Large Eddy Simulation of Pulverized Coal Jet Combustion and Flame Propagation

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The characteristics of a pulverized coal jet flame ignited by a preheated gas flow are modeled with large eddy simulation (LES) method. An open-source computational fluid dynamics (CFD) code –OpenFOAM (open field operation and manipulation) is applied to predict the instantaneous temperature, pressure, vortices and species mass fraction of the whole combustion process. The sub-grid scale (SGS) turbulence and combustion models based on the one-equation eddy-viscosity model and the kinetic-diffusion limited rate surface reaction model are used in the modeling process. Jet combustions with different inlet velocities are simulated to get an optimal value under the condition that a good combustion kinetic filed can be established. In order to prove the advantages of LES on the predictions of turbulent combustion, Reynolds-averaged Navier-Stokes (RANS) simulation has been performed and compared with the results of LES. The results suggest that LES can predict the instantaneous values of turbulent combustion while RANS can only get average effects. The ability of LES to capture the high and low values of temperature and species concentrations is better, and it can capture the flame centre and predict the recirculation flows more accurately than RANS. Furthermore, the effect of coal particle diameters on the flame characteristics is also investigated by LES. It has been observed that the region of high temperature is wider, the flame center is closer to the nozzle exit, and the local temperature is higher for smaller particles. The results also show that the combustion is more intensive and complete for smaller particles, which are coincident with the combustion theory.

Keywords: OpenFOAM; Pulverized coal combustion; Large eddy simulation; Jet combustion; Turbulence
1. Introduction

Numerical simulation has been regarded as one of the most powerful tools for analyzing the characteristics of industrial systems recently. A great number of commercial computational fluid dynamics (CFD) software have been developed. However, in practical two-phase combustion devices such as pulverized coal combustion furnace and propulsive devices, the combustion process is a very complex phenomena in which dispersion of fuel particles, evaporation (devolatilization), inter-phase chemical reaction and so on take place interactively at the same time.

To get the details of the whole turbulent combustion process, the direct numerical simulation (DNS) method which solves the governing equations directly is developed. Although DNS can predict the flow physics and chemical reactions accurately, it needs to handle all the governing equations with different length scales, from the largest scale (characteristic length of the computational domain) to the smallest scale of turbulence (Kolmogorov scale) [1], almost without any model assumptions. The demand of computing consumption and computer memory is so high that it is restricted to solve turbulence even with low Reynolds numbers and simple geometries under the existing calculation condition [2, 3] As the flow in combustion furnace is commonly high Reynolds number, markedly nonlinear and multiphase, DNS would not be widely used in researching of practical industry phenomenon for a long time in the future.

Since multi-phase reacting flow process is much more complex than single-phase process, the computational cost is also much higher. For such complex process, RANS (Reynolds-Averaged Navier-Stokes) simulation method is commonly utilized. In this approach, the mass, momentum and energy transport equations are averaged statistically. The Reynolds stress tensor and mean reaction rate terms which are included in the conservation equations are modeled by turbulence model and combustion model, respectively. Although the computer capacity and calculation time
of this approach are reasonable [4-7], the reacting flow behavior cannot be analyzed in
detail, because RANS can only get time averaged solutions and is unable to get the
characteristics of small length or small time scales, which play important roles in
reacting flows. In many cases, RANS is far from enough for prediction and design in
engineering applications.

Besides DNS and RANS, large eddy simulation (LES) plays a more and more
important role in reacting flow. The restrictions of DNS are overcome by LES, in which
the flow field is spatially filtered into large scales and small scales. The large scale
motions in the flow are directly solved, whereas the effect of the small scale motions is
modeled by the sub-grid scale (SGS) models. It can get the instantaneous turbulent
flame construction, and analyze the interacted effect mechanism between turbulent flow
and chemical reaction. Compared with RANS, LES can get useful information of
unsteady turbulent motions accurately, and examine the turbulent and combustion
models of RANS. Therefore, an increasing number of attentions are taken to the LES of
turbulent combustion. Similar to the computations using RANS, SGS models for
combustion flows are divided into SGS turbulence model and SGS combustion model.
The former is needed to determine the terms related to the SGS stress tensor [8, 9] the
latter is needed to solve the momentum and energy source terms [10, 11] in reacting
flows. However, although an increasing number of studies on LES for gas combustion
have been reported recently [12-15], to the author’s knowledge, little attention has been
focused on LES for coal combustion [16-19].

The purpose of this paper is to apply LES employing an open-source CFD code
–OpenFoam [20] (open field operation and manipulation) to pulverized coal turbulent
horizontal jet combustion. The SGS turbulence model and char combustion model are
based upon the one-equation eddy viscosity model and kinetic-diffusion limited rate
surface reaction model, respectively. The devolatilization model and radiation model are
based upon the constant rate devolatilization model and P-1 model, respectively. The
gas phase combustion model is based upon a simplified turbulent combustion model
proposed by K. Yamamoto [18]. Jet combustions with different jet velocities are
simulated to get an optimal value under the condition that the flame center is in the
central regime. Different particle size distributions are simulated to predict their
influence on flame characteristics. Furthermore, the simulated results of LES are
compared with those of RANS using k-ε model. The results show that LES has higher
accuracy.

2. Numerical Simulation

2.1 Flow field description and computational conditions

In this study, LES is applied to predict the characteristics of a pulverized coal jet flame.
Figure 1 shows the schematic drawing of the test furnace. The mixture of coal and air is
injected through the nozzle (diameter: 10mm) horizontally and ignited by the preheated
gas automatically. The combustion gas flows to the outlet. The velocity of primary jet is
10 m/s and the preheated gas temperature is 1000K. The test furnace is a cuboid
furnace, whose dimension is 0.3m×0.1m×0.5m. The coal combusted is a kind of
bituminous coal with 21.1% of volatile matter, 65.9% of fixed carbon, 10.4% of ash and
2.6% of moisture.

The computational domain and grids are also shown in figure 1. The
computational domain is divided into about 11,090 hexahedra volumes and the
minimum cell is located near the nozzle exit for both LES and RANS simulation. The
coal particle distribution uses the Rosin Rammler type of pdf model, the min and max
diameters of which are 5μm and 565μm, respectively. The CPU time required for this
computation is about 90h on one CPU.
2.2 Governing equations of LES

The turbulent flow is composed by many vortices of different scales. The large scale vortices influence the average flow, and the small scale vortices influence dissipation. The basic idea of LES is to decompose the turbulence into large scale and small scale motions, solve Navier-Stokes equations directly for the large scale motions, and solve the small scale motions and their interaction with large scales by establishing the SGS models.

The LES equations, which are derived from spatial filtering of Navier-Stokes equations with a filtering width, are given as [21],

\[
\frac{\partial \overline{\rho}}{\partial t} + \frac{\partial \rho \overline{u_i}}{\partial x_j} = 0 \quad (1)
\]

\[
\frac{\partial \overline{\rho u_i}}{\partial t} + \frac{\partial (\overline{\rho u_i u_j})}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \overline{u_i}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} \right) \quad (2)
\]

\[
\frac{\partial \overline{\rho Y_s}}{\partial t} + \frac{\partial (\overline{\rho u_i Y_s})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \overline{Y_s}}{\partial x_j} - \frac{w_s}{S_c} - \frac{q_{sgs}}{S_c} \right) \quad (3)
\]

\[
\frac{\partial \overline{\rho h}}{\partial t} + \frac{\partial (\overline{\rho u_i h})}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \mu \frac{\partial \overline{h}}{\partial x_j} - \frac{g_{sgs}}{Pr} \right) \quad (4)
\]

Where

\( \overline{\cdot} \) denotes the spatial filtering terms,

\( \overline{Y_s} \) is the mass fraction of species s,

\( \text{Pr} \) is the Prandtl number,

\( S_c \) is the Schmidt number,

\( q_{sgs} \) is the SGS heat flux,

\( g_{sgs} \) is the SGS mass flux,

\( w_s \) is the reaction rate of species s.
\[ \tau_{ij} = \rho \overline{u_iu_j} - \rho \overline{u_iu_j}, \] is the SGS stress tensor, which is the momentum transport between the filtered small scales and the solved large scale motions, and modeled by the one-equation eddy-viscosity model [22, 23].

