THE ASYMPTOTIC STABILITY OF THE TAYLOR-SERIES EXPANSION METHOD OF MOMENT MODEL FOR BROWNIAN COAGULATION

by

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In the present study, the linear stability of population balance equation due to Brownian motion is analyzed with the Taylor-series expansion method of moment. Under certain conditions, the stability of the Taylor-series expansion method of moment model is reduced to a well-studied problem involving eigenvalues of matrices. Based on the principle of dimensional analysis, the perturbation equation is solved asymptotically. The results show that the Taylor-series expansion method of moment model is asymptotic stable, which implies that the asymptotic solution is uniqueness, and supports the self-preserving size distribution hypothesis theoretically.

Key words: *linear stability, moment method, population balance equation, Brownian motion; asymptotic solution*

Introduction

The population balance equation (PBE) forms a general mathematical framework for modeling of particulate systems in a wide range of physical [1], technological and environmental applications. In a spatially homogeneous system, the PBE reads:

$$\frac{\partial n(\upsilon,t)}{\partial t}=\frac{1}{2}\int\limits_0^{\nu}\beta(\upsilon_1,\upsilon-\upsilon_1)n(\upsilon_1,t)n(\upsilon-\upsilon_1,t)\mathrm{d}\upsilon_1-\int\limits_0^{\infty}\beta(\upsilon_1,\upsilon)n(\upsilon,t)n(\upsilon_1,t)\mathrm{d}\upsilon_1 \tag{1}$$

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, and β – the collision frequency function of coagulation. Generally, the PBE with physically complicate kernels (*e. g.* Brownian coagulation) are not solvable directly. The moment method is a preferred tool to investigate the PBE numerically [2-5]. In mathematically, the moment method is a kind of integral transformation defined as:

$$M_k=\int\limits_0^{\infty}\upsilon^k n(\upsilon)\,\mathrm{d}\upsilon_1 \tag{2}$$

The PBE can be converted to moment equation as:

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

Recently, Yu *et al.* [5, 6] have proposed a moment-based approach the Taylor-series expansion method of moment (TEMOM) to approximate PBE. This approach makes no prior assumption on the shape of particle size distribution (PSD), and provides high computational efficiency and acceptable accuracy compared with other numerical method. Moreover, the form of TEMOM model for Brownian coagulation is simple enough to be solved asymptotically and analytically [7-11]. These solutions have also been verified by the quadrature method of moments (QMOM) numerically [12]. Therefore, TEMOM is not only a numerical method, but also a powerful tool to investigate the PBE theoretically.

The starting point to obtain the asymptotic solution of TEMOM model is the self-preserving distribution (SPSD) hypothesis, which implies that the standard deviation of PSD tends to a constant as time advances. In dynamical system, the asymptotic self-similar size distribution can be considered as an equillibrium point of Brownian coagulation. In the present study, the properties of the equilibrium point will be addressed based on the linear stability theory.

Mathematical model of linear stability theory

The linear stability theory decomposes the dynamical systems into a mean field and a disturbance superimposed on it. For PBE, the particle number density and its k^{th} moment can be expressed as:

$$\begin{aligned}n(\upsilon,t)&=\overline{n}(\upsilon,t)+n'(\upsilon,t)\\ M_k(t)&=\overline{M_k}(t)+M_k{}'(t)\end{aligned}\tag{4}$$

where the bar and prime represent the mean and disturbance quantities, respectively. In most cases, it is assumed that the quantities of disturbance are small compared with the corresponding quantities of the mean field. Substituting eq. (4) into the PBE and neglecting quadratic terms in the disturbance component, the linearized dynamics equations for small disturbances can be obtained if the mean field itself satisfies the PBE:

$$\begin{aligned}\frac{\partial n'(\upsilon,t)}{\partial t}=&\frac{1}{2}\int_0^v\beta(\upsilon_1,\upsilon-\upsilon_1)\overline{n}(\upsilon_1,t)n'(\upsilon-\upsilon_1,t)\mathrm{d}\upsilon_1-\int_0^\infty\beta(\upsilon_1,\upsilon)\overline{n}(\upsilon,t)n'(\upsilon_1,t)\mathrm{d}\upsilon_1+\\&+\frac{1}{2}\int_0^v\beta(\upsilon_1,\upsilon-\upsilon_1)n'(\upsilon_1,t)\overline{n}(\upsilon-\upsilon_1,t)\mathrm{d}\upsilon_1-\int_0^\infty\beta(\upsilon_1,\upsilon)n'(\upsilon,t)\overline{n}(\upsilon_1,t)\mathrm{d}\upsilon_1\end{aligned}\tag{5}$$

