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AN IMPROVED PARTICLE POPULATION BALANCE EQUATION IN THE CONTINUUM-SLIP REGIME

by

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An improved moment model is proposed to solve the population balance equation for Brownian coagulation in the continuum-slip regime, and it reduces to a known one in open literature when the non-linear terms in the slip correction factor are ignored. The present model shows same asymptotic behavior as that in the continuum regime.

Key words: *Taylor series expansion, moment method, population balance equation, slip correction factor*

Introduction

Population balance equations (PBE) are general mathematical framework for modeling of particulate systems [1]. The behavior of these systems is largely governed by the collision rate, *i. e.*, the number of collisions per unit time per unit volume of aerosol. The calculation of collision rate is simplified by the fact that particles are typically found at low volume fractions in the gas phase. Under such dilute conditions, collision can be modeled as two-body interactions wherein thermal/Brownian motion drives collisions. In the framework of mono-variants internal co-ordinate and time for each particle, the PBE characterized as Smoluchowski equation, which takes the form:

$$\frac{\partial n(\upsilon,t)}{\partial t} = \frac{1}{2}\int_0^\upsilon \beta(\upsilon,\upsilon-\upsilon_1)n(\upsilon_1 t)n(\upsilon-\upsilon_1,t)\mathrm{d}\upsilon_1 - \int_0^\infty \beta(\upsilon_1,\upsilon)n(\upsilon,t)n(\upsilon_1,t)\mathrm{d}\upsilon_1 \qquad (1)$$

in which $n(\upsilon,t)\mathrm{d}\upsilon$ is the number of particles per unit spatial volume with particle volume from υ to $\upsilon + \mathrm{d}\upsilon$ at time t; and β is the collision kernel/collision rate coefficient of coagulation.

The PBE can be viewed as the Boltzmann's transport equation in form. For its own non-linear integro-differential structure, only a limited number of known analytical solutions exist for simple coagulation kernel. The analytical solution of PBE, especially in terms of a particle size dependent coagulation kernel, still remains a challenging issue. Because of the relative simplicity of implementation and low computational cost, the moment method has been extensively used to solve most particulate problems, and has become a powerful tool for investigating aerosol microphysical processes in most cases [2-4]. In the conversion from PBE to the moment equation, the *k*-th order moment M_k is defined:

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$$M_k = \int_0^\infty \upsilon^k n(\upsilon) \mathrm{d}\upsilon \qquad (2)$$

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. In a spatially homogeneous system, the particle moments evolving with time due to the Brownian coagulation can be expressed:

$$\frac{\mathrm{d}M_k}{\mathrm{d}t} = \frac{1}{2}\int_0^\infty\int_0^\infty[(\upsilon+\upsilon_1)^k - \upsilon^k - \upsilon_1^k]\beta(\upsilon,\upsilon_1)n(\upsilon,t)n(\upsilon_1,t)\mathrm{d}\upsilon\mathrm{d}\upsilon_1, \quad (k=0,1,2,...) \qquad (3)$$

The minimum set of moments required to close the particle moment equation is the first three, M_0, M_1, and M_2. The zeroth moment represents the particle number concentration, the first moment represents the particle volume concentration, and the second moment is a poly-dispersity variable. It should be pointed out that M_1 remains constant due to the mass conservation requirement, and its initial conditions for the particle moment evolution equation can be note das M_{00}, M_1, and M_{20}, respectively.

Accurate calculation of particles moment evolution requires accurate collision kernel coefficient. When the particle radius of at least one object is large relative to the mean persistence distance of the colliding entities, the continuum approximation is satisfied and Smoluchowski's β applies:

$$\beta = 4\pi\left(\frac{k_\mathrm{B}T}{f_i}+\frac{k_\mathrm{B}T}{f_j}\right)(a_i+a_j) \qquad (4)$$

where f_i and f_j are the friction factors of type i and j entities, a_i and a_j – the radii of type i and type j entities, respectively, k_B – the Boltzmann's constant, T – the temperature of colliding entities and background fluid. The friction coefficient is a quantity fundamental to most particle transport processes. In the continuum regime, the Stokes law form holds for a rigid sphere as $f_i = 6\pi\mu a_i$, and μ is the gas viscosity.

