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Differentially weighted operator splitting Monte Carlo method for simulating complex aerosol dynamic processes

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Abstract

A differentially weighted operator splitting Monte Carlo (DWOSMC) method is developed to solve complex aerosol dynamic processes by coupling the differentially weighted Monte Carlo method and the operator splitting technique. This method is validated by analytical solutions and a sectional method in different aerosol dynamic processes, respectively. It is firstly validated in coagulation and condensation processes, and nucleation and coagulation processes, and is then validated through simultaneous nucleation, coagulation and condensation processes. The results show that this DWOSMC method is a high computationally efficient and quantitatively accurate method in simulating complex aerosol dynamic processes.

Keywords: Differentially weighted Monte Carlo, operator splitting, aerosol dynamics, particle size distribution

Nomenclature

d	average particle diameter (m)
D	diffusion coefficient (m^2/s)
i, j	particle label
I	condensation kernel (m^3/s)
J	nucleation kernel (/s)

K	coagulation kernel (m^3/s)
k_B	boltzmann constant (J/K)
K_n	Knudsen number
M_2	the second moment
n	number density of aerosol particles
N	particle number concentration during the simulation interval
N_0	initial particle number concentration
N_p	number of simulation particles
r	random number
t	time (s)
T_K	temperature (K)
Δt	time-step (s)
δt	time-step (s)
$\vec{u}$	velocity of the gas (m/s)
$v,\tilde{v}$	particle volume (m^3)
V	the volume of the aerosol system in simulation; or total particle volume during the simulation interval (m^3)
V_0	initial total volume of the aerosol particles (m^3)
w_i	weight of the simulation particle
X	the total process
X_d	deterministic process
X_s	stochastic process

Subscripts

coag	coagulation
cond	condensation
d	deterministic
nucl	nucleation
i, j, k	section number
i , j, m, n	index of simulation particle
p	simulation particle
s	stochastic

Superscripts

m	step number

Greek letters

α	correction factor
ε	relative error
τ	normalized computational time

Abbreviations

DWOSMC	differentially weighted operator splitting Monte Carlo Method
GDE	general dynamics equation
MC	Monte Carlo
MOM	method of moment
PBE	population balance equation
SM	sectional method

1. Introduction

The problem of air pollution is increasingly severe in recent years, resulting in all kinds of acute and chronic diseases of human beings, i.e., lung cancer, asthma, leukemia, etc. Therefore, the study of atmospheric science has been more and more important. The air pollution indexes (i.e., PM_1, $PM_{2.5}$, PM_{10}), refers to the diameter size of the particulate matters (PMs) in the air. The US Environmental Protection Agency has listed the reduction of $PM_{2.5}$ emissions as an important item for controlling air pollution (Raman & Fox, 2016). The ultra-fine, submicron and fine particles suspended in the air are also called aerosols (Friedlander, 2000; Gelbard, 1979). Considering their impact on climate and health, it is significant to understand the evolution and distribution of aerosol particles (Tie, 2015). Therefore, more and more researchers have drawn their attention to the study of aerosol dynamics in recent decades. The research of aerosols is highly related to polymerization processes, dispersion of aerosols in the atmosphere, chemical reactions involving surface growth, precipitation of particles, and processes for the production of pharmaceuticals. (Madadi-Kandjani & Passalacqua, 2015). Besides doing experiments for describing the aerosol dynamics and chemical reactions, numerical modelling also becomes a very useful tool to predict and describe the aerosol dynamic processes including nucleation, coagulation, condensation, etc. (Chan et al., 2006; Liffman, 1992; Qamar & Warnecke, 2007; Zhou & Chan, 2011). In different kinds of developed numerical models, the most popular ones are sectional method (Dergaoui et al., 2013; Gelbard, Fitzgerald, & Hoppel, 1998), the method of moment (Chan, Liu, & Chan, 2010; Liu, He, & Chan, 2011; McGraw, 1997; Yu & Chan, 2015; Yu et al., 2015), and Monte Carlo method (Fede, Simonin, & Villedieu, 2015; He et al., 2015; Zhang & You, 2015).

Sectional method (SM) is a kind of discrete aerosol size distribution approach. In a sectional representation, the size of the particles is divided into a certain number of sections and all the particles in one section have the same component composition (Chen, Lin, & Yu, 2014; Lu, 2005). While in the method of moments (MOM), the governing equation of the particles is transformed into a set of ordinary differential equations regarding the moments (Settumba & Garrick, 2004). Both of the SM and MOM are deterministic methods, and are effective tools to describe or predict the evolution of aerosol particle size distribution, and technically easy to be coupled with Eulerian-Eulerian models of multiphase flows (Vlieghe et al., 2016; Zhang & You, 2015). However, these two methods have their own advantages and disadvantages in accuracy and efficiency (Wei, 2013; Chen et al., 2014), for example, SM tends to be more accurate, however the sectional representations may lead to complicated algorithms; MOM is relatively efficient, but the main difficulty is to obtain the closure of the moment equations. Some researchers (Lee, Chen, & Gieseke, 1984; Pratsinis, 1988) achieved the closure of the moment equations by making a prior assumption of the initial form of the particle size distribution (PSD), and some other researchers have developed different methods to realize the closure of the moment equations without prior requirement for PSD (Chan et al., 2010; Frenklach, 2002; Yu & Chan, 2015; Yu, Lin, & Chan, 2008).

Besides MOM and SM, Monte Carlo (MC) method arises remarkably because of its advantage of stochastic characteristics (Hussain, Kumar, & Tsotsas, 2015; Kruis et al., 2012; Sun, Axelbaum, & Huertas, 2004). MC

method is a stochastic algorithm which is based on probabilities of different outcomes in a process which could not be easily predicted because of its randomness. Instead of solving directly the general dynamic equation, MC method imitates the formation, movement and dynamic behaviors of simulation particles based on the happening probabilities of these behaviors (Bird, 1976; Liu & Chan, 2016).

Metropolis and Ulam (1949) first proposed MC method applying the laws of probability and statistics to the natural sciences. Bird (Bird, 1963, 1976, 1994) developed the direct simulation Monte Carlo (DSMC) method for modeling rarefied gas flows. Different MC methods have been proposed to study the aerosol dynamics, which can be generally classified into time-driven MC method (Liffman, 1992; Liu & Chan, 2017b) and event-driven MC method (Mendoza-Coto, Díaz-Méndez, & Pupillo, 2016; Zhao & Zheng, 2009) with respect to the advancement method of the algorithm, or constant-number MC method (Lin, Lee, & Matsoukas, 2002; Liu & Chan, 2016) and constant-volume MC method (Yamakov, 2016; Zhao & Zheng, 2009) with respect to the variation of computational domain. Kostoglou and Konstandopoulos (2001) identified the characteristics of different MC approaches and classifications. Weighted MC methods (Boyd, 1996; Liu & Chan, 2017a; Zhao, Kruis, & Zheng, 2010) have also been proposed to increase the resolution and efficiency of MC method.

Since MC methods simulate directly the dynamic behavior of particles, it can approximate the population balance equation (PBE) solution through a large number of random samplings from the particle system. The stochastic nature of the MC method adapts itself naturally to the stochastic processes. It is also relatively simple to implement MC algorithm in multi-dimensional, multi-scale, and polydispersed systems (Xu et al., 2014). Kostoglou & Konstandopoulos (2001) and Kostoglou, Konstandopoulos & Friedlander (2006) successfully used MC method in solving bivariate coagulation equation. Generally, a classical MC simulation consists of the following steps：

1. Define a probabilistic process which can describe the studied problem;
2. Generate inputs randomly from the known probability distribution over the computational domain;
3. Perform computation on the established model to get the random solutions; and
4. Repeat the simulation and average the results.

Compared with other methods, MC methods are becoming more and more preferred, because of the following advantages (Wei & Kruis, 2013):

a). The stochastic nature of MC makes it ideally suitable to deal with the stochastic event;

b). MC method can solve the closure problem of general dynamic equation (GDE);

c). Each simulation particle can have its unique size, composition and morphology, i.e., any information about the particles can be obtained; and

d). It is simple and robust to code numerically.

