STEADY-STATE SOLUTIONS FOR PARTICLES UNDERGOING BROWNIAN COAGULATION AND BREAKAGE BY THE TEMOM MODEL

by

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When coagulation and breakage proceed simultaneously, a steady-state distribution may exist due to the opposite effects on particle size. In this paper, a moment model using Taylor-series expansion technology for particles undergoing Brownian coagulation and equal size multiple breakage is proposed, then the steady-state solutions of this model are obtained.

Key words: *Brownian coagulation, breakage, steady-state solution, moment model*

Introduction

Particle coagulation and breakage play an important role in many fields of aerosol science, and may occur simultaneously in some cases, such as the last steps of nucleation, combustion, and molecular growth [1, 2]. The earliest studies about these problems usually focused either on coagulation or breakage alone, except the well-known Blatz-Tobolsky model [3]. Using a similarity transform, the asymptotic solutions for Brownian coagulation both in the continuum and free molecule regime and breakage with a power-law breakage rate kernel at long times are obtained respectively [4-6]. Furthermore, Pulvermacher and Ruckenstein [7] shows that the similarity transform can be also explored to homogenous coagulation kernels.

When coagulation and breakage simultaneously occur, a steady-state distribution may exist due to the competition between these two processes. Considering some simple kernels, Vigil and Ziff [8] conjectured that the stable condition should satisfy $1 + \eta - \lambda > 0$ for particle systems with homogeneous rate kernels of order η (fragmentation) and λ (coagulation). Then Diemer and Olson [9] explored similarity transform to more general coagulation kernels, and yield the steady-state distribution for very large and very small particles.

With the relative simple construction, the Taylor-series expansion method of moments (TEMOM) has a great advantage on the analytical and asymptotic analysis of particle size evolution [10-23]. In this paper, we will develop a TEMOM model considering Brownian coagulation both in the free molecule and continuum regime in coincidence with an equal size multiple breakage process, and the corresponding steady-state solutions are obtained.

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Mathematical model

The particle balance equations for particles undergoing coagulation and breakage can be represented:

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

$$+\int_v^\infty a(v_1)b(v;v_1)n(v_1,t)\mathrm{d}v_1-a(v)n(v,t) \tag{1}$$

where $n(\upsilon, t)\mathrm{d}\upsilon$ is the number of particles per unit spatial volume with particle volume from υ to $\upsilon + \mathrm{d}\upsilon$ at time t, β – the collision kernel of coagulation, $a(\upsilon)$ – the breakage rate kernel, $b(\upsilon, \upsilon_1)$ – the probability of making a daughter of size υ from a parent of size υ_1. The first two terms of RHS represent the birth and death of particles with volume υ due to coagulation respectively and the latter two terms for breakage. With the definition of k^{th} order moment M_k:

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

equation (1) can be transformed into a set of moment equations:

$$\frac{\partial M_k}{\partial t}=\frac{1}{2}\int_0^\infty\int_0^\infty\left[(\upsilon+\upsilon_1)^k-\upsilon^k-\upsilon_1{}^k\right]\beta(\upsilon,\upsilon_1)n(\upsilon,t)n(\upsilon_1,t)\mathrm{d}\upsilon\mathrm{d}\upsilon_1+$$

$$+\int_0^\infty \upsilon^k\int_0^\infty a(\upsilon_1)b(\upsilon,\upsilon_1)n(\upsilon_1,t)\mathrm{d}\upsilon_1\mathrm{d}\upsilon-\int_0^\infty \upsilon^k a(\upsilon)n(\upsilon,t)\mathrm{d}\upsilon \tag{3}$$

There are several different mechanisms which lead to particle coagulation and breakage, for example, Brownian coagulation based on the random motion of particles, shear coagulation resulted from the fluid viscosity gradient, and a summary of breakage can be found in [24]. Here the Brownian coagulation in the free molecule and continuum regime and the self-similar equal size breakage with a power-law breakage rate are considered, in which cases the kernels are:

$$\beta_{FM}=B_1\sqrt{\frac{1}{\upsilon}+\frac{1}{\upsilon_1}}\left(\sqrt[3]{\upsilon}+\sqrt[3]{\upsilon_1}\right)^2 \tag{4a}$$

$$\beta_{CR}=B_2\left(\frac{1}{\sqrt[3]{\upsilon}}+\frac{1}{\sqrt[3]{\upsilon_1}}\right)\left(\sqrt[3]{\upsilon}+\sqrt[3]{\upsilon_1}\right) \tag{4b}$$

$$a(\upsilon)=k_1\upsilon^\eta \tag{4c}$$

$$\begin{aligned}&b(\upsilon;\upsilon_1)=l;\quad \upsilon=\frac{\upsilon_1}{l}\\&b(\upsilon;\upsilon_1)=0;\quad \text{otherwise}\end{aligned} \tag{4d}$$

