Aggregate Geometry Generation Method using a Structured Light 3D Scanner, Spherical Harmonics based Geometry Reconstruction and Placing Algorithms for Mesoscale Modelling of Concrete

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ABSTRACT

Mesoscale numerical modelling is an effective method of representing concrete as a three-phase material. Accurate aggregate geometry representation is an important aspect in numerical mesoscale modelling of concrete to predict mechanical properties as well as the damage initiation and fracture propagation. In this paper, a novel approach of 3D scanning of aggregates using a structured light 3D scanner is presented and parametric geometry reconstruction of aggregate geometries using spherical harmonics is carried out. This novel method of scanning aggregates is a faster, safer, economical and a convenient method of obtaining the 3D geometry compared with other methods. A comprehensive database of aggregate geometries is developed and an innovative aggregate placing algorithm for these aggregates is presented to develop the mesostructure. In addition to the proposed geometry generation method, a novel parametric based geometry generation and distribution method for polyhedral aggregate shapes is presented including flaky and elongated particles. Finally, aggregate transferring methods to finite element software and mesh generation methods are discussed with the challenges and possible methods to overcome these issues.

AUTHOR KEYWORDS : Mesoscale Modelling; Spherical Harmonics; Take and Place Method; 3D Scanning; Aggregate Shape Analysis; X-Ray Computed Tomography

1 INTRODUCTION

Mesoscale modelling of concrete represents concrete in the mesoscale as a three-phase material consisting of aggregates, mortar and Interfacial Transition Zone (ITZ) and this technique is an efficient method to investigate about fracture and damage mechanics of concrete, local deformation mechanisms, durability characteristics of concrete and various concrete formulations (Comby-Peyrot et al. 2009). Mesoscale modelling is the most useful and practical method to model the heterogeneities in concrete and understand how these heterogeneities affect the macro behavior of concrete (Thilakarathna et al. 2020a).

Coarse aggregate is one of the three phases in the mesoscale which significantly contributes to the performance of concrete (Shanaka 2016). In mesoscale models, only coarse aggregates are modelled due to the limitations in computational capacity and fine aggregates are assumed to be contained in the mortar phase (Li et al. 2019). Aggregate characteristics such as aggregate shape, aggregate size, aggregate volume fraction, mechanical properties of aggregate and particle size distribution curve (PSD) will influence the nonlinear behavior of concrete in mesoscale and hence representation of aggregates accurately is important (Kristombu Baduge et al. 2018; Trawiński et al. 2018).

To investigate the effect of aggregate parameters on the stress-strain behavior of the concrete, a robust methodology of aggregate shape generation and placing algorithms according to any given PSD is needed. These aggregate assemblies will serve as the core of the geometry in the mesoscale models. Mesoscale aggregate assemblies can be generated in 2D (Jiang et al. 2019; Rodrigues et al. 2016; Snozzi et al. 2012; Wang et al. 2015; Zhou et al. 2019) as well as in 3D (Häfner et al. 2006; Li et al. 2016; Pan et al. 2018; Zhang et al. 2018b; Zhou et al. 2017). With the increasing computational capacities and some limitations of 2D models, 3D mesoscale modelling has become prevalent and hence in this paper, generation of 3D aggregate assemblies are discussed.

This paper presents comprehensive shape generation algorithms for polyhedral shaped aggregates as well as a spherical harmonics-based algorithm to reconstruct the exact geometric shapes of real aggregates using the scanned aggregate geometries using a structured light 3D scanner. Also, an algorithm is proposed to disperse the 3D scanned aggregates until a particular volume fraction is achieved. Challenges of generating and placing aggregate particles to achieve a prescribed volume fraction are also discussed and methods to overcome those challenges are presented.

2 METHODOLOGY

Aggregate generation procedures, placing algorithms, aggregate shape analysis and geometry reconstruction methodologies are discussed in this section for scanned aggregate shapes as well as parameterized aggregate shapes. Results of the aggregate generation procedures and shape analysis are also included in this section.

2.1 3D SCANNING OF AGGREGATE GEOMETRIES

There are numerous methods to model aggregate geometry in mesoscale models and 3D scanning is one of the main techniques. X-ray computed tomography (XCT) scanning is a widely used 3D scanning method to scan aggregates and concrete samples to generate the mesostructure of concrete (Huang et al. 2015; Liu et al. 2018a; b; Ren et al. 2015; Shuguang and Qingbin 2015; Thilakarathna et al. 2020b). However, it is time-consuming and costly to scan aggregate particles using XCT (Anochie-Boateng et al. 2013) and XCT has a strict safety and radiation monitoring specifications (Anochie-Boateng et al. 2012). Hence, a more convenient method is needed to obtain the actual aggregate shapes. 3D laser scanning is another method used to scan and obtain 3D aggregate shapes (Kim et al. 2003; Lanaro and Tolppanen 2002; Mazzucco et al. 2018). However, these 3D laser scanners are comparatively slower than the structured light scanners (Laga et al. 2019).

