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# Methods of Moments for Resolving Aerosol Dynamics

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<http://dx.doi.org/10.5772/65565>

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## Abstract

The study on aerosol dynamics processes, such as formation of nano/microscale aerosol particle and its subsequent growth in quiescent or evolving flows, has received much attention from both chemical engineering and atmospheric environment communities. The suitable theoretical method for resolving aerosol dynamical processes is widely known as population balance modeling (PBM), which is based on solving the population balance equation (PBE) in terms of particle number concentration. The study on the solution of the PBE has undergone rapid development in last several decades. In this chapter, the development of the method of moments for solving the PBE is presented. Three main methods of moments, including the Taylor series expansion method of moments, log-normal method of moments, and quadrature method of moments, are discussed.

**Keywords:** aerosol dynamics, method of moments, population balance equation

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## 1. Introduction

Aerosol particles usually refer to fine particles in air whose size is smaller than micrometer [1]. This type of particles can be found in a wide range of industrial and natural phenomena such as nanoparticle synthesis [2, 3], aerosol sciences and air pollution [4–7], contamination control in the microelectronics and pharmaceuticals industries [8], and diesel particulate formation [9]. The dynamics characteristics of size of these particles spans from free molecular size regime much less than Kolmogorov length scale to inertial range. Due to Brownian motion, aerosol varies greatly in the degree of stability, even though the aerosol flow convection transport is not involved. Although this type of multiphase system widely emerges in industries and our surroundings, some key issues including the conversion from gas to particle and the subsequent particle growth affected by the surroundings remain unresolved [10]. Unlike some common

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techniques used in the multiphase flow community, the task of the study on aerosol dynamics is to grasp the interaction between the dispersed particles and the carrier phase and also to obtain the fundamentals of internal processes such as nucleation, condensation, coagulation, and breakage [11].

If the particle formation and subsequent growth are studied theoretically, the theory should cover from simple kinetics theory to continuum theory. The Stokes' law needs to be modified as applied in this field because aerosol particles are usually smaller than molecular mean free path [1]. Some common methodologies in multiphase flow community, such as Euler-Lagrange and Euler-Euler, are unsuitable to be used in this field. In fact, in the first decades of last century, studies on dynamics of micro- and nanoscale particles are always the focus of physical science [12]. With further requirements of modern industrial nanoparticle synthesis and atmospheric observation, the study on interaction between fine particles and the surrounding becomes more and more important, and thus, it needs to combine the methodology in modern multiphase flow theory with aerosol dynamics to resolve complicated micro- and nanoscale particle multiphase problems [13]. The object of these studies is to capture the property, behavior, and physical principle of aerosol particles in air and further apply this knowledge to their measurement and control.

Besides convection and diffusion transport, the evolution of aerosol particle dynamics arises mainly from internal mechanisms, including homogeneous or heterogeneous nucleation, condensation, coagulation, and breakage. Among these internal mechanisms, coagulation occurs most commonly, but it is yet the most difficult to be treated from the viewpoint of mathematics, because the correlation among all the particles must be concerned separately [14]. Since the pioneering work of Smoluchowski in 1917, the mean-field theory has been introduced in aerosol collision problems and has been basis for numerous theoretical applications. These applications include the derivation of coagulation kernel under different mechanisms, the solution of the governing equations within the Smoluchowski mean-field theory, and the application of Smoluchowski mean-field theoretical model to predict the behavior of aerosol multiphase system. In fact, within the Smoluchowski mean-field theory, some important phenomena such as self-preserving distribution [15–17], and gelation or asymptotic behavior [18–21] have been thoroughly studied using state-of-the-art technologies such as the method of moments (MOM) [17, 19–23], sectional method (SM) [24–30], stochastic particle method [31–35], and Monte Carlo method [36–42]. The method of moments is more widely used than other methods due to that it requires the least requirement for computational cost as well as the relative simplicity of implementation [36].

Although the method of moments has become a powerful tool for investigating aerosol chemistry physical processes since it was first used in aerosol community by Hulburt and Katz [22], the closure of governing equations in terms of  $k$ th moment is not easy to achieve. Up to now, there have been five main techniques proposed to achieve the closure of moment equations, namely the Taylor series expansion MOM (TEMOM) [43], the predefined size distributed method such as log-normal MOM (log MM) [44, 45] and Gamma MOM [46], Gaussian quadrature MOM (QMOM) and its variants [47, 48],  $p$ th-order polynomial MOM [49], and MOM with interpolative closure (MOMIC) [23]. In recent years, the PBM scheme,

which couples the PBE with the Computational Fluid Dynamics (CFD), has been increasingly received attention, and accordingly, it is possible to simultaneously capture the details of the fluid flow and transport, the evolution of the particle size distribution and complex chemical kinetics. For any techniques, consuming computational cost has to be concerned as the solution of Navier-Stokes equations is involved. Thus, the efficiency of solving the PBE in the implementation of the PBM is another important issue besides the accuracy of numerical calculation. Although the QMOM and its variants are the most used scheme for solving the PBE today, it shows disadvantage in efficiency as compared to the TEMOM and log MM. It needs to note here in the log MM, and the log-normal size distribution has to be employed in the construction of the model, which inevitably weakens its reliability and capability for solving the PBE. It is necessary to construct a new approach with respect to moment equation, which is easy to implement with low computational cost like the log MM and has not the prior requirement for particle size spectrum like the QMOM, to adapt to the requirement of modern complicated particulate industries. In particular, there needs a suitable technique capable of providing explicit moment governing equations for further asymptotic analysis for the PBE [50]. In order to accomplish it, a new promising method of moments based on Taylor series expansion technique has been proposed and successfully applied to resolve some aerosol engineering problems [43]. Relative to the QMOM and log MM, the TEMOM has advantage to give explicit moment governing equations, making it suitable as basis equation for further analytical solution or asymptotic solution of the PBE.