### 2.3 SGS turbulent flow model

Recent years, some inherent limitations of the SGS models used in LES have been found. For example, it has been demonstrated that the coefficient in the algebraic eddy-viscosity model of Smagorinsky [8] has to be fine tuned for different flows [24]. Moreover, the coefficient is strongly dependent on the Reynolds number [25, 26]. To overcome the deficiencies of these models, the one-equation eddy-viscosity model (OEEVM) [22, 23] has been developed.

The SGS models of the eddy-viscosity model are based upon the hypothesis that the deviatoric part of the SGS stress tensor dev(\(B\)) is aligned with the filtered deviatoric part of the rate of strain tensor dev(\(D\)) locally, while the normal stress is assumed to be isotropic and thus can be represented by the SGS kinetic energy \(k\) [26],

\[ B = \frac{2}{3} kI + \text{dev}(B) = \frac{2}{3} kI - 2\nu_{sgs}\text{dev}(D) \quad (5) \]

Here,

\[ \text{dev}(D) = D - \frac{1}{3} tr(D)I, \quad tr(D) = D_{11} + D_{22} + D_{33} \]

\[ k = \frac{1}{2} tr(B), D = \text{symm}(\text{grad}(u)) = \frac{1}{2} (\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}) \quad (6) \]

Where \(B\) is the SGS stress tensor, \(k\) is the SGS kinetic energy, \(I\) is the unit tensor, \(D\) is the strain rate tensor, \(\nu_{sgs}\) is the SGS viscosity, \(tr(D)\) is the trace of tensor \(D\).
In the one-equation eddy-viscosity model, an exact balance equation for \( k \) can be derived from the exact balance equation for \( B \). It could be assumed that the terms of diffusion and dissipation are reasonably well modeled by terms of the form 
\[
\text{div}(\nu_k \text{grad} k) \quad \text{and} \quad \varepsilon = c_\varepsilon k^{3/2} / \Delta \quad \text{[26]}. \]
Hence,
\[
\frac{d}{dt}(\rho k) + \text{div}(\rho \nu k) - \text{div}(\rho \nu_{\text{eff}} \text{grad}(k)) = -\rho \textbf{D} \cdot \textbf{B} - \rho \varepsilon \tag{7}
\]

Here,
\[
\nu_{\text{eff}} = \nu_{\text{gs}} + \nu, \nu_{\text{gs}} = c_k \sqrt{k} \cdot \Delta, \varepsilon = c_\varepsilon k^{3/2} / \Delta \tag{8}
\]

Where \( \nu_{\text{eff}} \) is the effective viscosity, \( \Delta \) is the filtering width. The dimensionless model coefficients are given the values \( c_k = 0.094 \) and \( c_\varepsilon = 1.048 \).

### 2.4 The radiation model

A radiation heat transfer equation considering the radiation recuperation between particles and fluid is solved by the P-1 model [27]. The governing equation goes as follows:
\[
q_s = -\frac{1}{3(\alpha + \sigma_s) - C \sigma_s} \nabla G \tag{9}
\]

Where \( \alpha \) is the absorption coefficient, \( \sigma_s \) is the scatter coefficient, \( G \) is the radiation input, \( C \) is the linear-anisotropic phase function.

### 2.5 Coal combustion models

In turbulent reacting flows, the chemical reactions occur only when the molecules of fuel and oxidizer mixing together. Since the mix of molecules is in small gas mass, the
SGS models considering the combustion features are needed to be developed.

Generally, coal combustion process includes three steps, first the volatile fraction giving off, then the gas phase combustion, and finally the char combustion [28]. The three kinds of combustion models are introduced in the following passages.

2.5.1 Devolatilisation model

There are many sophisticated devolatilization models, such as the FLASHCHAIN model [29], the distributed activation energy model (DAEM) [30] and the chemical percolation devolatilization (CPD) model [31], which require large computational resources. Therefore, those sophisticated models are not applicable to LES. An accurate and computational inexpensively devolatilization model is required for turbulent reacting flow simulation in LES.

