



An analytical solution for the population balance equation using a moment method



Mingzhou Yu^{a,b}, Jianzhong Lin^{a,*}, Junji Cao^b, Martin Seipenbusch^c

^a Department of Physics, China Jiliang University, Hangzhou 310028, China

^b Institute of Earth Environment, Chinese Academy of Sciences, Xi'an 710075, China

^c Institute for Mechanical Processes Engineering and Mechanics, Karlsruhe Institute of Technology, Germany

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ABSTRACT

Brownian coagulation is the most important inter-particle mechanism affecting the size distribution of aerosols. Analytical solutions to the governing population balance equation (PBE) remain a challenging issue. In this work, we develop an analytical model to solve the PBE under Brownian coagulation based on the Taylor-expansion method of moments. The proposed model has a clear advantage over conventional asymptotic models in both precision and efficiency. We first analyze the geometric standard deviation (GSD) of aerosol size distribution. The new model is then implemented to determine two analytic solutions, one with a varying GSD and the other with a constant GSD. The varying solution traces the evolution of the size distribution, whereas the constant case admits a decoupled solution for the zero and second moments. Both solutions are confirmed to have the same precision as the highly reliable numerical model, implemented by the fourth-order Runge–Kutta algorithm, and the analytic model requires significantly less computational time than the numerical approach. Our results suggest that the proposed model has great potential to replace the existing numerical model, and is thus recommended for the study of physical aerosol characteristics, especially for rapid predictions of haze formation and evolution.

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Introduction

The population balance equation (PBE) has become a fundamental equation in the study on aerosol dynamical processes (Friedlander, 2000). In mathematics, the PBE is a strong non-linear equation with the same mathematical structure as Boltzmann's transport equation. Thus, an exact analytical solution cannot be achieved. Because of the relative simplicity of implementation and low computational cost, the method of moments has been extensively used to solve the PBE, especially when coupling the PBE to the computational fluid dynamics (Buesser & Pratsinis, 2012; Fox, 2012; Murfield & Garrick, 2013; Yu & Lin, 2010a). Unfortunately, in almost all cases, the method of moments must be executed as an iterative numerical calculation, which inevitably becomes computationally expensive. Although some studies have solved the PBE analytically, they assume that the aerosol size follows a log-normal

distribution, which limits the applicability of these analytical models (Park & Lee, 2002).

The Taylor-expansion method of moments (TEMOM) was first proposed to solve the PBE under Brownian coagulation (Yu, Lin, & Chan, 2008). This method has received considerable attention from aerosol scientists, and is advantageous for resolving multiple dynamical processes, such as coagulation, condensation, and nucleation (Goo, 2012; Yu & Lin, 2010a). In particular, the method possesses the novel feature that it does not require any assumptions about the aerosol size distribution. To date, the asymptotic behavior of the TEMOM has been analyzed mathematically (Chen, Lin, & Yu, 2014a; Lin & Chen, 2013; Xie, 2014), and a variant version has been developed (Chen, Lin, & Yu, 2014b). The efficiency and precision of TEMOM over the entire size regime has been verified by comparing its output with those from the generally acknowledged methods of moments as well as the sectional method (Yu & Lin, 2009a,b). However, similar to other successful methods of moments, such as the quadrature method of moments (QMOM) and direct QMOM (DQMOM) (Marchisio, Pikiurna, Fox, Vigil, & Barresi, 2003; McGraw, 1997), the ordinary differential equation (ODE) of the TEMOM has to be solved by an iterative numerical calculation

* Corresponding author.

E-mail addresses: mecjlin@zju.edu.cn, yumz@ieeas.acn (J. Lin).

Nomenclature

r	particle radius, m
n	particle number concentration density, m^{-3}
B_2	collision coefficient for the continuum-slip regime
C	Cunningham correction factor
k_b	Boltzmann constant, J/K
Kn	particle Knudsen number
m_k	k th moment of particle size distribution
g	$= m_0 m_2 / m_1^2$
M_k	dimensionless k th moment
t	time, s
T	temperature, K
u	the point of Taylor-series expansion (m_1/m_0)
v	particle volume, m^3
v_g	geometric mean particle volume, m^3
N_0	total particle number concentration, m^{-3}

Greek letters

ν	kinematic viscosity, m^2/s
β	particle collision kernel
μ	gas viscosity $\text{kg}/(\text{m s})$
λ	mean free path of the gas, m
σ_g	geometric standard deviation of particle size distribution
τ	dimensionless coagulation time: tN_0B_2 in the continuum regime; $tNB_1(v_{g0})^{1/6}$ in the free molecular regime

Acronyms

PBE	population balance equation
TEMOM	Taylor-expansion method of moments
QMOM	quadrature method of moments
DQMOM	direct quadrature method of moments
ODE	ordinary differential equation
GSD	geometric standard deviation
NM	numerical method
AM	analytical method
AMV	analytical method with a varying g
AMC	analytical method with the constant g
SPSD	self-preserving size distribution

(Yu et al., 2008). This inevitably increases the computational cost, especially when coupled with the flow field calculation used in many engineering particulate models and global aerosol models (Lu & Bowman, 2010; Seinfeld & Pandis, 2012; Yu & Lin, 2010b). Thus, an analytical solution to the TEMOM ODEs becomes necessary.

