler, that use atmospheric air for burning the coal, in comparing to combustion processes using the oxyfuel conditions, considering the same hypothetical thermal power plant for both cases. Results include the residence time of the coal particles into the combustion chamber, temperature fields, flow fluid mechanics, heat transfer and pollutant formation, like CO and NO<sub>x</sub>, aiming to indicate possibilities for implementing the oxyfuel processes in this thermal power plant. Considering the characteristics of the blend CE3100 used at this power plant, with this study was possible to achieve data on the oxyfuel operation for this boiler, indicating that is possible to operate the thermal power plant with this new combustion method, being possible to convert this unit. It was verified, if compared with the atmospheric air combustion, that the oxyfuel processes demand different operation conditions to maintain stable the combustion processes to the same thermal power plant.*

**Keywords:** *Computational Fluid Dynamic, Thermal Power Plant, Oxyfuel.*

### 1. INTRODUCTION

In the last decades researches have been developed in order to search new ways to produce electrical energy with minimal environmental impact, mainly related to emissions of carbon dioxide into the atmosphere, the main gas responsible for the so called greenhouse effect. However, the worldwide increase of energy production is mainly due to fossil fuel exploitation, like mineral coal and natural gas, in combustion processes in furnaces from large scale boilers of thermal power plants. At this way, the search for new technologies to meet the low emission goals while increasing the net energy production is of great importance, considering that in conventional processes the conciliation of such factors is almost impossible.

In Brazil, that in the last years has reached significant levels of economic growth, new energetic alternatives need to be developed in order to keep or improve the economic growth, as expected. This way, more specifically in the southern region, where impressive coal reserves are available, installation of new thermal power plants to use this fuel is a good investment alternative. However, as said above, this kind of plant concentrates high levels of pollutant emissions, mainly carbon dioxide. So, aiming to reach better incomes to these plants, the conventional burning processes need to be improved and, if possible, even be replaced through the use of new technologies.

The oxyfuel technologies are very attractive to power plants supplied by pulverized coal, which, as a retrofitting option, can be implemented even so from existing plants, because the use of enriched flames with oxygen diluted in the combustion gases, along with the parallel operation of purification plants, drying and liquefaction of carbon dioxide, performs the Carbon Capture and Storage (CCS) and allows a significant decrease of the problems of these power plants operation related to global warming. However, the biggest problem of this kind of operation is related to the cost of oxygen energetic production, and the cleaning and the liquefaction of CO<sub>2</sub>.

The oxyfuel processes were first applied in the fifties (Gitman, 1986). Since then many studies have been conducted and developments achieved. At first, mainly due to the oil crisis and the decreasing cost of oxygen production due to the advance techniques of cryogenic air separation, the enriched flames emerged as a strong alternative to improve the efficiency of combustion processes at industrial level (Shahani et al., 1994, 1996). But recently, mainly due to environmental constraints, is increasing the economic viability of the process of oxy-

