V International Conference on Particle-based Methods – Fundamentals and Applications
PARTICLES 2017
P. Wriggers, M. Bischoff, E. Oñate, D.R.J. Owen, & T. Zohdi (Eds)

NUMERICAL STUDY ON THE EFFECT OF PARTICLE SHAPE ON MIXERS

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Key words: DEM, Graphical Processing Unit, Interactive Design, Interactive Simulation, Tumbling Mill, Numerical Multi-Fidelity Models

Abstract. Homogenization of particulate systems is a critical part in the processing of particulate materials to achieve consistency and ensure product quality. Homogenization is achieved by mixing, the aim is to obtain a final mixture that is homogeneous when mixing individual particulate constituents, in the sense of a uniform spatial mass distribution. Although there is always some measure of heterogeneity in a mixture this can be quantified by Gys sampling theory. This is critical for pharmaceutical industries in which it is essential that the variance of the active ingredients between tablets are within specified bounds. Although there have been numerous numerical studies on mixing using the Discrete Element Method (DEM), most studies to date have incorporated significant simplifications to reduce the computational time such as using mono-disperse size distributions, scaling up of particle size and spherical estimations of shape. The development of GPU based DEM simulations in the past few years significantly increased the number of spherical particles however most often at the expense of simplifying the physical interaction between particles. This oversimplification of particle shape has much wider primary implications as primary contact mechanisms such as angularity and locking are omitted. This is important in the pharmaceutical industry where the feed powders are often made from crystalline solids in which the shape of the individual particles are polyhedral. As this study demonstrates, this is significant in that the underlining dynamics of polyhedral particles is vastly different to that of spherical particles, resulting in tighter packing fractions different flow patterns, and percolation. In this paper we use the GPU based DEM code BlazeDEM3D-GPU to study and quantify the effect of particle shape in a high shear blade mixer.

1 INTRODUCTION

Homogenization of particulate materials such as powders is critical in numerous industries ranging from civil engineering to pharmaceuticals to food processing. All these industries include homogenization which is the process of mixing various constituents to obtain a final product where each constituent is distributed uniformly. The homogeneity of the final product depends on both the quality of the constituents in terms of the heterogeneity of particle sizes (particle dispersity), shape uniformity, moisture content and the primary mixing method and device used. Particle dispersity between constituents results in segregation occurring due to percolation [16] which can drastically influence mixing of the constituents and compromise the final product. Consequently, in mixing there is an equilibrium point that limits stable homogenization due to segregation and other processes. This can have devastating consequences in pharmaceutical industries when the active ingredient is not uniformly dispersed throughout a mixture. It is paramount to understand the underlying dynamics of the particles and the effect of a particular mixing device. Influencing the physical properties such as particle shape of the constituents can help shift this equilibrium point to achieve better and more stable homogenization to reduce waste and consequently production costs. There has been limited success in improving the design of mixing devices via experimental means, owing to the difficulties in obtaining unbiased samples of a mixed product either due to the sampling technique or insufficient statistics. Furthermore detailed experimental information on the relationship between the particles with the mixer geometry and the particles themselves is difficult to obtain. Particulate materials exhibit of both solids and fluids behaviour in different flow regimes, making the prediction of the dynamics via empirical means also extremely difficult. Numerical modelling offers a means of investigating the problem, and in particular the potential effect of the various particle properties on mixing. Two numerical approaches are readily available to simulate particulate systems which are 1. continuum models [19], and 2. discrete element models[4]. Continuum models are computationally cheap to evaluate but offer no means to incorporate properties at particle scale naturally and reliably. Hence, although continuum methods can model problems at an industrial scale their inability to accurately predict the macroscopic responses for variations at the particle-scale has only seen limited continuum solutions [20]. Limitations include, the failure to reliably predict the transitional flow regime in which both the collisional and frictional interactions drive flow behaviour [19], in addition to being unable to predict percolation which drives mixing. The underlying material models that are computationally tractable usually require re-characterization once particle scale properties are modified. In addition, the predictive capability of continuum models are limited to a small domain localized around which a solution has been calibrated and computed. The discrete element models are computationally expensive but readily allows for particle scale properties to be modified and investigated. In addition, the discrete element models are generally predictive over larger domains that continuum models [20]. The discrete element method is the only simulation approach that is capable of capturing microscopic and particle-scale effects to accurately predict the macro-scale of bulk behaviour but requires significant computational resources [12]. The discrete element method however is able to reliably predict all three flow regimes and in turn accurately quantifying mixing properties. As a result the discrete element method (DEM) has be- come the de facto standard to simulate particulate materials for which the discrete nature of particles and importance of quantifying particle-scale effects cannot be neglected. Consequently, the need for large scale discrete element simulations that can quantify the effect of particle-scale changes on the macro-scale response is becoming increasingly more important in industrial bulk material handling applications where simulations of lab-scale devices is not sufficient, poorly understood or not repeatable Ding et al. [23]. In addition, the demand to consider the poly-dispersed nature and shape non-uniformity of particulate systems in simulation has been well-established for a number of years by Clearly and Sawley [4], and recently reiterated by Höhner et al. [9] and Zhong et al. [22]. However, numerical studies to date that consider shape non-uniformity and polydispersity of polyhedral Figure 1 particle systems have been limited in scope due the large computational cost and lack of suitable codes to efficiently handle the associated geometrical complexity [6]. As a result the particle shape Figure 1 is often simplified as either spheres or by the multi-sphere approach that approximates a non-spherical particle as multiple spheres that are glued together [2], as depicted in Figure 1. Although the multi-sphere approximation is an improved description for complex particle shapes and allows for particle fragmentation to be taken into account [14], it is limited in the number of spheres that can be used to represent complex particle shapes, while being unable to accurately capture the particle angularity that may have a significant effect on the behaviour of the particulate system. Both the spherical and multi-spherical simplifications significantly reduce the complexity of inter-particle contact detection that results in a significant computational saving. In addition the constitutive models of interacting spheres has been well established and as a result has been used extensively simulations [18, 7]. Since the influence of particle shape and angularity on the mechanical behaviour of particle systems is well known [4, 10], the validity of approximate particle representations remains refutable [8, 13, 21]. To compute industrially

