Research Article

The Fundamental Aspects of TEMOM Model for Particle Coagulation due to Brownian Motion—Part II: In the Continuum Regime

He Qing and Xie Mingliang

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China

Correspondence should be addressed to Xie Mingliang; mlxie@mail.hust.edu.cn

The fundamental aspects of the Taylor-series expansion method of moment (TEMOM) model proposed to model the aerosol population balance equation due to Brownian coagulation in the continuum regime is shown in this study, such as the choice of the expansion point u, the relationship between asymptotic behavior and analytical solution, and the error of the high-order moment equations. All these analyses will contribute to the buildup of the theoretical system of the TEMOM model.

1. Introduction

The population balance equations (PBE) are used to describe the evolution process of aerosol particles in a wide range of physical, chemical, and environmental subjects, such as nucleation, coagulation, diffusion, convection, and so on. When the Brownian coagulation plays a dominant role in such cases where aerosol particles at a high concentration are concerned or where suspended particles have evolved for a long time [1], the PBE for a monovariants system can be written as [2]

$$\frac{\partial n(v,t)}{\partial t}$$
$$= \frac{1}{2} \int_0^v \beta(v_1, v-v_1)\, n(v_1,t)\, n(v-v_1,t)\, dv_1 \qquad (1)$$
$$- \int_0^\infty \beta(v_1,v)\, n(v,t)\, n(v_1,t)\, dv_1,$$

in which $n(v,t)$ is the number density concentrations of the particles with volume from v to $v+dv$ at time t, $\beta(v,v_1)$ is the collision frequency function between particles with volumes v and v_1.

Because of its strong nonlinear partial integral-differential structure, the direct solution is very complicated and only a limited number of analytical solutions exist for simple

coagulation kernel [3]. So several methods are proposed to solve this equation numerically, such as the sectional method (SM) [4], the Monte Carlo method (MCM) [5], and the method of moment (MM) [6]. With lower computational cost compared to the SM and MCM, the moment method has been widely used and become a powerful tool for investigating evolution processes of aerosol particles [7, 8].

By multiplying v^k both the sides of (1) then integrating over the entire particle size distribution (PSD) [9], the growth rate of the particle moment can be obtained as follows:

$$\frac{dM_k}{dt} = \frac{1}{2} \iint_0^\infty \left[(v+v_1)^k - v^k - v_1^k \right]$$
$$\times \beta(v,v_1)\, n(v,t)\, n(v_1,t)\, dv\, dv_1, \qquad (2)$$
$$(k = 0, 1, 2, \ldots),$$

where the moment M_k is defined as

$$M_k = \int_0^\infty v^k n(v)\, dv. \qquad (3)$$

One main difficulty of the moment method is the closure of the moment equations. There exist several methods to overcome this bottleneck, including but not limited to the quadrature method of moment (QMOM) [10], the direct quadrature

method of moment (DQMOM) [11], and the Taylor-series expansion method of moment (TEMOM) [3, 12].

It should be pointed out that the TEMOM has no prior assumption for the PSD using the Taylor-series expansion to achieve the closure and is considered as a promising approach to approximate the PBE for its relative simplicity of implementation and high accuracy [13]. Based on TEMOM model, the important information about the PSD, namely, the particle number density, particle mass, and geometric standard deviation, can be obtained for Brownian coagulation over the entire size regimes, and its results have a great agreement with other moment methods [3, 12–16]. But in these works, some fundamental problems are not clarified, for example, why the expansion point u is set to be M_1/M_0 instead of other formulas; why the Taylor-series are truncated just at the first three terms; and what about the errors estimation of the present TEMOM model. In the present study, mainly as a methodological introduction, we would like to demonstrate the theoretical analysis to answer these questions for Brownian coagulation in the continuum regime.

