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HIGH CONCENTRATION BROWNIAN COAGULATION IN JET FLOW USING TWO ENHANCEMENT FORMULATIONS

by

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Ultra-fine particle coagulation by Brownian motion at high concentration in planar jet flow is simulated. A Taylor-Series Expansion Method of Moments is employed to solve the particle general dynamic equation. The volume fraction gets high value, very closes to that at the nozzle exit. As the vortex pairing develops, the high volume fraction region rolls out and mixes with the low value region. The enhancement factor given by Trzeciak et al. will be less than one at some specific outer positions, which seems to be less accurate than the one given by Heine et al.

Key words: *large eddy simulation, planar jet, high concentration enhancement factor*

Introduction

Most works about particle coagulation [1-4] were carried out based on the classic Smoluchowski theory. This classic theory cannot predict the coagulation rate of highly concentrated particle (*e. g*. the volume fraction above 1%) [5], a transition from dilute to high volume concentration may be frequently present at the industrial scale manufacture of oxide particles [6]. Several researches have carried out focusing on the influence of high particle volume concentration in the processes of coagulation [7-10]. Furthermore, Heine *et al*. [11], Buesser [12], and Trzeciak *et al*. [13], gave out the correction overall in their works by direct numerical simulating (DNS) the particle trajectories. Their works mainly agree with each other, and show the coagulation rate is about 2-30 times fast of that calculated by the classic Smoluchowski theory at high concentration. But there are few deep analyses about the different influence of these two formulas in a high concentration particle coagulation flow field. This paper pays attention to the concentrated particles Brownian coagulation in a planar jet

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turbulence flow, and uses both of these two formulas when the simulation is proceeding, the different high concentration enhancement factor at the same position of the flow filed will be given out to show the details difference of the two formulas.

Mathematics formulation

In the flow filed x and y are the stream- and cross-stream direction, respectively. The width of the nozzle L is 5 mm. The inlet velocity at the nozzle U_0 is 6 m/s. The computational domain is $x \times y = 20L \times 20L$. The control equations are solved by the large eddy simulation. The particle general dynamic equation is adopted to trace the evolution of particles. A moment method is employed and the transformed moment equations based on the size distribution are obtained:

$$\frac{\partial M_k^*}{\partial t^*} + \frac{\partial(\overline{u_j^* M_k^*})}{\partial x_j^*} = D_0 \frac{\partial^2 M_k^*}{\partial x_j^* \partial x_j^*} + \dot{\omega}_k^* \quad (k = 0, 1, 2, \cdots), \tag{1}$$

where the k-th moment M_k^* is defined as:

$$M_k^* = \int_0^\infty v^{*k} n^*(v^*)\, \mathrm{d}v^* \tag{2}$$

In classic Smoluchowski Brownian coagulation theory, the collision kernel can be shown as [14]:

$$\beta_\mathrm{c}(v^*, v_1^*) = B_2 \left[\frac{C(v^*)}{\sqrt[3]{v^*}} + \frac{C(v_1^*)}{\sqrt[3]{v_1^*}} \right] \left(\sqrt[3]{v^*} + \sqrt[3]{v_1^*} \right) \tag{3}$$

The classic Smoluchowski Brownian coagulation collision kernel, $\beta_c\,(v_1^*, v^*)$, is accurate only for particle volume concentration, f, below 0.1%. The high concentration enhancement correction factor given by Heine *et al*. [11], Buesser [12], and Trzeciak *et al*. [13] are:

$$\gamma_\mathrm{HEINE} = \frac{\beta_\mathrm{h}}{\beta_\mathrm{c}} = 1 + \frac{2.5}{(1-f)(-\lg f)^{2.7}}, \quad \gamma_\mathrm{TRZECIAK} = \frac{1}{1.0734}\left[1 + 12f + \sqrt{24f(1+6f)}\right] \tag{4}$$

We can expand the coagulation source term $\dot{\omega}_k^*$ and obtain the full expression of the moment equations and the Taylor's Expansion Moment method model [15-19] is utilized. The source terms $\dot{\omega}_k^*$ in eq. (1) is:

$$\dot{\omega}_0^* = -B_2\gamma \left[\frac{M_0^{*2}\left(151 M_1^{*4} - 2M_0^{*2} M_2^{*2} + 13 M_0^* M_2^* M_1^{*2}\right)}{81 M_1^{*4}} - \right.$$

$$\left. - \frac{\sqrt[3]{M_0^{*7}}\left(5M_0^{*2} M_2^{*2} - 64 M_0^* M_2^* M_1^{*2} - 103 M_1^{*4}\right)\phi}{81\sqrt[3]{M_1^{*13}}} \right] \tag{5}$$

$$\dot{\omega}_1^* = 0 \tag{6}$$

$$\dot{\omega}_2^* = B_2\gamma\left[\frac{-2}{81}\cdot\frac{-151M_1^{*4} + 2M_0^{*2}M_2^{*2} - 13M_0^*M_2^*M_1^{*2}}{M_1^{*2}} - \right.$$

$$\left. -\frac{4}{81}\cdot\frac{\sqrt[3]{M_0^*}\,\phi\left(-2M_0^*M_2^*M_1^{*2} + M_0^{*2}M_2^{*2} - 80M_1^{*4}\right)}{\sqrt[3]{M_1^{*7}}}\right] \tag{7}$$

Results and discussions

The turbulence intensity is given to be 5%, and the Smoluchowski model constant $C_s = 0.1$. The SIMPLE scheme is used. The dimensionless time step Δt is 0.024. The fluid is isothermal at $T = 288$ K. The particle distributes always keep monodisperse with the initial size of $d_0 = 100$ nm. When focusing the effect of the high concentration, the initial volume concentration f_0 is given as 0.1%. M_1 is the particle volume fraction. Figure 1 shows M_1 at $T = 2000$.

