Calculated suspension density and temperature over boiler combustion chamber height

Numerical simulations of the industrial circulating fluidized bed boiler under air- and oxy-fuel combustion

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Abstract

Measured and numerical results of air-fuel combustion process within large scale industrial circulating fluidized bed (CFB) boiler is presented in this paper. For numerical simulations the ~~middle size~~ industrial compact CFB boiler was selected. ~~which is built at Turow Power Plant in Poland. The set of~~ Numerical simulations were carried out using three-dimensional model where the dense ~~particulate~~ ~~particle~~ transport phenomenon was simultaneously modelled with combustion process. The fluidization process was modelled using the hybrid Euler-Lagrange approach. ~~In order to investigate the impact of geometrical model simplifications on predicted~~ The impact of the geometrical model simplification on predicted mass distribution and temperature profiles over CFB boiler combustion chamber two kinds of geometrical models were used, namely the complete model which consist of combustion chamber, solid separators, external solid super-heaters and ~~sim-~~ ~~simplified~~ ~~reduced~~ ~~only~~ boiler geometry which was ~~simplified~~ ~~reduced~~ ~~only~~ to the combustion

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chamber. The evaluated temperature and pressure profiles during numerical simulations were compared ~~to~~ against measured data collected during boiler air-fuel operation. ~~combustion process.~~ Collected data ~~These data~~ was also used for validating numerical model of the oxy-fuel combustion model. ~~In order to check developed model stability several numerical simulations were carried out for different input data.~~ Stability of the model and its sensitivity on changes of several input parameters were studied. ~~This simulations were evaluated to check the response of the numerical model on changing some boiler operating conditions. The investigated oxy-fuel combustion process should be seen as hypothetical one.~~ The comparison of the pressure and temperature profiles for all considered cases gave comparable trends in contrary to measured data. Moreover, some additional test was carried out the check the influence of radiative heat transfer on predicted temperature profile within the CFB boiler.

Keywords:

Oxy-Fuel Combustion, Fluidization, Particles, CFB, Multifluid, hybrid Euler-Lagrange

1. Introduction

The fluidized bed boilers, due to their maturity, have many applications within industry. The fluidization process is often used in gasification, coating of particles, drying of solids, combustion, incineration, and many others. These technology finds many application for ~~The possibility of application the fluidization technology for~~ combustion low quality fuels like lignite coal, biomass, sewage slugs and waste material leads to increase role of this tech-

nology in the electricity generation sector. Due to relatively low combustion temperature within the combustion chamber, which varies between 800 °C to 950 °C, the level of thermal NO_x in fluidized bed boilers is considerably reduced without introduction complex burners or additional flue gas treatment facilities like it has to be done for the Pulverized Coal boilers. Additional advantage of fluidization technology is its possibility to in-situ SO₂ removal during combustion process by direct injection of the limestone stone into the boiler combustion chamber. All mentioned aspects, nowadays makes this technology very attractive in energetic sector.

The modelling of the particle transport and combustion processes within Circulating Fluidized Bed (CFB) boilers are computationally very ~~expensive and~~ demanding. The difficulties come from the complexity of particles interactions in dense beds, the interrelation between the chemistry of combustion and the particle movement. ~~—mainly due to a high concentration of the particle material and complexity of the reacting flow, as well as the strong relationships between them.~~ Frequently, the CFD simulations are usually limited to 2D geometry where multiphase flow is modelled using standard Euler-Euler approach [1]. Abundant application of Euler-Euler technique for modelling dense solid flows can be found in book [2]. One of the example has been well described in work [3] where two-fluid approach has been applied for modelling particle transport within the NETL pilot scale CFB system. A common challenge for Euler-Euler approach is high numerical cost in terms of wall clock time to reach accurate solution due to necessity of ensuring fine mesh at the bottom part of the riser in order to accurate predict drag between phases. A numerous of wok has been focused on decreasing simulation

time without losing model accuracy. One of the possibility is application of the Energy-Minimization Multi-Scale (EMMS) technique, which has been presented in reference [4]. In works [5] and [6] the EMMS technique has been future extended and used for modelling particle transport in large scale industrial boilers, where good accuracy of the model has been presented. Other problem which has to be resolved when CFB boilers are modelled, is connected with accurate prediction of the Particle Size Distribution (PSD). In many application the real PSD is simplified to one characteristic diameter which significantly reduce calculation time. Reference [7] describes prediction of the flow field within the large scale CFB furnace where the effect of particle polydispersity has been analysed. ~~to better understand the CFB boiler behaviour two dimensional geometry should be extended to a three dimensional model in order to capture spatial flow effect for the solid-solid and solid-gas mixing process.~~ The biggest challenge when the CFB boiler are simulated is the simultaneous modelling of the particle and reacting flows. The literature reports only a few cases devoted to the 3D full-loop simulation of the industrial CFB boilers where the combustion process has been accounted for. Nikku et. al (2014) [8] and Mohanen and Hyppanen (2011) [9] applied semi-empirical, steady state, three-dimensional Eulerian approach for modelling particle and combustion process inside commercial CFB furnaces. This model yields the temperature profile and species concentrations along the boiler height in relatively short time. The weak point of this model is that the inert material is modelled using empirical correlations, while only fuel particles are tracked in Lagrangian frame of reference. Nevertheless, the developed pseudo steady state model finds many applications in simulations

