NANOPARTICLE COAGULATION AND DISPERSION IN A TURBULENT PLANAR JET WITH CONSTRAINTS

by

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Numerical simulations of coagulating and dispersing nanoparticles in an incompressible turbulent planar jet with constraints are performed. The evolution of nanoparticle field is obtained by utilizing a moment method to approximate the particle's general dynamic equation. The spatio-temporal evolution of the first three moments along with the mean particle diameter and geometric standard deviation of particle diameter are discussed.

Keywords: *nanoparticles, coagulation, turbulent jet, numerical simulation*

Introduction

Many applications of nanoparticle-laden flow can be found in the field of engineering. In the actual condition the various variations of nanoparticles are always related to the flow status, among which the jet flow is very common. Therefore, it is of great importance for both scientific research and engineering application to study the nanoparticle coagulation and dispersion in the jet flow. Though many investigations have concerned with the dispersion of particles in jet flows [1-5], only limited attention has been devoted to the case of nanoparticles. Bessagnet *et al.* [6] showed that the number of particles formed during the plume development and sulfate concentration in nanoparticles are strongly dependent on the sulfur content in fuels. Wu *et al.* [7] showed reasonable predictions of the aerosol number density, aerosol surface density and critical gas species in the exhaust plume. Zhang *et al.* [8] examined the synthesis of nanophase silver particles using an evaporation/condensation aerosol process in a jet flow reactor. Yu *et al.* [9] showed that as jet travels downstream, the time-averaged particle number concentration becomes lower in the jet core and higher outside. Yu *et al.* [10] indicated that the change of Schmidt number has an influence on the number concentration of nanoparticles only when the particle diameter is less than 1 nm. Yin *et al.* [11] found that the ratio of the ambient wind velocity to exhaust gas velocity greatly affects the nanoparticle concentration and size distribution. Yu *et al.* [12] showed that the evolution of particle dynamics in the whole flow field is strongly related to the Re number and nozzle-to-plate distance. Yu *et al.* [13] indicated that the maximum particle number occurs in front of the high zone because of high precursor reaction rate, and then decreases due to coagulation.

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Yin *et al.* [14] found that the nucleation in sulfuric acid/water system will generate large number of nanoparticles. Yu *et al.* [15] showed that increasing the precursor loading leads to the larger agglomerated particles with larger size distribution. Xiong *et al.* [16] predicted the trajectory, velocity and temperature of the in-flight nanoparticles for different initial size and presented the distributions of the particle characteristics for multiple particles in the spray. Although coagulation and dispersion of nanoparticles in the jet have been studied as mentioned above, it has been relatively lacking in turbulent jet with constraint. Particle distribution is different in the turbulent flow with that in the laminar flow [17]. And the coherent structures in the jet with constraint are different that in free jet [18]. Therefore, the objective of present study is to help shed some lights on the coagulation and dispersion of nanoparticles in the turbulent jet with constraint.

Governing equations

The general dynamic equation for nanoparticles is:

$$\frac{\partial \bar{n}}{\partial t}+\bar{u}_i\frac{\partial \bar{n}}{\partial x_i}=\frac{\partial}{\partial x_i}\left[(D+D_t)\frac{\partial \bar{n}}{\partial x_i}\right]+\frac{1}{2}\int_0^v \beta(\tilde{v},v-\tilde{v})\,\bar{n}(\tilde{v})\bar{n}(v-\tilde{v})\,\mathrm{d}\tilde{v}-\int_0^\infty \beta(v,\tilde{v})\bar{n}(v)\bar{n}(\tilde{v})\,\mathrm{d}\tilde{v} \quad (1)$$

where $\bar{n}$ is particle size distribution function, $\bar{u}_i$ – the flow velocity, D – the coefficient of diffusivity, D_t – the turbulent diffusivity for the concentration, β – the collision coefficient, and v and $\tilde{v}$ are the particle volume.