The corresponding perturbation equations for moment are:

$$\begin{aligned}\frac{\partial M_k{}'}{\partial t}=&\frac{1}{2}\int_0^\infty\int_0^\infty[(\upsilon+\upsilon_1)^k-\upsilon^k-\upsilon_1{}^k]\beta(\upsilon,\upsilon_1)\overline{n}(\upsilon,t)n'(\upsilon_1,t)\mathrm{d}\upsilon\mathrm{d}\upsilon_1+\\&+\frac{1}{2}\int_0^\infty\int_0^\infty[(\upsilon+\upsilon_1)^k-\upsilon^k-\upsilon_1{}^k]\beta(\upsilon,\upsilon_1)n'(\upsilon,t)\overline{n}(\upsilon_1,t)\mathrm{d}\upsilon\mathrm{d}\upsilon_1\qquad(k=0,1,2,...)\end{aligned}\tag{6}$$

In dynamical systems, various criteria have been developed to prove the stability or instability of an equilibrium point. Under favorable circumstances, the question may be reduced to a well-studied problem involving eigenvalues of matrices. In the TEMOM model for Brownian coagulation, the minimum set of moments required to close the particle moment equations is the first three, *i. e.* M_0, M_1, and M_2, which are the most important moments describing the aerosol dynamics [13]. Because of mass conservation, the mean and disturbance quantities of first order moment remain constants in the coagulation process. Therefore, the evolution of dynamical equation is mainly concerned with the 0th and second order moment, and then the perturbation equation can be rewritten as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} M_0' \\ M_2' \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}\begin{bmatrix} M_0' \\ M_2' \end{bmatrix} \quad \text{or} \quad \frac{\mathrm{d}\mathbf{X}}{\mathrm{d}t} = \mathbf{AX} \tag{7}$$

where A is the linear operator whose eigenvalues characterize the behavior of the nearby equilibrium points. If all the eigenvalues of A have negative real part, then the equilibrium point is called linearly stable; otherwise, the equilibrium point is unstable.

In the free molecule regime, the elements of matrix A based on TEMOM are (for briefly, the bar in the superscript is omitted thereafter):

$$\begin{aligned} A_{11} &= \frac{\sqrt{2}B_1(2\cdot 65M_C - 1210)M_0^{11/6}M_1^{1/6}M_2}{5184M_1^2} + \\ &+ \frac{11\sqrt{2}B_1(65M_C^2 - 1210M_C - 9223 = M_0^{5/6}M_1^{1/6}}{5184\times 6} \\ A_{12} &= \frac{\sqrt{2}B_1(2\cdot 65M_C - 1210)M_0^{17/6}M_1^{1/6}}{5184M_1^2} \\ A_{21} &= -\frac{\sqrt{2}B_1(2\cdot 701M_C - 4210)M_0^{-1/6}M_1^{13/6}M_2}{2592M_1^2} + \\ &+ \frac{\sqrt{2}B_1(701M_C^2 - 4210M_C - 6859)M_0^{-7/6}M_1^{1/6}}{2592\times 6} \\ A_{22} &= -\frac{\sqrt{2}B_1(2\cdot 701M_C - 4210)M_0^{5/6}M_1^{1/6}}{2592} \end{aligned} \tag{8}$$

where $B_1=(3/4\pi)^{1/6}(6k_\mathrm{B}T/\rho_p)^{1/2}$, k_B is the Boltzmann constant, T – the temperature; and ρ_p – the particle density, and the dimensionless particle moment is defined as:

$$M_C = \frac{M_0M_2}{M_1^2} \tag{9}$$

If the particle size distribution assumed to be lognormal, the standard deviation can be expressed as $\ln^2\sigma = \ln(M_C)/9$. For Brownian coagulation in the continuum regime, the elements of matrix A are:

$$
\begin{aligned}
\mathrm{A}_{11} &= -\frac{B_2 M_0 (-8M_C^{\,2} + 39M_C + 302)}{81} \\
\mathrm{A}_{12} &= -\frac{B_2 M_0^{\,3} (-4M_C + 13)}{81 M_1^{\,2}} \\
\mathrm{A}_{21} &= \frac{2B_2 (-4M_C + 13) M_2}{81} \\
\mathrm{A}_{22} &= \frac{2B_2 (-4M_C + 13) M_0}{81}
\end{aligned} \tag{10}
$$

where $B_2 = 3k_\mathrm{B}T/2\mu$, and μ is the gas viscosity.

Substituting the analytical solution of TEMOM [14] into the elements of linear operator A, the eigenvalues of dynamic equation for small disturbance can be calculated numerically as shown in fig. 1. The results show that the evolution of eigenvalues of perturbation equation in the free molecule regime is almost the same as that in the continuum regime. There is an approximate relationship between eigenvalues at long time as:

$$\lambda_1 t = -2.4082, \qquad \lambda_2 t = +0.2308 \tag{11}$$

in the free molecule regime, and:

$$\lambda_1 t = -2.0575, \qquad \lambda_2 t = +0.0575 \tag{12}$$

in the continuum regime. As time advances, the eigenvalues approach to zeros, which means that the dispersion system is neutral stable. Therefore, from the point of view of positive and negative of eigenvalues, it cannot judge the stabilities obviously. Moreover, its asymptotic characteristics are more important in aerosol science and technology. Therefore, the linear stability will appeal for the qualitative theory to deal with the asymptotic properties of the perturbation equation after a long period of time.

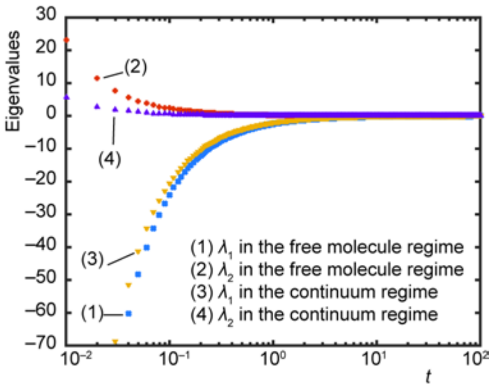

Figure 1. The evolution of eigenvalues as time advances

The asymptotic stability of TEMOM

At long time the asymptotic solution of TEMOM model for Brownian coagulation in the free molecule regime are [7]:

$$M_0 = 0.3133 B_1^{-6/5} M_1^{-1/5} t^{-6/5}, \qquad M_2 = 7.0222 B_1^{6/5} M_1^{11/5} t^{6/5}, \qquad M_C = 2.2001 \quad (13)$$

Substituting it into the dynamic equation, the magnitude order of the elements in the linear operator matrix A can be obtained based on the principle of dimensional analysis as:

$$\mathrm{A}_{11} \sim -\frac{11}{5} t^{-1}, \qquad \mathrm{A}_{12} \sim -t^{-17/5} \ll \mathrm{A}_{11}\mathrm{A}_{21} \sim t^{7/5}, \qquad \mathrm{A}_{22} \sim t^{-1} \ll \mathrm{A}_{21} \quad (14)$$

Then the perturbation equation can be simplified as:

$$\frac{\mathrm{d}M_0'}{\mathrm{d}t} \sim -\frac{11}{5} t^{-1} M_0', \qquad \frac{\mathrm{d}M_2'}{\mathrm{d}t} \sim t^{7/5} M_0' \quad (15)$$

and the solution can be found as:

$$M_0' \sim t^{-11/5}, \qquad M_2' \sim t^{1/5} \quad (16)$$

The results show that small disturbance for zeroth order moment will decrease with time, but the second one will increase. It should be noted that the mean quantities of particle moments are the function of time. For time-varying systems, the asymptotic stability of equilibrium point requires additional justification. Based on the limiting operation:

$$\lim_{t\to\infty} \frac{M_0'}{M_0} = \lim_{t\to\infty} \frac{M_2'}{M_2} \sim \lim_{t\to\infty} \frac{1}{t} = 0 \quad (17)$$

It can be found the TEMOM model for PBE in the free molecule regime is asymptotic stable. Analogously, the asymptotic solution of the particle moment in the continuum regime is:

$$M_0 = \frac{81}{169} B_2^{-1} t^{-1}, \qquad M_2 = \frac{338}{81} B_2 M_1^2 t, \qquad M_C = 2 \quad (18)$$

Substituting it into eq. (6), the dynamic equations for small disturbance are reduced to:

$$\frac{\mathrm{d}M_0'}{\mathrm{d}t} = -\frac{338 B_2 M_0 M_0'}{81}, \qquad \frac{\mathrm{d}M_2'}{\mathrm{d}t} = +\frac{10 B_2 M_0' M_2}{81} \quad (19)$$

The corresponding solution can be found as:

$$M_0' \sim \frac{1}{t^2}, \qquad M_2' \sim \ln t \quad (20)$$

The limits of the ratio between small disturbance and mean field are:

$$\lim_{t\to\infty}\frac{M_0{}'}{M_0}=\lim_{t\to\infty}\frac{M_2{}'}{M_2}\sim\lim_{t\to\infty}\frac{1}{t}=0 \tag{21}$$

The result is similar with that in the free molecule regime.