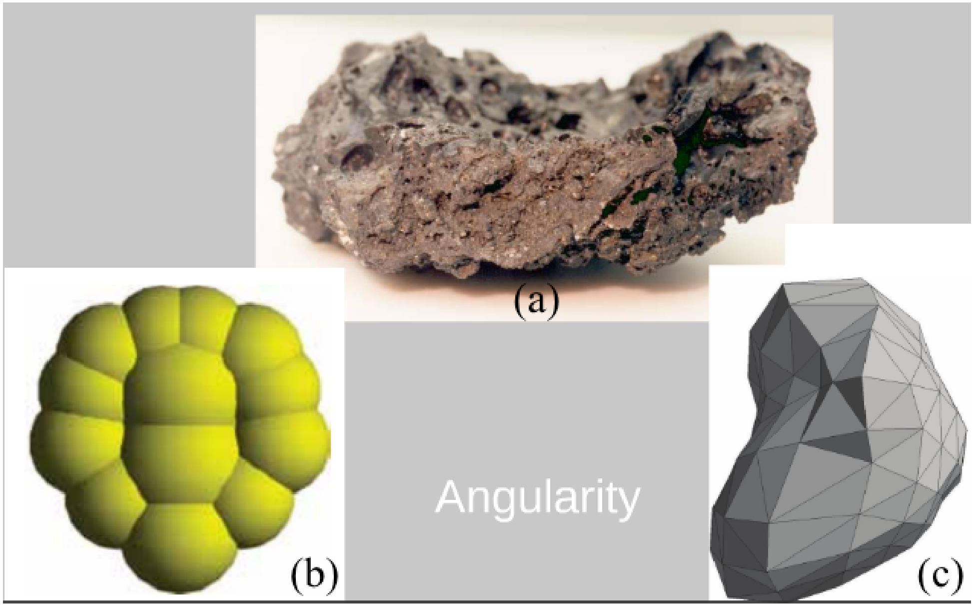

Figure 1: (a) Actual particle [1] represented using (b) a lumped sphere particle representation or (c) a polyhedron representation..

relevant discrete element simulations within a realistic time frame remains a challenging computational endeavour. Radeke et al. [15] performed the largest DEM simulation of a mixing device using 8 million spherical particles. This is still far from the hundreds of millions to billions of particles required for the simulation of industrially relevant mixing devices which have capacities of hundreds of litres. While the utilization of the Graphics Processing Units (GPU) in DEM simulations has resulted in simulations up to 50 million particles on a single computer and a billion particles using multiple computers with 256 GPUS, these simulations drastically oversimplify particle shape by modelling only spheres with simplistic contact models. In the case of Ge et al. the parallelization over multiple GPUs is highly problem specific.