It is generally acknowledged that the TEMOM is preferable to other methods of moments because of its simple mathematical form (Yu et al., 2008). Besides the first three moments (m_0 , m_1 , and m_2), there is only one explicit variable, i.e., $g = m_0 m_2 / m_1^2$. This variable is commonly used as an index to represent the polydispersity of aerosol size distribution, and possesses the property that it only varies over a very limited range, as shown in Fig. 1. In particular, in the free molecular regime and the continuum regime, where the geometric standard deviation (GSD) of the size distribution can be represented by $\ln^2 \sigma_g = (1/9)\ln g$, the variable g has been shown to be constant. Thus, it is reasonable to treat g as a constant. Consequently, it is possible to find an analytical solution for the TEMOM ODEs. Unfortunately, this analytical solution has not yet been calculated.

The aim of this study is to obtain analytical solutions of the PBE involving the Brownian coagulation mechanism. In our derivation,

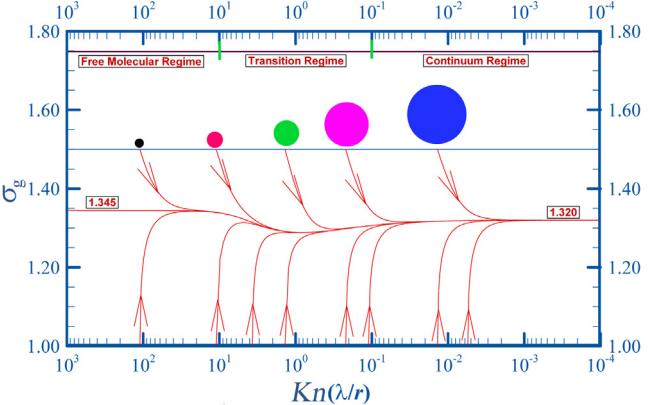


Fig. 1. Variation of geometric standard deviation σ_g with Knudsen number Kn . λ is the free molecular path (68.41 in this study) and r is the geometric mean radius of an aerosol particle. Aerosols with different initial size distributions (certain value for (σ_g, Kn)) converge finally to the self-preserving status with a definite σ_g , which is represented by $\ln^2 \sigma_g = (1/9)\ln g$.

the PBE is first converted to the moment ODEs using TEMOM, and then resolved by separating the variables. To distinguish the analytical method from the numerical method, the solution for the TEMOM ODEs using the fourth-order Runge–Kutta algorithm is called the numerical model (NM), and the solution using separation of variables is called the analytical model (AM). A brief description of the model is given in Background section, including the theory relevant to the new model and its detailed derivation. The computational parameters used in the calculation are presented in Computations section. In Results and discussion section, we verify the performance of the new model for aerosols at self-preserving size distributions, and discuss the scope of its application.

Background

The theory relevant to the method of moments, as well as a detailed derivation of TEMOM, was presented in our previous work (Yu et al., 2008). Thus, only a brief description of TEMOM is given here. The integro-differential PBE was first proposed by Müller (1928), and has the following form:

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

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' . The TEMOM ODEs have different forms in the free molecular regime and the continuum regime with respect to the coagulation kernel. Therefore, the analytical solution must be treated differently in each regime.

(1) Free molecular regime ($Kn > 100$)

The collision kernel in the free molecular regime was derived from gas kinetic theory, and is expressed as:

$$\beta(v, v') = B_1 \left(\frac{1}{v} + \frac{1}{v'} \right)^{1/2} (v^{1/3} + v'^{1/3})^2, \quad (2)$$

where $B_1 = (3/4\pi)^{1/6} (6k_B T / \rho)^{1/2}$, k_B is the Boltzmann constant, T is the gas temperature, and ρ is the mass density of the particles. The TEMOM is introduced to solve Eq. (1) with a closure model for the

kth moment:

$$\begin{aligned} m_k &= \left(\frac{u^{k-2}k^2}{2} - \frac{u^{k-2}k}{2} \right) m_2 + (-u^{k-1}k^2 + 2u^{k-1}k)m_1 \\ &\quad + \left(u^k + \frac{u^kk^2}{2} - \frac{3u^kk}{2} \right) m_0, \end{aligned} \quad (3)$$

where u is the Taylor expansion point. In this work, u is defined as m_1/m_0 . The TEMOM ODEs take the following form:

$$\begin{cases} \left(\frac{dm_0}{dt} \right)_f = \frac{\sqrt{2B_1}(65g^2 - 1210g - 9223)}{5184} m_1(t)^{1/6} m_0(t)^{11/6} \\ \left(\frac{dm_1}{dt} \right)_f = 0 \\ \left(\frac{dm_2}{dt} \right)_f = \frac{\sqrt{2B_1}(701g^2 - 4210g - 6859)}{2592} g^{1/6} m_1(t)^{11/6} m_2(t)^{1/6} \end{cases}, \quad (4)$$

