Modelling of interactions between variable mass and density solid particles and swirling gas stream

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Abstract. The aim of this work is to investigate the solid particles – gas interactions. For this purpose, numerical modelling was carried out by means of a commercial code for simulations of two-phase dispersed flows with the in-house models accounting for mass and density change of solid phase. In the studied case the particles are treated as spherical moving grains carried by a swirling stream of hot gases. Due to the heat and mass transfer between gas and solid phase, the particles are losing their mass and they are changing their volume. Numerical simulations were performed for turbulent regime, using two methods for turbulence modelling: RANS and LES.

1. Introduction

Two-phase flow with dispersed particles in the swirling jet is important in power engineering (Moin & Apte, 2006); moreover, it is interesting from research reasons. The interactions between the “cold” solid phase and the “hot” gas phase lead to shape, mass and volume changes of the solid particles. Those parameters have an impact on the aerodynamic properties determining for example the residence time of particles in combustion chamber. It is a main parameter which influences the whole combustion process efficiency. The mass exchange between solid particle and surrounding gases results in the additional mass, momentum and energy source in the flow; moreover, violent volume changes of the particle may significantly modify its trajectory. The modelling of turbulence in such case becomes an important issue. Different methods of turbulence modelling give different results (Apte et al, 2003). The values of particles concentrations or velocity field of continuous phase become significant informations. Results for the specifications about the differences between these approaches turn out to be very interesting from the research point of view. The problem described in the present work stems for an important practical situation: the pulverized coal combustion in real industry boilers. In this process, in its first stage called pyrolysis, such phenomena as vaporization and devolatilization (mass changes) (Tomeczek, 1992), and swelling or shrinking of grains (volume changes) (Fu et al, 2007), take place.

2. Numerical simulations

In this paper the analysis of the influence of turbulence model on the solid particles concentration in dispersed flow is presented. For this purpose, the numerical modelling was carried out by
the commercial code using two methods of turbulent flow modelling: RANS (two-equation $k - \epsilon$ model) and LES. The simulations concern the carrier phase motion (swirling flow of hot gases) two-way coupled with the Lagrangian tracking of the dispersed phase (solid particles). In contrast to other studies where the case of periodic heated channel flow (Pozorski & Luniewski, 2011), (Jaszczur, 2010) was considered; here, solid particles are treated as an open system, since the interphase mass transfer and particle material density changes take place as a result of heat transfer with the surrounding hot gases.

The simplified burner geometry of radius 0.15 m ($X, Z$ plane) and length $Y = 0.88$ m was considered. The burner was situated vertically and the flow was directed according to gravity. The appropriate conditions for mass and density changes were obtained by different temperatures of streams. The streams were injected coaxially, the core “cold” gas of the temperature 473 K and the inlet velocity 3 m/s, and the external “hot” jet (secondary air) with 1273 K and 8.6 m/s, respectively. Solid particles were at 300 K and they were mixed with cold gas and flow into the chamber with primary jet, which had a temperature of 573 K and inlet velocity 4m/s.

In both studied variants of turbulence models, the particle temperature increases due to the heat transfer from the hot jet, and in consequence the particle mass and density is changing (pyrolysis process). Mass transfer between particle and the surrounding fluid becomes the additional gas source term for the flow. The fluid is treated as a mixture of two components: air and volatiles (the gases released during particle heating). At this stage of analysis, the chemical reactions are not considered. In all simulations the uniform size of solid particles (200 $\mu$m diameter) was assumed. To get better mixing conditions the primary air was swirled (the swirl number was set to 0.54). Basing on experimental data received from the Institute for Chemical Processing of Coal in Zabrze, concerning the particle mass and diameter evolution under the heating conditions (Ściążko, 2005), the density and mass change functions were determined. It should be emphasized that the density of particles was obtained in a wide temperature range. In calculation the ideal spherical particle was assumed.

The mass loss process caused by heating can be described by the following equation:

$$\frac{dZ}{dt} = -k(Z - Z_e)H(Z - Z_e),$$

where $k = k(T)$ is the rate coefficient defined by the Arrhenius formula; $Z$ is the pyrolysis progress expressed as an instantaneous to initial mass ratio; $Z_e = Z_e(T)$ is an equilibrium function of pyrolysis progress (confer Figure 1 left picture, solid line), which refers to the slow pyrolysis process (heating rate tending to zero); $H$ denotes the Heaviside function determining the mass loss process direction, which means that for the negative values, the mass change does not occur. The mathematical formula for $Z_e$ function was determined basing on experimental data (Ściążko, 2005). The numerical simulations concern the particle mass and density changes which are modeled in terms of the apparent coal density and mass change defined by equation (1). To deal with these terms, the User Defined Functions (UDF) were written and implemented in the commercial solver.