2 OVERVIEW OF MIXING SIMULATIONS

The importance of considering particle shape in mixing has been demonstrated by Cleary et al. [5] for cubic salt particles being modelled as spherical particles. To correctly predict the mixing rate order and flow patterns required to consider the cubic salt particles as super-quadrics. The higher shear resistance of angular particles over spherical particles being the dominant reason for the observed differences. Laurent and Cleary [11] showed that approximating particles as spherical in a ploughshare mixer under-predicted the free surface angles, indicating again to lower shear resistance. In addition, particle shape can vary substantially between different types of particles and between particles from the same sample. Particle shape is known to be important to consider to accurately quantify mixing of even rotating drums. Chandratilleke et al. [3] found that when fluidization of the bed occurs, the effect of air drag on the particles becomes important. As drag depends on particle shape the mixing and segregation may exhibit shape dependence. However, particle shapes are usually modelled as spheres and modifications to properties made due to the associated computational cost of non-spherical particle shapes. For example small values of rolling friction are often added in an attempt to account for mild departures from sphericity. However, Zhou et al. [23] showed that mixing kinetics were enhanced for low friction materials. Since, particle shape influences shear resistance it directly affects the ability to predict mixing. In addition, they reported that the particles flowing over the paddle was the mechanism responsible for segregation effects. The implication being again that particle shape directly influences the ability to predict and model segregation effects. However, to what extent particle shape needs to be considered remains poorly studied since most researchers simulate mixing processes in three dimensions use spherical particles citing computational expense as the primary limitation to investigate other particles shapes.

3 DETAILS OF CONTACT MODEL

Contact between spherical and polyhedral particles are resolved using a sliding-sticking friction model where the tangential force is coupled to the normal force through Coulomb's law. The initial tangential force is computed as the sum of the tangential spring force and a tangential viscous force

$$\mathbf{f}_0^t = -k_t \mathbf{L}^k - \gamma_t \mathbf{v}_t, \tag{1}$$

with $\mathbf{L}$ the tangential spring displacement from its equilibrium position, k_t the tangential spring parameter and γ_t the tangential dissipation parameter, and $\mathbf{v}_t$ the relative tangential velocity. For the static friction case, below the Coulomb limit, the tangential spring magnitude is incremented by

$$L^{k+1} = L^k + v_t \Delta t, \tag{2}$$

whereas for sliding friction

$$\mathbf{L}^{k+1} = -\frac{1}{k_t}(f_C^d \mathbf{n} + \gamma_t \mathbf{v}_t), \tag{3}$$

along the tangential unit vector $\mathbf{t} = \frac{\mathbf{f}_0^t}{\|\mathbf{f}_0^t\|}$. The contact volume is resolved for the polyhedral shaped particles as outlined in Figures 2(a)-(d). Specifically, a Kelvin-Voigt linear viscoelastic spring dashpot for rigid particles is considered. This results in an elastic force that stores energy and a dissipative Coulomb force that dissipates energy given by

$$\mathbf{F}_{\mathrm{N}} = (\mathrm{K_n} \mathit{\Delta V})\mathbf{n} - \mathrm{C_n}(\mathbf{V}_{\mathrm{R}} \cdot \mathbf{n})\mathbf{n}, \tag{4}$$

where K_n is the volumetric spring stiffness ($\frac{N}{m^3}$), $\mathbf{n}$ the normal direction along which the force acts, C_n the damping coefficient ($\frac{Ns}{m}$) and $\mathbf{V_R}$ the relative velocity between the

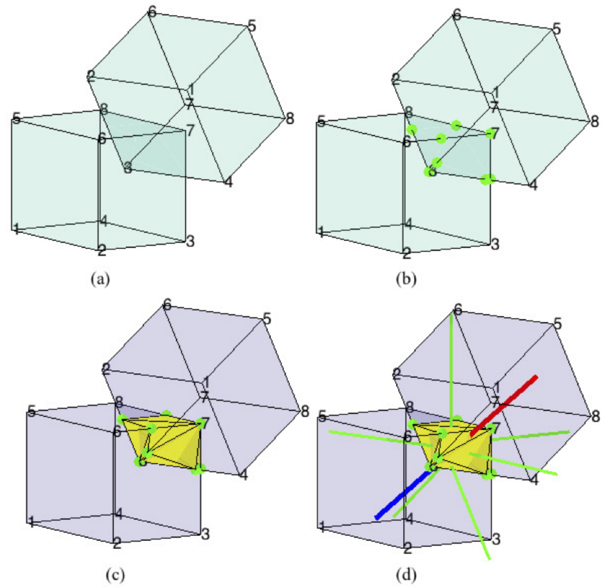

Figure 2: Contact resolution (a) between two intersection polyhedra by resolving the (b) contact points from which the (c) convex hull is constructed to compute the contact volume and (d) contact normals.

contacting particles. Given the overlap volume ΔV and contact normal that is resolved exactly for two polyhedral shaped particles as depicted in Figures 2(a)-(d).

In this study a normal spring stiffness of 100 N/m and tangential spring stiffness of $\frac{2}{7}$ of the normal stiffness is selected. In addition a coefficient of restitution (COR) of 0.9, friction coefficient of $\mu = 0.5$ and tangential viscous force of $\gamma_t = 0$ is selected.

4 SIMULATION OF A HIGH-SHEAR MIXER

The drum diameter is 13.5 cm with a single blade 0.80 cm high with a width of 0.10 cm as used by Sinnot et al. [17], the height of the particles is ≈2 cm. In this study two particles are considered, namely, spherical and tetrahedral shaped particles to fill a mixer volume of 100 cm^3 with a total mass of 240 g. In the high-shear mixer, mixing is done at 100 RPM for 10 seconds. The spherical particles are modelled as poly-dispersed by selecting 12 000 of the following diameters 0.14 cm, 0.1475 cm, 0.15 cm, 0.1525 cm and 0.155 cm for particles for a density of 2.5 g/cm^3. In turn , 60 000 truncated tetrahedral shaped particles are modelled using a particle volume of 0.001665 g/cm^3 and particle mass of 4.16×10^{-6} kg bounded with a radius of 0.0994 cm. The particle surface area is given by 0.08757 cm^2. The tetrahedral shaped particles are modelled with full angularity. The systems are colored initally in a left (green) right (red) split. The results for spherical shaped particles at various time instances is presented in Figures 3(a), (c) and (e), while the truncated tetrahedra is presented in Figures 3. The lower shear resistance of the spherical particles allowing for faster mixing to occur.

In order to quantify the mixing, the relative standard deviation (RSD) is reported as a function of time. $\sigma = \sqrt{\frac{1}{m_s-1}\sigma_{m_s}(\bar{x} - x_{m_s})^2}$, mean value of $\bar{x}$, number of samples m_s and standard deviation σ. $RSD = \frac{\sigma}{\bar{x}}$. Evidently, the RSD reflects a higher mixing rate for the spherical particles than the truncated tetrahedra as presented in Figure 3. The spherical particle shapes tend to taper off around an (1-RSD) of around 0.92, while the truncated tetrahedra tapers off around (1-RSD) of 0.85 resulting in a difference of and RSD of 0.07 after 10 seconds. After 30s the values remained around these values and no further mixing occurred. The higher shear resistance that results from the angular truncated tetrahedra particle shape is evident and important to consider in that the rate of mixing achieved after 5 seconds with spheres is the maximum value acheived after 10 seconds for the polyhedra.