In this study, a constant rate devolatilization model is proposed, of which the vaporization temperature needs to be set as 600 K. The volatile residual coefficient $C_{res}$ is set to be 0.001.

\[
m_{vol,0} = Y_{vol,0}m_0, m_{vol} = Y_{vol}m
\]  

(10)

Once the fraction of volatile $\frac{m_{vol}}{m_{vol,0}}$ is depleted below the threshold $C_{res}$, combustion occurs.

The matter volatilized from coal particles to carrier gas phase is:

\[
d_m = \min(dtA,m_{vol,0},m_{vol})
\]  

(11)

Where $m_{vol,0}$ and $m_{vol}$ are the initial and current mass of volatile matter (kg), respectively. $Y_{vol,0}$ and $Y_{vol}$ are the mass fraction of the initial and current volatile,
respectively. \( m_0 \) and \( m \) are the initial and current mass of coal (kg), respectively. \( A_0 \) is the devolatilization rate which is set to be 12 (1/s).

2.5.2 Gas phase combustion model

There are many turbulent combustion models for gas phase. For turbulent coal combustion, the eddy-break-up (EBU) model and the eddy dissipation model are based on intuitive arguments. The flamelet [32] model is one of the most promising models for gas fuel combustion but hasn’t been coupled with coal combustion model which takes both devolatilization and char oxidation into account. Therefore, a simplified turbulent combustion model [18] is adopted in this study,

\[
\bar{S}_{RK} = \rho(Y_k^* - \bar{Y}_k)/t_k
\]  

(12)

Where \( \bar{S}_{RK} \) is turbulent reaction rate, \( \bar{Y}_k \) is the mass fraction of gas species \( k \), \( \* \) denotes the values at chemical equilibrium. Combustion characteristic time \( t_k \) is assumed to be proportional to the Kolmogorov time scale:

\[
t_k = C(v/\varepsilon)^{1/2}
\]  

(13)

Where \( C \) is the model parameter set to be 1.0, \( v \) is the kinematic viscosity, and \( \varepsilon \) is the dissipation rate.

2.5.3 Char combustion model

For char combustion model, the kinetic-diffusion limited rate surface reaction model for coal parcels is used for a single reaction of \( C(s) + Sb*O2 \rightarrow CO2 \) to determine the consumption of char, where \( Sb \) is the stoichiometrical coefficient of the reaction.
\[ f_{\text{comb}} = \overline{Y}_{\text{solid}} \overline{Y}_c \quad (14) \]

If \( f_{\text{comb}} < \text{SMALL} \), the surface combustion active combustible fraction is consumed.

Here, \( f_{\text{comb}} \) is the fraction of remaining combustible material, \( \overline{Y}_{\text{solid}} \) is the solid mass fraction of mixture, \( \overline{Y}_c \) is the char mass fraction of solid. \( \text{SMALL} \) is an infinitesimal number.

Change in char mass (kg):

\[ d\overline{m}_c = \bar{A}_p \bar{\rho}_c R T_c \bar{X}_{O2} k_e dt = \bar{A}_p \bar{\rho}_c R T_c \overline{Y}_{O2} W_{O2} \frac{1}{D_0 + \frac{1}{R_k}} dt \quad (15) \]

And:

\[ D_0 = C_1 \bar{d} \left( \frac{T + \bar{T}_c}{2} \right)^{0.75}, R_k = C_2 e^{-E / R T_c}, \overline{A}_p = \pi \bar{d}^2 \quad (16) \]

Where:

- \( D_0 \) is the diffusion rate coefficient,
- \( C_1 \) is the mass diffusion limited rate constant (\( C_1 = 5 \times 10^{-12} \)),
- \( \bar{d} \) is the mean diameter of particles,
- \( \overline{T} \) and \( \bar{T}_c \) are the temperatures of gas and particles, respectively,
- \( R_k \) is the kinetic rate coefficient,
- \( C_2 \) is the kinetics limited rate pre-exponential constant (\( C_2 = 0.002 \)),
- \( E \) is the kinetics limited rate activation energy (\( E = 7.9 \times 10^7 \) J/mol),
- \( R \) is the general gas constant,
- \( \overline{A}_p \) is the Particle surface area.
3. Results and discussion