2. Brief Review of TEMOM Model and Its Solutions in the Continuum Regime

At the initial time, the particle size maybe small in the free molecule regime. As time advances, the particle volume will grow due to coagulation between particles, and the particle size will transform to the near continuum regime via the transition regime and finally will tend to the continuum regime [17]. Therefore, the characteristic of particle evolution in the continuum regime is important to understand the coagulation mechanism. The collision frequency function β in the continuum regime is

$$\beta = B_2 \left(\frac{1}{v^{1/3}} + \frac{1}{v_1^{1/3}} \right) \left(v^{1/3} + v_1^{1/3} \right), \tag{4}$$

where the constant $B_2 = 3k_B T / 2\mu$, k_B is the Boltzmann's constant, T is temperature, and μ is gas viscosity. Substituting (4) into (2), a set of moment equations including integral and fractional moments can be obtained. Using a Taylor-series expansion at $v = u = M_1/M_0$ for v^k, the fractional moments can be approximated by the combination of integral moments as follows:

$$v^k = u^k + u^{k-1} k (v - u)$$
$$+ \frac{u^{k-2} k (k-1)}{2} (v - u)^2 \tag{5}$$
$$+ \frac{u^{k-3} k (k-1) (k-2)}{3!} (v - u)^3 + \cdots ;$$

then the closure of the moment equations will be achieved automatically without any prior assumption about the particle size spectrum. The minimum number of moments for closing the equations is the first three-order moments M_0, M_1, and M_2, which represents or are proportional to the total particle number concentration, and the total particle mass

concentration, the total scattering light, respectively. According to the results derived by Yu et al. [3] and Xie and Wang [18], the equations can be rearranged as follows:

$$\frac{dM_0}{dt} = \frac{B_2 \left(2M_C^2 - 13M_C - 151 \right) M_0^2}{81},$$
$$\frac{dM_1}{dt} = 0, \tag{6}$$
$$\frac{dM_2}{dt} = -\frac{2B_2 \left(2M_C^2 - 13M_C - 151 \right) M_1^2}{81},$$

where the dimensionless moment M_C is defined as

$$M_C = \frac{M_0 M_2}{M_1^2}. \tag{7}$$

It is clear that M_1 remains constant due to the rigorous mass conservation requirement, and its initial conditions can be noted as M_{00}, M_{20}, and $M_{C0} = M_{00}M_{20}/M_1^2$. Equations in (6) are a set of ordinary differential equations and can be solved directly. The main process is described briefly as follows. Because of the same structures of the first and the third equations in (6), the following relationship can be obtained:

$$\frac{dM_2}{dM_0} = \frac{-2M_1^2}{M_0^2}. \tag{8}$$

This equation can be dissolved directly as follows:

$$M_2 = \frac{2M_1^2}{M_0} + C_1 M_1^2, \qquad C_1 = \frac{M_{20}}{M_1^2} - \frac{2}{M_{00}}, \tag{9}$$

where C_1 is the integration constant, and the dimensionless moment M_C can be expressed as

$$M_C = 2 + M_0 C_1. \tag{10}$$

Then substituting (10) into the first formula in (6), the relationship between M_0 and t can be obtained:

$$5 \ln M_0 + \frac{169}{C_1 M_0} - \frac{5}{2} \ln \left| 169 + 5C_1 M_0 - 2C_1^2 M_0^2 \right|$$
$$- \frac{701}{9\sqrt{17}} \operatorname{arctanh} \frac{\left| 4C_1 M_0 - 5 \right|}{9\sqrt{17}} = \frac{13^4 B_2}{3^4 C_1} t + C_2,$$
$$C_2 = 5 \ln M_{00} + \frac{169}{C_1 M_{00}} - \frac{5}{2} \ln \left| 169 + 5C_1 M_{00} - 2C_1^2 M_{00}^2 \right|$$
$$- \frac{701}{9\sqrt{17}} \operatorname{arctanh} \frac{\left| 4C_1 M_{00} - 5 \right|}{9\sqrt{17}}, \tag{11}$$

in which C_2 is the integration constant. Then the second moment M_2 and dimensionless particle moment M_C can be calculated by (9) and (10), respectively. As time advances, M_0 tends to zero due to coagulation; (11) can be simplified with some limit operation as

$$\lim_{M_0 \to 0} \frac{1}{M_0} = \lim_{t \to \infty} \frac{169 B_2}{81} t, \tag{12}$$

which is consistent with the asymptotic analysis shown by Xie et al. [18, 19].

