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Clustering Instabilities in Gas-Solid Systems: Role of Dissipative Collisions vs. Viscous Losses

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ABSTRACT

We assess via the lattice-Boltzmann method and dissipative molecular dynamics the relative importance of inelastic collision and viscous dissipation in gas-solid flow instabilities. We find that increasing dissipation enhances instabilities. Velocity-field instabilities precede concentration-field instabilities. Interestingly, enhanced instabilities can actually lead to long-term higher particle kinetic energy levels.

INTRODUCTION

Particulate flows are crucial to the chemical, energy, oil, and pharmaceutical industries. Despite this ubiquitous nature, such flows are not well understood (1-15). Unit operations involving particulates have typical downtimes of 40% (1). A 1-2% improvement in efficiency of the $60 billion US chemical industry that is linked to particulate technology will approach $1 billion in annual savings (4). For such efficiency to be obtained, a better understanding of particulate flows, in the form viable predictive models, is required (16,17).

Instabilities in particulate flows, such as particle velocity vortices (Fig. 1b-d) and particle clusters (Fig. 1c-d), are well known to occur in gas-solid risers and circulating fluidized beds. Such instabilities have been shown to manifest due to inelastic (collisional) dissipation (18) and also due to viscous losses (19) imposed by the fluid phase. In this work, we aim to address the relative importance of both viscous and inelastic energy dissipation in the formation of instabilities for a wide range of system parameters by performing lattice-Boltzmann simulations. We also analyze the resulting evolution of instabilities and long-term dynamics to find a counterintuitive interplay between dissipation and long-time particle kinetic energy levels.