In MC methods, simulation particles are used to represent the large number of real particles, and thus introducing the notion of "weighted simulation particles". In previous studies, the same weight for different simulation particles was used (Boyd, 1996; Liffman, 1992; Fox, 2003; Smith & Matsoukas, 1998; Zhao, Kruis, & Zheng, 2010). In order to reduce the statistical noise, Zhao et al. (Zhao & Zheng, 2011; Zhao, Zheng, & Xu, 2005b) developed a differentially weighted Monte Carlo method, which proves to be efficient and practical for simulating the coagulation process of aerosol particles. While deterministic method is more efficient for simulating the nucleation and condensation processes, in order to take advantage of both stochastic and deterministic methods, Zhou et al. (2014) and Liu and Chan (2017a) have successfully combined stochastic and deterministic methods by adopting the operator splitting technique. In the present study, a differentially weighted operator splitting Monte Carlo (DWOSMC) method coupling the operator splitting technique and the differentially weighted Monte Carlo method is proposed and validated through complex aerosol dynamic processes.

2. Methodology

2.1 General Dynamics Equation

In the past several decades, many researchers in aerosol science have introduced all kinds of ideas and concepts to describe the behavior of aerosol particles. The dynamic behaviors and the properties of the aerosol particles are usually described by a population balance equation (PBE) (Housiadas & Drossinos, 2005), which is also known as the general dynamic equation (GDE) (Friedlander, 2000), as is expressed in Eq. (1),

$$\frac{\partial n}{\partial t}+\nabla\cdot n\vec{u}=\nabla\cdot D\nabla n+\left[\frac{\partial n}{\partial t}\right]_{\text{nucl}}+\left[\frac{\partial n}{\partial t}\right]_{\text{coag}}+\left[\frac{\partial n}{\partial t}\right]_{\text{cond}} \tag{1}$$

where n is the size distribution function of the particles, $\vec{u}$ is the velocity of the gas, and D is the diffusion coefficient.

If the effects of convection and diffusion are not considered, Eq. (1) becomes,

$$\frac{\partial n}{\partial t}=\left[\frac{\partial n}{\partial t}\right]_{\text{nucl}}+\left[\frac{\partial n}{\partial t}\right]_{\text{coag}}+\left[\frac{\partial n}{\partial t}\right]_{\text{cond}} \tag{2}$$

2.1.1 Nucleation

Nucleation process refers to the process that the saturated vapours convert into particles of a critical size, v_0. Thus the number density of other particles (volume larger than v_0) does not change due to the nucleation process, and the nucleation process contributes to the variation of particle number concentration and the total particle volume fraction due to the production of new particles. The particle number concentration change due to nucleation is (Kalani & Christofides, 2002),

$$\left[\frac{\partial n}{\partial t}\right]_{\text{nucl}}=\delta_{v_0}(v)J_0(t) \tag{3}$$

The nucleation kernel, $J_0(t)$ describes the rate of formation of particles with volume, v_0. The $\delta_{v_0}(v)$ is the standard Dirac function, $\delta_{v_0}(v) = 0, (v \neq v_0)$.

In the present study, the new generated particles have the same volume of v_0, which is the initial volume of the particles, and are sorted into the weight of the corresponding simulation particle i which represents the real particles with volume v_0,

$$w_i^{'} = w_i + J_0(t)\delta t \tag{4}$$

where $w_i^{'}$ and w_i represent the weight of simulation particle, i, after and before the nucleation event, respectively, δt refers to one time-step. The definition of w_i is described in Section 2.3.

2.1.2 Coagulation

Coagulation process refers to that two particles collide and combine with each other to form a new bigger particle, it is described by the famous Smoluchowski's equation, which includes two terms and is expressed as Eq. (5) (Seigneur et al., 1986; Wei, 2016). The coagulation kernel, $K(v,\tilde{v})$ describes the rate of particles with volume, v coagulating with particles with volume, $\tilde{v}$. In different aerosol regimes, $K(v,\tilde{v})$ can be a constant value or a value that is dependent on the volume of particles.

$$\left[\frac{\partial n}{\partial t}\right]_{\text{coag}} = \frac{1}{2}\int_0^v K(v,\tilde{v})n(\tilde{v})n(v-\tilde{v})\mathrm{d}\tilde{v} - \int_0^\infty K(v,\tilde{v})n(\tilde{v})n(\tilde{v})d\tilde{v} \tag{5}$$

For the free molecule regime (where the diameter of particles is smaller than the mean free path of air), $K(\mathrm{v},\tilde{v})$ is expressed as Eq. (6) (Zhou et al., 2014),

$$K(v,\tilde{v}) = \left(\frac{6}{\pi}\right)^{2/3}\left(\frac{\pi k_{\mathrm{B}} T_{\mathrm{K}}}{2\rho}\right)^{1/2}\left(\frac{1}{v}+\frac{1}{\tilde{v}}\right)^{1/2}\left(v^{1/3}+\tilde{v}^{1/3}\right)^2 \tag{6}$$

The treatment of coagulation event in the present study is described in Section 2.3.

2.1.3 Condensation

Condensation process is the reverse process of evaporation, and the condensation rate, $I_0(v,t)$ is usually related to the surface area of the particles. Theoretically, the total particle number does not change due to the condensation process, while the size of all of the particles will be larger; therefore, the particle size distribution will change due to condensation process.

The change in particle size distribution due to condensation event (Ramabhadran, Peterson, & Seinfeld, 1976) is,

$$\left[\frac{\partial n(v,t)}{\partial t}\right]_{\text{cond}} = -\frac{\partial (I_0 n)}{\partial v}(v,t) \tag{7}$$

In the treatment of condensation event in the present study, the weights of the simulation particles remain the same value, which means condensation event does not change the total particle number, while the volume of simulation particle i will change accordingly as follows,

$$\frac{dv_i}{dt} = I(v) \tag{8}$$

where v_i represents the volume of simulation particle, i.

2.2 Operator splitting method

As can be seen in Eq. (2), it is a complicated equation which contains different processes, while an applicable strategy to deal with such complicated problems is to "divide and conquer". A rather successful approach in this spirit is an operator splitting technique. Operator splitting technique can separate the total process into multiple steps. It firstly solves different sub-processes and then combine the results (Carrayrou, Mosé, & Behra, 2004; McLachlan & Quispel, 2002), respectively. The second-order Strang splitting method (McLachlan & Quispel, 2002) is described by Eq. (9),

$$\exp(\delta tX)=\exp\left(\frac{1}{2}\delta tX_2\right)\exp(\delta tX_1)\exp\left(\frac{1}{2}\delta tX_2\right)+\mathcal{O}(\delta t^3) \tag{9}$$

where X refers to the total process, X_1 and X_2 refer to two different sub-processes respectively, δt refers to one-time step.

In the present study, X refers to the total aerosol dynamic process, X_1 refers to coagulation process, which is modelled by the stochastic method, X_2 refers to nucleation and condensation processes, which are solved by deterministic integration method. As X_2 includes two processes (i.e., nucleation and condensation processes), Eq. (9) becomes,

$$\exp(\delta tX)=\exp\left(\frac{1}{2}\delta tX_{\text{nucl}}\right)\exp\left(\frac{1}{2}\delta tX_{\text{cond}}\right)\exp\left(\delta tX_{\text{coag}}\right)\exp\left(\frac{1}{2}\delta tX_{\text{cond}}\right)\exp\left(\frac{1}{2}\delta tX_{\text{nucl}}\right)+\mathcal{O}(\delta t^3) \tag{10}$$

2.3 Differentially weighted Monte Carlo (DWMC) scheme

Because of its statistical character, the computational time consumption and accuracy of using Monte Carlo method are all related to the number of simulation particles (Filippov, Markus, & Roth, 1999; Maisels, Kruis, & Fissan, 2004). If high accuracy is needed for the simulation, Monte Carlo method usually has quite high requirement on computer memories and high computational time consumption. The concept of weight (Zhao et al., 2010) is widely used by Monte Carlo method to reduce the computational work and to resolve the conflict between the large amount of real particles and the limitation of computer capacity and central processing unit speed. The time-driven constant number differentially weighted Monte Carlo (DWMC) method developed by Zhao et al. (2005) is adopted herein. In this method, every simulation particle for calculation is weighted differentially with a number of real particles, which is the weight of the simulation particle, w_i (i = 0, 1, 2, 3...n), where n is the simulation particle number.

