Abstract: 3D–Finite Volume tool FLOREAN developed at the Institute for Heat and Fuel technology TU Braunschweig is used for simulations of combustion processes in industrial furnaces with different types of fuel and firing systems. Distributions of different characteristic parameters such as temperature, fluid flow properties like 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: CFD, Computational fluid dynamics, Combustion, Pollutant Emission, Furnace design, Furnace operation.

1 Introduction
In the last years Computational Fluid Dynamics - CFD has become a more and more reliable tool to check the design of furnaces. 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.

3D–Finite Volume 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. 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 [133]. 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 flux radiation model by Lockwood et al. [4]. The energy balance equation is written in terms of the enthalpy.

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.

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.

**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 [5].

*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.

**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 Lendt [6]. 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, De Soete [7] or the Mitchell-Tarbell [8] 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 (1975) [7] 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:

\[
R_1 = 1.0 \cdot 10^{10} \cdot X_{HCN} \cdot X_{O_2} \cdot \exp \left(-\frac{33732.5}{T}\right)
\]

\[
R_2 = 4.0 \cdot 10^6 \cdot X_{NH_2} \cdot X_{O_2} \cdot \exp \left(-\frac{16111.0}{T}\right)
\]

\[
R_3 = -3.0 \cdot 10^{13} \cdot X_{HCN} \cdot X_{NO} \cdot \exp \left(-\frac{30208.2}{T}\right)
\]

\[
R_4 = -1.8 \cdot 10^8 \cdot X_{NH_3} \cdot X_{NO} \cdot \exp \left(-\frac{13593.7}{T}\right)
\]

**Mitchell and Tarbell model.** A global model has been proposed by Mitchell and Tarbell [8], 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 CₓHᵧ.

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 [8], 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

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. These coals are considered to be low-rank coals. 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.

Fig.1 and Fig. 2 show a firing system with 12-swirl burners which is still in operation. The nozzles are located opposite to each other in two layers, 6 nozzles in each. The fuel in the layers is distributed equally, that caused the symmetrical flow fields (Fig.4 and 6). Recirculating regions are formed close to the walls and four strong recirculating regions are formed in the corner regions at the burner levels.

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 distribution (Fig.3). A significant increase of the flue gas temperature arises along the jets induced by the carbon monoxide combustion.

Temperature distributions in the furnace for full load operation (with coal and oil combustion) are presented in the Fig. 5-8. It’s seen that the zone of maximum temperatures are concentrated in the center of the fire-chamber on the level of the burners.

The minima in the presented temperature field are caused by the low temperatures of fuel and transporting gas supplied to the furnace through the burners nozzles. Calculated data show good agreement with experimental data (Fig.7) [9].
Fig. 3 - Velocity distribution in the level of the OFA jets during coal combustion at 100% load.

Fig. 4 – Horizontal component of the velocity parallel to the side wall at the level of the burners location during coal combustion at 100% load.

Fig. 5 – Temperature distribution at the burner level during coal combustion at 100% load.

Fig. 6 – Temperature distribution at the burner level for oil combustion at 100% load.
Fig. 7 – Simulated temperature distribution over furnace height during coal combustion at 100% load compared with experiment [9]

Due to the CO reactions also at lower temperatures CO concentration is further reduced in the gas path after the furnace outlet (Fig. 9).

The NOx 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. 8 – Temperature distribution in the middle vertical section during coal combustion at 100% load

Fig. 9 – CO concentration in the middle vertical section during coal combustion at 100% load

Fig. 10 – NO concentration at the burner level during coal combustion at 100% load
The NOx 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. 11 - NO-concentration distribution over furnace height during coal combustion at 100% load

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:

\[
\dot{q} = \alpha (T_{FG} - T_{Surface}) + C_{12}(T_{FG}^4 - T_{Surface}^4)
\]

where \( C_{12} = \varepsilon_{12} \sigma \).

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:

\[
\dot{q} = k (T_{surface} - T_{steam})
\]

\[
T_{surface} = \frac{\dot{q}}{k} + T_{steam}
\]

\( T_{surface} \) influences the heat flux \( \dot{q} \) and therefore an iteration is necessary:
- a) calculate heat flux;
- b) calculate \( T_{surface} \);
- c) recalculate heat flux with new surface temperature;
- d) recalculate \( T_{surface} \).

Fig.12 – 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;
\( \dot{q} \) – 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;
\( \alpha \) – heat transfer coefficient by convection, W/m2K;
\( \varepsilon_{12} \) – emissivity of the wall;
\( \sigma \) – Boltzmann constant, W/m2K4.
References: