Distribution of non-spherical nanoparticles in turbulent flow of ventilation chamber considering fluctuating particle number density*

Ruifang SHI¹, Jianzhong LIN^{1,†}, Hailin YANG¹, Mingzhou YU²

1. Department of Mechanics, State Key Laboratory of Fluid Power and Mechatronic Systems, Zhejiang University, Hangzhou 310027, China;

2. College of Mechanical and Electrical Engineering, China Jiliang University, Hangzhou 310028, China

(Received Nov. 18, 2020 / Revised Dec. 9, 2020)

Abstract The Reynolds-averaged general dynamic equation (RAGDE) for the nanoparticle size distribution function is derived, including the contribution to particle coagulation resulting from the fluctuating concentration. The equation together with that of a turbulent gas flow is solved numerically in the turbulent flow of a ventilation chamber with a jet on the wall based on the proposed model relating the fluctuating coagulation to the gradient of mean concentration. Some results are compared with the experimental data. The results show that the proposed model relating the fluctuating coagulation to the gradient of mean concentration is reasonable, and it is necessary to consider the contribution to coagulation resulting from the fluctuating concentration in such a flow. The changes of the particle number concentration M_0 and the geometric mean diameter d_g are more obvious in the core area of the jet, but less obvious in other areas. With the increase in the initial particle number concentration m_{00} , the values of M_0 and the standard deviation of the particle size σ decrease, but the value of d_g increases. The decrease in the initial particle diameter leads to the reduction of M_0 and σ and the increase in d_g . With the increase in the Reynolds number, particles have few chances of collision, and hence the coagulation rate is reduced, leading to the increase in M_0 and σ and the decrease in d_g .

Key words non-spherical nanoparticle, fluctuating particle concentration, ventilation chamber, particle distribution

Chinese Library Classification O358, O359

2010 Mathematics Subject Classification 76T20

1 Introduction

Nanoparticles are a kind of particles with the size less than 100 nm, which exist in different forms such as monomers, aggregates, and agglomerates. The nanoparticles suspended in

* Citation: SHI, R. F., LIN, J. Z., YANG, H. L., and YU, M. Z. Distribution of non-spherical nanoparticles in turbulent flow of ventilation chamber considering fluctuating particle number density. *Applied Mathematics and Mechanics (English Edition)*, 42(3), 317–330 (2021) <https://doi.org/10.1007/s10483-021-2707-8>

† Corresponding author, E-mail: mecjzlin@public.zju.edu.cn

Project supported by the Major Program of the National Natural Science Foundation of China (No. 91852102)

©The Author(s)

a turbulent flow are very common in many applications, e.g., nanoparticle synthesis^[1], heat transfer^[2], energy transport^[3], and turbine engines^[4]. In such a flow, one of the important factors is the evolution of nanoparticle concentration and size under the effects of convection, diffusion, and coagulation induced by Brownian motion and turbulence.

The general dynamic equation (GDE) for a particle distribution function is a basic equation for describing the evolution and distribution of nanoparticle concentration and size. In the turbulent flow, the fluid velocity and particle distribution function should be written as the sum of mean and fluctuating components and substituted into the GDE. The Reynolds-averaged GDE (RAGDE) can be derived by averaging the GDE with respect to time. In the RAGDE, the contribution to particle coagulation resulting from the fluctuating concentration, which is called the fluctuating coagulation term, is complex and usually neglected, but the importance of this term in the RAGDE has not been fully studied yet. Lin et al.^[5] assumed that the correlation of fluctuating coagulation is proportional to the ratio of turbulent kinetic energy to mean flow kinetic energy, and built the relation between the fluctuating coagulation term and the gradient of mean concentration. Based on the above-mentioned method, they solved numerically the RAGDE in a pipe flow and compared the numerical results with the experimental ones, showing that the fluctuating coagulation term in the RAGDE should be considered in the turbulent flow, especially when the Reynolds number is high. Although this method is applicable to the flow with obvious effects of walls such as pipe flows, there is a big error when this method is applied to the flow with negligible effects of walls. In this paper, therefore, we propose a model to establish the relationship between the fluctuating coagulation term and the gradient of mean concentration, and apply the model to the turbulent flow in a ventilation chamber.

