Directed clustering in driven compartmentalized granular gas systems in zero gravity

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Abstract. Clustering of shaken fluidized granular matter in connected compartments has been observed and studied in the laboratory. This clustering behavior in granular gas systems is related to the dissipative nature of granular system, and therefore shall not depend on gravity. This clustering phenomenon in compartmental configuration may provide a means for particle depletion and transportation in microgravity environment. In this work we propose different configurations for possible directed clustering in zero gravity. The related experiment has been planned for the Chinese satellite SJ-10.

1. Introduction
Clustering is one of the important features of granular gas systems [1–6]. It occurs spontaneously due to inelastic collisions among particles. On one hand, clustering is one kind of pattern formations commonly seen in non-equilibrium systems, which has caught much attention of physicists in recent years [7–15] using granular gases for understanding behaviors of non-equilibrium systems. On the other hand, granular matters have important industrial applications. Understanding the clustering mechanism can be economically and environmentally important.

In a vertically shaken two-compartment system, mono-dispersed particles will spontaneously cluster into one of the two compartments [16]. This clustering behavior demonstrates the “Maxwell’s demon” phenomenon, in which the energy dissipation between particles acts as the demon to preferentially let particles pass only in one direction to cluster in one compartment [17,18]. This kind of clustering behavior can also be found in N connected compartments [19,20], for example in three connected compartments it is found that for sufficiently strong shaking the granular gas will be equal-partitioned, but for some moderate shaking the gas will cluster in one of the compartments. For bi-dispersed particles, competitive clustering behavior will cause new phases [21,22], such as oscillatory clustering [23–29], degenerate oscillation state, and semi homogeneous state [30]. In a cyclic three-compartment system, a chaos-like clustering behavior, i.e., two kinds of particles cluster into compartments in a random order [31], is also observed.

In this paper, we will first review the clustering phenomena of mono-disperse granular gas in symmetric two-compartment system. We then propose and study possible directed clustering with asymmetric configurations for possible application of transporting particles under microgravity.
2. Clustering Phenomenon under Gravity

2.1. For cells with symmetric configuration: Maxwell Demon

A molecular dynamics simulation is performed for a container of two identical compartments, which are connected by an opening at the wall in between the compartments, as is shown in Fig.1. The ground area of each compartment is $26\sigma \times 26\sigma$, ($\sigma$ is the diameter of the particles). The lower edge of opening is $15\sigma$ above the bottom plate and the opening size is $26\sigma \times 30\sigma$. The bottom plate of the container provides a driving velocity $v_b$ in the unit of $\sqrt{2g\sigma}$ ($g$ is gravity acceleration) in a saw-tooth manner. Gaining kinetic energy by colliding with the bottom plate, particles may jump from one compartment to the other through the opening. Hard sphere method is used to describe collisions between particles. Particles are considered to be perfect hard sphere that the deformation during collision is ignored. Identical particles with unit mass and unit diameter are used, and the dissipation in a particle-particle collision is characterized by the coefficients of restitution. For simplicity, only the normal coefficient of restitution is considered, thus the particle-particle collision can be described as follows:

$$ \vec{v}'_i = \vec{v}_i - \frac{1 + e}{2} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n} \quad (1) $$

$$ \vec{v}'_j = \vec{v}_j + \frac{1 + e}{2} [(\vec{v}_i - \vec{v}_j) \cdot \hat{n}] \hat{n} \quad (2) $$

where $i, j$ refer to the two particles and $n$ the normal direction of their contact, $v$ and $v'$ are pre- and post-collision velocities, respectively, and $e$ is the normal coefficient of restitution, which is set to a constant value 0.9 throughout this paper. Particle-wall collisions are assumed to be elastic. Friction and rotation are ignored for all collisions. Each collision is considered to be a key event, and a standard event-driven algorithm [32] is adopted in our simulation.

![Figure 1](image1.png)

**Figure 1.** Homogeneous clustering state(HOM) (a) and asymmetric clustering state(ASY) (b) in mono-disperse two-compartment system by molecular dynamics simulation. Total number of particles $N_{tot}$ is 500. Shaking velocity $v_b$ is 0.90 (a) and 0.70 (b).