This chapter is outlined as follows: In Section 2, the review of the PBE as well as its solution is presented, in which three main techniques applied for solving the PBE, namely the method of moments, sectional method, and Monte Carlo method, are briefly presented; the method of moments is highlighted in Section 3, where three predominated methods of moments, including the QMOM, log MM, and TEMOM, are presented separately.

## 2. Methods for solving the PBE

The study of PBE dates back to 1917 when famous polish scientist, Smoluchowski, first established the discrete governing equation for colloid coagulation, that is, Smoluchowski equation [12]; then, Smoluchowski equation was further developed by Müller in its integral-differential form, which finally becomes the basis equation of the PBM [51]. Today, the Smoluchowski equation has developed from its original version only accounting for coagulation to the present version accounting to almost all aerosol dynamics, including external processes such as particle convection and diffusion transport in air, and internal processes such as nucleation, coagulation, condensation, and breakage [52, 53]. Without loss of generality, the general form of a PBE, accounting for both external and internal processes, can be expressed as: where  $n(v, x, t)$  is the particle number density for particle volume  $v$ , location  $x$ , and time  $t$ ;  $u_j$  is the particle velocity;  $u_{th}$  is the thermophoresis velocity;  $D_B$  is the Brownian diffusion coefficient;  $G_s$  is the particle surface growth rate;  $J$  is the nucleation rate for the critical monomer volume  $v^*$ ;  $\beta$  is coagulation kernel between two particles; and  $a$  and  $b$  are parameters accounting for the breakage rate associated with the turbulence shear force. Equation (1) encompasses

almost all physicochemical processes of aerosol with a size smaller than approximately  $1 \mu\text{m}$  and therefore is reliable for studying aerosol dynamics. In particular, an inherent advantage is that it can be coupled with the Navier-Stokes equation.

$$\begin{aligned}
 & \frac{\partial n(v, x_i, t)}{\partial t} + \frac{\partial (u_j n(v, x_j, t))}{\partial x_j} + \frac{\partial ((u_{th})_j n(v, x_j, t))}{\partial x_j} \\
 &= \frac{\partial}{\partial x_j} \left( D_B \frac{\partial n(v, x_j, t)}{\partial x_j} \right) + \frac{\partial (G_r n(v, x_i, t))}{\partial v} + J(v^*, x_i, t) \delta(v - v^*) \\
 &+ \frac{1}{2} \int_{v^*}^v \beta(v - v', v') n(v - v', t) n(v', x_i, t) dv' \\
 &- n(v, t) \int_{v^*}^{\infty} \beta(v, v') n(v', x_i, t) dv' + \int_v^{\infty} a(v') b(v|v') n(v', t) dv' \\
 &- a(v) n(v, t) + \dots,
 \end{aligned} \tag{1}$$

It needs to note here in Eq. (1), the coordinate (i.e., particle volume  $v$ ) of particle number concentration function might be other quantity, such as particle surface area or charge number, and coordinate number might be more, depending on the specific requirement of study. Even only the particle volume is selected as coordinate of particle number concentration function, the direct numerical solution of Eq. (1) is intractable for most applications due to the extreme large number of independent variables, and it should be further modified using suitable mathematical techniques. To solve the Eq. (1) numerically or analytically, several schemes by different researchers, including the method of moments, sectional method, and stochastic particle method, have been proposed and evaluated. Both advantages and disadvantages of these three methods have been compared in many review articles [36, 53]. In case the coagulation kernel is simplified with homogeneous assumption, the analytical solution of PBE can be achieved [54–57]. The analytical method has been used to study nanoparticle dynamics in an experimental chamber [58].

Because of relative simplicity of implementation and low computational cost, the method of moments has been extensively used to solve the PBE. In the application of this method, the fractal moment variables inevitably appear in the transfer from the PBE to moment governing equation, which needs to be further treated with different techniques. Due to the low requirement for computational cost, in the last decade, the combination of method of moments and Computational Fluid Dynamics (CFD) technique has been an emerging research field; the task is to investigate the temporal and spatial evolution of nanoparticles under turbulent conditions.

The information of particle size distribution is lost due to the integral in the transfer from the PBE to moment governing equations in the method of moments, and thus this method is unable

to trace the evolution of particle size distribution (PSD) if the reconstruct technique of PSD is not implemented [59]. The sectional method, which divides the PBE into a set of size classes, overcomes the limit of method of moments in tracing the PSD. This method was usually used as an exact solution to validate the method of moments [60] and also widely applied in studies on the evolution of particle size distribution at engineering conditions due to the different dynamical processes including coagulation, condensation, gas-particle conversion, etc.

An alternative to sectional method and method of moments for solving the PBE is stochastic particle method (or Monte Carlo method) [31–35]. The application of this method, however, is limited because of low efficiency. This method has advantage to capture the evolution of particle size distribution physically and also can be used to obtain some key kernels for aerosol dynamics such as coagulation. Up to now, there have been lots of versions of Monte Carlo methods for solving the PBE, but the coupling between the Computational Fluid Dynamics (CFD) and Monte Carlo method is still limited.

