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The oxy-combustion modeling in CFB using multiphase approach

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Abstract

Particle transport accompanied by air- and oxy-combustion in Circulating Fluidized Beds (CFB) installation has been simulated using ANSYS FLUENT commercial CFD package. The results concern a 3D model of a pilot-scale CFB installation built at Czestochowa University of Technology. In numerical simulations the mutual interactions between particles have been taken into account as well as the particle-wall collisions and friction. The granular flow has been predicted using a combination of Euler-Euler and Euler-Lagrange model, known as the Dense Discrete Phase Model (DDPM). This technique has common roots with the Multiphase Particle in Cell (MP-PIC) technique. In this approach the gaseous phase is modeled using a standard Eulerian approach while the particles are traced in a Lagrangian frame of reference. The particle-particle collisions effect have been modeled using a continuum model, based on a kinetic theory of granular flows. The main advantage of the DDPM in contrary to the Euler-Euler approach is that it gives possibility of modeling particle size distributions directly. However, the cost of numerical calculations in the Lagrangian technique strongly depends on the number of the tracked particles (characteristic diameters), whereas in Euler-Euler numerical cost is associated with mesh size, their quality and number of resolved phases. The validation of the numerical results have been carried out using experimental data delivered by researchers from Czestochowa University of Technology.

Key words: computational fluid dynamics, oxy-combusion,CFB, mulifluid

INTRODUCTION

Circulating Fluidized Bed (CFB) combustors, due to their robustness and insensibility to the quality of fuel became a popular alternative to traditional Pulverized Coal Boilers. The simulations of such devices require a solution of complex multiphase transport phenomena in gas-particulate mixtures with high solid phase loading. High concentration of particulate matter results in a significant influence of the particles mutual interactions due to collisions, frictions and combustion conditions in the CFB. The published models of CFB boilers are still in their infancy, as they are based on plug flow in 2 zones: near wall and core (Myöhänen K., 2011). This approach requires many empirical data and cannot account for the complex mixing of polydisperse granular flows. Additional difficulties during the CFB numerical modeling appears when the fuel combustion is taken into account. The complex reacting flow in dense solid bed requires advanced numerical techniques.

The gas and solid flow in the CFB is frequently modeled using two fluid model (TFM). The basic assumption of TFM is that the gas flow is modeled as continuum, whereas the second phase (solid phase) is treated as disperse. The TFM uses the extension of the kinetic theory for granular flow (KTGF) (Chapman, 1970) to represent particle-flow and particle-particle interactions within the disperse phase. The KTGF relies on the analogy of the Chapman-Enskog theory for dense gases. The KTGF theory describes the particle transport phenomena using solid phases stress tensor, where the momentum transfer between particles is represented by the granular pressure, viscosity and friction. The energy of particle velocity

fluctuation in fluid has been described using granular temperature Θ which has analogous to the thermodynamic temperature of dense gases. The granular temperature $\Theta = 1/3\left\langle C_x^2 + C_y^2 + C_z^2 \right\rangle$ is associated with random velocities of the particles $\bar{C}$. More information about the KTGF can be found in (Chapman, 1970) and (Gidaspow D., 1994). The main disadvantage of the Euler-Euler approach is that the real distribution of particle diameters, due to involved numerics, is not modeled directly. To cope with this difficulties additional models are required for the correct prediction of particle size distribution of the disperse phase (Marchisio et al., 2005). This becomes important when the combustion and gasification in the CFB is investigated. In such cases the distribution of particles changes significantly during the process and the range of diameters spans several orders of magnitudes. The easiest way of resolving the particle distribution is to use several disperse phases. Each additional disperse phase corresponds to a selected characteristic diameter. This approach is from computational point of view, very expensive especially when the large CFB boilers are simulated. An alternative approach to Euler-Euler is the Dense Discrete Phase Model (DDPM) (ANSYS-FLUENT, 2010) which combines the Euler-Lagrangian and Euler-Euler approaches. The idea behind this method is to trace particles motion and the energy exchange between the particles and the fluid using Lagrangian frame of reference, while the mutual interaction and friction between particles are calculated in continuous phase using Eulerian scheme. The DDPM can be used for volume fractions of particulate phase extending from 0 to the packing limit. Using the DDPM the particles distribution is solved in natural way. Moreover, the combustion phenomena of particles can be modeled relatively easy using standard combustion models derived for single fuel particle.