where $g = m_0 m_2 / m_1$. It is necessary to use the same characteristic variables to normalize the quantities appearing in Eq. (4). The initial particle size distribution is generally considered to follow a log-normal distribution. In this case, the k th moment is represented by $m_k = M_k m_{k0}$, with $m_{k0} = Nv_{go}^k$, N and v_{go} are the total particle number concentration and the geometric mean size of the initial aerosol, respectively. Then, Eq. (4) becomes:

$$\begin{cases} \left(\frac{dM_0}{d\tau_1} \right)_f = \frac{\sqrt{2}(65g^2 - 1210g - 9223)}{5184} M_1(\tau_1)^{1/6} M_0(\tau_1)^{11/6} \\ \left(\frac{dM_1}{d\tau_1} \right)_f = 0 \\ \left(\frac{dM_2}{d\tau_1} \right)_f = \frac{\sqrt{2}(701g^2 - 4210g - 6859)}{2592} g^{-1/6} M_1(\tau_1)^{11/6} M_2(\tau_1)^{1/6} \end{cases} \quad (5)$$

where $\tau_1 = tNB_1(v_{go})^{1/6}$. The theory of self-preserving size distribution (SPSD) indicates that self-preserving characteristics occur in almost all aerosol systems (Friedlander, 2000). Thus, by employing SPSD theory in this case, the variable g can be represented as $\ln^2 \sigma_g = (1/9)\ln g$, where σ_g is a constant of the self-preserving system.

For an aerosol in which Brownian coagulation is the only process, the first moment $M_1(\tau_1)$ is a constant. Thus, Eq. (5) can be solved analytically using the method of separation of variables:

$$\begin{cases} (M_0(\tau_1))_f = \left(-\frac{5}{6}a_f \tau_1 + M_{00}^{-5/6} \right)^{6/5} \\ (M_1(\tau_1))_f = M_{10} \\ (M_2(\tau_1))_f = \left(\frac{5}{6}b_f \tau_1 + M_{20}^{5/6} \right)^{6/5} \end{cases} \quad (6)$$

where $a_f = (\sqrt{2}(65g^2 - 1210g - 9223)/5184)M_{10}^{1/6}$ and $b_f = -((\sqrt{2}(701g^2 - 4210g - 6859))/2592)/g^{-1/6}M_{10}^{11/6}$.

In the dynamical process of Brownian coagulation, the zero moment M_0 must decrease with time while the second moment M_2 must increase with time. Thereby, the derivative of the zero moment with respect to time will be negative, and the derivative of the second moment positive. Therefore, the following criterion must be satisfied:

$$\begin{cases} 65g^2 - 1210g - 9223 < 0 \\ 701g^2 - 4210g - 6859 < 0 \end{cases}. \quad (7)$$

The solution to Eq. (7) is $g \in (0, (2105 + 36\sqrt{7129})/701)$. Correspondingly, the valid range for the GSD is $\sigma_g \in (1.000, 1.601)$, as we know that $\ln^2 \sigma_g = (1/9)\ln g$. In the free molecular regime, the GSD of an aerosol with SPSD is 1.345 (Lee, Chen, & Gieseke, 1984), which is within the valid range of the GSD.

(2) Continuum regime ($Kn < 1$)

In the continuum regime, the coagulation kernel was derived from Fick's law of diffusion:

$$\beta(v, v') = B_2 \left(\frac{1}{v^{1/3}} + \frac{1}{v'^{1/3}} \right)^{1/2} (v^{1/3} + v'^{1/3})^2, \quad (8)$$

where $B_2 = 2k_B T / 3\mu$, and μ is the gas viscosity. In this regime, the TEMOM ODEs have the following form:

$$\begin{cases} \left(\frac{dm_0(t)}{dt} \right)_c = \frac{B_2(2g^2 - 13g - 151)}{81} m_0(t)^2 \\ \left(\frac{dm_1(t)}{dt} \right)_c = 0 \\ \left(\frac{dm_2(t)}{dt} \right)_c = \frac{2B_2(2g^2 - 13g - 151)}{2592} m_1(t)^2 \end{cases}. \quad (9)$$