### 3. Method of moments

The evolution of aerosol particle behavior arises from the interaction between particles and surrounding air; these small particles share energy with gas molecules and exhibit Brownian motion. With the exception of convection and diffusion transport, the nucleation and condensation mechanisms account for the mass or energy transfer from gas vapors to particle system, while coagulation and breakage mechanisms account for particle number variance. In theory, all the mechanisms can be defined as a function of time from a macroscopic probability view. Within the Smoluchowski mean-field theory, all aerosol dynamics processes can be invoked into the particle general dynamic equation, that is, the PBE. Except nucleation and condensation mechanisms, some difficulties are from closure of unresolved moment, which limits the application of moment methodology in this field. This is not only because there is nonintegral form in coagulation or breakage kernel, but also because there are much more specific mechanisms to concern.

Typically, turbulence is the driving force for particle radii of about 1–10  $\mu\text{m}$ , while smaller particles are driven by Brownian motion and larger particles by differential sedimentation [61]. Here, coagulation receives much more attention by scientists than other dynamics processes such as nucleation and condensation because coagulation mechanism is harder to dispose in mathematics [14, 62]. The collision between interparticles is assumed to be instantaneous with spherical shape, while the mathematical description for agglomerate structures composed of noncoalescing spheres should be specially disposed [17, 63–65].

#### 3.1. Closure of moment equations

The key task of the method of moments for solving the PBE is to convert the PBE to moment governing equations, during the conversion some approximations have to be employed to achieve the closure of the moment governing equations. Once the closed moment governing equations were established, they can be solved by some common

numerical techniques, such as the fourth-order Runge-Kutta method. In the past, some techniques have been proposed to implement the method of moments. In this section, we only focus on coagulation and present how these different methods of moments are implemented for resolving this issue.

In order to represent the evolution of particle number, it is necessary to define particle concentration as a function of time and particle volume. This disposition was first proposed by Smoluchowski [12] for coagulation in dilute electrolytes, which has been basis for solving micro- and nanoparticle multiphase problems in modern aerosol or colloid science. The integral form of Smoluchowski equation is: where  $n(v,t) dv$  is the number of particles whose volume is between  $v$  and  $v+dv$  at time  $t$ , and  $\beta(v,v')$  is the collision kernel for two particles of volumes  $v$  and  $v'$ . If the method of moments is used, the general disposition for this problem is to convert Eq. (2) into an ordinary differential equation with respect to the moment  $m_k$ . The conversion involves multiplying Eq. (2) by  $v^k$  and then integrating over the entire size distribution, and finally the converted moment equation based on the size distribution is obtained where

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2} \int_0^v \beta(v-v',v') n(v-v',t) n(v',t) dv' - n(v,t) \int_0^\infty \beta(v,v') n(v',t) dv', \quad (2)$$

$$\frac{dm_k}{dt} = \frac{1}{2} \int_0^\infty \int_0^\infty \kappa(v,v',k) n(v,t) n(v',t) dv dv', \quad (3)$$

$$\kappa(v,v',k) = \left[ (v+v')^k - v^k - v'^k \right] \beta(v,v').$$

During the implementing conversion from the Smoluchowski equation, or PBE, to the moment governing equation, a definition for  $m_k$  should be

$$m_k = \int_0^\infty v^k n(v) dv. \quad (4)$$

The key task of all methods of moments, including the TEMOM, QMOM, MOMIC, and log MM, is to convert the integral term on the right hand of Eq. (3) to polynomials, and thereby, the numerical calculation can proceed. In this chapter, only the TEMOM, log MM, and QMOM will be presented. If readers have interests to other methods of moments, they are recommended to read articles for the MOMIC [23], the Gamma method of moments [66], and the DQMOM [48].

### 3.2. Taylor series expansion method of moments

The TEMOM was first proposed in 2008 in its numerical version for dealing with coagulation due to the Brownian motion [43]; since then, it was further developed [60, 64, 67]. On the basis of governing equations obtained from the TEMOM, researchers have found that it is easy to achieve analytical and asymptotic solutions of the PBE [19, 20, 56, 57, 68–70]. The TEMOM has been applied in many aerosol-related problems and has also successfully been used for the realistic environmental and engineering problems where multidynamics are involved [71, 72]. However, all of these quoted studies were only taken into consideration for three-order Taylor series expansion using integer moment sequence. The recent study shows that this kind of solution leads to shortcoming of the existing TEMOM, that is, the initial geometric standard deviation is limited, and the fractional moment at an initial stage cannot be accurately captured. Both shortcomings indeed greatly weaken the capability of the TEMOM. To overcome the shortcoming of the TEMOM in this aspect, a generalized TEMOM was currently proposed [60], in which the accuracy of numerical calculation is increased with increasing the orders of Taylor series expansion.

Here, we select coagulation in the continuum-slip regime as an example to present how the TEMOM is implemented. The coagulation kernel for agglomerates in the continuum-slip is [64] where  $v_{p0}$  is the volume of primary particles,  $B_2 = 2k_b T / 3\mu$ ,  $\psi = \lambda A / (3/4\pi)^{1/3}$ ,  $A = 1.591$ ,  $f = 1/D_f$ . To implement the TEMOM, we need to substitute Eq. (5) in Eq. (3) and then multiply  $v^k$  on both sides, and we can obtain the following expression, where

$$\beta(v, v') = B_2 \left( \frac{1}{v^f} + \frac{1}{v'^f} \right) (v^f + v'^f) + B_2 \psi v_{p0}^{f-\frac{1}{3}} \left( \frac{1}{v^{2f}} + \frac{1}{v'^{2f}} \right) (v^f + v'^f), \quad (5)$$