of industrial scale CFB boilers. Comparable model has been presented in reference [10], where semi-empirical approach has been utilized for simulating local conditions inside combustion chamber of industrial boiler. Detail description of the semi-empirical model can be found in work [9] where developed mathematical model is widely described. Based of this information it can be seen that the three-dimensional model which give possibility to predict flow field within the CFB boiler taken into account combustion process and particle interaction is still sought, mainly for prediction particle erosion process. To deal with this issues the Lagrangin based models have to be used. Snider et. al (2011) [11] applied the MultiPhase - Particle in Cell method (MP-PIC) [12] for simultaneous modelling coal gasification process. This method gives possibility to track group of particles in relatively low numerical cost. This computational technique has been future tested by Wang et. al (2014) [13] where close loop of the pilot-scale CFB installation has been modelled. ~~For more information the reader is send to work and where CPFD software is used for modelling reacting flow within the fluidized bed. Nevertheless, expect of this implementations the three dimensional model of the fluidized bed boiler still has to be improved and validated against measured data.~~

The paper presents simulations of the air- and oxy-fuel combustion processes within an industrial CFB boiler installed in Poland. Develop model gave possibility to simultaneously simulate particle transport, real PSD and air/oxy combustion process within large scale CFB boiler. The computations were carried out using commercial Ansys-FLUENT package [14]. The interactions between particles and phases were accounted for via hybrid Euler-

Lagrange approach. The original code was augmented with a set of User Defined Functions (UDF). The implemented UDFs were used for several purposes like, solid phase recirculation procedure, calculating of gas properties for radiation model, monitoring mass of solid material, etc. The model was tested in Ref. [15] where particle transport was modelled under isothermal conditions with temperature taken from measurements. The evaluated pressure profile well reproduced the measured data of a pilot scale CFB experimental rig built at Częstochowa University of Technology [16]. In the next step, the developed model was used to simulate the oxy-fuel combustion process using geometrical model of the pilot installation [17]. Subsequent step of the model development was to apply it to conventional air-combustion process inside a large scale CFB boiler, with the computational domain limited to the combustion chamber [18].

The present paper shows results of simulations of a boiler, which operates in air- and oxy-fuel combustion modes. The measured data collected during boiler air-combustion mode were used as a benchmark for validation of the numerical results. Hypothetical behaviour of the same boiler in oxy-combustion mode has been studied then, by appropriate modification of combustion kinetics and composition of the gaseous phase.

The objective of the research was the comparison of the performance of the CFB boiler operating in oxy-fuel mode for different oxidizer compositions. In order to investigate the impact of various oxy-fuel operating condition on predicted temperature, pressure, concentration and burn-out profiles within the boiler, several oxy-fuel cases were simulated. As claimed in [19] the behaviour of a Pulverized Coal (PC) boiler operated under oxy-fuel mode

is similar to air-combustion, when the oxygen volume fraction in oxidizer mixture is of the order of 30%. There are good reasons to expect, that CFB boilers would behave in a similar way. Thus, simulations have been carried out for oxygen concentration within the range of 27% to 32% by volume. Similarly, the influence of the concentration of moisture in the oxidizer, has been investigated. O_2 and H_2O fractions have been controlled by adjusting the recirculation ratio and drying intensity of the flue gases.

Other question appears when the CFB numerical model is used, namely the influence of the boiler geometrical model simplification on predicted material distributional within the combustion chamber and its influence on the temperature profile over combustion chamber. ~~Moreover,~~ In order to check geometrical model simplification on calculated flow field within combustion chamber the set of numerical simulation was performed using complete boiler geometrical model consisted of combustion chamber, solid separators, external solid super-heaters and simplified boiler geometry which included only combustion chamber. ~~Moreover,~~ the effect of radiation on predicted temperature profile within combustion chamber was also taken into consideration using only air-fuel combustion case. Based on carried out simulation comparable trends between numericals results and measured data have been observed.

Other problem, which has to be addressed when modelling combustion, mass, energy and momentum transfer in CFB boilers, is the influence of radiation on predicted temperature distribution. In order to investigate this issue, additional simulations were carried out for air-fuel mode, where the combustion process was simulated with and without invoked radiation trans-

fer solver. An original procedure of evaluation of the radiative properties based on spectral atomic data has been developed and implemented in the model [20]. The radiative solver used in the study was the Discrete Ordinates, while the spectral, temperature and composition dependence of the absorption coefficient has radiative properties were embedded into the Weighted Sum of Gray Gases model.

2. Geometrical and numerical model of CFB boiler

To check the response of the existing industrial CFB boiler at the changes of the operating conditions from air- to oxy-fuel mode the middle size compact CFB boiler was selected. This unit is installed in Poland at Turow Power Plant. The complete boiler geometrical models is illustrated in Fig. 1.

Figure 1: Geometrical model of the simulated unit

~~Used CFB boiler~~ Selected unit is equipped with four external solid separators located on the both boiler side walls. During boiler operation the separated solid material within solid separators is recirculated back to the combustion chamber through 8 External Steam Super-Heaters (ESSH). The rectangular cross section of the boiler combustion chamber is 22x10 m, while the height is 42 m.