Using the same procedure as in the free molecular regime, the non-dimensional form of Eq. (9) is:

$$\begin{cases} \left(\frac{dM_0(\tau_2)}{d\tau_2} \right)_c = \frac{(2g^2 - 13g - 151)}{81} M_0(\tau_2)^2 \\ \left(\frac{dM_1(\tau_2)}{d\tau_2} \right)_c = 0 \\ \left(\frac{dM_2(\tau_2)}{d\tau_2} \right)_c = \frac{2(2g^2 - 13g - 151)}{81} M_1(\tau_2)^2 \end{cases} \quad (10)$$

where $\tau_2 = NB_2 t$. Similarly, an analytical solution of Eq. (10) can be obtained by separating the variables, where g is regarded as a constant:

$$\begin{cases} (M_0(\tau_2))_c = \frac{1}{-a_c \tau_2 + (1/M_{00})} \\ (M_1(\tau_2))_c = M_{10} \\ (M_2(\tau_2))_c = b_c \tau_2 + M_{20} \end{cases} \quad (11)$$

with $a_c = (2g^2 - 13g - 151)/81$ and $b_c = -[2(2g^2 - 13g - 151)/81]M_{10}^2$. Using the same mathematical analysis as for the free molecular regime, the valid range of GSD in the continuum regime is confirmed to be $\sigma_g \in (1.000, 1.699)$. The GSD of an SPSD aerosol in the continuum regime is known to be 1.320 (Lee et al., 1984), which is within the valid range of the GSD.

Note that this derivation of the analytical model, both in the free molecular regime and in the continuum regime, is actually straightforward, and does not involve any asymptotic analysis. Thus, the model has the potential to overcome the limitation of asymptotic models, which are only valid at infinitely large times (Chen et al., 2014a; Xie, 2014).

Computations

Numerical computations were performed on an Intel (R) Core i7-3573U CPU 2.5 GHz computer with 4 GB RAM. The fourth-order Runge-Kutta method was employed with a fixed dimensionless time step of 0.001 to solve the ODEs for the NM. In all calculations, the total time was allowed to run to 100. The programs were written in C and compiled using Microsoft Visual Studio 2008. The relative error with respect to the reference numerical variables was calculated as:

$$\text{Error \%} = \frac{\phi - \phi_{NM}}{\phi_{NM}} \times 100\%, \quad (12)$$

where ϕ is an arbitrary variable and ϕ_{NM} is the reference numerical variable. In the present study, the criterion used to assess whether the analytical method solves the PBE with acceptable precision is

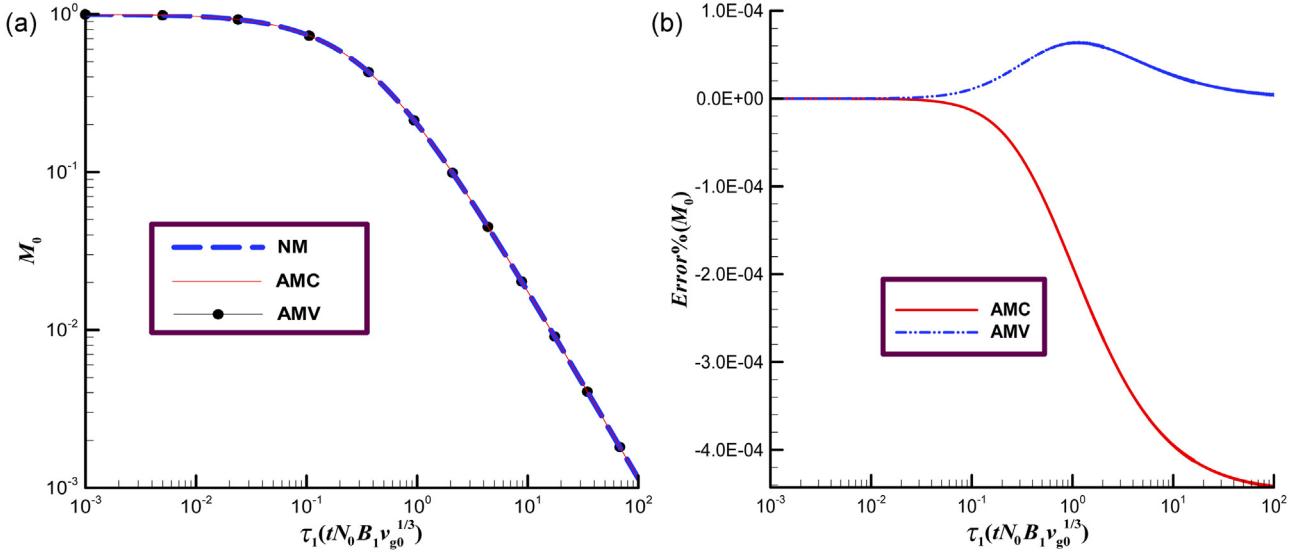


Fig. 2. (a) Variations of M_0 with time in the free molecular regime obtained from NM, AMV, and AMC; (b) relative errors of AMC and AMV with respect to NM.

that the absolute value of Error% must be less than 0.001. In the calculation, the initial dimensionless moments are set as:

$$\begin{cases} M_{00} = 1 \\ M_{10} = \chi \\ M_{20} = \chi^4 \end{cases} \quad (13)$$

where $\chi = e^{(3 \ln \sigma_{g0})^2/2}$, and σ_{g0} is the initial aerosol GSD.