Fig.1(a) shows the homogeneous distribution of particles in the two compartments when shaking strength is high enough. When shaking strength is getting lower, clustering in one compartments is observed (Fig.1(b)). A parameter $\varepsilon = \langle (N_l - N_r) / N_{tot} \rangle$ is defined to describe the asymmetric clustering phenomenon, where $N_l, N_r, N_{tot}$ are the distribution number of particles in left compartment, right compartment and the total number of particles, respectively. $\langle ... \rangle$ is averaged over time when system reaches stable state. Figure 2 shows a symmetry breaking...
transition from homogeneous clustering (HOM) to asymmetric clustering (ASY) with decreasing $v_b$.

2.2. Asymmetric structure: directed clustering

In the symmetric two-compartment system, the clustering can be in either compartment. By introducing an asymmetric structure, preferential directed clustering is possible [33]. One way to do it is by adding a slab into one of compartments (shown in fig. 3(a)). An experiment was performed. Our experimental setup consists of a glass cell with base size $2.5 \times 5 \text{cm}^2$ and height $15 \text{cm}$. The cell filled with $N_{\text{tot}} = 800$ glass beads of radius $r = 0.5 \text{mm}$, is mounted on a sinusoidal shaker. The cell is separated into two equal compartments by an aluminum plate, which has an opening of $2 \times 2.5 \text{cm}^2$. This opening is at a height with its lower edge $2 \text{cm}$ above the base. Different slabs of thickness $\delta h$ ranging from $6\text{mm}$ to $12\text{mm}$ are glued one at a time to the bottom of one of the two compartments. In this way the depth of the two compartments from the opening height become asymmetric. We refer the shallow one as compartment A and the deeper one as compartment B. The shaker frequency $f$ is fixed at $40 \text{Hz}$. Driving velocity $v_b = af$.

By changing the driving velocity, different clustering behaviors can be observed, as demonstrated in fig. 3(a)- (e). The demonstration is under an initial condition that all particles are put in compartment A (fig. 3(a)) with a slab of thickness $\delta h = 10\text{mm}$ in it. When the driving velocity is lower than a certain critical value $v_c$, a small percentage of beads are able to jump through the opening to compartment B, a large portion of beads remains in compartment A. This is the case shown in fig. 3(b). While the driving velocity reaches $v_c$, nearly all the beads initially in compartment A will cluster in compartment B, as shown in fig. 3(c). When driving velocity goes higher than $v_c$, beads in compartment B gradually flow back to A, and at large enough driving velocity the distribution will slowly approach homogeneous state (fig. 3(d)). When the driving velocity is reversed to a lower value, particles in compartment A will be relocated to compartment B. Instead of returning to the state as shown in fig. 3(a) even with same driving velocity, most of the particles would eventually cluster in the deeper compartment B, which is shown in fig. 3(e). But if we set the initial distribution for most of the beads originally to be located in compartment B, no abrupt phase transition would occur. The system would evolve along one phase trajectory without any bifurcation.

To get a clear view of the experimental observation, the number of particles in each compartment at any driving velocity is measured (fig. 4). After long enough time (usually several minutes after reaching a steady state), the shaker is turned off and the number of particles remaining in each compartment is counted. This procedure is performed several times with different initial conditions at each fixed driving velocity. A phase diagram of $N_A$ (the number of particles in compartment A) vs. $v_b$ is obtained. There are two regimes in this phase diagram as shown in fig. 4. In regime I (below $v_c$): for low shaking strength, particles can cluster in either compartment A or compartment B. While increasing the shaking strength, the state that most particles are in compartment A will suddenly change at a critical velocity $v_c$ to populate in compartment B; while in another state that most particles are in compartment B, they will evolve continuously without this sudden change. In regime II (above $v_c$): the system evolves in a relative simple and reversible way. It will eventually approach an asymptotically homogeneous distribution at high shaking strength.

