

Simulation of cohesive forces in rapid granular flow using a square-well potential

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Abstract

Cohesive interparticle forces have a significant effect in many granular flow applications. Consequently, many discrete-particle simulations of rapid granular flow have incorporated cohesive forces. On the other hand, efforts to incorporate cohesive interparticle forces into continuum models of rapid granular flow are limited. Continuum models use constitutive relations that are developed using kinetic theory, which assumes that all particle interactions are binary and instantaneous. This assumption of instantaneous particle interactions conflicts with cohesive force models that are typically a continuous function of particle separation distance. The square-well potential provides a way to incorporate cohesive interparticle forces into the system while still maintaining instantaneous, binary particle interactions.

In the present study, rapid granular flows with attractive inter-particle forces are investigated. In particular, cohesive forces are incorporated into hard-sphere (molecular dynamics) simulations via a square-well potential. For simple shear flows, an investigation of the input parameter space indicates that two distinct flow regimes are present. For relatively large cohesive forces, the formation of a large, single agglomerate is observed. For moderate cohesive forces, the sheared system is composed of mostly 2-particle, dynamic agglomerates that are fairly evenly distributed throughout the domain. Furthermore, the results for this latter regime indicate that cohesion attenuates the magnitude of the stress components at higher solids fractions (in the collisional regime) as compared to the non-cohesive case. At lower solids fractions (kinetic regime), however the presence of cohesive forces has little impact on the observed stress.

Key Words: Granular flows, cohesion, agglomeration, molecular dynamics, square-well potential