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PULVERIZED COAL UTILITY BOILER CFD MODELING OF A 360 MW POWER PLANT OPERATING WITH FAULTY OVER-FIRE AIR

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Abstract. *This work presents a numerical modeling applied on the real-scale geometry of a 360 MW steam generator to predict the behavior of coal combustion during an OFA maintenance. An Eulerian modeling of conservation equations of mass, momentum, energy and chemical species as well as the turbulence. For coal transportation and ash particles a Lagrangian modeling coupled with gas-phase was used. The objective is to develop a computational model capable of predict the behavior of reactive, turbulent and non-isothermal multiphase flow of a real-scale steam generator in order to investigate the influence of the OFA faulty operation. The results show that the reactive flow is bent towards the frontal wall, it implies an increased heat transfer on the water walls causing operation risks. Besides that, since the reaction implied by the burners is sub stoichiometric unburned combustion gases and coal particles remains in the flue gases, causing several hazards and efficiency loss.*

Keywords: *CFD, Coal Combustion, Utility Boiler, Turbulence, Sub Stoichiometric Operation, Faulty OFA.*

1. INTRODUCTION

There are several ways to produce energy. However, in the present days, coal is still present in the energy matrix of a considerable number of countries. This fuel meets the current demand but presents some negative characteristics. Coal combustion is highly harmful to the environment, sharing responsibility for the greenhouse effect impacts. Another negative particularity is that coal reserves are finite, which means that it will end up in few decades. Thus, studies to enhance the efficiency in coal combustion processes are extremely necessary, also aiming to understand the losses that faulty operational conditions can cause.

Several authors have been using CFD codes for boiler's arrangements studies, pulverized coal boilers with front burners, low NO_x burners (Kurose et al., 2004), variations in operating conditions, such as moisture content and size of coal particle (Bosoaga et al., 2006; Al-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 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 - Weighed-Sum-of-Gray-Gases were applied to the radiative 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), also using a commercial CFX code studied the behavior of pulverized coal combustion in a real boiler of a 160 MW thermal power plant in order to validate the model, simulate the operation and identify possible factors of inefficiency. In another work, Guo et al. (2015) simulated a 200 MWe tangentially fired boiler, which uses pulverized coal as fuel, to investigate the influence of the oxy-combustion process on boiler performance. Seven simulations were performed: one air-fired (reference case) and six others with oxy-fuel combustion.

In the same line of this research, Wenjing et al. (2015) developed a numerical investigation to study the pulverized coal combustion process in a 660 MWe tangentially-fired ultra-supercritical boiler. The authors, carrying out a three-dimensional numerical simulation based on the Eulerian-Lagrangian approach, used the k- ϵ turbulence model for the gas coupled phase, the P-1 radiation model for radiation, and a two-competing-rates model for the devolatilization. The purpose of the study was to investigate the effect of air distributions on boiler performance, evaluating flow, temperature,

species components and NOx emissions. As results, with the application of OFA (over-fire air) and AA (additional air), a little temperature decrease in the combustion zone occurs, which causes a reduction in NOx formation.

Silva, C.V. et al. (2019) studied the air leakage influence inside the boiler's furnace of a 160 MWe power plant. Three cases were studied concerning the amount of air leakage across the boiler water seal. The influence of the air leakage was analyzed with emphasis on temperature profiles, flow, wall heat flux, O₂, CO, NOx, Soot and CO₂ formation. As main results, it has been observed that air leakage across the water seal has influence over the profiles of temperature and concentration of oxygen and carbon dioxide. Significant amounts of air leakage can induce the plant staff to change the amount of air to be fed through the burners, changing the burning condition, thus impairing energy generation.

In this way, the present paper aims to study the influence of a faulty Over-Fire Air system over the profiles of temperature and mass fraction of oxygen, methane, carbon dioxide and carbon monoxide in a steam generator utility boiler of a 360 MWe power plant. To analyze the main combustion behavior, flue gas composition and thermal profile, a computational model capable of predict the behavior of reactive, turbulent and non-isothermal multiphase flow was used.

2. NUMERICAL METHOD

Property fields in the boiler were numerically determined using the commercial software Ansys CFX 19, 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. To compute the results a structured mesh was generated for the utility boiler and for the burners a hexahedral mesh, the total element number was about 41 million volumes. Table 1 show the methods used to evaluate mesh quality.

Table 1 – Mesh quality evaluate methods.

Criterion	Value	Percentual of Elements
Aspect Ratio – HEXA and QUAD	> 0.9	70%
Aspect Ratio – HEXA and QUAD	> 0.8	98%
Equiangle Skewness	> 0.9	50%
Equiangle Skewness	> 0.8	90%

3. MATHEMATICAL MODEL

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.

The kinetic scheme for coal particles pyrolysis used in this work was proposed by Silva et al. (2010), assuming that coal is composed of raw coal, ash and moisture. The raw coal decomposes into volatile gases and residual carbon by two devolatilization concurrent reactions, according to Ubayakar et al. (1976). The methane oxidation is modeled by two overall steps, the WD2 of Westbrook and Drier (1981). NOx formation is modeled through the NO-thermal, NO-prompt and NO-fuel mechanisms, according to the simplifications proposed by the methodology implemented in ANSYS - CFX (Ansys, Inc., 2019). Complementing this formulation, the drying of coal particles model proposed by Xianchun et al. (2009) was used. The kinetic parameters used in this reaction, namely the pre-exponential factor and the activation energy, are respectively $4.587 \times 10^{12} \text{ s}^{-1}$ and 78.995 kJ/kmol (Xianchun et al., 2009). For the residual char, the field char oxidation model (Ansys Inc., 2019) was adopted.

For a multicomponent fluid, scalar transport equations are solved for velocity, temperature and species mass fractions. 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 due to changes in composition. Each component has its own equation for mass conservation. After Favre-averaging the species conservation equation can be expressed in tensor notation as

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{U}_j \tilde{Y}_i) = \frac{\partial}{\partial x_j} \left(\left(\rho D_i + \frac{\mu_t}{Sc_t} \right) \frac{\partial \tilde{Y}_i}{\partial x_j} \right) + \bar{S}_i \quad (1)$$

where μ_t is the turbulent viscosity, Sc_t is the turbulent Schmidt number, \bar{S}_i is the source term for component i which includes the effects of chemical reactions, D_i is the mass diffusivity, $\bar{\rho}$ is the 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 $\tilde{Y}_i = \tilde{\rho}_i / \bar{\rho}$. Note that the sum of component mass fractions over all components is equal to one.

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

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{U}_i \tilde{U}_j) = -\frac{\partial p^*}{\partial x_j} \delta_{ij} + \frac{\partial}{\partial x_j} \left(\mu_{eff} \frac{\partial \tilde{U}_i}{\partial x_j} \right) + \frac{\partial \tilde{U}}{\partial x_j \partial x_i} + \bar{S}_U \quad (2)$$

where $\mu_{eff} = \mu + \mu_t$, μ is the mixture dynamic molecular viscosity and $\mu_t = C_\mu \rho k^2 / \varepsilon$ is the turbulent viscosity. The term $p^* = \bar{p} - (2/3)k$ is the modified pressure, $C_\mu = 0.09$ is an empirical constant of the turbulence model, \bar{p} is the time-averaged pressure of the gaseous mixture, and δ_{ij} 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 was used to represent the buoyancy force due to density variations. The $k-\omega$ model was used to model the turbulence on the flow (Wilcox, 1988). The energy conservation equation can be written as

$$\frac{\partial}{\partial x_j} (\bar{\rho} \tilde{U}_j \tilde{h}) = \frac{\partial}{\partial x_j} \left(\kappa \frac{\partial \tilde{T}}{\partial x_j} + \sum_i^{Nc} \tilde{h}_i \left(\rho D_i + \frac{\mu_t}{Sc_t} \right) \frac{\partial \tilde{Y}_i}{\partial x_j} + c_p \frac{\mu_t}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j} \right) + \bar{S}_{rad} + \bar{S}_{rea} + \bar{S}_T \quad (3)$$

where \tilde{T} , \tilde{h} and c_p are the average temperature, enthalpy and specific heat of the mixture, $C_{p,i}$ and \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, \bar{S}_{rad} , \bar{S}_{rea} and \bar{S}_T represent the sources of thermal energy due to the radiative transfer, the chemical reactions and sink our source of energy. The focus of this study was to evaluate the main reactive flow and species formation, so the radiative transfer was neglected. The term \bar{S}_{rea} can be written as

$$\bar{S}_{rea} = \sum_i \left[\frac{h_i^0}{MM_i} + \int_{T_{ref,i}}^{\tilde{T}} c_{p,i} d\tilde{T} \right] \bar{R}_i \quad (4)$$

where h_i^0 and $T_{ref,i}$ 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, 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. Close to the wall, the conventional wall logarithmic law is used (Nikuradse, 1933).