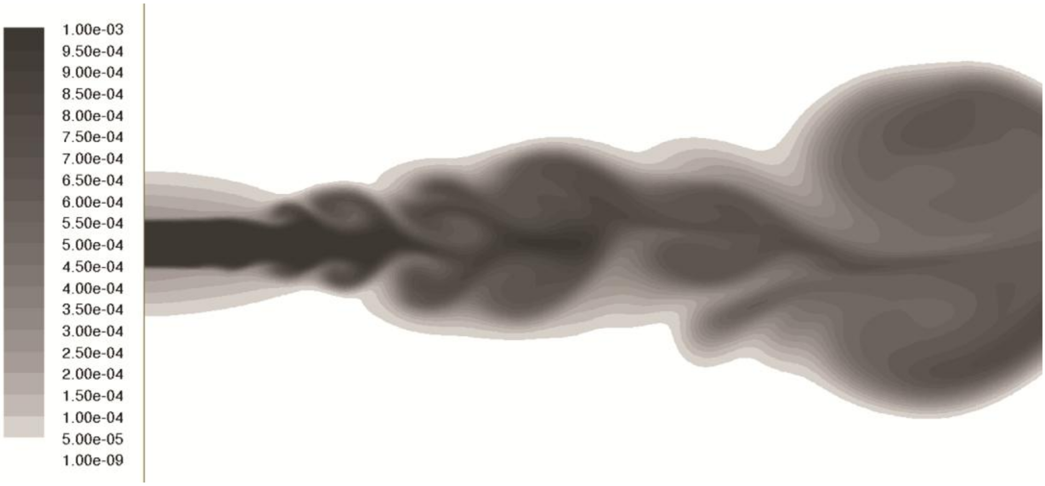

Figure 1. Particle volume fraction distribution

It's observed that the volume fraction gets high value, which very closes to that at the nozzle exit. As the process of vortex pairing goes on, the fluid in high value (of M_1) region is rolled out, elongated and mixed with that in low value region. The volume fraction is relative higher at the kernel region of the vortex than at the interface of mixing layer at the downstream. When the jet flow is developing on, the pairing vortexes always tend to transport the particle from upstream to downstream, from the core region to the mixing layer of jet, and make the volume fraction distribution much more uniform. Figure 2 gives out the comparison of the two correction factors at different flow positions when $T = 2000$. The nozzle exit is located at $y = -1$ to 1. Because the two factors are calculated at the same time, their patterns are basically consistent with each other at the same positions. The factors both show sudden drops from the nozzle exit region to outer field at $x \leq 5$ shown in fig. 2(a). When the flow going downstream, the high factor value region extends and approaches to two times in the width of the nozzle exit as shown in fig. 2(b). It can be found that all the curves calculated by Heine's equation are less steep than those by Trzeciak's equation. When $|y| > 2$ and $|y|$ keep increasing, the factor value calculated by Heine's equation approximates to one, which is the classic value, but always larger than one. In the opposite side, the curve calculated by Trzeciak's equation will traverse the Classic value line, $\gamma = 1$, when $|y|$ is large enough. It means that at these positions, the high concentration influence is not "enhance" any more, but "weaken", which seems to be less accurate than the one given by Heine *et al*. [11].

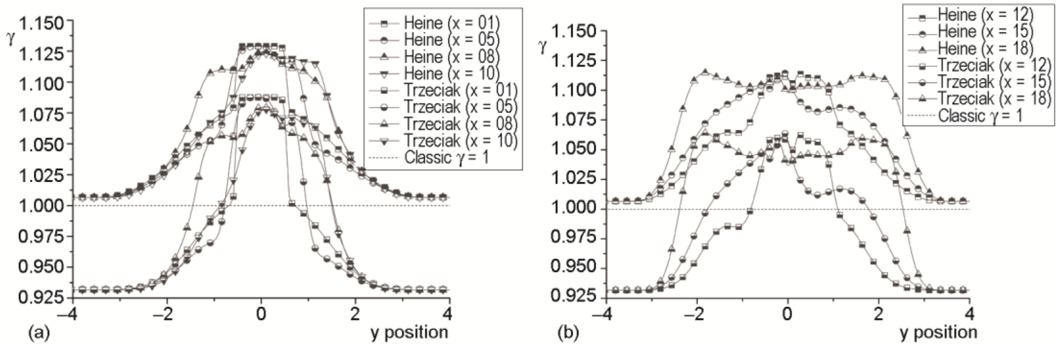

Figure 2. Different γ at the different flow positions when dimensionless time *T* = 2000; (a) *x* = 1 to 10, (b) *x* = 12 to 18

Conclusions

Particle volume fraction is only influenced by the flow transportation and particle diffusion but independent on particle coagulation. The volume fraction gets high value in the centerline core region. The pairing vortexes always tend to make the volume fraction distribution much more uniform. The enhancement factor given by Heine *et al.* [11] and Trzeciak *et al.* [13] are basically consistent with each other at the same flow positions. But the Trzeciak factor will be less than one at some specific outer positions, which seems to be less accurate than the one given by Heine *et al*. [11].

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