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ScienceDirect
Powder Technology 167 (2006) 10 – 19
POWDER TECHNOLOGY
www.elsevier.com/locate/powtec

Random particle packing with large particle size variations using reduced-dimension algorithms

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Received 18 October 2005; received in revised form 7 June 2006; accepted 7 June 2006
Available online 24 July 2006

Abstract

We present a reduced-dimension, ballistic deposition, Monte Carlo particle packing algorithm and discuss its application to the analysis of the microstructure of hard-sphere systems with broad particle size distributions.We extend our earlier approach (the "central string"algorithm) to a reduced-dimension, quasi-3D approach. Our results for monomodal hard-sphere packs exhibit a calculated packing fraction that is slightly less than the generally accepted value for a maximally random jammed state. The pair distribution functions obtained from simulations of composite structures with large particle size differences demonstrate that the algorithm provides information heretofore not attainable with existing simulation methods, and yields detailed understanding of the microstructure of these composite systems.

Keywords: Particle packing; Ballistic deposition; Pair distribution function; Packing fraction; Reduced-dimension algorithm

1. Introduction

Hard-sphere particle packing models have proven useful in the study of liquids and fluids [1–4], glasses [5,6], foams [7], granular flows [8,9], and amorphous solids [10,11], and have been extended to non-spherical particles as well [12,13]. Perhaps the most interesting application of particle packing is its use as a tool to understand the microstructure of particulate materials and powders. Understanding order in particulate systems is an outstanding question, and particle packing approaches have contributed to this line of research for some time [1,2,10,14–19,5,20,21]. Many researchers also use the tool to study a variety of related lines of research, including the interpretation of amorphicity as spatial chaos in one dimension [22], pressure and entropy in crystals [23], thermodynamics of slowly sheared granular systems [9], the onset of dilatancy in loose packings [24], transport properties [5], and porosity [25,26,5] to name a few. Of particular interest is the recent work on the concept of random close packing and the more rigorous definition of jamming in these systems [27,21,28,29].

Particle packing simulations take a variety of forms. Early attempts incorporated real particles such as powders [30], ball bearings [31,3,32], balls and spokes [1,2], and recently glass beads in a neutrally buoyant fluid [24], horizontally shaken beads [33], and M&M[1] chocolate candies [13]. Numerical and Monte Carlo techniques include seed aggregation [10] or variants thereof [34], growth in a unidirectional force field [35], shrinking of randomly placed spheres [36], growing spheres on the surface of a hypersphere [37], overlap relaxation followed by space expansion and vibration [38], conjugate gradient energy minimization [39,28], and various forms of molecular dynamics [40–42,6].

2. Motivation for this work

We seek to calculate the bulk and microstructural properties of particulate systems composed of rigid or semi-rigid particles embedded in an elastic or viscoelastic matrix [43,44]. This area of research demonstrates that the macroscopic properties of a composite material (e.g., the modulus) depend strongly on the microscopic details of the packing structure comprising the material [45,46]. For example, the bulk response of a highly

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doi:10.1016/j.powtec.2006.06.003

filled particulate system to an applied external stress can be determined in large part by particles in the pack that lie very near each other (i.e., within a fraction of a particle radius). For this reason, our desire to calculate bulk properties using a first-principles approach relies on a thorough understanding of the material microstructure. Moreover, detailed knowledge of the microstructure of such systems allows for related studies, such as combustion of solid rocket propellants [47].

For some systems of interest, the particulate ingredients that comprise the system may include particles with potentially very large size differences. Packing simulation of such systems with traditional methods can be problematic as the size difference increases. For example, a simulation of spherical particles with a size ratio of 100:1 would require 10^6 small spheres for each large sphere in the pack (assuming an equal mass ratio). Obtaining good statistics for such packs would require literally billions of particles in the pack, which is clearly unattainable with extant computational methods.

