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Large-scale GPU based DEM modeling of mixing using irregularly shaped particles

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ABSTRACT

Mixing of particulate systems is an important process to achieve uniformity, in particular pharmaceutical processes that requires the same amount of active ingredient per tablet. Several mixing processes exist, this study is concerned with mechanical mixing of crystalline particles using a four-blade mixer. Although numerical investigations of mixing using four-blades have been conducted, the simplification of particle shape to spherical or rounded superquadric particle systems is universal across these studies. Consequently, we quantify the effect of particle shape, that include round shapes and sharp edged polyhedral shapes, on the mixing kinematics (Lacey Mixing Index bounded by 0 and 1) that include radial and axial mixing as well as the inter-particle force chain network in a numerical study. We consider six 100 000 particles systems that include spheres, cubes, scaled hexagonal prism, bilunabirotunda, truncated tetrahedra, and a mixed particle system. This is in addition to two six million particle systems consisting of sphere and truncated tetrahedra particles that we can simulate within a realistic time frame due to GPU computing. We found that spherical particles mixed the fastest with Lacey mixing indices of up to 0.9, while polyhedral shaped particle systems mixing indexes varied between 0.65 and 0.87, for the same mixing times. In general, to obtain a similar mixing index (of 0.7), polyhedral shaped particle systems needed to be mixed for 50% longer than a spherical particle system which is concerning given the predominant use of spherical particles in mixing studies.

1. Introduction

Granular media is only second to water as the most manipulated substances on the planet [1]. Mixing forms part of the manipulation of granular media, which is essential in a number of industrial processes including civil engineering, pharmaceutical industry and food processing. Mixing is any process designed to combine two or more dissimilar granular materials uniformly to obtain a homogeneous product. The homogeneity of the final product depends on both material properties such as particle sizes (particle size polydispersity), particle shape, moisture content, the mixing method and mixing device. Particle size, volume, density and shape variations may result in demixing (segregation) occurring by percolation, flotation, elutriation, agglomeration, flow-induced or transport mechanisms [2,3]. Segregation may be highly sensitive to particle properties such as flow-induced segregation that is due to small differences in particle size or density when particles flow. Segregation can drastically influence the final product safety and quality.

A number of computational approaches have been developed [4–7] to predict particle mixing that include isolated cases of continuum models [8] and multi-scale continuum models [9], while the majority of studies considered discrete element models [10–19]. DEM has been shown to be capable to predict sensitive particle scale effects in mixing [10]. Discrete element particle mixing studies have been confined to the modeling of spherical particles [10–16,20], although the importance of particle shape and angularity from experimental [21,22] and discrete element studies [10] have

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highlighted the importance thereof. Laurent and Cleary [23] showed that approximating particles as spherical in a plough mixer under-predicted the free surface angles, leading to lower shear resistance. Cleary et al. [10] demonstrated qualitative agreement between flow patterns but mixing rates were poorly predicted, in particular for lower fill levels which were most likely due to the higher shear resistance of angular particles. This is highlighted by the excerpt and critical observation from Cleary et al. [10] made twenty years ago in 1998, "The most likely cause is in neglecting the real shape of the particles simulation". Hence the validity of studies [24–26], remain conditional.

Although numerous particle systems are representative of crystalline particles as shown in Fig. 1(a), only limited DEM studies have considered particle shape in mixing studies. Modifications to spherical particle properties are common to account for the effect of shape, for example, by adjusting rolling friction to account for a mild departure from sphericity [27]. This approach is limited as the relationship of rolling friction to particle shape is usually unknown requiring extensive characterization that diminishes the predictive ability of these models. Studies that considered particle shape usually limit themselves to ellipsoids [28], multi-sphere approximations [29], as depicted in Fig. 1(b), or smooth super-quadric particle representations [30–32], as depicted in Fig. 1(c). Polyhedral shape representation that captures the particle angularity as depicted in Fig. 1(d), has yet to be conducted for mixing studies.

One of the largest DEM simulation of a mixing device used 8 million spherical particles Radeke et al. [33], which is still far from the billions to trillions of particles required for the simulation of industrially relevant mixing devices. Recent advances in software and computing architectures have realized the utilization of the Graphics Processing Units (GPUs) to solve DEM models. This has resulted in simulations of up to 50 million particles on a single computer [34], and over a billion particles using up to 256 GPUs [35]. However, these large scale simulations drastically oversimplify particle shape by modeling only spheres with basic contact models due to the computational demands of DEM.