3.1 Comparisons among different inlet velocities

Images of pressure, velocity vector and temperature distributions on the central plane (x-y plane, z=0) with inlet velocity U0=10m/s are shown in figure 2. It is found in figure 2(a) that there is a negative pressure zone around the outlet of the nozzle, which might be caused by the entrainment of flue gas. From figure 2(b), it can be found that coal jets directly to the opposite wall, which causes large collision loss, and distorts the simulation results. From figure 2(c), the flame center located in the region of high temperature is found to be too close to the opposite wall, which is probably because the jet velocity is too high that there is no enough time for coal to be combusted near the nozzle exit. Accordingly, we need to reduce the inlet velocity to make the coal particles slow down towards the opposite wall, and to get the flame centre move forward to the furnace center to get a better combustion kinetic field.

Through tests of different inlet velocities, an optimal velocity 5 m/s is found. The distributions of pressure, velocity vector and temperature on the central plane with the optimal velocity are presented in figure 3. The negative pressure zone shown in figure 3(a) is similar to that in figure 2(a). Figure 3(b) shows the velocity vectors on the central plane. Coal jets to the central region of the furnace and then turns towards to the outlet instead of the opposite wall. Fig. 3(c) reflects the position of flame center, which is located in the central area instead of the opposite wall. All the comparisons indicate that the optimal velocity 5 m/s is appropriate for turbulent combustion simulation. Hereafter the simulations are performed with inlet velocity 5m/s.

3.2 Simulation results and comparisons between LES and RANS

In order to confirm the advantages of LES, the simulation results of LES are compared with those of RANS with the optimal velocity. The distributions are shown by
instantaneous value for LES and time-averaged value for RANS, respectively.

Figure 4 shows the comparison of temperature distributions predicted by RANS and LES. It is evident, as expected, that RANS gets a longer and narrower flame than the actual one, which is because RANS is not able to predict the turbulence structures that are generated downstream the burner. On the contrary, LES obtains a wider flame and a region of high temperature evidently. This means RANS can’t capture the flame centre and can’t describe the shape of flame after the nozzle exit but LES can predict these clearly.

Recirculation flow is very important for coal jet combustion. It can first lengthen the residence time of particles in the high temperature field near the nozzle exit, accelerate the evolution of volatile matter and the progress of char reaction, and then enhance the flame stability and combustion efficiency. Figure 5 shows the comparison of velocity vector distributions. It is found that a big backflow is formed above the nozzle for both LES and RANS. It is also found that a small backflow is formed below the nozzle for only LES, and the region of high velocity in recirculation zone is larger for LES than that for RANS. These probably stem from the fact that LES can predict the instantaneous turbulent accurately which influences the recirculation flows markedly while RANS can only get an average effect. Thus, LES has advantages in simulating coal combustion.

Figure 6 shows the mass fraction distributions of main gas species (CO2, CH4 and O2) on the central plane. Figure 6 (b) of LES demonstrates that the distributions of CH4 and CO2 are similar. Both mass fractions increase along the jet direction and reach the highest value in the flame center. Whereas the distribution of O2 is opposite, of which mass fraction is higher near the nozzle and decreases along the jet direction and reaches the lowest value in the flame center, which is corresponding to the coal combustion theory. Compare figure 6 (a) with figure 6 (b), it can be found that RANS
can only obtain an average effect of species concentrations. The ability of RANS to capture high and low concentrations is poor.

Figure 7 gives the scatter picture of species mass fractions along the jet direction obtained by LES and RANS, where the solid lines represent the results of LES, and the dotted lines represent the results of RANS. The peak values of CH4, CO2 and O2 are obtained around 0.15m from the nozzle exit for LES, while the three species mass fractions of RANS fluctuate around the respective average value.

3.3 Effect of the coal particle distributions

The study of combustion characteristics with three different particle distributions are also carried out by LES. The average diameters are 10 μm, 48 μm and 90 μm represented by Ptc1, Ptc2 and Ptc3 in the following figures, respectively.

