Modelling of pulverized coal injection combustion process in the validation test rig using the Euler-Lagrangian approach

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Abstract. The combustion of pulverized coal is widely used in ironmaking blast furnaces. The pulverized coal has become a very important fuel. Most of the combustion models for the domain zone blast furnaces are based on CFD-LPT approach. In the Eulerian-Lagrangian approach, the continuous phase is treated as a continuum by solving the Navier-Stokes equations and the conservation equations for mass momentum and heat; the dispersed phase is calculated by tracking a large number of particles that follow Newton second law. The coalChemistryFoam solver was used to calculate the flow parameters in the test blast furnace combustion chamber (validation test rig). A system of equations based on the URANS model and the k-ε model of turbulence was used. The gmsh utility was used to build the computational grid. The temperature, velocity fields for gas and solid particles, concentrations fields of gas in particles and ash in particles have been calculated for given flow rate of coal particles in the valid test rig. The calculations were run on a computing cluster of the web-laboratory of UNICFD ISP RAS. Each calculation was performed on 48-64 cpu cores.

1. Introduction
The combustion of pulverized coal is widely practiced in coal-fired power plants and ironmaking blast furnaces [1,2]. The pulverized coal has become a very important fuel which is used for generating heat and reductant in the raceway and for replacing expensive metallurgical coke, to lower the operating cost, stabilize the furnace operation and decrease the emission of carbon dioxide. However, as the rate of pulverized coal injection (PCI) increases, more unburnt char is generated. The unburnt char passes through the raceway boundary and is transported into the furnace, deteriorating the permeability of the surrounding coke bed. A high coal burnout in the raceway is desired.

The most of the combustion models for the domain zone of blast furnaces are based on the combined Computational Fluid Dynamics (CFD) approach for gas and Lagrangian Particle Tracking (LPT) for particles (CFD-LPT). In such a model, individual particles, which can be presented by a single particle or a group of particles, are simulated taking into account the interaction of particles with a liquid, but the collision of particles is ignored. This can be considered as a simplified model of CFD-Discrete Element Method (DEM). However, this simplification can significantly reduce computational costs. CFD-LPT combustion models appeared as 2D in the 1990s and became three-dimensional in the 2000s.

In the Eulerian-Lagrangian approach the continuous phase is treated as a continuum by solving the Navier-Stokes equations and the conservation equations for mass, momentum and heat; the dispersed phase is calculated by tracking a large number of particles that follow the Newton second law. When
modeling the granular flows, the discrete element method (DEM) and the Discrete Phase Model (DPM) are the models within the framework of the Eulerian-Lagrangian structure [3].

There is no strict distinction between DPM and DEM. The DEM describes the collision between individual particles, while the DPM describes the behavior of particles as groups. In a situation where the solid phase is sufficiently dense, for example, in a grid furnace, in the zone of the blast furnace tuyere camera, the compressibility and influence of the volume fraction of particles should be taken into account [1].

At present time the main research on modeling lies in the description of combustion and related phenomena occurring in the tuyere zone of the blast furnace. A detailed physical model in this regard was developed by a group of authors from the University UNSW (Australia, Sydney) [4-6]. In their model, the computational domain covered the tuyere, tuyere tube, tuyere zone, and coke layer. The blowing area was considered as a cavity. The coke layer was considered as a porous carrier, and the size and shape of the tuyere zone were determined in accordance with CFD-DEM calculation data [4].

The combustion model included reactions related to: (1) coal combustion (volatile removal, volatile combustion and charring reactions); (2) gas burning; and (3) coke combustion and gasification. Combustion models in the tuyere zone were used to obtain new useful results. In particular, through numerical and physical experiments, a simultaneous supply of pulverized coal, plastic, and gas fuel was simulated to increase the combustion efficiency.

It is noteworthy that 86% of the exhaust carbon can be reduced in an optimized blast furnace with gas processing and carbon dioxide fixation. This modification allowed an increase in the speed of the supply of pulverized coal injection (PCI). The authors of the UNSW University conducted a series of numerical calculations to quantify the impact of key parameters on coal burnout for PCI operations, including binary and ternary coal mixtures, evaluating coal properties and operating conditions such as explosion conditions and type of cooling gas.

2. Mathematical model
The mathematical model includes the equations for mass conservation, momentum conservation, energy equation for compressible flow. Under the assumption of a small volume occupied by particles, the gas phase equations have the form:

\[
\frac{\partial \rho_g}{\partial t} + \frac{\partial (\rho_g u_j)}{\partial x_j} = S_m
\]

\[
\frac{\partial (\rho_g u_j)}{\partial t} + \frac{\partial (\rho_g u_j u_j)}{\partial x_j} = \frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho_g g_i + S_{u,i}
\]

\[
\frac{\partial (\rho_g h)}{\partial t} + \frac{\partial (\rho_g u_j h)}{\partial x_j} + \frac{\partial (\rho_g k)}{\partial x_j} = \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j} \left( \alpha_{\text{eff}} \frac{\partial h}{\partial x_j} \right) + \rho_g u_j g_j + S_{\text{rad}} + S_{\text{ch}} + S_h
\]

\[
\frac{\partial (\rho_g Y_j)}{\partial t} + \frac{\partial (\rho_g u_j Y_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_{\text{eff}} \frac{\partial Y_j}{\partial x_j} \right) + S_l
\]

\[
p = \rho_g R T_g \mu_{\text{mix}}
\]

Where are t is time, \( \rho_g \) is density of gas, \( u_j \) is gas velocity vector components, \( x_j \) is Cartesian system coordinates, \( S_m \) is source describing mass transfer between two phases, \( p \) is gas pressure, \( \tau_{ij} \) is stress tensor, \( g_i \) is gravity vector component, \( S_{u,i} \) are components of the source of momentum transfer between two phases, \( h \) is enthalpy, \( k \) is kinetic energy of turbulence, \( \alpha_{\text{eff}} \) is effective thermal diffusivity, \( S_{\text{rad}} \) is radiation source, \( S_{\text{ch}} \) is chemical source due to chemical reactions, \( S_h \) is heat transfer source between gas and particles, \( Y_j \) is concentration of chemical component of gas, \( D_{\text{eff}} \) is effective diffusion coefficient, \( S_l \) is source term for concentrations, \( T_g \) is gas temperature, \( \mu_{\text{mix}} \) is molar mass of the mixture.
The trajectories and temperature of the particles are calculated by the equations:

$$\frac{dx_p^p}{dt} = u_p^p, m_p \frac{du_p^p}{dt} = F, m_p C_p \frac{dT_p}{dt} = Q_p$$ (6)

Where are $x_p^p$ represents particle coordinates, $u_p^p$ is particle velocity vector component, $m_p$ is particle mass, $F$ is the sum of various forces (Archimedes force, friction force, etc.), $C_p$ is particle specific heat, $T_p$ is particle temperature, $Q_p$ is a term describing convective, radiant and other heat exchange between the particle and the carrier gas.

In the gas phase, the following chemical components are assumed: nitrogen ($N_2$), oxygen ($O_2$), methane $CH_4$, hydrogen $H_2$, carbon dioxide ($CO_2$) and water vapor ($H_2O$). The two gross chemical reactions in a gas are determined by the Arrhenius law.

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$ (7)
$$H_2 + 0.5O_2 \rightarrow H_2O$$ (8)

To calculate the combustion of carbon (coke) in a particle, the kinetic and diffusion limited combustion model (KDLCCM) is used [8].

The global combustion reaction is assumed as:

$$C + O_2 \rightarrow CO_2$$ (9)

According to this model, the change in the mass of coke is determined by the formula:

$$\frac{dm}{dt} = A_p \left( \frac{1}{C_d} + \frac{1}{C_{ch}} \right)^{-1} \rho g RT_g \frac{Y_{O_2}}{\mu_{O_2}}$$ (10)

Where are $A_p$ is particle's surface area, $C_d$ is semi-empirical coefficient taking into account the diffusion on the particle surface, $C_{ch}$ is reaction rate calculated by the Arrhenius law.