The governing equations for the zeroth, first and second moments are:

$$\frac{\partial \bar{M}_0}{\partial t}+\bar{u}_i\frac{\partial \bar{M}_0}{\partial x_i}=\frac{\partial}{\partial x_i}\left[(D+D_t)\frac{\partial \bar{M}_0}{\partial x_i}\right]-AB_0(\bar{M}_{2/3}\bar{M}_{-1/2}+2\bar{M}_{1/3}\bar{M}_{-1/6}+\bar{M}_{1/6}\bar{M}_0) \quad (2)$$

$$\frac{\partial \bar{M}_1}{\partial t}+\bar{u}_i\frac{\partial \bar{M}_1}{\partial x_i}=\frac{\partial}{\partial x_i}\left[(D+D_t)\frac{\partial \bar{M}_1}{\partial x_i}\right] \quad (3)$$

$$\frac{\partial \bar{M}_2}{\partial t}+\bar{u}_i\frac{\partial \bar{M}_2}{\partial x_i}=\frac{\partial}{\partial x_i}\left[(D+D_t)\frac{\partial \bar{M}_2}{\partial x_i}\right]+2AB_2(\bar{M}_{5/3}\bar{M}_{1/2}+2\bar{M}_{4/3}\bar{M}_{5/6}+\bar{M}_1\bar{M}_{7/6}) \quad (4)$$

where $\bar{M}_0$ corresponds to the total particle number concentration, $\bar{M}_1$ is proportional to the total particle mass, $\bar{M}_2$ is proportional to the total light scattered. The A, B_0 and B_2 are:

$$A=\sqrt[6]{\frac{3}{4\pi}}\sqrt{\frac{6k_BT}{\rho_p}} \quad (5)$$

$$B_0=0.633+0.092\sigma_g^2-0.022\sigma_g^3,\quad B_2=0.39+0.5\sigma_g-0.214\sigma_g^2+0.029\sigma_g^3 \quad (6)$$

For the flow the continuity equation, Reynolds average Navier-Stokes equation and renormalization group k-ε model are used.

Flow parameters and numerical specifications

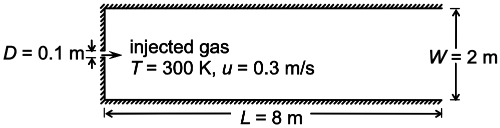

Figure 1. Flow and sketch of computation domain

The flow is shown in fig. 1. The medium is air with TiO_2 particles of 10 nm diameter. Particles number concentration is 10^{15}/m^3 and particle volume is $\pi/6 \cdot 10^{-24}$ m^3. $\bar{M}_0 = 10^{15}/\text{m}^3$, $\bar{M}_1 = \pi/6 \cdot 10^{-9}$ and $M_2 = (\pi/6)^2 \cdot 10^{-33}\text{m}^3$ at the gap exit, and $\bar{M}_0 = \bar{M}_1 = \bar{M}_2 = 0$ at wall. The initial conditions for are $\bar{M}_0 = 10^{12}/\text{m}^3$, $\bar{M}_1 = \pi/6 \cdot 10^{-12}$, $\bar{M}_2 = (\pi/6)^2 \cdot 10^{-36}\text{m}^3$. Schmidt number is $\text{Sc}_t = \mu_t / \rho D_t$ and $\text{Sc}_t = 0.7$ based on the experimental data. The mean particle volume is $v_{\text{mean}} = \bar{M}_1 / \bar{M}_0$, then the mean diameter of particle is $d_{\text{mean}} = (6 v_{\text{mean}} / \pi)^{1/3}$. The viscosity and density of air are $\nu = 1.46 \cdot 10^{-5}$ and $\rho = 1.225$ kg/m^3, respectively. The time step $\Delta t = 0.1$ s. Computations are performed on a domain of 8 m × 2 m in the stream and lateral rections, respectively. The computational grid is comprised of 320 × 80 grid points.

