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A simple method for determining sphere packed bed radial porosity

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ABSTRACT

A new and simple method is established to examine the radial porosity profile of mono-sized spheres in packed bed cylinders based on the sphere center coordinates. The method is derived from geometrical and analytical techniques and uses arc lengths to calculate the radial porosity profile at any given axial position, a given interval axial position, or the total axial position, thus evaluating the local, interval, or axially averaged radial porosity profile, respectively. The new method and analytical functions are simple and straightforward and provide an accurate representation of the radial porosity profile given the sphere center coordinates. The simple method is used to calculate the radial porosity profile for the fixed packing of identical spheres in cylindrical containers with $D/d \geq 1.0$. The evaluated results for the radial porosity profile are benchmarked with existing analytical equations and available experimental and numerical data, respectively, for mono-sized spheres in cylindrical containers. A concise FORTRAN program for the new arc length-based technique is presented for this simple method for calculating radial porosity profiles.

1. Introduction

Fixed packed bed structural properties of spherical and non-spherical particles have been widely examined for cylindrical containers. Both experimental and theoretical studies in support of transport modeling require a detailed description of the void space in the fixed packed bed structure. "The structures generated by tightly packed mono-sized spheres have been studied by scientists as model systems for understanding the emergence of order and crystallization or vice versa the appearance of disordered and amorphous phases in natural systems" [1]. Packed beds of spheres are particularly interesting structures for research in many contemporary scientific fields such as chemical, mechanical, and nuclear engineering, geology and geophysics, chemistry and physics. Even though the physical structure of an actual packed bed used for industrial and engineering applications may not contain spherical particles or may contain spheres with a given size and shape distribution the investigation and analysis for several centuries [1] and the large number of publications per year on the subject of packed beds of mono-sized smooth spheres for different cylinder-to-sphere diameter (D/d) ratios are measures of their utility as structural models for these and other types of packed bed systems.

Presently, to model and research fixed packed beds of spheres, numerically generated beds are obtained either by a packing algorithm [2–11] or by a dynamic simulation model [12–14]. Generally, the packing algorithm disregards the physical forces involved in the packing process and generates the packing structure by placing a sphere at a position based on a specific rule. Conversely, the dynamic simulation model is based on forces, such as gravity, friction, and contact, and uses Newton's second law to simulate the packing process. In either case, the result of the numerically generated bed is a detailed packing structure which provides the location (x, y, z center coordinates) of each sphere in the bed.

In general, one of the main structural parameters considered for fixed packed beds is the radial porosity variation, which is a characteristic quantity that is influenced by the physical connection of the particles with the container walls. The radial porosity profile consists of damped oscillations starting with large porosity values at the wall, which can be a significant component in the design and study of industrial fixed packed systems which include, for instance, chemical and nuclear pebble bed reactors, thermal solar heat exchangers, and environmental air scrubbers. In particular, mono-sized spheres in cylindrical containers are commonly used and the radial porosity variations have been investigated using a wide range of experimental methods by Roblee et al. [15], Benenati and Brosilow [16], Thadani and Peebles [17], Ridgway and Tarbuck [18], Martin [19], Cohen and Metzner [20], Goodling et al. [21], Kufner and Hofmann [22], Mueller [23], Govindarao et al. [24], Sederman et al. [25], Wang et al. [26], and Mariani et al. [27]. The accuracy of predictive fixed packing structural expressions for spheres in cylindrical containers can be assessed from these experimental packing data.

Efforts to predict the radial porosity profiles vary from entirely empirical in nature: Martin [19], Cohen and Metzner [20], Kufner and Hofmann [22], Mueller [23], de Klerk [28], and Bey and Eigenberger [29] to semi-analytical predictive expressions: Govindarao and Froment [30], Mariani et al. [31–33], and Mueller [34].

Traditionally, investigators have defined the local porosity or void fraction as the ratio of the void volume to the volume of the packing

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structure at a localized position within the packed bed. Once the particle positions are known, which can be obtained from a wide variety of methods, the local porosity can be calculated. Consequently, investigators initially developed porosity equations established on a volume-based approach. These volume-based equations characteristically are of an elliptic integral form. In the volume-based procedure, a cylindrical packed bed is divided into numerous concentric radial cylindrical volumes and the radial porosity in each volume is determined as a fraction of the void volume to the total radial cylindrical volume. Lamarche and Leroy [35] and Mueller [23] present the local radial porosity volume equation formulas for a cylindrical system with mono-sized spherical particles. Even though these void volume-based calculations are mathematically straightforward, this volume-based technique has a drawback in that elliptic integral equations must be numerically solved and the effort to solve these elliptic integral equations could be significant for extremely large fixed packed systems. In addition and more importantly, the volume-based technique provides an average value of the porosity at a radial position in the volume region that is defined. The smaller the radial cylindrical volume region the more accurate the volume-based technique becomes. Area-based porosity equations have also been presented in the form of analytical equations. In the area-based procedure, a cylindrical packed bed is divided into numerous concentric radial cylindrical surfaces and the radial porosity at each surface is determined as a fraction of the intersected void area to the total cylindrical surface area. Blum and Wilhelm [36] have proven that the mean area and volume void fractions are identically equal for packings of arbitrary cross-section for homogeneous packings. Mariani et al. [32] present area-based expressions for six geometrical quantities relating the intersection of a sphere and a cylindrical surface in terms of elliptic integrals. Mueller [34] has also recently presented the local radial porosity area-based analytical equation formulas for a cylindrical system with mono-sized spherical particles. These area-based equations for the local radial porosity greatly simplify the technique for determining the radial porosity while calculating the exact same results as the volume-based equations. It should be noted that the published volume-based and area-based methods determine the axially averaged radial porosity.

