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A new event-driven constant-volume method for solution of the time evolution of particle size distribution

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ABSTRACT

Direct simulation Monte Carlo (DSMC) method is an important approach for numerical solution of the population balance equation, which characterizes the dynamic evolution of particle size distribution in dispersed systems. One sample of the whole system (i.e., subsystem) is taken into account in most DSMC methods. It means that a spatially-isotropic whole system is considered, and simulation particles having same number weight are tracked. A new event-driven constant-volume (EDCV) method for population balance modeling is proposed to describe the dynamic evolution in dispersed systems under influence of coagulation, breakage, nucleation, surface growth/dissolution (condensation/evaporation) and deposition (settling). The method adopts the concept of differentially weighting simulation particles, and several schemes of sample restoration are developed to maintain simulation particle number within prescribed bounds, at the same time the constant-volume computational domain is tracked. By comparing of several popular Monte Carlo methods, it is concluded that the proposed EDCV method exhibits comparatively high precision and efficiency.

1. Introduction

Most recently, population balance modeling (PBM) of dispersed systems has attracted significant coverage from many different fields of science and engineering including combustion, chemical engineering, nanoparticle, and atmospheric physics [1–3]. Population balance modeling considers the dispersed system as a statistical ensemble in which each dynamic event has some known probability described by known frequency functions or kernels, and then obtains the dynamic evolution of particle size distribution (PSD) through the solutions of population balance equation (PBE). PBM is involved with at least two issues of fundamental importance [4]: the models of kernels of dynamic events, and the numerical solutions of the partial integro-differential PBE. Multi-dimensional PBM that describes the temporal-spatial evolution of PSD needs to be coupled with two-phase models and spatial coordinate systems. Most numerical approaches for the PBE focus on the temporal evolution of PSD, which factually describes a spatially zero-dimension system. This study only focuses on numerical method for zero-dimensional PBM. The following mathematical model represents the temporal evolution of particle size distribution function (PSDF) under influence of dynamic events including coagulation, breakage, nucleation, surface growth/dissolution (condensation/evaporation) and deposition (settling)

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$$\frac{\partial n(v,t)}{\partial t} = \left\{\frac{1}{2}\int_0^v \beta(v-u,u,t)n(v-u,t)n(u,t)\mathrm{d}u - n(v,t)\int_0^\infty \beta(v,u,t)n(u,t)\mathrm{d}u\right\}_{\text{coagulation}} + \left\{\int_v^\infty \gamma(u,v,t)b(u,t)B(u,t)n(u,t)\mathrm{d}u - B(v,t)n(v,t)\right\}_{\text{brakage}} + \{C_S K_S(v-v_S,t)n(v-v_S,t) - C_S K_S(v,t)n(v,t)\}_{\text{condensation/evaporation}} + \{J(v,t)\delta(v_{\min},v)\}_{\text{nucleation}} - \{E(v,t)n(v,t)\}_{\text{deposition}}, \quad (1)$$

in which v is the particle size expressed as the volume of the particle (μm^3, usually), $n(v,t)$ with dimension $\mu m^{-3}\cdot m^{-3}$ is the PSDF at time t, $n(v,t)\mathrm{d}v$ is the number concentration of particles with size range between v and $v+\mathrm{d}v$ at time t; $\beta(v,u,t)$ is coagulation kernel for two particles of volume v and u at time t, $m^3\cdot s^{-1}$; $B(v,t)$, $J(v,t)$, and $E(v,t)$ are the breakage, nucleation and deposition kernels for particle of volume v, respectively. They represent the rates of corresponding events at time t, with dimensions s^{-1}, $\mu m^{-3}\cdot m^{-3}\cdot s^{-1}$ and s^{-1}, respectively; C_S denotes the number concentration of condensing monomers, m^{-3}; $K_S(v,t)$ is the rate constant for condensation/evaporation (surface growth/dissolution) of particle v at time t, $m^3\cdot s^{-1}$; v_S is the volume of condensing monomers, μm^3. $\gamma(u,v,t)$ is the probability of making a daughter of volume v from a parent of volume u; $b(u,t)$ is the number of particles resulting from the breakage of a particle of volume u; $\gamma(u,v,t)b(u,t)$ describes size distribution of fragments of volume v resulting from the breakup of a particle of volume u.

Two classes of numerical solutions for the PBE can also be distinguished. One class directly solves the equation based on the Euler coordinate, including method of moments [5], sectional method [6], discrete method [7], discrete-sectional method [8,9], the entropy model [10], etc. These Euler solutions involve themselves in the discretization of PSD or, as in the case of the classical method of moments, in restriction on PSD-shape. Another class of solutions, Direct Simulation Monte Carlo (DSMC) method, which is first developed in rarefied gas dynamics [11] and directly solves the physical model of dispersed systems [12], has the same physical nature (chaotic and dilute systems) as the PBE [13]. The discrete nature of DSMC adapts itself naturally to dynamic processes. Although DSMC method is usually more computer-intensive than Euler approaches, it is capable of gaining the information about particle history, trajectory crossing and internal structure, and permits to study finite-size effects, spatial correlations and local fluctuations. Furthermore, DSMC method, which is easily programmed even for multivariate, multi-component case than Euler approaches, shifts the time spent on solving a problem from the programmer to the computer, and the drastic increase of CPU speed and memory capacity in the last decade allows for the fast development and wide application of DSMC method.

In "event-driven" DSMC technique (or no-time counter method in the nomenclature of Bird [11]), specific events are implemented stochastically with probabilities derived from mean-field rates of corresponding processes; following the implementation of an event, time is then incremented appropriately [14,15]. Kraft et al. [16] have proposed an efficient Monte Carlo (MC) method to examine the time evolution of the PSD with the concepts of majorant kernels and fictitious jumps. The MC is factually based on the event-driven technique. Another class of DSMC method, "time-driven" technique (or time counter method in the nomenclature of Bird [11]), takes account of all possible events within an adjustable time-step, where time-step must be less than or equal to the minimum time scale in which the number of every possible event must be less than or equal to one for every simulation particle [17]. Rajamanl et al. [18] had clearly presented a mathematical proof of the connection between event-driven and time-driven methods. Another way to classify MC methods is based on whether the total number of simulation particles is changed during simulation or not. If a constant computational domain is tracked, one calls it constant-volume method [19,20]; if, however, the domain is continuously adjusted so as to contain the constant-number of simulation particles, the MC method is known as constant-number method [21–23]. Other types of MC methods, direct simulation algorithm [24–26] or mass flow algorithm [27–30], have been examined and reviewed by Ref. [31].

A reasonably sized dispersed system (for example, as illustrated in Fig. 1(a)) contains approximately 10^{10} or more particles. However, DSMC code can only examine 10^3–10^7 particles at a time on fast PCs because of the limitation of CPU speed and memory capacity. Just as demonstrated in Fig. 1(b), a subsystem of the whole system is sampled in most DSMC methods, either implicitly or explicitly, where the fully-stirred and spatially-isotropic system is assumed and the periodic boundary conditions are adopted [17]. The subsystem concept indicates simulation particles having different sizes are assigned with same weight. In such a way, the behavior of the subsystem duplicates the dispersed system as a whole. However, it is impossible for these DSMC methods using the subsystem concept to simulate the whole system and to consider the space dispersion of PSDF, boundary conditions, and kernels with spatially anisotropic property.

The concept of differentially weighting simulation particle has been applied in solution of Boltzmann equation [32,33], numerical simulation of trace species [34] and Coulomb collisions in plasmas [35]. However, the concept is seldom used by DSMC method for PBM. In fact, PSD in dispersed systems is usually involved in polydispersed distribution where the number concentrations in different size sections vary greatly. Thus, keeping track of differentially weighting simulation particles with different sizes is conducive to improve the performance of DSMC for PBM. The multi-Monte Carlo (MMC) method [36–43] proposed by authors describes the time evolution of the PSD in the whole system through tracking differentially weighting simulation particles. The MMC method, however, demonstrates comparatively low computation precision and comparatively high computation cost on the whole [44]. Although it is possible to improve the MMC method through designing either right consequential treatment of a coagulation event or right coagulation rule for two differentially weighted simulation particles, the MMC method exhibits naturally some numerical errors which originate from the required uncoupling process of dynamic events within one time-step [44]. In fact, by analyzing qualitatively the computational accuracy and cost of some popular MC methods, it is found that an event-driven MC shows higher precision and lower cost than a time-driven

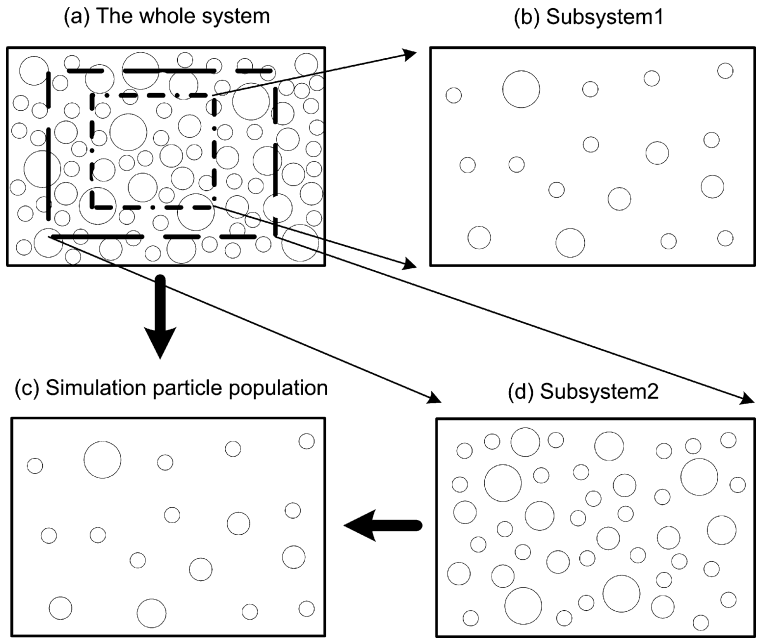

Fig. 1. Schematic program of the relation among the whole system, subsystem and simulation particle population.

