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Semi-analytical models of non-spherical particle shapes using optimised spherical harmonics

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ABSTRACT

Determining particle shape is vital for many industrial processes such as those found in the pharmaceutical, agricultural, and bioenergy industries. With modelling being an essential tool to acquire an understanding of the behaviour of particulates in industrial processes, numerical methods such as DEM are needing numerical solutions to formulate and implement particle shape models that overcome current limitations. Whereas pharmaceutical particles have a regular shape, agricultural and biomass particles often are specific, irregular and non-analytic. Because the diversity of real shapes is enormous, a variety of methods for describing particle shapes currently exist. Recently, the series of spherical harmonics (SHs) has gained much interest through their application in many other fields. This paper focuses on the application of the semi-analytical SH technique and addresses the development of a universal modelling tool for describing different particle shapes using a finite number of SHs. The results obtained from modelling pharmaceutical, agricultural, and biomass particles prove the applicability of SHs to regular as well as irregular shapes. In this regard, their optimised description by minimising the number of non-zero expansion coefficients is demonstrated. To proceed with a smaller number of low-order SHs, surface segmentation is introduced. Sufficient accuracy in the shape description of the particles selected was achieved with less than 16 SHs.

1. Introduction

Particle shape is an important attribute that plays an important role in many industrial processes (e.g., chemical, agricultural, and mining). Determining the particle shape is a very complex problem being closely related to the physical nature of particles, area of application, length scale, and other factors. Different aspects of particle shape are considered by Latham and Munjiza (2004) and Peña et al. (2007). The transition issue between the above scales is discussed by Cardoso et al. (2013), Felekoglu (2009), Kačianauskas et al. (2014), and Feinauer et al. (2015). The roughness has been analysed by Persson (2006).

The accuracy to be achieved in the description of real particle shapes is related to the accuracy demanded for the description of its physical behaviour. Such demands occur basically in the design and control of technological processes of particles in many technology-based areas including agriculture (Freireich et al., 2011; Ketterhagen, 2011) and pharmaceutics (Ren et al., 2012; Zhan et al., 2013). The particle shape directly affects the mechanical contact between particles (Kock

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and Huhn, 2007; Weis et al., 2017; Ng et al., 2018), the dosage of active pharmaceutical ingredients (Yu et al. 2017), heat and mass transfer between particles and environment (Gubba et al., 2011; Nemati Hayati et al., 2012), processes related to the thermal conversion of biomass (Cardoso et al., 2013), the relationship between iron ore granulation mechanisms, granule shapes, and sinter bed permeability (Nyembwe et al., 2017), particle packing, particle flow in hopper discharge of industrial processes, particle-fluid flows (fluidised bed, pneumatic conveying, channel flow), and vibration, coating, milling or mixing, among others (Zhong et al., 2016).

Digital, numeric and analytical descriptors are used for the description of shapes. Various digital descriptors such as voxels, clouds of points or wavelets (Masad et al., 2005) are used in the finer scale, mainly for the description of texture and roughness.

The numerical approach assumes the surface of a particle discretised by individual points. In particle analysis, this approach as proposed by Williams and O'Connor (1995) is termed the discrete function representation (DFR). The finite-element method (FEM) used for the description of particles belongs to the DFR category (Latham and Munjiza, 2004). The numerical approach is universal and shape-independent but also an expensive and time-consuming technique for 3D discretisation. The combined digital-numerical discretisation technique comprising a full sequence of numerical operations is available to transform scanned digital images to particle shape parameters yielding finally irregular-shaped particles (Johnson and Williams, 2009; Williams et al., 2014). The application of DFR though requires storage of a considerable amount of data.

In many cases, the mathematical description of particle shapes by analytical expressions, the so-called continuous function representation (CFR), can be more advantageous than numerical techniques. In practice, the CFR is synonymous with the smooth single-function approach. Perfect analytical shapes are seldom applicable to the physical characterisation of particles, but they are, for example, better suited for DEM applications. Critical reviews of recent developments in DEM with advances in the formulation and implementation of particle shape models are given in Lu et al. (2015) and Zhong et al. (2016).

In this regard, the perfect analytical shape is the sphere, which has been extensively used in DEM modelling. However, the use of other shapes is limited. Analytical representations of 3-D ellipsoids were proposed a couple of decades ago by Ting et al. (1993) and by Potapov and Campbell (1998). Other representations using super-quadric equations were proposed by Williams and Pentland (1992) and more recently by Lu et al. (2012) and Podlozhnyuk et al. (2017).

