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Technical note

A new analytical solution for solving the population balance equation in the continuum-slip regime

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ABSTRACT

A new analytical solution is first proposed to solve the population balance equation due to Brownian coagulation in the continuum-slip regime. An assumption for a novel variable g ($g=m_0m_2/m_1{}^2$, where m_0, m_1 and m_2 are the first three moments, respectively) is successfully applied in executing a separate variable method for ordinary differential equations of the Taylor expansion method of moments. The sectional method is selected as a reference to verify the new solution. The accuracy between the new solution and Lee et al. analytical solution (Lee et al., 1997, *Journal of Colloid and Interface Science, 188*, 486–492) is mainly compared. The geometric standard deviation of number distribution for the new analytical solution is revealed to be limited to 1.6583. Within the valid range of the geometric standard deviation, the new analytical solution is confirmed to solve the population balance equation undergoing Brownian coagulation with the very nearly same accuracy as Lee et al. analytical solution. For the total particle number concentration, the new solution usually yields higher accuracy. The new solution and Lee et al. analytical solution approximately become one solution as the Knudsen number is smaller than 0.1000. The new solution has the potential to become a competitive analytical solution for solving population balance equation regarding its accuracy and very straightforward derivation.

1. Introduction

A reliable prediction for aerosol properties including the total particle number concentration, the geometric mean size and the geometric standard deviation of number distribution has received much attention in emerging fields such as the risk evaluation of aerosols at workplace, the development of realistic exposure scenarios and the nanoparticle synthesis process (Buesser & Pratsinis, 2012; Vogel et al., 2014; Yu et al., 2008a, 2008b). For these aerosols, the evolution of particle size distribution due to Brownian coagulation is unavoidable (Lee & Wu, 2005; Upadhyay & Ezekoye, 2003), which usually leads to unsteady systems and has been confirmed to determine the aerosol characteristics in almost all ultrafine and nanoparticle processes(Crowe et al., 2011; Friedlander, 2000). When these processes are theoretically investigated, the evolution of the size distribution must be captured in mathematical models (Buesser & Pratsinis, 2012; Xie & Wang, 2013;

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Nomenclature

A	constant (=1.591)
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 of size distribution
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	initial total particle number concentration, m^{-3}

Greek letters

N	kinematic viscosity, $m^2\ s^{-1}$
B	particle collision kernel
M	gas viscosity kg $m^{-1}\ s^{-1}$
λ	mean free path of the gas, m
σ_g	geometric mean deviation of size distribution
τ	dimensionless coagulation time, tN_0B_2

Abbreviation

PBE	population balance equation
TEMOM	Taylor expansion method of moments
GSD	geometric standard deviation of number distribution
ODE	ordinary differential equation
SM	sectional method
QMOM	quadrature method of moments
SPSD	self-preserving size distribution
PSPSD	pseudo-self-preserving size distribution
Log-normal AMM	log-normal analytical method of moments
Log-normal NMM	log-normal numerical method of moments

Santos et al., 2013; Singh et al., 2013). To meet the requirement, Müller established the integral-differential equation for the dynamical process in 1928 based on the ground-breaking work of Smoluchowski (Müller, 1928; Smoluchowski, 1917), which was later called Population Balance Equation (PBE). The PBE has become a basic governing equation to study aerosol dynamics from then on. However, the analytical solution of this equation, especially in terms of a particle size dependent coagulation kernel, still remains a challenging issue.

The PBE is a strong non-linear equation with the same mathematical structure as Boltzmann's transport equation. Thus, an exact analytical solution for it cannot be achieved (Lee et al., 1997; Yu et al., 2008a, 2008b). To solve it analytically, the group of Prof. Lee in Kwangju Institute of Science and Technology, Korea has performed a series of ground-breaking works in different specific-size regimes with a log-normal distribution assumption (Lee et al., 1997, 1984; Otto et al., 1999; Park et al., 1999). These works received much attention because of their ability to capture the evolution of the size distribution. Another solution deserved to be mentioned to solve the PBE was proposed in 1964 by introducing a similarity transformation in the size distribution function (Swift & Friedlander, 1964), which is actually an asymptotic solution independent of the initial size distribution. The idea in the asymptotic solution was currently accepted in studies on Brownian coagulation processes using the Taylor expansion method of moments (TEMOM) (Chen et al., 2014a; Xie & Wang, 2013). In both the free molecular and continuum regimes, asymptotic solutions exist because the asymptotic status for the size distribution, i.e., self-preserving size distribution (SPSD), has been verified in both the regimes (Friedlander, 2000). However, in the continuum-slip regime, especially as the Knudsen number ranges from ~0.1000 to ~5.0000 (also called the near-continuum regime), the geometric standard deviation (GSD) of number distribution always varies with the Knudsen number (Otto et al., 1994; Park et al., 1999; Yu et al., 2011). In this case, the asymptotic solution will no longer exist. In fact, the asymptotic solution has a fatal shortcoming in that it is not able to capture the evolution of size distribution for the time period before the self-preserving size distribution is achieved (Lee et al., 1997). Therefore, an alternative solution beyond the asymptotic status and without the requirement for the pre-defined size distribution becomes necessary.

The TEMOM exhibits a huge potential to achieve the time-dependent analytical solution for the PBE due to its very simple mathematical structure of equations (Chen et al., 2014b; Xie et al., 2012; Yu et al., 2011; Yu & Lin, 2009a, 2009b). The key of the TEMOM is that fractal moments in the ordinary differential equations (ODEs) for moments can be replaced by the following expression (Yu et al., 2008a, 2008b):

$$m_k = \left(\frac{u^{k-2}k^2}{2} - \frac{u^{k-2}k^2}{2}\right) m_2 + \left(-u^{k-1}k^2 + 2u^{k-1}k\right) m_1 + \left(u^k + \frac{u^k k^2}{2} - \frac{3u^k k}{2}\right) m_0 \tag{1}$$

where u is the Taylor expansion point, k is the fractal number, and m_0, m_1 and m_2 are the first three moments. The zeroth and the first moments represent the total particle number concentration and the total volume concentration, respectively, while the second moment is a polydispersity variable. In the continuum-slip regime, the TEMOM (Yu et al., 2011) can be used for the Knudsen number up to 5.0000 (Lee et al., 1997). This method is valid for particles with diameter larger than ~27 nm; thus, this method can be used to resolve almost all Brownian coagulation issues, as shown in Fig. 1. The TEMOM ODEs have been successfully numerically solved using a highly reliable Runge–Kutta algorithm (Yu et al., 2011).