Nanoparticles in the ventilation chamber have attracted a lot of scientific attention with regard to their negative impacts on human health^[6–7]. The distribution of nanoparticles in a ventilation chamber varies in time and space under the influence of turbulent transport and Brownian motion^[8–9]. Kim et al.^[10] measured the turbulent and Brownian coagulation rates of polydisperse nanoparticles in a closed chamber at the atmospheric pressure, and showed that larger turbulent coefficients make the turbulent coagulation process become stronger. Cho et al.^[11] used the Brownian dynamics method to simulate particle sintering and collision. They observed the variations in the fractal dimension of agglomerates, and proposed the coagulation coefficient of agglomerates with two different fractal dimensions. Anand et al.^[12] carried out a comprehensive study on the nanoparticle coagulation in a ventilation chamber, and focused on the effects of the particle injection rate, the fractal dimension of the coagulated particles, and the ventilation removal rate on the particle distribution. They found that the total number concentration reaches a peak soon after particle emission starts, and the number size distribution can be assumed as a bimodal shape. Guichard and Belut^[13] combined the quadrature method of moments with a diffusion inertia model to simulate the dispersion of small and medium inertial aerosols in a ventilation chamber, and evaluated it in various test cases. Guichard and Belut^[14] simulated numerically the nanoparticle distribution in a chamber ventilated by a turbulent flow at moderate Reynolds numbers, and showed that the highest reduction of particle number corresponds to the smallest and least compact nanoparticles.

As mentioned above, the studies on the nanoparticle distribution in the ventilation chamber have not considered the effect of the contribution to coagulation resulting from the fluctuating concentration (the fluctuating coagulation term in the RAGDE), and the effects of the initial particle number density, the initial particle size, and the Reynolds number on the particle distribution are also lack of in-depth research. Therefore, the aims of this study are as follows: (i) to propose a model to establish the relationship between the fluctuating coagulation term and the gradient of mean concentration; (ii) to apply the model to the turbulent flow in a ventilation chamber for verifying its effectiveness; (iii) to assess the effects of the initial particle number density, the particle size, and the Reynolds number on the particle distribution.

2 Governing equations

2.1 RAGDE for nanoparticles

By using the Reynolds-averaged hypothesis, the fluid velocity and particle distribution function in a turbulent flow are expressed as the superposition of the mean and fluctuating components. Substituting the superposition into the GDE and averaging it with respect to time, we have the RAGDE,

$$\begin{aligned} & \frac{\partial \overline{n}(v, t)}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \overline{n}(v, t) - \nabla \cdot D_B \nabla \overline{n}(v, t) + \nabla \cdot \overline{n'(v, t) \mathbf{u}'} \\ &= \frac{1}{2} \int_0^v \beta(v - v_1, v_1) \overline{n}(v_1, t) \overline{n}(v - v_1, t) dv_1 - \int_0^\infty \beta(v, v_1) \overline{n}(v_1, t) \overline{n}(v, t) dv_1 \\ &+ \frac{1}{2} \int_0^v \beta(v - v_1, v_1) \overline{n'(v_1, t) n'(v - v_1, t)} dv_1 - \int_0^\infty \beta(v, v_1) \overline{n}(v_1, t) \overline{n'(v_1, t) n'(v, t)} dv_1, \quad (1) \end{aligned}$$

where the symbols with “—” and “'” represent the mean and fluctuating quantities, respectively, n is the particle distribution function, $\mathbf{u}$ is the fluid velocity, $\beta(v, v_1)$ is the coagulation kernel for two particles with volumes of v and v_1 , and D_B is the Brownian diffusion coefficient^[15], i.e.,

$$D_B = \frac{k_B T (1 + 1.591 \frac{2\lambda}{d})}{3\pi\mu d}, \quad (2)$$

where k_B is the Boltzmann constant, T is the temperature, λ is the mean free path of the gas molecules, μ is the fluid viscosity, and d is the equivalent volume diameter.

The last term on the left-hand side of Eq. (1) corresponds to the influence of turbulent diffusion on $\overline{n}$ and can be expressed as $\overline{n'(v, t) \mathbf{u}'} = -\nu_t \frac{\partial \overline{n}}{\partial x_i}$ ^[16], where ν_t is the eddy diffusivity and can be obtained by solving the equations of turbulent flow. The last two terms on the right-hand side of Eq. (1) are the contribution to particle coagulation resulting from the fluctuating concentrations and called the fluctuating coagulation term. In order to close Eq. (1), we propose a model to establish the relationship between the fluctuating coagulation term and the gradient of mean concentration,

$$\overline{n'(v_i, t) n'(v_j, t)} = \frac{k}{(\frac{\overline{u_i^2}}{2} + k)} \overline{n}(v_i, t) \overline{n}(v_j, t), \quad (3)$$

where k is the turbulent kinetic energy, and $\overline{u_i^2}$ is the mean flow kinetic energy.

