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Assessment of different coarse graining strategies to simulate polydisperse gas-solids flow

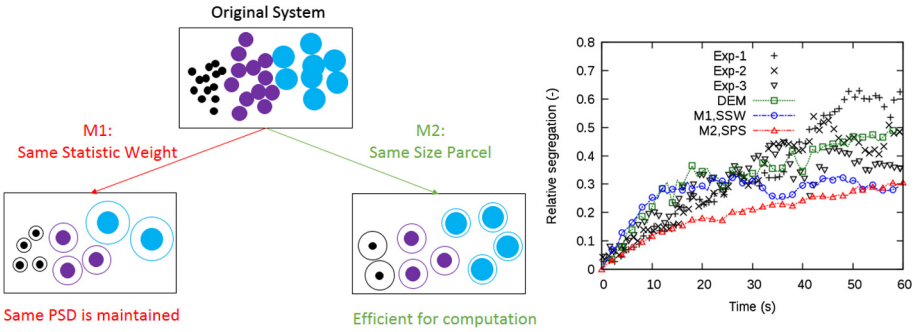
Liqiang Lu [a,*], Yupeng Xu [a], Tingwen Li [a,b], Sofiane Benyahia [a]

[a] National Energy Technology Laboratory, Morgantown, WV 26507, United States
[b] AECOM, Morgantown, WV 26505, United States

HIGHLIGHTS

- Two types of coarse grained CFD-DEM method for polydisperse system are compared.
- The same statistic weight method is more accurate for system with low gas velocity.
- The same parcel size method is more computationally efficient.
- They can predict similar and correct results when fully fluidized.

GRAPHICAL ABSTRACT



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ABSTRACT

Continuum methods require the additional development of solids stress closures for polydisperse powders based on complex kinetic theories that are non-trivial to develop, code, and numerically converge for the wide range of fluidization regimes from very dilute to dense/frictional flow limit. On the other hand, it is straightforward to model the flow of polydisperse granular materials by treating particles as discrete rigid bodies that are tracked following simple physical laws of motion. The coarsening of these discrete methods by lumping several particles in a parcel alleviates the significant computational cost associated with these discrete methods while introducing some inaccuracies in the numerical results. In this research, we explore two different coarse graining methods that can be applied to polydisperse powders, namely the same statistic weight method (SSW) and the same size parcel method (SSP), and assess their accuracy by comparison with the finest simulation results obtained with a discrete element method (DEM). For Geldart group B powders fluidized at a relative low superficial velocity, the numerical results indicate that the SSW is more accurate than the SSP method. For type A powders fluidized at relatively high velocity, these two methods predict similar results. Interestingly, up to four times increase in the speed of simulation of the SSP method was obtained because the original polydisperse powder is scaled to a mono-disperse system in terms of particle-particle collision. These results suggest that the SSP method is more favorable for the simulation of fluidized beds due to its accuracy and efficiency while the SSW method may be used for granular flow and dense fluidized bed systems where capturing the size segregation of particles due to collision is important.

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* Corresponding author.
E-mail address: Liqiang.Lu@netl.doe.gov (L. Lu).

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1. Introduction

Particulate matter is the second-most manipulated material in industry after water (Richard et al., 2005), and has been observed and studied by scientists and engineers since the earliest of human civilization. The particles used in industries like oil refinery and coal combustion are usually polydisperse with a continuous size distribution. This polydispersity can improve the fluidization state as summarized by Sun and Grace (1990): more close to ideal bubble-less fluidization and higher concentration of fines in the dilute regions. Thus, it is important to consider the influence of particle size distribution (PSD) when simulating polydisperse systems. By following the widely used two fluid model (TFM) (Anderson and Jackson, 1967) based on the continuum description of granular flows, it is necessary to develop polydisperse kinetic theories to close the granular stresses and solids-solids drag terms. In one of the simplest polydisperse TFM available in the literature, the particles are divided into several solids phases based on a discretized form of the PSD and the momentum equations for each solid phases are solved, which results in the so-called multi-fluid model (Syamlal et al., 1993). The momentum transfer between gas phase and each solids phase can be directly calculated; however, the momentum transfer due to particle-particle collisions among different solid phases is difficult to model. Syamlal (1987) developed a particle-particle drag term to account for this effect using kinetic theory of granular flow. For more complex systems where the PSD varies during the simulation (due to chemical reactions or crystallizations), the population balance method (Chen et al., 2011; Yang and Xiao, 2017) or a related quadrature method of moments (Fan et al., 2004) may be used to track spatial-temporal variations of PSD.

In computational fluid dynamic coupled with discrete element method (CFD-DEM) (Tsuji et al., 1993; Xu and Yu, 1997), the movement of each particle is directly tracked following simple physical laws of motion. Thus, no further physical model complexity is introduced for polydisperse systems (Zhang et al., 2017). The only issue requiring resolution is the computational cost due to the presence of large number of small particles in industrial systems requiring the resolution of small durations of particle collisions (Xu et al., 2011; Ge et al., 2015). To solve this problem, the coarse grained CFD-DEM (Patankar and Joseph, 2001) has been proposed to simulate large scale gas-solids flows like bubbling fluidized bed (Sakai et al., 2014; Lu et al., 2017b), circulating fluidized bed (Lu et al., 2014, 2016a, 2017a) and cyclones (Chu et al., 2016). In coarse grained CFD-DEM, several W real particles are lumped into a computation parcel. The voidage between original particles within a parcel was not considered in current model. The collision forces are calculated using an equivalent collision diameter d_{CGP}, calculated as $d_p W^{1/3}$. Other forces like drag, gravity, and pressure gradient forces are calculated at real particle scale. This method has recently been extended to solve for heat transfer (Lu et al., 2017d), chemical reactions (Lu et al., 2016b) and hard sphere methods (Lu et al., 2017c). There are only two publications in the literature that extend this method to polydisperse systems by employing the same strategy to represent the PSD (Chu et al., 2016; Verma et al., 2017). Both studies generate parcels of the same size to represent a PSD in order to calculate collision forces. In this research, we compare this coarse graining strategy to another one developed in this study in order to assess the accuracy and speed of simulation of Geldart type A (FCC particles) and type B (glass beads) particles. The comparison of these numerical results help us deduce best practices on how to lump particles into parcels for simulating polydisperse powders using a coarse discrete particle approach.

2. Method

2.1. Description of coarse graining methods for polydisperse powders

When dealing with polydisperse powders, we view the Same Statistic Weight (SSW) method for all particle types (method M1 in Fig. 1) as the most natural to implement because the shape of the PSD of the coarse grained powder remains identical to that of the original powder. One major issue of the SSW method is the fact that the solids phase time step is limited by the collision duration between the smallest coarse grained particles. To circumvent this issue, another option to coarsen a polydisperse powder is to use different statistic weights for particles with different diameters and scale the original polydisperse powder to a coarse monodisperse powder with Same Size Parcel (SSP). Unlike the SSW method, the SSP method was used recently in the literature to study the particle segregation in a rotating fluidized bed (Verma et al., 2017). To demonstrate one major benefit of using SSP over the SSW method, consider a coarsened granular system where the number of parcels is same for these two methods, then it is simple to deduce that the diameter of the mono-disperse system will be larger than the smallest diameter and smaller than the largest diameter in the polydisperse system. Because the same number of parcels can be used with a larger time step in the SSP method, it is easy to conclude that this method will lead to faster numerical simulation. Another benefit of the SSP method is the high efficiency of particle-particle collision detection in monodisperse system, which will lead to an even faster numerical simulation. In DEM where the particle-particle collision detections are carried only for a particle's neighbor list of particles, the neighbor list itself is constructed by mapping the particles into uniformly distributed cells with same sizes, which should be larger than the largest particle size. Thus, for polydisperse system, the cell size is larger than that of a mono-disperse system, which will lower the efficiency of constructing the neighbor list. Also, when the domain decomposition parallel method is used to speedup DEM simulation, there will be more ghost particles for polydisperse system due to the larger cell size (Berger and Hrenya, 2014).

2.2. Equations of motion for particles

Lagrange method is used to track the motion and collisions of fewer computational parcels. The governing equations for any real particle in a parcel takes the form:

$$m_{\mathrm{p}} \frac{d\mathbf{v}_{\mathrm{p}}}{dt} = m_{\mathrm{p}}\mathbf{g} - \frac{\pi}{6} d_p^3 \nabla P_f + \frac{\beta(\mathbf{v}_{\mathrm{f}}(\mathbf{x}^i) - \mathbf{v}_{\mathrm{p}})}{1-\varepsilon_f} \frac{\pi}{6} d_p^3 + \mathbf{F}_{\mathrm{c}} \tag{1}$$

$$I_{\mathrm{p}} \frac{d\boldsymbol{\omega}_{\mathrm{p}}}{dt} = \mathbf{T} \tag{2}$$

where m_{p} is the mass of the real particle and d_{p} is its diameter. On the right-hand side, the forces considered include gravity, pressure gradient, drag, and contact forces ($\mathbf{F}_{\mathrm{c}}$). The first three terms are calculated following the same process as in traditional CFD-DEM (i.e. these forces are calculated on a real particle). The contact force is calculated by the discrete element method (DEM) in normal ($\mathbf{F}^{\mathrm{n}}$) and tangential ($\mathbf{F}^{\mathrm{t}}$) directions using the parcel diameter (d_{CGP}) as collision diameter; this force is then divided by statistic weight to represent the force on a real particle:

$$\mathbf{F}_{\mathrm{c}} = \sum_{j=1\, j\neq i}^{N} (\mathbf{F}_{ij}^{\mathrm{n}} + \mathbf{F}_{ij}^{\mathrm{t}})/W \tag{3}$$

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