$$\left\{ \begin{array}{l} \frac{dm_0}{dt} = -\frac{B_2}{2} \int_0^\infty \int_0^\infty \left( \xi_1 + \psi v_{p0}^{f-\frac{1}{3}} \xi_2 \right) n(v, t) n(v', t) dv dv' \\ \frac{dm_1}{dt} = 0 \\ \frac{dm_2}{dt} = -\frac{B_2}{2} \int_0^\infty \int_0^\infty \left( \zeta_1 + \psi v_{p0}^{f-\frac{1}{3}} \zeta_2 \right) n(v, t) n(v', t) dv dv' \end{array} \right. \quad (6)$$

$$\xi_1 = 2 + v^f v'^{-f} + v^{-f} v'^f$$

$$\xi_2 = v^{-f} + v'^{-f} + v^{-2f} v'^f + v^f v'^{-2f}$$

$$\zeta_1 = 4vv' + 2v^{1+f}v'^{1-f} + 2v^{1-f}v'^{1+f}$$

$$\zeta_2 = 2v^{1+f}v'^{1-2f} + 2v^{1-2f}v'^{1+f} + 2v^{1-f}v' + 2vv'^{1-f}$$

Once the definition for  $k$ -th moment,  $m_k$ , shown in Eq. (4), is introduced, we can obtain the following expression for moment governing equation, where

$$\begin{cases} \frac{dm_0}{dt} = -\frac{B_2}{2}(\xi_1^* + \psi v_{p0}^{f-\frac{1}{3}}\xi_2^*) \\ \frac{dm_1}{dt} = 0 \\ \frac{dm_2}{dt} = -\frac{B_2}{2}(\zeta_1^* + \psi v_{p0}^{f-\frac{1}{3}}\zeta_2^*) \end{cases} \quad (7)$$

$$\xi_1^* = 2m_0m_0 + 2m_fm_{-f}$$

$$\xi_2^* = 2m_{-f}m_0 + 2m_fm_{-2f}$$

$$\zeta_1^* = 4m_1m_1 + 4m_{1+f}m_{1-f}$$

$$\zeta_2^* = 4m_{1-f}m_1 + 4m_{1+f}m_{1-2f}$$

It is obvious that Eq. (7) is not closed due to the appearance of some unexpected variables, such as  $m_{-f}$  and  $m_f$ . In the TEMOM, approximated functions are used to replace these unexpected variables, such as third-order Taylor series expansion function,

$$m_k = u_0^{k-2} \left( \frac{k^2 - k}{2} \right) m_2 + u_0^{k-1} (-k^2 + 2k) m_1 + u_0^k \left( \frac{2 + k^2 - 3k}{2} \right) m_0. \quad (8)$$

As the function shown in Eq. (8) is applied in Eq. (7), the final closed moment governing equation can be obtained where

$$\left\{ \begin{array}{l} \frac{dm_0}{dt} = -\frac{B_2}{2} (\eta_1 + \psi v_{p0} f^{-\frac{1}{3}} \eta_2) \\ \frac{dm_1}{dt} = 0 \\ \frac{dm_2}{dt} = -\frac{B_2}{2} (\eta_3 + \psi v_{p0} f^{-\frac{1}{3}} \eta_4) \end{array} \right. \quad (9)$$

$$\eta_1 = \frac{-m_0^2(-5f^2m_1^4 + f^4m_1^4 + 8m_1^4 + f^4m_2^2m_0^2 - 2f^4m_2m_1^2m_0 + 6f^2m_2m_1^2m_0 - f^2m_2^2m_0^2)}{4m_1^4}$$

$$\eta_2 = \frac{-m_0^{2+f}(\psi_4f^4 + \psi_3f^3 + \psi_2f^2 + \psi_1f^1 + \psi_0)}{2m_1^{4+f}}$$

$$\eta_3 = \frac{-5f^2m_1^4 + f^4m_1^4 + 8m_1^4 + f^4m_2^2m_0^2 - 2f^4m_2m_1^2m_0 + 6f^2m_2m_1^2m_0 - f^2m_2^2m_0^2}{2m_1^2}$$

$$\eta_4 = \frac{m_0^f(\psi_4f^4 - \psi_3f^3 + \psi_2f^2 - \psi_1f^1 + \psi_0)}{m_1^{2+f}}$$

$$\psi_4 = 2m_2^2m_0^2 + 2m_1^4 - 4m_2m_0m_1^2$$

$$\psi_3 = -m_2^2m_0^2 - m_1^4 + 2m_2m_0m_1^2$$

$$\psi_2 = -m_2^2m_0^2 - 7m_1^4 + 8m_2m_0m_1^2$$

$$\psi_1 = -2m_1^4 + 2m_2m_0m_1^2$$

$$\psi_0 = 4m_1^4$$

Equation (9) is a system of first-order ordinary differential equations, all the right terms are denoted by the first three moments  $m_0$ ,  $m_1$ , and  $m_2$ , and thus, this system can be automatically closed. It is clear in the derivation that no any physical assumption for the particle size distribution is introduced, making the TEMOM has more solid foundation in mathematics relative to the log MM.

The TEMOM was further developed to a much more general version, that is, generalized TEMOM. This newly developed version has some advantages as compared to old one. The new generalized TEMOM successfully overcomes the shortcomings of the old version whose

geometric standard deviation must be less than a certain value. In addition, the accuracy of numerical calculation for capturing fractional moments at an initial stage can be largely increased. In the generalized TEMOM, the closure function shown in Eq. (8) is changed, in which the moment sequence is composed not only by integer moments but also by fractional moments. Thus, higher-order Taylor series expansion can be achieved for the closure function, making it much more accurate function.

