A time-driven constant-number Monte Carlo method for the GPU-simulation of particle breakage based on weighted simulation particles

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ABSTRACT

Monte Carlo (MC) simulations based on weighted particles offer novel and more precise techniques for the solution of the population balance equation for particulate systems. A recent constant-number approach named stochastic weighted algorithm (SWA) (Lee et al. (2015), J. Comput. Phys. (303) 1–18) has been developed, which renders the breakage of a simulation particle by an alteration of its properties, without the creation of novel simulation particles. The theoretic justification of the general formulation for all possible SWAs is limited to binary breakage kernels. We present a novel approach for the derivation of the properties of the MC particles representing fragments, which is applicable for all sorts of breakage kernels. This general scheme encompasses the already introduced SWA schemes, especially a number-based (SWA1, named NBS in this paper) and volume-based (SWA2, named VBS in this paper) breakage scheme, and it makes novel formulations possible: the low volume scheme (LVS), which renders preferably lower fragment sizes, and the combination of LVS with the NBS (LVS-NBS) or VBS (LVS-VBS). The implementation of these breakage schemes in the context of a GPU-based time-driven method is presented and the gained results are validated by comparison with results of the analytic solutions of a homogeneous binary breakage kernel. It is found, that the SWA methods (NBS and VBS) are only able to render large particle sizes, and that LVS, NBS-LVS and VBS-LVS are able to render the whole spectrum of particle sizes. Smaller noise levels are found for VBS and specific VBS-LVS schemes, making both more suitable for prolonged simulations than the other presented methods.

1. Introduction

The solution of the Population Balance Equation (PBE) rendering the breakage of particles is not only interesting for the description of crushing and grinding processes, it is also used to understand liquid-liquid dispersions, polymer degradation and formulation of products through granulation. The most common approaches for the solution of the PBE are the methods of moments, discretization methods and Monte Carlo (MC) methods.

Sectional simulation methods encompass the discretization of the particle property space, which can be combined with deterministic formulations of the particle concentration in single sections [1,2], or with the mass-conserving form of the PBE for a finite volume

scheme [3,4]. Those approaches require the specific a priori designation of the interesting particle size domain, which can become problematic in a multidimensional property space. Additional processes like condensation and evaporation can only be incorporated with a great computational effort (via moving grids [5] or by a reformulation of the problem with the help of finite elements [6]) hence simpler implementations of growth processes lead to numerical diffusion [7].

Monte Carlo (MC) simulations render particle populations with the help of simulation particles, each simulation particle represents thereby a certain concentration (in m^{-3}) of real particles and avoid therefore the numerical diffusion characteristic for sectional approaches. The rendering of the large number of particles which are produced during the continuous breakage process poses a major problem for MC simulations, because large computational resources have to be provided for this purpose. In a typical milling process, for example, reductions of the particle diameters from 500 μm to 0.5 μm are encountered, the same amount of volume, which is

rendered by one simulation particle with a size of 500 μm has to be rendered by 10^9 simulation particles with a diameter of 0.5 μm, if all particles represent the same number concentration of real particles.

Early MC simulations solved this problem by a discretization of the particle property into bins and counting, how many MC particles [8] or the corresponding volume [9] or mass[1] [10] can be found within a specific bin. These approaches bear the same disadvantages as the sectional methods mentioned above.

An alternative concept in order to avoid large numbers of simulation particles is the constant-number MC approach developed by the Matsoukas group for the agglomeration [11], and extended to the simulation of breakage [12]. In the scope of this approach, the loss of simulation particles due to coagulation events could be compensated by a copy of randomly selected simulation particles - and the memory space for new simulation particles resulting from the breakage event could be created by the removal of randomly selected simulation particles. This method is known to produce a high level of statistical simulation noise [13,14].

The MC-simulation based on weighted particles allows the technique of merging two simulation particles into one ([15], introduced for the Multi-Monte Carlo approach). Although it was found that the Multi-Monte Carlo method led to systematic errors of the simulation [16], the merging methods can be combined with other simulation techniques based on weighted particles [14,17,18] or [13]. However, the resulting estimation of two suited simulation particles for a merge step has to be performed for each additional particle resulting from the breakage, leading to large computing times especially for particle systems describing the breakage of one particle into a large number of fragments - assuming that two particles suitable for the merging step can be found at all.