The reactions model employed in this work assumes finite rate reactions and a steady state turbulent combustion process to volatiles (CH₄ and CO) involving six species: O₂, N₂, CH₄, H₂O, CO₂ e CO. Thus, one has the conservation equation for the i -th chemical species, given by Eq. (3), where the source term, S_i , considers the average volumetric rate of formation or destruction of the i -th chemical species in 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, $\bar{R}_{i,k}$. Thus, $\bar{R}_i = \sum_k \bar{R}_{i,k}$. A combined Arrhenius-Magnussen model was used to obtain this rate (Eaton et al., 1999).

The kinetic scheme used in this paper for particle pyrolysis assumes that mineral coal is composed of raw coal, ash and moisture. Raw coal decomposes into char and volatile gases through two devolatilization competing reactions (R1 and R2, see Fig. 1), following the model proposed by Ubhayakar et al. Ashes and moisture present in the coal do not generate energy.

To increase the accuracy of the model, a reaction that predicts coal particles drying was implemented. This model, proposed by Xianchun et al., states that the wet coal particle undergoes a chemical reaction prescribed by the Arrhenius model, thus leading to moisture evaporation at a temperature of 373 K, resulting in dry raw coal and water vapor.

Table 1 presents the kinetic constants for the reactions involving coal particle.

Table 1 – Kinetic constants for coal particles reactions.

Reaction	$A_{r,i}$	$E_{r,i}$ or Activation Temperature
R_0	$4.5874 \times 10^{12} \text{ kg}^{-2} \text{ m}^6 \text{ s}^{-1}$	78,995 J/mol
R_1	$1.34 \times 10^5 \text{ 1/s}$	8,852 K
R_2	$1.46 \times 10^{13} \text{ 1/s}$	30,189 K

The conversion of raw coal into char and volatiles is done by

$$\frac{dC_o}{dt} = -(k_1 + k_2)C_o \quad (5)$$

where k_1 and k_2 are the reaction rates for the Arrhenius model [$\text{s}^{-1}(\text{mol m}^{-3})^{(1-n)}$]. Analogously, production rate of volatiles (dV/dt) [kg/s] and char formation [kg/s] can be determined by

$$\frac{dV}{dt} = (Y_1 k_1 + Y_2 k_2)C_o \quad (6)$$

$$\frac{dC_{ch}}{dt} = ((1 - Y_1)k_1 + (1 - Y_2)k_2)C_o \quad (7)$$

where k_1 and k_2 are the reaction rates for the Arrhenius model [$s^{-1}(\text{mol m}^{-3})^{(1-n)}$]. Analogously, production rate of volatiles (dV/dt) [kg/s] and char formation [kg/s] can be determined by

$$D_{O_2} = k_d(p_g - p_s) \quad (8)$$

where p_g is the O_2 partial pressure [Pa] in the hot gases away from the boundary layer of the particle and p_s is the oxygen pressure on the particle [Pa] surface. The value of k_d , which is the chemical reaction rate of oxygen diffusion [kg/(m² s)], can be obtained using

4. DESCRIPTION OF THE BOILER AND BOUNDARY CONDITIONS

The boiler studied is part of a power generation plant that use pulverized coal as fuel. The combustion chamber operates with frontal burning with colliding jets. The Fig. 1 show the boiler and burner geometry.