This proposed DWMC method is prominent for handling of the coagulation process. The occurrence probability of coagulation event on simulation particle, i within δt and V is,

$$P_i = 1-\exp(-VC_i\delta t/2) \tag{11}$$

where V is the volume of simulation system, δt is one time-step and C_i is the coagulation rate of simulation particle, i based on the probabilistic coagulation rule, and is described as,

$$C_i=\frac{1}{V^2}\sum_{j=1,j\neq i}^{N} K_{ij}^{'}$$

where N is the total number of simulation particles, and $K_{ij}^{'}$ is the normalized coagulation kernel for particle, i and particle, j ,

$$K_{ij}^{'}=2K_{ij}w_j\max(w_i,w_j)/(w_i+w_j)$$

Coagulation event will take place on simulation particle, i if a generated random number from a uniform distribution between 0 and 1, r_1 is less than P_i, and the choice of a pair particle, j is based on the acceptance-rejection method: the coagulation partner particle, j is decided if the following condition is satisfied,

$$r_2 \leq K_{ij}^{'}/\max(K_{mn}^{'})|_{\forall m,\forall n} \tag{12}$$

where r_2 is a generated random number. The condition in Eq. (12) is checked until a particle j is chosen.

When two simulation particles, i and j, have been selected to coagulate with each other, the previous particles are substituted by two new weighted simulation particles, which are also denoted as i and j, while the properties of these particles are changed. The calculations are formulated as the following equations (Zhao, Kruis, &Zheng, 2009):

$$\text{If } w_i=w_j, \begin{cases} w_i^{'}=w_i/2; v_i^{'}=v_i+v_j; \\ w_j^{'}=w_j/2; v_j^{'}=v_i+v_j; \end{cases} \tag{13a}$$

$$\text{If } w_i\neq w_j, \begin{cases} w_i^{'}=\max(w_i,w_j)-\min(w_i,w_j); v_i^{'}=v_m|_{w_m=\max(w_i,w_j)}; \\ w_j^{'}=\min(w_i,w_j); v_j^{'}=v_i+v_j; \end{cases} \tag{13b}$$

where $w_i^{'}$, $w_j^{'}$, $v_i^{'}$ and $v_j^{'}$ represent the weight or the volume of the new created simulation particles, i and j after the coagulation event.

2.4 Differentially weighted operator splitting Monte Carlo (DWOSMC) method

In the present study, a differentially weighted operator splitting Monte Carlo (DWOSMC) method is proposed and developed, using operator splitting technique to combine stochastic and deterministic methods, which makes the calculation more flexible and efficient. In this DWOSMC method, the stochastic Monte Carlo method is used for handling the coagulation process, while the deterministic integration method is utilised for deterministic processes (i.e., nucleation and condensation, etc.).

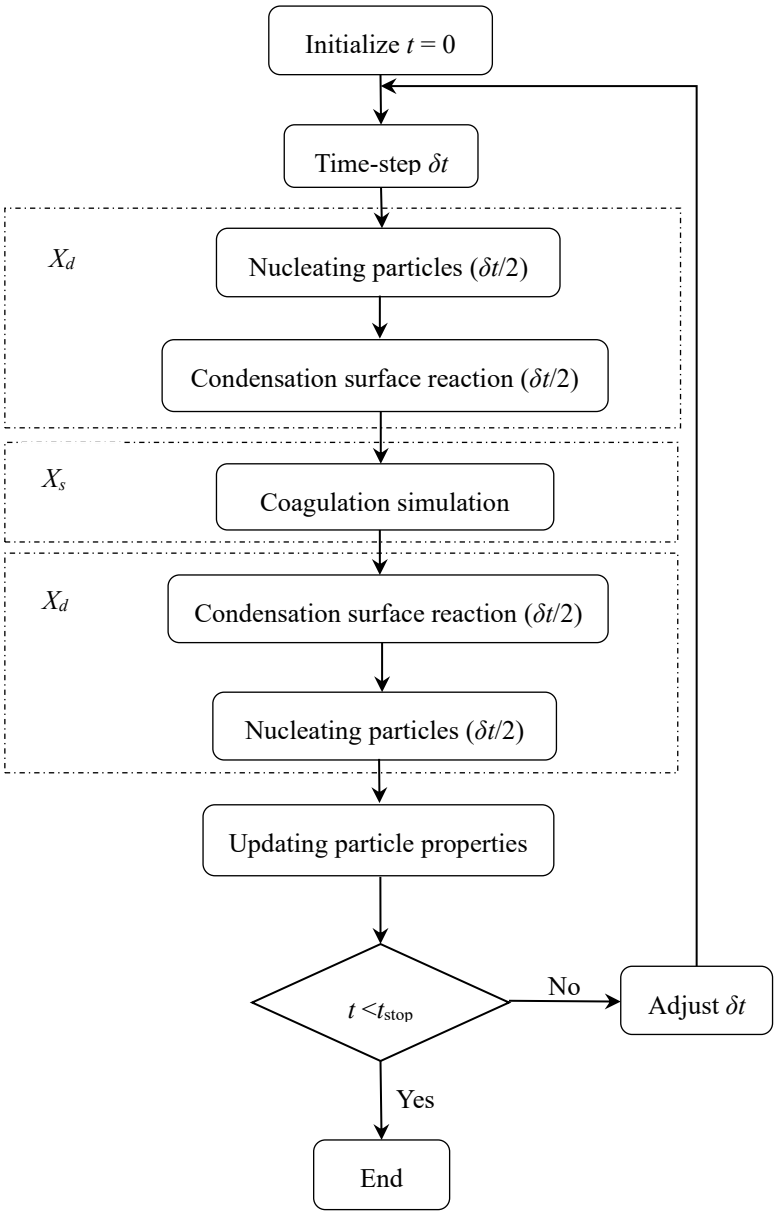


Fig. 1 Flowchart of DWOSMC algorithm (Liu & Chan, 2016).

Fig. 1 shows the flowchart of the full algorithm of DWOSMC method. The second order operator splitting in Eq. (10) is shown. Specifically, the full algorithm is as follows:

Step 1. Initialization. At the very beginning of the numerical simulation, i.e. when the integration time t=0, the properties (volume, diameter, weight, and number density etc.) of the simulation particles are initialized and stored in arrays.

Step 2. Generating time-step, δt. In the simulation process, the choice of an appropriate time step is vital. It is expected to be small enough to ensure that the successively happened coagulation events are uncoupled and that the integration of other physical processes is accurate. The time scale for different aerosol dynamic processes can be determined as the following:

(i) Coagulation

For all of the simulation particles in the system, the time-step for the coagulation event should be determined as (Zhao et al., 2010),

$$\Delta t_{\text{coag}} = \min(V/\sum_{i=1}^{N}\sum_{j=1,j\neq i}^{N} K_{ij}^{'})$$

where V is the volume of simulation system, N is the total number of simulation particles, , and $K_{ij}^{'}$ is the normalized coagulation kernel for particle, i and particle, j,

$$K_{ij}^{'} = 2K_{ij}w_j\max(w_i,w_j)/(w_i+w_j)$$

(ii) Nucleation

The time-step for the nucleation event should be determined by,

$$\Delta t_{\text{nucl}} = 1/(v_0 J_0(t))$$

where $J_0(t)$ is the nucleation kernel. v_0 is the volume of the new created particles.

(iii) Condensation

The time-step for the condensation event should be determined by (Debry, Sportisse, & Jourdain, 2003; Liu & Chan, 2017a),

$$\Delta t_{\text{cond}} = v_i/I_0(v,t)$$

where v_i is the volume of the particle, i, $I_0(v,t)$ is the condensation kernel.

In order to ensure the accuracy of the numerical simulation, the adopted time-step value, δt should be smaller than the minimum value of all the above time scales (Debry et al., 2003). δt is calculated as follows,

$$\delta t = \alpha \min(\Delta t_{\text{coag}}, \Delta t_{\text{nucl}}, \Delta t_{\text{cond}})$$

where α is constant with value of 0.01(Xu, Zhao, & Zheng, 2014; Zhao et al., 2009) during the calculation in order to ensure an accurate integration of all aerosol dynamic processes.

Step 3. Handling the aerosol dynamic processes. The second-order Strang splitting method is used herein. For nucleation and condensation processes, splitting the time-step into two parts, the simulation for nucleation and condensation processes is firstly calculated within the first $\delta t/2$, and then handling the coagulation process for the time-step, δt. At last, nucleation and condensation processes are then calculated within the second $\delta t/2$. The integration procedure in Eq. (10) from t^{m-1} to t^m (t is the total calculation time, m is the step number, and $t^m = t^{m-1}+\delta t$) is as follows,

(i) Integration of nucleation based on Eq. (4) for a time period of $\delta t/2$;

(ii) Integration of condensation based on Eq.(8) for a time period of $\delta t/2$;

(iii) Integration of coagulation based on Eqs. (11) to (13) for a time period of δt;

(iv) Integration of condensation based on Eq. (8) for a time period of $\delta t/2$; and

(v) Integration of nucleation based on Eq. (4) for a time period of $\delta t/2$;

Step 4. Updating the properties of the simulation particles, and obtain the information of the particles at time, t^{m}.

Step 5. Repeating Steps 2 to 4 if the accumulated simulation time, t^{m} is smaller than t_{stop}, otherwise, the current Monte Carlo simulation is finished and the next Monte Carlo simulation is then started. Eight Monte Carlo repetitions are used and the average results are obtained to reduce the stochastic errors.

3. Description of the studied cases

This developed DWOSMC method is validated by both corresponding analytical solutions (Maisels et al., 2004; Palaniswaamy & Loyalka, 2008; Ramabhadran et al., 1976) and a sectional method (Prakash, Bapat, & Zachariah, 2003), and three different test problems are considered in the present study, i.e., simultaneous coagulation and condensation processes, simultaneous nucleation and coagulation processes, and simultaneous nucleation, coagulation and condensation processes. For every test problem, the DWOSMC method is initially validated by the corresponding analytical solutions, and then the results obtained from DWOSMC method are compared with the sectional method for more complex studied cases. The studied cases are described as the following Sections 3.1 to 3.3.

In the present study, the sectional method adopted for the validation of DWOSMC which was developed by Prakash et al. (2003) based on the sectional method developed by Gelbard et al. (1980) and the coagulation nodal method developed by Lehtinen and Zachariah (2001). In this sectional method, particles only exit at discretized nodes, and by limiting the number of the particle parameters, this model makes the computational work quite simple and computational time-saving.

Specifically, the GDE at node k is given by,

$$\frac{\partial n_k}{\partial t} = \left[\frac{\partial n_k}{\partial t}\right]_{\text{nuc1}} + \left[\frac{\partial n_k}{\partial t}\right]_{\text{coag}} + \left[\frac{\partial n_k}{\partial t}\right]_{\text{cond}} \tag{14}$$

The population change due to nucleation, coagulation and condensation are respectively given by,

$$\left[\frac{\partial n_k}{\partial t}\right]_{\text{nuc1}} = \xi_k J_k(t) \tag{15}$$

$$\left[\frac{\partial n_k}{\partial t}\right]_{\text{coag}} = \frac{1}{2}\sum_{\substack{i=2\\ j=2}} \chi_{ijk} K_{i,j} n_i n_j - n_k \sum_{i=2} K_{i,k}\, n_i \tag{16}$$

$$\left[\frac{\partial n_k}{\partial t}\right]_{\text{cond}} = \frac{v_1}{v_k - v_{k\text{-}1}} K_{1,k\text{-}1}(n_1 - n^{s}_{1,k\text{-}1}) n_{k\text{-}1} - \frac{v_1}{v_{k+1} - v_k} K_{1,k}(n_1 - n^{s}_{1,k}) n_k \tag{17}$$

where ξ_k and χ_{ijk} are expressed as,

$$\xi_k = \begin{cases} \frac{v_0}{v_k}; & \text{if } v_{k-1} \le v_0 \le v_k, \\ \frac{v_0}{v_2}; & \text{if } v_0 \le v_1, \\ 0; & \text{otherwise.} \end{cases} \qquad \chi_{ijk} = \begin{cases} \frac{v_{k+1} - (v_i + v_j)}{v_{k+1} - v_k}; & \text{if } v_k \le v_i + v_j \le v_{k+1}, \\ \frac{(v_i + v_j) - v_{k-1}}{v_k - v_{k-1}}; & \text{if } v_{k-1} \le v_i + v_j \le v_k, \\ 0; & \text{otherwise.} \end{cases}$$

More detailed information about this method could be referred to Prakash et al. (2003). In the present study, 50 nodes are used in the programming.

3.1 Simultaneous coagulation and condensation processes

3.1.1 Constant rate coagulation and linear rate condensation case

For constant rate coagulation and linear rate condensation processes, the analytical solution (Ramabhadran et al., 1976) is available, and the parameters and initial conditions given by Palaniswaamy and Loyalka (2008) are selected as Case I for the numerical validation. When the coagulation kernel, K and the condensation kernel, I are given by $K = K_0$ and $I = \sigma_1 v$, respectively, the analytical solutions of the particle number concentration, $N(t)$ and the total particle volume concentration, $\emptyset(t)$ are derived as,

$$N(t) = \frac{N_0}{1 + K_0 N_0 t/2} \tag{18}$$

$$\emptyset(t) = \emptyset_0[\exp(\sigma_1 t)] \tag{19}$$

where N_0 represent the initial particle number concentration, and $\emptyset_0$ represent the initial total volume concentration of the particles.Specifically, K_0 and σ_1 are set as 5×10^{-6} m^3/s and 2×10^{-2}/s, respectively.

3.1.2 Free molecule regime rate coagulation and linear rate condensation case

Case II considers simultaneous free molecule regime rate coagulation and linear rate condensation process**,** where the coagulation kernel is given by Eq. (6) and condensation kernel is given by $I = \sigma_1 v$ ($\sigma_1 = 10$). The solutions of a sectional method from (Prakash et al., 2003) are also given to validate this DWOSMC method.

3.2 Simultaneous Nucleation and Coagulation Processes

3.2.1 Constant rate coagulation and constant rate nucleation case

For constant rate nucleation and constant rate coagulation processes, the analytical solution (Maisels et al., 2004) is available, and the parameters and initial conditions given by Maiselset al. (2004) are selected as Case III for the numerical validation. When the coagulation kernel, K and nucleation kernels, J are given by $K = A$ and $J = J_0$, respectively, the analytical solutions of N/N_0 and V/V_0 are derived as,

$$\frac{N}{N_0} = B\frac{1 + B\tanh(\tau/2)}{\tanh(\tau/2) + B} \tag{20}$$

$$\frac{V}{V_0}=1+\frac{1}{2}B\tau \tag{21}$$

where $\tau = t\sqrt{2AJ_0}$, $B=1/N_0\sqrt{2J_0/A}$ .Specifically, A and $J0$are set as 4×10^{-28} m^3/s and $1.91\times10^{28}/s$, respectively.

3.2.2 Free molecule regime rate coagulation and constant rate nucleation case

Case IV considers free molecule regime rate coagulation and constant rate nucleation processes**,** where the coagulation kernel is given by Eq. (6) and the nucleation kernel is given by $J=J_0$ ($J_0 = 1\times10^{20}/s$). The solutions of the sectional method (Prakash et al., 2003) are also given to validate this DWOSMC method.

3.3 Simultaneous Nucleation, Coagulation and Condensation Processes

3.3.1 Constant rate nucleation, constant rate coagulation and constant rate condensation case

For constant rate nucleation, constant rate coagulation and constant rate condensation processes, the analytical solution is available, and the parameters and initial conditions given by Maiselset et al. (2004) are selected as Case V for the numerical validation. When the nucleation, coagulation and condensation kernels, J, K and I are given by $J= J_0$, $K = A$ and $I=D$, respectively, the analytical solutions of N/N_0 and V/V_0 are derived as,

$$\frac{N}{N_0}=B\frac{1+B\tanh(\tau/2)}{\tanh(\tau/2)+B} \tag{22}$$

$$\frac{V}{V_0}=1+(\frac{1}{2}B+E)\tau+2E\ln(\frac{1+\exp(-\tau)}{2}+\frac{1-\exp(-\tau)}{2B}) \tag{23}$$

where $\tau = t\sqrt{2AJ_0}$, $B = 1/N_0\sqrt{2J_0/A}$, $E = DC_0/AN_0$. Specifically, A, J_0, C_0 and D are set as 4×10^{-28} m^3/s, $1.91\times10^{28}/s$, $1.91\times10^{28}/s$ and 2×10^{-28} m^3/s, respectively.

3.3.2 Constant rate nucleation, and free molecule regime rate coagulation and linear rate condensation case

Case VI considers constant rate nucleation, and free molecule regime rate coagulation and linear rate condensation.The coagulation kernel is given by Eq. (6), the nucleation kernel is given by $J = J_0 = 1\times10^{20}/s$, and condensation kernel is given by $I = \sigma_1 v$ ($\sigma_1 = 0.5$). The solutions of the sectional method (Prakash et al., 2003) are also given to validate this DWOSMC method. The present studied cases are summarized in Table 1.

