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Relationship between packing structure and porosity in fixed beds of equilateral cylindrical particles

Wenli Zhang[a], Karsten E. Thompson[a,*], Allen H. Reed[b], Liese Beenken[a]

[a] *Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA 70803, USA*
[b] *Naval Research Laboratory, Stennis Space Center, MS 39529, USA*

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Abstract

Fixed beds of cylindrical particles are important in chemical engineering applications, but their packing structures are not as well understood or as well characterized as sphere packings. In this work, X-ray microtomography is used to obtain 3D images of 1.8 mm diameter equilateral cylinders in a 23 mm cylindrical container over a range of bulk porosities. A novel algorithm is used to computationally reconstruct the packings, resulting in data sets that give the location and orientation of each cylinder in the imaged packings. Extensive analysis has been performed, including bulk and local porosities, radial distribution functions, and parameters describing local and global ordering. The major factors affecting packing structure are the overall packing density and the proximity to the wall. At the highest overall packing densities, near-wall porosity becomes nearly equal to interior porosity, and significant global ordering occurs near the wall. For a vertical container, global ordering is characterized by the alignment of the particles with an orthogonal coordinate system that has one axis coincident with r (as defined by the container) and the other two axes in the z–θ plane, but rotated 45° with the horizontal. The observed structures are relevant in the context of flow maldistribution and heat transfer in fixed beds.

Keywords: Packed bed; Tomography; Particulate processes; Granular materials; Packing structure; Wall effects

1. Introduction

The packing structure in fixed beds affects local fluid, heat, and mass transport, which in turn influences macroscopic parameters in many chemical engineering operations (e.g., separation and reaction processes). The packing structure for spherical particles is the most well studied and well understood of these systems. The minimum bulk porosity of sphere packings is 0.36 (for uniform-sized spheres), and the values for real packings typically fall into the range $\varepsilon = 0.36$–0.42. Packing structure near container walls exhibits partial ordering, because the locations (centers) of spheres in contact with the wall lie on a surface exactly $\frac{1}{2}$ diameter from the wall. Typically, this partially ordered structure propagates two to four diameters into the packing.

Like spheres, cylindrical particles are prevalent in chemical engineering. In fact, they are preferable to spheres in many applications because they can be extruded. However, the packing behavior of cylindrical particles is fundamentally different from spheres because cylinders exhibit orientational freedom, and their geometry contains a variety of surface elements (i.e., flat and curved surfaces as well as corners). These differences tend to produce more diverse packing structures as evidenced by the range of porosity values reported in the literature: for equilateral cylinders, porosities range from $\varepsilon = 0.25$ (Roblee et al., 1958) to $\varepsilon = 0.445$ (Coelho, 1997)—a much broader range than for spheres. Diversity in packing structure is also evident from a simple visual experiment: tapping or vibrating a vial of small equilateral cylinders causes many of the cylinders that are in contact with the wall to move into either parallel or perpendicular alignment with the wall, and also to move into end–end, end–side, or side–side alignment with one another. Continued vibration results in quite dramatic global alignment patterns such as what is seen in the photograph in Fig. 1. From a practical

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* Corresponding author. Tel.: +1 225 578 3069; fax: +1 225 578 1476.
E-mail address: karsten@lsu.edu (K.E. Thompson).

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Fig. 1. Photograph of a vial of cylindrical particles, which shows the high degree of ordering that occurs at the wall as a result of vibration.

standpoint, these observations are significant because they suggest that bulk transport properties may be harder to evaluate than for sphere packings.

Despite the importance of this problem, limited quantitative analysis has been performed on density and structure variations in packings of cylinders, especially at the particle scale. The primary reason is that particle-scale data for these structures is difficult to obtain. Most particle-scale analyses performed on sphere packings have relied on numerical simulations to produce the detailed packing structure. However, the computer simulations are difficult to implement with non-spherical particles, and the Monte-Carlo methods that are currently available do not reproduce the complex, semi-ordered structures that are observed experimentally (Zhang et al., in review). Conversely, experimental studies are able to create the complex packing structures of interest; however, recovering particle-scale data using traditional methods is difficult and time consuming.

In this work, we address this problem using a two-step process. First, X-ray microtomography imaging is performed on a series of packed beds of equilateral cylindrical particles. This approach allows real (rather than computer-simulated) packings to be used. At the same time, it provides the necessary resolution to obtain particle-scale data. Second, a novel computational method is used to reconstruct the packings from the microtomography images on a particle-by-particle basis. The resulting data sets contain the location and orientation of each cylinder in a packing, which is sufficient to completely characterize both the packing and void structure of the bed.

Using these data sets, we have analyzed changes in the packing structure as a function of increasing packing density. The cylindrical particles have dimensions $L \approx D \approx 1.8\,\mathrm{mm}$. The container is 23 mm in diameter. Hence, wall effects are significant, and much of the current analysis is aimed at this issue.

2. Background

2.1. *Packings of spheres*

Sphere packings are the most-studied type of particle packing. Ordered structures include rhombohedral packings and cubic packings, which bracket the range of attainable porosities at $\varepsilon_{\mathrm{min}} = 0.2595$ and $\varepsilon_{\mathrm{max}} = 0.4764$, respectively. Disordered packings exhibit a much smaller porosity range with most packings of interest falling into the range $\varepsilon = 0.36$–0.40. The terminology random close packed (RCP) is widely used to denote the highest packing density (lowest porosity) that can be achieved with spheres in the absence of global ordering. No theory has provided an exact value, but the well-accepted limit is $\varepsilon_{\mathrm{RCP}} = 0.36$, plus or minus some small amount that varies according to the source consulted.

The terminology *random* has been used rather loosely in sphere-packing studies, the implication being that packing structure remains random even as the porosity decreases over the commonly observed range. Although sphere packings are probably less susceptible to local or global ordering than are cylinder packings, there is evidence of structure as the packing density increases. Clarke and Jonsson (1993) observed a steady increase in the number of icosahedral clusters and icosahedral fragments in computer-generated sphere packings as the packing density increased. Torquato et al. (2000) studied jammed packings over a range of packing densities, and reported a steady increase in the parameter Q_6/Q_6^{fcc}, which quantifies the local bond-orientational order as compared to a perfect fcc crystal. Liu and Thompson (2000) used small periodic sphere packings (216 spheres) to achieve porosities as low as $\varepsilon = 0.3508$ (nearly 1% below the traditional RCP limit) and observed an onset of global ordering in these structures, even without the formation of a distinct lattice structure.

Torquato et al. (2000) addressed the ambiguity in the terminology *random packing* by proposing that the maximally random jammed (MRJ) state be used as a more rigorous definition to characterize dense, disordered structures. An MRJ value would be found by minimizing some measure of order over an ensemble of physically jammed states. For spheres, they obtained a value $\varepsilon_{\mathrm{MRJ}} = 0.36$, which is in agreement with the general definition of $\varepsilon_{\mathrm{RCP}}$, but is slightly greater than the