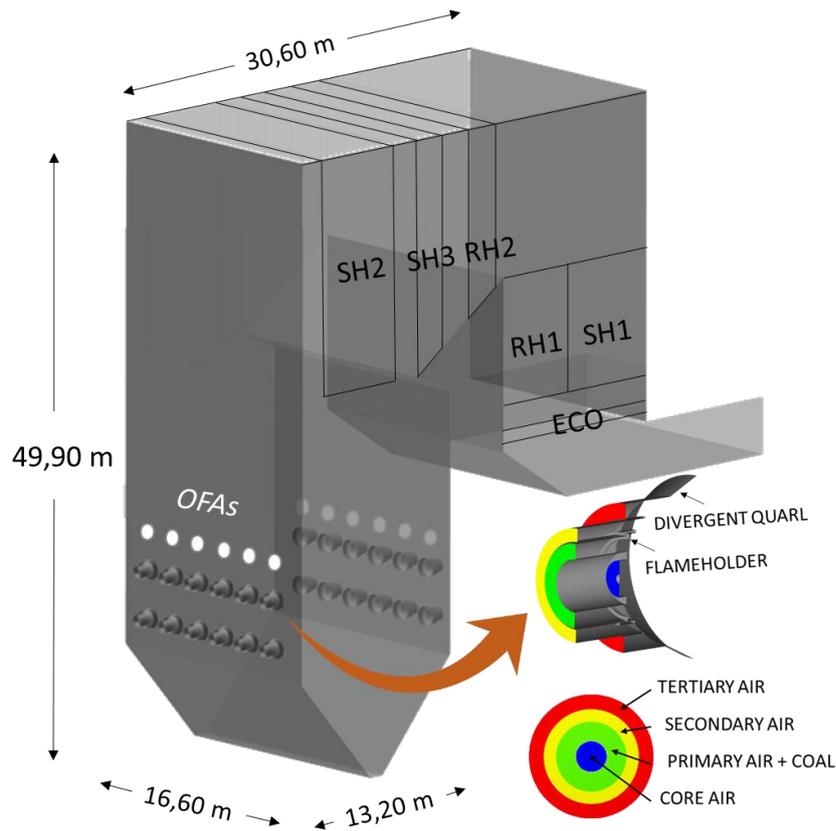


Figure 1 – Utility boiler components: Economizer (ECO), Re-Heater 1 (RH1), Re-Heater 2 (RH2), Super-Heater 1 (SH1), Super-Heater 2 (SH2), Super-Heater 3 (SH3), Over-Fire Air inlets (OFAs) and Burners as detailed.

The boiler furnace region is 16,60 m, 13,20 m and 49,90 m in width, depth and height, respectively. In the burners zone, 24 burners are arranged in 4 rows of 6 burners, 2 rows installed on the front wall facing the other 2 rows of the back wall. Twelve Over-Fire Air inlets are used in this boiler, they are arranged in 2 rows of 6 above the top row of burners on each wall.

The boundary conditions were presented at Tables 1 to 5. Values referring to mass flows, temperatures and compositions were provided by the power plant staff.

Table 1 – Boundary conditions for each burner.

Boundary	Mass Flow [kg s ⁻¹]	Temperature [K]	Swirl
Core Air	0.1	300	-
Primary Air	4	420	-
Coal	2*	650**	-
Secondary Air	3.5	620	0.45***
Tertiary Air	8.5	620	0.6***

Data obtained from the power plant staff. *Mass flow estimated equalizing the Calorific Power of the coal used in simulation to original one used by the plant. **Value used to increase devolatilization inside combustion chamber. *** Estimated values from the swirlers blade's angle drawings

Table 2 – Coal ultimate analysis and gross calorific value.

Component	Dry Basis
Total Moisture	6.23 %
Ash	11.98 %
Sulphur	0.34 %
Carbon	65.91 %
Hydrogen	4.59 %
Nitrogen	2.09 %
Oxygen	8.89%
Gross Calorific Value	27098 kJ/kg

Table 3 – Boundary conditions for the walls.

Variable	Temperature [K]	Mass and Momentum
Combustion chamber and SH2 region walls	608	No Slip
Heat exchangers walls	500*	No Slip
Burners walls	Adiabatic	Free Slip
OFA's	Adiabatic	Free Slip

*Estimated as the average value of flue gas temperatures at the volume after the RH2

Table 4 – Thermal exchange values for the heat exchangers.

Exchanger	Moment Loss Quadratic Coefficient [kg m⁻⁴]	Value [W m⁻³]
ECO	2.54	- 161,415.00
RH1	0.49	- 126,102.00
RH2	1.89	-99,229.00
SH1	0.48	-64,970.00
SH2	0.35	-104,026.00
SH3	0.15	-93,374.00

Data obtained from the power plant staff.