combustion in energy production in large coal power plants. Singh et al. (2003) presents a comparative study of the technical and economic performance of a 400MWe power plant retrofitted to operate in oxy-combustion. Two situations are analyzed: one starting from the separation of CO<sub>2</sub> from flue gas of its own process for insufflation after mixed with oxygen, the other considering the technique of recirculation of combustion gases by mixing pure oxygen. The results show that although both increase the cost of electricity to some 20 to 30%, the option of combustion gas recirculation and oxygen injection is presented as the most viable. However, to achieve the complete mastery of the technology application of oxy-combustion, and get really satisfactory results, it is still necessary an intense search for more knowledge on the process, especially for its application in the generation of steam in thermoelectric power plants. In this sense, the numerical simulation appears as a very effective tool for these studies. Several studies on the process of oxyfuel combustion in steam generators of power plants at full scale have been developed in recent years. Kass et al. (2008) have investigated the combustion of Lusitanian dried lignite and Polish hard coal in a 0.5 MWth test facility of CEBra. Pure oxygen (99.95 vol%) was supplied by a tank and mixed with hot flue gas in order to reach oxygen concentrations similarly to the atmospheric air. The effects of excess air and oxygen distribution between primary and secondary air on the maximization of CO<sub>2</sub> concentration in the flue gas as well as the minimization of gaseous pollutants (NO, CO, SO<sub>2</sub>) were among the goals of this research work. Excess air should correspond to an oxygen mole fraction of 3.24% in order to achieve high CO<sub>2</sub> levels in the range of 92.15 vol%. An increase in excess air also has a negative effect on NO<sub>x</sub> and SO<sub>x</sub> emissions. Staged combustion, e.g., lower oxygen content in the primary air compared to secondary air, was also found to minimize pollutant emissions. Vascellari and Cau (2009) performed 2D CFD investigations of a 2.4 MW furnace operating under two oxy-fuel combustion mode. Although the oxygen concentration was constant with respect to the reference, air-combustion case, two different oxy-fuel modes were examined: in the first, constant secondary molar flow rate was undertaken (21% O<sub>2</sub> and 79% CO<sub>2</sub> by volume), while in the second examined case, a constant secondary mass flow was maintained (30% O<sub>2</sub> and 70% CO<sub>2</sub> by volume). In another work Hjarstman et al. (2009) examined the influence of the flue gas recycle rate, which affects the O<sub>2</sub> fraction entering the furnace, in a 100 kW test unit. Three lignite-fired oxy-fuel flames were investigated (25, 27 and 29 vol% O<sub>2</sub>) under a constant stoichiometric ratio. Flame structure and gas concentrations for the oxy-fuel (OF) 25% case were similar to air-firing, while the reduced recycled rates corresponded to higher peak temperatures, lower gas velocities and faster gas burnout. CO levels in the furnace can reach locally high values for the OF 27 and 29 cases; however in the flue gas exiting the boiler, the mole fraction is lower than the air-firing case. NO<sub>x</sub> concentration in the exit is likewise decreased by 30% for all oxy-fuel cases. Similar results have been reached by Tan et al. (2006) for a 0.3 MWth boiler. Profiles of temperature and in-furnace heat transfer can match air-firing through O<sub>2</sub>/RFG reduction, while there is significant potential for NO<sub>x</sub> reduction which can be maximized by the appropriate burner design. Erfurth et al. (2009) performed CFD simulations for a 1200 MWth PF boiler with swirl burners. Several oxy-fuel scenarios, varying in O<sub>2</sub> mol fraction and whether wet or dry flue gas recycle is used, were investigated. Radiation modeling was based on the greyband version of the Exponential Wide Band Model (EWBM). In-furnace temperatures dropped when O<sub>2</sub> was 21 vol%. Similar flame behavior was reached by increasing the O<sub>2</sub> to 27% (wet) or 30% (dry), in order to maintain the same adiabatic flame temperature.

Liu et al. (2005) experimentally investigated the pulverized coal combustion in a 20 kW down-fired combustor for air and various mixtures of O<sub>2</sub>/CO<sub>2</sub>. Oxy-fuel combustion at O<sub>2</sub> levels comparable to air was found to result in significant temperature decreases and char burnouts, which may lead to destabilization of the flame. The increase of the O<sub>2</sub> to 30 vol% results in a temperature profile similar to air combustion, while coal burnout is improved. NO<sub>x</sub> and CO levels are high in the main combustion zone, within the vicinity of the combusting coal particles. At the same line, the work developed by Nikolopoulos et al. (2011) presents a three-dimensional numerical investigation of a pulverized-fuel, tangentially-fired utility boiler located at Florina/Greece under air, partial and full oxy-fuel conditions. The Computational Fluid Dynamic - CFD techniques was applied. At this work, the ECO-Scrub concept was compared with the standard air combustion operation, as well as with a full oxy-fuel combustion retrofit. Results are compared regarding the temperature and velocity fields, species concentrations, heat transfer, particle burnout and NO<sub>x</sub> emissions. The simulation results indicate that the implementation of oxy-firing conditions in large scale boilers is quite sensitive as far as its efficient operation is concerned. Phenomena such as char burnout percentage and hopper losses by solid particles having high temperatures cannot be taken into account by thermodynamics studies in contrast to CFD approaches.

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 for CE 3100 benefited coal, aiming to verify the possibility of retrofitting the boiler of this power plant to oxy-fuel process. It was considered the post-combustion CO<sub>2</sub> capture option, where this CO<sub>2</sub> is recycled and re-injected on the combustion processes in a mixture with pure oxygen, composing the oxidant for burning the pulverized coal. This situation was compared with the conventional combustion processes actually used on this boiler for the CE 3100 pulverized coal combustion. At both cases was used the same thermal load. Data about the pollutants formation, as NO<sub>x</sub> and CO, temperature and concentration fields for each case are obtained and compared.

## 2. MATHEMATICAL FORMULATION

A steady-state combustion 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 nitrogen was considered inert and the carbon monoxide oxidation is modeled by the second reaction above.

The hydrogen oxidation is modeled by:



When the atmospheric air is used as the oxidizer, the formation of NO<sub>x</sub> 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 NO-prompt 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. Here, on the coal devolatilisation process, is assumed that the 50% of the nitrogen of the fuel is instantly converted in HCN, and the complement is not oxidized, i.e., inert. At this way, the HCN oxidation to form NO is modeled to NO-fuel and NO-prompt by:



The HCN oxidation to consume the NO is



The HCO oxidation is modeled by



And, to the reburn of NO by the CH<sub>4</sub> fuel gas:



To oxy-fuel case was assumed that the nitrogen of the fuel is the unique source for NO<sub>x</sub> formation. 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 (Ansys 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:

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

where  $\tilde{U}_j = \sum \left( \tilde{\rho}_i \tilde{U}_{ij} \right) / \bar{\rho}$ ,  $\tilde{\rho}_i$  and  $\bar{\rho}$  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  $\bar{S}_i$  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,

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

where  $D_i$  is the kinetic diffusivity. The mass fraction of component  $i$  is defined as  $\tilde{Y}_i = \tilde{\rho}_i / \bar{\rho}$ . 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:

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

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.  $\bar{S}_v$  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- $\varepsilon$  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

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

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  $\bar{T}$  is the average temperature of the mixture,  $h_{\alpha}^0$  and  $\bar{T}_{ref,\alpha}$  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),  $\bar{\rho} = p \overline{MM} \left( \bar{R} \bar{T} \right)^{-1}$ , where  $p$  is the combustion chamber operational

pressure, which is here set equal to 101 kPa, and  $\overline{MM}$  is the mixture molecular mass. The aforementioned equations are valid only in the turbulent core, where  $\mu_i \gg \mu$ . 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 (Ansys 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 six species:  $\text{O}_2$ ,  $\text{CH}_4$ ,  $\text{N}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}_2$  and  $\text{CO}$ ,  $\text{NO}_x$ ,  $\text{HCN}$  and  $\text{HCO}$ . 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,  $\bar{R}_{\alpha,k}$ . Thus,  $\bar{R}_{\alpha} = \sum_k \bar{R}_{\alpha,k}$ . The rate of formation or destruction,  $\bar{R}_{\alpha,k}$ , 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.

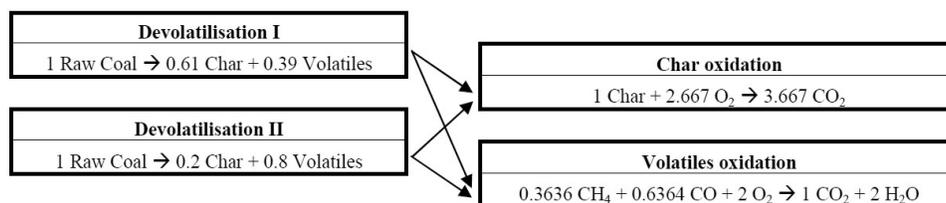


Figure 1. Basic scheme of the full chemical reactions of the raw coal.

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. 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.

### 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.

## 4. NUMERICAL METHOD

The flow fields inside the boiler (velocity, temperature, concentrations, etc.) were numerically determined with the commercial software Ansys CFX 11, 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 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 also the rectangular curve and the economizer tube bank. The outlet of the domain presents a pressure of -400 Pa (measured). 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, as 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.

