Chemical Engineering Science 94 (2013) 79–83

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Science

journal homepage: www.elsevier.com/locate/ces

Asymptotic solution of population balance equation based on TEMOM model

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HIGHLIGHTS

- ► The asymptotic solution for particle moment for PBE has been proposed.
- ► The asymptotic solution is an explicit exponential function of time.
- ► The asymptotic solution has been compared with numerical results.

ARTICLE INFO

Article history:
Received 24 July 2012
Received in revised form
1 February 2013
Accepted 8 February 2013
Available online 27 February 2013

Keywords:
Asymptotic solution
Aerosol
Nano-particle
Population balance equation
Coagulation
Brownian motion

ABSTRACT

In the present study, asymptotic solutions for particle moment and standard deviation due to Brownian coagulation have been obtained analytically, using a specific moment-based formulation known as the Taylor-series expansion method of moment (TEMOM). The derivation is rigorous, and the accuracy of the asymptotic solution is fully dependent on underlying approximations in an expanded Taylor series. The accuracy has been validated by a comparison with numerical results. The asymptotic solutions reveal that the long-time particle moments are an explicit exponential function of time and first particle moment.

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1. Introduction

It has been widely recognized that aerosol particles could be one of the most common unhealthy components of air pollution (Davidson et al., 2005). These particles may be generated by many natural and industrial sources. For example, aerosol particles are produced in a diffusion flame reactor by gas to particle conversion (Hulburt and Katz, 1964; Akhtar et al., 1991;Briesen et al., 1998; Giesen et al., 2004; Yu et al., 2008a, 2008b). The similar phenomenon occurs when manufacturing white pigment (Xiong and Pratsinis, 1991). Smoke ageing in wildfires is also a source of aerosols (Delichatsios, 1980). Particle size and concentration affect not only the environment and quality of a product but also the health of human beings. Researches have already shown that there is a strong correlation between mortality and particle size, with specific reference from nanoparticles (<50 nm) to fine particles (<2500 nm) (Kittelson, 1998; Jacobson et al., 2005).

Population balance equations (PBE) form a general mathematical framework for modeling of particulate systems (Friedlander, 2000) in a wide range of physical, technological and environmental applications. In the framework, a multi-dimensional vector of internal coordinates and time characterizes each particle. The general form of the population balance equation reads:

$$\frac{\partial n(\mathbf{x},t)}{\partial t} = B[n(\mathbf{x},t)] - D[n(\mathbf{x},t)] \tag{1}$$

where $n(\mathbf{x},t)$ is the number density of the particles, $B[n(\mathbf{x},t)]$ and $D[n(\mathbf{x},t)]$ are birth and death rates of the particles due to coagulation and breakage, respectively. For a mono-variants ($\boldsymbol{x}=\upsilon$) Smoluchowski equation, the formula for $B[n(\upsilon, t)]$ and $D[n(\upsilon, t)]$ are given as (Friedlander, 2000):

$$\begin{aligned} B &= \frac{1}{2}\int_0^{\upsilon} \beta(\upsilon_1,\upsilon-\upsilon_1) n(\upsilon_1,t) n(\upsilon-\upsilon_1,t) d\upsilon_1 \\ D &= \int_0^{\infty} \beta(\upsilon_1,\upsilon) n(\upsilon,t) n(\upsilon_1,t) d\upsilon_1 \end{aligned} \tag{2}$$