Table 1 characterizes inlet parameters at a stoichiometric value of 0.8, during operation core air is kept turned off but there's some always some mass flow directed to that duct, so it was considered a low mass flow to represent it. Primary air is fed with coal to the combustion chamber. Secondary air and tertiary air have a swirler installed on each inlet, this mechanism is composed by several blades that deflects the flow causing the swirl movement. The swirl movement represents a relation between axial and tangential velocities. Table 2 shows the coal chemical composition in dry and wet basis used in this simulation, Table 3 presents the assumed wall properties. The free sleep condition was assumed on burners walls to reduce perturbations of coal combustion area and the swirl movement formation. OFA's inlets were considered as walls with free slip conditions assuming there's an air pocket on caused by the faulty system.

Values in Tab. 4 indicate that energy is being transferred from the flue gases to the working fluid inside the heat exchanger tubes, this was obtained multiplying the steam mass flow by the delta enthalpy of inlet and outlet of each exchanger and the negative signal indicate the energy is leaving control volume. The domain outlet was set as being the opening located at the end of the volume control after ECO, having a prescribed pressure of -400 Pa. Steady state conditions were assigned for the computational simulations, together with a buoyancy of 9.81 m/s².

5. RESULTS

Figure 2 shows the velocity field in a vertical plane and horizontal sections along that plane in the combustion chamber, also SH2 and SH3 region.

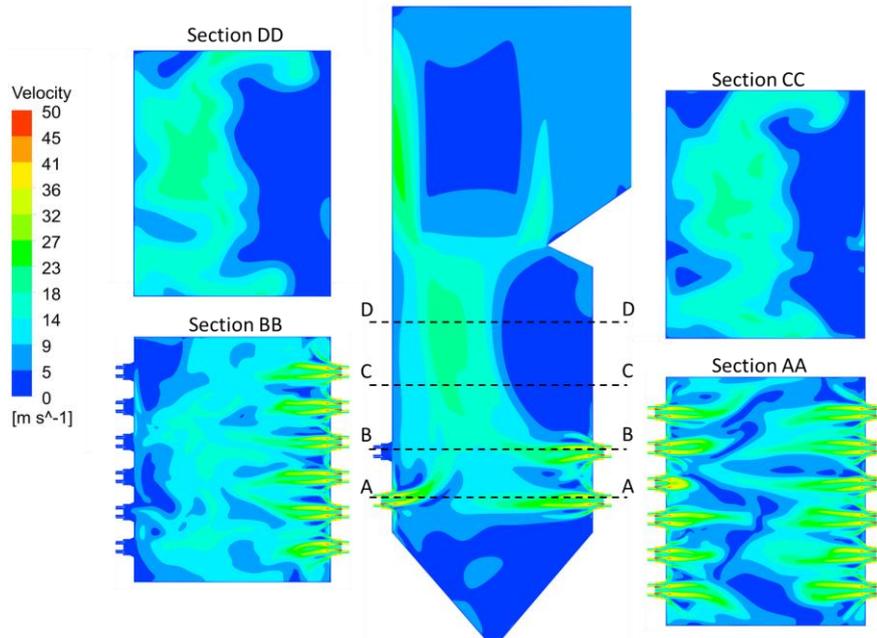


Figure 2. Velocity field of a transversal plane passing through the center of a burner. Horizontal sections are also shown for different heights of the combustion chamber: AA (9.2 m), BB (14.5 m), CC (17.5 m) and DD (19.2 m).

The highest speed is achieved at the primary air inlet of each burner, it's possible to see in this area a great speed difference between the air passing through the flame holders and the air stuck behind it. The acceleration is caused by the reduction of the passing area, and the flame holders are responsible for a recirculation to anchor the flame.

The speed's range from 60 ms^{-1} to zero on the walls of the equipment. In the figure is possible to observe that the flow is bent toward the boiler's front wall (left side of image), causing the flow to carry more energy to that area. Figure 3 shows the flow configuration of a single burner.