Even for smaller scale simulations only a limited number of investigations [31,32] have considered non-spherical particle shapes. In these studies, non-spherical particle shapes are restricted to super-quadric shapes [31,32] (see Fig. 1(c)) or multi-sphere shapes [36,37] (see Fig. 1(b)). The multi-sphere approach approximates a non-spherical particle using fused spheres [29], as depicted in Fig. 1(b). Although the multi-sphere approximation is an improved description for complex particle shapes and allows for particle fragmentation to be taken into account [38], it is limited in the number of spheres that can be used to represent complex particle shapes. It is also unable to accurately capture the particle angularity that may have a significant effect on the behavior of a particulate system. Both the spherical and multi-spherical simplifications significantly reduce the complexity of contact detection that results in significant computational savings. In addition, constitutive models for interacting spheres have been well established and as a result, have been used extensively [39,40]. Although super-quadric particles allow for improved particle shape representations over the multi-sphere approach they still lack proper angular representation of particles.

Due to the computational demand, polyhedral shaped particles have been limited in discrete element simulations, in particular, when considering proper constitutive models that rely on the overlap volume [41] as opposed to penetration distance [42]. Computing using the overlap volume for polyhedral shaped particles has been demonstrated to be computationally tractable [43] on graphical processing units (GPUs). This development is allowing for polyhedral shaped particles to be considered for industrial scale investigations.

This study therefore extends the envelope of discrete element simulations in mixing applications to include the effect of particle angularity and quantify the importance thereof. This is the first study to consider polyhedral particle shape representations that accounts for particle angularity in a mixing study.

2. BlazeDEM-GPU simulation framework

In this study we use BlazeDEM-GPU developed by Govender et al. [44] that solves Newton's equations of motion for soft particles using an explicit forward Euler time integration scheme on GPU architectures. In a BlazeDEM-GPU simulations, particles are confined by geometric boundaries that are denoted "world objects" to confine particle flow. The world objects are represented as closed-form expressions for curved or planar surfaces. Since, particle shapes can be either spherical or polyhedral that can interact with each other or world objects, requires contact detection to be split into particle-particle contact and particle-world. Recently, Govender et al. [43] demonstrated computational tractable simulations using spherical and polyhedral shaped particles on graphical processing units (GPUs), using the overlap volume to estimate contact force directions and magnitude.

Contact detection is computationally the most expensive part of a DEM simulation accounting for as much as 90% of the total simulation time for polyhedral shaped particles. Thus importance is placed on implementing algorithms to take full advantage of the parallel nature of the GPU. In addition, algorithms need to utilize memory correctly to minimize the number of memory transactions; otherwise the actual number of threads executing in parallel will be significantly reduced due to register pressure [45]. This is termed the occupancy of a particular method (kernel) executing on the GPU.While a detailed discussion is beyond the scope of this

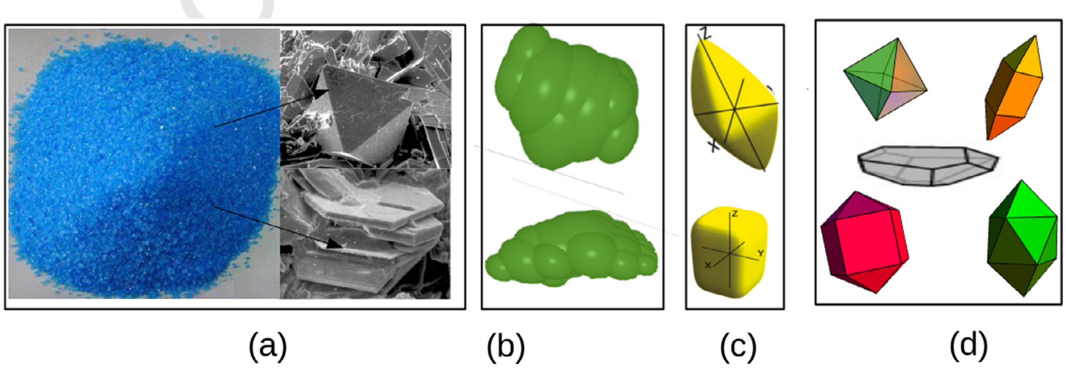

Fig. 1. (a) Typical crystalline powder with SEM scans at the particle scale, with associated DEM approximations using (b) clumped sphere (c) superquadrics and (d) polyhedral representations of particle shape.

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