As shown above, directed clustering occurs when $v_b$ is larger than $v_c$ that most particles will cluster in the lower compartment no matter what initiate distribution is. Such an asymmetric structure can be extended to N-compartment, which may be used as a method for directed transportation of granular particles.
3. Directed clustering in zero gravity

3.1. Symmetric structure

A 3-D molecular dynamics simulation is performed for a two-compartment cell connected by an opening on the sidewall, under zero gravity, with the top and bottom plates oscillating in saw-tooth manner. The size of each compartment is chosen to be $30\sigma \times 30\sigma \times 120\sigma$, and the connection opening at the sidewall is $30\sigma \times 30\sigma$, where $\sigma$ is the particle size. In a dilute system with small number of particles, the system is found to be homogenously distributed, as shown in Fig. 5(a). This symmetric distribution state is broken when more particles are added into the system. Particles will become asymmetrically distributed in the system and cluster in the middle part of one of the compartments (Fig. 5(b)). This phenomenon is very similar to the clustering behavior under gravity. Asymmetric factor $\varepsilon$ increases rapidly with total number of particles $N_{\text{tot}}$ as shown in Fig. 6. In this simulation the coefficient of restitution is assumed to be independent on relative velocity for particle-particle collisions. This final clustering state can be reached with any non-zero value of $v_b$ as long as the right $N$ is used.

3.2. Asymmetric structure

Similar directed clustering behavior can be found in zero gravity. Asymmetric configuration can be made by adding a slab in one of the two compartments, as shown in Fig. 7. If initially all particles are placed in compartment A, most of particles will remain in this compartment when the height of slab is not large enough (Fig. 7 (a)). Directed clustering can be observed by increasing the height of slab (Fig. 7(b)). The distribution can be clearly demonstrated in figure 8. Black square points represent the final distribution state with initial population of particles in compartment A; red circle points indicates the final population of initial state of particles in compartment B. When the height of slab $\delta h$ is not large enough, the final clustering state depend upon the initial clustering state (regime I). When $\delta h$ is above certain threshold value,
Simulation results of homogeneously clustering state (a) and asymmetric clustering state (b) in zero gravity. The total number of particles $N_{\text{tot}}$ in this simulation is 1500 (a) and 3000 (b).

Directed clustering is found: all particles will cluster in the deeper compartment (regime II).

Simulation result of different clustering state in asymmetric two-compartment system in zero gravity. Total number of particles is 5000, the height of slab $\delta h$ is (a) 5 and (b) 10 radii of the particle.

Asymmetric factor $\varepsilon$ changes with $N_{\text{tot}}$.

Number of particles remaining in compartment A vs. the height of slab $\delta h$ when initially all particles are in compartment A (black square points) or in compartment B (red circle points).

3.3. N-compartment configuration

With specially designed asymmetric N-compartment configuration, particles can be transported in a desired direction. Two examples are presented in Fig. 9. As shown in Fig. 9(a), ten compartments are connected with openings located near either end boundaries in an alternative manner. Particles will cluster around non-shaking boundaries (black lines). For example, particles will be pushed by the top boundary of compartment 1 and cluster around the bottom.
Because of large density gradient at the bottom boundaries of compartment 1, particles will diffuse into compartment 2 and then cluster around its top boundary. In this way, particles will flow from compartment 1 to compartment 10, and form a stable cluster at one end of compartment 10.

Fig. 9(b) shows another asymmetric configuration of ten compartments with two moving boundaries and opening in the middle wall. Particles initially cluster in the middle part of the compartment 1. Since the opening is set at the middle, particles will diffuse from compartment 1 into compartment 2, and through compartment 3, 4 ... and eventually to compartment 10.

The time evolution of the population can be obtained by simulation and is as shown in Fig. 10 (a) and (b). The system starts with all particles in compartment 1 (black curves), will populate through compartment 2 to 3, 4... and eventually evolve to compartment 10.

Figure 9. Two types of asymmetric N-compartment system in zero-gravity. In (a), red lines represent the moving boundaries. In (b), both top and bottom boundaries are moving. Particles are initially placed in compartment 1 and finally cluster into compartment 10.

Figure 10. Time evolution of number of particles in different compartments. Numbers in different compartments are indicated by different colors. Curves in (a) and (b) correspond to time evolution of configurations shown in Fig.9 (a) and (b), respectively.

4. Conclusion
Clustering occurs in compartmentalized granular gases due to the dissipative nature of the system. By constructing asymmetric configuration the cluster can be directed in a desired way. In this work MD simulation is performed and the directed clustering in zero gravity is achieved in some asymmetric two-compartment structure and in N-compartment cells with proper shaking strength.
5. Acknowledgement
This work is supported by the National Natural Science Foundation of China (Grant Nos. 10720101074 and 10874209), the Knowledge Innovation Program of the Chinese Academy of Sciences (Grant No. KJCX2-YW-L08), and grants from CSSAR and CNES.

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