THE VERIFICATION OF THE TAYLOR-EXPANSION MOMENT METHOD IN SOLVING AEROSOL BREAKAGE

by

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The combination of the method of moment, characterizing the particle population balance, and the computational fluid dynamics has been an emerging research issue in the studies on the aerosol science and on the multiphase flow science. The difficulty of solving the moment equation arises mainly from the closure of some fractal moment variables which appears in the transform from the non-linear integral-differential population balance equation to the moment equations. Within the Taylor-expansion moment method, the breakage-dominated Taylor-expansion moment equation is first derived here when the symmetric fragmentation mechanism is involved. Due to the high efficiency and the high precision, this proposed moment model is expected to become an important tool for solving population balance equations.

Key words: *Taylor-expansion moment method, breakage, aerosol particles, multiphase*

Introduction

Our surroundings are filled with thousands kinds of nanoparticles. There exist many researches on the property of nanoparticles, for example, particle nucleation [1], condensation [2], dispersion [3] coagulation [4], collision [5] and deposition [6]. The combination of the population balance equation for particle size distribution and the computational fluid dynamics (CFD) has become an emerging research field [7, 8]. The solution of the population balance equation is not easily to achieve. Although the method of moments, the sectional method, and the Monte Carlo method have been proposed when the first population balance equation (PSD) was proposed, the method of moments is always the most dominant method.

The Taylor-expansion moment method was firstly proposed for solving population balance equation dominated by coagulation process. Here, it is further applied to solve the population balance equation with respect to particle breakage. For non-spherical coagulation, the fractal dimension was usually used for fragmentation process by many researchers to characterize aggregate fractal-like properties [9-11]. In the existing studies, most researchers focus on simple breakage and erosion kinetics using SM method or QMOM method, whereas

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the application of TEMOM method in this field is not yet performed. Since the fragmentation occurs mainly in the size range approaching or beyond to Kolmogorov length scale where the effect of turbulence on interparticle collision surpasses completely Brownian motion, Brownian coagulation can be, of course, neglected for simplicity in the population balance equation as breakage process is involved. In fact, some researchers have followed this solution to study the dynamic behavior of aggregates [9, 12]. In this study, our emphasis is placed on how to construct the moment equations with respect to population balance equation as only breakage process is involved.

In the studies on particle coagulation using Taylor-expansion moment method, the closure of fractal moment variables is achieved by using the equation [10]:

$$m_k = \int_0^\infty v^k n(v)\,\mathrm{d}t =$$

$$= \left(\frac{u^{k-2}k^2}{2} - \frac{u^{k-2}k}{2}\right) m_2 + (-u^{k-1}k^2 + 2u^{k-1}k)\, m_1 + \left(u^k + \frac{u^k k^2}{2} - \frac{3u^k k}{2}\right) m_0 \tag{1}$$

where, m_k is the k^{th} moment, v is the particle volume, and u – the expansion point which will be replaced by $u = m_1/m_0$. Equation (1) will be used in the construction of breakage-dominated moment models.

The construction of moment model

The population balance equation dominated by the breakage process takes the equation:

$$\frac{\partial n\,(v,t)}{\partial t} = \int_v^\infty a(v_1) b(v\,|\,v_1) n(v_1,t) dv_1 - a(v)n(v,t) \tag{2}$$

The first term of the right-hand side (RHS) represent the rate of the birth of particles with volume v due to fragmentation of bigger particles, and the second is the rate of the death of particles due to fragmentation. The breakage kernel, $a(v)$, only power-law distribution is used and it takes the expression [9]:

$$a(v) = k_b \left[\frac{\eta(\phi_{\text{tot}})G}{\tau^*}\right]^q v_p{}^{1/3} \left[\frac{d_c(v)}{d_p}\right]^{3/D_f} \tag{3}$$

where the suspension effective viscosity $\eta(\phi_{tot})$, the shear rate G, the characteristic shear stress τ, and the constant variables (including k_b, q, v_p, d_p, D_f) are assumed to be independent on tracking variable v, and thus we can further simplify eq. (33) to be the form:

$$a(v) = k_b \left[\frac{\eta(\phi_{\text{tot}})G}{\tau^*}\right]^q v_p^{1/3-3/D_f^2} v^{3/D_f^2} \tag{4}$$

For fragment distribution function, $b\,(v|v_1)$, however, there are usually different mathematical forms due to specific breakage mechanism. Marchisio *et al*. [13] outlined five kinds of the fragment function in terms of particle length. In the study, however, we only focus one of them, as shown in tab. 1. Once the breakage kernel a (v), and the fragment distribution function, b ($v|v_1$), are provided, we can easily proceed to transfer eq. (2) to moment equations using the transforming equation of eq. (1). For two terms in the right-hand size in eq. (2), it is clear that they have an additive property in mathematical form, and thus it is feasible to be disposed separately.

