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A new analytical solution for agglomerate growth undergoing Brownian coagulation

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ABSTRACT

We proposed a new analytical solution for a population balance equation for fractal-like agglomerates. The new analytical solution applies to agglomerates with any mass fractal dimensions. Two well-known numerical methods, including the Taylor-series expansion method of moments and the quadrature method of moments, were selected as references. The reliability of the analytical solution with three mass fractal dimensions of 1.0, 2.0, and 3.0 in the continuum-slip regime was verified. The accuracy of the new analytical solution is affected by both the Knudsen number and the mass fractal dimension. The new analytical solution can be further improved in accuracy by introducing a correction factor to the originally derived mathematical formula. The new analytical solution was finally confirmed to possess potential for replacing the numerical solution in the continuum-slip regime.

1. Introduction

Aerosols are unstable in particle process engineering and the environment because of Brownian coagulation, which causes the particle size distribution to always vary with time [1]. This process can be characterized mathematically by solving the the population balance equation (PBE) [2,3]. The PBE was proposed by Smoluchowski and later developed by Müller in its integral-differential form [4,5]. However, the PBE associated with a particle-size-dependent coagulation kernel cannot be precisely solved. Various methods for solving the PBE have been proposed in the last century, including the method of moments [6–11], sectional method [12–15], and Monte Carlo method [16–19], with almost all methods belonging to the numerical solution. For the numerical solution, time-consuming iterative algorithms, such as the 4th-order Runge–Kutta method, must be performed. Although there are also some analytical solutions [20–22], the scope of their application is usually limited because of their inability to resolve time-dependent dynamical process or because of a prior assumption about size distribution. For fractal-like agglomerates, the analytical solution for the PBE is more difficult to achieve because of an additional variable(i.e., the mass fractal dimension) [2].

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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}
f	$1/D_f$
D_f	mass fractal dimension
Greek letters	
ν	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

Because of the relative simplicity of implementation and the low computational cost, the method of moments has been extensively used to resolve aerosol dynamical processes [23]. In the application of this method, the fractal moment variables inevitably appear in the conversion from the PBE to the ordinary differential equations (ODEs) for kth moments, the closure of which can be achieved using five techniques [23](i.e., pre-defined size distributed method [9,24], Gaussian quadrature method (QMOM) [8,10], pth-order polynomical method [25], interpolative method [7], and Taylor-series expansion method (TEMOM) [11,26]). To the best of our knowledge, the TEMOM has the simplest structure for governing equations among all the methods of moments. Compared with the QMOM and its variants, such as the direct QMOM, the TEMOM has an advantage in analytically expressing the time evolution of kth moments as polynomials composed of integer moments. Thus, the ODEs of the TEMOM are more easily solved analytically compared with their counterparts, especially for fractal-like agglomerates involving a very complex coagulation kernel.

Since being proposed in 2008 [11], the TEMOM has displayed potential to become a vital method in solving the PBE because it makes no assumptions for size distribution and generates very low computational costs. Two key physical quantities characterizing an aerosol property (the geometric standard deviation [GSD] of number distribution and geometric mean volume) [27] can be easily reconstructed using this method. In fact, the TEMOM, QMOM, and log-normal method of moments (log MM) [9] have been verified to yield nearly the same results for both quantities as well as for the first three moments [28]. Along with a mathematical analysis of the ODEs of the TEMOM, the governing equations for kth moments can be further simplified through introducing a novel variable $g(m_0 m_2/{m_1}^2$, where m_0, m_1, and m_2 are the first three moments, respectively). It was recently verified that if g is treated as a constant, then the ODEs of the TEMOM can be analytically resolved by executing a separate variable method (SPV) in both the continuum regime and free molecular regime [31]. Primarily because of the novel property of g, it only varies within a very small range, as illustrated in Fig. 1. This is consistent with the self-preserving size distribution theory first devised by Friedlander [22]. However, the feasibility of treating g as a constant in the derivation for fractal-like agglomerates in the continuum-slip regime has never been verified.

Therefore, the aim of this study was to verify the feasibility of an analytical solution for solving the PBE for fractal-like agglomerates in the continuum-slip regime. Here, fractal-like agglomerates represent particles composed of numerous smaller primary particles, the morphology of which can be characterized using fractal theory. Because the TEMOM and QMOM for numerically solving ODEs have been verified as reliable solutions [6–11], they were used here as references. Three key physical quantities, namely the total particle number concentration, GSD of the number distribution, and geometric volume concentration, were chosen for investigation. The structure of this paper is as follows. In Section 2, the mathematical equations are briefly discussed, and in Section 3, the specific calculation parameters are given. The results and discussion are presented in Section 4. Conclusions are given in Section 5.