2.2 Moment equation for nanoparticles

The RAGDE is usually solved numerically because of its own complexity. Among the numerical methods, the moment method, a kind of method that tracks the moment of the particle distribution^[17], has been used due to its relatively low computational cost. The k th moment of the particle distribution function is defined by

$$m_j = \int_0^\infty v^j n(v, t) dv, \quad j = 0, 1, 2, \quad (4)$$

in which m_0 , m_1 , and m_2 correspond to the particle number concentration, the total particle mass, and the particle polydispersity, respectively, and the particle diameter can be determined by the zeroth-order and first-order moments as $d = (6m_1/(\pi m_0))^{1/3}$. Based on Eq. (4), the RAGDE (1) can be transformed into the following moment equation:

$$\frac{\partial \overline{m}_j}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \overline{m}_j - \nabla \cdot (D_B + \nu_t) \nabla \overline{m}_j = \prod_{c,j} (t), \quad (5)$$

where $\prod_{c,j}(t)$ is the coagulation source term and can be given by the following population balance equation based on Eq. (3):

$$\prod_{c,j}(t) = \frac{1}{2} \int_0^\infty \int_0^\infty ((v+v_1)^j - v^j - v_1^j) \left(1 + \frac{k}{(\frac{v^2}{2} + k)}\right) \beta(v, v_1) \bar{n}(v, t) \bar{n}(v_1, t) dv dv_1, \quad (6)$$

where the coagulation kernel $\beta(v, v_1)$ has different forms for different particle sizes because the particle coagulation is induced by the Brownian motion or the turbulent shear depending on the particle size. The time scales for the Brownian coagulation and the turbulence coagulation are different. The former is much shorter than the latter when the Reynolds number is not so high, i.e., the particle coagulation induced by the Brownian motion plays a leading role. In the present study, we use the kernel for Brownian coagulation because the Reynolds number is not so high. The coagulation kernel $\beta(v, v_1)$, which is suitable for continuous and near-continuous regions (i.e., across a large particle size range), is used^[18], i.e.,

$$\beta(v, v_1) = B_2 \left(\frac{1}{v^f} + \frac{1}{v_1^f} \right) (v^f + v_1^f) + B_2 \phi v_{p0}^{f-\frac{1}{3}} \left(\frac{1}{v^{2f}} + \frac{1}{v_1^{2f}} \right) (v^f + v_1^f), \quad (7)$$

where $B_2 = 2k_B T / (3\mu)$, $f = 1/D_f$, D_f is the fractal dimension of particles for the characterization of particle morphology, v_{p0} represents the volume of primary particles (monomers), and $\phi = 1.591\lambda(4\pi/3)^{1/3}$.

2.3 Taylor-series expansion method of moments (TEMOM)

When the coagulation kernel (7) is substituted into Eqs. (1) and (6), the existence of its fractal dimension means that there is a fractional power of volume, and the integral result is that the fractional moment makes the equation unable to be closed. In the present study, the TEMOM^[19] is used to solve this problem. Expand v^j with Taylor-series about the point $v = u$ (where $u = m_1/m_0$ represents the mean volume of particles),

$$v^j = \frac{j(j-1)}{2} u^{j-2} v^2 - j(j-2) u^{j-1} v + \frac{(j-1)(j-2)}{2} u^j + O((v-u)^3). \quad (8)$$

Equation (8) can be transformed into the moment equation based on Eq. (4),

$$m_j = \frac{j(j-1)}{2} u^{j-2} m_2 - j(j-2) u^{j-1} m_1 + \frac{(j-1)(j-2)}{2} u^j m_0. \quad (9)$$

Then, the coagulation source terms in Eq. (6) with $j = 0, 1$, and 2 become

$$\begin{aligned} \prod_{c,0}(t) = & -\frac{B_2(1+\zeta_t)m_0^2}{4} \left(a_2 \left(\frac{m_0 m_2}{m_1^2} \right)^2 + a_1 \frac{m_0 m_2}{m_1^2} + a_0 \right) \\ & - B_2(1+\zeta_t) \phi v_{p0}^{f-\frac{1}{3}} \frac{m_0^{2+f} + m_1^{-f}}{2} \left(b_2 \left(\frac{m_0 m_2}{m_1^2} \right)^2 + b_1 \frac{m_0 m_2}{m_1^2} + b_0 \right), \end{aligned} \quad (10)$$