MC [44]. That is why in the fields of zero-dimensional PBM event-driven DSMC is more popular than time-driven DSMC, although the latter is at an advantage in the fields of multi-dimensional PBM because simulators of two-phase flow work with standard integrators that are time-driven.

Based on these understandings, we developed a new differentially weighting and event-driven DSMC in the paper. Constant volume, which is necessary for the purpose of considering the space evolution of the PSD, boundary condition and even particle-flow dynamics in multi-dimensional PBM in the next stage, is tracked in the method. The method is named event-driven constant-volume (EDCV) method. The EDCV method and MMC method (and its subsequent improved methods that will be next reported by us) differ in the manner in which the simulation clock is advanced. The EDCV method has been used to describe particle coagulation dynamics [45] and particle removal process by electrostatic precipitator [46]. The paper is organized as following. In the Section 2, the method is introduced in details. Then, the performance of the method is compared with other MC methods, and the numerical errors are analyzed qualitatively in Section 3. Lastly, some conclusions are made in Section 4.

2. Methodology

2.1. Weighting simulation particle population

Real particles having similar size are considered to have same properties and, hence, same behavior. These real particles are represented by several weighting simulation particles, where simulation particle is an indicator of these represented real particles. So the time evolution of simulation particles duplicates that of real particles. Here, the following steps are adopted to generate differentially weighting simulation particle population for a polydispersed real particle population:

(A) The real particle population is divided into C sections ($C = 1$ for an initial monodispersed real particle population), and the total number of real particles is N. The initial total number of simulation particles is set to N_{st}, and the initial common number weight is set to $w = N/N_{st}$ (w is not required to be an integral value); In order to conserve the statistical precision, the number of simulation particles representing a particle section must be greater than a minimum value, N_{min}; Generally speaking, N_{min} should be the magnitude of $O(10^1)$ or larger.

(B) Particle section looping;

I. As for particle section i in a given size range, the representative size is d_i, and the total number of real particles falling into the section is N_i. The number of simulation particles representing the particle section i is calculated by: $N_{si} = \text{integer}[N_i/w]$. If N_{si} is less than N_{min}, let $N_{si} = N_{min}$;

II. Some simulation particles, whose total number and size are N_{si} and d_i, respectively, are generated and indexed. As for one simulation particle whose index is j, its weight is updated: $w_j = N_i/N_{si}$;

(C) The total number of simulation particles is updated by: $N_{st} = \sum_i N_{si}$.

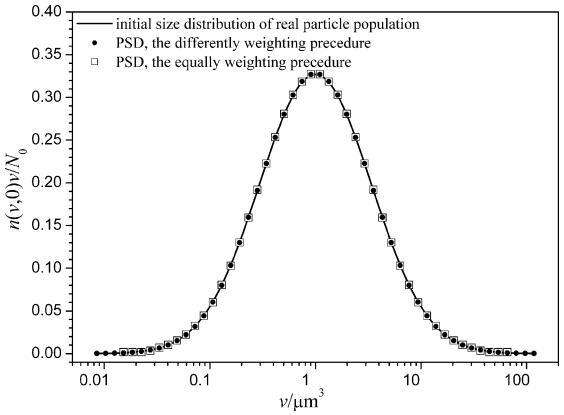

Fig. 2. Schematic representation of the equally and differentially weighting procedures.

The detailed description and a factual example are shown in references [38,39]. In fact, these simulation particles in same particle section are assigned with same number weight; however, those simulation particles in different size sections have different number weights. The generated simulation particle population has same statistical property of PSDF with the real particle population.

A real particle population, which is represented by a lognormal function, is demonstrated in Fig. 2. In the case, the size distribution is firstly divided into 50 sections, spaced logarithmically; and then only about 3000 simulation particles are utilized to represent about 10^6 real particles. Obviously, the equally weighting procedure loses some detailed information of the real particle population at the two edges of PSD, but the differentially weighting procedure duplicates the size distribution near exactly. On the other side, the equally weighting procedure also deteriorates statistical precision of stochastic approach, which is inversely proportional to the square root of simulation particle number. For example, only several equally weighting simulation particles are utilized to represent the two edges of PSD, as shown in Fig. 2. The differentially weighting procedure is capable of protecting against statistical fatigue, in which every section of real particle population is represented by more simulation particles. Last but not least, the equally weighting procedure constraints greatly the scope of MC method. For example, if a breakage event leads to some differentially sized particles, as it surely happens in nature, several differentially sized simulation particles having different number weights should be used to represent these fragments. If a nucleation event produces some unequally-sized particles, the same problem is solved by the differentially weighting procedure.

2.2. The rate of dynamic events

As far as an event-driven MC method is considered, the rate of dynamic event must be first calculated to determine the waiting time between two dynamic events and to select the main event and the main particle(s). There exist two cases.

2.2.1. Equally weighting simulation particle population

If the common number weight w is equal to 1, it means every simulation particle in a computational domain is tracked. Some usual event-driven MC methods (for example, the stepwise constant-volume method [20] and the constant-number method [21–23]) or time-driven MC methods (for example, the time-driven DSMC [17]) belong to the variant. In general, the common number weight w is unequal to 1, which means one simulation particle represents many real particles and number weight of each simulation particle is same.

The rates per unit volume for different dynamic events commonly encountered in particulate processes, R_l, are listed in Table 1. The calculation of R_l in the equally and differentially weighting procedures is equivalent for these events that are only associated with single particle, saying, breakage, condensation/evaporation, nucleation and deposition. However, the remarkable difference lies in two-particle event – coagulation event.

The coagulation of two simulation particles i and j is considered as the interaction between two groups of real particles. The coagulation event between two real particles is called "real coagulation event" in the paper. Thus the number of real coagulation events occurring among the ith-group real particles (these real particles are represented by simulation particle i, and number concentrations is w_i/V, V is the volume of simulated domain) and the jth-group particles (these real particles are represented by simulation particle j, and number concentrations is w_j/V) per unit time per unit volume is given by

$$\phi_{ij} = \beta_{ij} \times \frac{w_i}{V} \times \frac{w_j}{V}, \tag{2}$$

where β_{ij} is coagulation kernel of two particles i and j, and ϕ_{ij} is with the dimension of $\mathrm{m}^{-3} \cdot \mathrm{s}^{-1}$. One can call ϕ_{ij} the coagulation rate between real particle A and real particle B, where A and B are chosen randomly from the ith-group and the jth-group.

Table 1
The rate of dynamic events per unit volume.

Event	$R/s^{-1}\cdot m^{-3}$		
	Continuous expression	Discrete expression	
		The equally weighting procedure	The differentially weighting procedure
Coagulation	$\frac{1}{2}\int_{v_{min}}^{v_{max}}\int_{v_{min}}^{v_{max}}\beta(u,v)n(u)n(v)\mathrm{d}u\mathrm{d}v$	$\frac{w}{V^2}\sum_{i=1}^{N_{st}}\sum_{j=i+1}^{N_{st}}\beta_{ij}$	$\frac{1}{2V^2}\sum_{i=1}^{N_{st}}\sum_{j=1,j\neq i}^{N_{st}}\left[\frac{2\beta_{ij}w_j\max(w_i,w_j)}{w_i+w_j}\right]$
Breakage	$\int_{v_{min}}^{v_{max}}B(v)n(v)\mathrm{d}v$	$\sum_{i=1}^{N_{st}}B_i/V$	$\sum_{i=1}^{N_{st}}B_i/V$
Surface growth	$C_0\int_{v_{min}}^{v_{max}}K_S(v)n(v)\mathrm{d}v$	$C_0\sum_{i=1}^{N_{st}}K_{S,i}/V$	$C_0\sum_{i=1}^{N_{st}}K_{S,i}/V$
Nucleation	$VJ(v)\delta(v_{min},v)$	$VJ(v)\delta(v_{min},v)/w$	$VJ(v)\delta(v_{min},v)$
Settling	$\int_{v_{min}}^{v_{max}}E(v)n(v)\mathrm{d}v$	$\sum_{i=1}^{N_{st}}E_i/V$	$\sum_{i=1}^{N_{st}}E_i/V$