Table 1 A summary of the present studied cases.

Aerosol Dynamic Processes	Cases	Details
Coagulation + condensation	I	Constant rate coagulation $K = K_0$; and linear rate condensation $I = \sigma_1 v$
	II	Free molecule regime rate coagulation Eq. (6); and linear rate condensation $I = \sigma_1 v$
Nucleation + coagulation	III	Constant rate nucleation $J = J_0$; and constant rate coagulation $K = A$
	IV	Constant rate nucleation $J = J_0$; Free molecule regime rate coagulation Eq. (6)
Nucleation + coagulation + condensation	V	Constant rate nucleation $J = J_0$; constant rate coagulation $K = A$; and constant rate condensation $I=D$
	VI	Constant rate nucleation $J = J_0$; free molecule regime rate coagulation Eq. (6); and linear rate condensation $I = \sigma_1 v$

3.4 Assessment of the numerical simulation results

To assess the accuracy of this proposed and developed DWOSMC method, the relative error ε is utilized in the analysis of the simulation results. where ε is expressed as Eq. (24):

$$\varepsilon=|A(t)-A_0(t)|/A_0(t) \tag{24}$$

where $A(t)$ and $A_0(t)$ are the values obtained via the DWOSMC method and corresponding reference method at time t, respectively. The maximum relative error ε_{max} is calculated by taking the maximum value of the relative error in Eq. (24)

4. Results and Discussion

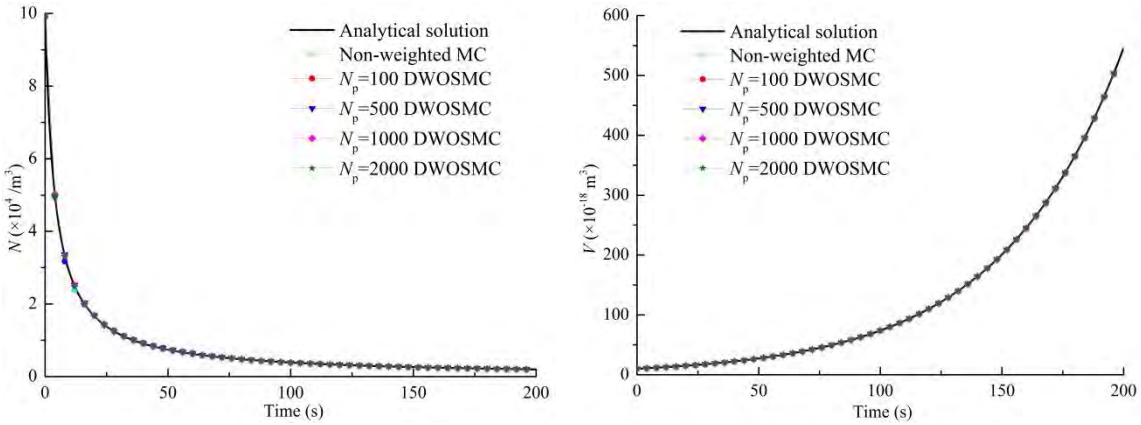
4.1 Simultaneous Coagulation and Condensation Processes

4.1.1 Constant rate coagulation and linear rate condensation case

For studied Case I, the initial particle number concentration, N_0 and initial total particle volume, V_0 are 10^5 and 10^{-17} m^3, respectively. The simulation time for Case I is t_{stop} = 200 s. Different numbers of simulation particles (i.e., N_p = 100, 500, 1000 and 2000) are used for the numerical simulation (the same simulation particles are used for the following studied Cases II to VI in the Sections 4.1.2 to 4.3.2).

In Case I, a non-weighted MC method (Liffman, 1992; Zhao et al., 2010) is used to show the computational efficiency and accuracy of this DWOSMC method. Generally speaking, the particle number concentration, N_0

decreases over time while the total particle volume concentration, V_0 increases over time for coagulation and condensation processes occurring simultaneously (Palaniswaamy & Loyalka, 2008), as is shown in Fig. 2(a) and 2(b). From Eqs. (18) and (19), it can be known that the particle number concentration changes due to the coagulation process, while the total particle volume changes due to the condensation process. Fig. 2(a) and 2(b) show that the simulation results obtained from DWOSMC method have excellent agreement with the analytical solutions even when only 100 simulation particles are used.



(a) (b)

Fig. 2 Evolution of (a) the particle number concentration, N and (b) the total particle volume, V from non-weighted MC method, DWOSMC method and analytical solutions (Ramabhadran et al., 1976) for simultaneous constant rate coagulation and linear rate condensation in studied Case I.

In Fig. 3, the relative error (%) of the particle number concentration and the normalized computational time, $\tau = t/t_{100}$, where t_{100} is the computational time when 100 simulation particles are used for Case I. It can be found that with the increase of the number of simulation particles, the relative error of the simulation results obtained from the DWOSMC method decreases. When the number of simulation particles reaches 1000, the relative error is basically within 1%, and the relative error obtained from the DWOSMC is much smaller with more even distribution than the non-weighted MC method. More importantly, the computational time of this proposed DWOSMC method is much smaller than the non-weighted MC method. When 1000 simulation particles are used, the computational time of DWOSMC method is less than one fifth of the non-weighted MC method.

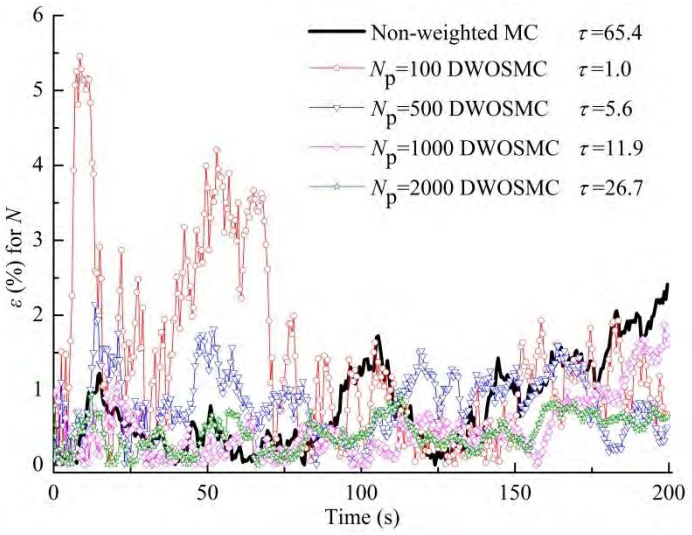


Fig. 3 Evolution of the relative error (%) for the particle number concentration, N obtained from the non-weighted MC method and DWOSMC method when compared with analytical solution (Ramabhadran et al., 1976) for studied Case I, and corresponding normalized computational time, τ.

A very satisfactory agreement on the variation of particle diameter distribution with time obtained from DWOSMC (i.e., $N_p = 2000$) and the sectional method (Prakash et al., 2003) for Case I is shown in

Fig. 4. At the beginning of the numerical calculation, the initial diameter of all the particles is set to be the same value. It can be seen from

Fig. 4 that the distribution function approximately evolves into a lognormal form and the result obtained from DWOSMC is consistent with the sectional method.

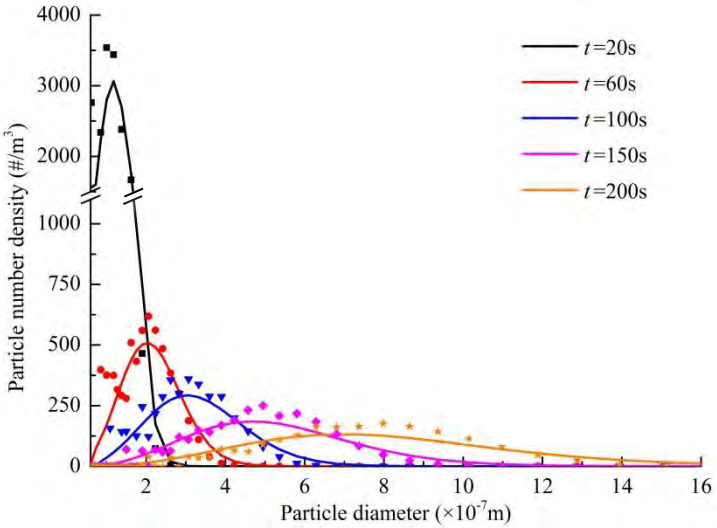


Fig. 4 Evolution of the particle diameter distribution obtained from DWOSMC method (scattered points) and sectional method (Prakash et al., 2003) (solid line) for simultaneous constant rate coagulation and linear rate condensation case processes in the studied Case I.

