Article

Direct numerical similarity solution of Smoluchowski equation for Brownian coagulation in the continuum regime

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Abstract: In this study, a simple and direct numerical scheme is proposed for the similarity solution of Smoluchowski coagulation equation based on Taylor series expansion method of moment. The results show that the present method is convergence with high accuracy by comparison with previous work in the literatures.

Keywords: similarity solution; Brownian coagulation; moment method; particle size distribution

1. Introduction

Smoluchowski coagulation equation (SCE) is a general mathematical framework for modeling of particulate system [1]. For its own nonlinear integrodifferential structure, only a limited number of known analytical solution exist for simple collision kernel [2-6]. The previous studies indicate that particle size distribution (PSD) of aged coagulation system approaches a universal asymptotic form called the self-preserving size distribution (SPSD) [7-9]. If the collision frequency is a homogeneous function of its arguments, the SCE can be converted into an ordinary differential equation by similarity transformation based on the assumption that the algebraic mean volution of PSD is unit, and the equation takes the form [1]:

$$(1+ab)\eta\frac{d\psi}{d\eta}+\left(2ab-b\eta^{1/3}-a\eta^{-1/3}\right)\psi+\int_0^{\eta}\psi(\eta-\tilde{\eta})\psi(\tilde{\eta})\left[1+\left(\frac{\eta-\tilde{\eta}}{\tilde{\eta}}\right)^{1/3}\right]d\tilde{\eta}=0 \tag{1}$$

For Brownian coagulation in the continuum regime. In which η is dimensionless particle volume, ψ is the dimensionless distribution function, parameters a and b are the origin moments of SPSD as

$$a=\int_0^{\infty}\eta^{1/3}\psi d\eta\,,\quad b=\int_0^{\infty}\eta^{-1/3}\psi d\eta \tag{2}$$

With the boundary condition

$$\eta=0:\psi(0)=0\,,\quad \eta=\infty:\psi(\infty)=0 \tag{3}$$

And the distribution function to be solved is restricted by the following mathematical and physical constraint as

$$\int_0^{\infty}\eta\psi d\eta=1\,,\quad \int_0^{\infty}\psi d\eta=1\,,\quad \psi\geq 0 \tag{4}$$

The similarity transformation represents a possible particular solution to the SCE, analytical solution to the governing equation of SPSD can be found for the upper and lower ends of the distribution by making suitable approximation. Landgrebe and Pratsinis [10] developed a discrete sectional model for the SCE for Brownian motion in the free molecule regime. This model makes no assumption about the shape of distribution, and it accurately reproduced the SPSD. Based on the results, Vemury et al. [11]

proposed an improved v^2-based discrete sectional model to calculate the SPSD both in the continuum and free molecule regimes, which is more accurately than the previous n-based or v-based sectional models. But the initial PSD is assumed to be lognormal in their calculations of SCE.

Since the solution of SPSD is of great practical interest in aerosol science and engineering, geophysics, meteorology, etc. in the present study, we will develop our previous work [12, 13], and obtain the similarity solution of SCE with a direct numerical method, its convergence and accuracy will be verified by comparing with previous results.

2. Numerical algorithm

The accuracy of initial value of parameters a and b is very important for solving the governing equation of SPSD. The Taylor-series expansion method of moment (TEMOM) is designed to obtain the initial value of parameters. In the TEMOM [14], the fractional and higher order moments of PSD can be represented by the first three integer order moments as

$$M_k = \frac{M_1^{\ k}}{M_0^{\ k-1}}\left[1+\frac{k(k-1)(M_C-1)}{2}\right] \tag{5}$$

In which the k-th order moment M_k of PSD is defined as

$$M_k = \int_0^\infty \eta^k \psi \, d\eta \tag{6}$$

And M_C is the dimensionless particle moment as

$$M_C = \frac{M_0 M_2}{M_1^{\ 2}} \tag{7}$$

Its asymptotic solution can be found as $M_C = 2$ [12,13]. Then the initial value of parameters can be obtained as a = 8/9 and b = 11/9, respectively.

Another key problem to solve the SPSD accurately is to obtain the value of sub-boundary condition $\psi(\Delta\eta)$, and $\Delta\eta$ is the numerical step. In the lower ends of SPSD, the convolution integral term in the governing equation can be approximately as zero as η~0, and the equation reduced to

$$(1+ab)\eta\frac{d\psi}{d\eta}+\psi(\eta)\left[2ab-b\eta^{1/3}-a\eta^{-1/3}\right]=0 \tag{8}$$

Its analytical solution can be found as

$$\psi = \exp\left[\frac{-2ab\ln\eta+3b\eta^{1/3}-3a\eta^{-1/3}}{(1+ab)}\right] \tag{9}$$

Therefore, the initial value of sub-boundary condition can be calculated as

$$\psi(\Delta\eta) = \exp\left[\frac{-2ab\ln(\Delta\eta)+3b(\Delta\eta)^{1/3}-3a(\Delta\eta)^{-1/3}}{(1+ab)}\right] \tag{10}$$

In order to ensure the computational accuracy of SPSD at low cost, the numerical step can be determined by the relationship $\psi(\Delta\eta) = \Delta\eta$, then the numerical step is about $\Delta\eta$ = 0.0005, which is also set as the error limit of the numerical algorithm.

The recursive relation of SPSD to be solved can be obtained by discretizing the governing equation as

$$\psi(\eta+\Delta\eta)=\frac{(1+ab)\eta\dfrac{\psi(\eta)}{\Delta\eta}-\left(2ab-b\eta^{1/3}-a\eta^{-1/3}\right)\psi(\eta)-s(\eta)}{(1+ab)\eta}\Delta\eta \tag{11}$$

In which s(η) is the convolution integral as

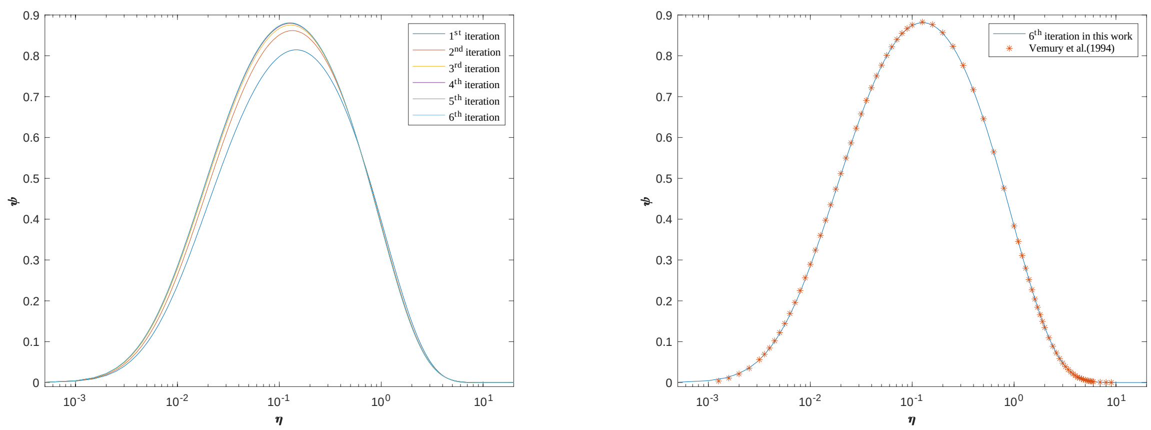
$$s(\eta)=\int_0^{\eta}\psi(\eta-\tilde{\eta})\psi(\tilde{\eta})\left[1+\left(\frac{\eta-\tilde{\eta}}{\tilde{\eta}}\right)^{1/3}\right]d\tilde{\eta} \tag{12}$$

And it can be discretized with trapezoidal integral formula as

$$s(\eta=k\Delta\eta)=\sum_{i=2}^{k-1}\psi(k\Delta\eta-i\Delta\eta)\psi(i\Delta\eta)\left[1+\left((k\Delta\eta-i\Delta\eta)/i\Delta\eta\right)^{1/3}\right]\Delta\eta \tag{13}$$

3. Results and discussions

The procedure is iterative and is repeated until an error value is smaller than a preset epsilon (0.0005), and the numerical solution of SPSD is shown in Figure 1. It can be found that the distribution functions between two adjacent iterations becomes closer and closer as the number of iterations increases, the curves of the fifth and sixth iterations almost coincide with each other, which is highly consistent with the data obtained by Vemury et al. [5]



(**a**) (**b**)

Figure 1. Numerical solution of SPSD: (**a**) The convergence of calculated SPSD with iteration; (**b**) The comparison between present results with previous work.

The changes of the values of the parameters in the governing equations of SPSD with iterations are shown in Table 1, they all tend to stable as iteration advances. The results illustrate that the present numerical method is convergence.

The significant moments of SPSD are compared with previous work as shown in Table 2. The present numerical solution best satisfies the physical constraint, namely, the requirement of zeroth and first order moment of SPSD to be equal to unit., and the error in the present work is about 0.0002. in addition, the asymptotic solutions of TEMOM are also listed in Table 2. Compared with the present numerical results, the maximum relative error is less than 10%. It shows that TEMOM model with first three integer order moments is a good approximation of Smoluchowski coagulation.

It should be pointed out that the present numerical method makes no assumption about the shape of distribution, and also reproduces the SPSD with high accuracy. Although the considerable mechanism is Brownian coagulation in the continuum regime.

The proposed numerical method is expected to develop into a general solver for the agglomeration problem with fractal spatial structures and other aerosol dynamics.

Table 1. The changes of parameters in the governing equation of SPSD

k-th iteration	a	b	M_0	M_1	M_2	M_C
0	0.8889	1.2222	1.0000	1.0000	2.0000	2.0000
1	0.9168	1.2415	1.0010	1.0001	1.5183	1.5193
2	0.9084	1.2585	1.0004	1.0000	1.8177	1.8184
3	0.9060	1.2638	1.0001	0.9997	1.8878	1.8878
4	0.9054	1.2654	1.0001	1.0000	1.9120	1.9121
5	0.9051	1.2659	1.0000	1.0000	1.9194	1.9193
6	0.9051	1.2660	1.0000	1.0002	1.9225	1.9218

Table 2. The moment, M_k, of SPSD in the continuum regime in the literature and present work

k	Vemury et al. [11]	Friedlander & Wang [7]	Present work	asymptotic solution [12]
-1/2	1.5181	1.4476	1.5160	1.3750
-1/3	1.2673	1.2393	1.2660	1.2222
-1/6	1.1046	1.0843	1.1038	1.0972
0	1.0003	0.9847	1.0000	1.0000
1/6	0.9373	0.9242	0.9372	0.9306
1/3	0.9049	0.8928	0.9051	0.8889
1/2	0.8973	0.8847	0.8977	0.8750
2/3	0.9112	0.8967	0.9117	0.8889
5/6	0.9451	0.9274	0.9458	0.9306
1	0.9994	0.9765	1.0002	1.0000
2	1.9234	1.7788	1.9225	2.0000

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