The total number of real coagulation events occurring among these real particles represented by simulation particle i and any other real particles per unit time per unit volume, saying, the total coagulation rate of one real particle from i per unit volume, is then calculated as follows:

$$\Phi_i=\sum_{j=1,j\neq i}^{N_{st}}\phi_{ij}=\frac{1}{V^2}\sum_{j=1,j\neq i}^{N_{st}}(\beta_{ij}\times w_i\times w_j). \tag{3}$$

Thus, the time interval of a real coagulation event that is associated with one real particle from i in the domain V, ζ_i, is followed as

$$\zeta_i=\frac{1}{V\Phi_i} \tag{4}$$

Since simulation particle i represent w_i real particles, a coagulation event of i means w_i real coagulation events of real particles from i. So the time interval of the coagulation event of i, Λ_i, is equal to $w_i\,\zeta_i$. And then, the total coagulation rate of simulation particle i (C_i with dimension of $s^{-1}\cdot m^{-3}$), which is the accumulative total of the coagulation rate between i and any one of the other simulation particles, is inversely proportional to Λ_i,

$$C_i=\sum_{j=1,i\neq j}^{N_{st}}C_{ij}^i=\frac{1}{V\Lambda_i}=\frac{1}{Vw_i\zeta_i}=\frac{\Phi_i}{w_i}=\frac{1}{V^2}\sum_{j=1,i\neq j}^{N_{st}}(\beta_{ij}\times w_j). \tag{5}$$

Note that $C_{ij}^i=\beta_{ij}w_j/V^2$. Since two simulation particles contain different numbers of real particles, for the same i–j coagulation event the coagulation rate of i (C_{ij}^i) is different from the coagulation rate of j ($C_{ij}^j=\beta_{ij}w_i/V^2$), and the time interval of i is also different from that of j.

Last, the rate of coagulation event occurring among two simulation particles per unit volume is calculated as

$$R_{coag}=\frac{1}{2}\sum_{i=1}^{N_{st}}C_i=\frac{1}{2V^2}\sum_{i=1}^{N_{st}}\sum_{j=1,i\neq j}^{N_{st}}(\beta_{ij}\times w_j) \tag{6}$$

The denominator "2" in Eq. (6) is for the purpose of the consideration of double counting of the particle pairs. In the equally weighting procedure, the coagulation rate per unit volume is simplified by

$$R_{coag}=\frac{w}{2V^2}\sum_{i=1}^{N_{st}}\sum_{j=1,i\neq j}^{N_{st}}\beta_{ij}=\frac{w}{V^2}\sum_{i=1}^{N_{st}}\sum_{j=i+1}^{N_{st}}\beta_{ij} \tag{7}$$

2.2.2. Differentially weighting simulation particle population

Firstly we investigate the coagulation process of two differentially weighting simulation particles. In fact, Eq. (5) formulizes one kind of coagulation rule for two differentially weighting simulation particles. The coagulation rule indicates that each real particle represented by simulation particle i undergoes a real coagulation event with probability 100% once the simulation particle is involved in one coagulation event with any other simulation particle. Here the number of real coagulation events is $w_i\times w_j$ once i coagulates with j. Since the total number of real particles from i and j is (w_i+w_j) and one coagulation event is related to two particles, the mean number of real coagulation events per real particle from i or j is

$$\Omega=\frac{2w_iw_j}{w_i+w_j} \tag{8}$$

Note that $\min(w_i,w_j)\leqslant\Omega\leqslant\max(w_i,w_j)$, and $\Omega=w$ if $w_i=w_j=w$. In the coagulation rule, the coagulation rate of simulation particle i is C_{ij}^i, and then the time interval of i is $1/(VC_{ij}^i)$. Since i contains Ω real coagulation events on average, the average time interval per real particle from i is given by $1/(V\Omega C_{ij}^i)$. Thus the mean coagulation rate of a real particle from i is (ΩC_{ij}^i). In

the same way, the mean coagulation rate of a real particle from j is (ΩC_{ij}^{j}). It is very intractable for the coagulation rule to treat the consequence of coagulation event between the two differentially weighting simulation particles, in which the mass, momentum and energy must be conserved during the coagulation process.

In this paper, we establish a new coagulation rule between two differentially weighting simulation particles. In the new coagulation rule, it is thought that one real particle represented by simulation particle i may interact with any one real particle among $\min(w_i, w_j)$ of simulation particle j, and one real particle of simulation particle j may coagulate with any one among $\min(w_i, w_j)$ of simulation particle i. Here the number of real coagulation events is $\Omega' = \min(w_i, w_j)$ once i coagulates with j. Obviously $\Omega' = w$ if $w_i = w_j = w$. The new coagulation rule will benefit the consequential treatment of coagulation event when considering the law of conservation of mass, momentum and energy, which will be explained in the next text. Let τ_d be the time increment of the coagulation event between simulation particle i and j in the new rule.

Similarly, in the new rule the coagulation rate of a real particle from i is $(\Omega' C_{ij}^{'i})$, and the coagulation rate of a real particle from j is $(\Omega' C_{ij}^{'j})$, where $C_{ij}^{'i}$ and $C_{ij}^{'j}$ is the coagulation rate of i and j for the i–j coagulation event in the new coagulation rule, respectively.

Whether any rule is adopted, the coagulation rate of a real particle from the same simulation particle should be same, that is, we can relate the two coagulation rules with the following equation:

$$\Omega C_{ij}^{i} = \Omega' C_{ij}^{'i}; \Omega C_{ij}^{j} = \Omega' C_{ij}^{'j} \tag{9}$$

So

$$C_{ij}^{'i} = \frac{\Omega}{\Omega'} C_{ij}^{i} = \frac{2 w_i w_j}{(w_i + w_j) \times \min(w_i, w_j)} C_{ij}^{i} = \frac{2 \max(w_i, w_j)}{w_i + w_j} C_{ij}^{i} \geqslant C_{ij}^{i} \tag{10}$$

Thus the total coagulation rate of simulation particle i with any other simulation particles is calculated by:

$$C_i' = \sum_{j=1, i\neq j}^{N_{st}} C_{ij}' = \frac{1}{V^2} \sum_{j=1, i\neq j}^{N_{st}} \left[\frac{2\beta_{ij} w_j \max(w_i, w_j)}{w_i + w_j} \right] = \frac{1}{V^2} \sum_{j=1, j\neq i}^{N_{st}} \beta_{ij}'. \tag{11}$$

Lastly, the rate of coagulation event occurring among two simulation particles per unit volume in the new coagulation rule is calculated by

$$R_{coag}' = \frac{1}{2} \sum_{i=1}^{N_{st}} C_i' = \frac{1}{2V^2} \sum_{i=1}^{N_{st}} \sum_{j=1, j\neq i}^{N_{st}} \left[\frac{2\beta_{ij} w_j \max(w_i, w_j)}{w_i + w_j} \right] = \frac{1}{2V^2} \sum_{i=1}^{N_{st}} \sum_{j=1, j\neq i}^{N_{st}} \beta_{ij}' = \frac{1}{2V_s^2} \sum_{i=1}^{N_{st}} S_i \tag{12}$$

where

$$S_i = \sum_{j=1, j\neq i}^{N_{st}} \left[\frac{2\beta_{ij} w_j \max(w_i, w_j)}{w_i + w_j} \right] = \sum_{j=1, j\neq i}^{N_{st}} \beta_{ij}', \beta_{ij}' = \frac{2\beta_{ij} w_j \max(w_i, w_j)}{w_i + w_j} \tag{13}$$

Obviously, if $w_i = w_j = w$, the coagulation rate in the differentially weighting procedure is same with that in the equally weighting procedure.

It is worth noting that

$$R_{coag}' = \frac{1}{2V^2} \sum_{i=1}^{N_{st}} \sum_{j=1, i\neq j}^{N_{st}} \beta_{ij}' \neq \frac{1}{V^2} \sum_{i=1}^{N_{st}} \sum_{j=i+1}^{N_{st}} \beta_{ij}'. \tag{14}$$

So calculating the coagulation rate in the differentially weighting procedure will consume CPU time of $O(N_{st}^2)$, which is about the twice of CPU time in the equally weighting procedure.

2.3. The waiting time between two events

The dynamic evolution of dispersed system is considered as a standard Markov process, in which the interval of quiescence of two events is distributed by an exponential function. According to Shah [47], the waiting time after (k-1) events is computed as following:

$$\Delta t_k = 1 \Big/ \left(V \sum_i R_{i,k} \right) \tag{15}$$

where $R_{i,k}$ is the rate per unit volume ($m^{-3} \cdot s^{-1}$) of event i after (k-1) events.

2.4. The selection of main event

The selection of dynamic event l is based on the probability of event l, P_l, which follows the relation:

$$P_l = \frac{R_l}{\sum_i R_i} = \frac{V R_l}{V \sum_i R_{i,k}} = V R_l \Delta t_k. \tag{16}$$

A stochastic process is used to select the main event, and Step 1 in Fig. 3 illustrates the process. Firstly, P_{depo}, P_{cond}, P_{brk}, P_{coag} and P_{nuc} (the probability of deposition, surface growth/dissolution (condensation/evaporation), breakage, coagulation, and nucleation) are computed, respectively. And then, if a random number r from a uniform distribution in the interval [0,1] satisfies the relation, $0 < r \leqslant P_{\text{depo}}$, deposition event occurs; if $P_{\text{depo}} < r \leqslant P_{\text{depo}} + P_{\text{cond}}$, the main event is condensation/evaporation; if $P_{\text{depo}} + P_{\text{cond}} < r \leqslant P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}}$, breakage event is selected; if $P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} < r \leqslant P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + P_{\text{coag}}$, coagulation event; if $P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + P_{\text{coag}} < r \leqslant P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + P_{\text{coag}} + P_{\text{nucl}} = 1$, nucleation event. It is worth noting that the sequence of these events observed in Fig. 3 can be stochastic.

2.5. The selection of main particle(s)

Once the main event is selected, the next issue is the implementation of the event. This selection can be done using either the inverse method (that is, the cumulative probabilities method) or the acceptance–rejection method [14], depending on the particulars of the problem. The case of coagulation event is used to demonstrate this selection.

In the inverse method, just shown in Step 2 of Fig. 3, the coagulation event of simulation particle i will be calculated when the random number r satisfies the following condition:

$$P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + \frac{1}{2V}\sum_{m=1}^{i-1} S_m \Delta t_k < r \leqslant P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + \frac{1}{2V}\sum_{m=1}^{i} S_m \Delta t_k. \tag{17}$$

And then, the same random number r is still used for the determination of the coagulation partner of simulation particle i, which is observed in Step 3 of Fig. 3. If the following relation:

$$P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + \frac{\Delta t_k}{2V}\left(\sum_{m=1}^{i-1} S_m + \sum_{m=1,m\neq i}^{j-1} \beta'_{im}\right) < r \leqslant P_{\text{depo}} + P_{\text{cond}} + P_{\text{brk}} + \frac{\Delta t_k}{2V}\left(\sum_{m=1}^{i-1} S_m + \sum_{m=1,m\neq i}^{j} \beta'_{im}\right) \tag{18}$$

is satisfied, it is decided that the simulation particle i will coagulate with simulation particle j.

As for the acceptance–rejection method, simulation particle i and j undergo the same coagulation event if a random number is less than the value $\beta'_{ij}/\beta'_{\max}$, where particles i and j are randomly chosen from simulation particle population, and $\beta'_{\max}$ is the maximum over all particle pairs in the new coagulation rule. If $\beta'_{\max}$ is overestimated, the acceptance–rejection method still describes the Markov process exactly but less efficiently.

2.6. The maintenance of constant-volume and the restoration of simulation particle number

When MC method describes the dynamic evolution in dispersed system, the total number of simulation particles and the volume of computational domain are two key issues. The excessive simulation particles will burden computation cost of MC

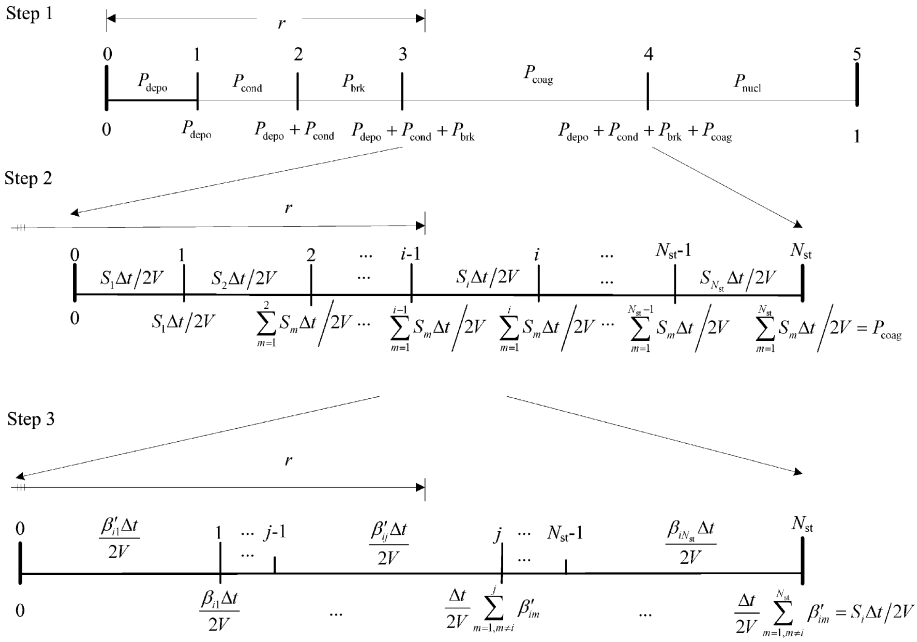

Fig. 3. The selection of main event and main particles.

simulation; however, the insufficient number of simulation particles will deteriorate computational precision of MC simulation. On the other hand, expansion or contraction of the domain results in the bad expansibility and applicability of MC. In the new MC method computational domain is always maintained; however the restoration of simulation particle number is different in the equally and differentially weighting procedures.

2.6.1. The equally weighting procedure

We found [44] the forcible maintenance of particle number will disturb the ensemble and then exhibit an error associated with "sample restoration"; and the doubling or halving scheme, which is adopted by the stepwise constant-volume method [19,20], the time-driven DSMC [17] and some other MC methods [48], demonstrates a weak influence on the precision of MC. So we develop two new schemes of sample restoration in special light of the equally weighting procedure. In the case, the number weight of each simulation particle is same at any time-point, and the total number of simulation particles is restored step by step, that is, the total number of simulation particles lies always between $N_{st,0}/2$ and $2N_{st,0}$, where $N_{st,0}$ is the initial total number of simulation particles.

2.6.1.1. Coagulation. The binary coagulation event between simulation particle i with volume of v_i and simulation particle j with volume of v_j results in a new simulation particle k with volume of v_k ($=v_i + v_j$). The number weight of the simulation particle k is still equal to the common value w. The old simulation particles j is abandoned, and the new simulation particle k is stored in the position of simulation particle i. The direct consequence of coagulation event is net depletion of the number of simulation particles.

2.6.1.2. Breakage. If simulation particle i of volume v breaks up, the following measures are adopted: fragment size distribution is gained according to $b(v)$ and $\gamma(v,u)$; and then, the parent particle i is replaced by the first fragment; next, the other fragments are put into the simulation particle population. The number weight of all fragments is equal to that of the parent particle i, saying, the common weight w. Attentively, the sum of simulation particles will be added $(b(v) - 1)$ along with one breakage event.

2.6.1.3. Surface growth/dissolution (condensation/evaporation). The occurrence of condensation/evaporation event does not disturb the total number of simulation particles. If the condensation event of simulation particle i with volume of v_i occurs, the volume of particle i is changed as $v_i + v_0$, where v_0 denotes the volume of the condensing monomer.

2.6.1.4. Nucleation. The nucleation event results in net generation of particles. The new simulation particle is endowed with volume of v_{min} and number weight of w, where v_{min} is the volume of nuclei or precursor.

2.6.1.5. Deposition (settling). If simulation particle i is settled, it is not tracked any longer. One deposition event means subtracting one from the total number of simulation particles.

The EDCV method develops two schemes to maintain the domain and treat the excessive or insufficient simulation particles. Stepwise constant-number scheme is firstly demonstrated. When the number of simulation particles reaches $N_{st,0}/2$, the surviving particles are duplicated and added into simulation particle population to restore the number of simulation particles. As a result, the number weight of each simulation particle is halved. When the number of simulation particles exceeds $2N_{st,0}$, one half of simulation particles, which are selected randomly, are excluded from the simulation particle population, while the number weight of each simulation particle is doubled. The halving/doubling of the common number weight is similar to the doubling/halving of the subsystem domain adopted by the time-driven DSMC [17] and the stepwise constant-volume method [20]; however the scheme adopted here maintains the computational domain. Nevertheless, we found the halving/doubling action exhibits some numerical errors. The errors are caused by two factors. On the one hand, if the total number of simulation particles is not just equal to the half/double of the initial number of simulation particles immediately before the doubling/halving action (for example, a multiple breakage case), several simulation particles must be added or discarded randomly to restore the sample of the computational domain, which generates numerical error. This error can be avoided through an appropriate choice of the number of simulation particles. If $N_{st,0} = i \times |z|$, where z is the stoichiometric coefficient of dynamic event [23], and i an integer, the simulation particle number immediately before the doubling/halving action would be always equal to the half/double of $N_{st,0}$. On the other hand, the removal of the randomly selected particles when treating the excessive simulation particles disturbs the statistics of the particle ensemble.