4.1.2 Free molecule regime rate coagulation and linear rate condensation case

For studied Case II, the initial particle number concentration, N_0 and initial total particle volume, V_0 are 1×10^{18} and 1.77×10^{-9} m^3, respectively. The simulation time for Case II is t_{stop} = 10 ms. The evolutions of particle number concentration, N, particle average diameter, d, total particle volume concentration, V, and the second moment, M_2, as a function of time for studied Case II are shown in Fig. 5(a) to 5(d), respectively, for simultaneous free molecule regime rate coagulation and linear rate condensation processes. The simulation results of a sectional method (Prakash et al., 2003) are used as a reference.

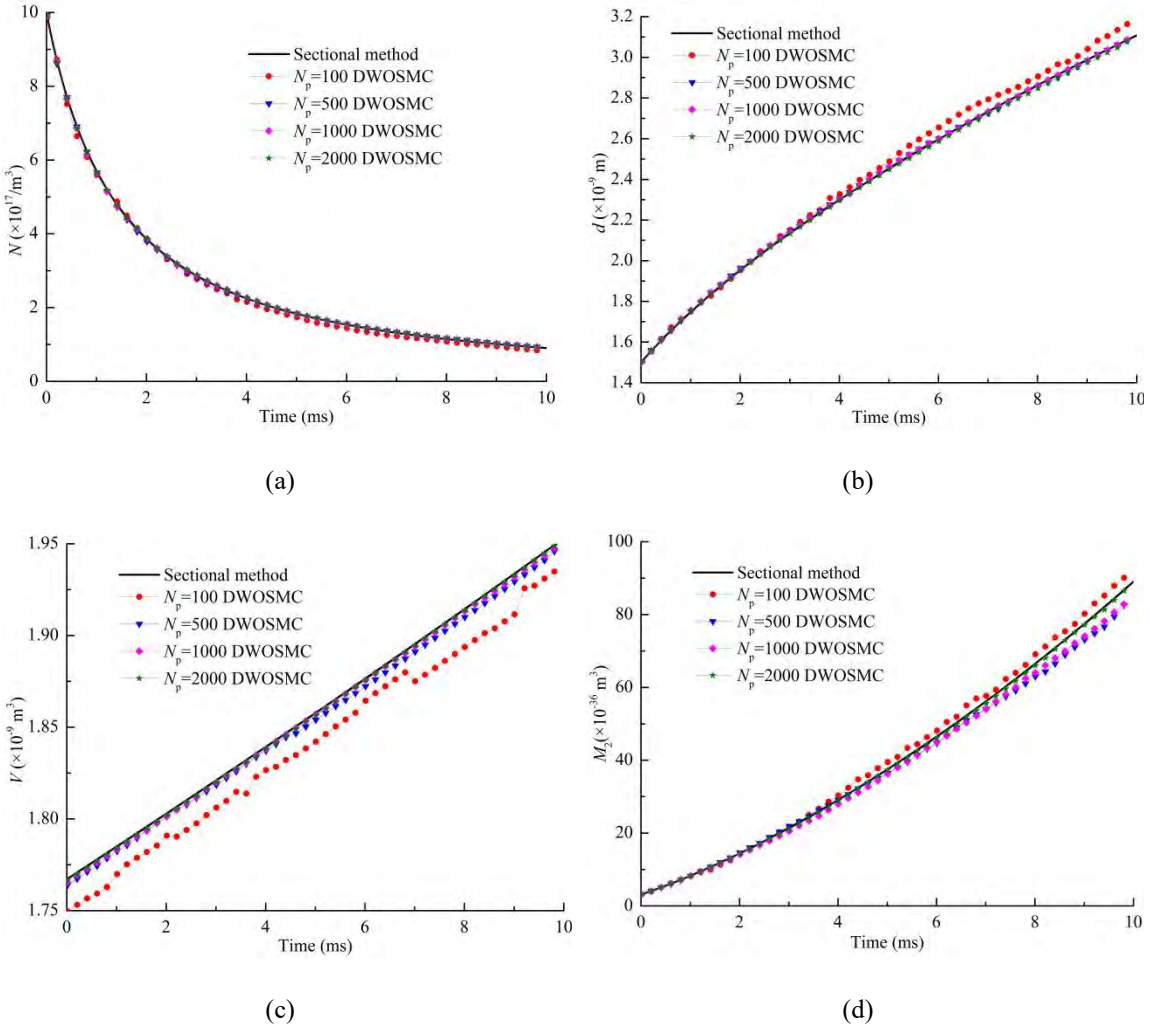


Fig. 5 Evolutions of (a) the particle number concentration, N, (b) the average particle diameter, d, (c) the total particle volume concentration, V, and(d) the second moment, M_2 obtained from DWOSMC method and sectional method (Prakash et al., 2003) for simultaneous free molecule regime rate coagulation and linear rate condensation processes in studied Case II.

From Fig. 5(a), it can be found that the particle number concentration decreases over time. It is because that the coagulation process makes the number of particles less, while the condensation process does not change the number of the particles. The numerical simulation results obtained from DWOSMC

method agree well with the sectional method even when only 100 simulation particles are used. For the evolutions of average particle diameter and the total particle volume, there are significant differences between the simulation results of DWOSMC and sectional method when only 100 simulation particles are used as shown in Fig. 5(b) and 5(c), respectively. While when the simulation particle number reaches 500 or 1000, the simulation results of DWOSMC method have good agreement with the sectional method. As the coagulation process does not change the total particle volume, the total particle volume shows approximate linear relationship over time because the condensation kernel is linear rate. As both of the coagulation and condensation processes contribute to the increase of the particle diameter, the average particle diameter increases quite fast and nonlinearly over time. For the evolutions of the second moment, there are relatively larger errors than other parameters. But it can be found that as the number of simulation particles increases, the relative error reduces. The relative error is rather small when 2000 simulation particles are used.

4.2 Simultaneous Nucleation and Coagulation Processes

4.2.1 Constant rate nucleation and constant rate coagulation case

For studied Case III, the initial particle number concentration, N_0 and initial total particle volume, V_0 are 1.91×10^{23} and 10^{-4} m^3, respectively. The simulation time for Case III is t_{stop} = 45 ms. The numerical simulation results of N/N_0 and V/V_0 are shown in Fig. 6(a) and 6(b), respectively. It can be found that the results show approximately linear relationship within a short period of time. The numerical simulation results obtained from DWOSMC method are consistent with the analytical solutions. When the simulation particle number reaches 500, both of the evolutions for the particle number concentration and the total particle volume show very few fluctuations and relative errors.

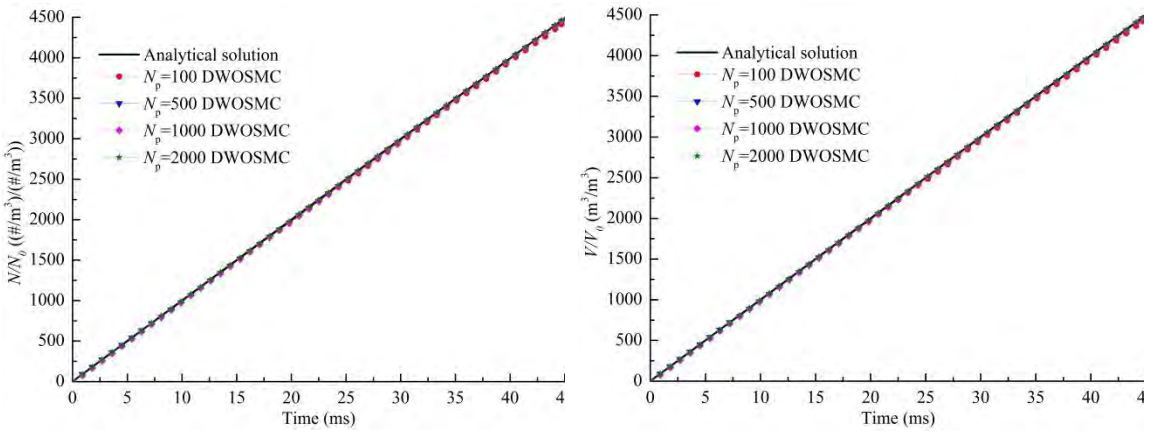


Fig. 6 Evolutions of (a) N/N_0 and (b) V/V_0 obtained from DWOSMC method and analytical solutions (Maisels et al., 2004) for simultaneous constant rate nucleation and constant rate coagulation processes in studied Case III.