In an earlier paper, one of us introduced the concept of the central string algorithm [48]. The key feature of that approach is the idea that some packing statistics near a line drawn through a composite material ought to mimic the three-dimensional statistics of the pack for a sufficiently long line. We emphasize that a reduced-dimension algorithm may not be able to supplant a 3D algorithm for all statistics of interest. In this paper, we focus on particle packing fraction and radial distribution functions; the treatment of other statistics is under investigation.

The appeal of the reduced-dimension approach is that, when correctly implemented, it should allow researchers to calculate certain statistics for packs with large particle size variations which would otherwise be unattainable due to the long computation times associated with a full three-dimensional packing of such composite materials.

The earlier work [48] demonstrated the promise of a reduced-dimension approach, but the central-string method exhibited shortcomings. The most serious shortcoming present in the previous model was that the perturbation approach was unable to prevent particle segregation during growth. Also, the earlier model was unable to provide detailed information about the microstructure because of the limited structure found around the central string. The present work seeks to overcome these shortcomings by extending the central-string approach to a quasi-3D method, thereby providing the ability to calculate detailed microstructure, including radial distribution functions and coordination numbers.

Our algorithm follows most closely that of Visscher and Bolsterli [35], and is in essence a ballistic deposition, reduced-dimension Monte Carlo simulation.

3. The concentric-cylinder, reduced-dimension approach

A natural extension of the central-string approach to reduced-dimension particle packing is to extend the central string into a cylinder, producing a quasi-3D packing algorithm. In effect, we extend the notion of a line drawn through the three-dimensional particle pack to a cylinder drawn through the particle pack. Whereas the particles that intersected the line represented the packing statistics (for a sufficiently long line), a cylinder of equivalent length which cuts through the pack should also represent the pack statistics, but with more accuracy (per unit length) because more particles are included in the cylinder than intersect the line. In particular, if properly simulated and interpreted, this approach should provide sufficient information to allow a detailed examination of the pack microstructure.

The key to this reduced-dimension approach is to represent each particle of a different size or density (a *mode*) in the pack by its own cylinder, scaled appropriately to the particle's size. We define a particle mode to be all particles in a pack that are indistinguishable relative to one or more properties of interest. A monomodal pack comprises a single cylinder (and is in fact equivalent to a three-dimensional pack). A binary pack includes two concentric cylinders, whose radii are scaled proportionally to the size of each particle. A ternary pack comprises three cylinders, and so on; see Fig. 1. All cylinders share a common axis, but the cylinder radii depend on each particle's size.

We construct the pack by dropping particles at a randomly chosen position within each particle's cylinder. When simulating more than one particle mode, the order in which the particles are dropped is also random (respecting the final number of each particle mode required to represent the desired mass fraction of each mode). Each particle is dropped above the pack and allowed to descend into the pack under the influence of a unidirectional force field (e.g., gravity) acting along the z-axis until the particle finds a contact stability point. Until the particle finds a stability point, it will roll along other particles or the roll corridor defined by one or more particles and/or the cylinder wall. Contact stability refers to whether the current sphere is in compressive contact with an object or in tensile contact. If it is in compressive contact with another sphere or the cylinder wall, the particles push against each other due to the current sphere's weight. When a particle touches three or more objects compressively, it is stable and is placed at that position.When in tensile contact with another particle or the cylinder wall, the current sphere will roll away from the object unless it already has three or more compressive contacts. After the particle is placed at a contact stability point, another particle is dropped and the sequence repeated until completion (all particles dropped and stable).

The dropping and rolling of pack particles does not include any dynamics. The particles do not bounce, do not gain speed or

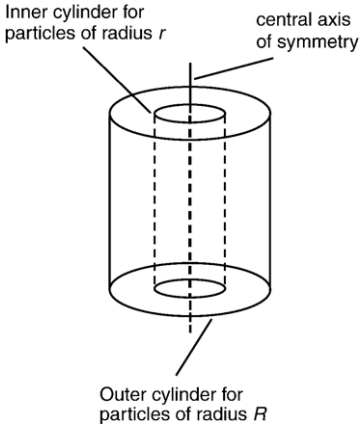

Fig. 1. Representation of the reduced-dimension, concentric-cylinder geometry.