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Multi-Monte Carlo method for particle coagulation: description and validation

Haibo Zhao *, Chuguang Zheng, Minghou Xu

State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China

Abstract

In the interest of decreasing computation cost and increasing computation precision of Monte Carlo method for general dynamics equation (GDE), a new multi-Monte Carlo (MMC) method for particle coagulation is prompted, which has characteristic of time-driven, constant-number and constant-volume Monte Carlo technique. The paper has described detailedly the scheme of MMC method, including the setting of time step, the choice of coagulation partner, the judgment the occurrence of coagulation event, and the consequential treatment of particle coagulation event. MMC method is validated by five special coagulation cases: (1) constant coagulation kernel of monodisperse particles; (2) constant coagulation kernel of exponential polydisperse particle distribution; (3) linear coagulation kernel of exponential polydisperse particle distribution; (4) quadratic coagulation kernel of exponential polydisperse particle distribution; (5) Brownian coagulation kernel of log-normal polydisperse particles in the continuum regime. The simulation results of MMC method for GDE agree with analytical solution well, and its computation cost is low enough to apply engineering computation and general scientific quantitative analysis.

* Corresponding author.
E-mail addresses: klinsmannzhb@163.com (H. Zhao), cgzheng@hust.edu.cn (C. Zheng), mhxu@hust.edu.cn (M. Xu).

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1. Introduction

Solid particles (or droplets) coagulation is an important mechanism in both nature and engineering, including formation and evolvement of air aerosols and emulsion droplets, manufacture of nanoparticle agglomerates. Because many important properties such as light scattering, electrostatic charging, toxicity, radioactivity of suspended particles, sediment and capturing strategy depend on their size distribution, the time evolution of size distribution due to the particle coagulation is of fundamental interest and a key issue (see [1]). Particle size distribution (PSD) along with time is described by general dynamics equation (GDE), which takes account of the physical processes such as coagulation, condensation/evaporation, nucleation, breakage and deposition (see [2]). So GDE is a key point describing those physical events of particulate matter. The paper focuses on algorithm solving GDE for particle coagulation, where GDE for particle coagulation is as follows:

$$\frac{\mathrm{d}n_p(v,t)}{\mathrm{d}t} = \frac{1}{2}\int_0^v \beta(v-u,u)n_p(v-u,t)n_p(u,t)\,\mathrm{d}u - n_p(v,t)\int_0^\infty \beta(v,u)n_p(u,t)\,\mathrm{d}u, \tag{1}$$

where $n_p(v,t)$ is the particle size distribution function at time t, so that $n_p(v,t)\mathrm{d}v$ is the number concentration of particles whose size range between v and $v + \mathrm{d}v$ per volume unit at time t; the dimension of $n_p(v,t)$ is particles/m^3/m^3, where "particles" denotes the number of particles; $\beta(v,u)$ is the coagulation kernel for two particle of volume v and u, describing the probability of a binary coagulation event in unit time; the dimension of $\beta(v,u)$ is m^3/particles/s. The terms on the left-hand side of Eq. (1) describes the change in the number concentration of particles of volume v with time, and the two terms on the right-hand side describe respectively the gain and loss in number concentration due to coagulation.

PSD is usually polydisperse and spans widely, for example, pulverized coal fly ash particle formation is accurately described as a tri-modal PSD that includes a submicron fume region centered at approximately 0.08 μm diameter, a fine fragmentation region centered at approximately 2.0 μm diameter, and a bulk or supermicron fragmentation region for particles of approximately 5 μm diameter and greater (see [3]). In addition, some kinds of mechanisms (such as coagulation and condensation/evaporation) have different and complicated nonlinear influence on PSD. The above complication leads to a condition

which normal numerical methods (such as finite volume method and finite difference method) are difficult to solve GDE. Nowadays the most popular numerical methods of GDE are moments of method (see [4]), Monte Carlo method (see [5,6]), sectional method (see [7]) and so on. Those methods have both advantages and disadvantages. The merit of moments method is less computation time; however its model is complicated and it assumes special particle initial size distribution. In addition there is no information about the history of each particle which collides to form a bigger particle. Sectional method has a receivable computation cost and computation precision, however, sectional representation results in very complex algorithms and it is difficult to handle multi-component, more-dimensional, chemical reaction and coating, etc. Monte Carlo method are time-consuming comparatively, whereas it can gain information about history, trajectory crossing and internal structure of particles; the Monte Carlo algorithms for solving polydisperse and multi-component particle GDE are easily programmed even considering restructuring, coating, chemical reaction and fractal aggregation. With more and more strong computer power, simulation with some 10^4–10^7 particles is possible on fast PCs, which relieves greatly the contradiction of expensive computation. So Monte Carlo methods are adapted more and more in solving GDE.