DESCRIPTION OF THE EXPERIMENTAL RIG

The geometry of circulating fluidized bed (CFB) used for simulations has been created based on the experimental rig installed at Czestochowa University of Technology. The installation is used for simulating combustion and granular transport in the small scale CFB unit. The thermal loading of this pilot-scale installation is estimated to be around 0.1 MW. This value can vary slightly depending on the calorific value of the combusted coal. The simplified scheme of the experimental rig is depicted in Fig. 1 (left). A three-dimensional numerical mesh has been applied to describe the CFB riser. The mesh consisting of 90 000 tetrahedral and hexahedral elements with the average size of elements ranged between 5 and 6 mm. The detailed view of the geometry and grid system is shown in Fig. 1 (right). The mesh is locally refined near injection of the solid and secondary gas ports. The main stream of oxidizer is supplied through the distributor located at the bottom of the combustion chamber. The secondary air is delivered using three ports which are installed above the inlet of a recirculation pipe. The combustion chamber (riser) is 4.98 m high and the internal diameter of the riser pipe is 9.8 cm. The secondary gas injection ports are located at 0.55 m above the distributor. The riser of the pilot-scale unit has been equipped with the temperature and pressure measuring ports located along riser height.

NUMERICAL MODEL

The particle transport in the CFB has been simulated using ANSYS/FLUENT commercial CFD package. The DDPM uses four-way coupling to take into account the relationship between continuum and disperse phases. The momentum exchange between the continuous phase and disperse phase is modeled using drag forces, solid stress tensor and source/sink terms in the momentum governing equations (2) and particle motion equation (5). At the present stage of the modeling tools development, the computational domain has been limited to the riser with a small part of recirculation zone including the solid injection port, see Fig. 1 (right). The complex flow through the cyclone is modeled separately in order to capture and

correctly predict its physics. In the simplified geometry the mass leaving the end of the riser has been returned to its bottom section. This mass flow between the parts of the installation has been simulated by a set of appropriate User Defined Functions (UDFs). At this stage of the model development, the gas flow in the distributor is greatly simplified.

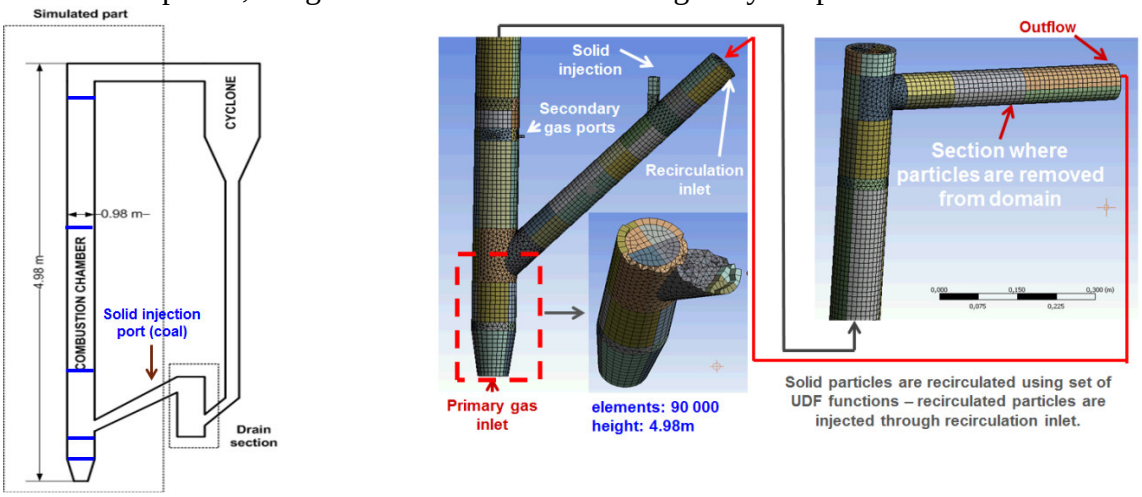

Figure 1: Simplified draft of the pilot-scale installation (left) and numerical geometry including mesh (right)

The DDPM approach solves the set of conservation transport equations of: mass Eq.(1), momentum Eq.(2), energy Eq.(3) and species Eq. (4). These equations are used for describing the flow of continuum phase in the Eulerian grid. The turbulent flow has been modeled using standard $k-\varepsilon$ approach. The two transport equations for turbulent model are not presented in this paper, their form can be found in (ANSYS-FLUENT, 2010).

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f) + \nabla \cdot (\varepsilon_f \rho_f \bar{u}_f) = \sum_{q=1}^{nphase} \left(\dot{m}_{qf} - \dot{m}_{fq} \right) \tag{1}$$

$$\begin{aligned} &\frac{\partial}{\partial t}(\varepsilon_f \rho_f \bar{u}_f) + \nabla \cdot (\varepsilon_f \rho_f \bar{u}_f \bar{u}_f) = -\varepsilon_f \nabla p + \varepsilon_f \rho_f \bar{g} + \nabla \cdot \tau_f + \\ &K_{DPM}(\bar{u}_{DPM} - \bar{u}_f) + S_{DPM} + \sum_{q=1}^{nphase} \left(K_{qf} \left(\bar{u}_q - \bar{u}_f \right) + \dot{m}_{qf} \bar{u}_{qf} - \dot{m}_{fq} \bar{u}_{fq} \right) \end{aligned} \tag{2}$$

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f h_f) + \nabla \cdot (\varepsilon_f \rho_f h_f \bar{u}_f) = \nabla \cdot (\varepsilon_f \Gamma_h \nabla \cdot h) + S_h + \sum_{q=1}^{nphase} \left(Q_{qf} + \dot{m}_{qf} h_{qf} - \dot{m}_{fq} h_{fq} \right) \tag{3}$$

$$\frac{\partial}{\partial t}(\varepsilon_f \rho_f Y_{f,k}) + \nabla \cdot (\varepsilon_f \rho_f Y_{f,k} \bar{u}_f) = \nabla \cdot \left(\varepsilon_f \rho_f D_k \nabla \cdot Y_{f,k} \right) + \nabla \cdot (\varepsilon_f \rho_f D_k \nabla \cdot Y_{f,k}) + S_{Y,k} \tag{4}$$

where ρ_s is the density of continuum phase, $\bar{u}_f$ is the velocity vector of fluid phase, p is the pressure, $\nabla \cdot \tau_f$ is the fluid stress gradient, S_{DPM} is the source term taken from the solution of the particle motion equation which includes acceleration of the fluid around particle due to pressure difference, K_{DPM} stands for the drag coefficient calculated for the granular phase, $K_{qf}\left(\bar{u}_q - \bar{u}_f\right)$ is the interface exchange force if more than one disperse Euler-Euler phases are considered in calculations, $\bar{u}_{DPM}$ is the solid velocity interpolated from parcels to cells. The terms $\dot{m}_{qf}\bar{u}_{qf} - \dot{m}_{fq}\bar{u}_{fq}$ in the momentum equation represent the mass transfer phases (continuum to disperse $\dot{m}_{qf}$ and vice versa $\dot{m}_{fq}$), h stands for the gas enthalpy, Y_k denotes the k-th species mass fraction, D_k is the diffusion coefficient and $\Gamma_h = \mu / \mathrm{Pr} + \mu_t / \mathrm{Pr}_t$ where

subscript t denotes the turbulent properties. When the reacting flow is taken into account the set of equation for continuous phase has to be averaged using Favre mass averaging in order to take into account density depends of temperature. The term Q_{fq} in Eq. (3) stands for intensity of heat transfer between continuum and solid phase, S_h denotes source term which includes source of enthalpy from radiation and chemical reactions. The terms $\dot{m}_{qf} h_{qf} - \dot{m}_{fq} h_{fq}$ in energy equation represent the enthalpy transfer between phases (continuum to disperse h_{fq} and vice versa h_{qf}). The set of equations related to the discrete phase is not solved directly in the continuous phase. The coal and inert particles in the riser were tracked in Lagrangian frame of reference with the particle momentum equation Eq. (5).

$$\frac{d\bar{u}_s}{dt} = F_D(\bar{u}_s - \bar{u}_f) + g - \frac{\nabla p_f}{\rho_s} - \frac{\nabla \cdot \tau_s}{\rho_s} \tag{5}$$

Where τ_s is the solid stress tensor, ρ_s the density of particles material, $F_D(\bar{u}_s - \bar{u}_f)$ is the acceleration due to drag force, ∇p_f is the pressure gradient calculated in parcel location which takes into account contribution from static and hydrostatic pressure $\nabla p + \rho_f g$. The momentum equation for continuum phase was solved using second order upwind differential scheme. The QUICK scheme was used for mass conservation equation. Due to high instability of the second order differencing scheme for k-ε model, the first order scheme was selected in the beginning of the simulation. This has been changed to second-order after an initial simulation period of rapid changes in the flow field. During calculations also the radiation model has been included. The radiation effect is dominating in the dilute regions of the riser, typically in the upper part of the riser. The radiation model that has been applied takes into account absorbing, emitting and scattering properties of gray gases. Currently two radiation models are often used for modeling the radiation in furnaces, namely P1 (Cheng, 1964) and the Discrete Ordinates (DO) (Backreedy et al., 2005 and Viskanta et al., 1987). In the present work DO model has been employed for radiation modeling. The radiation is important during coal combustion because of high concentration of CO_2 resulting from flue gases. Moreover, when the oxy-combustion is investigated, additional source of CO_2 is in the oxidizer mixture which contains high fractions of CO_2. The gas mixture absorption coefficient was calculated using the weighted sum of gray gases (WSGG) model (Węcel et al., 2009). Mathematical model also took into account the particles radiation interaction which is imporatnt in the dense part of the bed. For the oxy-combustion the impact of soot to the radiation properties has been neglected due to the lack of experimental data necessary for soot modeling. The solid stress tensor used in the particle motion equation (5) and momentum equation for continuum phase was modeled using the KTGF theory. The solid viscosity was calculated using Syamlal model (Syamlal et al., 1993), friction viscosity was included in the calculation using Schaeffer's model (Schaeffer, 1987) and the probability of particles collision was calculated based on the model described in (Lun et al., 1984) which was also used for modeling the solid bulk viscosity and momentum transfers between particles due to their collisions (solid pressure). The drag force between phases was calculated with Wen Yu model blended with Ergun, this model is known as Gidaspow drag model (Gidaspow, 1994). The transfer of information between cells and particles is accomplished by resorting to interpolation operators. In the presented paper all simulations were carried out using the standard DDPM volume fraction averaging where the parcel volume fraction is duped into one cell, however the gradients were calculated using node-based technique (ANSYS-FLUENT, 2010).

PARTICLE HEAT BALANCE EQUATION AND COMBUSTION MODELS

The particle temperature in the riser was calculated taking into account the heat transfer due to convection, radiation and the heat generated by chemical reactions. The energy equation for particles is given as

$$m_s c_s \frac{dT_s}{dt} = hS_{ext}(\tilde{T} - T_s) + S_{ext}\varepsilon_s\sigma(\Phi^4 - T_s^4) + Q_c \quad (6)$$

where c_s, T_s stands for the particles heat capacity and temperature respectively, h is the heat transfer coefficient, S_{ext} presents the external particle surface, $\tilde{T}$ denotes the mean gas temperature in the particle vicinity, Q_c is the heat transfer rate delivered to the particle due to chemical reactions and Φ stands for the irradiative temperature which can be determined from known particle irradiation G as $\Phi = \left(G/4\sigma\right)^{1/4}$ where $G = \int_{\Omega=0}^{4\pi} I d\Omega$, I is the radiation intensity and Ω stands for the solid angle. The combustion of coal particles is divided in several steps. The devolatilization and the temperature of the particles reaches 400K. In presented work the constant rate devolatilization model has been used (Baum, 1971) to predict mass changes of the particles due to this process $dm_s/dt = -A_0 Y_{vol,0}(1-Y_{w,0})m_{s,0}$, where $Y_{vol,0}$ and $Y_{w,0}$ tends for initial mass fraction of the devolatilization species and water respectively, $m_{s,0}$ represents the initial mass of the coal particle and A_0 is the constant, which for simulations was set to 40 1/s. The char combustion is the most important process, which directly influences the combustion conditions. The char combustion has been modeled using single heterogeneous reaction which oxidizes the coal to the carbon dioxide with stoichiometric burnout ratio equal to 2.66, whereas the combustion of volatiles has been modeled using a two-step homogenous reaction model. For char combustion the surface combustion as well as the diffusion of the combustion products to the particle surface has been included, so the char combustion rate can be calculated from Eq. (7)