The instantaneous temperature distributions on the central plane for three particle sizes are shown in figure 8. It can be seen that, compared to Ptc2 and Ptc3, high temperature region expands for Ptc1. It is also found that the smaller the coal particle is, the closer the flame centre moves to the nozzle exit, and the higher local temperature can reach. These probably be attributed to the reason that smaller coal particle can promote the reaction activity and the ejection of volatile matter, and shorten the delay time of ignition, which lead to a stronger combustion intensity and more stable combustion.

Figure 9 shows the velocity vectors on the central plane for three particle distributions. Compared to Ptc2 and Ptc3, the position at which the combustion gas begins to flow toward the outlet is closer to the nozzle, and the high velocity region is wider for Ptc1. These imply that the ignition place has moved forward because the mix of pulverized coal and gas is better for smaller coal particles.
Figure 10 presents the comparisons of main species concentrations with different particle sizes. The concentrations of CO2 and CH4 are much higher and the concentration of O2 is much lower for Ptc1 than those anywhere for Ptc2 and Ptc3. The widths of high concentration region for CH4 and CO2, and low concentration region for O2 are likely to spread widely for Ptc1. These may be caused by the reason that the decrease of the particle diameter leads to a bigger coefficient of heat transfer. The number of the particle with the same mass is bigger, the gas–solid contact area is larger and the gas–solid mixing is enhanced. This indicates that the combustion is more intensive and complete for small particles. Furthermore, the ignition and complete combustion of volatile can lead to good flame stabilization, which is agree with the results of figures 8 and 9.

4. Conclusions

A three-dimensional large eddy simulation method is applied to study the characteristics of pulverized coal turbulent jet flame. The validity is investigated by comparing with RANS simulation. In addition, jet combustion with different inlet velocities are simulated to get a good combustion kinetic filed. Different particle diameters are used in the simulations to analyze their effects on the flame characteristics. The following conclusions can be drawn from this study:

a. When the jet velocity is high, the coal jets directly to the opposite wall causing large collision loss, and the flame center is too close to the back wall. Therefore, we need to reduce the inlet velocity to make the coal particles slow down towards the opposite wall and to get the flame centre move forward to the furnace centre to get a better combustion condition. In this paper, it is found that 5m/s is an optimal jet velocity.

b. Compared with RANS, LES can predict the instantaneous values of turbulent combustion while RANS can only get average effects. The ability of LES to capture the
high and low values of temperature and species concentrations is better. LES can capture the flame centre and predict the recirculation flows more accurately than RANS. Shortly speaking, LES has advantages in simulating coal combustion.

c. From the comparisons of jet flame characteristics performed with different coal particle distributions, it is found that particle diameter plays an important part in reacting flow. The region of high temperature is wider, the flame centre is closer to the nozzle exit, and the local temperature is higher for smaller particles. These indicate that the combustion is more intensive and complete for small particles, which is corresponding to the combustion theory.

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**Figure Captions**

Figure 1: Schematics of the pulverized coal combustion test furnace and the numerical meshes.

Figure 2: The pressure (a), velocity vector (b) and temperature (c) distributions on the central plane (x-y plane, z=0) with inlet velocity U0=10m/s.

Figure 3: The pressure (a), velocity vector (b) and temperature (c) distributions on the central plane (x-y plane, z=0) with inlet velocity U0=5m/s.
Figure 4: Comparison of temperature (K) distribution on the central plane (x-y plane, z=0) between RANS (a) and LES (b).

Figure 5: Comparison of velocity vector distribution on the central plane (x-y plane, z=0) between RANS (a) and LES (b).

Figure 6: Comparison of mass fractions of main species on the central plane (x-y plane, z=0) between RANS (a) and LES (b).

Figure 7: Mass fraction distribution of main species along jet direction obtained by LES (solid line) and RANS (dotted line).

Figure 8: Instantaneous temperature distributions (x-y plane, z=0); (a) Ptc1; (b) Ptc2; (c) Ptc3.

Figure 9: Velocity vector distributions (x-y plane, z=0); (a) Ptc1; (b) Ptc2; (c) Ptc3.

Figure 10: Mass fraction distributions of main species (x-y plane, z=0). (a), (b) and (c) represent Ptc1, Ptc2 and Ptc3, respectively; 1, 2 and 3 represent CH4, CO2 and O2, respectively.