Journal of Computational Physics 303 (2015) 1–18

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Stochastic weighted particle methods for population balance equations with coagulation, fragmentation and spatial inhomogeneity

Kok Foong Lee [a], Robert I.A. Patterson [c], Wolfgang Wagner [c], Markus Kraft [a,b,*]

[a] Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge CB2 3RA, United Kingdom

[b] School of Chemical and Biomedical Engineering, Nanyang Technological University, 62 Nanyang Drive, Singapore, 637459, Singapore

[c] Weierstrass Institute for Applied Analysis and Stochastics, Mohrenstraße 39, 10117 Berlin, Germany

ARTICLE INFO

Article history:
Received 22 May 2015
Received in revised form 15 September 2015
Accepted 16 September 2015
Available online 25 September 2015

Keywords:
Stochastic weighted particle methods
Fragmentation
Coagulation
Weight transfer functions
Compartmental model

ABSTRACT

This paper introduces stochastic weighted particle algorithms for the solution of multi-compartment population balance equations. In particular, it presents a class of fragmentation weight transfer functions which are constructed such that the number of computational particles stays constant during fragmentation events. The weight transfer functions are constructed based on systems of weighted computational particles and each of it leads to a stochastic particle algorithm for the numerical treatment of population balance equations. Besides fragmentation, the algorithms also consider physical processes such as coagulation and the exchange of mass with the surroundings. The numerical properties of the algorithms are compared to the direct simulation algorithm and an existing method for the fragmentation of weighted particles. It is found that the new algorithms show better numerical performance over the two existing methods especially for systems with significant amount of large particles and high fragmentation rates.

1. Introduction

Population balance equations track the change in the particle population with time through different particle mechanisms like coagulation, nucleation, and fragmentation. Traditionally, population balance models are one-dimensional with particle size as the focus. However, when much more detail is required, sectional methods [1] which usually formulate a population balance equation for each size class are not computationally feasible.

Stochastic particle methods have received increasing interest because they can easily incorporate multiple internal co-ordinates and avoid the ‘curse of dimensionality’ which affects other numerical methods [2]. Stochastic simulation of high-dimensional particle models has been applied successfully in a wide range of areas including soot [3], granulation [4], snowflake structure [5], and formation of precipitation particles in clouds [6].

Stochastic particle methods can be loosely separated into two categories: direct simulation algorithm (DSA) and stochastic weighted algorithms (SWAs). In the DSA, the physical processes are directly simulated, e.g. a coagulation event deletes

* Corresponding author at: Department of Chemical Engineering and Biotechnology, University of Cambridge, New Museums Site, Pembroke Street, Cambridge CB2 3RA, United Kingdom.

E-mail address: mk306@cam.ac.uk (M. Kraft).

http://dx.doi.org/10.1016/j.jcp.2015.09.031
0021-9991/

the two original particles to form a new larger particle, and every computational particle represents the same number of physical particles. Although it is easy to implement, this method may allocate large amounts of computational resources to simulate the unimportant smaller particles and this leads to noisy estimates in the larger particle regions that dominate mass concentration [7–9].

To solve this issue, weighted particle methods, or SWAs may be used to utilise computational resources more efficiently. In SWAs, each particle is given a statistical weight which is proportional to the number of physical particles represented by the computational particle. Another key difference between the DSA and SWAs is that the coagulation and fragmentation processes do not require the number of computational particles to vary. Instead, the statistical weights are adjusted. In some way, SWAs are similar to the constant-N Monte Carlo method [10] which keeps the number of computational particles constant by resampling the ensemble after coagulation and fragmentation events, but this method is susceptible to noise especially for longer simulations.

The main challenge in the implementation of SWAs is the execution of processes which alter the number of particles, especially coagulation and fragmentation. In [11–13], a method called the Mass Flow Algorithm (MFA) is given for coagulation and fragmentation processes. The key difference between the MFA with the SWAs developed in this work is that the particles are not explicitly tagged with weights and the weights are implicitly determined as the inverse of the particle mass in the MFA. In systems with inception and frequent exchange of mass with the surroundings, frequent resampling of the particle ensemble is required and may be computationally inconvenient to implement. Nonetheless, successful attempts in extending the MFA to such systems have been reported [14–16].

The majority of previous studies involving SWAs with explicitly tagged weights focus on simulating coagulation accurately [7,17–20,9,6,21,22] and less attention is given to fragmentation. The fragmentation algorithm presented in [18] does not increase the number of computational particles where the weights of the resulting fragment particles are added onto similar particles which are already in the ensemble. However, this algorithm is not suitable for high-dimensional models because it is impossible to search for particles that are identical to the fragment particles [23]. On the other hand, a fragmentation algorithm suitable for high-dimensional models is presented in [23], but the algorithm is not suitable for applications with high fragmentation rates because it increases the number of computational particles. Thus, frequent resampling of the particle ensemble may be required to accommodate the new fragment particles and this may cause severe numerical errors.

The main purpose of this paper is to extend the work done in [17] and develop efficient algorithms for the fragmentation of weighted particles which do not increase the number of computational particles. By having particles tagged with statistical weights, a myriad of possible weight transfer functions can be constructed for coagulation and fragmentation. The flexibility of the weight transfer functions is mainly suited for multidimensional models where any quantity can be chosen to be conserved across the jump processes. In granulation applications for example, the binder content may be chosen to be the quantity to conserve when the statistical weight is adjusted in a coagulation process. Work has been done in [17] where a large family of coagulation weight transfer functions is presented and this paper focuses on a similar aspect for fragmentation.

Besides fragmentation, another aspect of this work is the application of stochastic particle methods in spatially inhomogeneous systems. Stochastic particle methods are traditionally used to simulate spatially homogeneous problems but the inhomogeneous behaviour of mixing processes should not be neglected in systems of practical interest, such as soot formation during combustion [21] and wet granulation [23]. Hence, this leads to a number of attempts to extend stochastic particle methods to spatially inhomogeneous systems [24,21,25,23,26]. One of the common findings among these studies is that the usage of SWAs significantly reduces the stochastic noise due to the spatial inhomogeneity, which is highlighted in this work as well.

This paper is structured as follows: In Section 2, a general population balance model with coagulation, fragmentation and spatial inhomogeneity is formulated. The stochastic particle methods used in this work are described in detail in Section 3. Then, a test system is constructed in Section 4 to investigate the numerical properties of the stochastic particle methods before applying the methods to a realistic multidimensional granulation model in Section 5.

2. Population balance model

In this work, population balance problems with particles undergoing inception, coagulation, breakage, and transport are considered. Particles take positions in a bounded domain of compartments, $\mathbb{Z}$, and the particles are elements of a type space $\mathbb{X}$ which may be multidimensional and either discrete or continuous. Particles are allowed to move from one compartment to another, where the direction and rate of flow are specified by the connections between the compartments. However, only particles within the same compartment are allowed to interact with each other and undergo coagulation. Lastly, the rates of the mechanisms in each compartment are allowed to be different in order to capture the inhomogeneous nature of most particle processes. The population balance problem is formulated for concentration measures $P(t, z, \mathrm{d}x)$, where $z \in \mathbb{Z}$ and $x \in \mathbb{X}$. So, $\int_U P(t, z, \mathrm{d}x)$ gives the number of particles with types $U \subset \mathbb{X}$ located in compartment z, and P is said to be a solution of the population balance problem if, for all $z \in \mathbb{Z}$: