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Original Research Paper

# Computer simulation-based method to predict packing density of aggregates mixture

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ABSTRACT

A key theory in concrete mix design is maximizing aggregate packing density (PD) of aggregate mixture. Different methods have been presented by researchers to estimate PD of aggregate mixture. One such method is computer simulation that has become increasingly common over the last decade; however, it is usually a time-consuming procedure. In the current study, a method based on computer simulation is proposed for estimating aggregate PD. In this method, aggregates with specific shapes, grading and PDs are substituted by monosized spherical aggregates. An equation is also presented for determining the diameter of equivalent monosized aggregates. The coefficient of friction between the equivalent monosized aggregates is determined in a way that the monosized aggregates will have a PD equal to that of actual aggregates. The proposed method is also used to simulate laboratory experiments conducted by the present authors and other researchers. Comparisons reveal the high accuracy of the proposed simple method in predicting the PD of aggregate mixtures.



## 1. Introduction

Particle packing density is an important factor affecting the behavior of composite materials produced in the different ceramics, concrete, asphalt and aluminum industries. Almost all research efforts in the field of concrete technology over the past century have been concentrated on obtaining proper aggregate proportions with minimal voids but with maximal packing density. This is especially advantageous because if aggregate blends of high packing density (PD) are achieved in concrete, the voids among the aggregates will then need only small amounts of paste, which makes the resulting concrete less expensive with few durability problems. Maximized PD of an aggregate mixture is, therefore, the key to desirable concrete mix designs [1–16]. A lot of research work has been accordingly devoted to the development of concrete mix designs based on minimized voids [4–6].

Aggregate features of great significance to their PD are grading and shape. Over the past couple of decades, many research efforts have been focused on determining the relationship between aggregate mixture PD and individual aggregate characteristics. However, while a lot of attention has been paid to aggregate grading, few studies have investigated the effect of aggregate shape on mixture PD. Three general approaches to the estimation of aggregate mixture packing density have been adopted in the studies conducted in this area:

(a) Using lab tests to develop optimized grading curves for each aggregate size range and aggregate mixture [8–12];
(b) Developing numerical models based on experimental results [3,5–7]; and
(c) Computer simulations [17–33].

## 2. Computer simulation

Advances in computer technology have encouraged researchers to explore the potentials of computer simulation for solving packing density problems. Simulations have been used to study aggregate arrangement and movement in containers and the interactions among them. Our literature review revealed that either of the following two methods are typically used for aggregate arrangement: (1) Ordered packing, in which aggregates are arranged in a manner to achieve maximum packing density [17–20]; and (2) Random packing, in which aggregates are

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randomly deployed in the container. Various versions of this method have been reported in the literature [21–25,27–31].

One of the following three approaches has been typically adopted in the literature to solving the equations of motion in packing problems with aggregates arranged by either of the ordered or random packing methods. The first, called the static approach, involves calculating the PD of aggregate arrangement so as to allow no movement of aggregates in the container while they still exert forces on each other. In the second, known as the semi-dynamic approach, each aggregate in the set of arranged aggregates is considered to be able to move under its own weight until stopped upon colliding with other aggregates [23]. In the third dynamic approach, aggregates are considered to be able to move under their own weight and to exert forces on each other upon collision. The discrete element method (DEM) is usually used for solving the equations of motion under the dynamic approach. Originally proposed by Cundall and Strack [34] for rock mechanics problems, this method differs from the finite element and finite difference methods in that it handles both the motion and rotation of particles [32,33].

In DEM, the second law of Newton and the force–displacement law are used alternatively. While the former is used to determine the motion of each particle due to the contact and body forces acting upon it, the latter updates the contact forces due to the relative motion at each contact. A time-stepping algorithm is used to solve the equation of motion that requires the iterative application of the law of motion to each particle and the force–displacement law to each contact. The set of contacts is updated at the onset of each time step from the known particle and wall positions of the container. This is followed by the application of the force–displacement law to each contact in order for the contact forces to be updated based on the relative motion between the two entities in contact and the contact constitutive model. The law of motion is finally applied to each particle and its velocity and position are updated based on the force due to the contact forces and any other forces acting on the particle. This stage needs in the onset of next time step. The cycle is repeated until a state is reached in which the differences between the forces or the coordinates relative to those of the previous step reduce to user-specified values.

Aggregates poured in the container collide with each other and exert forces on each other. At contact pint, normal force, $F^n$, and shear force, $F^s$, is developed. Using a friction coefficient, $\mu$, for that occurring between particles, Eq. (1) is employed to determine the relationship between the maximum shear force, $F^s_{max}$, and the normal force, $F^n$, between each two particles. The two aggregates will slip on each other when $F^s$ is greater than $F^s_{max}$ before an equilibrium is reached; i.e., $F^s = F^s_{max}$. The details of the algorithm used for calculating PD is reported in Ref. [29]. When two aggregates with different friction coefficient are in contact, the coefficient used for the slip calculation is the minimum of the two friction coefficients [35].

The friction coefficient between particles is an important parameter in DEM with significant effects on the packing density of aggregates [28–31]. Increasing friction coefficient between particles leads to enhanced frictional forces between them, which restricts their movement and rearrangement and, thereby decreasing their PD [28–31].

$$F^s_{max} = \mu F^n_i \quad (1)$$

Majidi et al. used DEM to simulate vibrated packing density of particles in their real shapes [30]. They also employed the PFC$^{3D}$ software [35] for both modeling the particles and solving the DEM equations. The friction coefficient of aggregates in the DEM model was estimated using the angle of repose test performed on aggregates both experimentally and by computer simulation. The friction coefficient between particles was calibrated in such a way that the angle of repose matched that obtained experimentally. The friction coefficient between particles and wall was adjusted in a way that the particles slip happens at the same angle as experimentally recorded. The results obtained showed that computer simulation was capable of estimating the vibrated bulk packing density (VBD) of aggregates. Moreover, aggregate shape was found to have a clear effect on the PD of particles. Increasing particle sphericity was also found to increase particle PD such that particles with a lower sphericity exhibited an enhanced rate of increase in VBD with decreasing friction coefficient. Thus, sphericity is capable of augmenting the effect of friction coefficient on VBD [30].

Modeling of aggregates in their actual shapes is a time-consuming and tedious procedure. Mostofinejad and Reisi developed a method in which aggregate could be modeled as spherical objects with their actual grading in the container [29]. In order to consider effect of aggregate shape in PD, an appropriate friction coefficient was selected for graded aggregate. Packing density test was used to calibrate friction coefficient. Packing density test was performed both experimentally and by simulation [29]. In this process, the friction coefficient between aggregates was selected in a way that the simulation PD measurement would be minimally different from the experimentally measured one. To verify the accuracy of the proposed method, the friction coefficient of each of six especially selected aggregates with different grading and shapes was determined using the method. Finally, simulated and experimental packing densities were determined for a mixture of two aggregates based on the calculated friction coefficient. Results indicated the high accuracy of the proposed method in predicting aggregate packing density. In sum, the results indicate that the aggregates can be considered as spherical in shape with appropriate coefficients of friction assigned to them. The friction coefficient accounts not only for the shape of the aggregates but also for the forces acting between them. Shen and Yu also reported that in order to consider effect of shape of aggregate in PD, it is possible to assign a suitable friction coefficient to each aggregate [27].

## 3. Research plan

### 3.1. Methodology

Using computer simulations to calculate the packing density of an aggregate mixture is a time-consuming procedure and sometimes the running time for each calculation takes more than a week. The situation becomes practically impossible with aggregate sizes in the range of 0–5 mm. It is, therefore, practically necessary to develop simple methods based on the results obtained from computer simulations capable of accurately predicting aggregate mixture PD over reasonable times.

It is, therefore, the objective of the current study to develop such a simple and accurate method drawing upon computer simulations using the PFC$^{3D}$ software.

#### 3.1.1. Substitution of graded aggregate with monosized spherical aggregate

In the proposed method, aggregates are modeled as spherical objects and each aggregate with specified grading and PD is substituted with a monosized aggregate so that the monosized aggregate will have a PD equivalent to that of the actual aggregate. In their numerical modeling, Dewar [6] and Golterman et al. [7] also took advantage of substituting graded aggregates to monosized ones.

In the proposed method, to determine equalized diameter for each graded aggregate, aggregates are poured on sieves and graded. The sieves are numbered from 1 to $n$, moving from the

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