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

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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.

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, Pikturna, Fox, Vigil, & Barresi, 2003; McGraw, 1997), the ordinary differential equation (ODE) of the TEMOM has to be solved by an iterative numerical calculation

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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	kth moment of particle size distribution
g	$= m_0 m_2/m_1^2$
M_k	dimensionless kth 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 kg/(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 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., $g = m_0m_2/m_1^2$. 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, 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.

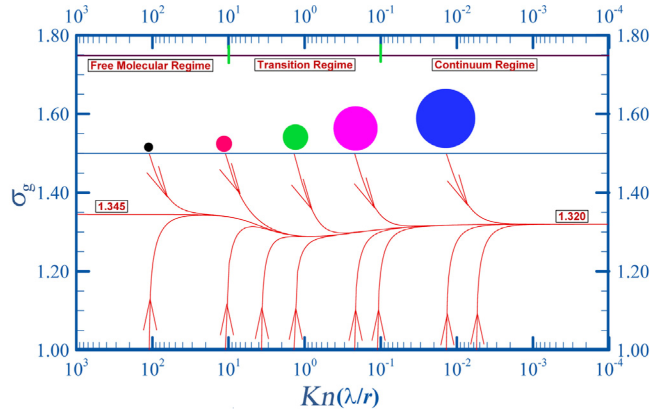

Fig. 1. Variation of geometric standard deviation σ_g with Knudsen number Kn. λ is the free molecular path (68.41 in this study) and r is the geometric mean radius of an aerosol particle. Aerosols with different initial size distributions (certain value for (σ_g, Kn)) converge finally to the self-preserving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

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 $B_1 = (3/4\pi)^{1/6}(6k_BT/\rho)^{1/2}$, 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