$$\frac{dm_s}{dt} = \pi d_p^2 \left[\frac{\rho_s R \tilde{T} Y_{O_2}}{M_{O_2}}\right] \frac{D_0 r}{D_0 + r} \quad (7)$$

where d_s is the particle diameter, M_{O_2} and Y_{O_2} stand for the molecular mass and mass fraction of oxygen in vicinity to the particle surface respectively, r denotes the kinetic rate $r = C_2 \exp\left(-\left(E/RT_s\right)\right)$ with zero order for the surface reaction and D_0 defines the diffusion coefficient and can be calculated as $D_0 = C_1/d_s\left(\left(T_s - \tilde{T}\right)/2\right)^{0.75}$. The kinetic/diffusion reaction model assumes that the particle diameter remains constant during char combustion (ANSYS-FLUENT, 2010), whereas the density of the particles decreases continuously to reach the ash density.

SETUP OF THE NUMERICAL MODEL

The main objective of this paper is to gain an understanding of the combustion behavior within the CFB riser under air and oxyfuel environments. For simulations and experiments the coal from Janina Polish coal mine has been selected. The proximate and ultimate analyses as well as the lower heat value (LHV) of simulated coal are shown in Tab. 1. The injected coal is partially dried in an atmospheric conditions so the coal composition as well LHV have to be recalculated to account for the new water content of the fuels well as the components of the coal. The raw coal contained 16% of H_2O, after drying the water content this value has been reduced to 5% approximately, which indicates that subsequent fuel components increase. The coal sieve analysis defined the range of fuel particle size 2500 μm with calculated mean diameter $\bar{d}_p$ =386 μm. The constants of the kinetic/diffusion model (7) C_1 and C_2 have been

evaluated based on the assumption that the coal particle should burn out in 4.89 s after it was injected into the riser, which is a typical residence time of the particle in the riser. The largest coal particle remained in the riser around 5-6s, so the model coefficients were set to C_1 = 2.0E-11 and C_2 = 0.05. The calculations have been performed for three cases: the case 1 simulated the coal combustion in air atmosphere, case 2 used oxyfuel environment with 30% O_2/CO_2, and case three 21% O_2/CO_2. For all cases the calculated BCs are specified in Tab. 2. The amount of oxidizer was calculated for an excess oxidizer ratio $\lambda = 1.25$. The total amount of oxidizer used for simulations has been depicted in Tab. 2.

Table 1: Coal analysis

Ultimate analysis, kg_i/kg_{fuel}		Proximate analysis, kg_i/kg_{fuel}	
	raw		***raw***
ASH	0.103	**C**	0.577
H2O	0.160	**H**	0.038
VOL	0.307	**S**	0.013
Char	0.430	**N**	0.009
LHV, MJ/kg	**22.49**	**O**	0.100

Table 2: BCs used for numerical simulations

	O_2	N_2	CO_2	Primary gas inlet		Secondary gas inlet		Solid injection		Recirculation inlet, kg/h	
				$\dot{m}_{oxy}$ kg/h	T_{oxy} T_{gas}K	$\dot{m}_{oxy}$ kg/h	T_{oxy} K	$\dot{m}_{oxy}$ kg/h	T_{oxy} K	$\dot{m}_{oxy}$, kg/h	T_{oxy}, K
Case 1 AIR	0.232	0.767	0	29.1	507	12.4	507	1.4	400	3.2	1045
Case 2 30%O_2	0.237	0	0.762	28.4	507	12.2	507	1.4	400	3.2	1045
Case 2 21%O_2	0.162	0	0.838	41.7	507	17.8	507	2.0	400	4.6	1005

