SPECIES SEGREGATION DRIVEN BY A GRANULAR TEMPERATURE GRADIENT

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Granular systems are typically characterized by some degree of polydispersity, which may lead to species segregation. A careful analysis of the equation governing segregation shows that lifting the equipartition-of-energy assumption gives rise to a previously unidentified driving force for segregation: gradient in species temperature. MD simulations, together with kinetic theory, indicate that this new driving force is significant for moderate values of mass differences and restitution coefficients.

IINTRODUCTION

Solid particulate flows occur in a wide variety of geological and engineering systems, such as in landslides, planetary rings, and pharmaceutical processing. Such flows may contain particles of varying sizes and densities. This non-uniformity may lead to species segregation, which is a complex phenomenon of importance to many industrial processes. The separation of dissimilar particles may be either desirable (as in mining operations) or detrimental (as in the mixing of pharmaceutical powders).

The focus of this work is on segregation in rapid granular flows (flows with nearly instantaneous collisions between grains in which the role of interstitial fluid is negligible). Continuum modeling based on dense-gas kinetic theory provides a means of investigating the different behaviors in rapid granular flow. For the case of binary granular mixtures, several kinetic based theories are available. Differences in these theories arise from the various assumptions used in the derivation process. Two simplifying assumptions are a Maxwellian velocity distribution and an equipartition of energy between unlike particles. Previous investigations show that a Maxwellian velocity distribution is not strictly upheld, and that a non-Maxwellian distribution is necessary for reliable stress predictions. Previous studies also indicate that an equipartition of energy is not strictly upheld, though the impact of incorporating a non-equipartition treatment on predictions is not as clear. Furthermore, no current theory exists in which both of these assumptions are lifted.

Of interest is how the equipartition assumption affects the predictive abilities of these models for systems in which segregation occurs. Previous theoretical investigations into the driving forces for segregation [1,2] are based on models in which equipartition of energy is assumed. These studies reveal several driving forces for segregation: external forces, pressure gradient (∇P_1, ∇P_2), species concentration gradient (∇n_1, ∇n_2), and mixture granular temperature gradient (∇T). In the current effort, a similar analysis based on a non-equipartition theory indicates that an additional driving force arises due to non-equipartition effects, namely a gradient in species temperature (∇P_{1n}, ∇P_{2n}). To evaluate the importance of this new driving force, results from molecular-dynamics simulations are applied to a segregating flow system and used together with Jenkins and Mancini [3] kinetic theory, which does not include an equipartition assumption. Segregation in binary mixtures is explored for various diameter ratios, density (mass) ratios, solids fractions, solids fraction ratios, and restitution coefficients. Results indicate that the new driving force is of similar magnitude to other driving forces for systems with moderate values of mass differences and restitution coefficients.

DISCRETE-PARTICLE SIMULATION

Two-dimensional, molecular-dynamics simulations are used to mimic the segregation of a binary mixture driven by a granular temperature gradient. The gravity-free domain is periodic in the y-direction and is bounded by 'walls' of a specified temperature in the x-direction. To establish a temperature gradient, the walls are set to unequal temperatures.

The simulation proceeds through time via a hard-sphere/overlap algorithm, where particle collisions are detected by searching for overlaps after each time step. The maximum allowed overlap between any two particles or a particle and a wall is 1% of either particle radius. After each successful step, collisions are resolved for particles exhibiting overlap. The post-collision speed of a particle colliding with a wall is taken from a Maxwellian distribution consistent with the set temperature of the given wall. The post-collision trajectory of the particle is reversed in the x-direction and unchanged or reversed in the y-direction. Correspondingly, a granular temperature gradient develops in the y-direction.

The simulation proceeds until a statistical steady state is reached. At this point data collection begins, during which 200,000 evenly spaced measurements of solids fraction, and granular temperature are made as a function of x-position by dividing the domain into a set number of vertical strips (parallel to the constant-temperature walls). The average of these 200,000 measurements is then reported for each parameter in a given data collection strip.

The dimensionless quantities that characterize the system include overall solids fraction (ϕ), solids fraction ratio of species 1 to species 2 (ϕ_1/ϕ_2), diameter ratio (d_1/d_2), material density ratio (ρ_{p1}/ρ_{p2}), restitution coefficient (e), granular temperature ratio of the hot wall to the cold wall (T_H/T_C), and ratio of domain size in the x and y direction to the diameter of species 1 (L_x/d_1) and (L_y/d_1). For all simulations, L_y/d_1 is set large enough such that the results are box-size independent. In the case where $L_y = L_x$, the characteristic dimension is simply referred to as L.