3. Results

The results of numerical simulations concerning the two-phase dispersed flows with mass and density changes are presented below. In Figure 1 (left picture) mass evolution of a chosen particle is presented. In both considered cases the particle mass is decreasing (due to release of gases). It can be seen that the total gas source in the flow differs depending on the turbulence model and the resulting fluid temperature field (the final points of the curves): ca. 20% of the total particle mass is transferred to the continuous phase for RANS (at the level of 820 K) and ca. 25% in the case of LES (at the level of 1015 K). Moreover, the mass change process is the most intensive
Figure 1. The particle mass determined by the pyrolysis progress (left picture) and particle diameter (right picture) for different turbulence models.

at the temperature of 800 K for RANS, and 850 K for LES. In Figure 1 (right picture) the particle diameter evolution is presented (also, the diameter varies with the temperature in both cases). The particle swells in the first stage of process (to the distance about 0.45 m for RANS and 0.3 m for LES) and shrinks afterwards. The ratio of the volume change for the swelling \( \left( \frac{d_{\text{swelling}}}{d_0} \right) \) is about 1.18 for RANS, and 1.2 for LES. For the shrinking \( \left( \frac{d_{\text{shrinkage}}}{d_{\text{swelling}}} \right) \) it is equal approximately 0.91 for RANS, and 0.83 for LES \( \left( d_{\text{swelling}} \right) \) is the maximum diameter of particle and \( d_{\text{shrinkage}} \) is the final diameter). Moreover, for LES simulations the final particle diameter is lower than its initial diameter.

In Figure 2 the fluid temperature distribution is presented. Comparison of plots shows that the mixture temperature in the external flow (close to the walls) for LES (left plots) is much higher than for RANS (right plots), ca. 200 K of difference. The gas mixture in the core flow has lower temperature in the case of LES (ca. 140 K) than for RANS, but only for distance of half the length of the combustion chamber. At the distance of \( y = 0.5 \) m, the core jet temperature for LES is higher, by about 100 K.

In Figure 3 in left plots the discrete phase concentration in the flow for LES are presented (instantaneous fields), right plots present the results for RANS. As it can be seen in the case of RANS, the maximum particle concentration has a higher value than for LES (but they have the same order of magnitude). In the LES, the value of instantaneous concentration obviously varies in time. For the RANS case, at the begining it increases with the flow and after that slowly decreases. Comparison of plots shows that at the distance of \( y = 0.5 \) m in the case of LES modelling the maximum concentration of the dicrete phase is about six times lower than for RANS.

In Figure 4 (left plots) the gas mass source in the flow for LES are presented (instantaneous fields), right plots present the results for RANS. As it can be seen in the case of LES, the mass source has a higher value than for RANS (one or even two orders of magnitude). This large difference between models results from the calculated fluid temperature profiles, which strongly depend on the used turbulence model. For LES much higher mean mixture temperature was obtained (ca. 1044 K vs. 872 K for RANS). Additionally, in the LES results the value of gas source is different for different flow times. Moreover, for each time flow the gas source slowly increases to the distance of \( y = 0.31 \) m, and after it decreases quickly. For the RANS case the mass exchanges intensify with the flow, and it can be said that this changes occur slowly. Comparison of plots shows that at distance of \( y = 0.5 \) m in the case of LES modelling the devolatilization process almost decays. The mass source volume integral was calculated at the level of 0.00029 kg/s for LES (from time \( t_3 \)), and 0.00022 kg/s for RANS. At this stage of LES calculation it can be concluded that the devolatilization process will be more intensive for LES.
Figure 2. The distribution of the fluid temperature in the combustion chamber for different distances from the inlet (in meters): from top $y = 0.27$, $y = 0.31$, $y = 0.5$, $t_1 = 7.8185 \cdot 10^{-2}$ s, $t_2 = 8.0185 \cdot 10^{-2}$ s, $t_3 = 8.2185 \cdot 10^{-2}$ s. Results for LES (left plots) and RANS (right plots).

turbulence modelling.
Generally, coupled effects of mass and density changes and turbulence modelling influence the dynamic parameters of the flow. In the case of RANS the particle velocity magnitude is lower, and in consequence the residence time is higher (about 10% difference).

4. Conclusions
The presented results show the influence of the turbulence model on the solid particles concentration in dispersed flow. The simulation results show that the intensity of the devolatilization process depends on the turbulence model, and it gives a higher value of the total amount of gases released from the particles for LES case. This difference comes from the calculated temperature, which is much higher for LES modelling. Additionally, for different models of turbulence with particle-fluid interactions different particle residence times were obtained. These results show the importance of appropriate physical and chemical data.
Figure 3. The distribution of the particle concentration in the combustion chamber for different distances from the inlet (in meters): from top $y = 0.27$, $y = 0.31$, $y = 0.5$, $t_1 = 7.8185 \times 10^{-2}$ s, $t_2 = 8.0185 \times 10^{-2}$ s, $t_3 = 8.2185 \times 10^{-2}$ s. Results for LES (left plots) and RANS (right plots).

implementation, especially the pyrolysis kinetic rate and the particle material density, in two-phase flow calculations.

Acknowledgments

The investigations presented in this paper have been carried out within a National Project POIG.01.01.02-00-016/08 “Model agroenergy complexes as an example of distributed cogeneration based on a local renewable energy sources”.

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Figure 4. The distribution of the volatile mass source in the combustion chamber for different distances from the inlet (in meters): from top $y = 0.27, y = 0.31, y = 0.5, t_1 = 7.8185 \cdot 10^{-2}$ s, $t_2 = 8.0185 \cdot 10^{-2}$ s, $t_3 = 8.2185 \cdot 10^{-2}$ s. Results for LES (left plots) and RANS (right plots).

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