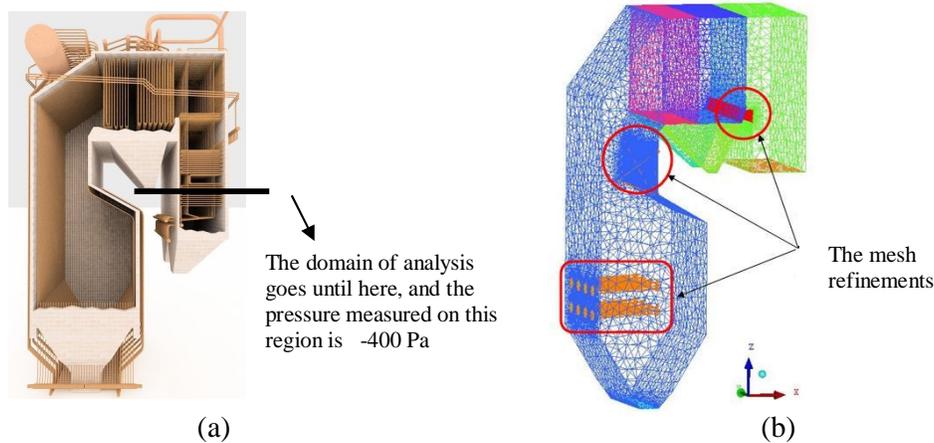


Figure 2 – (a) General disposition of the boiler components; (b) Mesh details: General view at the walls and refinements.

## 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 operation were considered for the coal blend as follows, as well as the chemical composition of the coal is show in Tab. 1. For both cases was considered the same excess air and the same thermal load.

### Case I: Conventional pulverized coal combustion for coal CE3100 from Brazil

**Inlet:** The inlet conditions are those for oxidizer and coal flows entering the domain from the burner nozzles. Here the oxidizer is the atmospheric air. 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: Oxy-fuel process for coal CE3100 from Brazil

**Inlet:** The inlet conditions are those for oxidizer and coal flows entering the domain from the burner nozzles. Here the oxidizer is a mixture of 30% of oxygen, 10% of moisture and 60% recirculation  $\text{CO}_2$  of the flue gas. Total primary and secondary oxidizer, 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 oxidizer and coal, and secondary oxidizer were set as 373 K and 550 K respectively. Pulverized coal size was modeled by Rosin-Rammler probabilistic distribution and limited between 50  $\mu\text{m}$  and 200  $\mu\text{m}$ .

Table 1 – Chemical composition of the coal blend.

Coal Chemical Species	CE3100 Dry Base	CE3100 Wet Base
Char	33.21 %	27.74 %
Ash	54.78 %	<b>45.76 %</b>
Oxygen	7.92 %	6.62 %
Hydrogen	2.34 %	1.95 %
Sulfur	1.14 %	0.95 %
Nitrogen	0.61 %	0.51 %
Humidity	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 temperature of the boiler walls, covered with slanting tubes from the bottom until the top, was set equal to 550 K, which is the saturation temperature to the pressure of vapor into the boiler tubes. The wall emissivity was set to 0.6 and all the other regions, as inlet and outlet regions, were considered as blackbodies. The methodology employed in the present work has been tested and validated in Silva et al. (2011), presenting good agreement with the validation data. In this work, the sulfur content of the coal was considered inert in the combustion processes. The continuation of the research will provide a chemical reaction for this species.

## 7. RESULTS

Here the simulation results were analyzed and compared for both cases. The main available parameters were the temperature and mass fraction of some chemical species, as well as the trajectories of the coal particles to 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  $O_2$  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 temperature ranges in this plane into the boiler are not similar for both cases, but they are physically coherent. To oxy-fuel process the higher temperature achieve levels above 1800 K. By Fennimore approach, used to predict the NO-prompt and NO-fuel on the combustion process, as mentioned by Lacava, 2000, this increases the levels of NOx production into the chamber, as can be verified in Fig. 6. At this way, for the operation conditions used at this work, the oxy-fuel process improve the combustion process, but produce higher levels of NOx.

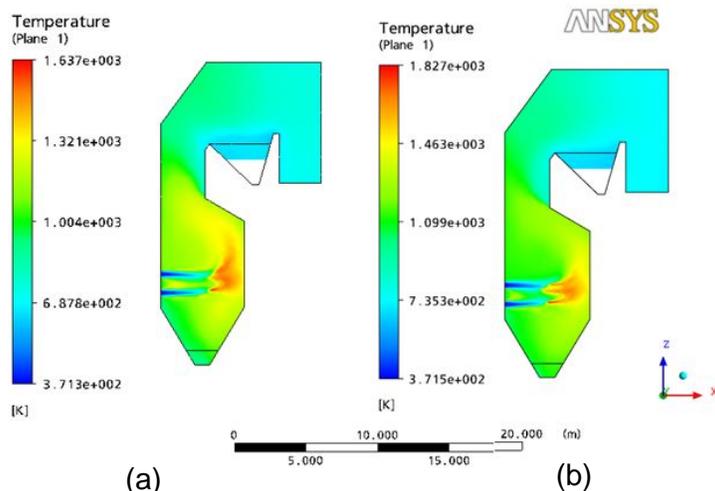


Figure 3 - Temperature field for a vertical plane into the boiler: (a) Conventional combustion; (b) Oxy-fuel

