PBM/LES Numerical Simulation of Vortex Structure and Fine Particles Agglomeration in Three-Dimensional Plate Jet

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The emission of fine particles has caused serious environmental problems due to the characteristics and the low removal efficiency of fine particles. The turbulent agglomeration is one of the most promising precondition techniques for guiding the growth and reunion of fine particles into larger particles, which is convenient to be captured by conventional precipitators when the size of particles increases to about $1 \times 10^{-6}$ m. This paper sets up a three-dimensional plane jet as a subject, we use the method of Population balance model (PBM) and Large eddy simulation (LES) to analyse the agglomeration of fine particles in this model. Furthermore, a study of the distribution of particle size via turbulent aggregation kernel function is presented. There are two main parameters which related to enlargement of fine particles, including the flow field of gas and the jet velocity. The simulated results show that there is a close relationship between particle distribution and jet vortex field. The agglomeration effect of fine particles increases with the increasing of jet velocity, and the influence of jet velocity is not obvious for particle enlargement.

1. Introduction

Atmospheric inhalable fine particles are the primary pollutant in urban air, having an important impact on the living environment. In particular, the current emissions of fine particles on the environment gets more heavy, causing a greater threat to human health. Vairo et al. (2014) used dispersion modelling to simulate the atmospheric emissions from a fossil fuel power station. Kumar et al. (2015) shows that coal combustion is the main source of Inhalable fine particles in the atmosphere, due to that the annual emissions of fine particles are as high as 63,400 – 79,200 t. Mancuso et al. (2014) analysed the factors of environment and safety in a power plant. Although fibre bag precipitators and electrostatic precipitators are equipped in almost all the coal-fired power plants, they can only remove coarse particles effectively, which directly leads to the emissions of fine particles are not effectively controlled. Moreover, the fine particles discharged into the environment are the most important pollutants. Recently, it has been shown that fine particles can be removed with enlarging the particles size by using some pre-treatment methods in order to achieve a removable the range of particle size through conventional precipitators. Turbulence agglomeration technology is one of the most economical and valuable technical means in the existing fine particles pre-treatment technologies. This technique takes full account of the interaction between the gas phase and the solid phase in the two-phase flow. The trajectory of the fine particles is changed under the influence of the follow-up characteristics of the fine particles and the entrainment of the vortex, this effect makes the size of fine particles are converted into larger particles size by the collision-coalescence. Finally, the increased particles can be effectively collected by conventional precipitators.

Turbulence agglomeration technique is receiving growing attention. Qi et al. (2015) used two-fluid model to study the movement of fine particles in pulverized coal separator, his result confirms the effect of flow field is important for the separation of fine particles. Cen et al. (2015) used the lattice Boltzmann method to simulate the gas-solid turbulent jet under high Reynolds number and found that different size of particles has different effect of diffusion in the flow field. Zhu et al. (2013) studied the dispersion and condensation of nanoparticles in a circular turbulent jet and verified that the production of bigger particles is attributed to turbulence. Zhang et al. (2016) reported the effect of different vortex structures on agglomeration of fine particles by adding vortex generators in the flow field and found that the turbulence energy dissipation rate has an important effect on the
intermolecular collision. Xu et al. (2013) coupled K-ε and PBM models to explore the effect of particle concentration on agglomeration. Yang et al. (2016) made a study about the abatement of fine particles by heterogeneous vapour condensation coupling two impinging streams, which confirmed the presence of turbulent effects contributes to the improvement of the removal efficiency of fine particles. According to the above study, the turbulence is mainly realized by two ways, vortex generators and the pattern of classical flow such as jet and impinging flow. Indeed, the latter for the resistance of flow field and the costs of production are better than the former. Considering the superiority of the flow field of the flat jet, the coupling of the large eddy simulation and population balance model are rarely reported for the study on agglomeration of fine particles. Therefore, the aim of this paper is to get help from LES and PBM. At the same time, the distribution of fine particles in the flow field is made a discussion, and the influence of jet velocity is investigated.

2. Particle Population Equilibrium Model and Agglomeration Kernel Function

2.1 Particle Population Equilibrium Model

The particle population equilibrium model describes the dynamics of particles in the discrete system. The discrete method proposed by Kumar and Ramakrishna (2000) has the advantages of low computational complexity and high computational precision. This paper chooses the discrete method to solve the PBM, it assumes that the particles are densely spherical. According to the particle size, the particles are divided into 12 groups as shown in Table 1. The population equilibrium model controlling equation is as follows (Ramakrishna, 2000):

\[
\frac{\partial}{\partial t} \left[ n(V,t) \right] = B_{ag,i} - D_{ag,i} - \frac{V}{2} \int_a \alpha(V'-V) n(V',t) n(V,t) dV' - \int_a \alpha(V,V') n(V',t) n(V,t) dV' - \int_a \alpha(V',V) n(V,t) n(V',t) dV' - \int_a \alpha(V,V') n(V',t) n(V,t) dV' 
\]

where \( n(V,t) \) is the unit concentration of particles of volume \( V \) at time \( t \), \( 1/m³ \); \( \alpha(V,V') \) is condensed nuclear of two particles, the volume of the particles is \( V \) and \( V' \), respectively; \( B_{ag,i} \) is condensate and generate items; \( D_{ag,i} \) is reunion and disappearance items

2.2 Agglomeration Kernel Function

The particle size distribution of the flue gas was measured by the electrostatic low-pressure impactor (ELPI). The range of distribution is from \( 0.021 \times 10^{-6} \) m to \( 6.256 \times 10^{-6} \) m. For turbulent agglomeration, the main influencing factor is the Stokes number, which reflects the dimensionless number of the particle inertia. In this paper, stokes number in the flue gas less than 1.0, which belongs to the finite inertial particle, and its corresponding turbulence kernel function is (Saffman and Turner, 1965):

\[
\beta(L_i, L_j) = \left( \frac{L_i + L_j}{8} \right) \frac{8\pi e \epsilon}{\sqrt{15} \nu} C_0 \left( \frac{2n}{\frac{L_i}{L_i + L_j}} \right)^{0.043 + 0.0315} \left( \frac{L_i}{L_i + L_j} \right)^{0.6}
\]

\( C_0 \) is a constant and its value is taken as 3.14. For Brown agglomeration, The Knudsen number characterizes the diffusion of particles. In this paper, Knudsen number in the flue gas is about \( 1.0 \sim 10.0 \), which belongs to the Brownian kernel function of the transition zone (Meyer and Deglon, 2011):

\[
\beta_B^{\alpha} = \beta_B^{\alpha} \cdot f(K_n)
\]

\[
f(K_n) = \frac{1 + K_n}{1 + 2K_n + 2K_n^2}
\]

\[
K_n = \frac{1}{2\beta_B^{\alpha}}
\]

where \( \beta_B^{\alpha} \) is the continuous region of Brownian reunion kernel function; \( \beta_B^{\alpha} \) is free molecular area Brownian kernel function; \( f(K_n) \) is the correct factor. We consider the agglomeration effect of coal-fired fine particles under turbulence agglomeration and Brownian agglomeration. Therefore, we introduce a more accurate reunion kernel function:

\[
\beta_{agg}^{\alpha} = \sqrt{\beta(L_i, L_j)^2 + \beta_B^{\alpha}^2}
\]
3. Physical model and Boundary conditions

The distance between the plates is represented by \( H \), whose value is 0.10 m, and \( X: Y: Z = 1.5: 1: 1 \) (in this paper, \( X = 96H, Y = 68H, Z = 68H \)) as shown Figure 1. The gas-solid two-phase flow is injected into the rectangular space with \( U = 10 \) m/s. This paper defines the characteristic time scale is \( T_0 = H/U \), the calculation time step is 0.001 s. The density of particle is 1,000 kg/m\(^3\).