Analytical models can grasp a limited number of particles shapes. Because of the lack of a unified methodology, composite approaches comprising various combinations of plane, spherical, and cylindrical segments prevail in DEM. This composite technique may be classified as a mixed technique, CFR/DFR, in which the particle surface is described by a non-smooth semi-discrete approximation. Polygonal (in 2D) and polyhedral (in 3D) formulations provide a high level of versatility in particle representation by cutting planes (Cundall, 1988; Chen et al., 2011; Alonso-Marroquín et al., 2013). The use of polygon formulations is a general approach to describe mathematically non-spherical particles having convex and concave shapes such as rocks, gravel, and sand that contain sharp edges. However, research is still ongoing to achieve an efficient determination of contact forces between two colliding polyhedral bodies.

Composite spheres technique termed multi-spheres allows to construct a non-spherical particle by "gluing" a specific number of spheres (Favier et al., 1999). Multi-spheres are successfully applied to represent gross shapes of complex-shaped particles, and agricultural shapes in particular (Horabik and Molenda, 2016). These models are a good alternative for polyhedral particles, where sharp-edge contacts are smoothed by spheres. Another smoothing alternative is related to the development of spheropolyhedral models (Alonso-Marroquín, 2008; Alonso-Marroquín et al., 2013), where sharp edges are replaced by cylindrical segments.

The advantages of an analytical CFR technique are retained by applying a semi-analytical approach. The corresponding model presents closed-form expressions containing a finite number of unknown coefficients. Such types of universal models grasp a substantially larger number of shapes. Development of a universal method for the description of all available shapes is still a challenge.

The Fourier series is probably the most popular and earliest semi-analytical method used for the description of particle shape (Bowman et al., 2001; Mollon and Zhao, 2012), but limited, however, to 2D particles. Recently, the use of spherical harmonics (SHs) has received increasing attention with their contribution in many fields, including modelling of molecules. SHs are the analogue of the 1D Fourier series and allow functions over a sphere to be defined in frequency space; even so, the sphere is the natural shape used in DEM. This has many advantages over discretisation of functions in real space, including rotational invariance and formulae for rapid integration (Hilton et al., 2013). The 3D mathematical analysis of particle shape using SHs with application to aggregates used in concrete was started by Garboczi (2002). The use of SH to describe the surface characteristics of granular material was presented by Masad et al. (2005). In their study, differences between the Fourier series and the SH series in 3D CT imaging was analysed, and a better accuracy was found with SHs.

The investigation of SHs, especially in combination with the available imaging techniques, was continued in a series of works (Garboczi, 2011; Liu et al., 2011; Garboczi and Kushch, 2015). The SH series as a universal technique is aimed at describing the so-called star-shaped particles (Bullard and Garboczi, 2013) and presents a tool suitable for a large group of shapes. The SH method was successfully applied in the description of sand (Zhou et al., 2015). Some illustrations of very complex shapes can be found in Mousa et al. (2008), whereas various shape indicators described in terms of SHs were considered in Feinauer et al. (2015). An application of SHs to describe agricultural grains is given in Radvilaitė et al. (2016a).

Generally, semi-analytical methods and SH methods, in particular, are universal modelling techniques that are independent of the area of application. Possible applications range from irregularly shaped rocks in macroscale to elongated airborne particles and even red blood cells in blood vessels on the micrometer scale. Recent developments indicate, however, that most of the achievements are concerned with accurate descriptions of the shape of various mineral particles. A large part of the above investigations deals with the generation of particles for which the statistical shape properties closely match the real particles, with the development of numerical methods and with the creation of large particle datasets (Garboczi, 2011; Liu et al., 2011; Garboczi et al., 2012).

Until now, direct use of the SH technique to DEM is still scarce. Contributions that use SH in DEM directly are scant and a universal approach does not exist. Available applications of SHs demonstrated the reconstruction of particle gross shape based on statistical data and mixed analytical-numerical results for calculations on the inter-particle contact (Garboczi and Bullard, 2013; Fu et al., 2017 Zhou and Wang, 2017). Descriptions of roughness needed for fluid interactions are demonstrated in Hilton et al. (2013).

The challenge is to overcome the drawbacks of the SHs and to explore their strength to satisfy DEM demands. The problem is that universal mathematical expressions used in the SH method, including their integration and differentiation, usually are complex and their implementation to exploit these main advantages is not simple; see discussion in Mollon and Zhao (2014). Therefore, essential issues are raised to motivate further research.

Non-star shapes and the presence of sharp edges are two main issues requiring novel solutions. The composite description seems to be suitable for capturing complex shapes, but new developments of SHs are required in the former instances. The angularity problem may be resolved by applying SHs in a natural way by rounding off sharp angles without needing spheres or cylinders as is usually done in composite methods.

It is necessary to prove that this relatively computationally intensive SH technique has sufficient efficiency to produce reliable accuracy within an acceptable cost. Here, optimising the number of harmonics may be used. A small number of low-order SHs was found to capture the gross shape, whereas the texture was captured using higher-order harmonics (Feinauer et al., 2015 Zhou and Wang, 2017). Consequently, full harmonic expressions using a large number of coefficients (of more