As it has been mentioned earlier in presented paper the combustion and gas-solid mixing processes have been simultaneously investigated applying ~~presented paper~~ full and simplified boiler geometries ~~were used~~. Selected CFB unit is equipped with fuel and solid injection ports located on both boiler side walls. The secondary oxidizer gas is injected to combustion cham-

ber through 26 ports distributed in three rows on trapped bed walls. The boiler geometrical model, with marked oxidizer injection ports, is illustrated in Fig. 2 (left). ~~full boiler geometry complete boiler geometrical model~~ part of the secondary gas was injected to the computational domain through the external solid super heaters. When the simplified boiler model was used, its computational domain has been limited to combustion chamber, which considerably reduce computational time and stabilized solution procedure . This exertion introduced to the boiler geometry considerable reduce required computational time in comparison to full boiler geometry. Comparable CFB numerical model was also used in earlier authors work [18], where it was used to simulate particle transport and air-fuel combustion process within large CFB unit.

In order to appropriately simulated material loop within the simplified boiler numerical model ~~for simplified boiler geometry is used~~, the recirculation procedure has been ~~replaced by~~ applied by set of proper user defined functions (UDFs) implemented into the solution procedure. The graphical illustration of the recirculation procedure is shown in Fig. 2 (right).

The set of UDFs consist of several sub-procedure. First procedure is responsible for collecting information at the boiler outlet. This function removes particles which touch the outflow boundary of the computational domain. For each removed particles the information like: mass, diameter, density, composition, temperature, etc. are collected and storage in the memory. The second procedure calculates overall mass of the removed particles, and redistributes the collected particles over appropriate recirculation inlets. The operating of this procedure depends on the boiler construction, and for

each boiler it has to be appropriately fitted. In used boiler configuration, the collected material was recirculated back to the combustion chamber through external solid super-heaters inlets located on side boiler walls. The temperature of recirculated material, as well as gases at the inlets was defined based on measured values collected during normal boiler operating. The last step of the recirculation procedure is injection of the material into the combustion chamber. This step has to be done before next time step for gaseous phase. Here only brief description of the recirculation procedure has been given, more information can be found in work [15].

The application of full boiler geometry has given possibility to capture the effect of mass accumulation within the solid separators and external solid super-heaters, and in consequences theirs influence on the solid distribution within the combustion chamber. Nevertheless, in order to simulate the CFB boiler loop seals their geometry has to be considerable simplified. This is no doubt that this simplification influences on the solid transport within the external solid super-heaters and amount of solid material transported back to combustion chamber. However, including detailed geometry of the recirculation loop has had huge impact on the required simulation time. In order to overcome this problem the external solid super-heaters can be simulated separately and calculated data can be then prescribed as the inlet to combustion chamber. **This idea can be tested in future works.** In case of decreasing calculation time additional simplifications were introduced to the boiler geometrical model, namely the grid was modelled as flat surface where the primary gas was injected to combustion chamber through its whole bottom cross section. Similar simplification can be found in reference [5] where

similar boilers were modelled. The boiler model were meshed using a combination of tetrahedral and hexahedral elements where full loop consist of 1,300,000, and simplified model was meshed with 600,000 elements. The numerical mesh was generated base on experience gained during work presented in paper [18] where boiler with similar construction was modelled using hybrid Euler-Lagrange technique.

Figure 2: Turow CFB boiler geometry with specified gas and solid injection ports and illustration of the recirculation procedure

The boiler input data is summarized in Table 1. When the oxy-fuel combustion process is investigated the composition of the oxidizer mixture injected to combustion chamber plays crucial role on the behaviour of the combustion process and heat exchange within the combustion chamber [21]. Based on the works [19] and [22] it can be observed that when the volume fraction of oxygen in oxidizer composition is kept close to 30% the combustion process under oxy-fuel mode has comparable trends with air-fuel combustion process. The idea behind selecting the oxygen fraction from range 27% to 32% was to check the numerical model flexibility and its possibility to follow the changing of oxidizer composition , and its influence on overall combustion process within the boiler.

2.1. Input data

The amount of oxidizer was calculated based on known low heating value of the burned lignite coal, his composition has been collected in Table 2, as well as overall boiler thermal load, and amount of burned coal. In simulated boiler the oxidizer is redistributed between grid, primary inlets, solid

injection ports, and secondary gas inlets. For oxy-fuel combustion cases it was assumed that the the amount of oxidizer used in combustion process was the same as that used in boiler under air mode. The same amount of oxidizer for both investigated cases maintained similar hydrodynamic conditions within the combustion chamber, **which is crucial when fluidization process is modelled** . The molar composition of the **gas produced in Air Separation Unit (ASU)-oxygen** used for mixing recirculated flue gases ~~was consisted of~~ 95% of O_2 and 5% of N_2 . In presented work the composition of oxidizer was calculated by changing amount of recirculated flue gases. Calculated compositions and other input parameters for all investigated cases are summarized in Table 1. The particle size distributions of the coal, sand, and ash for investigated boiler was modelled using Rosin-Rammler distribution, where the model parameters are shown in Table 3. At the recirculation inlet it was assumed that the temperature of injected oxidizer is the same as solid material. The boiler internal wall were simplified to flat walls where the heat transfer within the wall was treated as one-dimensional, with proscribed constant temperature (357 °C), thickens and material thermal properties. The set of numerical simulations carried out using boiler geometrical model with recirculation loop were performed applying the same parameter as for *AIR* case and *OXY 1 Case*.

