

CFD CODE FLOREAN FOR INDUSTRIAL BOILERS SIMULATIONS

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Abstract: - Computational fluid dynamics (CFD) becomes more and more reliable tool to analyze the furnace operation under different conditions. This paper provides an overview of the current possibilities of 3D-Finite Volume tool FLOREAN developed at the Institute for Heat and Fuel technology TU Braunschweig. This program is used for simulations of combustion processes in industrial furnaces. Distributions of different parameters such as temperature, fluid flow properties (velocities, pollutant substances such as CO, NOx) etc. are simulated. These simulations can be used to design furnaces, optimize furnace operation and minimize pollutant emissions.

Key-Words: Computational fluid dynamics, Combustion, Pollutant Emission, Furnace design and operation.

1 Introduction

In the last years Computational Fluid Dynamics - has become a more and more reliable tool to check the design of industrial furnaces and power plants [1-3]. The present paper provides an overview of the current capabilities of the CFD-computer code FLOREAN (acronym for FLOW and REAcTioN) developed at the Institute for Fuel and Heat Technology, Technical University of Braunschweig, Germany.

Simulation tool FLOREAN allows to get detailed information about furnace performance including velocities, temperature, thermal radiation and concentration distributions etc. within the furnace and along the walls. The efficient combustion of solid fuel in combustion chambers and the efficient heat transfer to water and steam in steam generators are essential for the economical operation of power plants. This information is useful to evaluate the combustion process and to design optimal furnaces. FLOREAN will also be very useful in improving combustion process of different fuels in industrial boilers, optimizing operation and minimizing pollutant emission.

2 Mathematical model

A three-dimensional computational fluid dynamics code was used to analyze the performance of

different boilers with pulverized coal combustion at different operation modes. The main objective of this study was to show a number of possibilities of this three-dimensional furnace modeling as an effective method for design, optimization and problem solving in power plant operation.

Consequently, the FLOREAN - code was used to predict thermal and hydrodynamic aspects of flue gases mixing in the near wall region and inside the furnace. In the case of Over Fire Air (OFA) technology the simulations show that effective mixing between flue gases and overfire air is of essential importance for CO reburning and low NOx emissions.

Program FLOREAN is based on the numerical solution of the Reynolds averaged balance equations for mass, species, energy and momentum [1-4]. It predicts gas flows, species concentrations, temperature fields due to combustion, radiation and convective heat transfer and the pollutant formation and destruction in furnace chambers.

The transport by diffusion of each value is calculated by an effective exchange coefficient, based on the effective viscosity and the empirical Prandtl-Schmidt number. The mean flow equations are closed by the k-ε turbulence model.

The changes of the concentrations of the flue gas components and the fuel due to the combustion are taken into account in the source/sink terms by

appropriate submodels. In addition, in the source/sink term the heat balance takes into account the energy release due to the combustion reactions and the significant heat transfer due to radiation using a six flux radiation model by Lockwood etc [5].

The energy balance is written as follows:

$$\frac{\delta}{\delta x_i}(\rho U_i h) = \frac{\delta}{\delta x_i} \left\{ \frac{\mu_{\text{eff}}}{Pr} \left(\frac{\delta h}{\delta x_i} \right) \right\} + S_{\text{comb}} + S_{\text{rad}} \quad (1)$$

The right hand side of the energy equation contains the source term S_{comb} due to the combustion of volatiles, char and formed carbon monoxide. The source/sink term due to radiation is calculated using the six flux model of Lockwood and Shah [6]. It's mentioned that radiative heat exchange is one of the three basic ways of heat exchange and some researcher successfully couple computer methods and radiative heat exchange phenomena [7]. The time mean temperature is obtained from the calculated enthalpy using polynoms taken out of [8].

In many practical combustion processes the fuels are liquids or solids, which have to be evaporated, and/or gasified usually prior combustion. The additional consideration of a phase change leads to more complex heterogeneous combustion processes than combustion processes in the gas phase. In FLOREAN models for combustion of heavy fuel oil and different coal types are included.

Coal Combustion Model. The coal particle size distribution is modeled through different mean diameters. During the combustion process the coal particle diameters changes. The change depends on the coal type e. g. swelling coal. At the end ash and unburnt carbon is left.

The coal combustion model is divided into five submodels for drying, pyrolysis, combustion of volatiles, carbon monoxide and residual char. The drying model considers the heat necessary for evaporating the moisture content. The pyrolysis model is usually a first order reaction model; more detailed models are available. Three different reactions between char and flue gas are considered. The oxidation of the char to carbon monoxide or carbon dioxide and the reduction of carbon dioxide at the surface of the char particle to carbon monoxide. The model incorporates the different effects of oxygen and carbon dioxide diffusion to the particle surface and in the pores and the kinetics of the chemical reaction at the surface as a function of temperature and particle diameter.

The Eddy Dissipation Model according to Magnusson et al. is used to predict the combustion of the volatiles and the carbon monoxide formed during

char combustion. Gaseous fuels are treated like volatiles [9].

In the case of coal combustion the two phase flow can be treated using the Eulerian or the Lagrangian approach to calculate the flow pattern of the solid phase.

Multi diameter model. In the multi diameter model for each particle class the energy balance of the solid phase is solved. It is assumed that there is neglectable slip between gas and particles. Therefore no additional momentum balance is needed. The source/sink term is calculated by:

$$\dot{Q}_{P,1} = \dot{Q}_{C,1} + \dot{Q}_{R,1} + \dot{Q}_{Ch,1} - \dot{Q}_{D,1} - \dot{Q}_{MI,1} \quad (2)$$

$\dot{Q}_{C,1} \Rightarrow$ heat flux due to convection

$\dot{Q}_{R,1} \Rightarrow$ heat flux due to radiation

$\dot{Q}_{Ch,1} \Rightarrow$ heat generation due to char combustion

$\dot{Q}_{D,1} \Rightarrow$ heat loss due to vaporization of water

$\dot{Q}_{MI,1} \Rightarrow$ heat loss due to mass loss of the particle, e. g. drying, pyrolysis etc.

The convective heat flux is calculated under the assumption of spherical particles:

$$\dot{Q}_{C,1} = n_{P,1} \cdot \pi \cdot d_{P,j}^2 \cdot \alpha_i (T_G - T_P) \quad (3)$$

There is $n_{P,1}$ the number of particles in the control volume.

$$n_{P,1} = \frac{V \cdot \rho_S \cdot m_{P,1}}{\rho_{P,1} \cdot \frac{\pi}{6} \cdot d_{P,j}^3} \quad (4)$$

$V \Rightarrow$ volume

$\rho_S \Rightarrow$ density of suspension

$\rho_{P,1} \Rightarrow$ density of particles

$m_{P,1} \Rightarrow$ mass fraction of the particles

The heat transfer coefficient α_i between particle and gas has been calculated using constant Nusselt Number of magnitude two.

The radiative heat flux to the particles is calculated from the difference of absorbed and emitted radiation:

$$\dot{Q}_{R,1} = V \cdot K_{a,P,1} \cdot \left(\frac{4}{3} \pi \sum B_i - 4\sigma T_{P,1}^4 \right) \quad (5)$$

Here B_i is the heat flux of the six flux radiation model and $K_{a,P,1}$ the absorption coefficient of the particles.

The sink term in the particle energy balance due to mass loss is calculated as follows

$$\dot{Q}_{Ml,l} = c_{P,l} \cdot T_{P,l} \cdot (\dot{m}_{D,l} + \dot{m}_{V,l} + \dot{m}_{Char,Ch,l}) \quad (6)$$

$\dot{m}_{D,l} \Rightarrow$ mass loss due to vaporization

$\dot{m}_{V,l} \Rightarrow$ mass loss due to devolatilization

$\dot{m}_{Char,Ch,l} \Rightarrow$ mass loss due to char burnout

Devolatilization, char burnout and changing of particle diameter and density are calculated using models described above. In the Arrhenius expressions of the combustion model the particle temperature is used calculated from the energy balance of each particle class. The number of particle classes is arbitrary but increasing number of classes means increasing memory demand and computation time.

Fuel Oil Combustion Model. Three phases of droplet combustion are considered:

Heating phase: heat from the gas phase causes the droplet surface to heat up. Much of the energy is convected into the droplet until the entire droplet is approaching the boiling temperature.

Fuel evaporation stage: Fuel evaporates into the gas phase and a combustible mixture is formed; the droplet diameter decreases in time. The droplet evaporation model includes heat and mass transfer. Usually the continuous gas phase is at a higher temperature than the fuel droplets [10].

Combustion phase: The oil combustion model uses the Eddy Dissipation Model for the combustion of evaporated combustible species in the gas phase.

The changes of the concentrations of the flue gas components and the fuel due to the combustion are taken into account in the source/sink terms.

Chemically Reactive Species (Combustion).

Five gaseous Species are considered: oxygen, volatile matter, carbon monoxide and final combustion products consisting of carbon dioxide and water vapour. Three solid species char, coal and ash are taken into consideration. The mass balance of each species k is as follows:

$$\frac{\delta}{\delta x_i} (\rho U_{i,mk}) = \frac{\delta}{\delta x_i} \left\{ \frac{\mu_{eff}}{Sc} \left(\frac{\delta m_k}{\delta x_i} \right) \right\} + S_k \quad (7)$$

with m_k being the mass fraction of species k . Sc is the Schmidt number and S_k the source/sink term due to the reaction.

NOx formation model. Within the combustion of fossil fuels, nitric oxide is built up through different reaction paths. The main reactions are the oxidation of molecular nitrogen (thermal NO-formation) and the oxidation of the fuel

bounded nitrogen (fuel-NO).

Detailed kinetic models for predicting fuel NO with 29 elementary reactions are used, for example, by Ro and Lendt [11-12]. In the case of three-dimensional simulation, such models consume too much CPU-time. Therefore global mechanisms are used. In FLOREAN for simulation of nitrogen oxides formation the Zel'dovich mechanism for thermal NOx [13], De Soete [14] or the Mitchell-Tarbell [15] mechanisms for fuel NOx formation are applied.

Depending on the coal type, fuel-bound nitrogen is released during pyrolysis and char burnout. It is supposed that the main gas species containing nitrogen produced during coal combustion are HCN and NH3. In some modeling approach, volatile and char nitrogen is released only as HCN proportional to the char burnout rate. In FLOREAN, both HCN and NH3 release is possible.

De Soete mechanism. Recognizing the importance of HCN as a precursor to the subsequent nitrogen compound intermediates, De Soete [14] correlated the rate of NO formation and decay with a pair of competitive parallel reactions, each first order in HCN and NH3. This model describes the gas phase reaction of HCN and NH3 with an oxidation rate to NO and a reduction rate to N2. HCN and NH3 are competitively oxidized and reduced according to the following generic scheme involving four reactions:

$$\begin{aligned} R_1 &= 1.0 \cdot 10^{10} \cdot X_{HCN} \cdot X_{O_2}^a \cdot \exp\left(\frac{-33732.5}{T}\right) \\ R_2 &= 4.0 \cdot 10^6 \cdot X_{NH_3} \cdot X_{O_2}^a \cdot \exp\left(\frac{-16111.0}{T}\right) \\ R_3 &= -3.0 \cdot 10^{12} \cdot X_{HCN} \cdot X_{NO} \cdot \exp\left(\frac{-30208.2}{T}\right) \\ R_4 &= -1.8 \cdot 10^8 \cdot X_{NH_3} \cdot X_{NO} \cdot \exp\left(\frac{-13593.7}{T}\right) \end{aligned}$$

Mitchell and Tarbell model. A global model has been proposed by Mitchell and Tarbell [15], involving NH3, HCN, NO and N2 as N-containing species. The first reaction step is the conversion of HCN to NH3 by an attack of an oxidizing agent.

The NH3 forms and destructs NO within a pair of competitive parallel reactions. In their global model, Mitchell and Tarbell propose the recycling of NO back to HCN through hydrocarbons CxHy.

The postulated reaction rate of the NO recycling is not temperature dependent. The suggested value of the C atom number x in the hydrocarbons is eight [15], the value of y is calculated from coal analysis. The H2-concentration is calculated from equilibrium. In addition NO is reduced by a heterogeneous reaction between NO and char particles.

3 Results of CFD Studies

Kazakhstan has huge stocks of power resources, sufficient for covering own needs and export to other regions, both in a natural, and in the form of electric power. About 3,3 % of world industrial stocks of coals are concentrated in Kazakhstan. More than 70 % of the electric power in Kazakhstan are generated in Thermal Power Plants.

FLOREAN has been applied for the calculation of a furnace chamber of Aksu power station fired with low grade coal of Ekibastuz (Kazakhstan). It has to be emphasized that in Kazakhstan thermal power plants predominantly use bituminous and sub-bituminous coals from Ekibastuz, Karaganda, Kuuchekinsk.

Coals from these basins have almost the same characteristics. All Kazakhstan coals are considered to be low-rank. The moisture content varies from 5 to 40% and the high ash content is up to 55%. The volatile matter content reaches up to 28%. High ash content results in high fly ash contents in flue gases, which reach up to 60-70 g/m³ for high ash coals.

Figure 1 – 3 show a firing system with 12-swirl burners which are all in operation. The nozzles are located opposite to each other in two layers, 6 nozzles in each. In order to intensify the ignition process the air is fed to the chamber in such a way that oxygen, it contains, comes into reaction gradually.

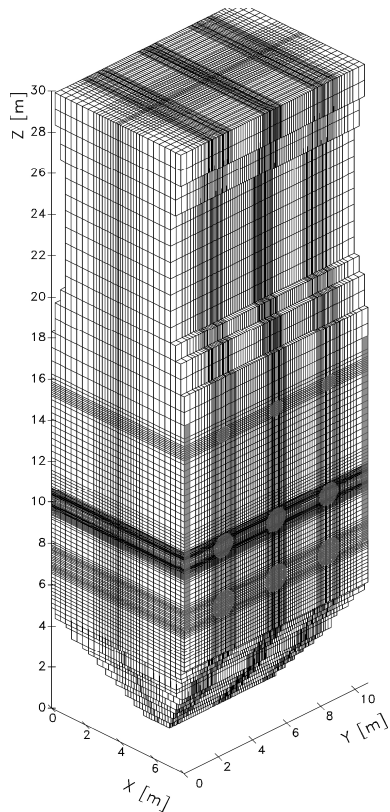


Fig. 1 -

Fig. 1 – Finite volume discretization grid of the furnace of the PK39 steam generator

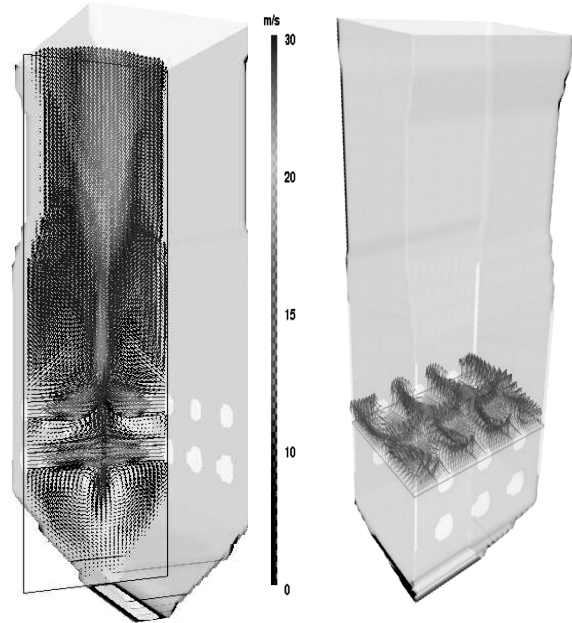


Fig. 2 - Velocity distribution in the vertical mean cross section during coal combustion at 100% load

The fuel in the layers is distributed equally, that caused the symmetrical flow fields (Fig.2 and Fig.3). Recirculating regions are formed close to the walls and four strong recirculating regions are formed in the corner regions at the burner levels (Fig.2).

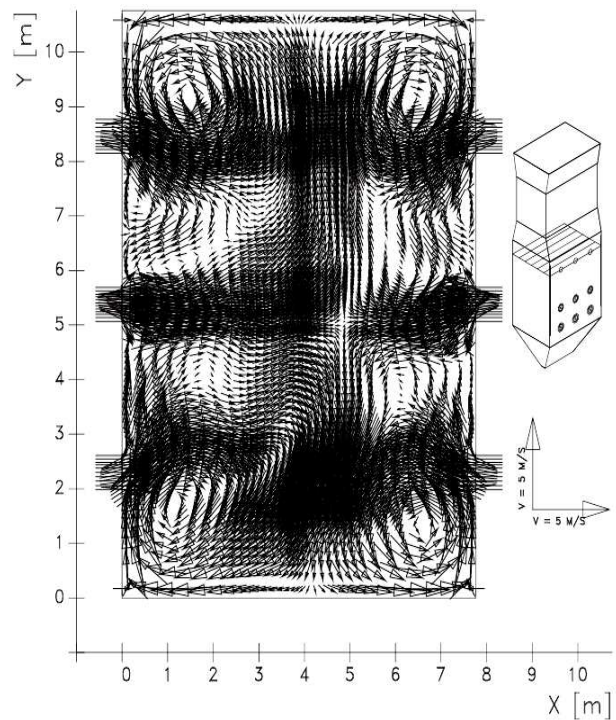
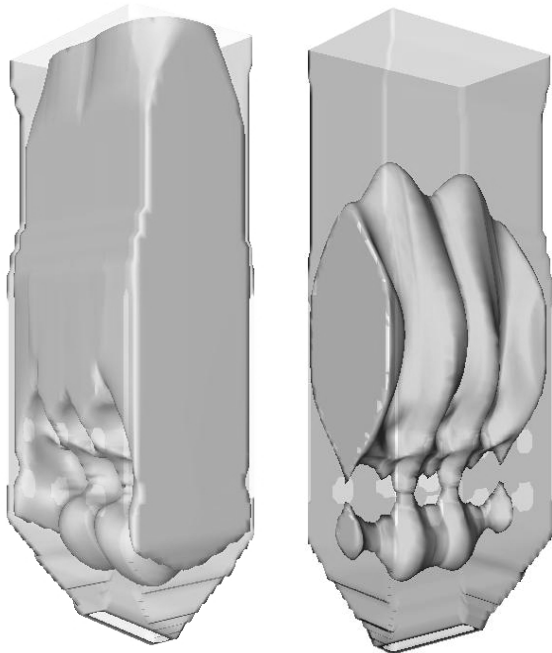