A resetting scheme is also proposed in the paper. Once the total of simulation particles is greater than $2N_{st,0}$ or less than $N_{st,0}/2$, a new simulation particle population with number of $N_{st,0}$ is generated to represent real particle population at the current time-point so as to restore the sample number. The PSDF of real particle population is first obtained through counting old simulation particle population, and then new simulation particle population is generated to duplicate the obtained PSDF as possible according to the steps described in Section 2.1. The PSDF information of old simulation particle population can not be fully transferred to the new simulation particle population, so the scheme also exhibits some numerical error. Both the stepwise constant-number scheme (the halving/doubling of number weight of simulation particles) and the resetting scheme (the resetting of simulation particle population) can be adopted by the EDCV method, depending on the choice of user and the particulars of the problem.

2.6.2. The differentially weighting procedure

In the case, both the computational domain and the total number of simulation particles are automatically maintained through the following constant-number scheme.

2.6.2.1. Coagulation. When the main simulation particle i coagulates with its coagulation partner j, it means that some real particles of simulation particle i coagulate with these of simulation particle j; however, it does not mean every real particle of simulation particle i or j undergoes coagulation event in the new coagulation rule. In fact, it is thought that the number of real coagulation events is $\min(w_i, w_i)$ in the new coagulation rule. After the coagulation event between simulation particles i and j, all of consequent real particles are divided into two parts: these "coagulated" real particles and these "non-coagulated" real particles. The two parts of real particles are re-represented by the two simulation particles i and j respectively, which is shown in Fig. 4. Two involved simulation particles are both conserved in order to maintain the total number of simulation particles; accordingly, their number weight (w_i and w_j), and size (v_i and v_j) are adjusted to satisfy the law of conservation of mass:

$$\begin{aligned}
&(1)\ \textit{if}\ (w_i)_{\text{old}} > (w_j)_{\text{old}},\ \begin{cases} (w_i)_{\text{new}} = (w_i)_{\text{old}} - (w_j)_{\text{old}}; (v_i)_{\text{new}} = (v_i)_{\text{old}} \\ (w_j)_{\text{new}} = (w_j)_{\text{old}}; (v_j)_{\text{new}} = (v_i)_{\text{old}} + (v_j)_{\text{old}} \end{cases} \\
&(2)\ \textit{if}\ (w_i)_{\text{old}} < (w_j)_{\text{old}},\ \begin{cases} (w_i)_{\text{new}} = (w_i)_{\text{old}}; (v_i)_{\text{new}} = (v_i)_{\text{old}} + (v_j)_{\text{old}} \\ (w_j)_{\text{new}} = (w_j)_{\text{old}} - (w_i)_{\text{old}}; (v_j)_{\text{new}} = (v_j)_{\text{old}} \end{cases}
\end{aligned} \tag{19}$$

where the subscript "old" and "new" denote the conditions before and after the dynamic event, respectively.

In some sense, the constant-number scheme is a simplified version of conservative weighting scheme proposed by Boyd [34]. In the conservative weighting scheme, both linear momentum and energy is explicitly conserved during collisions by introducing the "split-merge" scheme. The paper only considers zero-dimensional PBM where mass conservation of particle population is necessary. As for multi-dimensional PBM where the conservation of mass, momentum, and energy must be considered, the conservative weighting scheme could be further adopted by the differentially weighting method.

With respect to other dynamic events, the constant-number scheme developed in the MMC method [38,39] can be transplanted to the EDCV method.

2.6.2.2. Breakage. Here the total number of simulation particles is conserved at any time by the following so-called "merging" measure that is also adopted by the MMC method for simultaneous particle coagulation and breakage [38]. The first fragment is stored in the position of the parent particle i and other fragments are merged respectively with randomly selected simulation particle whose size most closely matches that of the fragment. One binary breakage event is used to illuminate the maintenance of simulation particle number. Let i be the index of the parent simulation particle, let l be the index of the randomly selected simulation particle, and let the index j and k represent the first and second fragment, respectively. The size and number weight of these particles are related by: $(v_i)_{\text{old}} = v_j + v_k$, $(w_i)_{\text{old}} = w_j = w_k$, $(v_l)_{\text{old}} = v_k$. After the breakage event, the merging measure is taken in order to maintain the total of simulation particles

$$\begin{aligned}
&(v_i)_{\text{new}} = v_j; \quad (w_i)_{\text{new}} = (w_i)_{\text{old}} \\
&(v_l)_{\text{new}} = (v_l)_{\text{old}}; \quad (w_l)_{\text{new}} = (w_l)_{\text{old}} + (w_i)_{\text{old}}
\end{aligned} \tag{20}$$

These "new" simulation particles are tracked in the next time-step. By these measures is the simulation particle number conserved on the cost of some systematic errors. The systematic errors directly originate from the disturbed number weights of simulation particles and the non-conserving mass during the mergence action, which is qualitatively analyzed in Ref. [44].

2.6.2.3. Surface growth/dissolution (condensation/evaporation). The measures in the equally and differentially weighting procedures are equivalent because the event does not change the number of simulation particles.

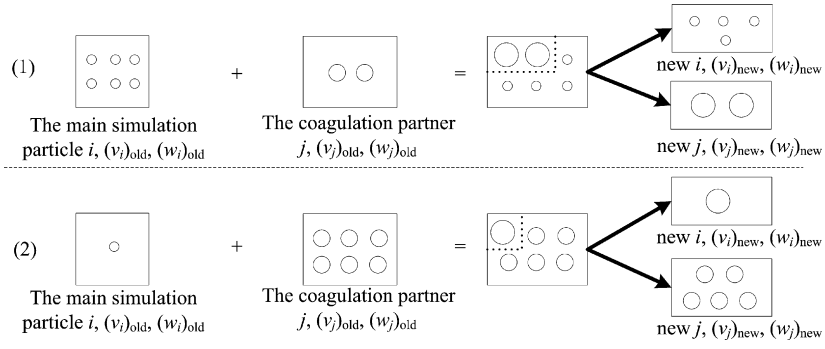

Fig. 4. The coagulation between two differentially weighting simulation particles.

2.6.2.4. Nucleation. One new nucleus will generated after one nucleation event. Firstly the nucleus is represented by one new simulation particle with size of $v_{\min}$. Then the simulation particle is merged with one simulation particle whose size most closely matches $v_{\min}$, which is similar with these measures that are adopted in the binary breakage event.

2.6.2.5. Deposition (settling). The vacancy of the deposited simulation particle i should be filled in order to maintain the total of simulation particles. The simulation particle j is selected by a stochastic process, and then these real particles which are represented by simulation particle j are halved to two groups, and then are represented by two new simulation particles k and l, respectively, where $w_j = 2w_k = 2w_l$, and $v_j = v_k = v_l$. And then simulation particles i and j are replaced by simulation particles k and l, respectively. Factually, these measures mean that the leaving vacancy of the settled simulation particle i is filled with the half of the randomly selected simulation particle j. The same measures have been presented in the MMC method [41,42]. These measures also introduce some systematic errors which directly originate from the disturbed number weights of simulation particles [44].

2.7. The flowchart of the event-driven constant-volume method

Up to now, we can draw the flowchart of the EDCV method, as shown in Fig. 5. There exist three alternative "switches" that are represented by the symbol "Δ" in the figure, that is, the equally or differentially weighting procedure, the inverse or acceptance–rejection method, the stepwise constant-number or resetting or constant-number scheme. User can turn on/off these alternative "switches", depending on the particulars of the problem. For example, if the equally weighting procedure is

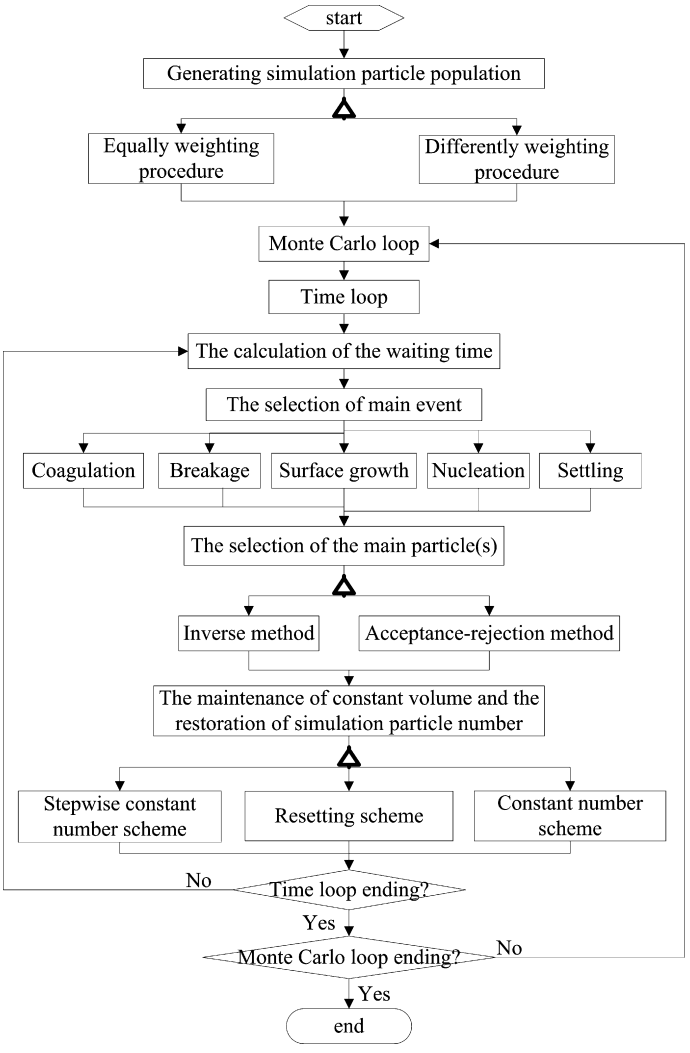

Fig. 5. The flowchart of event-driven constant-number method.

selected, and in particular the common number weight is equal to 1, the EDCV method is similar to the popular stepwise constant-volume method [20,23].