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0009-2509/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.ces.2013.02.025

in which $n(\upsilon,t)d\upsilon$ is the number of particles per unit spatial volume with particle volume from υ to $\upsilon+d\upsilon$ at time t; and β is the collision frequency function of coagulation. In free molecule regime, the collision frequency function is given by:

$$\beta_{FM}=B_1\left(\frac{1}{\upsilon^{1/3}}+\frac{1}{\upsilon_1{}^{1/3}}\right)^{1/2}(\upsilon^{1/3}+\upsilon_1{}^{1/3})^2 \tag{3a}$$

where the constant $B_1=(3/4\pi)^{1/6}(6k_BT/\rho_p)^{1/2}$; k_B is the Boltzmann's constant; T is the temperature; and ρ_p is the particle density. In the continuum regime, the collision frequency function is:

$$\beta_{CR}=B_2\left(\frac{1}{\upsilon^{1/3}}+\frac{1}{\upsilon_1{}^{1/3}}\right)(\upsilon^{1/3}+\upsilon_1{}^{1/3}) \tag{3b}$$

where the constant $B_2=3k_BT/2\mu$, and μ is the gas viscosity.

The PBE can be viewed in form as the Boltzmann's transport equation. Unfortunately, only a limited number of known analytical solutions exist due to its own non-linear integro-differential structure (Yu et al., 2008c, 2009). Lage (2002) and Patil and Madras (1998) have derived a particular solution for PBE with simultaneous aggregation (coalescence) and fragmentation (breakage), but for the special case where the total number of particles is constant. The more general reversible case, when either fragmentation or coalescence can dominate, has numerous applications, and thus is of considerable importance (McCoy and Madras, 1998, 2001; McCoy, 2001). McCoy and Madras, 2003 have derived an analytical solution of PBE by Laplace transformation when both coalescence and breakage occur. For an initial exponential distribution, the solution is always exponential and has a similarity form. This solution is applicable for the general case when the number of particles is not constant, and thus when breakage and coalescence rates are not equal. For other initial conditions, they have presented the asymptotic solution.

In general, PBE must be solved numerically either by direct bin methods or moment-based methods. In bin based methods, the number density $n(\upsilon,t)$ is solved directly by introducing discrete bins (Wang et al., 2007), while in moment-based method, the equations for the moments of $n(\upsilon,t)$ are numerically solved (e.g., see Xie et al., 2012). It is well known that the moment equations derived from PBE depend on unsolved higher-order moments, and approximations of one kind or another are introduced in each moment-based method to close the moment equation. These include, for example, lognormal distribution (Lee et al., 1984), bin-wise quasi-linear distribution (Wang et al., 2007), Gauss Quadrature approximations (McGraw, 1997; Fox, 2003), moment-conservative fixed pivot technique (Kumar and Ramkrishna, 1996), the cell average technique (Kumar et al., 2006), and direct quadrature spanning tree method (Vikhansky, 2013).

Recently, Yu et al. (2008c) have presented a new, moment-based numerical approach termed as the Taylor-series expansion method of moment (TEMOM) to solve the coagulation equation. In the TEMOM, the moment equations are closed using a Taylor-series expansion technique. Through constructing a system of the first three order ordinary differential equations, the most important moments for describing the aerosol dynamics, namely, the particle number density, particle mass and geometric standard deviation, are obtained. This approach makes no prior assumption on the shape of the particle size spectrum, therefore, the limitation inherent in the lognormal distribution theory automatically disappears, several studies have demonstrated that it is a promising method to approximate the aerosol PBE, with high degrees of physical accuracy and computational efficiency (Yu and Lin, 2010a, 2010b). Xie et al. (2012) applied this method to study the evolution of particle coagulation in a temporal mixing layer obtained from direct numerical simulation, their results reveal that the relative growth rate is slow at long times, and the system bottleneck is the advection and diffusion, this explains why the distributions in space are self-similar as the coherent vortex structure of temporal mixing layer develops. The self-similarity also implies that the effect of coagulation and effect of mixing by advection and diffusion on particle growth could be modeled separately.

In this study, we will show that the TEMOM model provides an elegant analytical framework to examine analytically the asymptotic solution of PBE for Brownian coagulation, and the asymptotic results show that all moments at long times depend explicitly on time and particle first moment (i.e., particle mass concentration). Because no additional physical assumption is introduced in the derivation, and the accuracy of the asymptotic solution is only depends on the underlying approximations in the expanded Taylor series. The asymptotic results can be used to model particle coagulation coupled with time-dependent non-uniform fluid flow, as only the first particle moment needs to be numerically solved and all other particle moments can be calculated through the asymptotic solutions. This could significantly reduce the overall computation cost.