Fig. 3 - Velocity distribution in the level of the OFA jets during coal combustion at 100% load

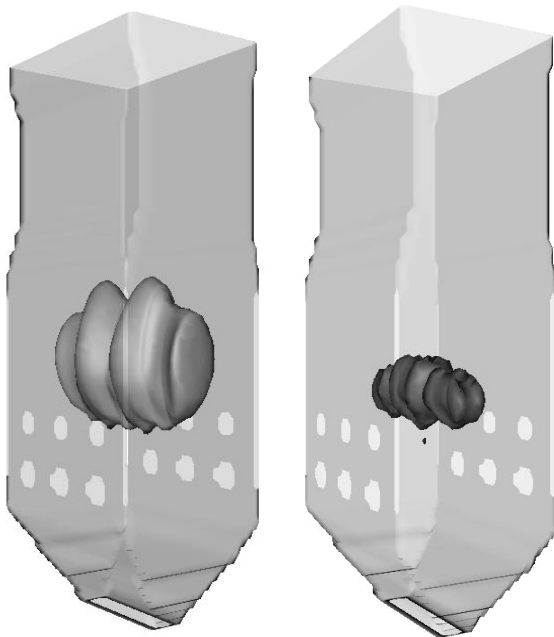
Temperature distributions in the furnace for full load operation (with coal and oil combustion) are presented in the Fig. 4-9.

Temperature distribution in furnace volume for full load boiler operation with coal combustion are given on Figure 4 in the shape of temperature isosurfaces. It's seen that zone of maximum temperatures are concentrated in the center of the fire-chamber on the level of the burners.



T = 1200 grad C

T = 1400 grad C



T = 1600 grad C

T = 1750 grad C

Fig. 4 - Temperature isosurfaces

Fig. 5 and Fig. 6 show the temperature distribution different cross sections of the furnace: in the lower level of the burners and in vertical sections due to symmetry plane of combustion chamber.

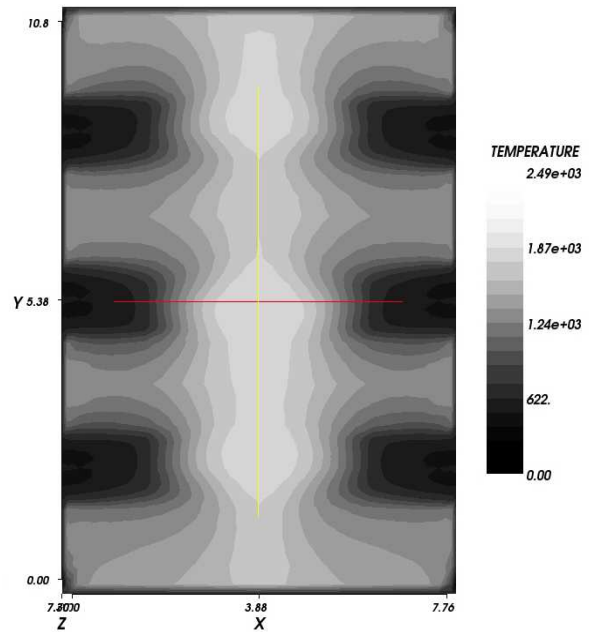


Fig. 5 - Temperature distribution in cross section of the furnace in the lower level of the burners

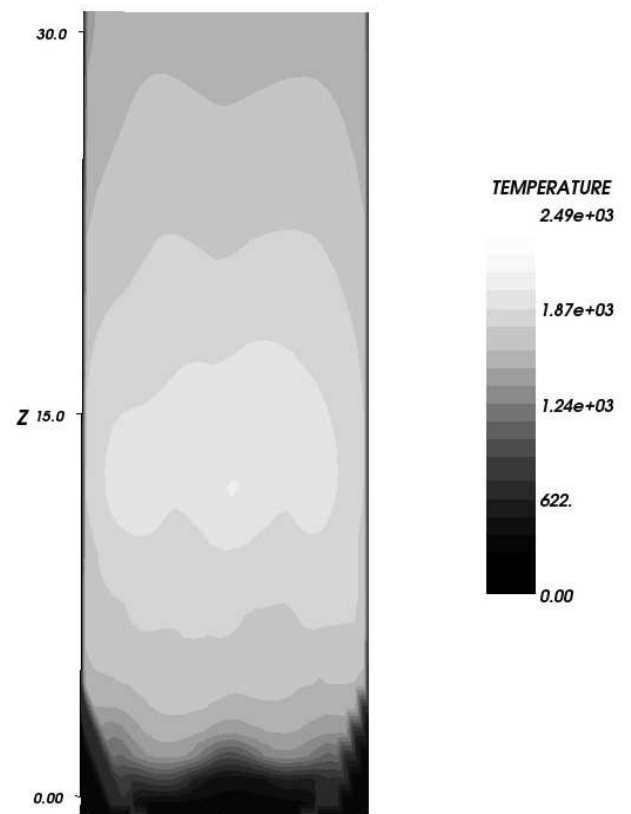


Fig. 6 - Temperature distribution in cross section of the furnace in the lower level of the burners

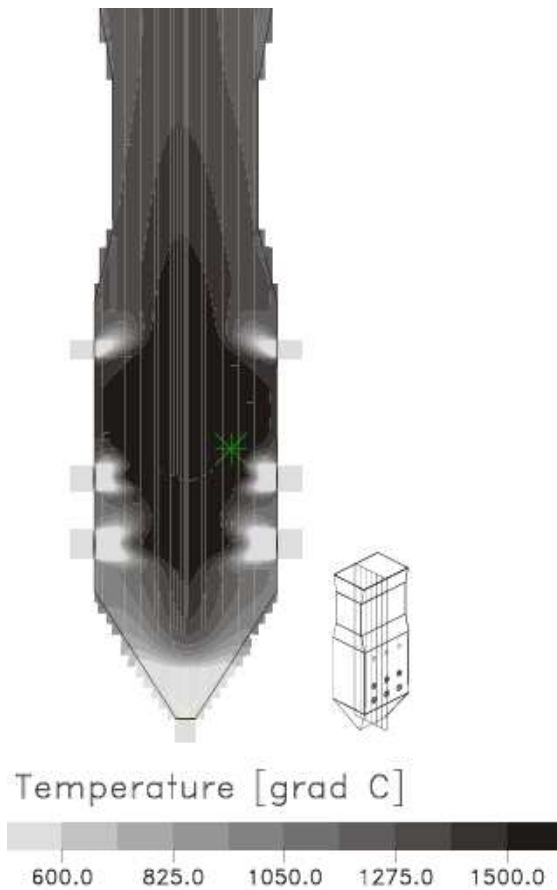


Fig. 7 – Temperature distribution in the middle vertical section during coal combustion at 100% load

To reduce NO emissions air staging was used. The penetration of the over fire air jets into the furnace can be seen in the velocity (Fig.3) and temperature (Fig.8) distribution. A significant increase of the flue gas temperature arises along the jets induced by the carbon monoxide combustion. Calculated data show good agreement with experimental data (Fig.8) [17].

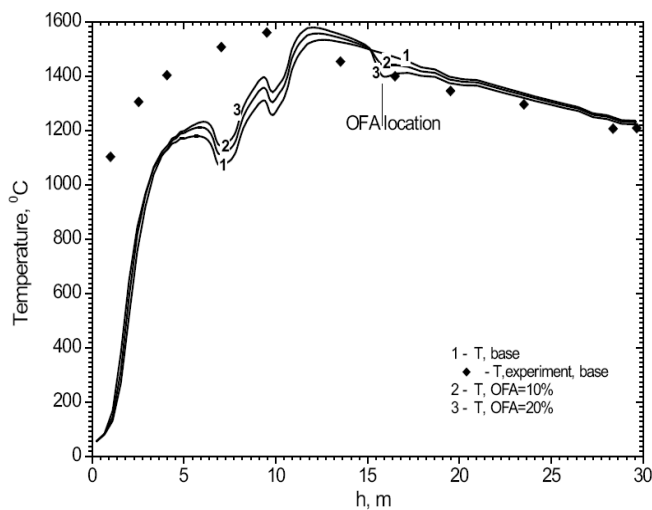


Fig. 8 – Simulated temperature distribution over furnace height during coal combustion at 100% load compared with experiment [17]

It's seen that maximum temperatures are in the center of the fire-chamber on the level of the burners. Here the intensive combustion took place. The existing of minima in presented temperature field caused by low temperature of fuel and transporting gas supplied to furnace through the burners nozzles.

Temperature distributions in the furnace for full load operation with oil combustion are given at Figure 9.

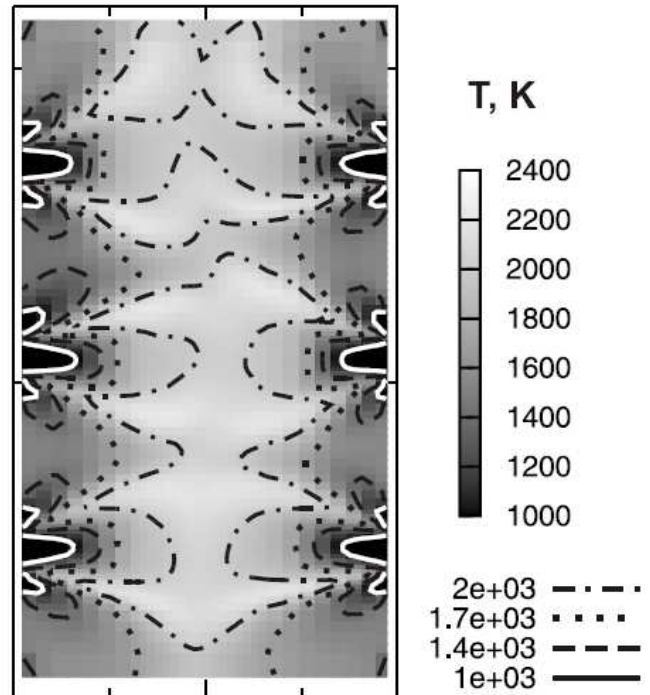


Fig.9 – Temperature distribution at the burner level for oil combustion at 100% load

Fig. 10-18 shows results of combustion products calculations for low grade Kazakhstan hard coal power station. Concentration isosurfaces show concentration of O₂ (Fig.10), CO (Fig.12) and CO₂ (Fig.15) distribution inside of the furnace space and over furnace height.

The picture of fuel burning out is shown in Figure below by fields of concentration of oxygen O₂ (Fig.11), carbon monoxide CO (Fig.13) and carbon dioxide CO₂ (Fig.16) over furnace height during coal combustion at 100% load.

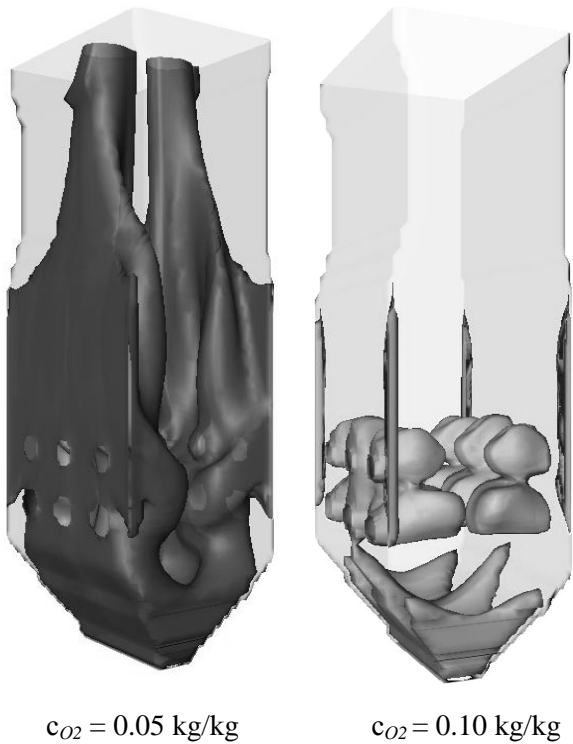


Fig. 10 – Oxygen isosurfaces

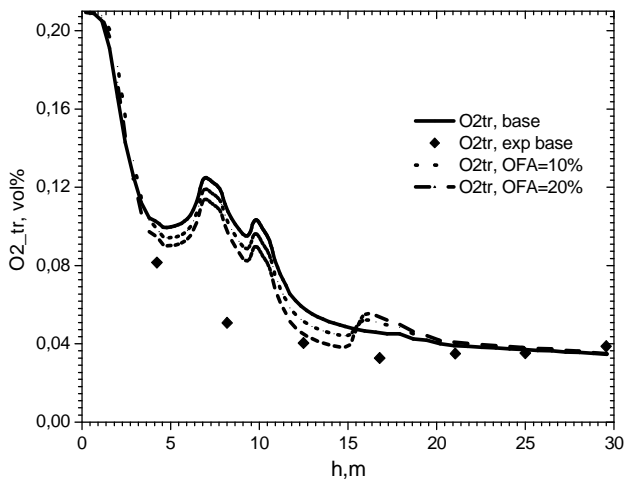


Fig. 11 – Simulated oxygen distribution over furnace height during coal combustion at 100% load compared with experiment [17]

In the model for combustion products formation three different reactions between char and flue gas are considered. The oxidation of the char to carbon monoxide or carbon dioxide and the reduction of carbon dioxide at the surface of the char particle to carbon monoxide.

The model incorporates the different effects of oxygen and carbon dioxide diffusion to the particle surface and in the pores and the kinetics of the chemical reaction at the surface as a function of temperature and particle diameter.

Due to the CO reactions also at lower temperatures CO concentration is further reduced in the gas path after the furnace outlet.

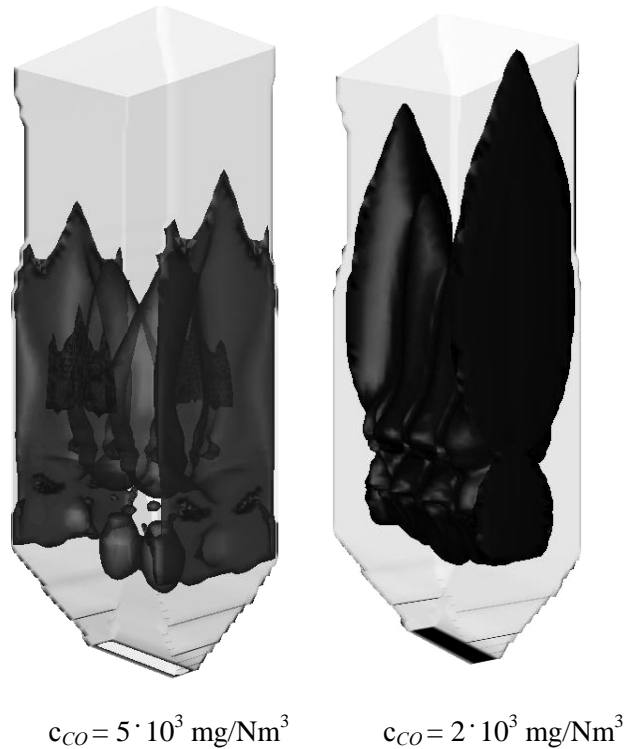


Fig. 12 – Carbon monoxide isosurfaces

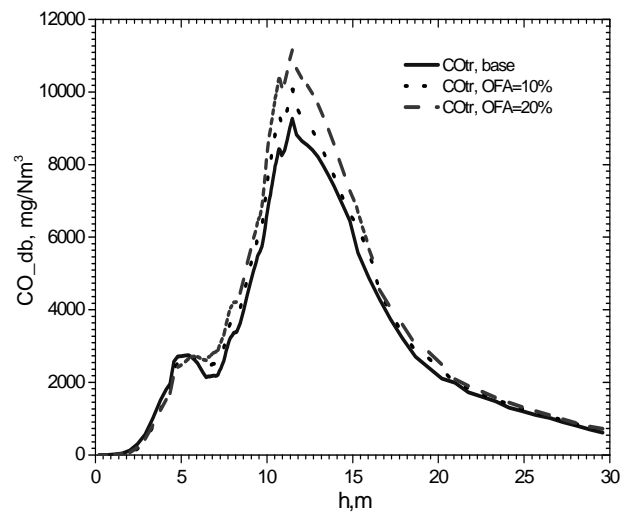


Fig. 13 – Simulated carbon monoxide distribution over furnace height during coal combustion at 100% load

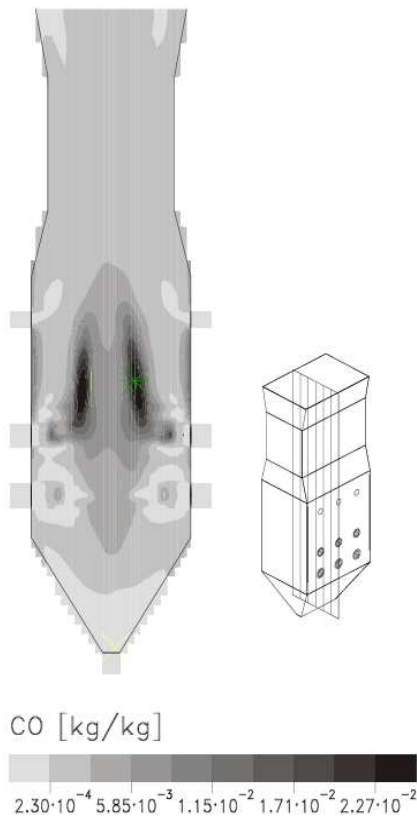


Fig. 14 - CO concentration in the middle vertical section during coal combustion at 100% load

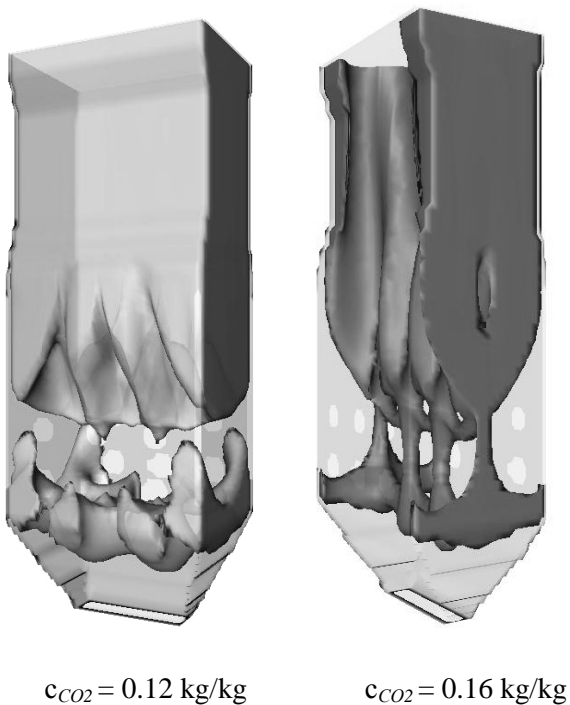


Fig. 15 - Carbon dioxide isosurfaces

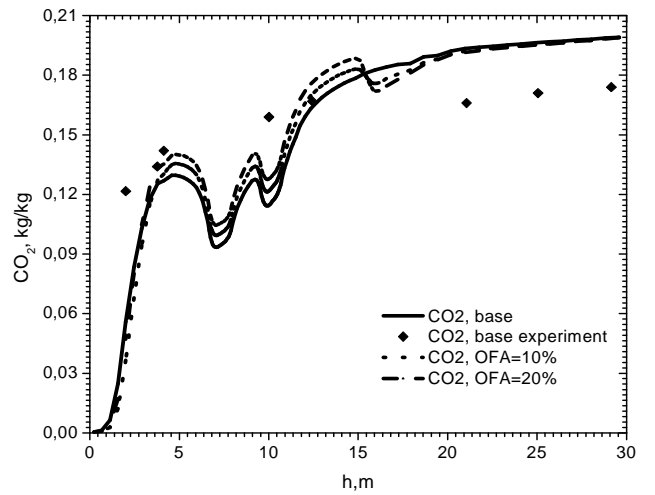


Fig. 16 – Simulated carbon dioxide distribution over furnace height during coal combustion at 100% load compared with experiment [17]

The NO_x model is realized separately as post-processing. It's made under the assumption that the pollutant formation has no influence on the fluid flow, temperature distribution etc. This assumption is reasonable due to the small concentrations of the pollutants.

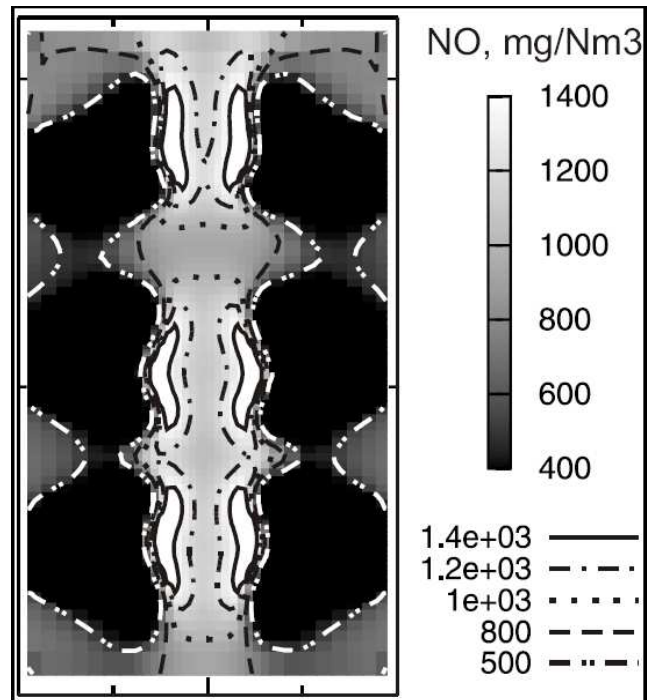


Fig. 17 – NO-concentration at the burner level during coal combustion at 100% load

The NO_x formation in the furnace has been investigated by applying a mathematical model with two kinetics. This model also helps to study the influence of various parameters on the net production of NO (for example influence of OFA etc).