3. Results

Particle size distribution, particle number concentration N (M_0, the zero-order moment of PSDF) and particle volume (mass) concentration M (M_1, the first-order moment of PSDF) are counted throughout simulation particle population, and they are considered as reference for evaluating MC methods. Particle coagulation and breakage are difficult points for MC methods all the while, and the two events are chosen in the paper for numerical comparison. Other dynamic events such as surface growth/dissolution (condensation/evaporation), nucleation and settling are concerned with only one "parent" simulation particle and/or one "son" simulation particle. They can also be realized numerically by MC methods more easily; however these results are not shown here because of the limit of space.

3.1. Case1, constant coagulation kernel, initial monodispersed population

The precision and operability of MC method do not depend on the forms of kernel model. In the paper, the constant coagulation kernel is selected. The constant kernel enables a rough estimation of the particle number concentration in the Brownian coagulation. In the case, coagulation kernel $\beta_{ij} = A = 10^{-10}\ \mathrm{m^3 \cdot s^{-1}}$, the initial number concentration $N_0 = 10^{10}\ \mathrm{m^{-3}}$, the initial volume $v_0 = 1$ (dimensionless) and the characteristic coagulation time is defined as $\tau_{\mathrm{coag}} = 1/(N_0 A)$. The initial number of simulation (fictitious) particles for all MC methods is chosen as 1000.

In the case, simulation particles are weighted either equally or differentially, and the acceptance–rejection method is used to select the main particles. Here we presented two kinds of the EDCV method: EDCV-1 (the differentially weighting procedure and the constant-number scheme are adopted), EDCV-2 (the equally weighting procedure and the stepwise constant-number scheme are adopted). The performance of the two EDCV methods is compared with that of the MMC, constant-number and stepwise constant-volume methods. The multiplicative constant in the MMC method, α, is set as 0.01. The constant-number method is realized numerically by the mass method, and it adopts the acceptance–rejection method to select the main particles. The inverse method is adopted by the stepwise constant-volume method.

In the case of initial monodispersed particle population, we quantified the accuracy of MC methods on basis of standard deviations in calculation of properties of PSD, that is, σ_N (the standard deviation of the fluctuation of N/N_{theory}), σ_M (the standard deviation of the fluctuation of M/M_{theory}), and σ_d (the overall error in the size distribution) [44]. The approach is also used for accuracy analysis of the new MC method. Numerical results of several MC simulations are compared with analytical solutions [49], which is shown in Fig. 6. In Fig. 6(c), the abscissa k is the number of elementary particles, and P_k is the probability of obtaining a cluster obtaining k elementary particles. The computation cost of these MC methods is listed in Table 2, where the length of time evolution is $1000\tau_{\mathrm{coag}}$ and computational environment is Athlon Xp2500+, 512M.

The results of EDCV-2 method are very similar to that of the stepwise constant-volume method, which indicates that the stepwise constant-volume method is a special case of the EDCV method. In fact, the EDCV-2 method tracks the whole system, and every simulation particle is assigned with the same number weight, in which the halving of the common weight is adopted to restore the number of simulation particles in the case of coagulation event. As far as the stepwise constant-volume method is considered, the subsystem is tracked and the tracked simulation particles in the subsystem are equally weighted with value "1". However, from the point of view of the whole system, every simulation particle has the common weight of $w_{\mathrm{a}} = V/V_{\mathrm{s}}$, where V_{s} is the volume of subsystem. The stepwise constant-volume method restores the number of simulation particles by means of the doubling of the subsystem domain V_{s} in the coagulation case, that is, the halving of the common weight w_{a} from the point of view of the whole system. So the two MC methods are equivalent in some sense, and the differences lie in the tracked computational domain and the scheme of sample restoration.

However, with respect to the number concentration N, the EDCV-1 method, which keeps the number of simulation particles constant, exhibits the lower precision than the EDCV-2 method, which is attributed to the the number weights of simulation particles are frequently disturbed when automatically conserving the number of simulation particles in the differentially weighting procedure. It is noted that the EDCV-1 method shows a few higher precision than the MMC method and the constant-number method. The two EDCV methods and two other event-driven MC methods (the stepwise constant-volume method and the constant-number method) describe perfectly the mass concentration M due to the mass conservation, which contrasts with the lower precision of the MMC method. Among the five MC methods, the two MC methods adopting the differentially weighting procedure, the EDCV-1 and MMC methods, exhibit the least error at the high-end of the size distribution, as shown in Fig. 6(c). This is because the differentially weighting procedure allows more simulation particles with lower number weight to represent these few real particles at the high-end of the size distribution.

The EDCV-1 method shows the lowest efficiency, which is attributed to at least two factors. On the one hand, the EDCV-1 method that adopts the differentially weighting procedure takes the CPU time of $O(N_{\mathrm{st}}^2)$ to calculate the coagulation rate R'_{coag}; however, these MC methods that adopts the equally weighting procedure only cost one half of CPU time, as indicated in Eqs. (7) and (14). On the other hand, the number of the tracked simulation particles is $N_{\mathrm{st},0}$ in the EDCV-1 method but $N_{\mathrm{st},0}/2 \sim N_{\mathrm{st},0}$ in the stepwise constant-volume method and the EDCV-2 method.