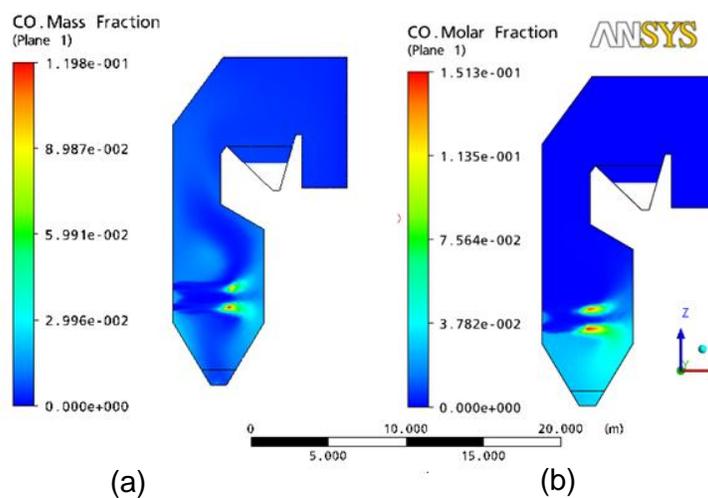


Figure 4 - CO mass fraction for a vertical plane into the boiler: (a) Conventional combustion; (b) Oxy-fuel.

In Fig. 4 is possible to see that the CO concentration at the burners inlet jet is almost null in practically its entire extension, and increases until its maximum value next to the end of the jets (in flame, region of high temperatures), as a result of pre-heating and coal devolatilisation on the process. Note, at oxy-fuel case, that at the region below of jets, and also immediately above them, exists a high quantity of this chemical species, product of coal devolatilisation and also of the partial combustion of methane, also devolatilised in this same process. However, for both cases, this CO recirculates at the combustion chamber, again passing through the flame region that is rich in oxygen (see Fig. 5), being practically burnt on the process.

Figure 5 shows a comparison between oxygen concentration fields for the conventional CE 3100 pulverized coal burning process, and for the oxy-fuel process, under the same vertical transversal plane. Note that for the case of oxy-fuel was injected a higher quantity of oxygen on the oxidant, 30% of the mixture, while the conventional combustion has 23% of  $O_2$ , i.e., for the oxy-fuel process the flame in oxygen richer. One can observe that the higher oxygen concentration is in the inlet jet regions for both cases. Also note that the oxygen is consumed more intensely in the conventional process of firing than in the oxy-fuel process, thus leaving a lower concentration of oxygen in the flue gases. The fact of increasing the oxygen concentration in the oxidant from 23% to 30% improves the burning efficiency and produces higher temperature levels into the chamber, as verified in Fig. 3.

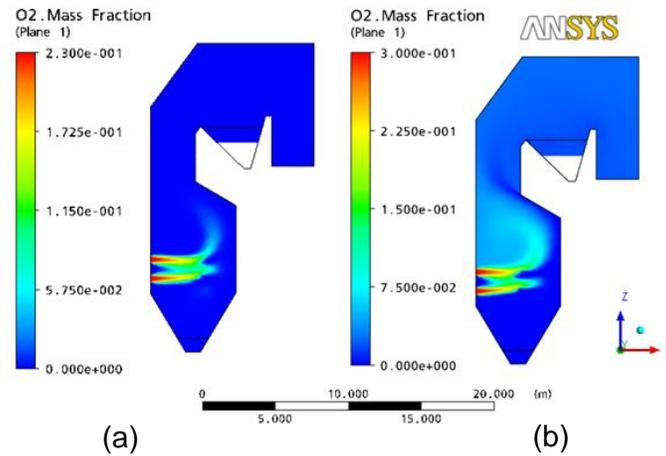


Figure 5 - O<sub>2</sub> mass fraction for a vertical plane into the boiler: (a) Conventional combustion; (b) Oxy-fuel.