Results and discussion

Free molecular regime

In the free molecular regime, the GSD is constant as the aerosol has SPSD (Lee et al., 1984). In the present study, the value of GSD under this SPSD status is 1.345, which is the value verified by TEMOM, QMOM and log-normal method of moments (Lee, Lee, &

Han, 1997; Yu et al., 2008). Fig. 2(a) shows a comparison of the total particle number concentrations given by NM and AM. The analytical model gives two different specific solutions, i.e., one with the constant GSD (AMC) and another one with a varying GSD (AMV). AMV is actually a finite analytical solution. The GSD is fixed to 1.345 in the AMC; thus, the solutions for M_0 and M_2 are decoupled. In the AMV, the variable g is updated at the end of each iterative calculation. Hence, the solutions for M_0 and M_2 must be coupled (Lee et al., 1997, 1984). Updates of the variable g in the AMV are performed according to the following algorithm procedure:

- (i) Initialize $M_0(0)$, $M_1(0)$, and $M_2(0)$ using Eq. (13).
- (ii) Determine $g(\tau_1)$ at time τ_1 using $g(\tau_1) = (M_0(\tau_1 - \Delta t)M_2(\tau_1 - \Delta t))/M_1(\tau_1 - \Delta t)^2$, where $M_0(\tau_1 - \Delta t)$, $M_1(\tau_1 - \Delta t)$, and $M_2(\tau_1 - \Delta t)$ are the first three moments from the previous time step.
- (iii) Update the first three moments as follows:

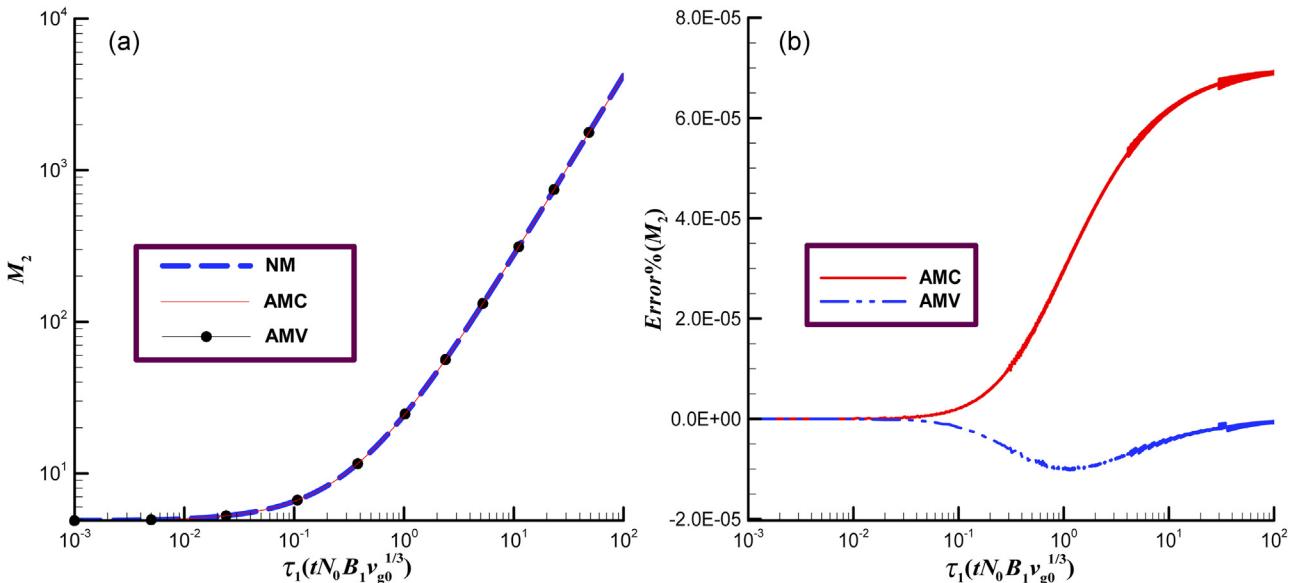


Fig. 3. (a) Variations of M_2 with time in the free molecular regime obtained from NM, AMV, and AMC; (b) relative errors of AMC and AMV with respect to NM.