$$\prod_{c,1}(t) = 0, \quad (11)$$

$$\begin{aligned} \prod_{c,2}(t) = & \frac{B_2(1+\zeta_t)m_1^2}{2} \left(a_2 \left(\frac{m_0 m_2}{m_1^2} \right)^2 + a_1 \frac{m_0 m_2}{m_1^2} + a_0 \right) \\ & - B_2(1+\zeta_t) \phi v_{p0}^{f-\frac{1}{3}} \frac{m_0^f + m_1^{2-f}}{2} \left(d_2 \left(\frac{m_0 m_2}{m_1^2} \right)^2 + d_1 \frac{m_0 m_2}{m_1^2} + d_0 \right), \end{aligned} \quad (12)$$

where

$$\begin{aligned} a_0 &= f^2(f^2 - 5) + 8, & a_1 &= -2f^2(f^2 - 3), & a_2 &= f^2(f^2 - 1), \\ b_0 &= 2f^4 - f^3 - 7f^2 - 2f + 4, & b_1 &= -2(2f^4 - f^3 - 4f^2 - f), & b_2 &= 2f^4 - f^3 - f^2, \\ d_0 &= 2f^4 + f^3 - 7f^2 + 2f + 4, & d_1 &= -4f^4 - 2f^3 + 8f^2 - 2f, & d_2 &= 2f^4 + f^3 - f^2. \end{aligned}$$

Assume that the evolution of particle distribution satisfies the log-normal distribution,

$$n(v, t) = \frac{N}{3\sqrt{2\pi} \ln \sigma} \exp\left(\frac{-(\ln^2(v/v_g))}{18 \ln^2 \sigma}\right) \frac{1}{v}, \quad (13)$$

where v_g and N represent the geometric mean volume and the total number of particles, respectively, and σ is the geometric standard deviation of the particle size,

$$v_g = \frac{m_1^2}{\sqrt{m_0^3 m_2}}, \quad \ln^2 \sigma = \frac{1}{9} \ln\left(\frac{m_0 m_2}{m_1^2}\right). \quad (14)$$

Accordingly, the initial particle geometric mean volume is v_{g0} , the initial geometric standard deviation is σ_0 , the initial total particle number is N_0 , and the initial value of the k th-moment is denoted by $m_{j0} = N_0 v_{g0}^j e^{9j^2 \sigma_0^2 / 2}$.

2.4 Dynamic shape factor of particles

Primary spherical nanoparticles will become non-spherical due to particle coagulation. Non-spherical particles include two types^[20], i.e., one has a regular geometric shape such as cube, cylinder, single crystals, and clusters of spheres, and the other has an irregular shape, e.g., agglomerates composed of spherical particles. For the agglomerates composed of nanoparticles, the dynamic shape factor χ is used to characterize the sphericity of agglomerates ($\chi = 1$ for a sphere). Therefore, the equivalent volume diameter for an agglomerate is defined as d . In order to compare the present numerical results with the experimental ones, we adopt a relationship between the equivalent volume diameter used in the numerical simulation and the mobility diameter d_m used in the experiment^[21], i.e.,

$$\frac{d_m}{Cu(d_m)} = \chi \frac{d}{Cu(d)}, \quad (15)$$

where Cu is the Cunningham coefficient, and

$$Cu(d) = \left(1 + 1.591 \frac{2\lambda}{d}\right), \quad Cu(d_m) = \left(1 + 1.591 \frac{2\lambda}{d_m}\right). \quad (16)$$

For an agglomerate system, the following power law relationship is satisfied^[16]:

$$N_p = \frac{v}{v_{p0}} = k_f \left(\frac{v_c}{v_{p0}}\right)^{D_f}, \quad (17)$$

where N_p is the number of primary particles contained in a single agglomerate, v_c is the solid volume, and k_f is 1.47.

2.5 Flow field

Consider that the particle phase is a low-inertia particle with a volume fraction of less than 10^{-5} and a diameter of less than 100 nm, and hence the effect of particles on the flow field can be ignored, and the one-way coupling method is selected for simulation. Assume that the fluid is at a constant temperature and incompressible. Expressing the instantaneous fluid velocity as the superposition of the mean and fluctuating components, substituting the superposition

into the continuity equation and the Navier-Stokes equation, and averaging it with respect to time, we have the mean continuity equation and the Reynolds-averaged Navier-Stokes (RANS) equation,