3. The Choice of Expansion Point u

In the TEMOM model, the choice of the expansion point at $u = M_1/M_0$ is not arbitrary. Some researchers think that the expansion for the characteristic size should take account of dispersion in the size spectrum and that is best done by using the well-known log-normal based expression $u = M_0^{-3/2}M_1^2M_2^{-1/2}$ in a second order closure formalism [6]. Using the expansion point, the corresponding moment equations based on TEMOM in the continuum regime are rewritten as

$$\frac{dM_0}{dt}$$

$$= -\frac{B_2 M_0^2\left(-2M_C^4+17M_C^{5/2}-4M_C^2-35M_C+35M_C^{1/2}+151\right)}{81},$$

$$\frac{dM_1}{dt} = 0,$$

$$\frac{dM_2}{dt}$$

$$= -\frac{2B_2 M_1^2\left(2M_C^4-8M_C^{5/2}-5M_C^2-145M_C-8M_C^{1/2}+2\right)}{81M_C}.$$

(13)

The detailed derivation is provided in the appendix. The comparison of numerical results between (6) and (13) is shown in Figure 1. And the initial conditions are selected as lognormal distribution: $M_{00} = 1$; $M_1 = 1$; $M_{20} = 4/3$. The results show that the relative errors are small, and the two sets of equations are equivalent approximately. However, this selection results in more complicated moment equations. In fact, for any expression, when it is operated using the Taylor expansion technique, the selection of the expansion point is not unique. In mathematics, we only need to make sure in the targeted range than the Taylor-series expansion is convergent, and the final constructed moment equations are simple in the form. From this viewpoint, the selection of $u = M_0^{-3/2}M_1^2M_2^{-1/2}$ cannot be considered to be prior to the selection of $u = M_1/M_0$.

4. The High-Order Moment Equations

The accuracy of the TEMOM model largely depends on the truncation errors of Taylor-series expansion. One method to determine the truncated errors is comparing the results of different TEMOM models, for example, the first three-moment model, the first four-moment model, the first five-moment model, and so forth. Similar to the derivation of the first three moment equations, v^k is expanded at $v = u$ and truncated at the first four terms as

$$v^k = u^k + u^{k-1}k(v-u)$$

$$+ \frac{u^{k-2}k(k-1)}{2}(v-u)^2$$

$$+ \frac{u^{k-3}k(k-1)(k-2)}{3!}(v-u)^3 + \cdots;$$

(14)

then the closed first four-moment equations can be obtained as follows:

$$\frac{dM_0}{dt} = \frac{B_2}{6561}\left(\frac{70M_0^6M_3^2}{M_1^6} - \frac{636M_0^5M_3M_2}{M_1^5}\right.$$

$$+ \frac{1440M_0^4M_2^2}{M_1^4} + \frac{1225M_0^4M_3}{M_1^3}$$

$$\left.- \frac{5160M_0^3M_2}{M_1^2} - 10061M_0^2\right),$$

$$\frac{dM_1}{dt} = 0,$$

$$\frac{dM_2}{dt} = \frac{B_2}{6561}\left(\frac{-32M_0^4M_3^2}{M_1^4} + \frac{408M_0^3M_3M_2}{M_1^3}\right.$$

$$- \frac{1260M_0^2M_2^2}{M_1^2} - \frac{344M_0^2M_3}{M_1}$$

$$\left.+ 3570M_0M_2 + 23902M_1^2\right),$$

(15)

$$\frac{dM_3}{dt} = \frac{B_2}{2187}\left(\frac{76M_0^3M_3^2}{M_1^3} - \frac{348M_0^2M_3M_2}{M_1^2}\right.$$

