

A BIMODAL TEMOM MODEL FOR PARTICLE BROWNIAN COAGULATION IN THE CONTINUUM-SLIP REGIME

by

Qing HE, Jin LI, Tingting KONG, and Mingliang XIE*

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology,
Wuhan, China

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In this paper, a bimodal Taylor-series expansion moment of method is proposed to deal with Brownian coagulation in the continuum-slip regime, where the non-linear terms in the Cunningham correction factor is approximated by Taylor-series expansion technology. The results show that both the number concentration and volume fraction decrease with time in the smaller mode due to the intra and inter coagulation, and the asymptotic behavior of the larger mode is as same as that in the continuum regime.

Key words: *modal aerosol dynamics, Taylor-series expansion, moment method, continuum-slip continuum*

Introduction

Aerosol particles are increasingly recognized as one of the most common unhealthy components of air pollution, it has an awful impact not only on the environment but also on the health of human beings. Meanwhile, there is also a strong relationship between visibility and particle size distribution (PSD), especially the particle size from 0.1 to 100 μm [1]. Particle evolution involves a wide range of physical-chemical reaction process, and the detailed information of PSD can be derived from the particle balance equation (PBE), which is characterized as the Smoluchowski equation of irreversible coagulation in terms of one-particle density depending on particle size and time:

$$\frac{\partial n(v, t)}{\partial t} + \frac{1}{2} \int_0^v \beta(v_1, v - v_1) n(v_1, t) n(v - v_1, t) dv_1 - \int_0^\infty \beta(v_1, v) n(v, t) n(v_1, t) dv_1 \quad (1)$$

where $n(v, t)$ is the number density concentration of the particles with volume from v to $v + dv$ at time t , and $\beta(v, v_1)$ is the collision frequency function between particles with volume v and v_1 .

The equation is usually dissolved by numerical method due to the complicated non-linear partial differential-integral construct, such as the moment method. It is to transform the PBE into a series of moment equations and has become a powerful tool for investigating aerosol microphysical processes in most cases for its relative simplicity of implementation and low computational cost, even though it is the particle moment obtained but not the real PSD. Recently, Yu *et al.* [2] proposed a new moment method called as the Taylor-series expansion mo-

* Corresponding author; e-mail: mlxie@mail.hust.edu.cn

ment of method (TEMOM), which could achieve the closure of moment equations without any other prior assumption of PSD, and has been recognized as a promising method [3-5].

Most studies focus on the evolution of particle systems with unimodal size distribution, which limits the application of these technologies in some cases, for example, a smaller nucleation mode with newly formed particles and a larger accumulation mode with particles generated earlier may coexist when the particle formation is not instantaneous [6, 7]. Moreover, removing fine particles through inter-coagulation with coarse particles also can't be represented by a unimodal model because of the wide range of PSD [8]. Modal aerosol dynamics (MAD) models represent the PSD as a sum of two or more distinct modes, in which each mode is represented by a separate size distribution function and governed by the PBE [9]. This method is successfully performed for particles undergoing nucleation, coagulation, and surface growth simultaneously with the assumption that the PSD of each mode is monodisperse or log-normal distribution [7, 10]. In the framework of moment method, Lin and Gan [11] firstly investigated the Brownian coagulation of particles in the entire size regime with initial bimodal log-normal distribution. Recently, MAD models are applied to the TEMOM model in both the (near) continuum regime and free molecule regime for Brownian coagulation and agglomeration [12-14]. In this work, we will propose an improved bimodal TEMOM model for Brownian coagulation in the continuum-slip regime without neglecting the non-linear terms in the Cunningham correction factor.

Modal and theory

For a bimodal model composed of mode i (the smaller mode) and mode j (the larger mode), the number density concentration can be expressed as: $n(v, t) = n_i(v, t) + n_j(v, t)$, and the corresponding Smoluchowski equation takes the following form:

$$\frac{\partial [n_i(v, t) + n_j(v, t)]}{\partial t} = \frac{1}{2} \int_0^v \beta(v_1, v - v_1) [n_i(v_1, t) + n_j(v_1, t)] [n_i(v - v_1, t) + n_j(v - v_1, t)] dv_1 - \int_0^v \beta(v, v_1) [n_i(v, t) + n_j(v, t)] [n_i(v_1, t) + n_j(v_1, t)] dv_1 \quad (2)$$