$$\frac{\partial \bar{u}_i}{\partial x_j} = 0, \quad (18)$$

$$\rho \left(\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_k \frac{\partial \bar{u}_i}{\partial x_k} \right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu \frac{\partial \bar{u}_i}{\partial x_j} \right) + \frac{\partial R_{ij}}{\partial x_j}, \quad (19)$$

where u_i is the fluid velocity, p is the pressure, and the Reynolds stress R_{ij} is

$$R_{ij} = -\rho \overline{u'_i u'_j} = \rho \nu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij}, \quad (20)$$

where $\nu_t = C_\mu k^2 / \varepsilon$, ε is the turbulent dissipation rate, and

$$\frac{\partial k}{\partial t} + \bar{u}_j \frac{\partial k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\nu + \frac{\nu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right) + 2\nu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \varepsilon, \quad (21)$$

$$\frac{\partial \varepsilon}{\partial t} + \bar{u}_j \frac{\partial \varepsilon}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\left(\nu + \frac{\nu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right) + \frac{\varepsilon}{k} \nu_t C_{\varepsilon 1} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \rho C_{\varepsilon 2} \frac{\varepsilon^2}{k}, \quad (22)$$

where ν is the fluid viscosity, $C_\mu = 0.09$, $C_{\varepsilon 1} = 1.44$, $C_{\varepsilon 2} = 1.92$, $\sigma_k = 1$, and $\sigma_\varepsilon = 1.3$.

3 Numerical simulation

3.1 Flow in ventilation chamber and numerical specification

As shown in Fig. 1, the low-inertia nanoparticles suspended in a turbulent gas flow are injected into the ventilation chamber from the inlet on the left side, and flow out from the outlet on the right side. The evolution and distribution of particle concentration and size in the ventilation chamber depend on the particle convection, diffusion, and coagulation.

Fig. 1 Flow in ventilation chamber (color online)

Equations (5), (10)–(12), and (18)–(22) are solved numerically with the finite volume method in OpenFOAM-5, and the term of velocity-pressure coupling and the convection term are dealt with OpenFOAM SIMPLE algorithm. The no-slip boundary condition for the gas and the zero-gradient boundary condition for the particle number density are applied to the wall, respectively. The moments are dimensionless with initial values, i.e., $M_j = m_j / m_{j0}$. Parameters are as follows: $T = 293$ K, $k_B = 1.38 \times 10^{-23}$ J/K, $\chi = 1.08$, $\rho = 1.205$ kg/m³, and $\nu = 1.5 \times 10^{-5}$ m²/s. The other parameters used in the computation under different conditions are listed in Table 1, where the subscript “0” represents the initial value, and d_g is the geometric mean diameter of particles.

Table 1 Parameters used in computation under different conditions

Re_D	Inlet velocity/($\text{m}\cdot\text{s}^{-1}$)	d_{g0}/nm	σ_0	m_{00}/m^{-3}	Mobility density/($\text{kg}\cdot\text{m}^{-3}$)	Monomer diameter/nm	Fractal dimension
1 500	0.589	41.9	0.5	6.3×10^{12}	2 170	6.09	2.85
1 917	0.7	41.9	0.5	6.3×10^{12}	2 170	6.09	2.85
2 465	0.9						
				6.3×10^{11}			
1 500	0.589	41.9	0.5	3.15×10^{12}	2 170	6.09	2.85
				12.6×10^{12}			
1 500	0.589	30	0.5	6.3×10^{12}	2 170	1	2.85
		50					

3.2 Mesh independence test and validation

A grid independence test is performed by changing grid points. Figure 2 shows the comparison of velocity profiles between numerical results with a coarse mesh (230 720 cells) and a fine mesh (518 400 cells) and experimental results^[21]. The experiment is performed for the NaCl nanoparticles in a chamber ($0.8\text{ m}\times 0.4\text{ m}\times 0.4\text{ m}$), and the inlet and the outlet with a diameter of 0.04 m are located at 0.055 m from the top to the bottom in the plane of $y = 0$ as shown in Fig. 1. Almost no difference is observed for the cases of coarse and fine meshes. Therefore, 230 720 cells are used in the simulation. In addition, agreement between numerical and experimental results indicates that the numerical method is reasonable and reliable.

Fig. 2 Comparison of velocity profiles between numerical and experimental results for $x = 3/8$ (color online)

4 Results and discussion

4.1 Effects of fluctuating coagulation term on particle distribution

Figures 3 and 4 show the numerical results of the particle number concentration M_0 and the geometric mean diameter d_g along the z -direction at different streamwise positions, respectively. The corresponding experimental results are also presented in the figures, where we can see that the numerical results with consideration of the fluctuating coagulation term are more consistent with the experimental results than that without consideration of the fluctuating coagulation term. Therefore, it is concluded that the established relationship between the fluctuating coagulation term and the gradient of mean concentration is reasonable, and it is necessary to consider the contribution to coagulation resulting from the fluctuating concentration in such a flow. In addition, the particle number concentration is reduced from $M_0 = 1.0$ to 0.78 (see Fig. 3), and the geometric mean diameter is increased from $d_g/d_{g0} = 1$ to 1.14 (see Fig. 4) along the jet centerline between the inlet and the area near the center of the chamber ($x/X = 0.375$), indicating the effect of particle coagulation on the distributions of number concentration and size.

Fig. 3 Distributions of particle number concentration along z -direction at $y = 0$ (color online)

Fig. 4 Distributions of geometric mean diameter of particles along z -direction at $y = 0$ (color online)

4.2 Distribution of particles

After particles are injected into the ventilation chamber as shown in Fig. 1, their concentration and size will change under the coupled action of convection, diffusion, and coagulation induced by fluid motion, Brownian motion of particles, and flow shear-induced force. Particles diffuse from a high concentration region to a low concentration region because of Brownian motion, resulting in a uniform particle distribution. Therefore, a spatial inhomogeneity of particle distribution mainly results from the flow shear-induced force, which is related to the mean velocity gradient and the turbulent dissipation rate. The distributions of the particle number concentration M_0 and the geometric mean diameter d_g at the xz -plane are shown in Fig. 5,

where we can see that the values of M_0 and d_g are the largest and smallest, respectively, in the core area of the jet at the inlet, and then decrease and increase gradually along the flow direction and the z -direction because of particle coagulation and diffusion. The changes of M_0 and d_g are more obvious in the core area of the jet, but less obvious in other areas. The reason is that the particle coagulation and diffusion are dependent on the mean velocity gradient $\frac{\partial \bar{u}_i}{\partial x_j}$ and the turbulent dissipation rate ε , and both $\frac{\partial \bar{u}_i}{\partial x_j}$ and ε are the largest in the core area of the jet, leading to a more frequent coagulation and a stronger diffusion.

4.3 Effects of initial number concentration of particles

The evolution of the particle number concentration M_0 along the streamwise direction for different values of the initial number concentration m_{00} is shown in Fig. 6. It can be seen that the values of M_0 do not change basically at $0 < x/X < 0.2$, then decrease rapidly at $0.2 < x/X < 0.9$, and finally increase at $0.9 < x/X < 1$. This is because there is a backflow vortex at $0.9 < x/X < 1$, causing particles to backflow and accumulate there. M_0 decreases with increasing the initial number concentration m_{00} , which indicates that particle coagulation occurs more frequently when the initial number concentration is higher, thus leading to a decrease in the particle number concentration.

Fig. 5 Distributions of (a) particle number concentration and (b) geometric mean diameter at xy -plane for $d_{g0} = 50$ nm and $m_{00} = 3.15 \times 10^{12} \text{ m}^{-3}$ (color online)

Fig. 6 Evolution of particle number concentration along x -direction for different values of initial number concentration (color online)

Figure 7 shows the distributions of the particle number concentration M_0 , the geometric mean diameter d_g , and the standard deviation of particle size σ along the z -direction for different values of the initial number concentration m_{00} at $x/X = 0.375$. We can see the significant influence of the initial number concentration on M_0 , d_g , and σ . With the increase in the initial number concentration m_{00} , the values of M_0 and σ decrease but the value of d_g increases. The reason is that the increase in the initial number concentration enhances the probability

of inter-particle collision, thus shortening the time scale required for particle coagulation, intensifying particle coagulation, leading to the reduction of particle number concentration and polydispersity, and resulting in the increase in the geometric mean diameter. In addition, the distributions of M_0 , d_g , and σ become more uniform along the z -direction with decreasing the initial number concentration.

4.4 Effects of initial mean particle size

The distributions of the particle number concentration M_0 for the initial particle diameter of $d_{g0} = 30$ nm at the xz -plane are shown in Fig. 8. By comparing it with the case for the initial particle diameter of $d_{g0} = 50$ nm as shown in Fig. 5(a), we can find that, at the same location, the value of M_0 is larger for the case with a larger initial particle diameter ($d_{g0} = 50$ nm), because small particles are more likely to coagulate and thus reduce the number of particles. With the development along the downstream, the difference in M_0 between the cases with different initial particle diameters gradually becomes smaller.