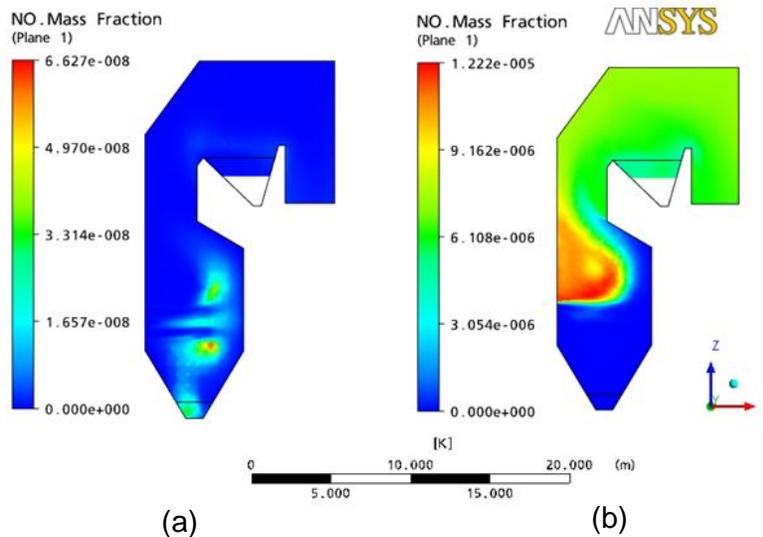


Figure 6 - NO mass fraction for a vertical plane into the boiler: (a) Conventional combustion; (b) Oxy-fuel.

Table 2 shows the average mass fraction of the chemical species of flue gases in the outlet region for both cases. It may be noted that for some chemical species the mass fraction shows a large variation between the cases, for example, the CO mass fraction, that decreases, and NO<sub>x</sub> that, conversely, suffers a relative increase, as expected due to the oxy-fuel conditions here studied.

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

	Conventional pulverized coal combustion to CE 3100		Oxi-fuel combustion process to CE 3100	
	Absolute value	Relative	Absolute value	Relative
Temperature	712.8 K	-	715.3 K	-
CO*	0.0033 [kg/kg]	0.33 %	1.32x10 <sup>-6</sup> [kg/kg]	1.32 ppm
CO <sub>2</sub> *	0.2571 [kg/kg]	25.7 %	0.8315 [kg/kg]	83.15 %
CH <sub>4</sub> *	0.0016 [kg/kg]	0.15 %	3.07x10 <sup>-8</sup> [kg/kg]	0.0307 ppm
H <sub>2</sub> O*	0.0591 [kg/kg]	5.9 %	0.1461 [kg/kg]	14.6 %
N <sub>2</sub> *	0.6804 [kg/kg]	68 %	3x10 <sup>-4</sup> [kg/kg]	0.03%
NO <sub>x</sub> *	1.12x10 <sup>-9</sup> [kg/kg]	1.12x10 <sup>-3</sup> ppm	6.66x10 <sup>-6</sup> [kg/kg]	6.66 ppm
O <sub>2</sub> *	~0 [kg/kg]	~0 %	0.0217 [kg/kg]	2.17 %
H <sub>2</sub> CN*	3.4x10 <sup>-4</sup> [kg/kg]	0.034 %	3x10 <sup>-4</sup> [kg/kg]	0.03 %
HCO*	4.47x10 <sup>-9</sup> [kg/kg]	4.47x10 <sup>-3</sup> ppm	1.62x10 <sup>-11</sup> [kg/kg]	1.1x10 <sup>-5</sup> ppm
Total	1 [kg/kg]	100 %	1 [kg/kg]	100 %

\*All absolute data are mean values.

## 8. CONCLUSIONS

Based on the study realized in this work, the main conclusion is that the boiler operation conditions for the CE3100 are not the best ones, resulting in inefficiencies at combustion process, confirming that the conventional pulverized coal combustion really presents some problems to the boiler operation. Thus, the retrofit of this unit to an oxy-fuel process can be an alternative to improve the performance of the equipment using this type of coal; can also be a good solution for reducing pollutant emissions to the atmosphere. However is necessary to make an economical analysis to verify a viability of this retrofit.

## 9. ACKNOWLEDGEMENTS

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