In this study, a novel aggregate scanning method using a handheld structured light scanner is proposed to obtain the accurate geometries of aggregate particles. Previous researchers have mainly used XCT and laser scanning methods to obtain the accurate aggregate geometries and the proposed scanning method has numerous advantages compared to those scanning methods. Structured light scanners are much safer than the 3D laser scanners and XCT scanners. These scanners also produce a higher detail level with dense and accurate data compared with the laser scanners. This scanner is very convenient to operate due to its portability. However, this does not penetrate the samples as in XCT to produce a comprehensive 3D mesh with internal heterogeneities and number of particles. The number of particles which can be processed per hour depends on the 3D scanner type and the portable one can process around 500 particles per hour and this is comparatively lower than the XCT. For mesoscale modelling purposes, aggregates are assumed to be homogenous and hence this is a safer, less expensive and a convenient method of obtaining the accurate 3D geometry.

Schematic diagram of 3D scanning process of aggregates is shown in ***Fig. 1***. Artec Space Spider 3D scanner was used in this study to scan aggregates placed on a turntable. This scanner has a 3D resolution of 0.1 mm and a 3D point accuracy of 0.05 mm. This has a linear field of view of 90 × 70 mm at the closest range and 180 × 140 mm at the furthest range.

3D scanning and processing sequence using the structured light scanner is shown in ***Fig. 2***. Each of the steps in the sequence of scanning the aggregates are further described in the next sub-sections.

2.1.1 Scanning

This step involves taking the 3D scans of the aggregates using the structured light scanner and transferring those scans to the computer for further processing. An aggregate was placed on the turntable as shown in ***Fig. 1*** and then it was scanned by rotating the turntable slowly until a sufficient number of frames were scanned to capture the surface variations of the aggregate. ***Fig. 3*** shows a collection of scanned frames.

After completing this scan, the aggregate was turned upside down and followed the same procedure to capture the areas which were not scanned in the previous step. Additional scans can be done to make sure all the surfaces are included in the scans. However, in this scenario two scans per aggregate were sufficient.

Ambient lighting was used for the scans and structured light scanner uses LED flashes to illuminate the scanning area and hence, scans can be obtained even in a completely dark environment. Capture rate of the scanner in this study was 7.5 frames/second and while scanning captured frames are automatically aligned using the features in overlapping areas. Rotating speed of the turntable was approximately 4 rpm and the scanner is incapable of capturing important features if the turntable is rotated too fast. Optimal distance between the scanner and the object for was around 250 mm and a 3D resolution of 0.2 mm was used.

2.1.2 Cleaning

It can be seen from ***Fig. 3*** that parts of the turntable have also been scanned and some outliers are clearly visible. In this step, rough cleaning of the scans was done by removing outliers and the parts of the scanned turntable.

Outliers are unnecessary noise visible in the scanned frames and if these are not removed, they can be attached on to the final 3D geometry as fragments. Parts of the scanned turntable were also deleted in this step. Aggregate scans after deleting the outliers and the base are shown in ***Fig. 4***.

Artec Studio (Artec3D 2020) software uses a statistical algorithm to determine the mean distance and standard deviation between each point in the model and a set of adjacent points and compares that with an interval defined by considering global mean distances and standard deviations. If the distances of the considered points are greater than the distances defined in this interval, it is considered as an outlier and removed from the model.

2.1.3 Alignment

In this step, different scans were aligned to make one complete scan. Data in the scans were converted into one coordinate system using pairs of points. At least three sets of points are needed to carry out the alignment step. Selection of points need not to be precise in this step as in the registration step, accurate registration is done.

2.1.4 Registration

After aligning the scans, global registration of the frames was carried out. In this step, the global registration algorithm present in Artec studio (Artec3D 2020) uses all the frames captured by the scanner and converts the object surfaces in these frames in to a single coordinate system by identifying the mutual positions of the features present in the surfaces. This is done by picking a set of geometry points in one frame and searching for matching pairs of points present in the other frames. For this, an initial approximation is required, and this initial approximation is obtained by the selected points in the aligning step.

2.1.5 Fusion

In the fusion step, a 3D polygonal model of the scanned geometry was created. In this step, the resolution of the model can be specified to define the mean distance between the two points of the model. When generating the polygonal model, defects can appear on the reconstructed geometry due to incomplete scans and these can be avoided by ensuring the quality of the scans and number of scans are sufficient. To improve the quality of the scan, speed of rotation of the turntable can be reduced or the rate of capture can be increased.

If these defects are minor, these can be repaired to obtain a defect-free polygonal model. If there are holes that can't be mitigated by increasing the number of scans, those can be filled to obtain a watertight mesh. In this hole-filling algorithm, edge fragments are connected by a surface which follows the curvature of the neighboring surfaces. Some of the scanned aggregates after fusion are shown in ***Fig. 5***.

2.1.6 Postprocessing

The scanned geometry consists of a significant number of polygons and the number of polygons needs to be reduced to be used in the mesoscale model. This mesh simplification was done using meshlab software (Cignoni et al. 2008). A Database of aggregates was developed by scanning various aggregates with different sizes. Also, using meshlab software, some of the obtained meshes were scaled uniformly to ensure that an aggregate particle database with a wide range of sizes was obtained.

It should be noted that to numerically model a concrete specimen, a large number of aggregate particles with different shapes and sizes are needed. It is time-consuming to scan a massive number of aggregate particles. Hence, a mathematical representation of the real shape of aggregates is vital so that varying the parameters, different shapes and sizes can be generated.