Fig. 7 Distributions of (a) particle number concentration, (b) geometric mean diameter, and (c) standard deviation of particle size along z -direction for different values of initial number concentration and $x/X = 0.375$ (color online)

Fig. 8 Distributions of particle number concentration for initial particle diameter of $d_{g0} = 30$ nm (color online)

The distributions of the particle number concentration M_0 , the geometric mean diameter d_g , and the standard deviation of particle size σ along the z -direction for different values of the initial particle diameter d_{g0} at $x/X = 0.625$ are shown in Fig. 9. The obvious effects of the initial particle diameter on M_0 , d_g , and σ can be observed. The decrease in the initial particle diameter leads to the reduction of the particle number concentration and the standard deviation of particle size (polydispersity), and the increase in the geometric mean diameter, because the particles diffuse faster and are easier to coagulate when the initial diameter is smaller.

Fig. 9 Distributions of (a) particle number concentration, (b) geometric mean diameter, and (c) standard deviation of particle size along z -direction for different values of initial particle diameter and $x/X = 0.625$ (color online)

Fig. 10 Distributions of particle number concentration along z -direction for different Reynolds numbers (color online)

4.5 Effects of Reynolds number

Figures 10, 11, and 12 show the distributions of the particle number concentration M_0 , the geometric mean diameter d_g , and the standard deviation of particle size σ along the z -direction for different Reynolds numbers at different streamwise positions. With the increase in the Reynolds number, the flow convection effect is larger than the diffusion effect as shown in Eq. (5), and the particles have few chances of collision and hence the coagulation rate is reduced, leading to the increase in the particle number concentration and the standard deviation of particle size. Accordingly, the geometric mean diameter of particles is decreased due to low coagulation rates.

Fig. 11 Distributions of geometric mean diameter of particles along z -direction for different Reynolds numbers (color online)

Fig. 12 Distributions of standard deviation of particle size along z -direction for different Reynolds numbers (color online)

5 Conclusions

The RAGDE for the particle distribution function is derived, including the contribution to particle coagulation resulting from the fluctuating concentration. A model to establish the relationship between the fluctuating coagulation term and the gradient of mean concentration is proposed. The RAGDE together with the equations of turbulent gas flow is solved numerically with the Taylor-series expansion moment method in a ventilation chamber. Some results are compared with the experimental data. The conclusions are summarized as follows.

The established model relating the fluctuating coagulation term to the gradient of mean concentration is reasonable, and it is necessary to consider the contribution to coagulation

resulting from the fluctuating concentration in such a flow. The changes of the particle number concentration M_0 and the geometric mean diameter d_g are more obvious in the core area of the jet, but less obvious in other areas. The initial particle number concentration m_{00} has a significant effect on M_0 , d_g , and the standard deviation of particle size σ . With the increase in m_{00} , the values of M_0 and σ decrease but the value of d_g increases. Particle coagulation occurs more frequently when m_{00} is larger, leading to a decrease in the particle number concentration. The decrease in the initial particle diameter leads to the reduction of the particle number concentration and polydispersity and the increase in the geometric mean diameter. With the increase in the Reynolds number, particles have few chances of collision and hence the coagulation rate is reduced, leading to the increase in M_0 and σ , and the decrease in d_g .