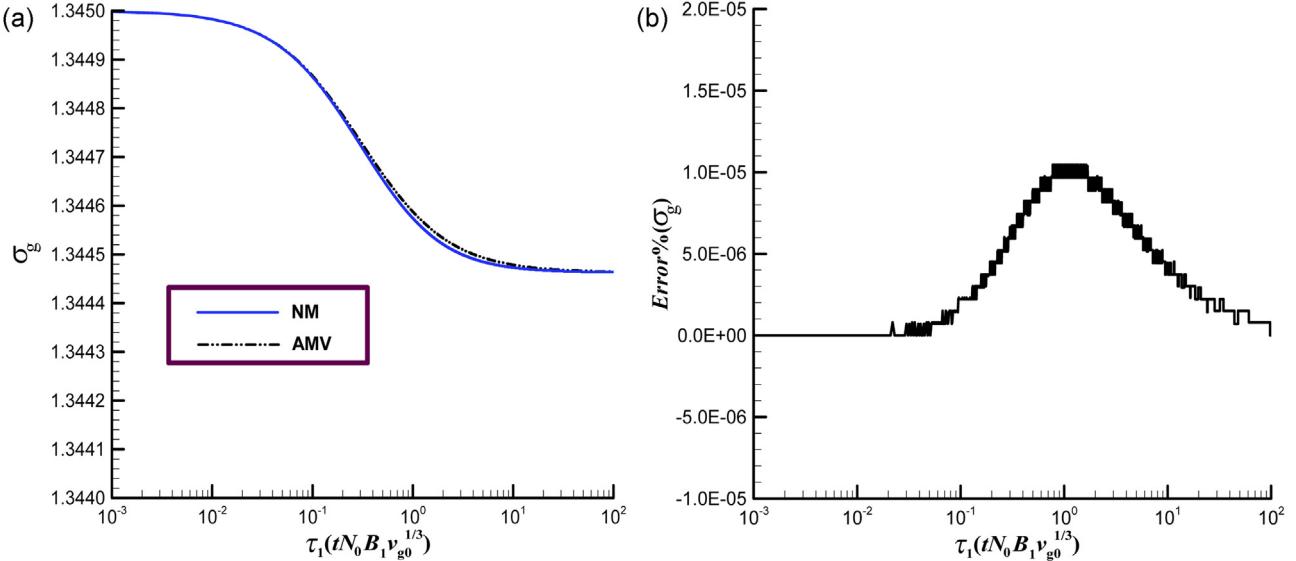


Fig. 4. (a) Variations of σ_g with time in the free molecular regime obtained from NM and AMV; (b) relative error of AMV with respect to NM.

- $(M_0(\tau_1))_f = \left(-\frac{5}{6}a_f \tau_1 + M_{00}^{-5/6} \right)^{-6/5}$,
 - $(M_1(\tau_1))_f = M_{10}$,
 - $(M_2(\tau_1))_f = \left(\frac{5}{6}b_f \tau_1 + M_{20}^{-5/6} \right)^{6/5}$.
- (iv) Go to Step (ii), i.e., the time step is updated and the calculation proceeds to the next time step.

In Fig. 2(a), the NM, AMC, and AMV solutions produce nearly the same total particle number concentration. The relative errors of the two analytical solutions with respect to the NM for the total particle number concentration are shown in Fig. 2(b). Up to $\tau = 100$, the relative errors are limited to a negligible absolute value ($<4.0 \times 10^{-4}$), implying that both analytical solutions have the same precision as the NM under the criterion proposed in Computations section. Fig. 2(b) also shows that the absolute values of relative error of the

AMC are always larger than that of the AMV, which is consistent with the theoretical analysis.

The variations of M_2 with time and the relative errors of the AMC and AMV with respect to the NM are displayed in Fig. 3. It is impossible to distinguish the three solutions shown in Fig. 3(a). In Fig. 3(b), we can see that the absolute values of relative error of the AMC and AMV are always limited to a negligible regime, i.e., 7.0×10^{-5} . As for M_0 , the AMV generates a smaller absolute error % than AMC.

Although the GSD has been verified as 1.345 in the free molecular regime, this value decreases with time as the aerosol approaches or enters the transient regime, i.e., the GSD decreases as the Knudsen number becomes smaller, as shown in Fig. 1. In our previous work, it was shown that the NM captures this change in the GSD (Yu et al., 2008). Fig. 4(a) illustrates the variations of GSD with time given by both the NM and the AMV. Surprisingly, the AMV produces the same results as the NM. Fig. 4(b) shows the relative error of AMV