Results and discussions

As shown in fig. 2, $\bar{M}_0$ is affected by particle coagulation and dispersion. $\bar{M}_0$ is the largest at the gap exit, then reduces to the relatively low value. The total particle number concentration decreases along stream. The distribution for total particle mass is only affected by flow transportation and turbulent dispersion. As shown in fig. 3, $\bar{M}_1$ decreases continuously along stream and is obviously affected by coherent vortices, and $\bar{M}_1$ is high within the vortices. This fact clarifies that the high total particle mass appears in the center of the vortices. Coagulation creates new particles of different sizes. This, together with the increase in particle size, alters $\bar{M}_2$. The evolution of $\bar{M}_2$ is shown in fig. 4. $\bar{M}_2$, contrast to $\bar{M}_0$ and $\bar{M}_1$, increases along stream direction. The distribution of $\bar{M}_2$ is obviously affected by coherent structure, and $\bar{M}_2$ is high within the vortices.

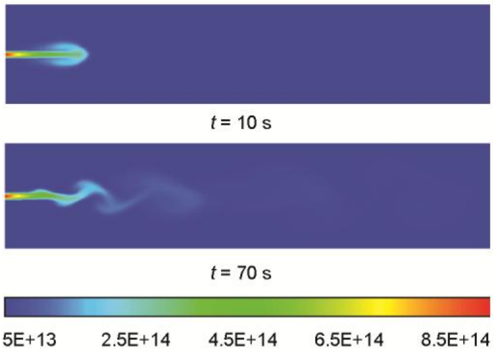

Figure 2. Total particle number concentration

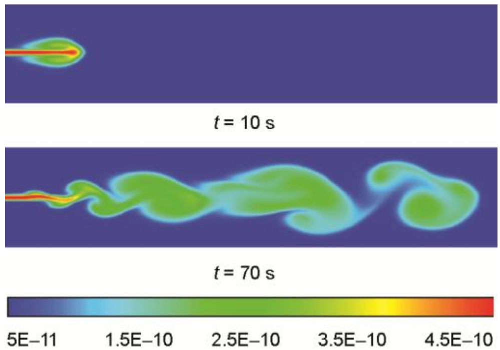

Figure 3. Total particle mass

Figure 5 shows distribution of d_{mean}. d_{mean} increases along stream direction. The distribution of d_{mean} is asymmetric with respect to the centerline. The variation of d_{mean} is dependent on the particle coagulation. The coherent structures result in the increase of particle number concentration and enhances the possibility of collision between particles as well as enforces the particle coagulation. Therefore, the largest particles are found within the center region of the jet.

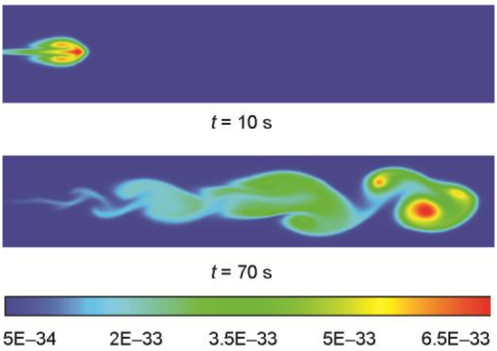

Figure 4. Total light scattered

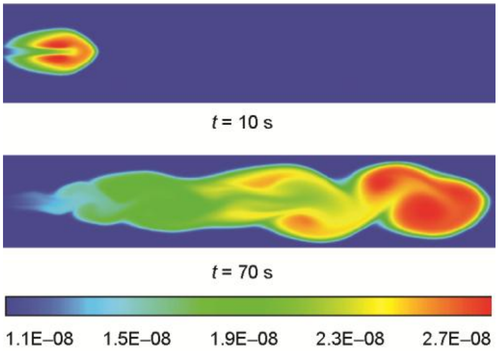

Figure 5. Mean diameter of particles

Conclusions

The distribution for total particle number concentration is affected by particle coagulation and dispersion as well as the flow entrainment, and decreases along stream directions. The total particle mass decreases continuously along stream direction, and the area of the particles increases. The total particle mass is obviously affected by coherent vortices. The mean particle diameter increases along stream direction. The variation of mean particle diameter is dependent on particle coagulation, the largest particles are found within the center region of the jet.

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