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- [1] DADA, L., LEHTIPALO, K., KONTKANEN, J., NIEMINEN, T., BAALBAKI, R., AHONEN, L., DUPLISSY, J., YAN, C., CHU, B. W., PETAJA, T., LEHTINEN, K., KERMINEN, V. M., KULMALA, M., and KANGASLUOMA, J. Formation and growth of sub-3-nm aerosol particles in experimental chambers. *Nature Protocols*, **15**(3), 1013–1040 (2020)
- [2] ZHU, J., WANG, S. N., ZHENG, L. C., and ZHANG, X. X. Heat transfer of nanofluids considering nano-particle migration and second-order slip velocity. *Applied Mathematics and Mechanics (English Edition)*, **38**(1), 125–136 (2017) <https://doi.org/10.1007/s10483-017-2155-6>
- [3] SHEHZAD, S. A., MUSHTAQ, T., ABBAS, Z., RAUF, A., KHAN, S. U., and TLILI, I. Dynamics of bioconvection flow of micropolar nanoparticles with Cattaneo-Christov expressions. *Applied Mathematics and Mechanics (English Edition)*, **41**(9), 1333–1344 (2020) <https://doi.org/10.1007/s10483-020-2645-9>
- [4] SAFFARIPOUR, M., THOMSON, K. A., SMALLWOOD, G. J., and LOBO, P. A review on the morphological properties of non-volatile particulate matter emissions from aircraft turbine engines. *Journal of Aerosol Science*, **139**, 105467 (2020)
- [5] LIN, J. Z., PAN, X. J., YIN, Z. Q., and KU, X. K. Solution of general dynamic equation for nanoparticles in turbulent flow considering fluctuating coagulation. *Applied Mathematics and Mechanics (English Edition)*, **37**(10), 1275–1288 (2016) <https://doi.org/10.1007/s10483-016-2131-9>
- [6] DONALDSON, K., TRAN, L., JIMENEZ, L. A., DUFFIN, R., NEWBY, D. E., MILLS, N., MACNEE, W., and STONE, V. Combustion-derived nanoparticles: a review of their toxicology following inhalation exposure. *Particle and Fibre Toxicology*, **2**, 10 (2005)
- [7] YI, J. H., CHEN, B. T., SCHWEGLER-BERRY, D., FRAZER, D., CASTRANOVA, V., MCBRIDE, C., KNUCKLES, T. L., STAPLETON, P. A., MINARCHICK, V. C., and NURKIEWICZ, T. R. Whole-body nanoparticle aerosol inhalation exposures. *Journal of Visualized Experiments*, **75**, e50263 (2013)
- [8] CHAN, T. L., LIU, S. Y., and YUE, Y. Nanoparticle formation and growth in turbulent flows using the bimodal TEMOM. *Powder Technology*, **323**, 507–517 (2018)
- [9] KYLAFIS, G. F., TOMLIN, A. S., SLEIGH, P. A., and VIGNES, A. Evolution of particle interactions between accidentally released aerosol particles generated from powdered engineered nanomaterials into a simulated workplace atmosphere. *Journal of Aerosol Science*, **129**, 98–115 (2019)
- [10] KIM, D. S., HONG, S. B., KIM, Y. J., and LEE, K. W. Deposition and coagulation of polydisperse nanoparticles by Brownian motion and turbulence. *Journal of Aerosol Science*, **37**(12), 1781–1787 (2006)

-
- [11] CHO, K., CHUNG, K., and BISWAS, P. Coagulation coefficient of agglomerates with different fractal dimensions. *Aerosol Science and Technology*, **45**(6), 740–743 (2011)
 - [12] ANAND, S., MAYYA, Y. S., YU, M., SEIPENBUSCH, M., and KASPER, G. A numerical study of coagulation of nanoparticle aerosols injected continuously into a large, well stirred chamber. *Journal of Aerosol Science*, **52**, 18–32 (2012)
 - [13] GUICHARD, R. and BELUT, E. Evaluation of a moments-based formulation for the transport and deposition of small inertia aerosols. *The Journal of Computational Multiphase Flows*, **6**(4), 407–418 (2014)
 - [14] GUICHARD, R. and BELUT, E. Simulation of airborne nanoparticles transport, deposition and aggregation: experimental validation of a CFD-QMOM approach. *Journal of Aerosol Science*, **104**, 16–31 (2017)
 - [15] LEE, K. W., LEE, Y. J., and HAN, D. S. The log-normal size distribution theory for Brownian coagulation in the low Knudsen number regime. *Journal of Colloid and Interface Science*, **188**(2), 486–492 (1997)
 - [16] FRIEDLANDER, S. K. *Smoke, Dust and Haze: Fundamentals of Aerosol Behavior*, John Wiley & Sons, New York (2000)
 - [17] BARRETT, J. C. and JHEETA, J. S. Improving the accuracy of the moments method for solving the aerosol general dynamic equation. *Journal of Aerosol Science*, **27**(8), 1135–1142 (1996)
 - [18] YU, M. and LIN, J. Z. Binary homogeneous nucleation and growth of water-sulfuric acid nanoparticles using a TEMOM model. *International Journal of Heat and Mass Transfer*, **53**(4), 635–644 (2010)
 - [19] YU, M. Z., LIN, J. Z., and CHAN, T. L. A new moment method for solving the coagulation equation for particles in Brownian motion. *Aerosol Science and Technology*, **42**(9), 705–713 (2008)
 - [20] HINDS, W. C. *Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles*, 2nd ed., John Wiley & Sons, New York (1999)
 - [21] BELUT, E. and THÉO, C. A new experimental dataset to validate CFD models of airborne nanoparticles agglomeration. *9th International Conference on Multiphase Flow*, Firenze, Italy (2016)