where the constants $B_1 = (3/4\pi)^{1/6}(6k_BT/\rho_p)^{1/2}$ and $B_2 = 2k_BT/3\mu$, k_B is the Boltzmann's constant, T – the temperature, ρ_p – the particle density, μ – the gas viscosity, k_1 is a constant independent of particle size, and η ranges between 0 and 1, l ($l \geq 2$) – the number of daughter particles υ resulting from a breakage event of a single particle with volume υ_1. The TEMOM models for Brownian coagulation have been investigated in many studies [12, 15, 20], and now only a brief derivation for breakage process is showed. Substituting eqs. (4c) and (4d) into eq. (3), we can get:

$$\left.\frac{\partial M_0}{\partial t}\right|_{BR} = (l-1)k_1 M_\eta ; \left.\frac{\partial M_1}{\partial t}\right|_{BR} = 0; \left.\frac{\partial M_2}{\partial t}\right|_{BR} = (l^{-1}-1)k_1 M_{\eta+2} \tag{5}$$

Using the three order Taylor-series expansion approximation, the k^{th} fractional order moment can be approximated as [20, 25]:

$$M_k = \frac{M_1^k}{M_0^{k-1}}\left[1 + \frac{k(k-1)(M_C-1)}{2}\right] \tag{6}$$

where $M_C = M_0M_2/M_1^2$ is a dimensionless moment indicating the dispersity of the system. Thus eq. (5) can be enclosed without any prior assumption about the particle size distribution:

$$\begin{aligned}
\left.\frac{\mathrm{d}M_0}{\mathrm{d}t}\right|_{BR} &= \frac{k_1(l-1)}{2}\left(\frac{M_1}{M_0}\right)^\eta M_0\left[\eta(\eta-1)M_C - (\eta+1)(\eta-2)\right] \\
\left.\frac{\mathrm{d}M_1}{\mathrm{d}t}\right|_{BR} &= 0 \\
\left.\frac{\mathrm{d}M_2}{\mathrm{d}t}\right|_{BR} &= -\frac{k_1(l-1)}{2l}\left(\frac{M_1}{M_0}\right)^\eta \frac{M_1^2}{M_0}\left[(\eta+1)(\eta+2)M_C - \eta(\eta+3)\right]
\end{aligned} \tag{7}$$

Steady-state solution of TEMOM model in the free molecule regime with breakage

Whether the steady-state distribution exists depends on the ratio γ of $\mathrm{d}M_0/\mathrm{d}t_{FM}$ to $\mathrm{d}M_0/\mathrm{d}t_{BR}$:

$$\gamma = \left|\frac{\sqrt{2}B_1}{2592k_1} f(M_C, \eta, l) M_0^{5/3+\eta}\right| \tag{8}$$

where $f(M_C, \eta, l)$ is a function of M_C, l and η:

$$f(M_C, \eta, l) = \frac{65{M_C}^2 - 1210M_C - 9223}{(l-1)M_1^{\eta-1/6}\left[(\eta+1)(2-\eta) - \eta(1-\eta)M_C\right]} \tag{9}$$

For a given case, l and η are invariable and M_C tends to a constant at long time, which means $f(M_C, \eta, l)$ is also a fixed value. Thus the ratio γ can be simplified:

$$\gamma \propto M_0^{5/3+\eta} \tag{10}$$

When $\gamma > 1$, that means the rate of coagulation is larger than that of breakage and M_0 decreases, then γ will decrease. When $\gamma < 1$, that means the rate of coagulation is smaller than that of breakage, and γ will increase as M_0 increases. This suggests that the evolution tends to an equilibrium state at which $\gamma = 1$, and in this case we can get:

$$-\frac{\sqrt{2}B_1(65M_C^2-1210M_C-9223)M_1^{1/6}M_0^{11/6}}{5184}=$$
$$=\frac{k_1(l-1)}{2}\left(\frac{M_1}{M_0}\right)^{\eta}M_0\left[\eta(\eta-1)M_C-(\eta+1)(\eta-2)\right]-$$
$$-\frac{\sqrt{2}B_1(701M_C^2-4210M_C-6859)M_1^{11/6}M_2^{1/6}}{2592M_C^{1/6}}=$$
$$=\frac{k_1(l-1)}{2l}\left(\frac{M_1}{M_0}\right)^{\eta}\frac{M_1^2}{M_0}\left[(\eta+1)(\eta+2)M_C-\eta(\eta+3)\right] \tag{11}$$