Using spherical harmonics, the scanned aggregate surfaces can be mathematically represented, and this method can be used to regenerate new aggregates with realistic aggregate shapes and sizes by adjusting the parameters of the Fourier expansion. To reconstruct the accurate aggregate shapes, SPHARM-MAT (Shen et al. 2009b) code was used. This method is further explained in the following section.

2.2 AGGREGATE GEOMETRY BY SPHERICAL HARMONICS

Spherical harmonic is an effective method of accurately representing 3D geometries based on Fourier expansion. Spherical harmonics has been used to represent and reconstruct geometries in various fields including civil engineering (Lu and Garboczi 2014; Qian et al. 2016), medical image analysis (Chung et al. 2007; Gerig et al. 2001), graphics (Bülow 2004; Funkhouser et al. 2003; Gu et al. 2003; Shen and Makedon 2006; Zhou et al. 2004), biology (McPeek et al. 2008, 2009; Shen et al. 2009a) and bioinformatics (Cai et al. 2002; Ritchie and Kemp 1999; Shen et al. 2007b).

3D spherical harmonic representation of aggregates was pioneered by Garboczi (Garboczi 2002) where aggregates were scanned by a XCT scanner and SH was used to reconstruct the aggregates. Since then, Combination of XCT and SH has been used to reconstruct many particle shapes for coarse aggregates (Erdogan et al. 2006; Thomas et al. 2016), fine aggregates (Erdoğan et al. 2017; Erdoğan et al. 2007; Lu et al. 2020; Taylor et al. 2006) cement particles (Bullard and Garboczi 2013; Erdoğan et al. 2010; Holzer et al. 2010), slag (Liu et al. 2011) etc. . Shape analysis of particles (Garboczi and Bullard 2004; Mahmoud et al. 2010), effect of aggregate shapes on concrete rheology (Erdogan 2005) and effect of aggregate shapes on damage and fracture propagation are some of the main applications of the generated aggregates using SH. Most of the previous studies (Erdogan 2005; Erdoğan et al. 2017; Erdoğan et al. 2007; Garboczi and Garboczj 2002) have used a voxel mesh resulting from the scanning to fit the SH series to the geometry. However, the proposed method in this paper using the SPHARM code can fit a SH series to voxel mesh as well as a triangular mesh. In this paper, SH series is fitted to a triangular mesh obtained using the structured light 3D scanner.

Also, most of the previous researchers have used SH to model star shaped particles only (Garboczi and Bullard 2017) and in the parameterized method used in this study which was initially proposed by Brechbuhler et al. (Brechbuhler et al. 1995) can generate non-star shaped particles compared to the conventional spherical harmonic method (Ballard and Brown 1982). Hence, particles with overhanging protrusions can be modelled using this method and this is important to obtain the accurate geometries for mesoscale simulations.

Three steps are needed to obtain a spherical harmonics shape description of the input mesh (Shen et al. 2009d). Those are 1) Spherical parameterization 2) Spherical harmonic expansion and 3) Spherical harmonic alignment.

2.2.1 Spherical Harmonic Parameterization

The first step is to parameterize the input shape using the spherical parameterization. In this step, a uniform and continuous bijective mapping was created from the object surface to the surface of a unit sphere so that every vertex v in the input mesh is assigned to a pair of spherical coordinates (θ,φ) in the unit sphere (Shen et al. 2009c, 2017).

$$v(\theta,\varphi)=(x(\theta,\varphi),y(\theta,\varphi),z(\theta,\varphi))^T \tag{1}$$

Spherical coordinates (θ,φ) convention as shown in ***Fig. 6*** is used in this parameterization process. In this coordinate system, θ is taken as the colatitudinal coordinate and φ is taken as the longitudinal coordinate. Here, θ is in the range of $[0, \pi]$ and φ is in the range of $[0, 2\pi)$.

When this bijective mapping of each vertex of input mesh to the unit sphere is done, distortions of the length, angles, and the areas of the triangles can occur. However, these distortions need to be minimized for a good mapping. Three types of mappings are there to minimize these distortions (Shen and Makedon 2006). Those are 1) isometric mapping where the length of the arc in the input mesh and the unit sphere is equal 2) conformal mapping where the angles between a pair of intersecting arcs in the input mesh is the same as that of the unit sphere 3) equiareal mapping where each part on the input mesh is mapped on to the unit sphere with the same area.

In the SPARM-MAT code, an equiareal mapping algorithm proposed by Shen and Makedon (Shen and Makedon 2006) called CALD (Control of Area and Length Distortions) has been used. This algorithm attempts to minimize the area distortions when the bijective mapping is done at the same time attempting to minimize the length distortions (Shen and Makedon 2006). This algorithm consists of mainly three steps. The first step is the initial parameterization step where each vertex of the input triangular mesh is mapped on to a unit sphere. This step is an extension of the method proposed by Brechbuhler et al. (Brechbuhler et al. 1995) to a triangular mesh. In the initial mapping of the mesh to the unit sphere, north pole ($\theta = 0$) and the south pole ($\theta = \pi$) of the sphere are selected as two vertices such that their projections to the principle axis of the scanned aggregate are furthest apart. Then, in the next step, two systems of equations are solved to obtain the colatitudinal coordinates (θ) and the longitudinal coordinates (φ) for the all the mesh vertices (Shen and Makedon 2006).