In fluid dynamics, the Cunningham correction factor or Cunningham slip correction factor is used to account for non-continuum effects when calculating the drag on small particles. The derivation of Stokes Law, which is used to calculate the drag force on small particles, assumes a no-slip condition, which is no longer correct at high Knudsen number. The Cunningham [5] slip correction factor allows predicting the drag force on a particle moving a fluid with Knudsen number between the continuum regime and free molecular flow. The slip correction factor C_c is given by:

$$C_c = 1 + \mathrm{Kn}\left(A_1 + A_2 \mathrm{e}^{\frac{A_3}{\mathrm{Kn}}}\right) \qquad (5)$$

with $A_1 = 1.165$, $A_2 = 0.483$, and $A_3 = 0.997$ obtained in experiments [6]. The Knudsen number is a dimensionless number defined as the ratio of the molecular mean free path length, λ, to a representative physical length scale (the particle radius, a, in the present study), *i. e.*, $\mathrm{Kn} = \lambda/a$.

Recently, Yu *et al.* [7] proposed a moment mode for particle PBE in the continuum-slip regime with a linearized slip correction factor as $C_c = 1 + A\mathrm{Kn}$ ($A = 1.591$), and have solved it analytically. In the present work, we will improve their moment model in the continuum-slip regime without neglecting the non-linear terms in the slip correction factor, and analyze its asymptotic behavior. The results show that both the improved moment model and its simplified forms have the same asymptotic solution as that in the continuum regime [8].

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Mathematical formulations

The collision kernel in the continuum-slip regime can be re-written based on particle volume:

$$\beta = \frac{2k_B T}{3\mu}[C_c(\upsilon_i)\upsilon_i^{-1/3} + C_c(\upsilon_j)\upsilon_j^{-1/3}](\upsilon_i^{1/3} + \upsilon_j^{1/3}) \tag{6}$$

The slip correction factor can be expanded with Taylor series at the point (the particle mean volume $u = M_1/M_0$):

$$C_c(\upsilon) = 1 + g_0(u) + g_1(u)(\upsilon - u) + g_2(u)(\upsilon - u)^2 + \cdots \tag{7}$$

and the corresponding functions g_0, g_1, and g_2 are defined:

$$g_0(u) = \frac{B}{u^{1/3}} + A_1 + A_2 e^{-\frac{A_3 u^{1/3}}{B}} \tag{8a}$$

$$g_1(u) = -\frac{1}{3}\frac{A_2 e^{-\frac{A_3 u^{1/3}}{B}} A_3}{u} - \frac{1}{3}\frac{B}{u^{4/3}} + A_1 + A_2 e^{-\frac{A_3 u^{1/3}}{B}} \tag{8b}$$

$$g_2(u) = \frac{2}{9}\frac{B}{u^{7/3}} + A_1 + A_2 e^{-\frac{A_3 u^{1/3}}{B}} + \frac{1}{18}\frac{A_2 e^{-\frac{A_3 u^{1/3}}{B}} A_3(4B + A_3 u^{1/3})}{Bu^2} \tag{8c}$$

where the constant is defined as $B = Kn_0(M_1/M_{00})^{1/3}$, with the initial Knudsen number based on particle moment is $Kn_0 = \lambda/u_0 = \lambda(4\pi M_{00}/3M_1)^{1/3}$. Then the ordinary differential equation for particle moment evolution can be obtained:

$$
\begin{aligned}
\frac{dM_0}{dt} = -B_2 M_0^2 & \left\{ [1 + g_0(u)]\left(1 + \frac{M_{-1/3}M_{1/3}}{M_0^2}\right) + g_1(u)u\left(\frac{M_{2/3}M_{1/3}}{M_1 M_0} - \frac{M_{-1/3}M_{1/3}}{M_0^2}\right)\right. \\
& \left. + g_2(u)u^2\left(\frac{M_2 M_0}{M_1^2} + \frac{M_{5/3}M_{1/3}}{M_1^2} - 2\frac{M_{2/3}M_{1/3}}{M_1 M_0} + 1 + 1 + \frac{M_{-1/3}M_{1/3}}{M_0^2}\right)\right\}
\end{aligned}
$$

$$\frac{dM_1}{dt} = 0 \tag{9}$$

$$
\begin{aligned}
\frac{dM_2}{dt} = 2B_2 M_1^2 & \left\{ [1 + g_0(u)]\left(1 + \frac{M_{2/3}M_{4/3}}{M_1^2}\right) + g_1(u)u\left(\frac{M_2 M_0}{M_1^2} + \frac{M_{5/3}M_{4/3}M_0}{M_1^3} - 1 - \frac{M_{2/3}M_{4/3}}{M_1^2}\right)\right. \\
& + g_2(u)u^2\left(\frac{M_3 M_0^2}{M_1^3} + \frac{M_{8/3}M_{4/3}M_0^2}{M_1^4} + 1 + \frac{M_{2/3}M_{4/3}}{M_1^2}\right. \\
& \left.\left. - 2\frac{M_2 M_0}{M_1^2} - \frac{M_{5/3}M_{4/3}M_0}{M_1^3}\right)\right\}
\end{aligned}
$$

with the constant $B_2 = 2k_B T/3\mu$. Using the Taylor series expansion, the higher and fractal particle moment can be calculated by the first three-particle moments M_0, M_1, and M_2 [9]:

$$M_k = \frac{1}{2}u^{k-2}k(k-1)M_2 - u^{k-1}k(k-2)M_1 + \frac{1}{2}u^k(k-1)(k-2)M_0 \tag{10}$$

Their accuracy has been discussed in our previous work [10, 11], and then the ordinary differential equations for particle moment can be obtained:

$$\frac{\mathrm{d}M_0}{\mathrm{d}t} = -B_2 M_0^2 \left\{ \begin{array}{l} \frac{1}{81}[1-g_0(u)](2M_C^2 - 13M_C + 151) \\ -\frac{1}{27}g_1(u)u(M_C^2 - 11M_C + 10) \\ +\frac{1}{9}g_2(u)u^2(M_C^2 - 20M_C + 19) \end{array} \right.$$

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = 0 \tag{11}$$

$$\frac{\mathrm{d}M_2}{\mathrm{d}t} = 2B_2 M_1^2 \left\{ \begin{array}{l} \frac{1}{81}[1-g_0(u)](2M_C^2 - 13M_C + 151) \\ -\frac{1}{27}g_1(u)u(4M_C^2 - 37M_C + 41) \\ +\frac{2}{9}g_2(u)u^2(M_C^2 - 7M_C + 8) \end{array} \right.$$

with the dimensionless particle moment $M_C = M_0 M_2 / M_1^2$. The geometric standard deviation, σ, of particle size distribution is the function of dimensionless particle moment can be noted as $\ln^2\sigma = \ln(M_C)/9$ [2]. The ordinary differential eq. (11) can be solved numerically with fourth Runge-Kutta method with its initial conditions [9, 12].

Simplified moment model

In the case of neglecting the non-linear term in the slip correction factor, the functions g_0, g_1, and g_2 are simplified:

$$g_0(u) = \frac{BA_1}{u^{1/3}}; \quad g_1(u)u = \frac{1}{3}\frac{BA_1}{u^{1/3}}; \quad g_2(u)u^2 = \frac{2}{9}\frac{BA_1}{u^{1/3}} \tag{12}$$

and the corresponding moment model is reduced to:

$$\frac{\mathrm{d}M_0}{\mathrm{d}t} = -B_2 M_0^2 \left[\frac{1}{81}(2M_C^2 - 13M_C + 151) - \frac{1}{81}\frac{BA_1}{u^{1/3}}(5M_C^2 - 64M_C + 103) \right]$$

$$\frac{\mathrm{d}M_1}{\mathrm{d}t} = 0 \tag{13}$$

$$\frac{\mathrm{d}M_2}{\mathrm{d}t} = 2B_2 M_1^2 \left[\frac{1}{81}(2M_C^2 - 13M_C + 151) - \frac{1}{81}\frac{BA_1}{u^{1/3}}(2M_c^2 - 4M_C + 160) \right]$$

The simplified moment model is that Yu *et al.* [9] have obtained in their work, but with a little difference in the coefficient (*i. e.*, $A_1 = 1.257$ or $A_1 = 1.165$, but $A = 1.591$).

In some cases, the collision kernel may be written [13]:

$$\beta = B_2 C_c(u)(\upsilon_i^{-1/3} + \upsilon_j^{-1/3})(\upsilon_i^{1/3} + \upsilon_j^{1/3}) \tag{14}$$

which means

$$C_c(\upsilon_i) \approx C_c(\upsilon_j) \approx C_c(u) \tag{15}$$

It is only suitable for narrow particle size distribution or small Knudsen number. And the corresponding ordinary differential equation for particle moment evolution can be simplified:

$$\frac{dM_0}{dt} = \frac{(2M_C^2 - 13M_C + 151)}{81} B_2 M_0^2 C_c(u)$$
$$\frac{dM_1}{dt} = 0 \qquad\qquad\qquad\qquad\qquad (16)$$
$$\frac{dM_2}{dt} = \frac{2(2M_C^2 - 13M_C + 151)}{81} B_2 M_1^2 C_c(u)$$

The asymptotic analysis of moment model

It can be found that:

$$\lim_{t \to \infty} u = \lim_{t \to \infty} \frac{M_1}{M_0} = \infty; \ \lim_{u \to \infty} g_0(u) = 0; \ \lim_{u \to \infty} g_1(u)u = 0; \ \lim_{u \to \infty} g_2(u)u^2 = 0; \ \lim_{t \to \infty} C_c(u) = 1 \ (17)$$

then the particle moment evolution eq. (11) and its simplified models, eqs. (13) and (16), are also reduced to the same as the moment model in the continuum regime, and its analytical and asymptotic solutions have been obtained by Xie and He [14] and Xie and Wang [8], respectively.

Discussion and conclusions

In the present study, we have proposed an improved moment model for particle PBE in the continuum-slip regime. This model can be simplified to the existing models in the literatures [7, 9] using the linearized slip correction factor. It has the same asymptotic behavior as that in the continuum regime. The linearized moment model becomes simpler so that its analytical solution can be obtained. Due to the introduction of non-linear terms in the slip correction factor, the analytical solution of present moment model is difficult to obtain. Even if the analytical solution is obtained with some special mathematical technique, *e. g.*, the exponential function substituted by a polynomial or a Taylor series [14], it can only proof that the present model has some advantages in mathematics, but the structure of the analytical solution will become too complicated to be used in practice. Moreover, the expansion of the exponent function will bring more constraints in physics and mathematics, which makes the effective interval for particle dimensionless moment, M_C, of the analytical solution much smaller [7, 11, 14]. In theory, the geometric standard deviation of aerosol particle size distribution can be an arbitrary value; this confined interval of M_C reveals the inherent drawback in the moment method.

Another reason for the unnecessary to obtain the present model's analytical solution is that the relative error of the solution becomes much larger at high Knudsen number. In essence, the slip correction factor is a drag correction [15], rather than the correction of the collision kernel itself. Although the corrected formula of particle resistance in fluid can be well applied in the wide range from free molecular to continuum regime, the collision kernel based on the slip correction factor will become infinite and unreasonable in physics at higher Knudsen number. Our previous works [16], have provides a useful attempt to deal with the non-physical phenomenon, but the analysis and calculation of the moment model have introduced some empirical formula. A better approach of mathematical physics to calculate the moment model accurately across the entire particle size regime will be presented in the future.

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