### 3.3. Log-normal method of moments

Unlike the TEMOM, the closure of moment governing equations in the log MM is achieved by assuming the PSD to log-normal size distributions. This method was first investigated by Cohen and Vaughan whose work covers both Brownian and gravitational coagulation [73]. This work forms the basis of the computer code HAARM and aerosol dynamics model MAD [74], and the latter finally became key part in some atmospheric forecast models, such as WRF/chem. Thanks to works from scientists, including Lee [44, 75], and Pratsinis [14], the log MM becomes one of several main methods of moments today, and especially, it has been applied in computational fluid dynamics software, Fluent.

Similar to the TEMOM, the log MM also requires to first obtain the moment equations as shown in Eq. (7). Then, the task is to use its own closure function to achieve the closure of moment equations. In this method, the closure function is obtained on basis of the log-normal size distribution assumption, which has the following expression, where

$$m_k = m_0 v_g^k \exp\left(\frac{9}{2} k^2 \ln^2 \sigma\right) \quad (10)$$

$$v_g = \frac{m_1^2}{m_0^{3/2} m_2^{1/2}}$$

$$\ln^2 \sigma = \frac{1}{9} \ln\left(\frac{m_0 m_2}{m_1^2}\right).$$

In theory, once the PBE was converted to forms such as Eq. (7), in which unresolved moments are involved, it can be further numerically solved together with Eq. (10).

### 3.4. Quadrature method of moments

The QMOM and its variants such as DQMOM are regarded as the mostly used method of moments in the implementation of the PBM [47, 48]. This method achieves great success in that it has no any physical assumptions and has no requirement for the form of dynamics kernels. Thus, this method can deal with all relevant aerosol dynamics problems. Unlike the

log MM, this method does not need to first convert the PBE to unresolved moment equations, which needs further closed by approximated closure functions, such as Eqs. (8) and (10). Therefore, this method can be regarded as the most ideal scheme for solving the PBE if the numerical efficiency is not considered. In this method, the closure problem of the PBE is solved with a quadrature approximation. However, the weights and abscissas of the quadrature approximation need to be additionally obtained by suitable mathematical techniques, such as the product-difference algorithm. This increases the computational cost in contrast to the log MM and TEMOM. In fact, the numerical efficiency is similar important to the accuracy for simulation; especially, the coupling between the PBM and the computational fluid dynamics is considered.

Same as discussed in Sections 3.3 and 3.4, coagulation in the continuum-slip regime is selected as an example to present how the QMOM is implemented. To implement the QMOM, Eq. (3) needs to be disposed using Gaussian quadrature approximation as below, where  $v_i$  is the  $i$ th quadrature point, and  $\omega_i$  is the corresponding weight in the quadrature formula. This method has insensitive form of kernel  $\beta(v_i, v_j)$ , and thus, extremely complicated kernel can be used. The method requires two times of quadrature point number to attain expected moments, for example, governing equations for moment  $m_0, m_1, \dots, m_5$  need to be simultaneously solved as  $N_Q = 3$ .

$$\frac{dm_k}{dt} = \frac{1}{2} \sum_{i=1}^{N_Q} \sum_{j=1}^{N_Q} \left[ (v_i + v_j)^k - v_i^k - v_j^k \right] \beta(v_i, v_j) \omega_i \omega_j \quad (11)$$

To implement the QMOM, the quadrature abscissas and weights are obtained from lower-order radial moment sequence by solving Eq. (11). During the implementation, the key task is to construct a symmetric tridiagonal matrix whose diagonal elements and off-diagonal elements are derived from the calculated moments. The symmetric tridiagonal matrix is diagonalized to obtain the abscissas and weights. It needs to note here that the number of abscissas and weights are dependent on  $N_Q$ . More details about the implementation of the QMOM are recommended to see the original work of this method.