This problem is avoided by the mass-flow algorithm (MFA) which was introduced for the coagulation process [19] and extended to the breakage process [20] as well. In the scope of this approach, the resulting fragments are represented by only one MC-particle which replaces the original particle, selected for breakage, leading thus to a constant-number scheme. The simulation particles used by the MFA are differentially weighted (i.e. each simulation particle represents a different concentration of real particles) but renders the same amount of mass concentration, so that the statistical weight is defined by the property (mass) of the simulation particle. This causes the incorporation of growth processes to be difficult, hence specifically defined statistical weights as a second particle property are needed [21]. This problem has been solved by the formulation of stochastic weighted algorithms (SWA) [18] for the coagulation, which could be extended to the breakage process [13].

A general breakage scheme is presented in the scope of the SWA for breakage [13], consisting of two parts. The first part describes the probability distribution function (PDF) with which the new volume of the simulation particle is selected. The second part describes how to calculate the statistical weight of the simulation particle depending on the selected volume. This derivation was performed for a binary breakage kernel and is founded on symmetry arguments. In this paper, we present an alternative approach for the derivation of the breakage scheme in Section 2 by resorting to the argument, that the breakage of many MC-particles with equal properties and weights has to lead to a particle size distribution (PSD) of fragments, which is described by the corresponding breakage kernel. The implementation of the gained results on the GPU in the scope of a time-driven MC simulation will be discussed in Section 3.

2. Theory

In order to provide a higher level of clarity, it will be distinguished between particles and differentially weighted simulation entries (SE) in the following. The particles refer to existing physical objects, whose behavior is described by kinetic equations. The SE are representations of the PSDs of the particles stored on the computer. A SE i contains the properties of the particles (in the here presented case the volume v_i) and an additional property: the statistical weight W_i, which is a concentration (in units m^{-3}).

The existing number-based and volume-based formulations for (real) particles of the breakage process are summarized in Section 2.1. Section 2.2 presents different selection schemes for the properties of the fragment SEs in order to render the breakage process.

The formulation of the population balance equation (PBE) used in this work is based on one particle property, the volume v (the term 'size' is used synonymously).

2.1. Formulations of the PBE for breakage

2.1.1. Number-based formulation

The number-based PBE [2], for breakage describes the temporal change of the number-based PSD[2] $n(v)$ of the particle population:

$$\frac{\mathrm{d}n(v)}{\mathrm{d}t} = -S(v) \cdot n(v) + \int_v^\infty n(v') \cdot S(v') \cdot b_n(v, v') \mathrm{d}v'. \tag{1}$$

The breakage rate of a particle with the volume v_P is denoted by $S(v_P)$. The number-based distribution of the resulting fragments is described by the breakage function $b_n(v_F, v_P)$ which states, that $b_n(v_F, v_P)\mathrm{d}v_F$ fragments with the volume between v_F and $v_F + \mathrm{d}v$ are created due to the breakage of a parent particle with the volume v_P. The mean total number of fragments resulting from the breakage of one parent particle is:

$$B(v_P) = \int_0^{v_P} b_n(v_F, v_P) \, \mathrm{d}v_F. \tag{2}$$

In the special case of a binary breakage, there are exactly two fragments, so that: $B(v_P) = 2$ for all v_P.

The conservation of the volume during the breakage poses a restriction on all possible formulations for $b_n(v_F, v_P)$ by the following formula:

$$v_P = \int_0^{v_P} b_n(v_F, v_P) \cdot v_F \mathrm{d}v_F. \tag{3}$$

2.1.2. Volume-based formulation

The volume-based formulation of the PBE [1] can be gained by setting the volume-based PSD $M(v)$ to $M(v) = v \cdot n(v)$:

$$\frac{\mathrm{d}M(v)}{\mathrm{d}t} = -S(v) \cdot M(v) + \int_v^\infty M(v') \cdot S(v') \cdot b_m(v, v') \, \mathrm{d}v'. \tag{4}$$

The thus resulting volume-based breakage kernel b_m is written in accordance to [1] as:

$$b_m(v_F, v_P) = \frac{v_F}{v_P} \cdot b_n(v_F, v_P).$$