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A Monte Carlo method for coagulation of charged particles

Jianming Wei *

Institute for Nanostructures and Technology, Faculty of Engineering Science, and CENIDE (Center for Nanointegration, Duisburg-Essen), University of Duisburg-Essen, 47057 Duisburg, Germany

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ABSTRACT

A simple, straightforward Monte Carlo method for handling coagulation of charged particles has been presented in this note, which is essentially by extending a differentially weighted Monte Carlo method. Then the Monte Carlo scheme is applied to a case study of coagulation of bipolarly charged particles. It is shown that the Monte Carlo method proposed can achieve satisfactory results with a very straightforward algorithm and greatly minimized programming efforts.

1. Introduction

Coagulation of charged particles is widely used in various fields such as aerosol science (Labowsky et al., 2006), materials synthesis processing (Kruis et al., 1996), air pollution control (Ylatalo et al., 1992), etc. For example, differential mobility analyzer (DMA) sort charged particles according to their different electrical mobility. Electrostatic precipitators (ESP) remove the charged particles using the electrical force. In order to improve the separation efficiency of small particles in ESPs, one may convert those particles into larger ones through coagulation. Hence, it is of great interest to study the behavior of particle sizes and charges in the course of coagulation. To this end, a variety of deterministic models, including moment methods (Park et al., 2005) and sectional methods (Oron & Seinfeld, 1989a, 1989b; Vemury et al., 1997), have been proposed. However, these methods either need considerable computer time or bear rather algorithm complexity. On the other hand, it is well known that Monte Carlo (MC) methods are a kind of effective method for population balance problems of neutral particles (Efendiev & Zachariah, 2002; Garcia et al., 1987; Kruis et al., 2000; Lee & Matsoukas, 2000; Liffman, 1992; Zhao & Kruis, 2008). Compared with their deterministic counterparts, MCs offer several remarkable advantages, e.g. they impose no *in prior* requirements on particle properties (such as particle size distribution), allow to provide information about particle history, and from computing point of view, they are quite easy to code and simple to implement.

In view of those characteristics abovementioned, a MC scheme for handling coagulation of charged particles is presented; more precisely, it is based on an extension of a differentially weighted Monte Carlo (DWMC) (Zhao & Kruis, 2008). The MC proposed is then applied in a case study of coagulation of bipolarly charged particles and compared to a sectional method.

* Tel.: +49 203 3946279; fax: +49 203 379268.
E-mail address: wei@uni-duisburg.de

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Nomenclature

e	electronic charge (C)
$k_{i,j}$	interact potential (m^2 kg s^{-2})
K_f	coagulation coefficient in free-molecular regime ($m^{5/2}$ s^{-2})
n_r	average number of trials for a coagulation event
n_s	number of simulation particles
q_i	number of elementary charge carried by a particle
T	temperature (K)
r	random number in-between 0 and 1
v_i	particle volume (m^3)
w_i	particle weight
β	coagulation rate function (m^3 s^{-2})
β'	coagulation rate function used by DWMC (m^3 s^{-2})
β'_{max}	maximum coagulation rate (m^3 s^{-2})
γ	collision efficiency due to the electrostatic interaction
ε	permittivity of air (F m^{-1})
κ_B	Boltzmann constant (m^2 kg s^{-2} K^{-1})
ρ	particle density (kg m^{-3})

2. Theory

2.1. Monte Carlo method

Unlike other MC methods such as constant-N or constant volume method, which describe coagulation process by adjusting either particle number or volume of the simulation box; DWMC has introduced weight to accommodate the changes of particle number or volume of the system. By this method, the coagulation kernel should be modified, and it takes the form

$$\beta'(v_i, v_j) = \beta(v_i, v_j)\frac{2w_j max(w_i, w_j)}{w_i + w_j}, \tag{1}$$

where $\beta(v_i, v_j)$ is the (conventional) coagulation rate function, $\beta'(v_i, v_j)$ is the corrected coagulation kernel by DSMC, v_i and v_j are volume associated with particle i and j, w_i and w_j are their weight value. Mathematically, the weight w_i and w_j, of particle i and j, can be regarded as the number of real particles that are represented by the two particles in a unit volume. For dealing with coagulation of neutral particles, the following formulae are used by DWMC to evaluate the changes in particle size and weight once a coagulation event occurs (Zhao & Kruis, 2008):

$$\begin{cases} w'_i = max(w_i, w_j) - min(w_i, w_j), & v'_i = w_i > w_j ? v_i : v_j \\ w'_j = min(w_i, w_j), & v'_j = v_i + v_j \end{cases} \quad \text{if } w_i \neq w_j \tag{2}$$

and

$$\begin{cases} w'_i = w_i/2, & v'_i = v_i + v_j \\ w'_j = w_j/2, & v'_j = v_i + v_j \end{cases} \quad \text{if } w_i = w_j, \tag{3}$$

where $w'_i(w'_j)$ and $v'_i(v'_j)$ are weight and volume of particle $i(j)$, respectively, after the coagulation event. Expression $v'_i = w_i > w_j ? v_i : v_j$ says that v'_i takes either v_i or v_j, depending upon which weight, w_i or w_j, is larger. One can easily see from (2) and (3) that total particle mass is conserved before and after a coagulation event.

Evidently, only two properties, i.e. particle size and weight, are necessary when DWMC is applied to coagulation of neutral particles. In order that DWMC can accommodate coagulation of charged particles, we have introduced the third property, namely charge, q, and assigned it to each individual particle. Here, q stands for the number of elementary charge that a particle is carrying. Furthermore, we have designed the following rules to which charged particles in the course of coagulation should be subjected

$$\begin{cases} q'_i = w_i > w_j ? q_i : q_j \\ q'_j = q_i + q_j \end{cases} \quad \text{if } w_i \neq w_j \tag{4}$$

and

$$\begin{cases} q'_i = q_i + q_j \\ q'_j = q_i + q_j \end{cases} \quad \text{if } w_i = w_j \tag{5}$$

where q'_i (q'_j) represents the particle charges of particle $i(j)$ after the coagulation event. The most important principle to follow is that the variation of particle charges should conform to charge conservation. With this principle one can easily verify the correctness of (4) and (5). Suppose that the chosen particles $(i,\ j)$ have different weights, i.e. $w_i \neq w_i$. The total charges carried by them before the coagulation can be computed as $w_i q_i + w_j q_j$; whilst after the coagulation event their total charges are given by

$$w'_i q'_i + w'_j q'_j = (max(w_i,\ w_j) - min(w_i,\ w_j))q'_i + min(w_i,\ w_j)(q_i + q_j) \tag{6}$$