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Technical note

A Metropolis scheme for Monte Carlo methods for the solution of particle population balance

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ABSTRACT

A Metropolis scheme that can be used by various Monte Carlo methods for solving particle population balance equations has been proposed and verified. A detailed derivation of the scheme is presented. The computational accuracy of the proposed scheme is tested under various coagulation kernels. The computational performance of the scheme is also measured and compared to that of Inverse and acceptance–rejection scheme.

1. Introduction

Coagulation is of great fundamental and practical interest owning to a rich variety of processes such as nanoparticle synthesis (Hawa & Zachariah, 2005), colloidal suspensions (Yasrebi, Shih & Aksay, 1991), combustion (Khan, Wang & Langridge, 1971; Lehtinen & Zachariah, 2002), catalytic chemical process, and so on. Indeed, coagulation process of particles in these processes influences not only the evolution of particle number, size distribution, but also the morphology of aggregates. Quantitatively, the following population balance equation (PBE), introduced by Smoluchowski (Friedlander, 1997), is well known for characterizing the evolution of particles in a coagulation process,

$$\frac{\partial n(v,\ t)}{\partial t} = \frac{1}{2}\int_0^v \beta(v-u,\ u)n(u,\ t)n(v-u,\ t)du - n(v,\ t)\int_0^\infty \beta(v,\ u)n(u,\ t)du \tag{1}$$

where $n(v_p,\ t)$ is in general the number concentration of particles with size at v_p time t, $\beta(u, v)$ is the coagulation rate describing the frequency that two particles with volume u and v collide with each other. The first term on the right-hand side describes the rate of production of particles of volume v due to the coagulation event between a particle of volume u and a particle of volume $(v-u)$; the coefficient $1/2$ is introduced to avoid counting collisions twice in the integral. The second term indicates the rate of disappearance of particles of volume v due to collisions with any other particles.

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Nomenclature

A	kernel-related constant
B_1	modified Bessel function of the first kind
C_c	Cunningham correct factor
d_0	initial particle diameter (m)
d_p	particle diameter (m)
$K_f(K_c)$	coagulation coefficient in different regimes ($m^{5/2}\ s^{-1}$)
K_n	Knudsen number
M_0	0th moment
n_r	times of simulation runs
n_s	simulation particle number
n_t	total number of time points
$n(v, t)$	particle number concentration ($\#/m^3$)
N_0	initial number concentration ($\#/m^3$)
N_p	total number of particle pairs
$N(t)$	Particle number concentration at time t
P_k	probability of finding particle with k primary particles
R_c	threshold value in $(0,\ 1)$
r	random number in $(0,\ 1)$
t	time (s)
v	particle volume (m^3)
v_0	initial particle volume (m^3)
$v_{min}(v_{max})$	minimum (maximum) particle volume (m^3)
v_t	total particle volume (m^3)
W	transition probability
W^{acc}	acceptance probability
W^{prop}	proposal probability
β_c	Brownian kernel in the continuum regime ($m^3\ s^{-1}$)
β_{fm}	Brownian kernel in the free-molecule regime ($m^3\ s^{-1}$)
β_{max}	the maximum coagulation rate ($m^3\ s^{-1}$)
ϵ_{mean}	mean calculation error
σ_g	geometric standard deviation of particle size
τ	average coagulation time step (s)
τ_{char}	characteristic time of coagulation (s)

Various methods have been developed to tackle the foregoing PBEs. Broadly, these methods can be categorized into two types depending on their different mathematical nature: the deterministic and non-deterministic methods. The typical methods falling into the first category includes sectional method (Jeong & Choi, 2001; Landgrebe & Pratsinis, 1990; Mitrakos, Hinis & Housiadas, 2007; Wu & Biswas, 1998), moments method (Brown, Kauppinen, Jokiniemi, Rubin & Biswas, 2006; Terry, McGraw, & Rangel, 2001; Yamamoto, 2004; Yu, Lin & Chen, 2007; Yu, Lin & Chan, 2008), wavelet method (Liu & Cameron, 2001), etc. The non-deterministic methods involve primarily Monte Carlo (MC) methods (Efendiev & Zachariah, 2002; Garcia, Broeck, Serneels & Aertsens, 1987; Gillespie, 1976; Goodson & Kraft, 2002; Kruis, Maisels & Fissan, 2000; Lee & Matsoukas, 2000; Liffman, 1992; Zhao, Kruis & Zheng, 2009). Owing to its stochastic nature, MC method is extremely suitable for describing discrete, stochastic processes, such as particle coagulation, coalescence, etc. By converting coagulation process into a statistical computer game, the numerical difficulties encountered in solving the complicated integro-differential equation such as Eq. (1) are dramatically reduced, and the corresponding efforts in coding is also minimized. Some advantages of a MC method over its deterministic counterparts can be summarized as: (1) it describes particle dynamic event in a discrete manner without relying on a priori knowledge of particle system to be studied (e.g. particle size distribution), therefore it is able to describe a dispersed system intrinsically and more accurately; (2) new property/function with respect to simulation particles can be easily incorporated into the existing MC frameworks because each simulation particle is treated as an individual, independent object in the context of a MC scheme; (3) MCs are simple in concept and implementation.

One crucial step centered in various MC methods is how to pick a desired coagulation pair with some schemes that can reflect the dynamical nature of particle coagulation processes. Two commonly used schemes by various MC methods are the Inverse and acceptance–rejection (AR) scheme (Garcia et al., 1987). Each scheme has its pros and cons. Inverse scheme chooses a coagulation event from among a given number of different possibilities by comparing a random number with a sequence of accumulative coagulation probabilities (Garcia et al., 1987; Jacoboni & Reggiani, 1983). When no acceleration technique is used (Kruis et al., 2000), the complexity of this scheme is of the order $O(n_s^2)$, where n_s is the number of simulation particles.

Comparing with Inverse scheme, AR scheme selects a coagulated particle pair by means of a much simpler rule such as (Garcia et al., 1987),

$$r < \frac{\beta(i,j)}{\sum_{m=1,m\neq n}^{n_s}\sum_{n=1}^{n_s}\beta(m,\ n)}, \tag{2a}$$

or

$$r < \frac{\beta(i,j)}{\beta_{max}}, \tag{2b}$$

where r is a random number which is uniformly distributed in the interval $(0, 1)$, β_{max} is the maximum coagulation rate evaluated from the total particle pairs, $\beta(i,j)$ is the coagulation rate followed from the chosen particle pair (i,j).