Divide the first equation of eq. (11) by the second one for both the sides, a third-order algebraic equation of M_C can be obtained after some operation:

$$c_1M_C^3+c_2M_C^2+c_3M_C+c_4=0 \tag{12}$$

in which the coefficients c_1, c_2, c_3, and c_4 are:

$$\begin{aligned}
c_1&=-1402l\eta^2+65\eta^2+1402l\eta+195\eta+130\\
c_2&=9822l\eta^2-1275\eta^2-9822l\eta-3825\eta-2804l-2420\\
c_3&=5298l\eta^2-8013\eta^2-5298l\eta-24039\eta+16840l-18446\\
c_4&=-13718l\eta^2+9223\eta^2+13718l\eta+27669\eta+27436l
\end{aligned} \tag{13}$$

Its solution can be obtained as [14]:

$$M_C=\frac{1}{6c_1}\left[(d_1+d_2)^{1/3}-\frac{4d_3}{(d_1+d_2)^{1/3}}-2c_2\right] \tag{14}$$

where the parameters d_1, d_2, and d_3 are:

$$\begin{aligned}
d_1&=12c_1\sqrt{3(27c_1^2c_4^2-18c_1c_2c_3c_4+4c_1c_3^3+4c_2^3c_4-c_2^2c_3^2)}\\
d_2&=-108c_1^2c_4+36c_1c_2c_3-8c_2^3\\
d_3&=3c_1c_3-c_2^2
\end{aligned} \tag{15}$$

Then the solution of M_0 and M_2 can be also gotten together with eq. (11). The relationship between M_C and η with different l at a steady-state are showed in fig. 1(a). In general, we observe that M_C decreases monotonically when l equals to 2 with η varying from 0 to 1, but for a larger l, M_C will decrease first and then increase.

Steady-state solution of TEMOM model in the continuum regime with breakage

In this case the ratio γ of $\mathrm{d}M_0/\mathrm{d}t_{CR}$ to $\mathrm{d}M_0/\mathrm{d}t_{BR}$ is:

$$\gamma\propto M_0^{1+\eta} \tag{16}$$

This suggests that the evolution will also tend to an equilibrium-state and steady-state equation can be written:

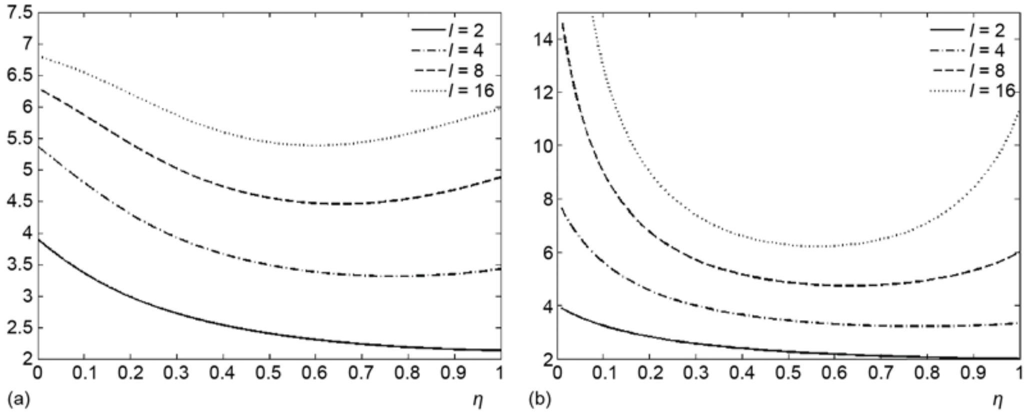

Figure 1. The relationship between M_C and η with different l at a steady-state; (a) in the free molecule regime, (b) in the continuum regime

$$-\frac{B_2(2M_C{}^2-13M_C-151)M_0{}^2}{81}=\frac{k_1(l-1)}{2}\left(\frac{M_1}{M_0}\right)^{\eta}M_0\left[\eta(\eta-1)M_C-(\eta+1)(\eta-2)\right] \quad (17a)$$

$$-\frac{2B_2(2M_C{}^2-13M_C-151)M_1{}^2}{81}=\frac{k_1(l-1)}{2l}\left(\frac{M_1}{M_0}\right)^{\eta}\frac{M_1^2}{M_0}\left[(\eta+1)(\eta+2)M_C-\eta(\eta+3)\right] \quad (17b)$$

With the same derivations, we can get:

$$M_C=\frac{2l(\eta+1)(\eta-2)-\eta(\eta+3)}{2l\eta(\eta-1)-(\eta+1)(\eta+2)} \quad (18)$$

The results are showed in fig. 1(b), which have the similar varying curves but with steeper slope as those in the free molecule regime, especially for a larger *l*.

Conclusion

In this work, the steady-state solutions for particles undergoing Brownian coagulation and breakage are proposed based on TEMOM model. The results imply that the increasing of the number of daughter particles from a breakage event would enhance the dispersity of the system, and in the continuum regime, the effect of η on M_C is more strengthened than that in the free molecule regime.

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