Even though meaningful advancements have been made in simplifying the procedure for calculating the radial porosity for mono-sized spherical particles in cylindrical containers for both volume-based and area-based methods, further improvements can certainly be accomplished by analyzing the particular geometry from a unique perspective. The additional simplification of the radial porosity calculation procedure will greatly enhance the computer simulation environment for investigators working in this research domain.

It is for this reason the objective of this study is to present a new and simple method for calculating the radial porosity profile for mono-sized spheres in cylindrical containers. The new method is derived from geometrical and analytical techniques and uses arc lengths to calculate the radial porosity profile. To the author's knowledge, this is the first time a length-based technique has been used to calculate the radial porosity. Given the sphere center coordinates, the presented analytical equations are easy to use and provide accurate results for the radial porosity profile. The simple arc length-based technique is used to calculate the radial porosity profile for the fixed packing of identical spheres in cylindrical containers with $D/d \geq 1.0$. The evaluated results for the radial porosity profile are benchmarked with existing analytical equations and available experimental and numerical data, respectively, for mono-sized spheres in cylindrical containers. In addition, a concise FORTRAN program is presented for the new arc length-based technique so investigators can immediately make use of this simple method.

2. Radial porosity elements

Traditionally, the local radial porosity is represented as a dimensionless packing system volumetric structural property having a mathematical value between 0 and 1. This type of volumetric analysis has been analytically derived by Mueller [23] for the axially-averaged local radial porosity of mono-sized spheres in cylindrical containers. Nevertheless, recently Mueller [34] has analytically established an area-based analysis such that the axially-averaged local radial porosity of mono-sized spheres in cylindrical containers can be obtained from the intersection of a radial cylindrical surface of radius, r, from the origin, O, with that of any sphere with a radial center position, r_p, within a particle radius, R_s, on either side of this radial cylindrical surface. This particular geometrical condition is shown in Fig. 1 for the x–y view. An analogous type of a sphere–cylinder geometrical surface interaction has also been recognized and analyzed by Mariani et al. [31] together with geometrical expressions and quantities that were defined and derived in the investigation. However, for this most recent analysis, the local radial porosity at a particular axial position, $\varepsilon_z(r)$, is defined and evaluated in terms of an arc length, s, intersecting a sphere such that $\varepsilon_z(r) = s_{void}/s_{total} = (s_{total} - s_{solid})/s_{total} = 1 - s_{solid}/s_{total}$, where s_{solid}, s_{void}, and s_{total} are the solid arc length (intersecting arc length), void arc length (non-intersecting arc length), and total arc length (total radial arc length, i.e. circumference), respectively, at the given radial distance and axial position. The local radial porosity, which is a function of the radial position, for a cylindrical packed bed system of mono-sized spheres at a specific axial position is given by:

$$\varepsilon_z(r) = 1 - \frac{s_{solid}}{s_{total}} = 1 - \sum_{n=1}^{N(R_s)} \frac{s_n(r)}{s_T(r)}, \tag{1}$$

where $N(R_s)$ is the number of sphere particles located within a sphere particle radius, R_s, on either side of the radial arc length, at a specific axial position, at the radial position, r, $s_n(r)$ is the intersecting arc length of an nth-sphere at the radial location, r, and $s_T(r)$ is the total radial arc length at a radial location, r, and is easily found to be $2\pi r$.

The intersecting arc length of an nth-sphere, $s_n(r)$ at a specific axial location, z, and at the radial location, r, is shown in Fig. 1 and in Fig. 2 as the arc length, s. This arc length can be analytically determined exactly from one principal equation for all intersecting geometries that arise in a packed bed regardless of the location of the sphere and the axial–radial arc length intersection. The principal analytical equation for determining the intersecting arc length, s, is

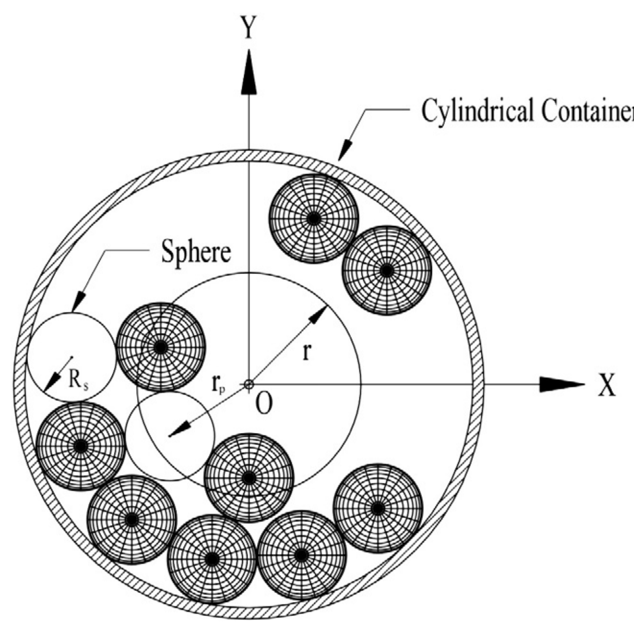

Fig. 1. X–Y plane of intersecting sphere at radial position r.