4.2.2 Free molecule regime rate coagulation and constant rate nucleation case

For studied Case IV, the initial particle number concentration, N_0 and initial total particle volume,V_0 are 1×10^{18} and $1.77\times10^{-9}\,m^3$, respectively. The simulation time for Case IV is $t_{stop}=4.5$ ms. The evolutions of particle number concentration, N, particle average diameter, d, total particle volume concentration, V, and the second moment, M_2, as a function of time for Case IV are shown in Fig. 7(a) to 7(d), respectively, for simultaneous free molecule regime rate coagulation and constant rate nucleation processes.

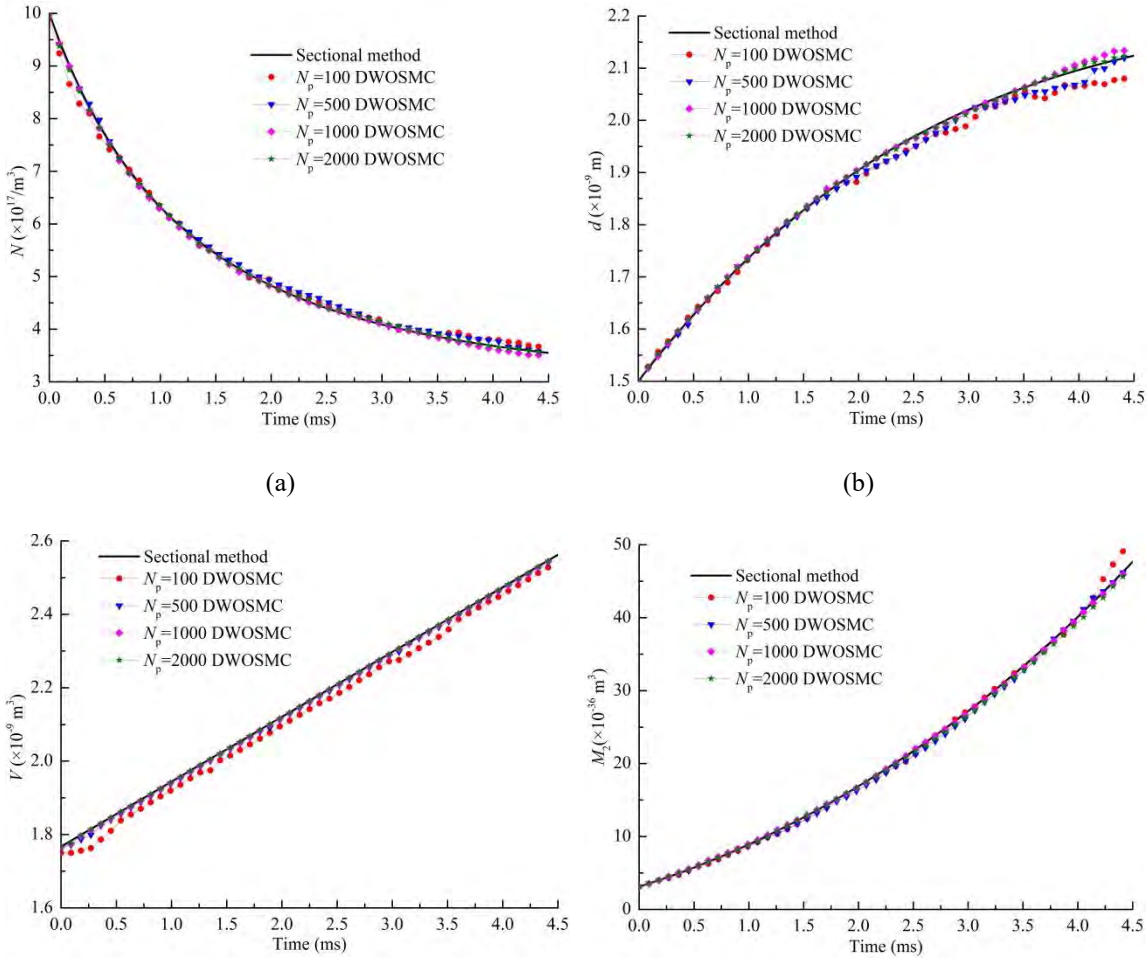


Fig. 7 Evolutions of (a) the particle number concentration, N, (b) the particle average diameter, d, (c) the total particle volume concentration, V, and(d) the second moment, M_2 obtained from DWOSMC method and sectional method (Prakash et al., 2003) for free molecule regime rate coagulation and constant rate nucleation processes in studied Case IV.

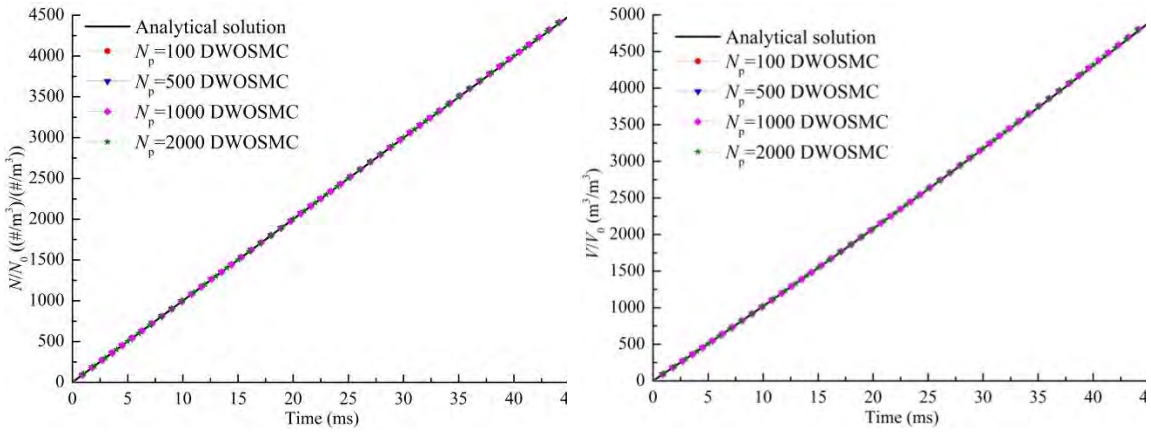
From Fig. 7(a) and 7(b), it can be found that the coagulation process dominates the whole process, because the particle number concentration decreases and the average particle diameter increases over time. But for the nucleation process, the particle number concentration increases and the average particle diameter decreases over time. Hence, the coagulation process completely eliminates the effect of the nucleation process. While from Fig.

7(c) and 7(d), the effect of nucleation process can be clearly found as the total particle volume and the second moment increase over time. From Fig. 7(a) to 7(d), it can also be found that when 1000 simulation particles are used, the numerical simulation results obtained from DWOSMC method agree well with the sectional method (Prakash et al., 2003), with very few fluctuations and errors.

4.3 Simultaneous Nucleation, Coagulation and Condensation Processes

4.3.1 Constant rate nucleation, constant rate coagulation and constant rate condensation case

For studied Case V, the initial particle number concentration, N_0 and initial total particle volume, V_0 are 1.91×10^{23} and 10^{-4} m^3, respectively. The simulation time for Case V is t_{stop} = 45 ms. The numerical simulation results of N/N_0 and V/V_0 are shown in Fig. 8(a) and 8(b), respectively. Similar to Case III, both of the evolutions of N/N_0 and V/V_0 exhibit nearly linear relationship within a very short period of time. Even when only 100 simulation particles are used, the numerical simulation results remain very high consistency with the analytical solutions for constant rate nucleation, coagulation and condensation processes.



(a) (b)

Fig. 8 Evolutions of (a) N/N_0 and (b) V/V_0 obtained from DWOSMC method and analytical solutions (Maisels et al., 2004) for simultaneous constant rate nucleation, constant rate coagulation and constant rate condensation processes in studied Case V.

4.3.2 Constant rate nucleation, free molecule regime rate coagulation and linear rate condensation case

For studied Case VI, the initial particle number concentration N_0 and initial total particle volume V_0 are 1×10^{18} and 1.77×10^{-9} m^3, respectively. The simulation time for Case VI is t_{stop} = 3 ms. The evolutions of the particle number concentration, N, the average particle diameter, d, the total particle volume concentration, V, and the second moment, M_2, as a function of time for Case VI are shown in Fig. 9(a) to 9(d), respectively, for simultaneous constant rate nucleation, free molecule regime rate coagulation and linear rate condensation processes.

