Particuology xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Particuology

journal homepage: www.elsevier.com/locate/partic

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

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ARTICLE INFO

Article history:
Received 7 December 2016
Received in revised form 17 March 2017
Accepted 10 April 2017
Available online xxx

Keywords:
Differentially weighted Monte Carlo
Operator splitting
Aerosol dynamics
Particle size distribution

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. It is first validated in coagulation and condensation processes, and nucleation and coagulation processes, and then validated through simultaneous nucleation, coagulation, and condensation processes. The results show that the DWOSMC method is a computationally efficient and quantitatively accurate method for simulating complex aerosol dynamic processes.

Introduction

The problem of air pollution has become increasingly severe in recent years and contributes to several types of acute and chronic diseases in human beings, for example, lung cancer, asthma, and leukemia. Therefore, the study of atmospheric science has become increasingly important. The air pollution indices (i.e., PM_1, $PM_{2.5}$, and PM_{10}) refer to the diameters of particulate matters (PMs) in the air. The US Environmental Protection Agency has listed the reduction of $PM_{2.5}$ emissions as an important task to control air pollution (Raman & Fox, 2016). Ultrafine, submicron, and fine particles suspended in the air are also called aerosols (Friedlander, 2000; Gelbard, 1979). Considering their impact on the climate and health, it is significant to understand the evolution and distribution of aerosol particles (Tie, 2015). Therefore, increasing numbers of researchers have studied aerosol dynamics in recent decades. The research into aerosol dynamics 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). In addition to performing experiments to describe aerosol dynamics and chemical reactions, numerical modeling has become a very useful tool to predict and describe aerosol dynamic processes, including nucleation, coagulation, and condensation (Chan, Lin, Zhou, & Chan, 2006; Liffman, 1992; Qamar & Warnecke, 2007; Zhou & Chan, 2011). Among different types of developed numerical models, the most popular ones are the sectional method (SM) (Dergaoui, Sartelet, Debry, & Seigneur, 2013; Gelbard, Fitzgerald, & Hoppel, 1998), method of moments (MOM) (Chan, Liu, & Chan, 2010; Liu, He, & Chan, 2011; McGraw, 1997; Yu & Chan, 2015; Yu, Lin, Cao, & Seipenbusch, 2015), and Monte Carlo (MC) method (Fede, Simonin, & Villedieu, 2015; He, Zhao, Wang, & Zheng, 2015; Zhang & You, 2015).

The SM is a type of discrete aerosol size distribution approach. In a sectional representation, the size of the particles is divided into a certain number of sections, where all the particles in one section have the same component composition (Chen, Lin, & Yu, 2014; Lu, 2005). For the MOM, the governing equation of the particles is transformed into a set of ordinary differential equations regarding the moments (Settumba & Garrick, 2004). Both the SM and MOM are deterministic methods, effective tools to describe or predict the evolution of aerosol particle size distribution (PSD), and technically easy to couple with Eulerian–Eulerian models of multiphase flows (Vlieghe, Coufort-Saudejaud, Liné, & Frances, 2016; Zhang & You, 2015). However, these two methods have advantages and disadvantages in terms of accuracy and efficiency (Wei & Kruis, 2013; Chen et al., 2014). For example, the SM tends to be more accurate; however, the sectional representations may lead to complicated algorithms. The MOM is relatively efficient; however, the main difficulty is obtaining 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 regarding the initial form of the PSD, and other researchers have developed methods to achieve the closure of the

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http://dx.doi.org/10.1016/j.partic.2017.04.002

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^{-1})
K	Coagulation kernel (m^3/s)
k_B	Boltzmann constant (J/K)
K_n	Knudsen number
M_2	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 in DWOSMC simulation (s)
$\vec{u}$	Velocity of gas (m/s)
$v,\tilde{v}$	Particle volume (m^3)
V_s	Volume of the aerosol system in simulation (m^3)
V	Total particle volume during the simulation interval (m^3)
V_0	Initial total volume of aerosol particles (m^3)
w_i	Weight of the simulation particle
X	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

Acromyms

DWOSMC	Differentially weighted operator splitting Monte Carlo
GDE	General dynamic equation
MC	Monte Carlo
MOM	Method of moment
PBE	Population balance equation
SM	Sectional method

moment equations without a prior requirement for the PSD (Chan et al., 2010; Frenklach, 2002; Yu & Chan, 2015; Yu, Lin, & Chan, 2008).

In addition to the SM and MOM, the MC method has become popular because it has the advantage of stochastic characteristics (Hussain, Kumar, & Tsotsas, 2015; Kruis, Wei, van der Zwaag, & Haep, 2012; Sun, Axelbaum, & Huertas, 2004). The MC method is a stochastic algorithm that is based on the probabilities of different outcomes in a process that could not be easily predicted because of their randomness. Instead of directly solving the general dynamic equation (GDE), the MC method imitates the formation, movement, and dynamic behavior of simulation particles based on the happening probabilities of the behavior (Bird, 1976; Liu & Chan, 2016).

Metropolis and Ulam (1949) first proposed the MC method to apply the laws of probability and statistics to the natural sciences. Bird (1963, 1976, 1994) developed the direct simulation MC method to model rarefied gas flows. Different MC methods have been proposed to study aerosol dynamics, which can generally be classified as the 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 the computational domain. Kostoglou and Konstandopoulos (2001) identified the characteristics of different MC approaches and classifications. Weighted MC methods (Boyd, 1996; Liu & Chan, 2017a; Zhao et al., 2010) have also been proposed to increase the resolution and efficiency of the MC method.

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

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

Compared with other methods, MC methods are increasingly preferred because of the following advantages (Wei & Kruis, 2013).

(a) The stochastic nature of the MC method makes it ideally suitable to manage a stochastic event.
(b) The MC method can solve the closure problem of the GDE.
(c) Each simulation particle can have a unique size, composition, and morphology, that is, any information about the particles can be obtained.
(d) The MC method is robust and simple to code numerically.

In MC methods, simulation particles are used to represent the large number of real particles, and thus introduce 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 et al., 2010). For reducing statistical noise, Zhao and Zheng (2011) and Zhao, Zheng, and Xu (2005) developed a differentially weighted MC (DWMC) method, which proved to be efficient and practical for simulating the coagulation process of aerosol particles. However, the deterministic method is more efficient for simulating the nucleation and condensation processes. Taking advantage of both

Please cite this article in press as: Liu, H., & Chan, T.L. Differentially weighted operator splitting Monte Carlo method for simulating complex aerosol dynamic processes. *Particuology* (2017), http://dx.doi.org/10.1016/j.partic.2017.04.002