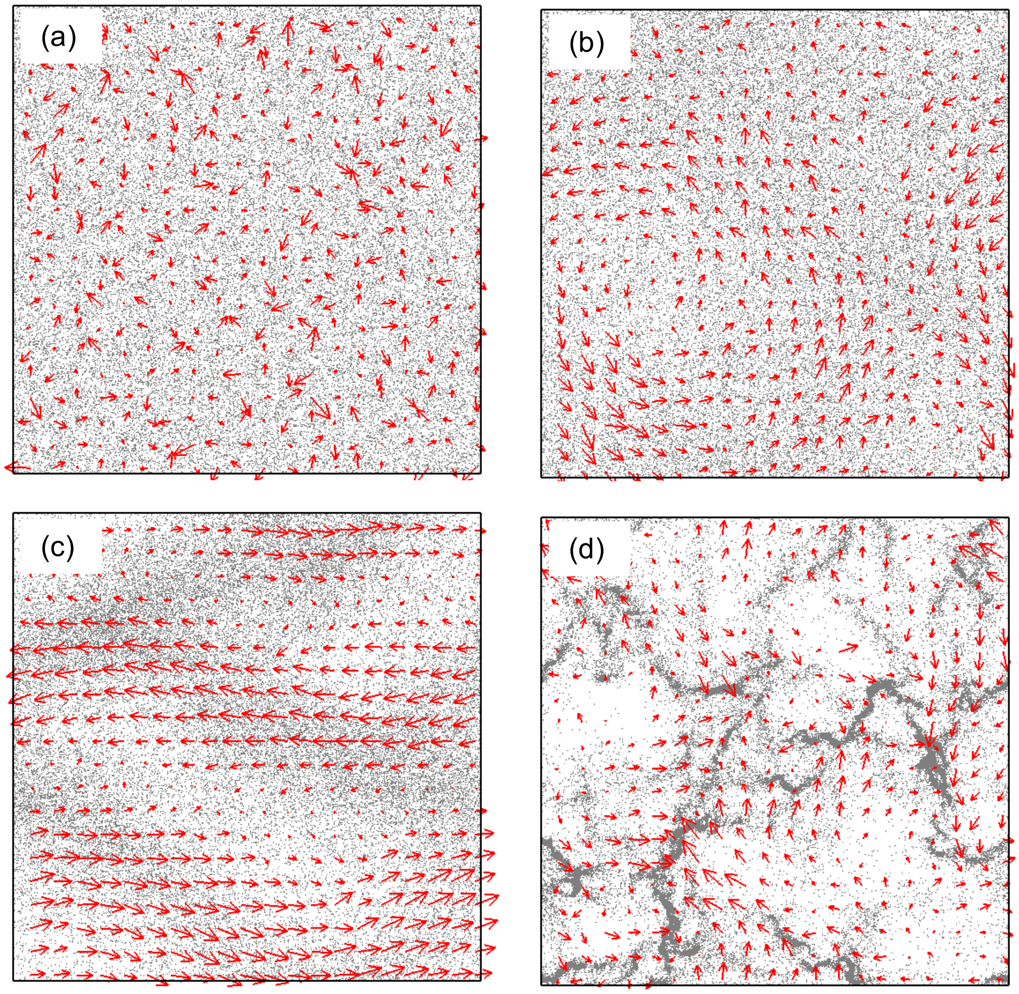

Figure 1. Visualizations of particle positions (gray dots) and velocity vectors (red arrows) from two-dimensional molecular dynamics simulations with *N*=40,000 particles and a solids volume fraction $\phi = 0.05$ in a square domain with length of 793*d, where *d* is the particle diameter. Snapshots correspond to varied normal restitution coefficient 0.6 < *e* < 0.98 and simulation duration, expressed in collisions per particle *C/N*, as follows: (*a*) *e*=0.98 and *C/N*=10, (*b*) *e*=0.98 and *C/N*=210, (c) *e*=0.98 and *C/N*=380, (d) *e*=0.6 and *C/N*=34.

METHODS

A combination of lattice-Boltzmann method and molecular dynamics simulations are used to assess the influence of viscous and inelastic dissipation on the formation of instabilities. Each method is described below.

Lattice-Boltzmann Method

Lattice-Boltzmann simulations, which resolve the flow dynamics around each moving particle (20), have been performed in a rectangular and periodic domain with dimensions $L_x \times L_y \times L_z$ = 29.7*d* × 29.7*d* × 4*d*, where *d* is the particle diameter. Simulations have been performed for a range of Reynolds numbers $1 \le \mathrm{Re}_T \le 30$, particle-fluid material density ratios $800 \le \rho_s/\rho_g \le 1500$, normal restitution coefficients $0.8 \le e \le 1$, and solids volume fractions $0.1 \le \phi \le 0.4$. Here, the Reynolds number is defined by the particle fluctuating velocity: $\mathrm{Re}_T = \frac{\rho_g d}{\mu_g}\sqrt{\frac{T}{m}}$, where ρ_g is the gas material density, *T* is the granular temperature, μ_g is gas viscosity, and *m* is the particle mass. From the system parameters, Eq. 1 gives the total number of particles *N*,

$$N = \frac{\phi V}{\left(\pi d^3 / 6\right)} , \quad (1)$$

where $V = L_x L_y L_z$ is the total domain volume. Instabilities in the velocity and concentration fields in the forms of vortices and clusters, respectively, are assessed via Fourier analyses, the processes of which have been described in detail in Ref. (21).

Molecular Dynamics Simulations

Event-driven, hard-sphere molecular dynamics simulations, which track discrete particles and resolve collisions via a constant normal restitution coefficient and momentum conservation, have been performed in an analogous *granular* system. Such simulations of a granular flow provide analysis in the limit of negligible fluid for corresponding ranges of e and ϕ. Instabilities in molecular dynamics simulations are analyzed in the same manner as for the lattice-Boltzmann method; see (21).

RESULTS

Instabilities are enhanced and onset more quickly with increasing viscous dissipation and also with increasing inelastic (i.e., collisional) dissipation, as expected. Either form of dissipation works to dissipate particle kinetic energy by decreasing the normal component of particle velocities, resulting in alignment of the tangential motion. This alignment of tangential velocities is associated with velocity vortices (Fig. 2a) and, eventually, gives to cluster formation (Fig. 2b).