The k^{th} order moment is defined: $M_k = \int_0^\infty v^k n(v) dv$, and M_0 represents the total particle number concentration and M_1 the total particle volume fraction, while M_2 is a poly-dispersity variable and $v = M_1/M_0$ is the mean volume, noting that the initial condition is $M_{00}, M_{10}, M_{20}, u_0$. Then eq. (2) can be transformed into two sets of moment equations with the assumption that the newborn particles produced by inter-coagulation between particles in mode i and j belong to the larger mode j ,

$$\frac{dM_{ik}}{dt} = \frac{1}{2} \int_0^\infty \int_0^\infty [(v - v_1)^k + v^k - v_1^k] \beta(v, v_1) n_i(v, t) n_i(v_1, t) dv dv_1 - \int_0^\infty \int_0^\infty v^k \beta(v, v_1) n_i(v, t) n_j(v_1, t) dv dv_1 \quad (3a)$$

$$\frac{dM_{jk}}{dt} = \frac{1}{2} \int_0^\infty \int_0^\infty [(v - v_1)^k + v^k - v_1^k] \beta(v, v_1) n_j(v, t) n_j(v_1, t) dv dv_1 + \int_0^\infty \int_0^\infty [(v - v_1)^k + v^k - v_1^k] \beta(v, v_1) n_i(v, t) n_j(v_1, t) dv dv_1 \quad (3b)$$

Obviously, the first term in the right side of eqs. 3(a) or 3(b) represents intra-coagulation in mode i or j and has no difference with the original unimodal moment equations, while the second term indicates the change by particle migration from mode i to mode j due to inter-coagulation.

In the continuum-slip regime, the collision kernel function can be expressed:

$$\beta(v, v_1) = B_2 [C(v)v^{1/3} C(v_1)v_1^{1/3}] (v^{1/3} + v_1^{1/3}) \quad (4)$$

in which $B_2 = 2K_b T/3\mu$, K_b is the Boltzmann's constant, T – the temperature, μ – the gas viscosity, and C – the Cunningham correction factor:

$$C = 1 + \text{Kn} \left(A_1 + A_2 \exp \frac{A_3}{\text{Kn}} \right) \quad (5)$$

where $\text{Kn} = \lambda/r$ is Knudsen number defined as the ratio of the molecular mean free path length to the particle radius; $A_1 = 1.165$, $A_2 = 0.483$, and $A_3 = 0.997$ [15]. In some works, the non-linear term in C is neglected, then C can be approximated as $(1 + A\text{Kn})$ with $A = 1.591$ in case of $\text{Kn} < 5$ [13, 16, 17]. Knudsen number can also be written: $\text{Kn}_0(u_0/v)^{1/3}$ if Kn_0 is set to be $\lambda/(3u_0/4\pi)^{1/3}$, thus we can approximate the non-linear term $g(v) = \exp[-A_3(v/u_0)^{1/3}/\text{Kn}_0]$ at the point u using the Taylor-series expansion:

$$g(v) = g(u) + g'(u)(v - u) + \frac{1}{2} g''(u)(v - u)^2 + \dots \quad (6)$$

in which $g(u)$, $g'(u)$, $g''(u)$ are the zeroth, first and second derivative of $g(v)$, respectively. Truncate the right side of eq. (6) at the first three terms, and then C can be arranged:

$$C(v) = 1 + f_0(u)v^{5/3} + f_1(u)v^{2/3} + f_2(u)v^{-1/3} \quad (7)$$

where $f_0(u)$, $f_1(u)$, and $f_2(u)$ are functions of u :

$$\begin{aligned} f_0(u) &= \frac{1}{18} \frac{A_2 A_3}{\text{Kn}_0} u^{5/3} + A_3 \frac{u}{u_0} + 2\text{Kn}_0 g(u); \\ f_1(u) &= \frac{1}{9} \frac{A_2 A_3}{\text{Kn}_0} u^{2/3} + A_3 \frac{u}{u_0} + 5\text{Kn}_0 g(u); \\ f_2(u) &= \frac{1}{18} \frac{A_2 A_3}{\text{Kn}_0} u^{1/3} + A_3 \frac{u}{u_0} + 8\text{Kn}_0 \frac{18\text{Kn}_0^2}{A_3} \frac{u}{u_0} + g(u) + A_1 \text{Kn}_0 u_0^{1/3} \end{aligned} \quad (8)$$

