Abstract

Geometry and Topology of Model Sediments and Their Influence on Sediment Properties

Cynthia Gabrielle Thane, M.S.E.
The University of Texas at Austin, 2006

Supervisor: Steven L. Bryant

The focus of this study has been to analyze the geometry and topology of model sediments. The geometry is determined by the spatial locations of the grains. The effect of packing geometry on porosity, pore throat distributions, floating grains, contact statistics and mechanical stiffness is presented. The contacts between grains establish a structure whose topology influences mechanical properties of the sediment. In order to create the packings for this study, a cooperative rearrangement sphere packing algorithm was developed. The algorithm was extended to simulate the deformation of ductile grains in sediments. The packing is validated by the experimental Finney Pack for mono-dispersed cases.
The study focuses on mono-dispersed and bi-dispersed packings. The porosity of the mono-dispersed packs of rigid grains was 0.359±0.002, averaged over all simulations. The porosity of the experimental Finney Pack is ~0.36. The porosities of bimodal packs exhibit a minimum at 40% small spheres by volume. The porosity trend is similar to experimental data from sand-clay mixtures under a confining pressure of 20 MPa reported in the literature (Koltermann and Gorelick, 1995). The lowest porosity obtained for the bi-dispersed case was ~0.28 for a radius ratio of 5. A radius ratio (RR) is the ratio of the large grain size to the small grain size.

A model that approximates a ductile grain was created. In this model, a ductile grain behaves as a rigid core with a soft outer shell. When a rigid grain overlaps with the soft shell, the radius of the ductile grain is changed so that it occupies the same total volume. Properties are determined as the volume percent of grains that are ductile and the thickness of the ductile shell are varied. For simulations of bi-dispersed packings with ductile grains, the lowest porosity (~0.19) is obtained for a RR of 3 and 40% small grains by volume. The packings that produced the lowest porosities had 100% ductile grains by volume. Ductile packings for the bi-dispersed case had a rigid core that was 95% of the size of the sphere. The porosity trend observed in the rigid grain packings was more pronounced when ductile grains were included, in agreement with experiments.

A method of calculating pore throats for heterogeneous packings was developed. For mono-dispersed packings, the maximum inscribed circle in a Delaunay face is traditionally used to represent the pore throat size. However, this is not always a useful definition in bi-dispersed packings. The method created for this study was based on the idea that the pore throat can be defined using a near-by fourth sphere in conjunction with the three other spheres that create the Delaunay face.
The volume of loose grains found in a packing of mono-dispersed spheres was 0.67 +/- 0.05%. This is slightly larger than the Finney pack which has ~0.55% loose grains by volume. In bi-dispersed case, the packings generally exhibit a peak in the number of loose grains at 20% by volume of small grains. The presence of ductile grains greatly decreases the volume of loose grains.

The average coordination number for the mono-dispersed packings is 5.61 +/- 0.03, agreeing well with the value of 5.61 for the Finney Pack. Coordination numbers in bi-dispersed packings were studied by examining the specific contact statistics between large and small spheres, instead of using the average coordination number.

A hypothesis is proposed that certain short-range configurations may lead to mechanically weaker packing. One such configuration two larger spheres (in a bi-dispersed packing) forced apart by one or more nearby small spheres. A commercial simulator, Particle Flow Code in 2 Dimensions (PFC$^{2D}$), was used to test this idea on a few ordered packing structures. Bi-dispersed packings were studied to determine what radius ratios had the highest occurrence of these weak configurations. The presence of loose grains and weak local configurations could explain certain acoustic velocity trends in unconsolidated sediments.