Many researchers have investigated Monte Carlo method for solving GDE. To sum up, MC method can be divided into two classes according to approach of time-step setting: one is referred to as ''time-driven'' Monte Carlo, which takes into account all of possible event such as coagulation and breakage within a special adjustable time step, and time step must be less than or equal to minimum time in which every possible event takes place once for every simulation particle; the other more common Monte Carlo is called ''event-driven'' Monte Carlo. In general especial events are implemented stochastically with probabilities derived from the mean-field rates of the corresponding process. In simulation of event-driven MC, a single event is selected to occur, and the time is advanced by an appropriate increment. In contrast to time-driven MC, this MC does not need explicit time discretization and its time step, which is calculated during the simulation, adjusts itself to the rates of the various event processes. On the other hand, MC method can also be classified into two general classes according to whether the number of simulation particles and simulation volume are changed along with the evolvement of time. The first approach is to track a constant volume and thus grow or shrink the number of simulation particle in direct proportion to the number concentration of the physical system, while conserving the mass, this method is sometimes referred to as ''constant-volume MC'', which cannot maintain constant statistical accuracy. The second class is ''constant-number MC'' prompted by Matsoukas etc. [8–10], in which the number of simulation particles is kept constant and the simulation volume is continuously adjusted so as to contain the same

number of particles. The constant-number method maintains constant statistical accuracy and can simulate growth over arbitrarily long times with a finite number of simulation particles. Nevertheless, it is difficult for constant-number MC to take account of space dispersion of size function because of the expansion and contraction of the simulated subsystem volume. Furthermore, ''event-driven'' Monte Carlo method can hardly consider particle Lagrangian tracking, which is important in coupling with two-phase Euler/Lagrange model to investigate particle-flow interaction and particle motion.

In order to decrease computation cost and increase computation accuracy of Monte Carlo method for solving general dynamics equation (GDE) for coagulation, a new multi-Monte Carlo (MMC) method for coagulation is prompted. Firstly the MMC method is described detailedly; and then five special cases for which complete or partial analytical solutions exist are chosen to validate the MMC method; lastly some conclusions is drawn.

2. Description for multi-Monte Carlo method

In the first place, fictitious particles, of which the number is far less than real particles, are created by handling real particles. Those real particles which have same or similar volume can be considered to have the same properties and hence the same behaviors. Those real particles can be represented by one or several simulation particles (naming ''weighted fictitious particle'') according to local particle size distribution. One fictitious particle, whose serial number is i, is endowed with a transform-weight ''kwt_i'', and the physical meaning of kwt_i is the number of local real particles. Since less number of fictitious particles (or called simulation particles) is tracked and evolved circularly, computation cost of MMC method will decrease accordingly, especially when the number of real particles is large within computational domain. Furthermore, within time step Δt which is set real-timely, ''time-driven'' Monte Carlo method is developed to consider possible binary coagulation events. Although the total number of real particles cuts down continuously along with the occurrence of the coagulation event, the total number of fictitious particles is constant by means of adapting the transform-weight kwt_i of fictitious particle i. In addition, the volume of computational domain is conserved. Those techniques are integrated a whole, which is named with multi-Monte Carlo (MMC) method. In fact, MMC method here has characteristic of the time-driven, constant-number and constant-volume technique. The key points of MMC method include the real-time setting of time step, the choice of fictitious coagulation partner, the judgement of the occurrence of coagulation event, and consequential treatment of particle coagulation, which are described detailedly in the following text. Flow chart and schematic diagram of MMC method for particle coagulation is shown in Fig. 1.

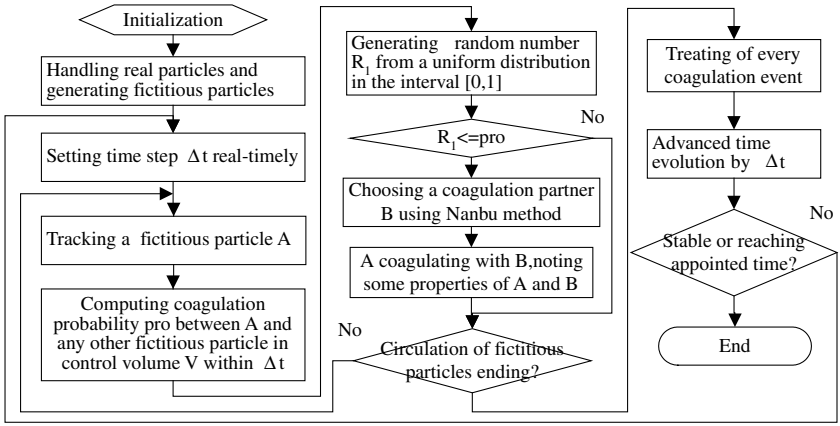

Fig. 1. Flow chart and schematic diagram of multi-Monte Carlo method.

2.1. Setting of time step

On the one hand, time step is supposed to be small enough compared to time scales of physical processes in order to allow an accurate integration, on the other hand it is expected to be large enough to avoid a prohibitive computational cost. The rule of setting of time step is as follows: within time step Δt, the number of coagulation event of any fictitious particle must be less than or equal to 1. The rule can assure that every coagulation event can be counted. Within computational domain V, one assumes the number of real particles is N and the number of fictitious particles as N_f. The coagulation time of fictitious particle i (occurring one coagulation event) is as follows:

$$t_{i,\mathrm{coag}} = 1 \Big/ \sum_{j=1,j\neq i}^{N_f} \beta_{i,j} \times \min(\mathrm{kwt}_i, \mathrm{kwt}_j), \tag{2}$$

where $\beta_{i,j}$ is the coagulation kernel (or collision kernel) for particle i and j in a volume V, represented the probability of a binary coagulation in unit time.

Time step Δt should be less than or equal to the minimum value among the coagulation time of any fictitious particle in MMC method, that is:

$$\Delta t \leqslant 1 \Big/ \max\left(\sum_{j=1,j\neq i}^{N_f} \beta_{i,j} \times \min(\mathrm{kwt}_i, \mathrm{kwt}_j) \right). \tag{3}$$

In addition, as all know, along with the occurrence of coagulation, particle size distribution must have been changed, which makes minimum coagulation time change. So Δt must be adjusted real-timely, not just as a fixed value.

2.2. Coagulation event judgement

Let us note the coagulation probability "pro" for the occurrence of a coagulation event between the tracked fictitious particle i and any other fictitious particle in control volume V within Δt. A random number R_1 from a uniform distribution in the interval $[0,1]$ is generated. A coagulation event is calculated when the random number R_1 becomes smaller than the coagulation probability "pro", i.e. if

$$R_1 \leqslant \sum_{j=1,i\neq j}^{N_f} (\beta_{i,j} \times \mathrm{kwt}_j) \times \Delta t = \mathrm{pro}. \tag{4}$$

Because of the limitation of time step setting Eq. (4), the coagulation probability "pro", i.e., the right side of Eq. (5), must be less than or equal to 1. If adopting jointly both Eqs. (3) and (4) to set time step and judge the occurrence of a coagulation event, computation cost will reach $\mathrm{O}(2 \times N_f^2)$.

To decrease computation cost, one stores the sum of possible coagulation kernel of fictitious particle i and any other fictitious particle (see [5]), i.e.

$$S_i = \sum_{j=1,i\neq j}^{N_f} (\beta_{i,j} \times \min(\mathrm{kwt}_i, \mathrm{kwt}_j)). \tag{5}$$

The physical meaning of S_i is coagulation probability of fictitious particle i within Δt and in V. Accordingly, the limitation of time step Eq. (3) is as follows:

$$\Delta t \leqslant 1/\max(S_i). \tag{6}$$

And then, the mathematic relation for judging whether or not coagulation event occurs is:

$$R_1 \leqslant S_i \times \Delta t. \tag{7}$$

Now the computation cost reaches only $\mathrm{O}(N_f + N_f^2)$ and the storage space of computer memory needs only $\mathrm{O}(N_f)$.

2.3. Choice of coagulation partner

Once coagulation event occurs, the next issue is choosing coagulation partner of the tracked fictitious particle i. Firstly, the probability of fictitious particle i coagulating with any fictitious particles j is expressed as $P_{ij} = \min(\mathrm{kwt}_i, \mathrm{kwt}_j) \times \beta_{ij} \times \Delta t$. Secondly the random number R_1 is still used for the determination of true coagulation partner. If the relation

$$\sum_{k=1}^{j-1} P_{ik} \leqslant R_1 \leqslant \sum_{k=1}^{j} P_{ik}, \quad j \in [1, N_f] \tag{8}$$

is satisfied, it is decided that the tracked particle i coagulate with fictitious particle j.

2.4. Sequential treating of particle coagulation

The direct result of particle coagulation is that two smaller particles become one bigger particle, and one coagulation event means subtracting one from the sum of particles. Along with the occurrence of particle coagulation event, the total number of real particle cuts down continuously, so does the total number simulation particle in ordinary Monte Carlo methods. If the dimension of sample space decreases continuously, computation precision of Monte Carlo method will decrease accordingly. In order to counter it, in Ref. [9], the domain V and the number of tracked particles N_f are doubled when the concentration has dropped by half. Although the evolution can carry through a long time, computation precision cannot be conserved. Matsoukas and his cooperators [8–10] had put forward the so-called "constant-number" Monte Carlo, which was applied to event-driven Monte Carlo technique. A Monte Carlo technique named by "constant fictitious particle number technique" is developed and is coupled with time-driven Monte Carlo technique and constant-volume Monte Carlo technique in this paper.

Every fictitious particle represents some real particles, where fictitious particle "A" and "B" corresponds respectively to collection "a" and "b" of real particles. When the tracked fictitious particle "A" coagulates with coagulation partner "B", it means, some real particles in collection "a"(its particle number is $\mathrm{kwt_A}$) coagulate with those in collection "b" (its particle number is $\mathrm{kwt_B}$). The number of coagulation event is the minimum between transform-weight $\mathrm{kwt_A}$ and $\mathrm{kwt_B}$, that is, $\min(\mathrm{kwt_A}, \mathrm{kwt_B})$. In order to conserve the total number of fictitious particles, the tracked fictitious particle is not replaced by a newborn fictitious particle, neither the coagulation partner is discarded. Instead the tracked fictitious particle A and its coagulation partner B are both conserved. Accordingly their transform-weight kwt and their volume are adjusted to satisfy the law of conservation of mass and the rule of change of number. Because during each time step Δt a coagulation event of particle pairs is double counted, only some properties of the current tracked particle is changed and there are no changes in its partner. That is, when the tracked fictitious particle is "A", the following measures of three cases are taken according to difference between "$\mathrm{kwt_A}$" and "$\mathrm{kwt_B}$":

$$\begin{aligned}
&\text{if } \mathrm{kwt_A} = \mathrm{kwt_B} \quad (\mathrm{kwt_A})_{\mathrm{new}} = \mathrm{kwt_A}/2; \quad (v_A)_{\mathrm{new}} = v_A + v_B,\\
&\text{if } \mathrm{kwt_A} > \mathrm{kwt_B} \quad (\mathrm{kwt_A})_{\mathrm{new}} = \mathrm{kwt_A} - \mathrm{kwt_B}; \quad (v_A)_{\mathrm{new}} = v_A,\\
&\text{if } \mathrm{kwt_A} < \mathrm{kwt_B} \quad (\mathrm{kwt_A})_{\mathrm{new}} = \mathrm{kwt_A}; \quad (v_A)_{\mathrm{new}} = v_A + v_B.
\end{aligned} \tag{9}$$

When the tracked fictitious particle is assigned to "B" in turn, the same coagulation event "A–B" will be checked and its coagulation partner will be "A" in theory. The same measure is adopted:

$$\begin{aligned}
&\text{if } \mathrm{kwt_B} = \mathrm{kwt_A} \quad (\mathrm{kwt_B})_{\mathrm{new}} = \mathrm{kwt_B}/2; \quad (v_B)_{\mathrm{new}} = v_A + v_B,\\
&\text{if } \mathrm{kwt_B} > \mathrm{kwt_A} \quad (\mathrm{kwt_B})_{\mathrm{new}} = \mathrm{kwt_B} - \mathrm{kwt_A}; \quad (v_B)_{\mathrm{new}} = v_B,\\
&\text{if } \mathrm{kwt_B} < \mathrm{kwt_A} \quad (\mathrm{kwt_B})_{\mathrm{new}} = \mathrm{kwt_B}; \quad (v_B)_{\mathrm{new}} = v_A + v_B.
\end{aligned} \tag{10}$$

Although the total number of real particles cuts down continuously along with the occurrence of coagulation event, the total number of fictitious particles is constant by the means of adapting the transform-weight "kwt" of the tracked fictitious particle, no matter how many coagulation event and how long evolution time. The technique is named as "constant fictitious particle number technique".

It is noticeable that coagulation event does not influence immediately properties and behaviors of the tracked fictitious particles and the related fictitious particles within a time step. The influence will occur in next time step. So treating of particle coagulation should be delayed until the end of current time step, which can be referred to Fig. 1.

3. Computational cases

Because GDE describes the evolution of particle size distribution with time, few experiment result or even numerical simulation can be referred. In general the best usual and effective measure of validating algorithm for GDE is comparison with analytical solution in some special cases.

3.1. Case 1, constant coagulation kernel of monodisperse particles, $\beta_{ij} = A$

Here A is a constant. Constant coagulation kernel indicates that the rate of coagulation is independent of particle volume, i.e., particle size distribution. The constant kernel reproduces the integral value behavior in the Brownian coagulation. The initial particle size distribution is monodisperse. If one defines N_0 as the initial number of primary particles at $t = 0$, the total number of particles $N(t)$ at time t is (see [5])

$$N(t) = N_0/(1 + AN_0t/2). \tag{11}$$

And then the mean mass ($\overline{M}(t)$) and the normalized variance (σ) are given theoretically (see [8]):

$$\begin{aligned}
&\overline{M}(t)/\overline{M}_0 = 1 + AN_0t/2,\\
&\sigma^2 = \overline{M(t)^2}/\overline{M(t)}^2 - 1 = AN_0t/(AN_0t + 2).
\end{aligned} \tag{12}$$

3.2. Case 2, constant coagulation kernel of exponential polydisperse particle distribution, $\beta_{ij} = A$

In this case the initial particle size distribution is polydisperse and is represented by an exponential function:

$$n_p(v,0) = \frac{N_0}{v_{g0}} \mathrm{e}^{-\frac{v}{v_{g0}}}, \tag{13}$$

where the initial total number is N_0, and the initial mean size is v_{g0}.

Coagulation kernel constant A is chosen as the Brownian constant for average atmospheric conditions. The analytical solution of time evolution of PSD is as follows (see [11,12]):

$$n_p(v,t) = \frac{N_0}{v_{g0}(1+AN_0t/2)^2} \exp\left(-\frac{v}{v_{g0}(1+AN_0t/2)}\right). \tag{14}$$

3.3. Case 3, linear constant kernel of exponential polydisperse particle distribution, $\beta_{ij} = A(v_i + v_j)$

The initial particle size distribution in both Case 3 and Case 4 is the same with those in Case 2. Here v_i and v_j is respectively the volume of two coagulation particles, i and j. The setting of A in both Case 3 and Case 4 is for the purpose of same time scale of Case 1. The linear coagulation kernel is frequently used to approximate turbulent gravitational coagulation, as the kernels have about the same degree of growth with increasing particle size. The analytical solution of time evolution of PSD is (see [11,12])

$$\begin{aligned} n_p(v,t) = {} & N_0 \frac{\exp(-AN_0v_{g0}t)}{v\sqrt{1-\exp(-AN_0v_{g0}t)}} \exp\left(-[2-\exp(-AN_0v_{g0}t)]\frac{v}{v_{g0}}\right) \\ & \times I_1\left(2\sqrt{1-\exp(-AN_0v_{g0}t)}\frac{v}{v_{g0}}\right), \end{aligned} \tag{15}$$

where I_1 is the modified Bessel function of the first kind and the first order.

3.4. Case 4, quadratic coagulation kernel of exponential polydisperse particle distribution, $\beta_{ij} = Av_iv_j$

The quadratic coagulation kernel leads to critical phenomena (''gelation'') during coagulation and its study is useful for methodological purposes. The exact analytical solution is provided (see [12]):

$$n_p(v,t) = \frac{N_0}{v_{g0}} \exp\left(-\left\{1+AN_0v_{g0}^2t\right\}\frac{v}{v_{g0}}\right) \sum_{m=0}^{\infty} \frac{(AN_0v^3t/v_{g0})^m}{(m+1)!(2m+1)!}. \tag{16}$$

3.5. Case 5, Brownian coagulation kernel of log-normal polydisperse particles in the continuum regime

When particle diameter is so small that its Knudsen number ($=\lambda/r$) is about 1, where r is the particle radius ($=(3v/4\pi)^{1/3}$) and λ is the mean free path length of the gas molecules, particles enter into continuum regime. The coagulation kernel for Brownian diffusion are given (see [13]):

$$\begin{aligned}\beta(u,v) &= \frac{2k_{\mathrm{B}}T}{3\mu}\left[2+\left(\frac{u}{v}\right)^{1/3}+\left(\frac{v}{u}\right)^{1/3}\right]\\ &= \frac{2k_{\mathrm{B}}T}{3\mu}\left[(u)^{1/3}+(v)^{1/3}\right]\left[\frac{1}{(u)^{1/3}}+\frac{1}{(v)^{1/3}}\right],\end{aligned} \tag{17}$$

where k_{B} is Boltzmann's constant ($1.38054\times 10^{-23}\,\mathrm{J\,K}$), T is the temperature and μ is the viscosity of the medium.

The initial particle size distribution is log-normal polydisperse particle size distribution, and in the course of particle evolution, particle size distribution is self-preserving log-normal size distribution, that is, at any time t,

$$n_p(v,t) = \frac{1}{3v}\frac{N(t)}{\sqrt{2\pi}\ln\sigma(t)}\exp\left\{-\frac{\ln^2[v/v_g(t)]}{18\ln^2\sigma(t)}\right\}. \tag{18}$$

Lee et al. [14] had gained analytical solution:

$$\begin{aligned}&N(t) = \frac{N_0}{1+a'KN_0t};\quad Z = \ln^2\sigma(t) = \frac{1}{9}\ln\left[2+\frac{\exp(9Z_0)-2}{1+a'KN_0t}\right],\\ &\frac{v_g(t)}{v_{g0}} = \frac{(1+a'KN_0t)\times\exp\left(\frac{9}{2}Z_0\right)}{\left[2+\frac{\exp(9Z_0)-2}{1+a'KN_0t}\right]^{1/2}};\\ &a' = 1+\exp(Z_0),\qquad K=\frac{2k_{\mathrm{B}}T}{3\mu};\quad Z_0=\ln^2\sigma_0,\end{aligned} \tag{19}$$

where $v_g(t)$ is the geometric number mean particle volume, $\sigma(t)$ is the geometric standard deviation based on particle radius, and v_{g0}, N_0, Z_0, σ_0 is the initial value for v_g, $N(t)$, Z, $\sigma(t)$, respectively.

It is noticeable that coagulation kernel β_{ij} is generally bounded as follows: $A \leqslant \beta_{ij} \leqslant A(v_i+v_j)$ or Av_iv_j.

4. Simulation

Computational conditions of five cases are listed in Table 1, where N_{f} is the total number of fictitious particle. For collecting statistics properties such as

Table 1
Computational conditions for Cases 1–5

Case	Parameters	v_{g0}	Bin discretization	N_0	N_f	Time evolution (s)	CPU time (s)
1	$A = 10^{-9}$	1.0	Monodisperse	10^8	10^3	1000	1091
2	$A = 6.405 \times 10^{-10}$	0.029	200 Classes, equally spaced	10^6	10^4	≈1561.3	13
3	$A = 1.115 \times 10^{-8}$	0.029	200 Classes, equally spaced	10^6	10^4	≈1561.3	131
4	$A = 3.808 \times 10^{-7}$	0.029	200 Classes, equally spaced	10^6	10^4	≈1561.3	401
5	$\sigma_0 = 1.5$, $\mu = 1.83 \times 10^{-7}$, $T = 2500$	1.0	200 Classes, logarithmically spaced	10^8	10^4	5×10^6	1105

particle size distribution, polydisperse particles must explicit particle bin discretization. For Cases 2–5, polydisperse particles are divided into 200 classes between the largest and smallest particle volume in the simulation. (Noting: no information about bin discretization needs during simulating, which will avoid numerical diffusion as possible (see [15]).)

Fig. 2 shows the comparison of the time evolution of some parameters for Case 1 between analytical and MMC solution, including the curve of relative total number concentration $N(t)/N_0$ along with time t, relative geometric mean particle mass $M(t)/M_0$ along with t and geometric standard deviation σ along with t. Although time evolution is continued to a long times, and particle total number decrease sharply, computation precision is conserved well because of constant fictitious particle number. The agreement between MMC solution and analytical solution is exact. The difference of $N(t)/N_0$ along with t between MMC solution and analytical solution is even less than the thickness of the line.

The results of numerical simulation for Cases 2–4 are shown in Figs. 3–5, respectively. As we can see, the simulation result of MMC method for GDE agrees with analytical solution well. During the evolution, PSD remains basically the exponential distribution for three cases, which is called by "self-preserving" curve (see [13,16]).

Fig. 6(a) illustrates the evolution of the size distribution for Brownian coagulation of polydisperse particles. The agreement between MMC solution and analytical solution is mostly good. Along with the evolution of time, the peak value of size distribution curve is descending, which means particle number

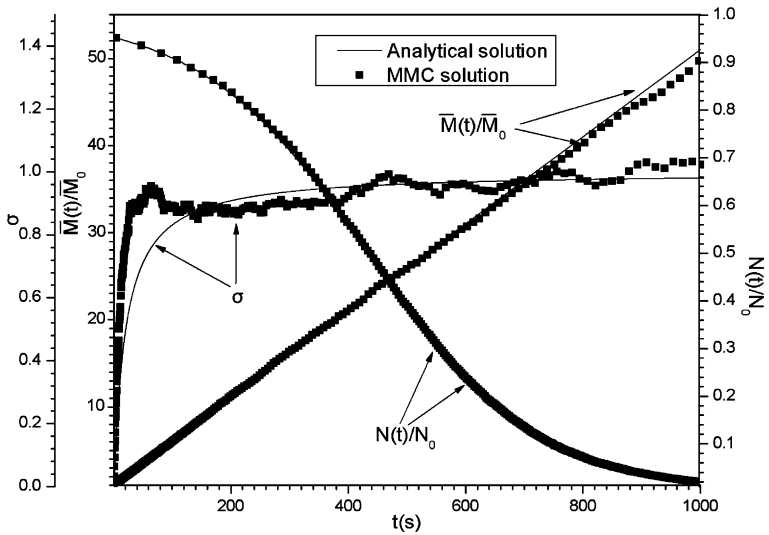

Fig. 2. The time evolution of parameters for Case 1.

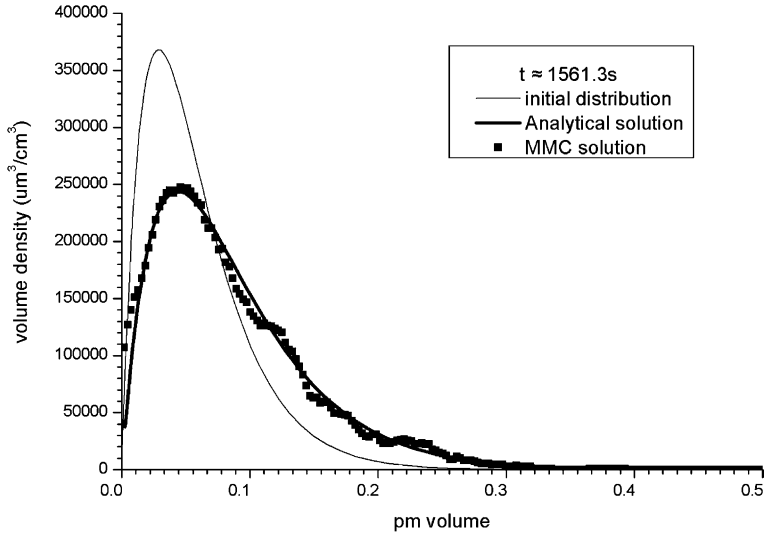

Fig. 3. The time evolution of PSD for Case 2.

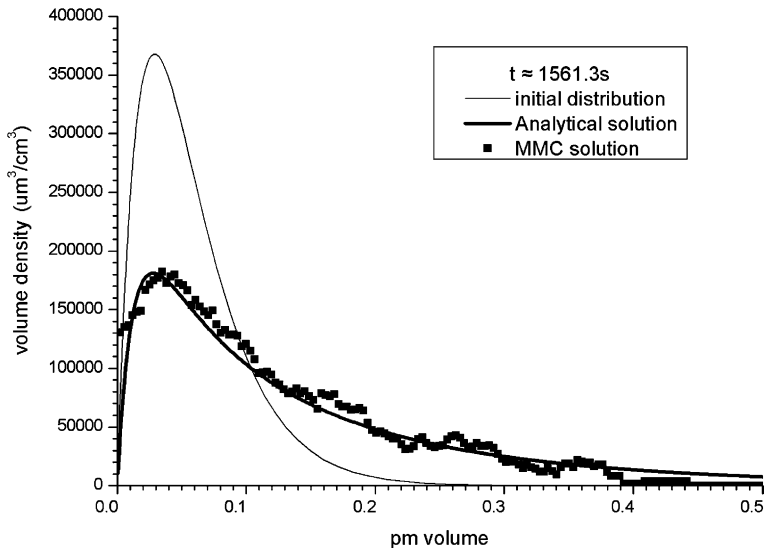

Fig. 4. The time evolution of PSD for Case 3.

decreases continuously; and the location of peak is moving to right side—the side of bigger particles, which means the particle volume is more and more bigger. During the evolution, the particle size distribution remains basically the

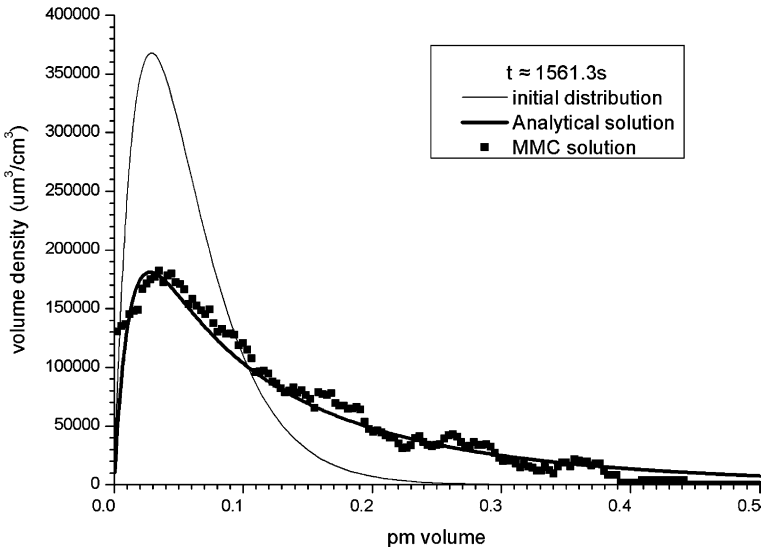

Fig. 5. The time evolution of PSD for Case 4.

"self-preserving" log-normal distribution (see [13,16]). However, along with advancing of time evolution, the agreement for size distribution between MMC solution and analytical solution becomes more and more worse. The inapplicable measure of particle bin discretization and the insufficient number of fictitious particles may contribute partly to it, and certain additional approximations and simplifications of analytical solution may also contribute partly to those bias. Those need validate and probe farther. The striking difference of σ in Fig. 6(b) between analytical and MMC solution inherits the difference of size distribution in Fig. 6(a).

In order to control computation precision, ordinary Monte Carlo methods have to increase the number of simulation particles because of decreasing real particles and simulation particles continuously along with time evolution, which leads to a dissatisfactory computation cost. So there is an antinomy of computation cost and computation precision in ordinary Monte Carlo methods. For Case 1, the simulation particle number given by literature [5] is 10^3–10^5 at the same computational condition, and 15000 in literature [8] for Case 4. Although no comparison about computation cost can be taken because there are no data about computation cost in literature [5,8], it can be confirmed that MMC method can save computation cost because of less number of simulation particle. Computation cost of MMC method is listed in Table 1 (hardware and software environment are as follows: Athlon Xp2500+, 512M, Visual Fortran 6.0, Windows Xp professional).

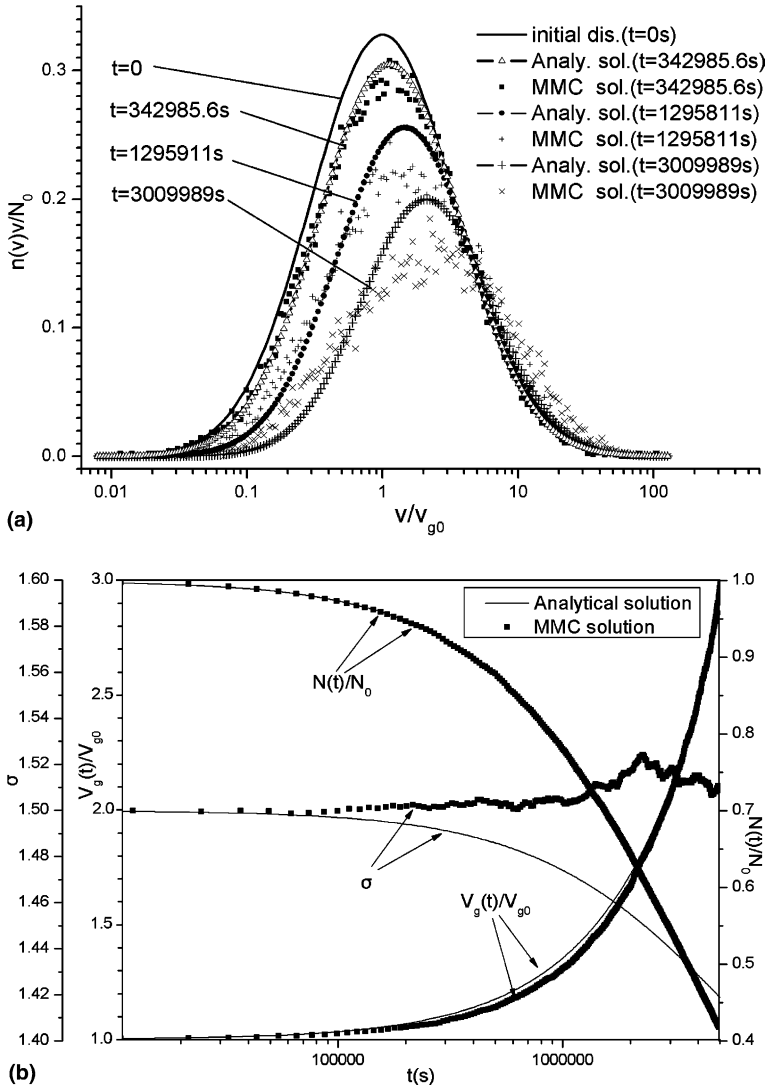

Fig. 6. The comparison between analytical and MMC solution of Case 5 for (a) the time evolution of particle size distribution (PSD); (b) $N(t)/N_0 \sim t$, $v_g(t)/v_{g0} \sim t$ and $\sigma \sim t$.

5. Conclusion

Multi-Monte Carlo (MMC) method for general dynamics equation (GDE) is performed in the paper. Its characteristics are as follows: handling fictitious particles of which the number is far less than that of real particles to decrease

computation cost, coupling "time-driven" Monte Carlo technique and constant-number Monte Carlo technique, and conserving computational domain. MMC method had been used to simulation five special coagulation cases. The agreement between MMC solution and analytical solution is mostly good, which validated computation precision of the MMC method. Furthermore the computation cost of the MMC method is receivable for engineering application engineering computation and general scientific quantitative analysis. Those may make the MMC method a standard solution for solving GDE.

Computational bias of MMC methods will be advanced by means of applicable measure of particle bin discretization, the apposite number of fictitious particle and the more times of MMC simulation. The mutual relation of time step, fictitious particle number and computation cost, computation precision will be very significative. Those works will further go along.

MMC method can expand to take account of other event such as condensation/evaporation, nucleation, deposition, breakage, space dispersion, particle phase properties evolution and so on. Of course some technique must be coupled, for instance, cell plotting technique for space dispersion and two-phase flow model for particle and medium velocity field. MMC method can also be applied to consider GDE for multi-component, more-dimensional and polydisperse particle. Those works will be developed in the next stage.

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