After the initial parameterization, global mesh smoothing, and local mesh smoothing steps were initiated to improve the parameterization quality. Using the CALD algorithm a mapping with high quality can be achieved. It should be noted the above-mentioned mapping is only applicable to genus-zero objects. Aggregates are genus zero objects and hence aggregates surface mesh can be mapped using this method. A mapping of a scanned aggregate particle to a unit sphere using the CALD algorithm is shown in ***Fig. 7***.

2.2.2 Spherical Harmonic Expansion

The second step is the spherical harmonic expansion where the input mesh surface is expanded into a complete set of spherical harmonic basis functions Y_m^l. If x, y and z are Cartesian input mesh coordinates and θ and φ are polar coordinates in the parameter space, above parameterization process will result in three explicit functions $x(\theta,\varphi), y(\theta,\varphi)$, and $z(\theta,\varphi)$ which describe the input mesh surface. These three explicit functions can be described using Fourier spherical harmonic functions as given in Equations *(2)*, *(3)* and *(4)*.

$$x(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lx}^{m} Y_l^m(\theta,\varphi) \quad (2)$$

$$y(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{ly}^{m} Y_l^m(\theta,\varphi) \quad (3)$$

$$z(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{lz}^{m} Y_l^m(\theta,\varphi) \quad (4)$$

Above three equations can be combined into one equation as given in Equation *(5)*.

$$v(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{l}^{m} Y_l^m(\theta,\varphi) \quad (5)$$

where $v(\theta,\varphi) = (x(\theta,\varphi), y(\theta,\varphi), z(\theta,\varphi))^T$ and $c_l^m = (c_{xl}^m, c_{yl}^m, c_{zl}^m)^T$. In the above equations c_l^m are the Fourier coefficients and $Y_l^m(\theta,\varphi)$ is the spherical harmonic basis function which is given by Equation *(*6).

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\varphi} \quad (6)$$

where $P_l^m(\cos\theta)$ are the associated Legendre polynomials. In these basis functions, spherical harmonic degree is denoted by *l* and order is denoted by *m*. Hierarchy of the spherical harmonic functions can be depicted using ***Fig. 8***. Zero-degree spherical harmonic is represented by a sphere and higher degree harmonics represent a distortion of the shape.

The ultimate objective is to calculate the Fourier coefficients $c_l^m = (c_{xl}^m, c_{yl}^m, c_{zl}^m)^T$ to a user-specified maximum degree. These Fourier coefficients will determine the shape of the regenerated aggregate particles and these coefficients can be complex numbers. These Fourier coefficients c_l^m can be solved using standard least-squares estimation. The process of obtaining these Fourier coefficients are described below by taking $x(\theta,\varphi)$ as an example.

If the functional values for an input spherical function $x(\theta,\varphi)$ are given by $x_i = x(\theta_i,\varphi_i)$ for $1 \leq i \leq n$ where n is the number of points, a linear system as given in Equation *(7)* can be developed according to Equation *(2)*.

$$\begin{pmatrix} y_{1,1} & y_{1,2} & y_{1,3} & \cdots & y_{1,k} \\ y_{2,1} & y_{2,2} & y_{2,3} & \cdots & y_{2,k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ y_{n,1} & y_{n,2} & y_{n,3} & \cdots & y_{n,k} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \\ a_k \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} \tag{7}$$

In the above linear system, $y_{i,j} = Y_l^m(\theta_i, \varphi_i)$, $j = l^2 + l + m + 1$ and $k = (L_{max} + 1)^2$. Unique index j is assigned for each pair of (l, m). For almost all the scenario $k < n$ and hence the above linear system can be solved using least square fitting. For example, in this study the simplified mesh of the scanned aggregates had around 100,000 vertices (i.e. n=100,000) and the maximum degree considered was 30 ($L_{max} = 30$). So, k =961 and k < n, and hence the linear system could be solved using least square fitting. study Hence, $(a_1, a_2, a_3, \dots, a_n)^T$ can be obtained and these are estimates for the original coefficients c_{lx}^m and using these coefficients the geometry can be reconstructed according to the following equation.

$$\check{x}(\theta, \varphi) = \sum_{l=0}^{L_{max}} \sum_{m=-l}^{l} \check{c}_{lx}^m Y_l^m(\theta, \varphi) \approx x(\theta, \varphi) \tag{8}$$

From spherical harmonic expansion using the estimated coefficients, x, y, z coordinates of the regenerated aggregate particle can be obtained and using Matlab, the mesh can be generated using the triangular elements once the coordinates of the regenerated particle is known.

When a higher number of degree is specified (i.e. L_{max} is increased) geometry reconstruction is more accurate. In terms of the coefficients, the absolute value of the coefficients decreases when the number of degrees increases implying that when the number of degrees increases, the geometry converges to the actual geometry. Matlab data files for these coefficients for different degrees are attached in the supplementary materials. The same procedure is applied to obtain coefficients $\check{c}_{ly}^m$ and $\check{c}_{lz}^m$ and these coefficients are used to reconstruct the geometry in 3D.

2.2.3 Spherical Harmonic Alignment

The third step of the process is spherical harmonic alignment. In this step, the reconstructed object is placed into a common reference system as the original scanned object mesh. This is beneficial when comparing the reconstructed surface and the original scanned surface (Shen et al. 2007a). However, this is not discussed in this paper in detail because when mesoscale model is generated, a random rotation is assigned to the reconstructed aggregate shapes when aggregate is placed and hence this step is not essential.

2.2.4 Case Study of Reconstruction of Aggregate Geometry

Spherical harmonic reconstruction of a scanned aggregate particle is shown in ***Fig. 9***. When the spherical harmonic degree was increased, a more accurate geometry could be obtained. It should be noted that, if the number of degrees is L then the number of coefficients in the spherical harmonic expansion is $(L+1)^2$. Hence, the computation time increases when the number of degrees is increased. It could be observed that the number of degrees around 30 can accurately represent the geometry of the aggregates.

2.3 PLACING ALGORITHMS FOR SCANNED AGGREGATES

In this section, a placing algorithm is proposed to develop the mesoscale aggregate distribution using the scanned aggregates or the reconstructed aggregates using the spherical harmonics. Previous researchers have used various algorithms to distribute the aggregates inside the bounding geometry as reviewed in (Thilakarathna et al. 2020b). However, most of the algorithms are for parameterized aggregate shapes such as spheres (Shahbeyk et al. 2011; Wriggers and Moftah 2006), ellipsoids (Häfner et al. 2003), convex polyhedrons (Zhou et al. 2017) etc. and placing algorithms for scanned particles with realistic shapes are not yet established properly. Qian et al. (Qian et al. 2016) proposed an algorithm to distribute star-shaped particles with realistic aggregate geometry obtained using XCT and the intersection checking algorithm in that study was based on solving contact equations. However, the proposed algorithm in this paper uses a different particle intersection checking algorithm based on the face-vertex data of the mesh and hence can be used to generate aggregate packing assemblies with non-star shaped particles and particle shapes where the parameterized equation is unknown.

A database of aggregates was created using the scanned aggregates. Polygon number of the scanned aggregates were reduced before generating the aggregate filled cylinder to reduce the computational demand. This database consists of 52 scanned aggregate particles with diameters spanning from 6mm to 25mm and some of the aggregate sizes are shown in ***Fig. 10***. Some of the aggregates were scaled to ensure that there is a wide range of diameters within the database. This scaling and polygon reduction procedure was implemented in meshlab software (Cignoni et al. 2008).

Aggregates were distributed inside a cylinder with a radius of 50mm and a height of 200mm in this scenario. Any type of geometry such as a cylinder, cube etc. can be selected as the bounding geometry. Following three conditions were satisfied when aggregates were distributed inside the cylinder.

- Placed aggregates should be completely inside the bounding cylinder
- There should not be any overlaps between placed aggregate particles
- There should be a minimum distance between two aggregate particles to represent the coating of mortar in between aggregate particles

Aggregate distribution process was carried out according to a Particle Size Distribution (PSD) curve. In this investigation, Fuller's particle size distribution curve (W.B. and S.E. 1907) was used. Fuller's curve is widely regarded as the grading curve which gives the optimum compaction, density and strength in concrete and also a good workability and a good segregation resistance (Wriggers and Moftah 2006) and hence it has been used by many researchers to develop aggregate assemblies for mesoscale models (Zhang et al. 2019a, 2017).

Aggregate percentage by weight passing through a sieve diameter D according to the Fuller's curve can be calculated from Equation *(9)*.

$$Y = 100\left(\frac{D}{D_{max}}\right)^{\mathrm{n}} \tag{9}$$

In the above equation, D_{max} is the diameter of the largest aggregate and Y is the percentage of aggregate by weight passing through a sieve with diameter D aperture and n is a constant parameter generally between 0.45 and 0.7 (Sheng et al. 2016). In this paper, n was taken to be 0.5.

Volume of the aggregates within a grading segment between the sieve diameters d_s and d_{s+1} is given by Equation (10).

$$V_p[d_s, d_{s+1}] = \left(\frac{P(d_s) - P(d_{s+1})}{P(d_{max}) - P(d_{min})}\right) \times v_p \times V \tag{10}$$

where, $V_p[d_s, d_{s+1}]$ is the volume of aggregate within the grading segment $[d_s, d_{s+1}]$, d is the sieve diameter, d_{max} and d_{min} are the largest and smallest sieve diameter v_p is the volume fraction of aggregates and V is the total volume of the concrete.

The above-mentioned aggregate database consists of .stl files and face-vertex information of all the aggregates in the database were read and stored. While reading the face-vertex information of the aggregate particles, the minimum bounding box of the aggregate particle in 3D was determined using the vertices of the aggregate particle as shown in ***Fig. 11***. In this scenario, it is assumed that a particle passes through a sieve with a diameter D if the second-largest length of the bounding box (L) is less than D. After reading all the aggregates in the database, those aggregates were sorted according to dimension L.

Aggregate distribution inside the cylinder was done until a required volume fraction is achieved. However, it should be noted that due to the large number of polygons in the scanned aggregates, the time to generate the aggregate filled geometry will be increased with the increasing volume fraction.

Sieve diameters were specified, and Fuller's PSD was used in this scenario to calculate the volume of aggregates within each sieve segment. Aggregates in the database were then classified into the sieving sections and number of aggregates in each grading segment was calculated using the previously read data.

Then, the aggregates were randomly distributed from the largest particle to the smallest particle. Efficiency of the algorithm increases when the distribution is carried out from the largest particle to the smallest particle rather than selecting a random particle within the grading segment. Random position inside the cylinder was selected by first selecting a point on the vertical axis of the cylinder as the z coordinate and then randomly generating a radius and a rotating angle to define the x and y coordinates. Bounds of the x, y and z coordinated were decided so the aggregate is completely inside the cylinder by considering the largest length of the aggregate bounding box.