RESULTS AND DISCUSSION

Molecular dynamics simulations were used to investigate the behavior of a binary mixture in the presence of a granular temperature gradient. Previous investigations into such "thermal diffusion" indicate that larger particles tend to congregate in the cooler regions of the domain. The current simulations reveal similar findings. Namely, under the influence of a granular temperature gradient, all particles tend to concentrate in the coolest region though the more massive particles have a higher affinity for this region (i.e., species segregation occurs). A quantitative measure of segregation is provided by the local solids fraction of a species over that of the expected species solids fraction in a homogeneous mixture (ϕ/ϕ_E). For example, for $\phi = 0.1$, $\phi_1/\phi_2 = 4$, $d_1/d_2 = 2$, $\rho_{p1}/\rho_{p2} = 8.0$, $e = 0.9$, $T_H/T_C = 10$, and $L/d_1 = 62.6$, the solids fraction of the large particles is found to be 4.7 times greater than would be expected in a homogenous mixture at $x/L = 0.15$ (near the cold/left wall), but 0.13 times less than would be expected at $x/L = 0.85$ (near the hot/right wall). In contrast, the solids fraction of the small particles stays more homogenous across the domain with $\phi_2/\phi_E = 2.1$ at $x/L = 0.15$ and $\phi_2/\phi_E = 0.45$ at $x/L = 0.85$.

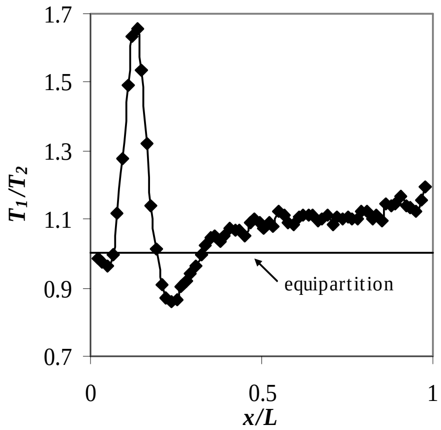

Figure 1. Granular temperature ratio of species 1 to species 2 (T_1/T_2). Relevant parameters: $\phi = 0.1$, $\phi_1/\phi_2 = 4.0$, $d_1/d_2 = 2.0$, $\rho_{p1}/\rho_{p2}, = 8.0$, $e = 0.9$, $T_H/T_C = 10$, and $L/d_1 = 62.6$

The newly-identified driving force for segregation arises from the presence of non-equipartition. The degree of non-equipartition is demonstrated in figure 1, which displays the granular temperature ratio (T_1/T_2) as a function of x-position. Non-equipartition is seen to exist near the cold wall, specifically in the region around $x/L = 0.14$ where $T_1/T_2 = 1.66$. It is also worthwhile to note the non-equipartition is atypical at $x/L \sim 0.23$; namely $T_1/T_2 < 1$, which implies that the more massive particle is cooler than its lighter counterpart.

A new aspect of this work concerns the presence of non-equipartition driving forces ($CP_{1n}\nabla P_{1n}$ and $CP_{2n}\nabla P_{2n}$) and their magnitude relative to previously identified driving forces ($Cn_1\nabla n_1$, $Cn_2\nabla n_2$, $CT\nabla T$, $CP_1\nabla P_1$ and $CP_2\nabla P_2$). The 'C' terms represent the transport coefficients associated with the segregation driving forces (for details see [3]). Simulation with theory was used to evaluate the importance of the new driving forces. Specifically, the profiles in species number density, species temperature, and mixture temperature obtained from the simulations were used to evaluate the magnitude of the driving forces in the diffusion equation from [3]. An examination of figure 2 reveals that the larger of the two newly identified driving forces arising from non-equipartition is that associated with the lighter particle ($CP_{2n}\nabla P_{2n}$). More importantly, the magnitude of this driving force is similar to that of the other driving forces

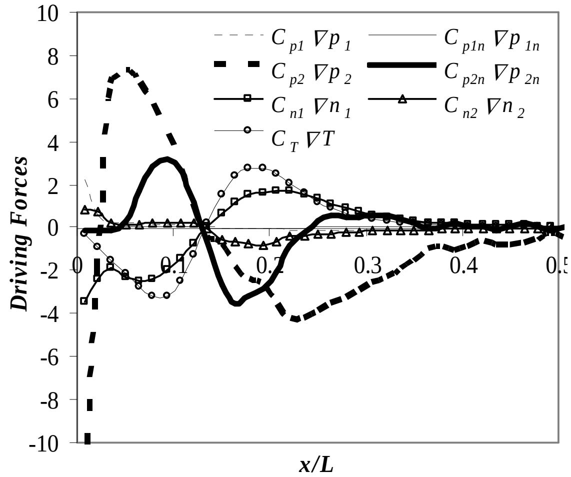

Figure 2. Driving forces for segregation using a form of Jenkins and Mancini [3] diffusion of velocity equation and simulation results. Relevant parameters: $\phi = 0.1$, $\phi_1/\phi_2 = 4.0$, $d_1/d_2 = 2.0$, $\rho_{p1}/\rho_{p2}, = 8.0$, $e = 0.9$, $T_H/T_C = 10$, and $L/d_1 = 62.6$

CONCLUSIONS

Discrete-particle simulations were employed to simulate segregation of a binary granular mixture driven by a granular temperature gradient. The results from these simulations were then used in conjunction with Jenkins and Mancini [3] theory to assess the various driving forces for segregation. Specifically, the magnitude of a newly identified driving force arising from a non-equipartition of energy was evaluated. Results indicate that the new driving force is of similar magnitude to other driving forces for systems with moderate values of mass differences and restitution coefficients. In many cases, a non-equipartition driving force was the second largest driving force present.

References

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