3. Numerical model

The gas and solid particles flow in the CFBs is frequently modelled by means of the so called Euler-Euler two-fluid approach. Detailed description of the this approach, can be found in the literature [1]. Alternatively to two-

Table 1: Input data for numerical model

	AIR	OXY 1	OXY 2	OXY 3	OXY 4
Oxidizer mass flow rate, kg/s	274.5				
X _{O₂,oxi} , %	20.92	32.09	28.81	27.31	28.19
X _{CO₂,oxi} , %	0.00	62.22	61.69	63.11	54.86
X _{H₂O,oxi} , %	0.00	1.92	2.30	2.32	8.24
X _{N₂,oxi} , %	78.78	3.77	7.20	7.26	8.71
H ₂ O reduction in rec. flue gases, %		70			30
Temp. of rec. material, °C	800 - 900				
Oxidizer temp., °C	277				
Coal temp., °C	100				

Table 2: Ultimate and proximate analysis of the lignite coal burned in Turow boiler

Proximate, %		Ultimate, %	
Ash	21.8	C	28.82
Water	40.5	H	2.32
Vol	22.3	S	0.31
Char	15.4	N	0.29
		O	5.96
Low Heating Value (LHV _{AR}), kJ/kg		10 600	
Coal flow rate, kg/s		~52.6	

Table 3: Material properties for fluidization process

	coal	inert
Density, kg/m ³	1300	1800
Mean diameter, μm	325	330
Max diameter, μm	2000	1000
Min diameter, μm	50	50
Distribution parameter	1.25	1.35
Number of diameters	6	8

fluid model the methods of moments like Quadrature or Direct Quadrature Methods of Moments can be used, however they introduce additional complexities [23] which exclude them from application to large scale CFB boilers [24]. Instead of using the Eulerian approach the hybrid Euler-Lagrange technique can be used for modelling the granular flow in the CFB units, which has common roots with the Multiphase Particle in Cell (MP-PIC) technique [25]. The characteristic features of this model is that it takes into account the real Particle Size Distribution (PSD), the combustion process is considered in level of single particle, and can be used for detecting corrosion at the boiler walls. In the hybrid Euler-Lagrange approach the four-way coupling [26] has been taken into account to represent the relation between continuous and dispersed phases in the mass, momentum and energy transfer. The interactions between particles have been taken into account applying the Kinetic Theory of Granular Flow (KTGF) [1].

The hybrid Euler-Lagrange approach does not track each of individual

particles, instead of groups of particles called parcels are tracked. Each parcel contains several particles of identical mass, velocity, position, temperature, composition, etc. which significantly decrease computational time. The number of individual particles contained in the injected parcel can be easily calculated from

$$n_p = \frac{\dot{m}_{\text{par}} \Delta t}{m_p} \quad (1)$$

where Δt is the time step in transient calculation, $\dot{m}_{\text{par}}$ is the mass flow rate of a single parcel and m_p is the mass of an individual particle evaluated based on the particle diameter and density $m_p = \pi \frac{d^3}{6} \rho_s$. In order to calculate the parcel/particle position the particle equation of motion which is prescribed for one particle in parcel has to be calculated [14]

$$\frac{d\mathbf{u}_p}{dt} = F_D(\mathbf{u}_f - \mathbf{u}_p) + \frac{\mathbf{g}(\rho_p - \rho_f)}{\rho_p} - \frac{\nabla p}{\rho_p} - \frac{\nabla \cdot \sigma_s}{\rho_p} \quad (2)$$

where subscript p denotes the particle data, f stands for gaseous phase, $\mathbf{u}_f$ and $\mathbf{u}_p$ are the velocity vectors of the gaseous phase and particle, respectively, $\mathbf{g}$ is the local gravitational acceleration, ρ is the density, p is the pressure of gaseous phase. The term $F_D(\mathbf{u}_f - \mathbf{u}_s)$ defines the particle acceleration due to the drag. The term $-\nabla p/\rho_p$ in the above equation defines the particle acceleration due to the pressure difference at the particle location. σ_s is the granular stress tensor which represents particles interactions, its value is calculated based on the KTGF in the Eulerian grid for known solid volume fraction within the numerical cells and position of parcel. The granular stress tensor for presented particle motion equation Eq. (2) can be calculated as

$$\sigma_s = -p_s \bar{\mathbf{I}} + \varepsilon_s \mu_s (\nabla \mathbf{u}_s + \nabla \mathbf{u}_s^T) + \varepsilon_s \left(\lambda_s - \frac{2}{3} \mu_s \right) \nabla \cdot \mathbf{u}_s \bar{\mathbf{I}} \quad (3)$$

where λ_s is the bulk viscosity, $\bar{\mathbf{I}}$ is the unit tensor, p_s is the granular pressure, μ_s represents the solid dynamic viscosity, and $\mathbf{u}_s$ stands for the average velocity vector of the solid phase acquired at the particle location. The parcel position is calculated for known parcel velocity (2) as

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p \quad (4)$$

After obtaining the particle position, the solid volume fraction in a given numerical cell can be calculated as

$$\varepsilon_s = \frac{\sum_{i=1}^{N_{\text{parcels}}} V_{p,i} n_{p,i}}{V_{\text{cell}}} \quad (5)$$

where ~~is the considered particle volume~~, V_{cell} is the numerical cell volume, $V_{p,i}$ is the volume of individual particle in parcel. The calculated solid volume fraction is assigned to Eulerian grid where the void fraction can be determined as $\varepsilon_f = 1 - \varepsilon_s$. The particle velocity and position obtained by solving Eqs. (2) and (4), strongly depends on the evaluated solid stresses σ_s (see Eq. (3)) in the Eulerian grid. In order to calculate the solid stress tensor several closure terms have to be calculated. Closure terms are used in the description of the granular pressure p_s , granular viscosity μ_s , solid bulk viscosity λ_s , frictional pressure p_{fr} and granular temperature θ_s . The set of models which were used for modelling closure terms for calculating particle-particle and gas-particle interactions for both investigated boiler models are shown in Table 4.

When the hybrid Euler-Lagrange model is used for reactive flow simulation, transport equations for mass, momentum, species, energy are solved within the Eulerian grid for continuous phase only. The set of equations is supplemented with the selected turbulence model transport equations. The transport equations can be written as [14, 30]

Table 4: Closure models for the Euler-Euler and hybrid DDPM approaches

Solid pressure	Lun et al. [27]
Solid viscosity	Gidaspow [1]
Bulk viscosity	Lun et al. [27]
Friction viscosity	Schaeffe [28]
Friction pressure	Based on KTGF [29]
Granular temperature	Algebraic - Syamlal et al. [29]
Drag model	Gidaspow [1]
Restitution coefficient: e_{ss}	0.95
Friction package limit: ε_s^{fr}	0.61
Package limit: ε_s^*	0.63
Transition factor (hybrid model)	1.0

$$\frac{\partial}{\partial t} (\varepsilon_f \rho_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f) = S_{\text{mass}} \quad (6)$$

$$\frac{\partial}{\partial t} (\varepsilon_f \rho_f \mathbf{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f \mathbf{u}_f) = -\varepsilon_f \nabla p + \nabla \cdot \tau_f + \varepsilon_f \rho_f \mathbf{g} + K_{DDPM} (\mathbf{u}_s - \mathbf{u}_f) + S_{\text{mom}} \quad (7)$$

$$\frac{\partial}{\partial t} (\varepsilon_f \rho_f h_f) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f h_f) = \varepsilon_f \frac{\partial p}{\partial t} + \tau_f : \nabla \mathbf{u}_f - \nabla \cdot \mathbf{q}_f - \nabla \cdot \left[\sum_{k=1}^m \varepsilon_f h_{f,k} \mathbf{J}_k \right] + S_{f,\text{rad}} + S_{f,\text{rec}} + S_{\text{en}} \quad (8)$$

$$\frac{\partial}{\partial t} (\varepsilon_f \rho_f Y_{f,k}) + \nabla \cdot (\varepsilon_f \rho_f \mathbf{u}_f Y_{f,k}) = \nabla \cdot \varepsilon_f \mathbf{J}_k + \varepsilon_f R_{f,k} + \mathcal{R} + S_{\text{sp}} \quad (9)$$

where the subscripts f denote the fluid phase, k is the species index, h is the enthalpy, ε denotes the phase volume fraction, ρ is the density, $\mathbf{u}$ defines the velocity vector, $\mathbf{g}$ is the gravity, τ_f is the fluid stress tensor which represents

viscous forces in fluid phase, $Y_{f,k}$ stands for the mass fraction of species k in fluid phase, K_{DPM} is the drag coefficient calculated for the average value of the solid volume fraction in a numerical cell, $\text{Sc}_{f,k}$ is the Schmidt number, m stands for the number of species in resolved flow, $\mathbf{J}$ is the diffusion flux of species k , and $\mathbf{q}$ is the heat flux. The source term $S_{f,\text{rad}}$ defines the contribution to the energy equation due to the radiation. The source term $S_{f,\text{rec}}$ stands for the amount of energy released from chemical reactions. The $R_{f,k}$ represents the net rate of production of homogeneous species k , whereas $\mathcal{R}$ is the heterogeneous reaction rate in case of modelling surface combustion. The S_{mass} , S_{mom} , S_{en} and S_{sp} are sources due to exchange of mass, momentum energy and species between the continuous phases and particles in discrete phase, respectively. The energy source S_{en} includes the enthalpy transfer due to convection, chemical reactions and radiation from discrete phase. The momentum source term S_{mom} determines the change of momentum in the gaseous phase due to particles movement.

For above set of equations different discretization models can be selected during solution procedure. In this work the QUICK discretization scheme was used for the mass conservation equation [31], whereas the second order upwind scheme was selected for the remaining equations excluding turbulent equations. The turbulence was modelled using standard k - ε model with *dispersed* option [32] for hybrid Euler-Lagrange derived based on the Tchen theory of dispersion described in [33]. Detailed derivation of the turbulent equations and closure model for the *dispersed* k - ε model can be found in [34].

One of the important issue during modelling multiphase flows is the prediction of the mass distribution over computational cell. In this work for all

presented simulations the node based averaging process was applied. In default model settings the total solid volume fraction from all parcels in given cell is mapped into the center of computational grid, which is numerical very unstable. In order to stabilize the solution procedure the node based averaging procedure was used which ensure smooth distribution of the solid material over the nodes of the computational grids. For that purpose the Gaussian Averaging kernel [35, 36] was selected, where the Gaussian Factor was set to 6 [35].

3.1. Modelling combustion process

When the combustion process is taken into account by the hybrid Euler-Lagrange approach, the particle mass and temperature changes are tracked by solving the mass and energy balance equations for individual particle. The particle mass changes during combustion process can be described as

$$\frac{dm_p}{dt} = \frac{dm_{\text{char}}}{dt} + \frac{dm_{\text{vol}}}{dt} + \frac{dm_{\text{water}}}{dt} \quad (10)$$

where m_{char} , m_{vol} and m_{water} are the mass of the char, volatile and water in combustible particle, respectively. The convective and radiative heat transfer between surrounding gases and the particle is taken into account by solving particle balance equation

$$m_p c_p \frac{dT_p}{dt} = A_{\text{ext}} h (T_f - T_p) + Q_c + A_{\text{ext}} \epsilon_p \sigma (\Phi^4 - T_p^4) \quad (11)$$

where c_p and T_p stands for the particle heat capacity and temperature respectively. T_f is the temperature of gases inside a cell where the particle is located. h denotes the heat transfer coefficient, ϵ_p is the particle emissivity, σ is the Stefan-Boltzmann constant and A_{ext} represents the particle surface

area. The incident radiation temperature Φ on the particle can be calculated as

$$\Phi = \left(\frac{G}{4\sigma} \right)^{1/4} \rightarrow G = \int_{\Omega=0}^{4\pi} I d\Omega \quad (12)$$

where I stands for the radiation intensity, Ω is the solid angle, Q_c represents the changes of energy due to the evaporation and surface combustion processes and G represents the particle irradiation.

Due to the lack of exact kinetic data, the reaction rates for the homogeneous reaction were mixing controlled using the Eddy Dissipation Model proposed by [37]. The combustion processes modelled using EDM are mixing-limited so the complex chemical kinetic rates can be neglected [38]. The coal combustion process was modelled using two-step homogeneous reactions for the gaseous phase (13), (14) and one heterogeneous reaction (C(S)-O₂) for char combustion (15).

The stoichiometric coefficients (ν_{O_2} , ν_{CO} , ν_{H_2O} , ν_{N_2} , ν_{SO_2}) for homogeneous reaction (13) have been calculated by applying mass balance to each of the elements of volatile species $C_iO_jH_kN_mS_n$.

In order to calculate fraction of volatile components reference to total molar mass of volatile, the carbon fraction (kgC/kgCoalDAF) has to be reduced by the mass fraction of the fixed carbon expressed in kgChar/kgCoalDAF. Making this calculation the amount of component C fixed only with volatiles can be retrieved. ~~has been calculated assuming that contains only volatile~~

~~fraction without fixed carbon (char).~~ Calculated composition of the volatile and stoichiometric coefficients lignite coals are shown in Tables 5.

Table 5: Elementary composition of the volatile and stoichiometric coefficients used by the homogeneous reaction of lignite coal

composition of volatile			stoichiometric coefficients	
i	1.511	$\text{kmol}_C/\text{kmol}_{VOL}$	ν_{CO}	1.511
j	0.502	$\text{kmol}_O/\text{kmol}_{VOL}$	ν_{O_2}	1.289
k	3.103	$\text{kmol}_H/\text{kmol}_{VOL}$	ν_{H_2O}	1.551
m	0.028	$\text{kmol}_N/\text{kmol}_{VOL}$	ν_{SO_2}	0.009
n	0.009	$\text{kmol}_S/\text{kmol}_{VOL}$	ν_{N_2}	0.014

The particle combustion process, where heterogeneous reaction took place was divided into several submodels shown in Table 6. Typically the combustion model constants should be determined based on experiments performed for a given coal (e.g. in a drop tube facility [39]). Nevertheless, for fluidized bed combustion this technique cannot be directly used, due to large particles diameter. ~~For that particles the falling velocity is high~~, which requires special design of the test apparatus. Nowadays, such devices ~~which can generate comparable combustion conditions to those which exist in the CFB unit are not~~ ~~has not been directly~~ available. ~~for coal burned within similar conditions as those which exist in CFB boiler.~~ One of the possibility to determine the combustion model constant is application of numerical technique combined with experiment, using a kind of an inverse approach. Based on the experiments carried out on the well measured CFB experimen-

tal facility and numerical simulations the model constants can be evaluated iteratively during simulations in order to fulfil experimental conditions [17]. ~~The model constants for char combustion, namely the mass diffusion limited rate constant and kinetic limited rate (pre-exponential factor), as well as devolatilization rate were derived iteratively during simulations. These model constants were selected under assumption that the injected coal should burn before it exits the combustion chamber.~~ The final model constants for both burned coals were collected in Table 7.

Table 6: Models used for particle combustion

Heating	Heat transfer (convection and radiation)
Evaporation	Diffusion Controlled Model
Devolatilization	Constant Rate Devolatilization Model [40]
Char combustion	Kinetic/Diffusion Surface Reaction Rate Model [40],

Table 7: Model constants used for combustible particles

			Lignite Coal
Devolatilization rate, 1/s	A_0		80
Swelling coefficient	C_{sw}		1.4
Activation energy, J/kmol	E		$7.9 \cdot 10^{-7}$
Specific heat, J/kgK	c_s		1680
Pre-Exp. Factor			0.1
Mass Diff. Rate Constant			$5 \cdot 10^{-12}$

4. Sample results

4.1. Effect of radiation

The first set of simulations ~~was~~ performed using simplified boiler geometry in order to check the influence of radiation on evaluated temperature profile within the boiler. It is no doubt that the radiative heat transfer plays important role within the Pulverized Coal (PC) boilers where ~~high~~ non-uniform temperature and presence of participating gases makes the heat exchange mode important in simulations of the energy transfer in the PC boiler. In contrary to the PC boiler the temperature within the combustion chamber of the CFB boiler is much smaller (800-950 °C) and it is uniform, which attenuates the effect of radiation. ~~Additional factor which mitigate the radiation effect within the CFB~~ is the presence of the high concentration of the particulate mater. ~~which mitigate influence of radiative heat transfer.~~ Based on these features it can be assumed that the effect of radiation within the boiler can be safely neglected. Nevertheless, to confirm this ~~assumption~~ hypothesis the air-combustion process was modelled with and without activated radiation model. The radiative heat transfer in presented work was modelled using the Discrete Ordinate (DO) method which in Ansys FLUENT is programmed in Finite Volume form [41]. The influence of radiation on predicted temperature profile within the pilot instillation was also investigated within other authors work [17]. Calculated temperature profiles over boiler combustion chamber with and without activated radiation model are depicted in Fig. 3. Some discrepancies can be observed at the bottom and upper zones of the combustion chamber in contrary to measured data. These differences can be attributed to the introduced truncation of the com-

putational domain and artificial boundary conditions (outlet) prescribed at the top surface of the domain. Generally, the differences between the profiles plotted in Fig. 3 are very small which confirms the hypothesis that radiation modelling within the CFB boiler can safely be neglected.

~~Comparing both calculate profiles similar tendencies can be observed with some discrepancies. However, the difference between plotted profiles on Fig are very small which confirm that the the necessity of radiation modelling within the boiler can be safely neglected.~~ When the heat transfer due to radiation was not taken into account, the required simulation time was considerable reduced. Moreover, the solution procedure was stable. The distributions of temperature on selected planes over boiler combustion chamber for both investigated cases are illustrated in Fig. 4.

Figure 3: Calculated temperature profiles ~~calculated~~ over combustion chamber ~~of the simplified boiler geometry~~ with and without activated radiation model

Figure 4: Calculated temperature distribution on selected planes with and without activated radiation model

4.2. Comparison of the complete and simplified CFB geometrical models

Next set of simulation was performed using complete and simplified boiler **geometrical models** in order to check the influence of the geometrical model simplification on calculated pressure and temperature profiles within the boiler. The comparison of the pressure profile within the combustion chamber along boiler height for simplified and complete boiler geometry applying

Figure 5: Scaled pressure profile calculated for simplified and complete boiler model compared ~~with~~ against measured data ~~evaluated for the CFB-Turow boiler~~

Figure 6: Scaled temperature profile calculated for simplified and complete boiler model compared ~~with~~ against measured data ~~evaluated for the CFB-Turow boilers~~

air and *OXY 1* cases are depicted in Fig. 5, whereas the temperature profiles are illustrated in Fig. 6.

It can be seen that for each boiler model (simplified and complete) the difference between calculated temperature profiles for *AIR* and *OXY 1* cases are comparable. However, the pair of temperature profiles for complete boiler geometry is lower in contrary to measured data and this calculated using simplified model. This situation is caused by higher amount of solid material within the combustion chamber for complete boiler geometry which can be seen on the pressure profile in Fig. 5. With increasing the amount of solid material within the combustion chamber the heat transfer to the boiler walls also increase. This caused decreasing temperature of the gaseous phase within the combustion chamber. For complete boiler geometry it was very difficult to stabilize amount of solid material due to introduced geometrical model simplification within external solid super-heaters geometries. This is no doubt that taken more detailed geometry of the boiler recirculation section the amount of solid material within combustion chamber should be easier stabilized. Additional difficulties with mass stabilization were connected with variation of temporal and spacial scales within the boiler individual zones. In order to exactly simulated flow pattern within the solid separators they should by modelled separately using different turbulent model and time

steps than these used within the combustion chamber and solid super-heaters. When simplified boiler geometry was used the amount of solid material within the combustion chamber was controlled by the recirculation procedure implemented into the solution procedure. Finally the amount of solid material within the combustion chamber for complete boiler geometry was stabilized at the level of 170 tones, whereas for simplified model it was 130 tones. The amount of solid material within the boiler was approximately 130 tones which was calculated applying simple manometry formula defined as [1]

$$\rho_{\text{sus}} = \varepsilon_s \rho_s = \Delta p / (g \Delta h) \quad (16)$$

where g is the gravitational acceleration, Δp is the pressure drop in the gaseous phase, h is the boiler height, ε_s , is the volume fraction of the solid material, and ρ_s denotes the average solid phase density.

The temperature profiles calculated for simplified boiler geometry for cases air and oxy 1 fit quite good to measured data. Some discrepancies can be observed between calculated and measured data for both cases, mainly at the upper boiler zone. For complete boiler geometry this situation is caused by presence of swirl dominated flow within the separators which influence at the pressure profile and temperature profile within the boiler [42]. In Fig. 7 the temperature distributions at the walls of the complete boiler geometry for air, and oxy 1 are illustrated. On this figure colder region at the solid separators walls can be observed. In this places the amount of solid material was very small which reduced heat transfer rate to the separators walls. In order to accurately predict flow field within the solid separators where the flow is dominated by the swirl, this boiler section should be modelled separately as it has been mentioned earlier. The flow field calculated within

the solid separators has also direct impact on the flow field within the combustion chamber. This issue can be resolved by applying more sophisticated turbulent model, which gives possibility to simultaneously demarcate temporal and spatial scales within all boiler sections, however such model is still sought for.

Figure 7: Scaled temperature distribution on external boiler walls for *AIR* and *OXY 1* cases

4.3. Results for oxy-fuel combustion

The temperature profiles calculated for the four *OXY* cases compared against measured data for boiler operated under air mode are presented in Fig. 8. The calculated profiles show comparable tendencies, similarly as for earlier described cases the temperature differences are observed at the upper boiler zone. Some discrepancies are also observed for at the bottom zone for case *OXY 4*. This situation was caused by increasing fraction of water in oxidizer composition. In Table 8 the average composition of the wet flue gases at the combustion chamber outlets for all investigated oxy cases are collected.

Figure 8: Scaled temperature profiles for *OXY* cases 1, 2, 3, and 4 compared with measured data

5. Conclusions

This work was focused on testing and validating a CFD model capable for solving particle transport phenomena combined with air- and oxy-fuel combustion process within the large scale CFB boiler. Several known numerical

Table 8: Flue gases composition for all investigated *OXY* cases in wet molar basis

	AIR	OXY 1	OXY 2	OXY 3	OXY 4
$X_{O_2,fg}, \%$	2.7	5.8	2.8	1.7	2.71
$X_{CO_2,fg}, \%$	13.6	67.1	68.9	70.1	64.8
$X_{H_2O,fg}, \%$	14.6	21.6	21.3	21.6	25.7
$X_{N_2,fg}, \%$	69.1	5.5	7.0	6.6	6.8

approaches can be used to deal with the complex reacting multifluid flow within the CFB boiler. The core computer code used in the research was commercial Ansys FLUENT code, the underlying research required modification of the existing code via the User Defined Function (UDF) mechanism. Moreover, the application of the methods implemented in the Ansys FLUENT was associated with selecting of proper combination of submodels, numerical techniques and careful control of the solution convergence.

~~Numerical simulations presented in this paper were split in the three parts. The former part was focused on modelling the air combustion process within the industrial CFB boiler where the influence of the heat radiation on calculated temperature profiles was investigated. Within the second part the impact of geometrical model simplifications on calculated temperature and pressure profile within combustion chamber were investigated. Finally, the last part of the work was devoted to modelling oxy-fuel combustion process for several composition of the oxidizer mixture. Carried out numerical results were compared against measured data collected under normal boiler operating conditions in air-fuel mode.~~

~~Evaluated results with and without activated radiation mode shown comparable trends between measured and calculated data. Based on carried out simulation the minor influence of radiative heat transfer on evaluated temperature profile within the combustion chamber was observed.~~

Evaluated results with and without activated radiation mode show good agreement of measured and calculated data. Based on the carried out simulations minor influence of radiative heat transfer on temperature profile has been confirmed.

~~In order to speed up numerical simulations the boiler geometry was simplified to combustion chamber, including gas, fuel, and solid injection ports. Simplified geometrical model gave possibility to circumvent the problem with large difference of spatial and temporal scales in the transport phenomena occurring in the boiler.~~

The numerical results obtained using complete and simplified boiler model were compared against measured data. Numerical simulations shown that when the complete boiler model **was** used it was very difficult to stabilize the solution and control amount of solid material within the boiler. Introduced simplification to external solid super-heaters **geometry** had huge impact on the mass distribution over the boiler which **influenced in consequentness had impact** on the predicted temperature profile within the boiler. When the simplified boiler model was **used** this problem was solved by applying recirculation procedure which gave possibility to control amount of solid material within the boiler combustion chamber.

The carried out numerical simulations for different oxidizer composition produced negligible differences between cases. Nevertheless, with increas-

ing amount of water fraction in the oxidizer (controlled by concentration of water vapour in recirculated flue gases) the temperature at the boiler bottom decreases, however with increasing distance from the injection port, the temperature of gaseous phase tends to the measured data.

~~In the last set of simulations the impact of different oxidizer composition on predicted temperature profile within the combustion chamber was investigated. The carried out numerical results presented small difference between simulated cases. Nevertheless, with increasing amount of water fraction in oxidizer composition controlled by concentration of water vapour in recirculated flue gases the temperature at the boiler bottom decrease, however with increasing distance form the injection port the temperature of gaseous phase tends to measured data.~~

The main conclusion when summarizing the results of combustion process presented in this paper is that the very complex and non-uniform flow behaviour combined with combustion process within the large scale CFB boiler can be modelled using commercial CFD Ansys FLUENT package extended buy set of UDFs implemented into the solution procedure. ~~–was observed which was mainly caused by dense granular flow.~~ The disadvantages of the simulations carried out using a 3D geometry were associated with very long simulation time required to obtain stable solution. The required simulation time for the simplified boiler model necessary to obtain solution exceeded 350 s, which was adequate to 1 month of wall clock time simulation, whereas when complete boiler geometry was used this time increased to 3 months. In reality to reach the pseudo steady-state operating condition it can take minutes and even hours, which mean that the hybrid Euler-Lagrange model still

has to be developed in order to be seen as a engineering tool for CFB boiler construction optimization. Nevertheless, developed model can be used in hybrid numerical calculation, where hybrid Euler-Lagrange model can be used as a tool for calculating good input data to the semi-empirical models used for calculating combustion process within CFB boilers under steady-state conditions [9].

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