2. The TEMOM model for particle coagulation

The TEMOM is designed to solve the moment s of the size distribution, which could be a function of time and space. The k-th order moment M_k of the particle distribution is defined as:

$$M_k=\int_0^\infty \upsilon^k n(\upsilon)d\upsilon \tag{4}$$

By multiplying both sides of the PBE, Eq. (1), with υ^k and integrating over all particle sizes, a system of transport equations for M_k are obtained (Pratsinis, 1988). In a spatially homogeneous system, the particle moments evolve in time due to the Brownian coagulation and can be expressed as:

$$\frac{dM_k}{dt}=\frac{1}{2}\int_0^\infty\int_0^\infty[(\upsilon+\upsilon_1)^k-\upsilon^k-\upsilon_1{}^k]\beta(\upsilon,\upsilon_1)n(\upsilon,t)n(\upsilon_1,t)d\upsilon d\upsilon_1,\ (k=0,1,2,\cdots) \tag{5}$$

In the TEMOM, the minimum set of moments required to close the particle moment equations is the first three, M_0, M_1 and M_2. The zeroth order moment M_0 represents the total particle number concentration; the first order moment M_1 is proportional to the total particle mass concentration; the second order moment M_2 determines the total light scattered by the particle system (Friedlander, 2000). Based on the detailed derivations of TEMOM in Yu et al. (2008c, 2009, 2011) and Xie et al. (2012), the resulting closed-form equations for the first three moments equations for the collision frequency function in free molecule regime can be rearranged as:

$$\begin{aligned}
\frac{dM_0}{dt}&=\frac{\sqrt{2}B_1(65M_C{}^2-1210M_C-9223)M_1{}^{1/6}}{5184}M_0{}^{11/6}\\
\frac{dM_1}{dt}&=0\\
\frac{dM_2}{dt}&=-\frac{\sqrt{2}B_1(701M_C{}^2-4210M_C-6859)M_1{}^{11/6}}{2592M_C{}^{1/6}}M_2{}^{1/6}
\end{aligned} \tag{6a}$$

On the other hand, for collision frequency in the continuum regime, the first three moments equations are governed by:

$$\begin{aligned}
\frac{dM_0}{dt}&=\frac{B_2(2M_C{}^2-13M_C-151)M_0{}^2}{81}\\
\frac{dM_1}{dt}&=0\\
\frac{dM_2}{dt}&=-\frac{2B_2(2M_C{}^2-13M_C-151)M_1{}^2}{81}
\end{aligned} \tag{6b}$$

where the dimensionless moment M_C is defined as:

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

It is important to note that the derivation of particle moment equations does not involve any assumptions concerning the shape of the particle size distribution (PSD) (Yu et al., 2008c, 2009, 2011). If the particle size distribution assumed to be lognormal, then the mean particle volume and standard deviation of the lognormal distribution can be expressed as (Pratsinis, 1988)

$$V = M_1/M_0; \quad \ln^2\sigma = \frac{1}{9}\ln(M_C) \tag{8}$$

Clearly, these moment equations represent a system of coupled nonlinear differential equations. Since all terms are dependent on the first three moments M_0, M_1 and M_2, and thus the system can be automatically closed. In general, these equations can be solved numerically to determine the time evolution of the first three moments, which may be then used to further determine approximately higher order moments under the assumption of lognormal distribution.

3. Asymptotic behavior of the TEMOM model for collision frequency in free molecule regime

Here we shall show that, under certain conditions, the TEMOM moment equations lead to an explicit long time solution. The starting point is to assume that the shape of the size distribution becomes self-similar at long times. This shape preservation (Friedlander and Wang, 1966) implies that the standard deviation or dimensionless moment tends to a constant as time advances, this has indeed been observed in several numerical studies (Pratsinis, 1988; McGraw, 1997; Fox, 2003; Yu et al., 2008c, 2009, 2011; Xie al., 2012). Therefore, our key assumption is that the dimensionless moment tends to a constant denoted by $M_{C\infty}$. Furthermore, we note that M_1 remains constant due to the rigorous mass conservation requirement. Under these conditions, we seek a long time solution of the system Eq. (6a), using the form:

$$\begin{aligned} M_0 &\to \left(-\frac{5}{6}\times\frac{\sqrt{2}(65{M_{C\infty}}^2-1210M_{C\infty}-9223)}{5184}\right)^{-6/5} {B_1}^{-6/5}{M_1}^{-1/5}t^{-6/5} \\ M_2 &\to \left(-\frac{5}{6}\times\frac{\sqrt{2}(701{M_{C\infty}}^2-4210M_{C\infty}-6859)}{2592{M_{C\infty}}^{1/6}}\right)^{6/5} {B_1}^{6/5}{M_1}^{11/5}t^{6/5} \end{aligned} \tag{9}$$

several immediate predictions follow from this specific asymptotic solution. First, the asymptotic solution reveals an important long time growth time scale

$$\left|\frac{1}{M_0}\frac{dM_0}{dt}\right| = \left|\frac{1}{M_2}\frac{dM_2}{dt}\right| \to \frac{1.2}{t} \tag{10}$$

Namely, the growth is rather slow at long times. Second, the self-consistency requirement that M_C tends to a constant $M_{C\infty}$, yields a nonlinear algebraic equation for $M_{C\infty}$

$$M_{C\infty} = \left[\frac{2(701{M_{C\infty}}^2-4210M_{C\infty}-6859)}{(65{M_{C\infty}}^2-1210M_{C\infty}-9223){M_{C\infty}}^{1/6}}\right]^{6/5} \tag{11}$$

so the asymptotic value of the dimensionless particle moment $M_{C\infty}$ can be analytically determined. By trial and error, we found that $M_{C\infty}=2.200126847$, and the corresponding standard deviation is $\sigma=1.344462843$ according to Eq. (8). This prediction is in excellent agreement with the asymptotic values obtained numerically in the literature: McGraw (1997) of $\sigma=1.346$ using the QMOM method with 6 nodes; Yu et al. (2008c, 2009, 2011) found $\sigma=1.345$ by solving TEMOM numerically; and Pratsinis (1988) obtained $\sigma=1.355$ using MOM, which is close to the value given by Lee et al. (1984) who assumed that particle size distribution to be lognormal. It should be noted that the accuracy of the k-th moments and standard deviation only depends on the approximation in the expanded Taylor-series.

Finally, combining the above predictions, we obtain the following fully explicit asymptotic solution for the particle moments:

$$\begin{aligned} M_0 &\to 0.313309932\times{B_1}^{-6/5}{M_1}^{-1/5}t^{-6/5} \\ M_2 &\to 7.022205880\times{B_1}^{6/5}{M_1}^{11/5}t^{6/5} \end{aligned} \tag{12}$$

4. Asymptotic behavior of the TEMOM model for collision frequency function in the continuum regime

Under the same conditions and using the similar reasoning, the asymptotic solution can also be obtained in the continuum regime. In this case, the long-time particle moments can be written as:

$$\begin{aligned} M_0 &\to -\frac{81}{(2{M_{C\infty}}^2-13M_{C\infty}-151)}{B_2}^{-1}t^{-1} \\ M_2 &\to -\frac{2(2{M_{C\infty}}^2-13M_{C\infty}-151)}{81}B_2{M_1}^2t \end{aligned} \tag{13}$$

it follows that the asymptotic growth rate is:

$$\left|\frac{1}{M_0}\frac{dM_0}{dt}\right| = \left|\frac{1}{M_2}\frac{dM_2}{dt}\right| \to \frac{1}{t} \tag{14}$$

which is similar to that in the free molecule regime, but with 16.7% less in magnitude. The self-consistency requirement for $M_{C\infty}$ leads to

$$M_{C\infty} = \left.\frac{M_0M_2}{{M_1}^2}\right|_{t\to\infty} = 2 \tag{15}$$

This implies that the corresponding standard deviation is $\sigma=1.319850145$ according to Eq. (8). The asymptotic value can be compared to published numerical asymptotic values: the QMOM method predicts $\sigma=1.325$ with 2 nodes and $\sigma=1.315$ when 6 nodes are used (McGraw, 1997); the numerical asymptotic value from TEMOM is 1.319 (Yu et al., 2008c, 2009, 2011); in addition, the asymptotic value for MOM (Pratsinis, 1988) is close to the value of 1.32 reported by Lee et al. (1984) who assumed log-normal functions for particle size distribution.

Finally, putting all predictions together, we obtain analytically the following fully explicit asymptotic solution of the particle moments in the continuum regime

$$\begin{aligned} M_0 &\to \frac{81}{169}{B_2}^{-1}t^{-1} \\ M_2 &\to \frac{338}{81}B_2{M_1}^2t \end{aligned} \tag{16}$$

which is expected to be valid at long times.

5. Comparison with numerical results

To further illustrate the value and accuracy of the asymptotic solution, we shall compare them to numerical solutions at different times. Without loss of generality, three cases are selected, the first one is the mono-disperse system (Pratsinis, 1988), and the other two are multi-disperse systems (Barret and Jheeta, 1996). The numerical method used is the fourth-order Runge–Kutta method, and its accuracy has been well established by comparison with other methods, such as MOM (Pratsinis,

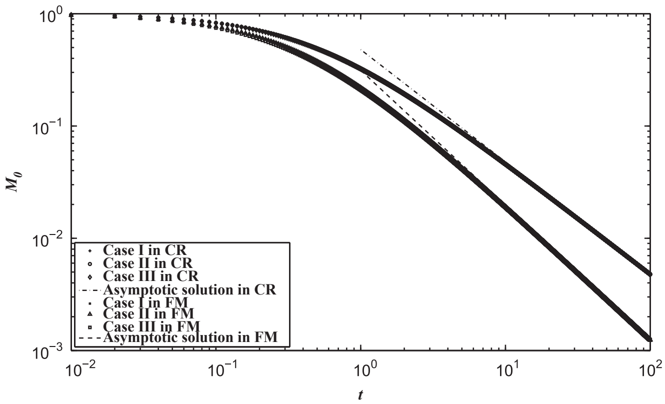

Fig. 1. The comparison of particle zeroth moment between asymptotic solution and numerical solution for different cases.

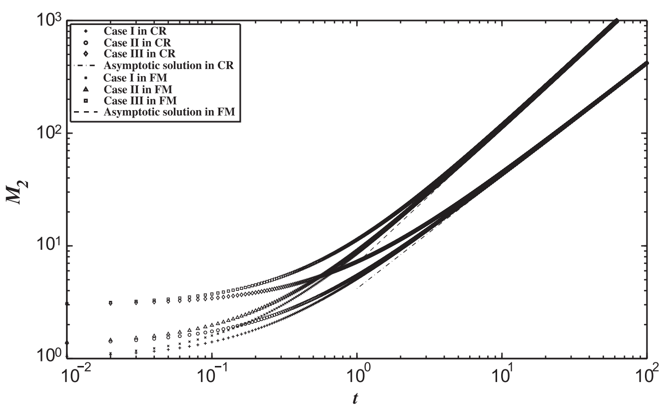

Fig. 2. The comparison of particle second moment between asymptotic solution and numerical solution for different cases.