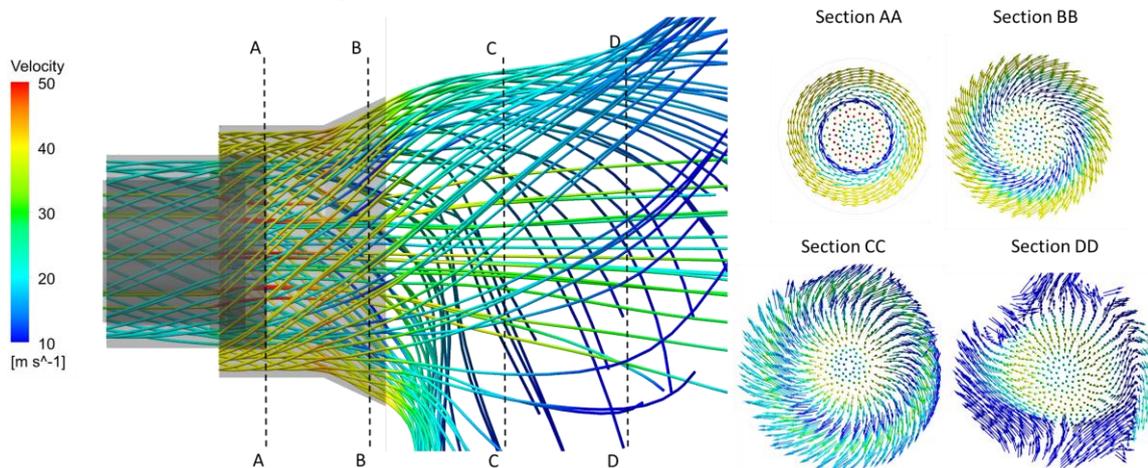


Figure 3. Streamlines of a single burner showing the flow profile and it's disturbance by the control volume. Sections show vectors in 4 different stages. Swirl can be seen at the vectors.

The streamlines show the overall flow and the sections show how it behaves inside and outside the burners. Is noticeable how the flow is perturbed by the turbulence present inside the furnace in the section DD.

Figure 4 shows the temperature field in a vertical plane and horizontal sections along that plane in the combustion chamber, also SH2 and SH3 region.

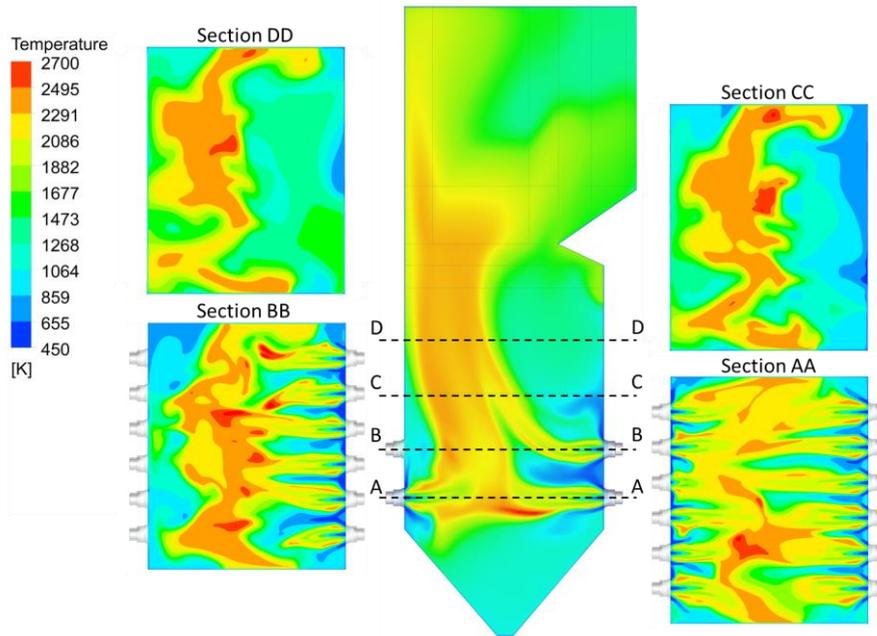


Figure 4. Temperature field of a transversal plane passing through the center of a burner. Horizontal sections are also shown for different heights: AA (9.2 m), BB (14.5 m), CC (17.5 m) and DD (19.2 m).

The highest temperatures are distributed along the main flow in the combustion chamber region reaching SH2 region, the fuel and air inlet jets at low temperatures characterizing the flame region. There is also a decrease in the temperatures in the flow path towards the exit region of the boiler promoted by the energy absorption of the heat exchangers (SH2 and SH3) located at the top of the area shown. Both exchangers are modeled with source terms where the volumetric rate of heat absorption and the corresponding loss of charge are prescribed for representing the tube banks of these heat exchangers.