According to the rule of linearization, the perturbation of dimensionless particle moment is:

$$M_C{}'=\frac{M_0M_2{}'+M_0{}'M_2}{M_1{}^2} \tag{22}$$

Substituting the solution of the perturbation moment equation into eq. (22), the solution together its limit can be obtained approximately both in free molecule and continuum regime as:

$$M_C{}'\sim\frac{1}{t}\xrightarrow{t\to\infty}0 \tag{23}$$

which means that the standard deviation is stable.

Conclusion

In a spatially homogeneous coagulation system, the particle size distribution will reach the self-similar form at long time, which can be considered as an equilibrium point in dynamical system. In the present study, the asymptotic properties of the equilibrium point are analyzed based on the linear stability theory. The results show that the dynamic equations together with dimensionless particle moment for small disturbance are asymptotic stable at long time both in the free molecule and continuum regime.

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References

[1] Friedlander, S. K., *Smoke, Dust, and Haze: Fundamentals of Aerosol Dynamics*, Oxford University Press, London, 2nd ed., 2000
[2] Pratsinis, S. E., Simultaneous Nucleation, Condensation, and Coagulation in Aerosol Reactor, *Journal of Colloid and Interface Science*, *124* (1988), 2, pp. 416-427
[3] McGraw, R., Description of Aerosol Dynamics by the Quadrature Method of Moment, *Aerosol Science and Techno*logy, *27* (1997), 2, pp. 255-265
[4] Marchisio, D. L., *et al.*, Quadrature Method of Moments for Population Balance Equations, *AICHE Journal*, *49* (2003), 5, pp. 1266-1276
[5] Yu, M. Z., *et al.*, A New Moment Method for Solving the Coagulation Equation for Particles in Brownian Motion, *Aerosol Science and Techno*logy, *42* (2008), 9, pp. 705-713
[6] Yu, M. Z., *et al.*, Generalized TEMOM Scheme for Solving the Population Balance Equation, *Aerosol Science and Techno*logy, *49* (2015), 11, pp. 1021-1036
[7] Xie, M. L., Wang, L. P., Asymptotic Solution of Population Balance Equation Based on TEMOM Model, *Chemical Engineering Science*, *94* (2013), May, pp. 79-83
[8] Chen, Z. L., *et al.*, Asymptotic Behavior of the Taylor-Expansion Method of Moments for Solving a Coagulation Equation for Brownian Particles, *Particuology*, *14* (2014), June, pp. 124-129

[9] Yu, M. Z., *et al.*, A New Analytical Solution for Solving the Smoluchowski Equation Due to Nanoparticle Brownian Coagulation for Non-Self-Preserving System, *Aerosol and Air Quality Research*, *14* (2014), 6, pp. 1726-1737
[10] Yu, M. Z., *et al.*, A New Analytical Solution for Solving the Population Balance Equation in the Continuum-Slip Regime, *Journal of Aerosol Science*, *80* (2015), Feb., pp. 1-10
[11] Yu, M. Z., *et al.*, An Analytical Solution for the Population Balance Equation Using a Moment Method, *Particuology*, *18* (2015), Feb., pp. 194-200
[12] Shen, X. T., Maa, J. P. Y., Numerical Simulations of Particle Size Distribution: Comparison with Analytical Solutions and Kaolinite Flocculation Experiments, *Marine Geology*, *379* (2016), Sept., pp. 84-99
[13] Zhang, X. T., *et al.*, Verification of Expansion Orders of the Taylor-Series Expansion Method of Moment Model for Solving Population Balance Equations, *Aerosol and Air Quality Research*, *15* (2015), 6, pp. 2475-2484
[14] Xie, M. L., He, Q., Analytical Solution of TEMOM Model for Particle Population Balance Equation Due to Brownian Coagulation, *Journal of Aerosol Science*, *66* (2013), Dec., pp. 24-30

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