$$+ 925M_3M_0 + \frac{36M_0M_2^2}{M_1}$$

$$\left.+ 25791M_1M_2 - \frac{236M_1^3}{M_0}\right);$$

with the same process, the closed first five-moment equations are

$$\frac{dM_0}{dt}$$

$$= \frac{B_2 M_0^2}{59049M_1^8}$$

$$\times\left(-59049M_1^8 + 8520M_0^4M_4M_2M_1^2\right.$$

$$- 11550M_0^3M_4M_1^4$$

$$- 45474M_0^3M_3M_2M_1^3 + 60060M_0^2M_3M_1^5$$

$$- 128700M_0M_2M_1^6 - 3745M_0^5M_4M_3M_1$$

$$+ 51480M_0^2M_2^2M_1^4 + 350M_0^6M_4^2$$

$$\left.+ 10010M_0^4M_3^2M_1^2\right),$$
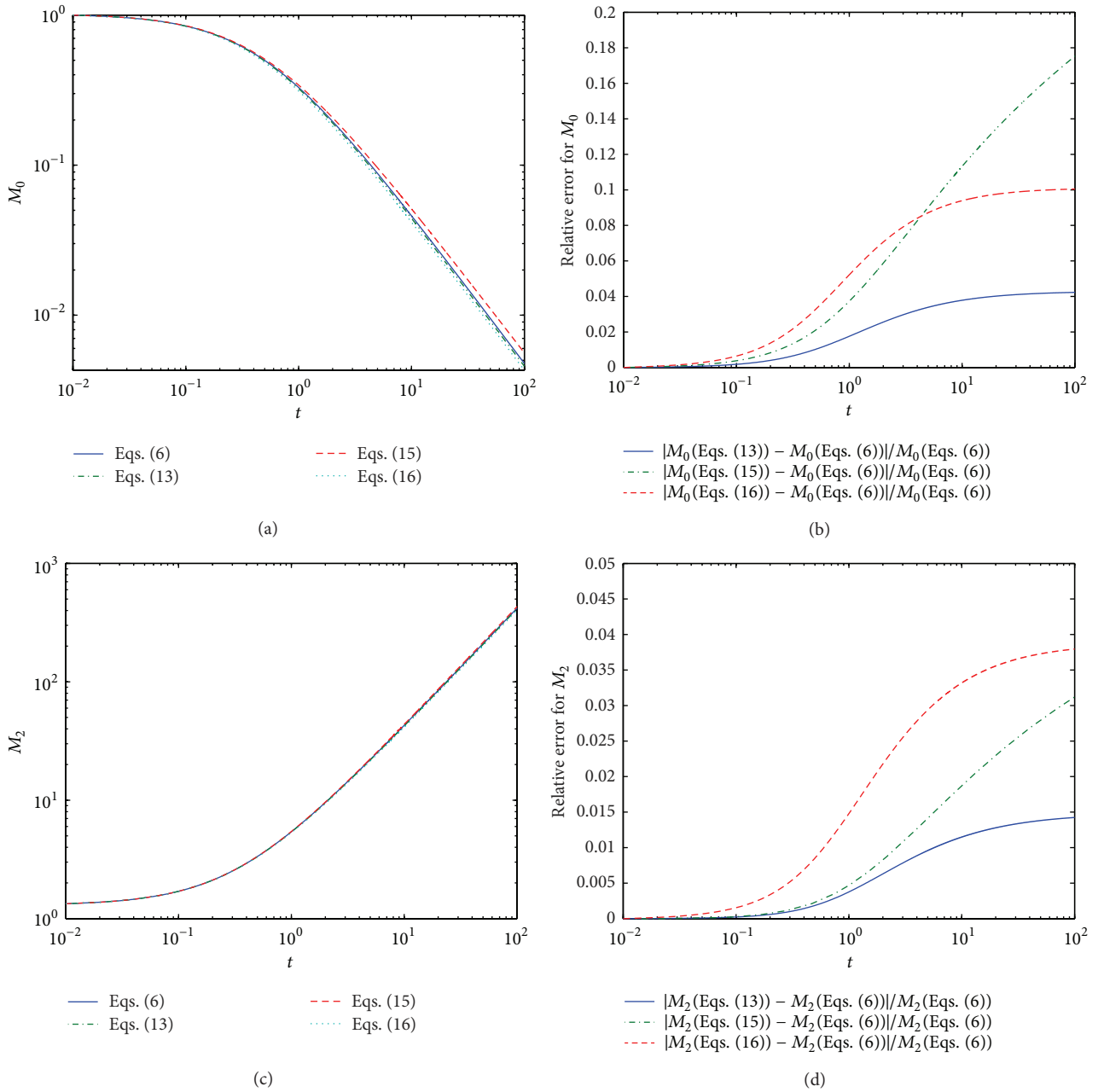
$$\frac{dM_1}{dt} = 0,$$

(a)

(b)

(c)

(d)

FIGURE 1: The comparison of numerical results among (6), (13), (15), and (16) with the initial condition $M_{00} = 1$, $M_1 = 1$, and $M_{20} = 4/3$; (a) the numerical results of M_0; (b) the relative errors for M_0; (c) the numerical results of M_2; (d) the relative errors for M_2.

$$\frac{dM_2}{dt}$$

$$= \frac{-2B_2}{59049 M_1^6}$$

$$\times \left(-525 M_0^3 M_4 M_1^4 - 8160 M_0^3 M_3 M_2 M_1^3 \right.$$

$$+ 4080 M_0^2 M_3 M_1^5$$

$$- 22050 M_0 M_2 M_1^6 - 106299 M_1^8$$

$$+ 12600 M_0^2 M_2^2 M_1^4$$

$$+ 1280 M_0^4 M_3^2 M_1^2 + 35 M_0^6 M_4^2$$

$$+ 1365 M_0^4 M_4 M_2 M_1^2$$

$$\left. - 424 M_0^5 M_4 M_3 M_1 \right),$$

$$\frac{dM_3}{dt}$$

$$= \frac{B_2}{19683 M_1^5}$$

$$\times \left(-1105 M_0^4 M_4 M_3 M_1 + 915 M_0^3 M_4 M_2 M_1^2 \right.$$

$$- 930M_0^2 M_4 M_1^4$$

$$- 9870M_0^2 M_3 M_2 M_1^3 + 13584M_0 M_3 M_1^5$$

$$+ 226458M_2 M_1^6$$

$$+ 3150M_0 M_2^2 M_1^4 + 3920M_0^3 M_3^2 M_1^2$$

$$+ 74M_0^5 M_4^2),$$

$$\frac{dM_4}{dt}$$

$$= \frac{-2B_2}{59049M_1^4 M_0^2}$$

$$\times \left(695M_0^6 M_4^2 - 2905M_0^5 M_4 M_3 M_1 \right.$$

$$+ 8340M_0^4 M_4 M_2 M_1^2$$

$$- 16545M_0^3 M_4 M_1^4 + 14430M_0^3 M_3 M_2 M_1^3$$

$$+ 22770M_0 M_2 M_1^6 - 481344M_0^2 M_3 M_1^5$$

$$- 360297M_0^2 M_2^2 M_1^4 - 7020M_1^8$$

$$\left. - 4810M_0^4 M_3^2 M_1^2 \right).$$

(16)

The comparison of numerical results among (5), (14), and (15) are also shown in Figure 1. The results show that the relative errors are small, and the three sets of equations can be considered equivalent nearly. Since the complexity of moment equations increases rapidly with the increasing number of reserved items but with little differences in the numerical results, we usually prefer using the first three-moment model proposed originally by Yu et al. [3].

5. Conclusion

Without a prior assumption for the shape of particle size distribution, the TEMOM has been considered as a promising method to model the aerosol population balance equation. In this study, the fundamental problems of the TEMOM model in the continuum regime due to Brownian coagulation are clarified, such as the choice of the expansion point u and the error of the high-order moment equations. It benefits the understanding of PBE and TEMOM model.

Appendix

With the same process as Yu et al. [3] shown, we can get the first three-moment equations as follows:

$$\frac{dM_0}{dt} = -B_2 \left(M_{1/3} M_{-1/3} + M_0^2 \right),$$

$$\frac{dM_1}{dt} = 0, \qquad (A.1)$$

$$\frac{dM_2}{dt} = 2B_2 \left(M_{4/3} M_{-2/3} + M_1^2 \right).$$

Then using (3) and (5), the fractional moments can be approximated by the combination of the first three integral moments, for example, the $M_{1/3}$ is

$$M_{-1/3} = \frac{1}{9u^{7/3}} \left(2M_2 - 7uM_1 + 14u^2 M_0 \right),$$

$$M_{1/3} = \frac{1}{9u^{5/3}} \left(-M_2 + 5uM_1 + 5u^2 M_0 \right)$$

$$M_{2/3} = \frac{1}{9u^{4/3}} \left(-M_2 + 8uM_1 + 2u^2 M_0 \right), \qquad (A.2)$$

$$M_{4/3} = \frac{1}{9u^{2/3}} \left(2M_2 + 8uM_1 - u^2 M_0 \right).$$

Now replacing all the fractional moments by the integral moments (i.e., M_0, M_1, and M_2) in (A.2) and substituting $u = M_1^2/(M_0^{3/2} M_2^{1/2})$ and $M_C = M_0 M_2/M_1^2$ into (A.1), (13) is obtained.

References

[1] S. H. Park, K. W. Lee, E. Otto, and H. Fissan, "The log-normal size distribution theory of Brownian aerosol coagulation for the entire particle size range. Part I: analytical solution using the harmonic mean coagulation kernel," *Journal of Aerosol Science*, vol. 30, no. 1, pp. 3–16, 1999.