The temperature adjacent to front wall is 1602.53 K while back wall's adjacent temperature is 1191.4 K. The average heat flux is $13,824.2 \text{ Wm}^{-2}$ and $5,630.1 \text{ Wm}^{-2}$, respectively.

Figure 5 shows the methane, carbon monoxide, dioxide and oxygen mass fraction fields in the combustion chamber.

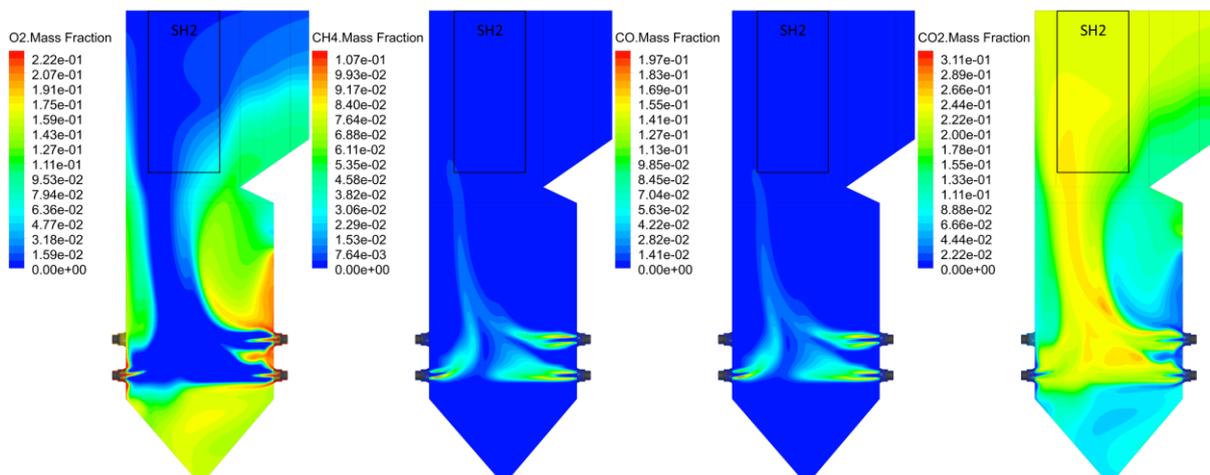


Figure 5. Oxygen, methane, carbon monoxide and dioxide mass fraction fields in the combustion chamber.

In the oxygen mass fraction field, it's possible to see that the higher concentration of oxygen is in the core, secondary and tertiary air inlets. The coal enters with primary air, so it also shows a fair concentration of oxygen before the oxidation region. The methane is the product of coal devolatilization, its highest concentration is present in the burner's primary air main flow and it's quickly converted to carbon monoxide and later to carbon dioxide. Carbon monoxide mass fraction field is very similar to methane field, since they have a close correlation. The last image shows the carbon dioxide field, its lowest concentration is close to the inlets and the highest in the main reactive flow.

These burners operate on a sub-stoichiometric regime usually between 0.8 and 1 oxidizer to fuel ratio, and the OFAs are responsible to provide more air until reach a 1.2 ratio. Since the OFAs aren't in operation, it is possible to see in the

oxygen mass fraction field image that all the oxygen was consumed in the main flow stream. That leads to unreacted and unburned fuel reaching the heat exchanger (SH2) region. For this simulation, even with a stoichiometry of 1, the air coming from secondary and tertiary inlets can't penetrate the main flow. In this type of situation, the operation becomes extremely unsafe, the excess heat in the front wall may damage the tubes causing water leakage and steam pressure loss and the unburned fuel may accumulate on the heat exchangers causing an explosion or outside the utility boiler's furnace, harming other equipment.

6. CONCLUSION

In this paper, a CFD code has been used to investigate the pulverized coal combustion process in a 360 MWe tangentially fired boiler, considering a faulty OFA operation. The results obtained showed that even with a stoichiometry of 1, the secondary and tertiary air can't mix with the main flow, thus can't guarantee a stoichiometry condition. The lack of oxygen in the main flow causes unburned fuel to reach heat exchangers (SH3), which may accumulate on the heat exchangers causing an explosion or outside the utility boiler's furnace, harming other equipment.

For future works a further investigation on a way to compensation the OFAs may be applied, increasing the swirl number and using the disabled row to provide air to the main flow.

7. RESULTS

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