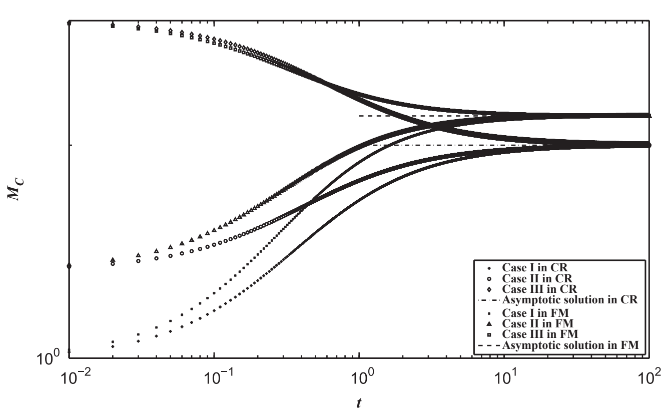

Fig. 3. The evolution of dimensionless particle moments with time for different cases.

1988), QMOM (McGraw, 1997), TEMOM (Yu et al., 2008c, 2009, 2011; Xie et al., 2012), etc.

Case I: For mono-disperse system, the initial conditions are $M_0(0)=1$; $M_1(0)=1$; $M_2(0)=1$
Case II: For multi-disperse system with an initially lognormal distribution, the initial conditions for moments are $M_0(0)=1$; $M_1(0)=1$; $M_2(0)=4/3$
Case III: For multi-disperse system with an initially Gamma distribution (i.e., the two parameter Gamma distribution with a shape parameter 0.5 and a scale parameter 2), the initial conditions for moments are $M_0(0)=1$; $M_1(0)=1$; $M_2(0)=3$

These different initial value for M_2 cover the different initial particle size distribution. For convenience, the constant in the collision frequency functions are set to $B_1=1$ and $B_2=1$. Figs. 1–3 show the time evolution of three particle moments, respectively, obtained from asymptotic solutions and numerical integration. Clearly, all the results are in excellent agreement at long times. The asymptotic growth rate in the free molecule regime with a slope of 6/5 is larger than that in the continuum regime with a slope of unit in the log–log coordinates. More importantly, the results reveal how for different initial conditions, the particle moments evolve smoothly from the initial condition to the asymptotic solution at about $t=10$.

6. Conclusion

The shape preservation of particle size distribution during the evolution of particle coagulation has been proposed by the researchers many years ago (Friedlander, 2000). In this paper, we combine this observation and the moment equations derived from the Taylor series expansion method of moments, to demonstrate that an asymptotic solution can be derived analytically. This is done for collision frequency functions in both the free molecular regime and the continuum regime. Several important predictions are made and are shown to be in excellent agreement with published numerical asymptotic results. The asymptotic solutions have also been compared to numerical solutions at different times for several initial distributions. Since the TEMOM method has no prior requirement for the shape of particle size distribution (PSD), it has been viewed as a promising method to model the aerosol population balance equation. The asymptotic solutions reveal that the long-time particle moments are an explicit function of time and particle mass concentration. The results can be used to model the long-time evolution of particle coagulation, which could reduce the computational cost greatly for certain applications (e.g., Xie et al., 2012).

Nomenclature

M_c	the dimensionless moment
M_k	the k-th order particle moment
T	the fluid temperature
V	the mean particle volume
k	the order of Taylor series expansion
k_B	the Boltzmann's constant
$n(\upsilon,t)$	the number density of particles
t	the time variant
$\mathbf{x}$	multi-dimensional vector

Greek letters

β	the collision frequency function
μ	the gas viscosity
υ	the particle volume
υ_g	the geometric mean volume
σ	the standard deviation

Acknowledgments

This work is supported by the National Natural Science Foundation of China with Grant nos. 50806023, and 50721005, and the Programmer of Introducing Talents of Discipline to Universities ("111" Project no. B06019), China.

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