![Figure 1: The schematic diagram of three-dimensional plate jet](image1)

### Table 1: Percentage of the number of particles in each scale

<table>
<thead>
<tr>
<th>Interval number</th>
<th>Particle size / (10^{-6}) m</th>
<th>Percentage of quantity/%</th>
<th>Interval number</th>
<th>Particle size / (10^{-6}) m</th>
<th>Percentage of quantity/%</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bin-0</td>
<td>6.256</td>
<td>0.10</td>
<td>Bin-6</td>
<td>0.314</td>
<td>0.88</td>
</tr>
<tr>
<td>Bin-1</td>
<td>3.074</td>
<td>0.38</td>
<td>Bin-7</td>
<td>0.200</td>
<td>8.26</td>
</tr>
<tr>
<td>Bin-2</td>
<td>1.945</td>
<td>0.77</td>
<td>Bin-8</td>
<td>0.120</td>
<td>39.02</td>
</tr>
<tr>
<td>Bin-3</td>
<td>1.224</td>
<td>1.15</td>
<td>Bin-9</td>
<td>0.073</td>
<td>18.57</td>
</tr>
<tr>
<td>Bin-4</td>
<td>0.758</td>
<td>1.02</td>
<td>Bin-10</td>
<td>0.041</td>
<td>16.85</td>
</tr>
<tr>
<td>Bin-5</td>
<td>0.481</td>
<td>0.82</td>
<td>Bin-11</td>
<td>0.021</td>
<td>12.18</td>
</tr>
</tbody>
</table>

3.1 Characteristics of jet inlet particles

It can be found from Figure 2 that most of the particles in the flue gas are in the submicron range. In addition, the number of particles is related to the percentage of the number of particles. Meanwhile, particle size is also a factor. So, the number of submicron particles decreases as the particle size increases. It can be founded that the number of submicron particles are more than \(10^{12}\), the maximum number can reach \(10^{20}\). It will be more meaningful for the pre-treatment of fine particles as well as the control of emissions in order to reduce the number of fine particles in the environment.

![Figure 2: The particle size of the jet inlet and the number of particles](image2)

4. Results and discussion

4.1 The distribution of continuous phase and particle phase

This section takes the jet velocity as 10 m/s and the inlet volume fraction is \(5 \times 10^{-3}\), the percentage of the number of inlet particles is set according to Table 1. The cross section of \( Z = 0.3 \) m is taken in the field. It can be seen from the Figure 3a that there is a large velocity gradient, the intensity of vorticity is obviously gradually
decreases in the direction of flow. At the shear layer of the jet, there is a symmetrical and rotational direction of the opposite direction of the vortex. The scope of the vortex is gradually expanding. The distance between the small plate and jet speed are the main reason for the formation of this phenomenon.

Figure 3: (a) The distribution of vortices in jet flow field (T=160T0). (b) The situation of vortex distribution

Figure 3b intercepts the five characteristic positions of X = 0.05, 0.2, 0.4, 0.6 and 0.8 to further reveal the change of the vortex, these sections are located in the jet inlet, the jet process and the jet vortex area. It can be observed that vorticity shows bimodal distribution. At the entrance of jet (X = 0.05), the intensity of vortex is largest and span of vortex is smallest, whose scope of influence is only about 7H. In the jet process (X = 0.2 ~ 0.6), the peak of the vortex intensity decreases in turn, and the range gradually increases. In the area of jet vortex (X = 0.8), the intensity of vortex is the lowest and the change of slope tends to be gentle, the most important is that the scope of influence increases to about 20 H. This result confirms the phenomenon in Figure 3a.

Figure 4a represents that the small particles near the axis have undergone dramatic changes. At the entrance of jet (X = 0.05), the volume fraction of fine particles does not change much. In the jet process (X = 0.2 ~ 0.6), the trend of symmetrical inverted single peak is more and more significant, showing that volume fraction of small particles is significantly reduced. During this process, the particles collide and agglomerate into larger particles. In the area of vortex (X = 0.8), the image does not appear at the unimodal distribution. The reason is that symmetrical vortex structure is formed, and most of small particles are drawn into the vortex. Also, Figure 4b shows the images of larger particles and small particles are up and down. The volume fraction of larger particles increases with the development of the jet. Especially in the area of the vortex, most of the larger particles are distributed on the outer edge of the vortex.