Fig. 9(a) to 9(d) show that for the particle number concentration, N, the average particle diameter, d, the total

particle volume, V, and the second moment of particles, M_2, the numerical simulation results of DWOSMC method agree well with the sectional method (Prakash et al., 2003) when 1000 to 2000 simulation particles are used.

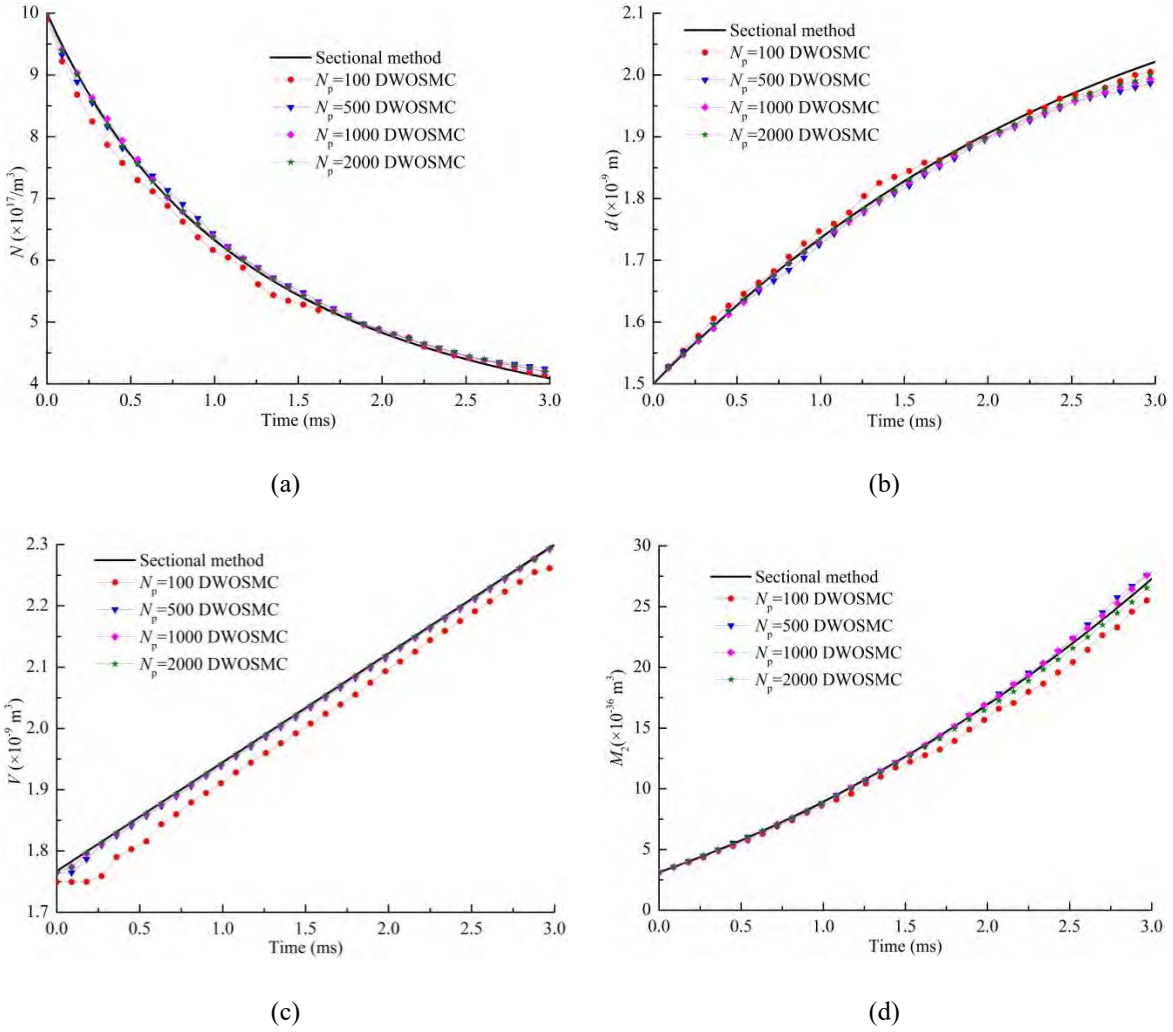


Fig. 9 Evolutions of (a) the particle number concentration, N, (b) the particle average diameter, d, (c) the total particle volume concentration, V, and (d) the second moment, M_2, obtained from DWOSMC method and sectional method (Prakash et al., 2003) for simultaneous constant rate nucleation, free molecule regime rate coagulation and linear rate condensation processes in studied Case VI.

4.4 Computational Efficiency and Accuracy Analysis

To further understand the computational efficiency and accuracy of this proposed and developed DWOSMC method, the maximum relative error for the particle number concentration and the total particle volume for different studied cases are shown in Tables 2 and 3. It can be clearly shown that, for the same case, the maximum relative error decreases when the number of simulation particles increases. For different studied cases, the more complicated the case is, the higher of the maximum relative error is. For constant rates in studied Cases III and V, the maximum relative errors are within 1% when only 500 simulation particles are used, while for other studied Cases IV and VI, more simulation particles are needed to reach the same accuracy.

Table 2 The maximum relative error (%) of N for different cases using DWOSMC method compared with the analytical solutions or the sectional method.

ε_{max}(%) for N / Case	Particle number N_p			
	100	500	1 000	2 000
I	5.51	2.22	1.71	0.80
II	8.22	2.33	1.51	1.00
III	2.31	0.15	0.16	0.03
IV	4.12	3.11	2.20	1.22
V	0.40	0.32	0.26	0.20
VI	5.53	3.22	2.21	2.00
Note: Cases I, III and V are evaluated by the analytical solutions (Ramabhadran et al., 1976 and Maisels et al., 2004), and Cases II, IV and VI are evaluated by the sectional method (Prakash et al., 2003). The maximum relative error (%) is calculated according to Eq. (24).				

Table 3 The maximum relative error (%) of V for different cases using DWOSMC method compared with the analytical solutions or the sectional method.

ε_{max}(%) for V / Case	Particle number N_p			
	100	500	1 000	2 000
I	1.51	0.22	0.20	0.08
II	1.20	0.27	0.15	0.10
III	2.46	0.19	0.21	0.07
IV	3.01	0.82	0.61	0.50
V	0.63	0.50	0.41	0.32
VI	3.20	1.52	0.61	0.58
Note: Cases I, III and V are evaluated by the analytical solutions (Ramabhadran et al., 1976 and Maisels et al., 2004), and Cases II, IV and VI are evaluated by the sectional method (Prakash et al., 2003). The maximum relative error (%) is calculated according to Eq. (24).				

For Tables 2 and 3, the numerical results show that the maximum relative errors obtained from the particle number concentration are commonly larger than those obtained from the total particle volume. For most of the cases, when the number of simulation particles reaches 2000, the maximum relative errors obtained from the particle number concentration are within 2%, while the maximum relative errors obtained from the total particle volume are within 1%. It is because the evolution of the particle number concentration is mainly due to the stochastic coagulation process, which is calculated by Monte Carlo method, which will bring some statistical errors. The evolution of the total particle volume is mainly due to the nucleation and condensation processes,

which are calculated by deterministic method with much smaller errors. It also indicates that for most of the classical and typical studied cases used in the present study, 2000 simulation particles are good enough with small errors, which indicates that this proposed and validated (DWOSMC) method proves very high computational efficiency and accuracy.

5. Conclusions

A differentially weighted operator splitting Monte Carlo (DWOSMC) method is developed and validated by the corresponding analytical solutions and a sectional method through different classical and typical studied cases, including two cases for simultaneous coagulation and condensation processes in different regimes, two cases for simultaneous nucleation and coagulation processes in different regimes, and two cases for different simultaneous nucleation, coagulation and condensation processes. For the relatively simple cases, the numerical simulation results of DWOSMC method show very good consistency with the analytical solutions. For the complex cases, the numerical simulation results of DWOSMC method are also consistent with the results obtained from the sectional method. In some cases, only 500 simulation particles are good enough for obtaining the maximum relative error within 1%. Even in the most complex case in the present study, 2000 simulation particles are good enough for simulating the particle number concentration, the total particle volume concentration, the average particle diameter and the second moment of particles. This developed and validated DWOSMC method proves to have very high computational efficiency and accuracy, and has high potential for solving complex aerosol dynamic problems.

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