Together with the eqs. (3-5), (7), the first three-order bimodal TEMOM model in the continuum-slip regime can be expressed as ($k = 0, 1, 2$):

$$\begin{aligned} \frac{dM_i^k}{dt} &= B_2 \sum_{l=0,1,2} [a_{kl} f_l(ui) - b_{kl} f_l(uj)] - c_i^k \\ \frac{dM_j^k}{dt} &= B_2 \sum_{l=0,1,2} [a_{kl} f_l(ui) - b_{kl} f_l(uj)] - c_j^k \end{aligned} \quad (9)$$

where $a_{i0l} = -(M_{i0} + M_{j0})M_{i_{5/3-l}} - (M_{i_{1/3}} + M_{j_{1/3}})M_{i_{4/3-l}}$, $a_{i1l} = -a_{j1l} = -(M_{i_{7/3-l}}M_{j_{1/3}} + M_{i_{8/3-l}}M_{j_0})$; $a_{i2l} = 2M_{i_1}M_{i_{8/3-l}} + 2M_{i_{4/3}}M_{i_{7/3-l}} - M_{i_{10/3-l}}M_{j_{1/3}} - M_{i_{11/3-l}}M_{j_0}$; $a_{j0l} = 0$; $a_{j2l} = 2M_{i_{7/3-l}}M_{j_{4/3}} + 2M_{i_{8/3-l}}M_{j_1} + M_{i_{10/3-l}}M_{j_{1/3}} + M_{i_{11/3-l}}M_{j_0}$; $b_{i0l} = -(M_{i_k}M_{j_{5/3-l}} + M_{i_{k+1/3}}M_{j_{4/3-l}})$; $b_{j0l} = -(M_{j_0}M_{j_{5/3-l}} + M_{j_{1/3}}M_{j_{4/3-l}})$; $b_{j1l} = -b_{i1l}$; $b_{j2l} = 2M_{j_1}M_{j_{8/3-l}} + 2M_{j_{4/3}}M_{j_{7/3-l}} + 2M_{i_1}M_{j_{8/3-l}} + 2M_{i_{4/3}}M_{j_{7/3-l}} + M_{i_2}M_{j_{5/3-l}} + M_{i_{7/3}}M_{j_{4/3-l}}$; $c_{i0} = -(M_{i0} + M_{j0})M_{i0} - (M_{i_{1/3}} + M_{j_{1/3}})M_{i_{-1/3}} - M_{i0}M_{j0} - M_{i_{1/3}}M_{j_{-1/3}}$; $c_{i1} = -c_{j1} = -(2M_{i_1}M_{j_0} + M_{i_{2/3}}M_{j_{1/3}} + M_{i_{4/3}}M_{j_{-1/3}})$; $c_{i2} = 2M_{i_1}^2 + 2M_{i_{2/3}}M_{i_{4/3}} - 2M_{i_2}M_{j_0} - M_{i_{5/3}}M_{j_{1/3}} - M_{i_{7/3}}M_{j_{-1/3}}$; $c_{j0} = -(M_{j_0}^2 + M_{j_{1/3}}M_{j_{-1/3}})$; $c_{j2} = 2M_{j_1}^2 + 2M_{j_{2/3}}M_{j_{4/3}} + 2M_{i_{2/3}}M_{j_{4/3}} + 4M_{i_1}M_{j_1} + 2M_{i_{4/3}}M_{j_{2/3}} + M_{i_{5/3}}M_{j_{1/3}} + 2M_{i_2}M_{j_0} + M_{i_{7/3}}M_{j_{-1/3}}$. The fractional moments can be approximated by combination of the first three integral moments:

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

Now the bimodal TEMOM model for particles by Brownian coagulation in the continuum-slip regime is gotten. Obviously, all the terms like as $Mi_{k1} Mi_{k2}$ or $Mj_{k1} Mj_{k2}$ represent the intra-coagulation in mode i or mode j , and the other terms like as $Mi_{k1} \cdot Mj_{k2}$ indicate the inter-coagulation of particles between mode i and mode j . Moreover, the value of (dMi_1/dt) is opposite to that of (dMj_1/dt) due to the total mass conservation requirement. If all of the terms $(Mi_{k1} Mj_{k2})$ are ignored, which means the inter-coagulation is not considered, the bimodal model will reduce to a unimodal model.