Aggregates were placed randomly until the calculated volume of each grading segment is achieved. This was done by calculating the enclosed volume of the selected aggregate mesh and reducing that volume from the required volume of that grading segment until the volume left is smaller than any aggregate particle within that grading segment. In that scenario, the volume left was transferred to the next grading segment and the process was repeated for the next grading segment. It should be ensured that there are enough aggregate particles in the database within a particular grading segment to achieve the calculated volume of the particles within that grading segment. However, if the number of particles is not sufficient, the same set of particles within the same grading segment were repeated.

Placing of the aggregates are done one after another sequentially. When placing the aggregates, first the aggregate was placed at the origin of the cylinder. Then this aggregate was rotated randomly around its centroid so that each placing aggregate has different orientations. Then this aggregate is translated to the random location which was determined initially. All these rotations and translations are done using matrix operations to the coordinates of the mesh.

This rotation was done using Euler's rotation theorem as shown in ***Fig. 12***. First rotation is by an angle of α around z-axis, second rotation is by an angle of β around former x-axis and the third rotation is by an angle of γ around Z' axis.

The rotation matrices corresponding to these three rotations can be specified as in Equations *(11)*, *(12)* and *(13)*.

$$Z(\alpha) = \begin{bmatrix} \cos\alpha & -\sin\alpha & 0 & 0 \\ \sin\alpha & \cos\alpha & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{11}$$

$$N(\beta) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\beta & -\sin\beta & 0 \\ 0 & \sin\beta & \cos\beta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{12}$$

$$Z'(\gamma) = \begin{bmatrix} \cos\gamma & -\sin\gamma & 0 & 0 \\ \sin\gamma & \cos\gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{13}$$

Hence, the combined rotation matrix can be specified as,

$$R = Z(\alpha)N(\beta)Z'(\gamma) \tag{14}$$

The coordinates of the nodes after rotating the particle can be obtained by *(15)*.

$$X_2 = RX_1 \tag{15}$$

Where X_2 is the coordinates after rotation, R is the rotation matrix and X_1 is the coordinates before the rotation. α, β and γ are randomly selected using a random number k using Equations *(16)*, *(17)* and *(18)*.

$$\alpha = k * 2 * \pi \tag{16}$$

$$\beta = k * \pi \tag{17}$$

$$\gamma = k * 2 * \pi \tag{18}$$

After rotating the aggregate, it was translated to the randomly selected location using the translation matrix given in *(19)*.

$$T = \begin{bmatrix} 1 & 0 & 0 & D_x \\ 0 & 1 & 0 & D_y \\ 0 & 0 & 1 & D_z \\ 0 & 0 & 0 & 1 \end{bmatrix} \qquad (19)$$

where, D_x, D_y, and D_z represent the displacements in x, y, and z directions respectively.

First aggregate was placed randomly inside the cylinder using the procedure described above and from the second aggregate onwards, intersection check between aggregates were checked to ensure that there will be no overlap between aggregate particles as well as there is a sufficient gap between aggregates to represent the mortar. For this intersection check, two-step procedure was followed.

First, the minimum bounding spheres of the aggregates were calculated using the vertices and then the intersection check was carried out by checking whether the sum of the two radii of the bounding spheres is less than the distance between the two centroids of the bounding spheres using Equation (20*)*.

$$\sqrt{(x_A - x_B)^2 + (y_A - y_B)^2 + (z_A - z_B)^2} \geq 1.1 \times [r_A + r_B] \qquad (20)$$

where x_A, y_A, z_A and x_B, y_B, z_B are the coordinates of the centers of the bounding spheres of aggregates A and B and r_A and r_B are the radii of the bounding spheres of aggregates A and B. It should be noted that a factor of 1.1 was used to multiply with the sum of radii of the bounding spheres to ensure that there is a sufficient gap in-between aggregates to represent the mortar. Allocating this gap is helpful when meshing the mortar phase in the meso scale model when finite element analysis is carried out and it should be noted that in reality the actual gap between the aggregates might be less than this. If the bounding spheres do not intersect with each other, the aggregates inside the bounding spheres will not intersect. Hence, if this criterion is satisfied for all the previously placed aggregates, then the aggregate is placed inside the cylinder. However, if that criterion is not satisfied, a further check is needed to check whether the aggregates inside the bounding spheres intersect with each other.

In the second step, first, it was checked whether the distance between the centroids of the bounding spheres of the aggregates is greater than the radius of the larger particle and if this condition was satisfied, the algorithm was proceeded to check whether the vertices of the two aggregates are inside the other aggregate. When this check was carried out, new aggregate was expanded by multiplying the vertices by a factor as shown in ***Fig. 13*** to ensure that there will be a sufficient gap between the aggregates to represent the mortar.

All the nodes in one aggregate were checked to see whether any of the vertices of one aggregate is inside the other aggregate. If any of the vertices is inside the other aggregate, two aggregates intersect with each other and the new aggregate position is discarded, and a new random position is sought. To check whether a vertex is inside the aggregate, rays were emanated from the all the vertices of one aggregate in X, Y and Z directions as shown in ***Fig. 14***. Since all the scanned aggregates are watertight geometries, if the checking node is inside the aggregate, number of intersections of the passing rays with the facets of the aggregates should be an even number (Patil and Ravi 2005). Also, the edge to tri mesh surface intersection check was carried out additionally using the algorithm proposed by Sunday (Sunday n.d.) to ensure that there will be no edge to face intersection.

After checking for the intersection of the new aggregate with the previously placed aggregates, new aggregate was placed in that position if it does not intersect with any of the previously placed aggregate particles. This process was repeated until the required volume fraction is achieved. Around 200 particles were needed to achieve 25% volume fraction and this test took few hours to complete. Generated aggregate assemblies inside a cylinder are shown in ***Fig. 15***.

2.4 SPHERICAL AND ELLIPSOIDAL PARTICLES

Parametric surfaces can also be used to generate aggregate particles instead of scanning the particles or reconstructing it. Real aggregate particles can be in various shapes and these shapes are represented using parameter-based equations.

Spherical (Gal et al. 2008; Li et al. 2016, 2019; Shahbeyk et al. 2011; Xu and Chen 2016) and ellipsoidal (Liu et al. 2014; Unger and Eckardt 2011; Xu and Chen 2012) particle shapes have been widely used by researchers due to the simplicity. However, generation of placing algorithms of these particles are well established and hence those are not discussed in this paper. Some of the generated spherical and ellipsoidal particles are shown in ***Fig. 16***.

2.5 POLYHEDRAL AGGREGATES GENERATION AND PLACEMENT

Convex polyhedrons can be used to represent the geometry of the crushed aggregates in mesoscale concrete models. In a convex polyhedron, a line connecting any two vertices of the polyhedron always lies in the interior of the polyhedron. A novel three-step procedure was proposed to check the intersection and place the polyhedral particles in this paper.

First, the aggregates were distributed randomly according to Fuller's curve. It was assumed that a polyhedral particle belongs to the grading segment of [d_s, d_{s+1}] if the diameter of the bounding sphere of the aggregate is less than the aperture of the sieve with diameter d_s and larger than the aperture of the sieve with diameter d_{s+1}. Spheres were generated according to the PSD and polyhedral particles were generated by randomly selecting 20 points on the surface of the spheres as the vertices of the polyhedrons so that the spheres would be circumscribed spheres of the polyhedrons. These vertices were selected so that the center of the circumscribed sphere is contained inside the polyhedron.

Three-step procedure was followed to check the intersection of the polyhedron aggregates. First, the intersection of the bounding spheres was checked. This check was carried out by checking whether the distance between the two aggregate particles is less than the sum of the radii of the bounding spheres. If the bounding spheres do not intersect, the aggregate particles also do not intersect and if the bounding spheres intersect with each other, a further check was done to investigate whether the polyhedrons would intersect.

In the second step, it was checked whether the distance between the two centers of the bounding spheres is greater than the radius of the larger particle. If this condition is not satisfied, then a new location for the placing aggregate is sought. If this condition is satisfied, then the third condition was checked.

The third condition was checked by checking the distance of nodes of one aggregate with respect to the triangular surfaces of the other aggregates. Normal vectors to the triangular faces were calculated by taking the cross product between the edge vectors and by convention, the surface normals are presumed to be pointed outwards from the aggregates. Equation of triangular mesh planes can be denoted by the following Equation *(21)*.

$$Ax + By + Cz + D = 0 \tag{21}$$

where A, B, C and D are the constant coefficients of the plane depending on the location and the orientation of the plane and x, y, z are the coordinates of any point lying in the plane.

If the above equation is not satisfied by a point in the space, then that point is either inside or outside depending on the sign of the distance to the point. In this scenario, nodes of one polyhedron are checked against all the triangular surfaces of the other expanded polyhedron to check whether those points are inside the polyhedron. This check was repeated by interchanging the nodes to the polyhedron and polyhedron to the nodes as shown in ***Fig. 17***. Also, edge to tri mesh surface intersection check was carried out additionally using the algorithm proposed by Sunday (Sunday n.d.) to ensure that there will be no edge to face intersection.

After the intersection check was done, the new aggregate was placed inside the cylinder if it does not intersect with previously placed particles and this process was repeated until the required volume fraction is achieved.

Generated aggregate assemblies using polyhedron particles inside a cylinder is shown in ***Fig. 18***. Using this new algorithm, polyhedral aggregate volume fractions up to 40% can be generated.

This volume fraction is sufficient to simulate mesoscale concrete in most of the general cases and if very high aggregate volume fractions are needed for specific investigations, polyhedral aggregate generation method proposed by Zhang et al. (Zhang et al. 2018a, 2019c; b) can be used.

It should be noted that, since the random points on the surface of the sphere are selected as the vertices of the polyhedron, generated aggregate particles generally have equal dimensions in each three directions. However, flaky aggregates and elongated aggregates can also be generated by scaling the generated aggregate along a dimension. Aggregates can be identified as flaky aggregates if the least dimension of the aggregate (thickness) is less than 0.6 times the mean sieve size of the aggregate grading segment and aggregates are elongated if the largest dimension of the aggregate is greater than 1.8 times the mean sieve size of the aggregate grading segment (Kwan et al. 1999). Generation of an elongated and a flaky aggregate using the same aggregate is shown in ***Fig. 19***.