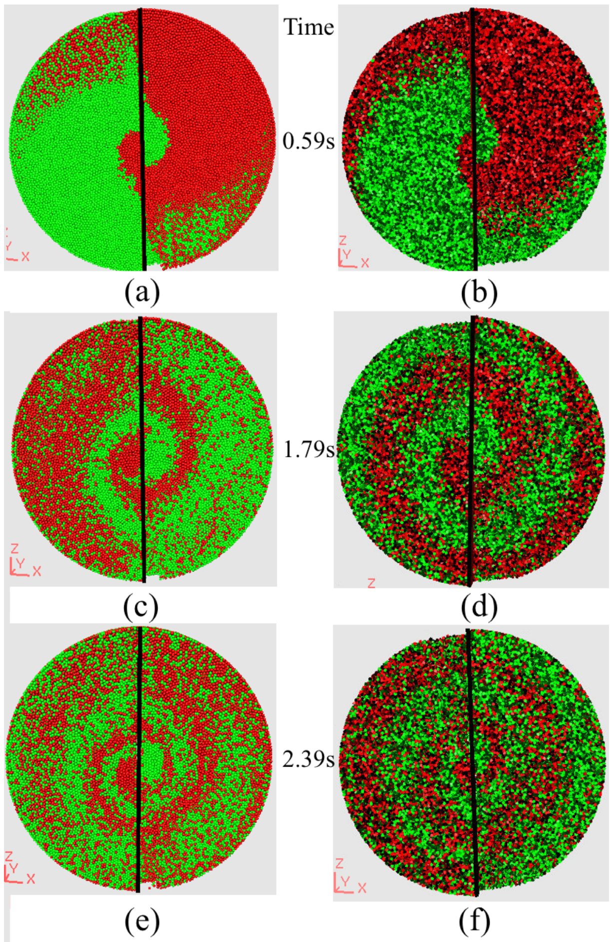

Figure 3: Mixing surfaces for the (a),(c),(e) spherical and (b),(d),(f) truncated tetrahedral particle shapes after 1 , 3 and 4 revolutions respectively.

One of the advantages of simulation over experiment which can greatly aid in the

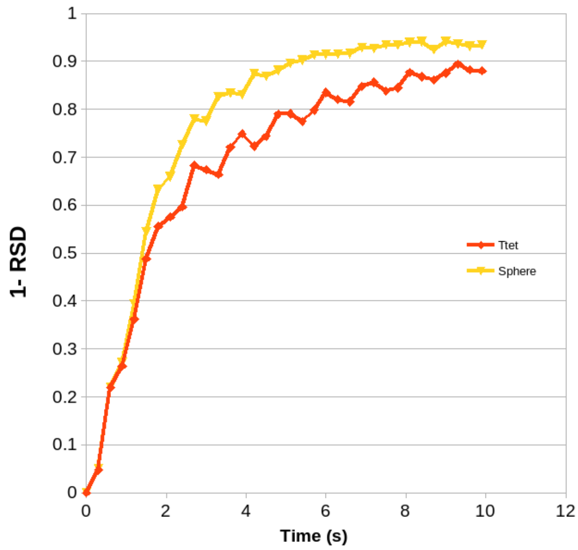

Figure 4: One minus the relative standard deviation as a function of time for the spherical and truncated tetrahedral shaped particles (1 rev = 0.60 s).

understanding mixers is that detailed information that would be tedious or difficult via experimental means is easily done in a computational environment. Consider Figure 5 which shows the RSD over a number of spatial cells, we see that while the average RSD indicates a fairly good mix for the truncated tetrahedral shaped particles, this mix is not as homogeneous in space as the spheres which is crucial for pharmaceuticals where differences of a few % leads to rejection of an entire batch due to regulatory requirements.

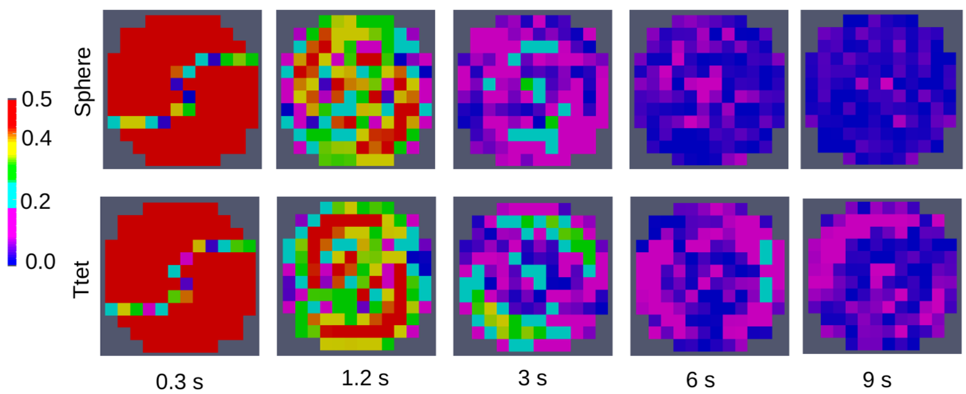

Figure 5: Relative standard deviation spatially distributed cells as a function of time for the spherical and truncated tetrahedral shaped particles (1 rev = 0.60 s).