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## References

- [1] S. K. Friedlander, *Smoke, dust and haze: fundamentals of aerosol behavior*, 2nd ed. John Wiley & Sons, Inc., New Jersey, 2000.
- [2] B. Buesser and S. E. Pratsinis, Design of nanomaterial synthesis by aerosol processes, *Annu. Rev. Chem. Biomol. Eng.*, vol. 3, pp. 103–127, 2012.
- [3] M. Yu, J. Lin, and T. Chan, Effect of precursor loading on non-spherical TiO<sub>2</sub> nanoparticle synthesis in a diffusion flame reactor, *Chem. Eng. Sci.*, vol. 63, no. 9, pp. 2317–2329, 2008.
- [4] M. Kulmala, Atmospheric science. How particles nucleate and grow, *Science*, vol. 302, no. 5647, pp. 1000–1001, 2003.
- [5] K. Savolainen, L. Pylkkänen, H. Norppa, G. Falck, H. Lindberg, T. Tuomi, M. Vippola, H. Alenius, K. Hämeri, J. Koivisto, D. Brouwer, D. Mark, D. Bard, M. Berges, E. Jankowska, M. Posniak, P. Farmer, R. Singh, F. Krombach, P. Bihari, G. Kasper, and M. Seipenbusch, Nanotechnologies, engineered nanomaterials and occupational health and safety – a review, *Saf. Sci.*, vol. 48, no. 8, pp. 957–963, 2010.
- [6] A. Joonas Koivisto, M. Yu, K. Hämeri, and M. Seipenbusch, Size resolved particle emission rates from an evolving indoor aerosol system, *J. Aerosol Sci.*, vol. 47, pp. 58–69, 2012.
- [7] M. Yu, A. J. Koivisto, K. Hämeri, and M. Seipenbusch, Size dependence of the ratio of aerosol coagulation to deposition rates for indoor aerosols, *Aerosol Sci. Technol.*, vol. 47, no. 4, pp. 427–434, 2013.
- [8] S. K. Friedlander and D. Y. Pui, Emerging issues in nanoparticle aerosol science and technology experimental methods and instrumentation, *J. Nanoparticle Res.*, no. 4, pp. 313–320, 2004.
- [9] P. Kumar, B. R. Gurjar, A. S. Nagpure, and R. M. Harrison, Preliminary estimates of nanoparticle number emissions from road vehicles in megacity Delhi and associated health impacts, *Environ. Sci. Technol.*, vol. 45, no. 13, pp. 5514–5521, 2011.
- [10] J. Kirkby, J. Duplissy, K. Sengupta, C. Frege, H. Gordon, C. Williamson, M. Heinritzi, M. Simon, C. Yan, J. Almeida, J. Tröstl, T. Nieminen, I. K. Ortega, R. Wagner, A. Adamov, A. Amorim, A. K. Bernhammer, F. Bianchi, M. Breitenlechner, S. Brilke, X. Chen, J. Craven, A. Dias, S. Ehrhart, R. C. Flagan, A. Franchin, C. Fuchs, R. Guida, J. Hakala, C. R. Hoyle, T. Jokinen, H. Junninen, J. Kangasluoma, J. Kim, M. Krapf, A. Kürten, A. Laaksonen, K. Lehtipalo, V. Makhmutov, S. Mathot, U. Molteni, A. Onnela, O. Peräkylä, F. Piel, T. Petäjä, A. P. Praplan, K. Pringle, A. Rap, N. A. D. Richards, I. Riipinen, M. P. Rissanen, L. Rondo, N. Sarnela, S. Schobesberger, C. E. Scott, J. H. Seinfeld, M. Sipilä, G. Steiner, Y. Stozhkov, F. Stratmann, A. Tomé, A. Virtanen, A. L. Vogel, A. C. Wagner, P. E. Wagner, E. Weingartner, D. Wimmer, P. M. Winkler, P. Ye, X. Zhang, A. Hansel, J.

Dommen, N. M. Donahue, D. R. Worsnop, U. Baltensperger, M. Kulmala, K. S. Carslaw, and J. Curtius, Ion-induced nucleation of pure biogenic particles, *Nature*, vol. 533, no. 7604, pp. 521–526, 2016.

- [11] M. Yu and J. Lin, Nanoparticle-laden flows via moment method: a review, *Int. J. Multiph. Flow*, vol. 36, no. 2, pp. 144–151, 2010.
- [12] M. von Smoluchowski, Versuch einer mathematischen Theorie der Koagulationskinetik kolloider Lösungen, *Z. Phys. Chem.*, vol. 92, no. 2, pp. 129–168, 1917.
- [13] D. Ramkrishna and M. R. Singh, Population balance modeling: current status and future prospects, *Annu. Rev. Chem. Biomol. Eng.*, vol. 5, pp. 123–146, 2014.
- [14] S. Pratsinis, Simultaneous nucleation, condensation, and coagulation in aerosol reactors, *J. Colloid Interface Sci.*, vol. 124, no. 2, pp. 416–427, 1988.
- [15] F. O. Ernst and S. E. Pratsinis, Self-preservation and gelation during turbulence-induced coagulation, *J. Aerosol Sci.*, vol. 37, no. 2, pp. 123–142, 2006.
- [16] S. Vemury and S. E. Pratsinis, Self-preserving size distributions of agglomerates, *J. Aerosol Sci.*, vol. 26, no. 2, pp. 175–185, 1995.
- [17] E. Goudele, M. L. Eggersdorfer, and S. E. Pratsinis, Coagulation–agglomeration of fractal-like particles: structure and self-preserving size distribution, *Langmuir*, vol. 31, no. 4, pp. 1320–1327, 2015.
- [18] Z. Varga, G. Wang, and J. Swan, The hydrodynamics of colloidal gelation, *Soft Matter*, vol. 11, pp. 9009–9019, 2015.
- [19] M. L. Xie, Asymptotic solution of moment approximation of the particle population balance equation for Brownian agglomeration, *Aerosol Sci. Technol.*, vol. 49, no. 2, pp. 109–114, 2015.
- [20] Z. Chen, J. Lin, and M. Yu, Asymptotic behavior of the Taylor-expansion method of moments for solving a coagulation equation for Brownian particles, *Particuology*, vol. 14, pp. 124–129, 2014.
- [21] S. Park and K. Lee, Asymptotic particle size distributions attained during coagulation processes, *J. Colloid Interface Sci.*, vol. 233, no. 1, pp. 117–123, 2001.
- [22] H. M. Hulburt and S. Katz, Some problems in particle technology: a statistical mechanical formulation, *Chem. Eng. Sci.*, vol. 19, no. 8, pp. 555–574, 1964.
- [23] M. Frenklach, Method of moments with interpolative closure, *Chem. Eng. Sci.*, vol. 57, no. 12, pp. 2229–2239, 2002.
- [24] H. Liu, M. Yu, Z. Yin, Y. Jiang, and M. Chen, Study on the evolution of nanoparticle size distribution due to continuous injection using the sectional method, *Int. J. Numer. Methods Heat Fluid Flow*, vol. 24, no. 8, pp. 1803–1812, 2014.