Table 1. Fragment distribution functions

Mechanism	$b(v/v_1)$	$\bar{b}_i^k$
Symmetric fragmentation	$\begin{cases} 2 & \text{if } v_1 = 2v \\ 0 & \text{otherwise} \end{cases}$	$2^{1-k} v_i^k$

First, we focus on the second term of RHS in eq. (2) and then write the population balance equation as the following simple form $\partial n(v, t)/\partial t = -a(v)\, n(v, t)$. If we multiply the equation v^k and then integrate over the entire size distribution as well as introduce eq. (1) to it, then we can finally obtain the corresponding moment equation: $\mathrm{d}m_k/\mathrm{d}t = -\varsigma m_{k+3/D_f^2}$, here, the fractal moment, m_{k+3/D_f^2}, can be achieved using eq. (1) if the three-order Taylor-series expansion is applied. Similarly, we can take the same procedure to dispose the first term of RHS in eq. (2) and finally the absolute moment equation is:

$$\frac{\mathrm{d}m_k}{\mathrm{d}t} = \varsigma 2^{1-k} m_{k+3/D_f^2} - \varsigma m_{k+3/D_f^2} \qquad (k = 0, 1, 2) \tag{5}$$

Results and discussions

For convenient analysis, in this study, all the quantities are scaled by the relationships: $m_k = M_k\, m_{k0}$ and and $\tau = t\zeta v_p^{3/D_f^2}$ where $m_{k0} = N v_p^{\,k} \chi^{k^2}$, $\chi = e^{w_g^2}$, $w_g = 3\log\sigma_g$, N is the total particle number concentration, and σ_g is the geometric standard deviation of particle size distribution. In the calculation, the diameter of primary particle is 3 nm, and the initial aggregate size distribution takes a log-normal distribution. The temperature of air is 300 K and the viscosity is $1.850772 \cdot 10^{-5}$ Pa·s, and correspondingly the gas mean free path is 68.41 nm.

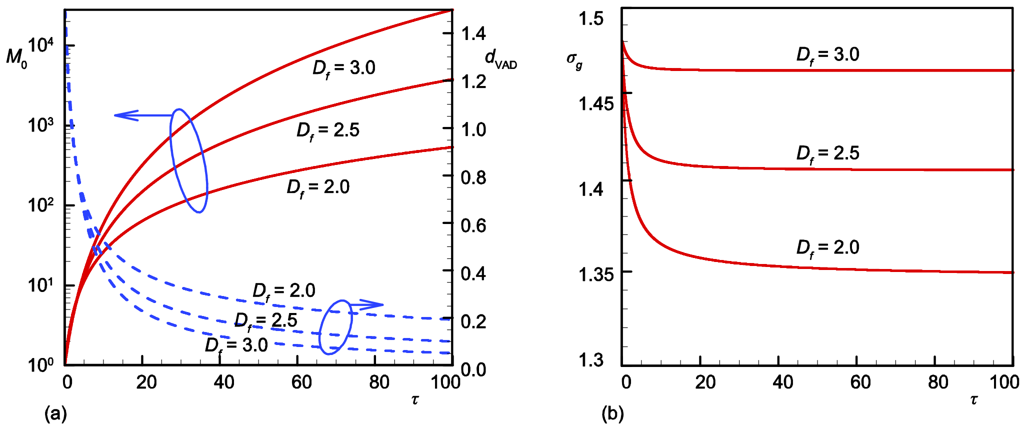

Figure 1. Evolution of scaled total particle number concentration (M_0) and scaled volume-averaged diameter (d_{VAD}) with time (a), and the geometric standard deviation with time (b)

In fig. 1(a) the fractal dimension is selected to be 2.0, 2.5, and 3.0. In the turbulent condition, when the particle breakage is dominated by the symmetric fragmentation mechanism, the birth of newly particles is increased with the increase of fractal dimension, and cor-

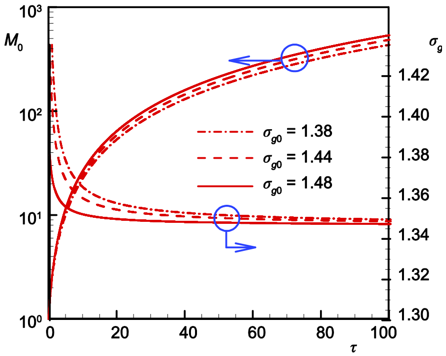

Figure 2. Evolution of total particle number concentration and geometric standard deviation with time

respondingly an inversed relationship between fractal dimension and the volume-averaged diameter was also observed. In this study, the scaled volume-averaged diameter takes the following expression $d_{\rm VAD} = (6M_1/\pi M_0)^{1/3}$.

In order to investigate the polydisperse characteristics of aerosol particles when the symmetric fragmentation breakage mechanism dominates, the geometric standard deviations are shown in fig. 1(b) when the fractal dimension varies. In this figure, it is clear that at three different fractal dimensions, all the particle size distributions finally achieve the self-preserving size distribution since the steady geometric standard deviation can be achieved for them. In addition, the comparison among three cases shows the aerosol has the greater polydisperse distributions when the fractal dimension is larger. For the same initial size distribution, it needs less time to approach the self-preserving size distribution for aerosols with larger fractal dimension.

The initial particle size distribution has an effect on the subsequent evolution of particle dynamics. In this study, three initial geometric standard deviations of 1.38, 1.44, and 1.48 were employed and compared as shown in fig. 2 which shows the total particle number concentration increases more quickly for aerosols with larger initial geometric standard deviation. In addition, it was observed that the final same geometric standard deviation was achieved, even though aerosol has the different initial particle size distribution. This is similar to the aerosol dynamics dominated by coagulation [10].

Conclusions

The moment equation based on three Taylor-expansion technique ever used in the TEMOM model was derived to study the evolution of particle dynamics due to breakage. The breakage mechanism is dominated by symmetric fragmentation. The self-preserving size distribution was observed. The fractal dimension and the initial particle size distribution were found to play important roles in determining the evolution of particle dynamics, including the particle total number concentration and the particle geometric standard deviation.

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