2.6 TRANSFERRING GEOMETRY TO FINITE ELEMENT PROGRAM

All the above discussed parameterized geometries were generated using MATLAB. These meshes are surface meshes with a set of vertices and faces. However, for finite element analysis of mesoscale concrete model, a solid mesh is needed and transferring surface mesh into solid mesh is a challenge. This section discusses effective methods to obtain a solid model using the surface meshes developed in MATLAB.

Geometry information from the MATLAB can be saved and then using another program, solid geometries can be generated. Most of the finite element software have the capability of generating simple shapes like spheres using inbuilt functions. For example, in spherical aggregate assemblies, center coordinates and diameters of the particles were saved and using this information solid spheres were generated to obtain the solid aggregate assemblies.

Another method is to save the face-vertex information from MATLAB and generate a solid mesh from bottom up using finite element programs. It should be noted that when placing the aggregates using previously discussed algorithms, for each aggregate vertex numbers start from 1 and the faces are defined according to these vertex numbers as shown in ***Fig. 20*** (a). However, to generate the full assembly of the aggregates, these nodes should be renumbered as shown in ***Fig. 20*** (b) depending on the number of vertices on each aggregate and then the faces should be defined using these renumbered vertices. Then this can be saved, and a bottom-up geometry can be generated in the finite element software.

Another method is to write these face vertex information directly to a standard mesh file such as *.stl* and *.ply* directly from MATLAB. However, these mesh files will be surface meshes and by using third-party software such as Ansys Spaceclaim and Freecad, these surface meshes can be volumized. When volumizing these surfaces meshes, errors can be occurred due to band mesh quality or defects in the surface meshes. In that case, the surface meshes need to be preprocessed before volumizing is carried out.

3 DISCUSSION

Aggregate shape, volume fraction and the distribution are important aspects of concrete and these aspects will affect the macroscopic behavior of concrete including fracture and damage initiation and propagation, strength in compression and tension, fracture energy of the concrete etc. Also, shape and the size of the interfacial transition zone (ITZ) will also depend on the aggregate shapes. ITZ has been found to be one critical aspect in concrete where the damage initiates and progresses and to accurately model the shape and volume of the ITZ, accurate shape of the aggregates is vital. 3D scanning of the aggregates as well as the spherical harmonic geometry reconstruction algorithm combined with the proposed aggregate distribution algorithm can be used in this scenario to accurately represent the aggregate geometry.

Different algorithms for placing different aggregate shapes were discussed in this paper and the efficiency of these algorithms depends on the aggregate shape, PSD, required volume fraction and volume of the bounding geometry. It was found that when the number of polygon count is higher in an aggregate, more time will be consumed to check the intersection of the aggregates and hence more time is needed to achieve a given volume fraction. However, it should be noted that too much reduction of polygon numbers will result in failure to capture important geometric features of the particles. Hence, a compromise is required to reduce the generation time while the important features of the geometry are present.

Aggregate volume fractions up to 40% can be achieved for polyhedral aggregate particles and up to 30% can be achieved for scanned aggregates. It should be noted that this is due to the increase of running time due to the complexity of the mesh of the aggregates with higher polygon number. Also, the volume fraction depends on the PSD and the sieve sizes as well. Higher volume fractions can be achieved when the PSD curve has a higher percentage of aggregates with small diameter because the packing and search for a location for the placing can be efficiently carried out.

According to AS 2758.1 (Standards Australia 2014), the flakiness index of the aggregates used in the concrete should not exceed 35% and using this algorithm, any specified percentage of flakiness index and elongation index can be achieved.

4 SUMMARY AND CONCLUSIONS

Aggregate generation is an important aspect for mesoscale modelling of concrete. In this paper, aggregates with various shapes were generated inside a cylinder and these aggregates were distributed without any overlap to achieve a realistic volume fraction. A novel method was proposed to scan aggregates with a 3D structured light scanner and distribute those aggregates inside a cylinder by creating a real aggregate shape database in 3D. Spherical harmonics-based parameterization method was proposed to reconstruct these actual aggregate geometries using parameters. Also, parametric aggregate shape generation for polyhedral shapes was discussed with an efficient placing algorithm. Following conclusions can be derived from this investigation.

- Accurate geometrical models of aggregates can be obtained using a 3D structured light scanner and this method is faster and convenient compared with the XCT scanning method.
- Mesh simplification should be carried out for the scanned aggregates because the scanned object mesh density is very high and after this simplification important features of the aggregate geometry should prevail.
- Accurate scanned geometry can be reconstructed using spherical harmonics based parametric method and various aggregate shapes can be generated by changing the parameters of the Fourier expansion.
- Crushed aggregate shapes can be accurately represented using convex polyhedrons and using the proposed algorithm aggregate volume fractions up to 40% can be obtained. Flaky and elongated particles can be generated by the proposed method for specific applications.
- Various methods can be obtained to transfer the surface geometries to finite element analysis software where solid geometries are used and errors when volumizing can be mitigated by improving the mesh quality.

5 Data Availability Statement

Some or all data, models, or code generated or used during the study are available in a repository or online in accordance with funder data retention policies. (Thilakarathna, S. (2020), “3D Scanned Aggregates ”, Mendeley Data, v1 http://dx.doi.org/10.17632/x5dbx8yxdw.1)

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