- [25] M. M. Attarakih, C. Drumm, and H. J. Bart, Solution of the population balance equation using the sectional quadrature method of moments (SQMOM), *Chem. Eng. Sci.*, vol. 64, no. 4, pp. 742–752, 2009.
- [26] M. C. Bruns and O. A. Ezekoye, Development of a hybrid sectional quadrature-based moment method for solving population balance equations, *J. Aerosol Sci.*, vol. 54, pp. 88–102, 2012.
- [27] S. H. Park, A moving sectional model for the formation and growth of soot particles, pp. 1–13, 2003.
- [28] J. D. Landgrebe and S. E. Pratsinis, A discrete-sectional model for particulate production by gas-phase chemical reaction and aerosol coagulation in the free-molecular regime, *J. Colloid Interface Sci.*, vol. 139, no. 1, pp. 63–86, 1990.
- [29] M. Kostoglou, Extended cell average technique for the solution of coagulation equation, *J. Colloid Interface Sci.*, vol. 306, no. 1, pp. 72–81, 2007.
- [30] F. Gelbard, Y. Tambour, and J. H. Seinfeld, Sectional representations for simulating aerosol dynamics, *J. Colloid Interface Sci.*, vol. 76, no. 2, pp. 541–556, 1980.
- [31] K. Sabelfeld, Stochastic models for coagulation of aerosol particles in intermittent turbulent flows, *Math. Comput. Simul.*, vol. 47, nos. 2–5, pp. 85–101, 1998.
- [32] F. E. Kruis, J. Wei, T. van der Zwaag, and S. Haep, Computational fluid dynamics based stochastic aerosol modeling: combination of a cell-based weighted random walk method and a constant-number Monte-Carlo method for aerosol dynamics, *Chem. Eng. Sci.*, vol. 70, pp. 109–120, 2012.
- [33] E. Debry, B. Sportisse, and B. Jourdain, A stochastic approach for the numerical simulation of the general dynamics equation for aerosols, *J. Comput. Phys.*, vol. 184, no. 2, pp. 649–669, 2003.
- [34] W. J. Menz, J. Akroyd, and M. Kraft, Stochastic solution of population balance equations for reactor networks, *J. Comput. Phys.*, vol. 256, pp. 615–629, 2014.
- [35] S. L. Rani, R. Dhariwal, and D. L. Koch, A stochastic model for the relative motion of high Stokes number particles in isotropic turbulence, *J. Fluid Mech.*, vol. 756, pp. 870–902, 2014.
- [36] M. Kraft, Modelling of particulate processes, *Kona*, vol. 23, no. 23, pp. 18–35, 2005.
- [37] N. Morgan, C. Wells, M. Goodson, M. Kraft, and W. Wagner, A new numerical approach for the simulation of the growth of inorganic nanoparticles, *J. Comput. Phys.*, vol. 211, no. 2, pp. 638–658, 2006.
- [38] J. Wei and F. E. Kruis, GPU-accelerated Monte Carlo simulation of particle coagulation based on the inverse method, *J. Comput. Phys.*, vol. 249, pp. 67–79, 2013.

- [39] S. Khalili, Y. Lin, A. Armaou, and T. Matsoukas, Constant number Monte Carlo simulation of population balances with multiple growth mechanisms, *AIChE J.*, vol. 56, no. 12, pp. 3137–3145, 2010.
- [40] H. Zhao and C. Zheng, A population balance-Monte Carlo method for particle coagulation in spatially inhomogeneous systems, *Comput. Fluids*, vol. 71, pp. 196–207, 2013.
- [41] A. Vikhansky and M. Kraft, A Monte Carlo methods for identification and sensitivity analysis of coagulation processes, *J. Comput. Phys.*, vol. 200, no. 1, pp. 50–59, 2004.
- [42] X. Hao, H. Zhao, Z. Xu, and C. Zheng, Population balance-Monte Carlo simulation for gas-to-particle synthesis of nanoparticles, *Aerosol Sci. Technol.*, vol. 47, no. 10, pp. 1125–1133, 2013.
- [43] M. Yu, J. Lin, and T. Chan, A new moment method for solving the coagulation equation for particles in Brownian motion, *Aerosol Sci. Technol.*, vol. 42, no. 9, pp. 705–713, 2008.
- [44] K. W. Lee, H. Chen, and J. A. Gieseke, Log-normally preserving size distribution for Brownian coagulation in the free-molecule regime, *Aerosol Sci. Technol.*, vol. 3, no. 1, pp. 53–62, 1984.
- [45] S. E. Pratsinis, Simultaneous nucleation, condensation, and coagulation in aerosol reactors, *J. Colloid Interface Sci.*, vol. 124, no. 2, pp. 416–427, 1988.
- [46] M. M. Williams, On the modified gamma distribution for representing the size spectra of coagulating aerosol particles, *J. Colloid Interface Sci.*, vol. 103, no. 2, pp. 516–527, 1985.
- [47] R. McGraw, Description of aerosol dynamics by the quadrature method of moments, *Aerosol Sci. Technol.*, vol. 27, no. 2, pp. 255–265, 1997.
- [48] D. L. Marchisio and R. O. Fox, Solution of population balance equations using the direct quadrature method of moments, *J. Aerosol Sci.*, vol. 36, no. 1, pp. 43–73, 2005.
- [49] J. C. Barrett and J. S. Jheeta, Improving the accuracy of the moments method for solving the aerosol general dynamic equation, *J. Aerosol Sci.*, vol. 27, no. 8, pp. 1135–1142, 1996.
- [50] M. L. Xie, Asymptotic behavior of TEMOM model for particle population balance equation over the entire particle size regimes, *J. Aerosol Sci.*, vol. 67, pp. 157–165, 2014.
- [51] H. Müller, Zur allgemeinen Theorie der raschen Koagulation, *Fortschrittsberichte über Kolloide und Polym.*, vol. 27, no. 6, pp. 223–250, 1928.
- [52] V. Raman and R. O. Fox, Modeling of fine-particle formation in turbulent flames, *Annu. Rev. Fluid Mech.*, vol. 48, no. 1, pp. 159–190, 2016.
- [53] U. Vogel, K. Savolainen, Q. Wu, M. van Tongeren, D. Brouwer, and M. Berges, *Handbook of Nanosafety: Measurement, Exposure and Toxicology*. Elsevier, Amsterdam, 2014.
- [54] S. Park, R. Xiang, and K. Lee, Brownian coagulation of fractal agglomerates: analytical solution using the log-normal size distribution assumption, *J. Colloid Interface Sci.*, vol. 231, no. 1, pp. 129–135, 2000.