Discussion and results

To simplify the computation, eq. (9) is non-dimensionalized through the following relations: $M_0^* = M_0/M_{00}$, $M_1^* = M_1/M_{10}$, $M_2^* = M_{C0}M_2/M_{20}$, $t^* = tB_2M_{00}$, $u^* = u/u_0$, where the dimensionless moment M_C is defined as $M_C = M_0M_2/M_1^2$, then the numerical solution can be obtained easily by means of fourth-order Runge-Kutta method with $\Delta t^* = 1e-2$. Note that the initial condition of mode i is $Mi_{00} = 1$, $Mi_{10} = 1$, $Mi_{20} = 4/3$ (the star symbol '*' is omitted thereafter), and the ratio of initial total number concentration, mean particle volume and M_C of mode j to mode i is set as $a = Mj_{00}/Mi_{00}$, $b = (Kni_0/Knj_0)^3$, and $c = [\ln(Mj_{C0})/\ln(Mi_{C0})]^{1/2}$, respectively, thus the first and second moment of mode j can be expressed: $Mj_{10}/Mi_{10} = a^*b$, $Mj_{20}/Mi_{20} = a^*b^{2*} Mi_{C0}(2^*c^2 - 2)$. In all of the cases, we set that $Kni_0 = 1$ and $c = 1$.

From fig. 1, we can see that both Mi_0 and Mi_1 decreases rapidly with a higher number concentration of mode j , especially in the earlier stage of coagulation, but the large Mj_0 also leads to greater decay rate of particle number concentration in mode j which will bring less effect on mode i as time goes on. With a reducing to 0.01, the discrepancy caused by different Knj_0 is very small, that means the number concentration plays a dominant role in inter-coagulation. But when a is larger than 0.1, the effect of particle size can not be neglected, at this point larger particle size difference results in increasing collision kernel function will enhance coagulation observably. Moreover, a larger particle from mode j provides a larger cross-section surface area which will also accelerate the coagulation rate. For convenience, the evolution of mode i is ignored when Mi_1 is small enough, such as less than $1e-5$.

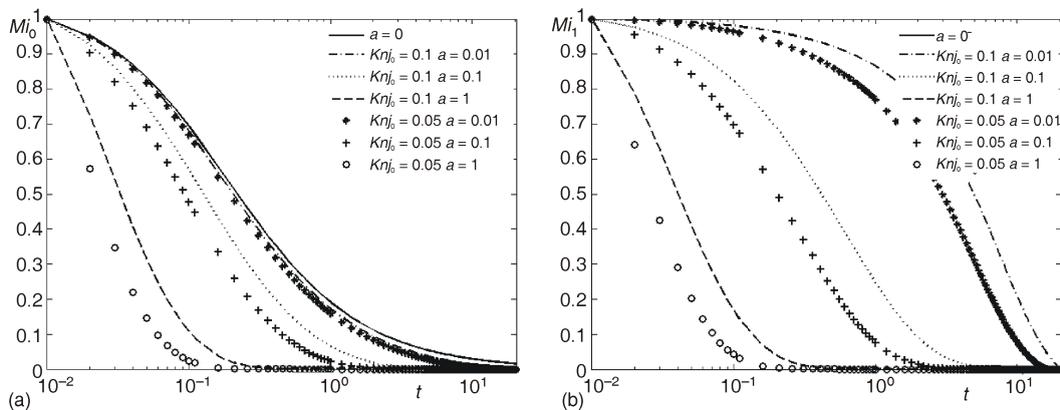


Figure 1. The particle moment evolution of mode i with different mode j ; (a) Mi_0 ; (b) Mi_1

Figure 2 shows the particle moment evolution of mode j with different Knj_0 and a , and the results of Mj_0, Mj_1, Mj_2 are normalized as $Mj_k(t)/Mj_k(0)$ for convenience. The decrease of Mj_0 is because of the intra-coagulation in mode j and mainly depends on the initial particle number, while the inter-coagulation has no direct effect on Mj_0 due to the assumption that the newborn particles belong to mode j , but the contribution to mean particle volume may have an influence. When $Knj_0 < 0.1$, the characteristic of mode j can be treated as the same as that in continuum regime (usually defines as $Kn < 1$ or 0.1), and the change caused by Knj_0 varying is negligible. The Mj_1 is increasing for the reason of particle migration from mode i to mode j , which will result in decreasing Mi_0 and Mi_1 and then weaken the significance of inter-coagulation, thus Mj_1 will tend to a constant $[Mj_1(0) + Mi_1(0)]$ as time advances. In fig. 2(d), the dimensionless moment Mj_C tends to two at long time, which is as the same as that of a unimodal model in the continuum regime [18].