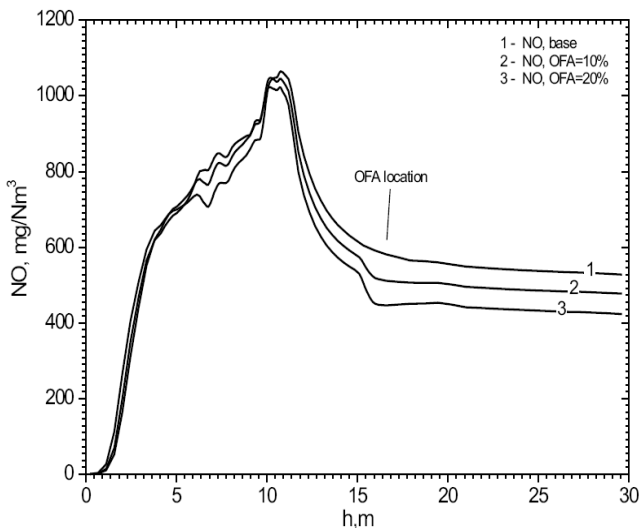


Fig. 18 - NO-concentration distribution over furnace height during coal combustion at 100% load

Heat flux distribution. Distribution of heat flux at the furnace walls is shown in fig. 12 depending on the wall conductivity (this example is using $k = 300 \text{ W/m}^2\text{K}$). Above the burners temperature increases due to reactions until they are finished and then decreases because of increased radiation heat transfer.

The heat flux received by the walls was calculated in relation to the measured temperature along the pipes. We can see the maximum heat flux predicted on the side walls above the main burners level.

The heat flux is calculated as:

$$\dot{q} = \underbrace{\alpha (T_{FG} - T_{Surface})}_{convection} + \underbrace{C_{12} (T_{FG}^4 - T_{Surface}^4)}_{radiation} \quad (8)$$

where $C_{12} = \epsilon_{12} \sigma$.

In FLOREAN two possibilities to define surface temperatures can be used:

- Fixed constant surface temperature $T_{surface} = \text{const.}$
- Calculated surface temperature with constant heat transfer and fixed constant evaporation temperature inside the tubes $T_{steam} = \text{const.}$

In the case, that the surface temperature $T_{surface}$ is to be calculated following formulas are used:

$$\dot{q} = k (T_{surface} - T_{steam}) \quad (9)$$

$$T_{surface} = \frac{\dot{q}}{k} + T_{steam} \quad (10)$$

$T_{surface}$ influences the heat flux \dot{q} and therefore an iteration is necessary:

- calculate heat flux;
- calculate $T_{surface}$;
- recalculate heat flux with new surface temperature;
- recalculate $T_{surface}$

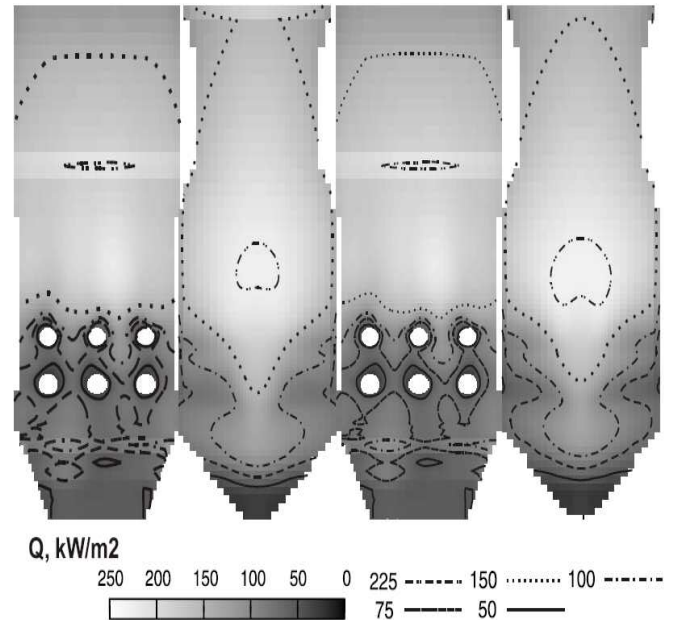


Fig.19 – Absorbed heat flux to the furnace walls

4 Conclusion

By means of the 3D CFD tool FLOREAN numerical simulations have been carried out to predict gas flow, species concentrations, temperature fields due to combustion, radiation and convective heat transfer and the pollutant formation and destruction in furnace chambers of Kazakhstan Power Plants.

The purpose of the presented research was to investigate numerically the characteristics of reacting flows and heat transfer due to oil and coal turbulent combustion in large-scale boiler furnaces. The data resulting from the present study allow an improved understanding of combustion processes and provide detailed description of furnace performance.

Results from CFD simulation can be useful for engineers to choose an appropriate burner and furnace design, to reduce pollutant emissions, as well as to optimize furnace operation.

5 Nomenclature

X_i – mole fraction, mol/mol;
 m_k – mass fraction of species k, kg/kg;
 $m_{p,i}$ – mass fraction of the particles;
 ρ_s – density of suspension, kg/m³;
 $\rho_{p,i}$ – density of particles kg/m³;
 Sc – the Schmidt number;
 Pr – the Prandtl number;
 S_k – the source/sink term due to the reaction;
 \dot{q} – heat flux received by the walls, kW/m²;
 R – reaction rate, 1/s;
 T – temperature, K;
 T_{FG} – flue gas temperature, K;
 $T_{Surface}$ – surface temperature, K;
 k – wall conductivity, W/m²K;
 α – heat transfer coefficient by convection, W/m²K;
 ϵ_{12} – emissivity of the wall;
 σ – Boltzman constant, W/ m²K⁴.

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