Finally, Figure 6 depicts our current investigation of a semi-industrial scale simulation of a mixer in which 10 million truncated tetrahedral particles, are simulated on a single computer using two GPUs at a rate of 1.5 s a day.

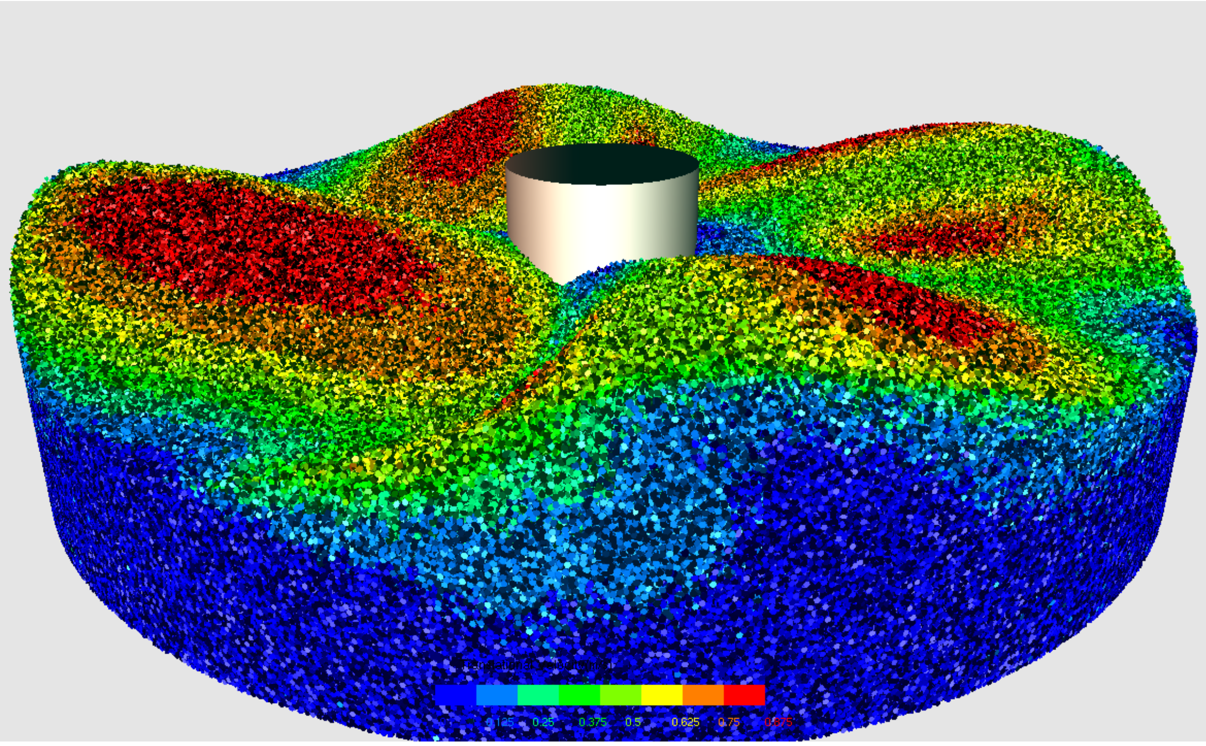

Figure 6: Semi-industrial scale simulation of a mixer using 10 million truncated tetrahedral particles.

5 CONCLUSIONS

This study quantified the difference in the relative standard deviation index of mixing between spherical particles and truncated tetrahedra. The importance of particle shape and angularity in the shear resistance of the particulate system is critical to consider as it has a significant effect on the mixing of the particulate system, highlighting again the importance of modelling particles with accurate geometry and angularity.

Acknowledgements

We gratefully acknowledge the support of NVIDIA Corporation with the donation of a Titan X Pascal GPU used for this research.

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