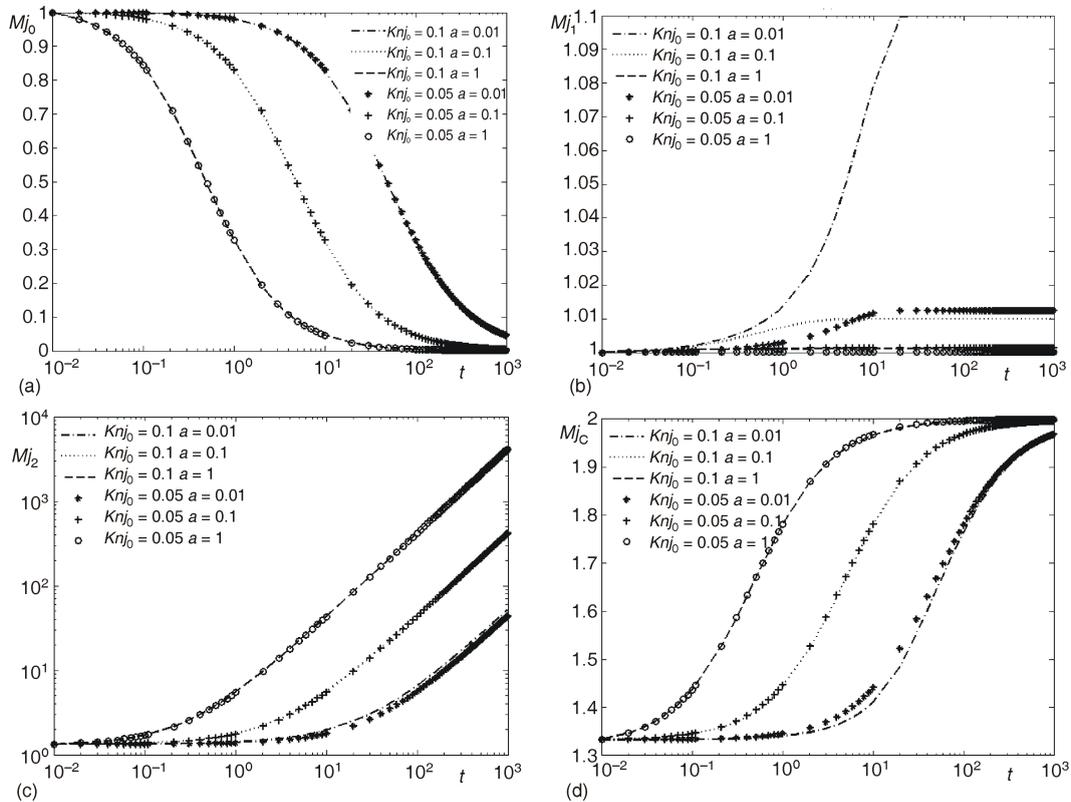


Figure 2. The particle moment evolution of mode j with different Knj_0 and a ;
 (a) Mj_0 ; (b) Mj_1 ; (c) Mj_2 ; (d) Mj_C

Conclusion

In this work, we propose a bimodal TEMOM model for Brownian coagulation in the continuum-slip regime without neglecting the non-linear terms in the Cunningham correction factor. The results show that number concentration is expected to have a major contribution to inter-coagulation, and the volume fraction of mode i will decrease with time due to the inter-co-

agulation. For mode j , the decrease of number concentration is only caused by the intra-coagulation, while the inter-coagulation will result in the increasing volume fraction. As time advances, the Mi_0 and Mi_1 become less and less, as well as the weakened effect of mode i on inter-coagulation, thus the evolution of mode j will tend to that of a unimodal model, and the asymptotic behavior becomes the same as that in the continuum regime.

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