- [55] E. Otto, H. Fissan, S. Park, and K. Lee, Log-normal size distribution theory of Brownian aerosol coagulation for the entire particle size range: part II—analytical solution using Dahneke's coagulation kernel, *J. Aerosol Sci.*, vol. 30, no. 1, pp. 17–34, 1999.
- [56] M. Yu, J. Lin, J. Cao, and M. Seipenbusch, An analytical solution for the population balance equation using a moment method, *Particuology*, vol. 18, pp. 194–200, 2015.
- [57] M. Yu, X. Zhang, G. Jin, J. Lin, and M. Seipenbusch, A new analytical solution for solving the population balance equation in the continuum-slip regime, *J. Aerosol Sci.*, vol. 80, pp. 1–10, 2015.
- [58] M. Seipenbusch, A. Binder, and G. Kasper, Temporal evolution of nanoparticle aerosols in workplace exposure, *Ann. Occup. Hyg.*, vol. 52, no. 8, pp. 707–16, 2008.
- [59] L. G. M. de Souza, G. Janiga, V. John, and D. Thévenin, Reconstruction of a distribution from a finite number of moments with an adaptive spline-based algorithm, *Chem. Eng. Sci.*, vol. 65, no. 9, pp. 2741–2750, 2010.
- [60] M. Yu, Y. Liu, J. Lin, and M. Seipenbusch, Generalized TEMOM scheme for solving the population balance equation, *Aerosol Sci. Technol.*, vol. 49, no. 11, pp. 1021–1036, 2015.
- [61] J. Chun and D. L. Koch, Coagulation of monodisperse aerosol particles by isotropic turbulence, *Phys. Fluids*, vol. 17, no. 2, pp. 027–102, 2005.
- [62] R. R. Upadhyay and O. A. Ezekoye, Treatment of size-dependent aerosol transport processes using quadrature based moment methods, *J. Aerosol Sci.*, vol. 37, no. 7, pp. 799–819, 2006.
- [63] M. M. Maricq, Coagulation dynamics of fractal-like soot aggregates, *J. Aerosol Sci.*, vol. 38, no. 2, pp. 141–156, 2007.
- [64] M. Yu and J. Lin, Taylor-expansion moment method for agglomerate coagulation due to Brownian motion in the entire size regime, *J. Aerosol Sci.*, vol. 40, no. 6, pp. 549–562, 2009.
- [65] M. Yu and J. Lin, Solution of the agglomerate Brownian coagulation using Taylor-expansion moment method, *J. Colloid Interface Sci.*, vol. 336, no. 1, pp. 142–149, 2009.
- [66] M. M. R. Williams, Some topics in nuclear aerosol dynamics, *Prog. Nucl. Energy*, vol. 17, no. 1, pp. 01–52, 1986.
- [67] Z. Chen, J. Lin, and M. Yu, A direct expansion method of moments for Brownian coagulation, *Phys. Scr.*, vol. 89, no. 12, pp. 125204, 2014.
- [68] M. Yu, Y. Liu, G. Jin, and H. Jin, A new analytical solution for agglomerate growth undergoing Brownian coagulation, *Appl. Math. Model.*, vol. 40, pp. 5497–5509, 2016.
- [69] M. Xie and Q. He, Analytical solution of TEMOM model for particle population balance equation due to Brownian coagulation, *J. Aerosol Sci.*, vol. 66, pp. 24–30, 2013.

- [70] M. L. Xie, Asymptotic behavior of TEMOM model for particle population balance equation over the entire particle size regimes, *J. Aerosol Sci.*, vol. 67, pp. 157–165, 2014.
- [71] M. Yu and J. Lin, Binary homogeneous nucleation and growth of water–sulfuric acid nanoparticles using a TEMOM model, *Int. J. Heat Mass Transf.*, vol. 53, no. 4, pp. 635–644, 2010.
- [72] M. Yu, J. Lin, and T. Chan, Numerical simulation for nucleated vehicle exhaust particulate matters via the TEMOM/LES method, *Int. J. Mod. Phys. C*, vol. 20, no. 3, pp. 399–421, 2009.
- [73] E. R. Cohen and E. U. Vaughan, Approximate solution of the equations for aerosol agglomeration, *J. Colloid Interface Sci.*, vol. 35, no. 4, pp. 612–623, 1971.
- [74] E. R. Whitby and P. H. McMurry, Modal aerosol dynamics modeling, *Aerosol Sci. Technol.*, vol. 27, no. 6, pp. 673–688, 1997.
- [75] K. Lee, Y. Lee, and D. Han, The log-normal size distribution theory for Brownian coagulation in the low Knudsen number regime, *J. Colloid Interface Sci.*, vol. 492, no. 188, pp. 486–492, 1997.