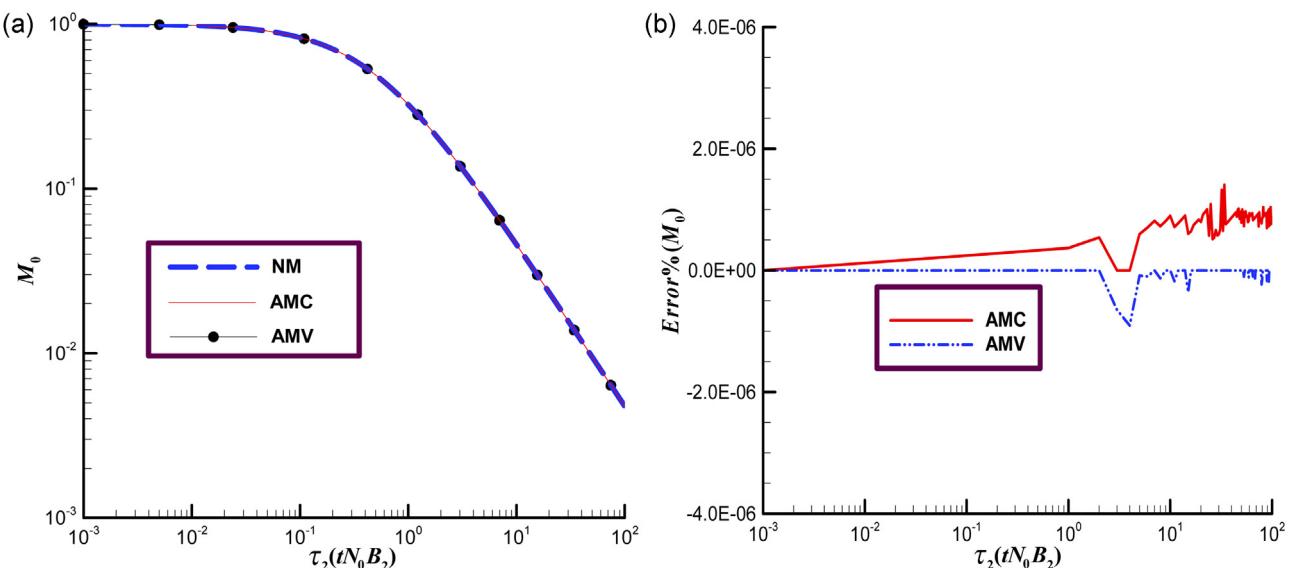


Fig. 5. (a) Variations of M_0 with time in the continuum regime obtained from NM, AMV, and AMC; (b) relative errors of AMC and AMV with respect to NM.

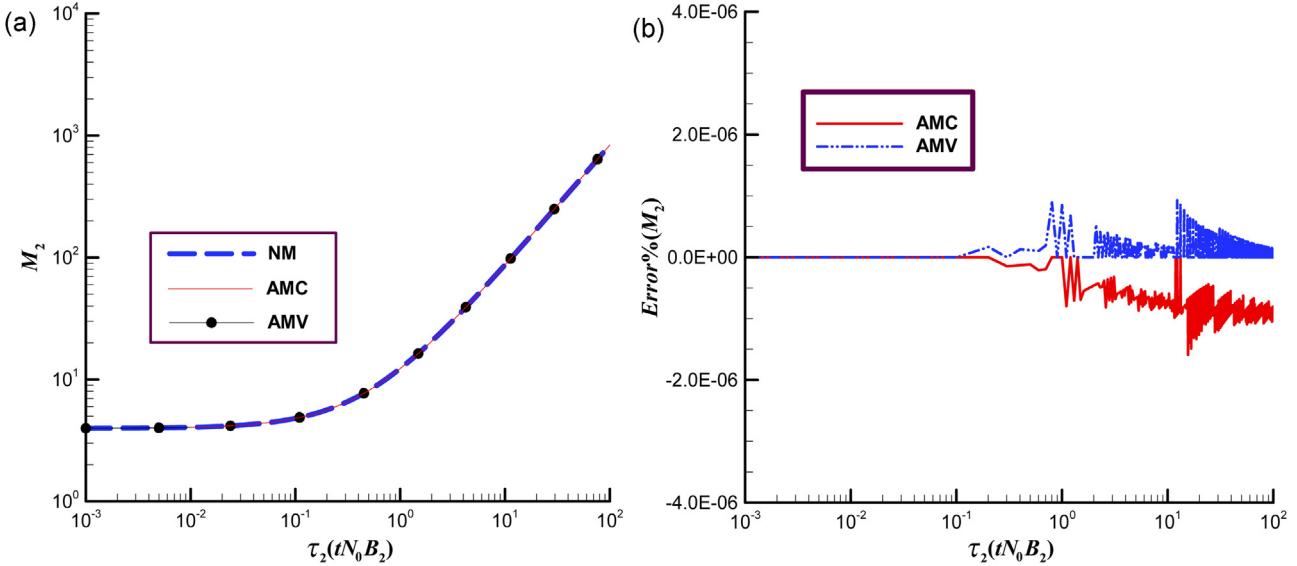


Fig. 6. (a) Variations of M_2 with time in the continuum regime obtained from NM, AMV, and AMC; (b) relative errors of AMC and AMV with respect to NM.

with respect to the NM for the GSD. The absolute value remains negligible at less than 1.0×10^{-5} . Therefore, we can conclude that the AMV has the ability of the NM to trace the variation of GSD, i.e., the variation of particle size distribution.

Continuum regime

Fig. 5(a) compares the particle number concentrations, M_0 , obtained from the three solutions. The initial size distribution is assumed to be a SPSD, i.e. the GSD is assigned a value of 1.32. In this figure, three curves cannot be distinguished from one another. Hence, we use the values of Error% shown in Fig. 5(b) to evaluate the precision of the different solutions. Up to $\tau = 100$, the absolute values of relative error of both analytical solutions remains below 1.0×10^{-6} , implying the difference between NM and AM is negligible. The variations of M_2 with time, as well as the relative error in AMC and AMV, are shown in Fig. 6. We can see that the absolute values of relative error of the analytical solutions have the same precision as the NM for M_0 and M_2 under the criterion proposed in Computations section.

In the continuum regime, the GSD is known to be 1.32. This value is retained over the whole evolution (Friedlander, 2000; Lee et al., 1984; Pratsinis, 1988). To verify the capability of the AMV to capture the evolution of GSD in this regime, we compare the GSDs given by the NM and AMV in Fig. 7. In this figure, both models produce the same results over the entire time range, with the GSD remaining fixed at 1.32. Because the GSD is 1.32 in the continuum regime of a self-preserving system, the AMC should have the same precision as the AMV, unlike in the free molecular regime (see Free molecular regime section) where aerosols inevitably enter the transient regime during their evolution and the GSD varies slightly with time. We therefore conclude that, in the continuum regime, both AMV and AMC produce the same results for the key characteristic quantities of M_0 and M_2 .

Efficiency

Compared with other numerical techniques, such as the sectional method and the Monte Carlo method (Kostoglou, Konstandopoulos, & Friedlander, 2006; Morgan, Wells, Goodson,

Kraft, & Wagner, 2006), the method of moments has a significant advantage in terms of efficiency. This ability to reduce the computational cost has received considerable attention in recent years, especially when coupled with computational fluid dynamics (Murfield & Garrick, 2013). However, to date, methods of moments, e.g. QMOM (McGraw, 1997), DQMOM (Marchisio & Fox, 2005), TEMOM (Yu et al., 2008) and MMIC (Frenklach, 2002), have required numerical solutions, which inevitably entail some computational cost. Our analytical solution is therefore superior to these numerical solutions as it does not require an iterative procedure. We now compare the computational time of the proposed AM and the NM with the fourth-order Runge–Kutta iterative algorithm. The total dimensionless computation time is 100, and the iterative time step is 0.001 for the NM. The data is written to file once per time step. All aerosols are self-preserving, meaning the initial GSD is 1.345 in the free molecular regime and 1.32 in the continuum regime. The

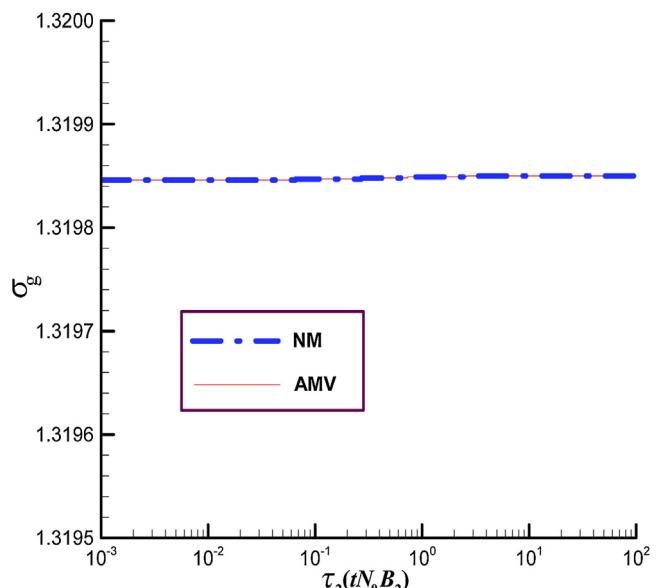


Fig. 7. Comparison of the evolutions of GSDs in the continuum regime obtained from NM and AMV. The initial GSD is set to be 1.319846.

Table 1

Comparison of computation time required by the NM, AMC, and AMV in the free molecular regime and continuum regime.

	NM	AMC	AMV
Free molecular regime	74.031	2.489	4.157
Continuum regime	36.449	2.458	4.130

computational cost of each model is listed in **Table 1**. In the free molecular regime, the computational cost of the NM is shown to be about 30 times that of AMC and 18 times that of AMV. In the continuum regime, the computational cost of the NM is about 15 times that of AMC and about 9 times that of AMV. It is clear that the analytical model reduces the computational cost by an order of magnitude or more. We can also see that AMV consumes much more computational time than AMC.

Conclusions

We have presented an analytical solution of the TEMOM ODEs for the PBE under Brownian coagulation. Our model separately considers the free molecular regime and the continuum regime of a self-preserving aerosol. We first verified a novel property of the variable $g = m_0 m_2 / m_1^2$, and this allowed us to treat this quantity as a constant in the model derivation. The scope of application of the newly proposed model was defined in terms of the GSD. In the free molecular regime and the continuum regime, the analytical model gives two specific solutions, one with a constant GSD and the other with a varying GSD. We verified that both the AMV and AMC have the same precision as a highly reliable numerical method under certain critical criteria. The AMV and AMC reduce the computational cost by an order of magnitude or more compared with the numerical method. The AMV solution has the ability to trace the evolution of size distribution, whereas the AMC solution admits a decoupled solution for the zero and second moment equations. There is a strong potential for the proposed model to replace the existing numerical model, and its use is recommended in the study of particulate matter characteristics in aerosols.

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