The external walls of the riser were insulated by a 10 cm insulation layer with thermal conductivity 0.04 W/m·K, outer conditions were simulated using Robin BC with the heat flux coefficient equal to 5 $W/m^2 \cdot K$ and surrounding temperature 25^0C. The internal walls of the riser for the continuous and disperse phase were treated as no-slip, where the restitution coefficient for disperse phase has been set to 0.85 for normal and tangential collision direction. The ash of a burned coal has been used as the inert bed material with the particle size in range 0-1000E-6 m with calculated mean particle diameter $\overline{d}_{inert}$ = 225E-6 m. The heat capacity of ash was set to 850 J/kg·K and density to 2000 kg/m^3. The ash was injected into the riser through the recirculation inlet, see Fig. 1 (right). The material recirculation has been modeled using set of appropriate UDFs. During simulations the total amount of the solid material (coal and ash) in the riser varied from 1.8 to 2.3 kg.

RESULTS

The simulations for three kinds of gaseous atmospheres have been performed in order to check the response of the low-scale installation form Częstochowa University of Technology when the combustion atmosphere has been switched from air to oxy. The simulation for oxy atmosphere has been performed for two kind of oxidizer mixtures having ratio of O_2/CO_2 equal to 30 and 21%. In order to solve complex granular flow including reacting transport of coal particles, it was required to perform all simulations in transient state which brought additional difficulties connected with long computational times. The simulation time for both

investigated cases was 39s, which corresponds to wall clock time of 38-44 days on computer equipped with 8 processor units. Moreover all simulations were split in two steps. The first step of simulations was focused on stabilization of the gas and particles flow pattern over riser. In this part the installation was loading with required amount of ash mixed with coal. When the total amount of solid material in installation reached around 3.8 kg, and 1.8-2.3 kg in the riser the injections of solid material were switched off and recirculation UDF has been activated to keep constant amount of solid material in installation. The properties of recirculated material has been described in previous section. All evaluated numerical results have been compared with experimental data. The comparison of temperature profile for oxidizer mixture 21% O_2/CO_2 with experimental results has been depicted in Fig. 2 (left). In Fig. 2 (right) the temperature profile calculated based on simulations for AIR and 30% O_2/CO_2 atmosphere has been compared with experimental data.

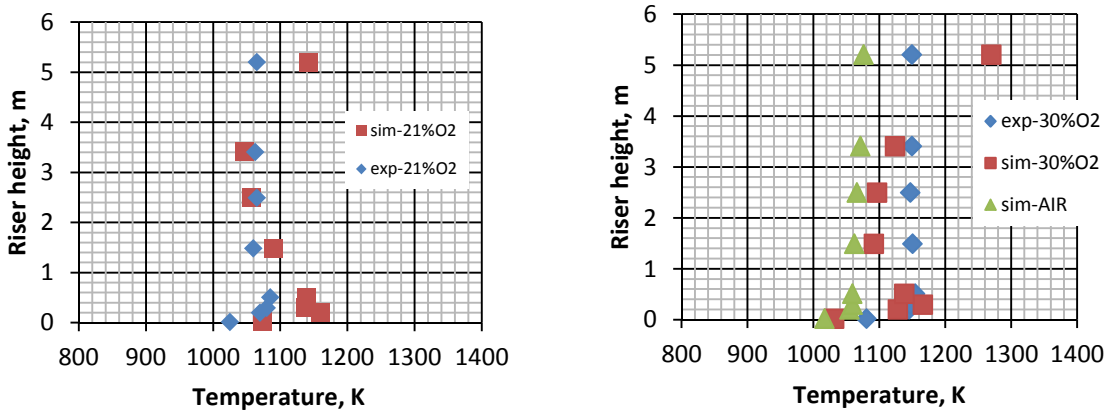

Figure 2: Temperature profile over riser height for 21%O_2/CO_2 (left) and 30%O_2/CO_2 (right)

Replacing N_2 by CO_2 in oxy combustion causes decrease in temperature of gases due to the higher specific heat and emissive properties of CO_2. This feature can be observed when the temperature profile from case 2 is compared with case 3 where high concentration of CO_2 in oxidizer is used. The average gas temperature in the CFB riser increases with increasing oxygen fraction in oxidizer mixture, however the oxygen concentration should not exceed 35% of O_2 due to the safety reasons. The differences between evaluated numerical results with experimental data for both oxy cases can be attributed to the fact that simple air kinetic model for both investigated oxy cases were used. Moreover the reaction kinetic constant have been set based on simple calculation performed for single particles due to the lack information about those constant for burned coal. Additional source of discrepancies between results can be connected with used kinetic/diffusion char surface combustion model which is dedicated for air atmosphere (in vicinity to the particles only oxygen is taken into model) does not properly work in oxyfuel atmosphere where large amount of oxygen is transported with CO_2. Numerical simulations assumed also that the recirculated coal burned out in the cyclone and the loop seal, so no coal was recirculated back to the riser with ash. The evaluated results for cases 1 and 2 give similar temperature profiles. The combustion conditions in the riser approaches the air case while increasing mass fraction of O_2 in oxidizer for case 2. The mass fractions of oxygen in the end of the riser pipe have been compared with experimental data. In Fig. 3 (left) and Fig. 3 (right) the mass fraction of oxygen evaluated for case 2 (30% O2/CO2) and case 3 (21% O2/CO2) is compared with experimental results respectively. The difference between oxygen concentration are mostly caused by the amount of not burned coal. The differences can be damped by changing amount of injected coal with fixed amount of delivered oxidizer. The amount of unburned coal is not known from experiments directly which introduces additional difficulties with selecting appropriate kinetic constant for coal combustion models.

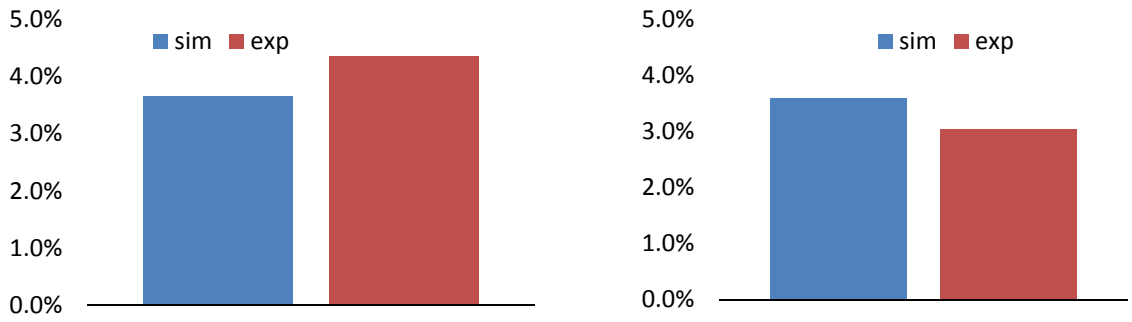

Figure 3: Oxygen concentration in the upper part of the riser for 21% O_2/CO_2 (left) and 30% O_2/CO_2 (right) combine with experimental data

CONCLUSIONS AND FINAL REMARKS

Particle transport and coal combustion under O_2/N_2, 21% O_2/CO_2 and 30% O_2/CO_2 conditions in the CFB has been simulated using ANSYS/FLUENT CFD package. The results concern the 3D model of the pilot scale CFB installation at Czestochowa University of Technology. Some discrepancies in the predicted temperature profiles between experimental data and simulated results were observed. This was associated with the lack of information concerning the reaction kinetics for burning coal. It is necessary to include in the future calculations a modified surface coal combustion model which will incorporate the influence of oxyfuel atmosphere into combustion conditions. The standard kinetic/diffusion model for coal combustion does not take into account CO_2 concentration in vicinity to the burned particles surface. Additionally in future calculations the reaction kinetic constants determined based on the experiments in a drop tube fluency will be used.

The biggest advantages of the DDPM over the standard Euler-Euler is the possibility of modeling combustion using the well-established DPM models. Moreover, the variation of the size distribution of particles can be modeled relatively easy. The weakness of the approach is the drag which does not predict formation of clusters of particles which is important in bottom part of the riser. The KTGF model used for calculation of mutual particles interaction also has to be improved. Obtained results using DDPM show that this technique can be seen as a appropriate approach for simulating gas-solid flows in the CFBs including reacting flows.

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