Volatile matter output is described by the constant rate devolatization model [8]. Components of volatile substances are methane ($CH_4$), hydrogen ($H_2$), and carbon dioxide ($CO_2$).

In this paper, the coalChemistryFoam solver was used to calculate the flow parameters in the blast furnace combustion chamber (validation test rig). A system of equations based on the URANS model and the $k-\varepsilon$ model of turbulence was used. The pulverized coal injection combustion model is based on the vortex dissipation model.

The Gauss upwind scheme was used for approximation of convective terms, the Gauss linear scheme was used for approximation of diffusion terms, the Gauss linear orthogonal scheme was used to approximate the Laplacian term. To solve linear system of equations, the GAMG method was used for pressure and the smoothSolver method was used for $U$, $h$, $Y$, $k$, $\varepsilon$ values. The tolerance was set to $10^{-6}$. The resulting equations for velocity and pressure coupling were solved by the iterative PIMPLE algorithm with nCorrectors equal to 3.

3. Definition of the problem

The geometric dimensions and modes of operation of the model camera were chosen according to the data of [6, 7]. The installation diagram is shown in Fig.1. The conveying air inlet gas velocity was $V = 10$ m/s, the air inlet velocity was $V = 50$ m/s. The spatial numerical domain with two planes of symmetry was used for numerical simulation (Fig. 2).

The distribution of particles in the entrance section is given using the Rosin-Rammler diameter distribution method with mean diameter $D_p = 40$ mm and spread parameter of 0.5. The inlet particle temperature coincides with the gas temperature $T_g=293$ K. Particles move at velocity $V = 10^5$ parcels/s and constant mass velocity of 12 kg/h in the area with a radius of 3 mm near the axis of symmetry. In terms of OpenFOAM the patchInjection input type is used.

The calculations were carried out for one of the cases of supply and combustion of pulverized coal. In the course of calculation, the fields of velocity, temperature, particle sizes and particle trajectories,
the distribution of the mass fraction of oxygen were determined. A comparison is made with the experimental results and a good match is obtained.

Figure 1. The scheme of the test rig.

The gmsh utility was used to build the computational grid. A special script has been developed for this utility, which has made it possible to build a regular grid for a given combustion chamber geometry with relatively little effort and adjust it by the number of nodes in each direction with the necessary compression or tension. In the radial direction, we had to enter four sections, in each the required grid parameters were set. Another advantage of the gmsh utility is that the grid generation process can be performed based on a cylindrical coordinate system, while the resulting grid will be in a Cartesian system. This is convenient when using the OpenFOAM package. The real calculations were performed on a 51 x 76 x 30 grid (in a cylindrical coordinate system).

Figure 2. The computational mesh.

4. Main results of simulation.
The simulations were run with time step $\Delta t = 2 \cdot 10^{-6}$ s and for the final time $T_{\text{end}} = 0.05$ s. The results of measuring the temperature, velocity fields for gas and solid particles are shown in Figure 3, 4. The concentration fields of gas in particles and ash in particles are shown in Figure 5. X axis is shown on a scale of 1: 5.
Figure 3. Temperature of a) gas and b) solid particles.

Figure 4. Velocity of a) gas and b) solid particles.

Figure 5. Concentration of a) gas in particles and b) ash in particles.

The burnout is a measure of the extent of coal combustion, calculated according to the ash balance. The burnout is calculated by the following formula [7]:

\[
B = \frac{1-Y_{a,0}}{1-Y_{a,0}}
\]  

(11)
Where $Y_{a,0}$ is ash content in the particle inlet, $Y_a$ is residue ash. The distribution of burnout along the length of the test setup is shown in Fig.6. Qualitatively, the picture coincides with the results of work [7]. For quantitative coincidence more detailed information is needed primarily on the composition of coal particles.

![Figure 6. Computed burnout evolution.](image)

The calculations were carried out on a computing cluster of the web-laboratory of UNICFD ISP RAS. Each calculation was performed on 48-64 computing cores.

**Conclusions**
For quantitative coincidence more detailed information is needed primarily on the composition of coal particles and more fine computational grids can be used in future work.

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