Velocity vortex instabilities precede particle clustering, as was previously observed in the granular case (18). Intuitively, adding to the level of viscous or inelastic dissipation will enhance instabilities and increase the initial rate of particle kinetic energy decay. However, somewhat surprisingly, systems with higher levels of dissipation can actually reach higher levels of particle kinetic energy at later times via the evolution of instabilities (Fig. 2c). This seemingly counterintuitive result is actually consistent with an understanding of particle dynamics in unstable systems. Specifically, the previously described aligned motion associated with velocity vortices gives to smaller relative normal particle velocities. Since inelastic dissipation is proportional to the relative normal velocity, this aligned motion actually serves to significantly reduce energy dissipation such that, in some cases, more dissipative systems actually end with highly energy levels than less dissipative counterparts. This behavior is depicted in Fig. 2c where the least dissipative system (blue) ends with the lowest energy level.

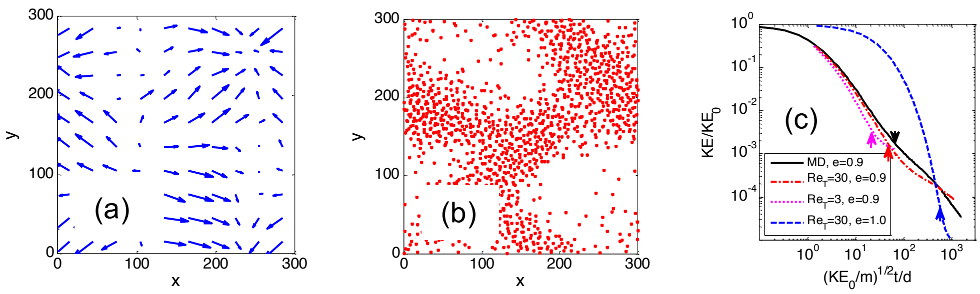

Figure 2. MD-DNS simulations of a gas-solid homogeneous cooling system. (*a*) Coarse-grained slice of the particle velocity field (showing vortices) in a system with *N* = 1340, ϕ = 0.2, and *e* = 0.9; (*b*) Particle center locations in the same x-y slice of the domain and time as snapshot (*a*). The dimensions in (*a*) and (*b*) correspond to the lattice spacing where $L_x = L_y = 300$ and *d* = 10.1. (*c*) Particle kinetic energy *KE* normalized to the initial value KE_0 as a function of a non-dimensional time in a system with *N* = 2680, and ϕ = 0.4. Arrows depict the onset of instability.

Additionally, we have assessed the relative importance of viscous vs. inelastic dissipation as a function of input parameters. Viscous dissipation becomes dominant for later times, as particle velocities decay since collisional dissipation has a higher order dependence on velocity than viscous dissipation. Decreasing *e* or Increasing ϕ increases the importance of inelastic dissipation by increasing the proportion of dissipation for each collision or by increasing the rate of collisions, respectively. Finally, increasing ρ_s/ρ_g or Re_T increases the role of collisions by diminishing the viscous effects of the fluid phase.

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NOTATION

C	Total number of collisions [collisions]
e	Normal restitution coefficient [dimensionless]
ϕ	Particle volume fraction [dimensionless]
$L_{x/y/z}$	Domain length in 3D simulations [meters]
m	Single-particle mass [kilograms]
μ_g	Gas viscosity [kilogram/ (meter second)
N	Number of particles [particles]
Re_T	Thermal Reynolds number [dimensionless]
ρ_g	Gas material density [kilogram/ cubic meter]
ρ_s	Particle material density [kilogram/ cubic meter]
T	Granular temperature [kilogram meter^2/ second^2]
V	Domain volume [cubic meters]

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