[2] S. K. Friedlander, *Smoke, Dust, and Haze: Fundamentals of Aerosol Dynamics*, Oxford University Press, London, UK, 2nd edition, 2000.

[3] M. Z. Yu, J. Z. Lin, and T. L. Chan, "A new moment method for solving the coagulation equation for particles in Brownian motion," *Aerosol Science and Technology*, vol. 42, no. 9, pp. 705–713, 2008.

[4] S. S. Talukdar and M. T. Swihart, "Aerosol dynamics modeling of silicon nanoparticle formation during silane pyrolysis: a comparison of three solution methods," *Journal of Aerosol Science*, vol. 35, no. 7, pp. 889–908, 2004.

[5] N. M. Morgan, C. G. Wells, M. J. Goodson, M. Kraft, and W. Wagner, "A new numerical approach for the simulation of the growth of inorganic nanoparticles," *Journal of Computational Physics*, vol. 211, no. 2, pp. 638–658, 2006.

[6] S. E. Pratsinis, "Simultaneous nucleation, condensation, and coagulation in aerosol reactors," *Journal of Colloid And Interface Science*, vol. 124, no. 2, pp. 416–427, 1988.

[7] E. Otto, F. Stratmann, H. Fissan, S. Vemury, and S. E. Pratsinis, "39 P 17 Brownian coagulation in the transition regime II: a comparison of two modelling approaches," *Journal of Aerosol Science*, vol. 24, no. 1, pp. S535–S536, 1993.

[8] M.-Z. Yu, J.-Z. Lin, and T.-L. Chan, "Effect of precursor loading on non-spherical TiO$_2$ nanoparticle synthesis in a diffusion flame reactor," *Chemical Engineering Science*, vol. 63, no. 9, pp. 2317–2329, 2008.

[9] R. R. Upadhyay and O. A. Ezekoye, "Evaluation of the 1-point quadrature approximation in QMOM for combined aerosol growth laws," *Journal of Aerosol Science*, vol. 34, no. 12, pp. 1665–1683, 2003.

[10] R. McGraw, "Description of aerosol dynamics by the quadrature method of moments," *Aerosol Science and Technology*, vol. 27, no. 2, pp. 255–265, 1997.

[11] R. O. Fox, *Computational Models for Turbulent Reacting Flows*, Cambridge University Press, Cambridge, UK, 2003.

[12] M. Z. Yu and J. Z. Lin, "Taylor-expansion moment method for agglomerate coagulation due to Brownian motion in the entire size regime," *Journal of Aerosol Science*, vol. 40, no. 6, pp. 549–562, 2009.

[13] M. Z. Yu and J. Z. Lin, "Solution of the agglomerate Brownian coagulation using Taylor-expansion moment method," *Journal of Colloid and Interface Science*, vol. 336, no. 1, pp. 142–149, 2009.

[14] M. Z. Yu and J. Z. Lin, "Binary homogeneous nucleation and growth of water-sulfuric acid nanoparticles using a TEMOM model," *International Journal of Heat and Mass Transfer*, vol. 53, no. 4, pp. 635–644, 2010.

[15] M. Z. Yu, J. Z. Lin, H. H. Jin, and Y. Jiang, "The verification of the Taylor-expansion moment method for the nanoparticle coagulation in the entire size regime due to Brownian motion," *Journal of Nanoparticle Research*, vol. 13, no. 5, pp. 2007–2020, 2011.

[16] M. L. Xie, M. Z. Yu, and L. P. Wang, "A TEMOM model to simulate nanoparticle growth in the temporal mixing layer due to Brownian coagulation," *Journal of Aerosol Science*, vol. 54, pp. 32–48, 2012.

[17] E. Otto, H. Fissan, S. H. Park, and K. W. Lee, "The log-normal size distribution theory of Brownian aerosol coagulation for the entire particle size range. Part II: analytical solution using Dahneke's coagulation kernel," *Journal of Aerosol Science*, vol. 30, no. 1, pp. 17–34, 1999.

[18] M. L. Xie and L. P. Wang, "Asymptotic solution of population balance equation based on TEMOM model," *Chemical Engineering Science*, vol. 94, pp. 79–83, 2013.

[19] M. L. Xie and Q. He, "Analytical solution of TEMOM model for particle coagulation due to Brownian motion," *Journal of Aerosol Science*, vol. 66, pp. 24–30, 2013.