Figure 4: The distribution of volume fraction of small particles (Bin-11) and large particles (Bin0)

To sum up, there is a close relationship between particle distribution and jet vortex field. The small particles are mainly distributed in the region of the vortex and show a symmetrical distribution with the structure of symmetrical vortex. In the outer edge of vortex, larger particles are mainly distributed especially between the vortexes. The reason that is the small particles have good follow-up characteristics. It is easy to fill the flow field along with the jet and the Brownian motion of the particles, especially in the vortex distribution. For larger
particles, because of their large inertia, the process of movement is not easy to change the trajectory, so most of the particles are distributed in the periphery of the vortex but they do not enter the whirlpool.

4.2 The influence of the velocity of jet

The velocity of jet is important parameters for three-dimensional flat jet. In this section, the volume fraction of fine particles was kept as 5·10⁻³. The turbulence energy dissipation rate of Z = 0.3 m cross section is obtained. And jet velocity of 6, 8, 10, 12, 14 m/s five conditions were calculated. Also, the turbulent kinetic energy dissipation rate is the only parameter of the reaction flow field performance in Eq(2).

According to the analysis of part 3.1, Figure 5a found that turbulence energy dissipation rate gradually weakened with the development of the jet, which is highly consistent with the distribution of particles. This result is mainly due to the distribution of the turbulent kinetic energy dissipation rate related to the average number of collisions of particles in the local volume per unit volume. Especially in the outer edge of the vortex, the turbulent kinetic energy dissipation rate is enhanced. Therefore, collision of the particles probability is larger, the agglomeration behavior of the particles is more obvious so as to the volume fraction of larger particles is relatively bigger as shown in Figure 4b.

Figure 5: (a) The distribution of turbulence energy dissipation rate in jet flow field (T=160T₀, V=10 m/s). (b) The turbulence energy dissipation rate at each velocity in the jet direction (T=160T₀)

Figure 6: The percentage of particle density at the exit of the jet

Figure 6 presents the change of the percentage of the number of particles at different jet speeds. When the velocity is 6 and 8 m/s, the decrease of the volume fraction of small particles is not obvious. As shown from Figures 5b, the velocity is small and the turbulent kinetic energy dissipation rate is weak, resulting in lower collision efficiency between particles and poor agglomeration. When the velocity reaches 10 m/s, the percentage of small particles decreases by 15 % compared with the inlet, and the increase of the large particle
size is obvious because the turbulence energy dissipation rate is strengthened. The effect of agglomeration between particles is significant. When the speed reaches 12 m/s and 14 m/s, the percentage of small particles decreases by about 2% compared with the speed of 10 m/s, the reason is that the initial velocity of the jet is large, so that the turbulence energy dissipation rate jet is very large, which affects the collision efficiency between the particles, but it is difficult to form the vortex in the limited space and stay time is relatively small.

5. Conclusions
For the control of fine particles emission, three-dimensional flat jet that combines large eddy simulation with the population balance model was simulated. The application of flat jet changes the trajectory of particles. Meanwhile, fine particles can be enlarged by the influence of turbulence and collision-coalescence in the area of jet. In this paper, it mainly studies the distribution of gas and particle phases in the process of jet, besides, the agglomeration behaviour of fine particles under different velocities of jet is analysed. The results that fine particles have good followability, and can respond well to the flow field. Especially in the region where the vortex exists, the small particles can enter the vortex area, Leading to behaviour of collision-coalescence. Turbulent energy dissipation rate is the only influent factor of turbulence agglomeration, the agglomeration effect of fine particles increased with the increase of jet velocity. Additionally, there is the best fit for jet speed for different size of the device. Compared to other pretreatment equipment, turbulent agglomeration chamber of the three-dimensional flat jet has a simple structure and no moving parts, which will be installed before the dust removal equipment in the process of industrial production and have good prospects of engineering application.

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