Molecular dynamics simulations of driven granular mixtures

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The Boltzmann kinetic theory is used as a starting point to model a suspension of bidisperse solid particles immersed in a viscous fluid. The grains are modeled as hard disks or spheres that undergo inelastic collisions characterized by velocity-independent coefficients of normal restitution. As a first approximation, the effect of the fluid on the grains dynamics is accounted for two terms: (i) a drag force, proportional to the velocity of particles (Stokes' law), that attempts to model the friction of the grains on the interstitial fluid and (ii) a stochastic force, where the particles are randomly kicked between collisions. The last contribution tries to simulate the kinetic energy gain due to eventual collisions with the (more rapid) particles of the surrounding fluid. Molecular dynamics simulations of the model are based on a event-driven algorithm where the two additional forces are incorporated, after a proper identification of the characteristic time scales of the system. Some numerical results are compared with the theoretical predictions [1, 2] obtained by solving the Boltzmann equation from the Chapman-Enskog method. Here, we focus on steady homogeneous states as they are fundamental for the construction of a hydrodynamic description of the system, see [1, 2].

References

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