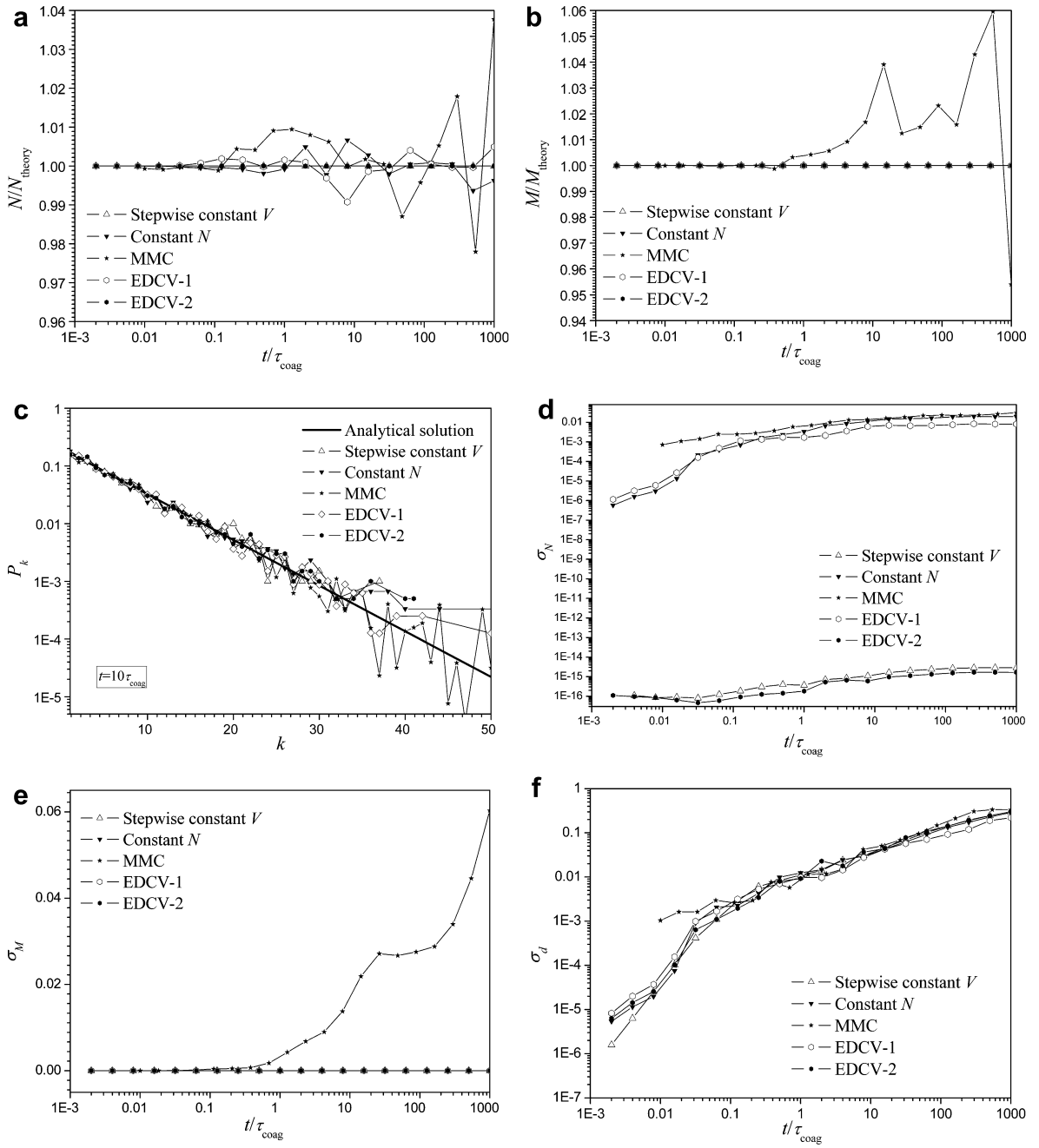

Fig. 6. Case 1, constant coagulation kernel with initial monodisperse population: (a) number concentration; (b) mass concentration; (c) size distributions; (d) error in number concentration; (e) error in mass concentration; and (f) error in size distributions.

Table 2
The comparison of computation cost.

Parameter	Stepwise constant V	Constant N	MMC	EDCV-1/EDCV-A/EDCV-I	EDCV-2/EDCV-B/EDCV-II
CPU t/s, Case1	18.07	45.15	13.01	331.04	20.27
CPU t/s, Case2	–	–	–	8392.72	144.02
CPU t/s, Case3	6.55	2.99	20.59	6.24	5.90

3.2. Case2, constant coagulation kernel, initial exponential distributed particle population

The case is utilized to validate the performance of the EDCV method in the case of initial polydispersed particle population. The initial size distribution is represented by an exponential function $n(v,0)=[N_0\exp(-v/v_{g0})]/v_{g0}$. Here coagulation kernel $\beta_{ij} = A = 6.405 \times 10^{-10}\text{cm}^3/\text{s}$, $N_0 = 10^6\ \text{cm}^{-3}$, the initial mean volume $v_{g0} = 0.029\ \mu\text{m}^3$, and $\tau_{coag} = 1/(N_0 A)$. The mean volume is calculated as $v_g = M_1/M_0 = M/N$. The numerical results of the EDCV method and analytical solutions [50] are shown in Fig. 7. Here, two MC methods utilize the inverse method; and the EDCV-A is implemented by the differentially weighted procedure and the "constant number scheme"; and the EDCV-B method is realized by the equally weighted procedure, where the "stepwise constant-number scheme" is adopted to restore the sample.

As shown in Fig. 7, the two EDCV methods exhibit the high precision of the moments of PSDF and PSDF at some special time-points. The EDCV-A method describes nearly perfectly the time evolution of the mass concentration; however it presents some numerical error for the number concentration after $t/\tau_{coag} \approx 0.1$, which is involved with the disturbance of statistic ensemble in order to forcibly maintain the constant-number of simulation particles in the differentially weighting procedure. The EDCV-B method performs a comparatively low accuracy of the mass concentration and a comparatively stable accuracy of the number concentration. In fact, the equally weighting procedure results in the deterioration of statistical ensemble when transforming the initial polydispersed particle population into the equally weighting simulation particle population. So, in the initial stage of numerical simulation, the EDCV-B method loses some information of real particle population on the edges of the PSD, which deteriorates the precision of the EDCV-B method for N, M and PSDF.

With respect to the PSDF at some special time-points, there is a little difference between the numerical results of the two MC methods and analytical solutions. In order to collect the detailed information of the PSD at some special time-points, the continuous polydispersed real particle population is discretized into several sections by certain kinds of law between the

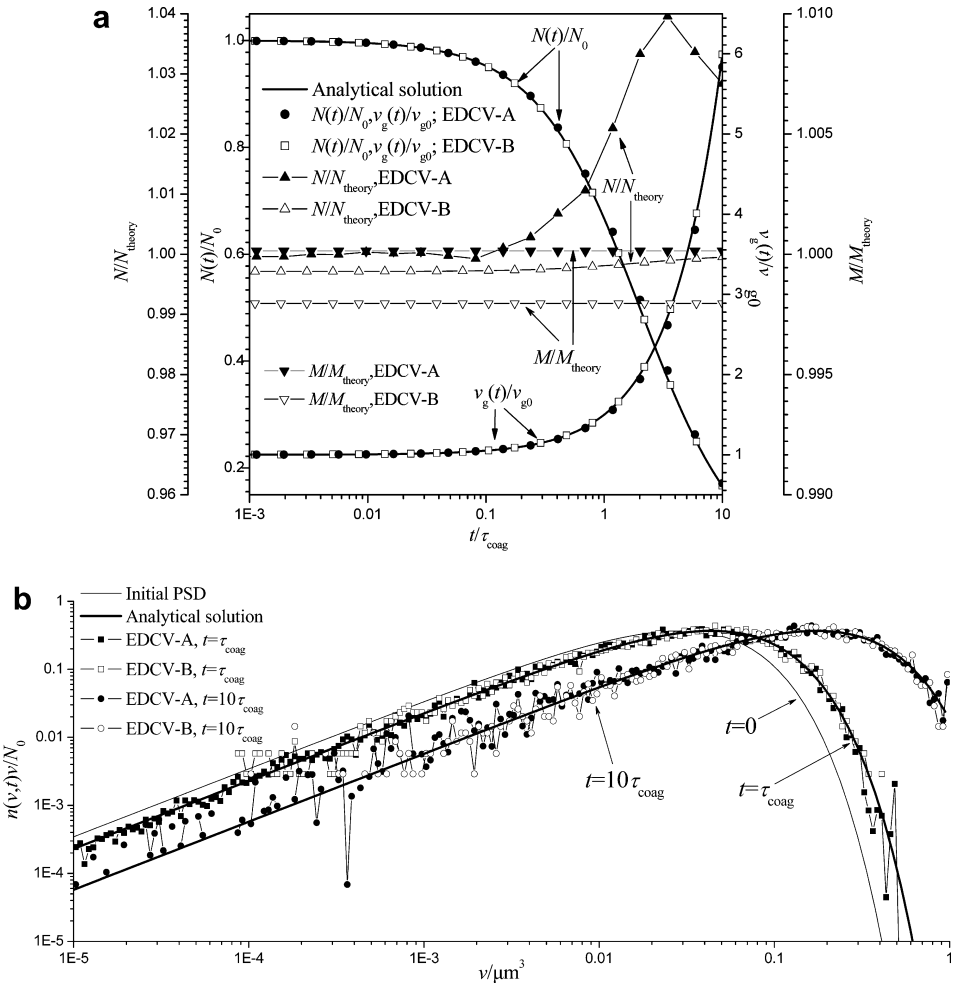

Fig. 7. Case 2, constant coagulation kernel with initial polydispersed population: (a) the time evolution of moments of PSD; and (b) the time evolution of PSD.

largest and smallest sizes. The particle number concentration in each section is counted at some special time-points, in such a way that the detailed information of PSD is obtained. The PSD calculated by the EDCV-A method oscillates around the analytical solution with smaller amplitude than the PSD calculated by the EDCV-B method. It is also worth noting that the EDCV-A method is capable of tracking the size distribution to smaller and larger sizes than the EDCV-B method. Two factors deteriorate the precision of the MC for the detailed information of the PSD. First, the total number of simulation particles plays an important role in the precision of the detailed information of the PSD when polydispersed population spans a wide range. Only when the number of simulation particles in each section reaches to the magnitude of $O(10)$ or more does a MC method protect well against the statistical fatigue of the PSD. To increase the total number of simulation particles will decrease the statistical error. Second, the number of sections and the law of discretization will also influence the calculation

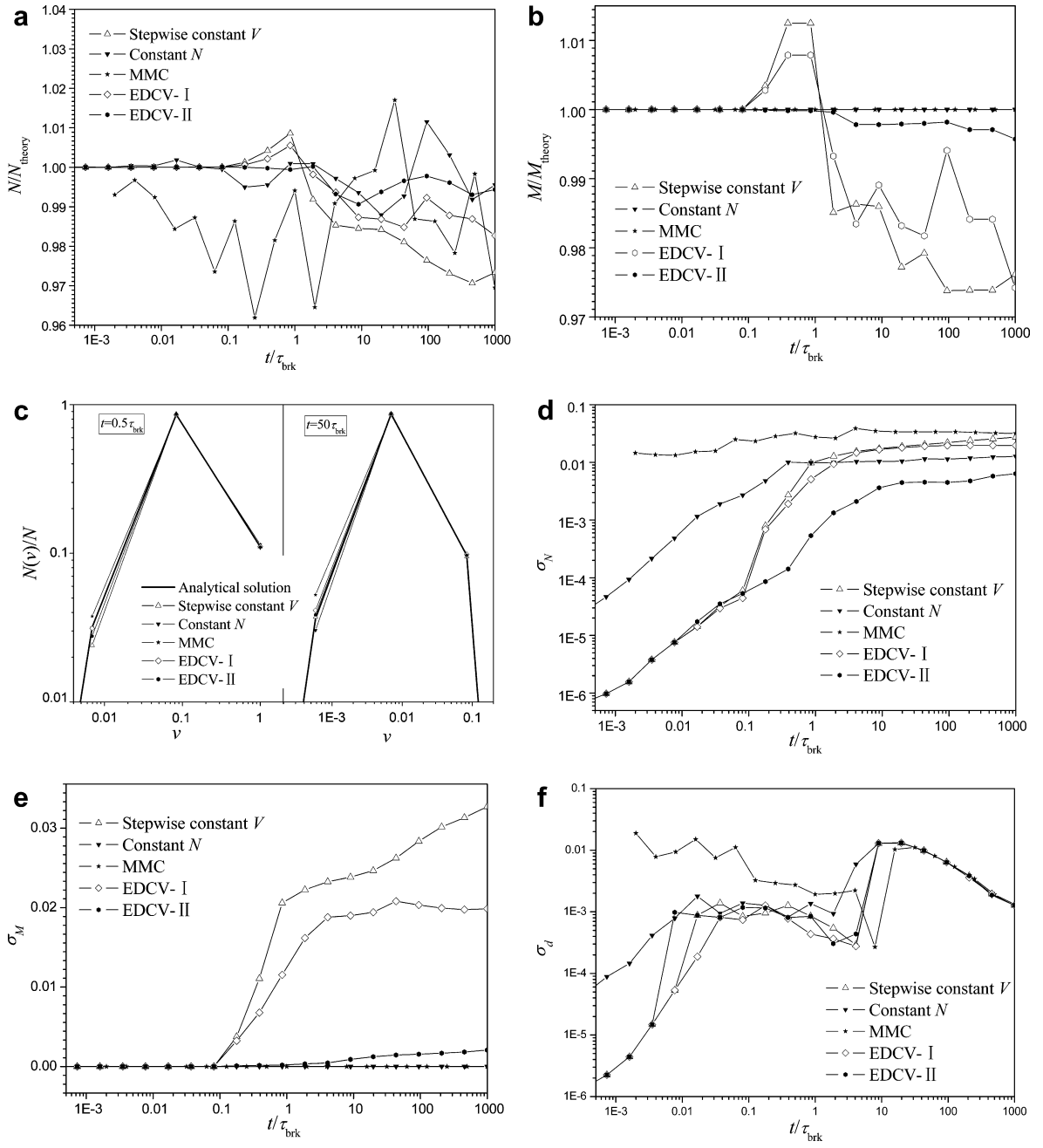

Fig. 8. Case 3, power-law breakage kernel with equal-size fragment size distribution: (a) number concentration; (b) mass concentration; (c) size distributions; (d) error in number concentration; (e) error in mass concentration; and (f) error in size distributions.

of PSD. The choice of sections and discretization laws controls the section range and the simulation particle number in the discretized sections and then the relative importance of different parts of the size range in the overall error calculation. The proper discretization method should depend on the particulars of the problem. In the case the number of discrete sections is 200, logarithmically spaced. With respect to the differentially weighting procedure, every section has at least 10 simulation particles at the beginning of MC simulation; and then the total number of simulation particles is 4040. If the initial polydispersed population in continuous spectrum form is exponentially discretized, or the number of discrete sections is greater or less than 200, for example, the calculated PSD at some special time-points may be different from the results shown in Fig. 7(b).

3.3. Case3, power-law breakage kernel with equal-size fragment size distribution

The MC method demonstrates a good performance for binary coagulation of an initial monodispersed or polydispersed population, and the statistical error when counting the PSD is analyzed. We also compare two approaches of selecting the main particles, i.e. the inverse method and the acceptance–rejection method. However, the numerical error, which originates from the maintenance of the computational domain, is not still analyzed. A complex breakage case, a parent particle breakage into 12 equally-sized fragments with power-law rate, is considered. Here $B(v) = v^{1.8}$, $b(v) = 12$, $\gamma(v,u) = \delta(v,u/12)$, $N_0 = 3000\ \mathrm{m}^{-3}$, $v_0 = 1$ (dimensionless), the characteristic breakage time is defined by $\tau_{\mathrm{brk}} = 1/B(v_0) = 1/(v_0^{1.8})$. In the case, only the equally weighting procedure and the inverse method are adopted, however either the stepwise constant-number scheme (noted as EDCV-I) or the resetting scheme (EDCV-II) is utilized to maintain the domain and restore the simulation particle number. Numerical results and analytical solutions [51] are shown in Fig. 8, where the ordinate "$N(v)/N$" of Fig. 8(c) is the relative number concentration of particle of volume v.

Any MC starts the simulation with 3000 simulation particles. Because every breakage event produces 12 fragments, the total number of real particles increases sharply along with breakage events. The number of simulation particles in the stepwise constant-volume method and the EDCV-I and EDCV-II methods is always between 3000 and 6000, but always maintains 3000 in the constant-number method and the MMC method. After 273 breakage events, the number of simulation particles in the stepwise constant-volume method and the EDCV-I and EDCV-II methods reaches to 6003, i.e., the number of simulation particles is not just equal to the double of the initial number of simulation particles, in which some procedures must be taken to restore the sample. In the stepwise constant-volume method and the EDCV-I method that adopts the stepwise constant-number scheme, three simulation particles are randomly selected and then are discarded in the first place, which will generate some errors; and then, the halving of the computational domain for the stepwise constant-volume method or the doubling of the common number weight for the EDCV-I is taken to restore the particle number, which will also generate some errors because 3000 simulation particles are also randomly selected and then are discarded. When the resetting scheme is adopted by the EDCV-II method, the first moment of the PSD (the mass concentration) is maintained. The EDCV-II method describes exactly the mass concentration, and shows a better performance of the number concentration than other MC methods.

Due to difference between particle concentrations in adjacent size sections by factor of 12 and power-law breakage rate, particle number concentrations in each section is enough high, in such a way that the statistical error degrades when counting the PSD. Under such conditions, all MC methods exhibit nearly the same accuracy.

4. Discussion and conclusions

A new MC method, event-driven constant-number (EDCV) method, is proposed to describe the time evolution of PSD. Generally speaking, the EDCV method has high precision and low cost in calculation of not only number and mass concentrations but also the detailed information of PSD. The numerical errors of the EDCV method are concluded as follows. Firstly, the equally weighting procedure will omit some detailed information of real particle population with polydispersed distribution. However, even though the differentially weighting procedure is adopted, the full duplication of the PSD information from real particle population to simulation particle population is impossible. Certainly, the differentially weighting procedure duplicates the real PSD comparatively exactly than the equally weighting procedure. Secondly, when the method has to restore the sample in the case of the equally weighting procedure, the numerical errors involved with the sample restoration is also inevitable. It should be noticed that the resetting scheme reduces greatly the errors in comparison to the stepwise constant-number scheme. When automatically conserving the simulation particles in the differentially weighting procedure, the constant-number scheme also exhibits some numerical errors which originate from number weights of simulation particles are frequently disturbed. Lastly but not least, any MC methods exhibit the errors associated the process of random sampling and statistics. The enough simulation particle number and the proper discretization method will help restrain the error efficiently.

The proposed EDCV method integrates the concept of equally and differentially weighting simulation particles. Depending on the particulars of the problem, users can choose different versions of the EDCV method, for example, the inverse method or the acceptance–rejection method, the stepwise constant-number scheme or the resetting scheme or the constant-number scheme. These alternative techniques can be packaged together to simulate the dynamic evolution in dispersed system with initial monodispersed or polydispersed distribution. Numerical simulation shows the new method

has same or higher precision than not only the time-driven MC methods such as the MMC method and time-driven DSMC method but also some popular event-driven MC methods such as the stepwise constant-volume method and the constant-number method. In general, the inverse method, which describes perfectly the Markov process of dynamic evolution and exhibits a determinate computation cost, is recommended; the differentially weighting procedure, which contains the equally weighting procedure and exhibits the wider scope of application, is the right selection; however, As for these coagulation cases of initial monodispersed or discrete-distribution particles, the EDCV method tracking equally weighting particles is recommended because of its higher precision and efficiency; furthermore, in the case of the equally weighting procedure, the resetting scheme, which conserves the mass concentration and reduces the fluctuation of the number concentration, is raised to handle excessive or insufficient simulation particles.

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