Segregation in Rapid Flows: Continuum and DEM

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1. Overview

2. Modeling Approaches
   • Discrete Element Models (DEM)
   • Continuum

3. Types of Polydispersity
   • Binary Mixture
   • Continuous PSD

4. Case Study: Lunar Regolith Ejection by Landing Spacecraft
Outline

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Hrenya Research Group: Current Thrusts

“De-mixing” of particles according to size/density/etc.

“Clustering” Instabilities

Agglomeration of Wetted Particles

Microgravity flows

Sticky balls

The popular desktop toy Newton's cradle consists of a row of suspended metallic spheres. When the sphere at one end is pulled back and released, it strikes the row, causing the sphere at the other end to fly up with a similar velocity.

Christine Hrenya and her colleagues at the University of Colorado at Boulder wanted
Polydispersity

**Definition:** Non-identical particles, that can vary in size, material density, shape, restitution coefficient, and/or friction coefficient, etc.

In nature…polydispersity is common

- sand
- Saturn’s rings
- asteroids
- lunar regolith

In industry…polydispersity is common

- characteristic of starting material
- desired for improved efficiency (e.g., fluid catalytic cracking unit)

- biomass
- coal
- FCC catalyst
How do polydisperse flows differ from monodisperse?

1) **Bulk flow behavior:** solid-phase viscosity, pressure, etc.

2) **Species segregation (de-mixing)**
   - no monodisperse counterpart!
   - ubiquitous!

- pouring
- shaking
- flowing
- low-velocity fluidization (bubbling)
- high-velocity fluidization (particle carryover)
So ….is species segregation good or bad?

**BOTH!!**

- Good for separation processes (e.g., mining on Mars!)

- Bad for mixing operations (e.g., mixing of pharmaceutical powders)

Either way, a better understanding of the segregation phenomenon will lead to improved processing...
Many, many causes…

- Percolation / sieving: *Nico Gray’s talk!*
- External forces (e.g., drag force)
- Granular temperature (KE of velocity fluctuations) gradient: *this talk*
- Etc…

Where to begin? Limit Scope! Here we will (mostly) consider “rapid granular flows”

- rapid: binary (“dilute”) and instantaneous contacts (not enduring)
- granular: role of interstitial fluid phase is negligible
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Modeling Approaches

**Discrete Element Method (DEM):** an equation of motion (Newton’s law) is solved for each particle in the system:

\[ \sum F = ma = m \frac{d\mathbf{V}}{dt} \]

\[ \longrightarrow \text{particles are treated as discrete entities} \]

**Continuum:** an averaging procedure is used to develop a single equation of motion for the particulate phase:

\[ \rho \frac{D\mathbf{u}}{Dt} = -\nabla \cdot \mathbf{P} + n \mathbf{F} \]

\[ \longrightarrow \text{particle phase is treated as a continuum} \]
Pros/Cons of DEM and Continuum Approaches

**DEM**

1) **Disadvantage:**
   Computationally intensive
   (tracking of individual particle trajectories requires solution of EOM for each particle present in system)

   *Current desktop (serial) capabilities:*
   ~10,000 particles

   *Pilot plant unit:*
   ~10,000,000,000 particles

**Continuum**

1) **Advantage:**
   Less computational overhead
   (single equation of motion for each particle phase)

   **BUT,** for more complex systems, however, the computational savings is not as great...

   Example (van Wachem et al., 2001):
   CPU time for transient, 3D simulation of fluidized bed with binary particle mixture (=4 weeks f/ 14s real time on 166 MHz IBM RS 6000) is one order of magnitude > monodisperse case.
### Pros/Cons (con’t)

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<tr>
<th><strong>DEM</strong></th>
<th><strong>Continuum</strong></th>
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<tbody>
<tr>
<td><strong>2) Advantage:</strong> “Straightforward” to incorporate complex physics</td>
<td><strong>2) Disadvantage:</strong> Averaging gives rise to unknown terms that require constitutive relations (e.g., stress)</td>
</tr>
<tr>
<td>• nonuniform size/density</td>
<td>Challenging to specify for “simple” systems (e.g., smooth, inelastic, monodisperse particles), and even more difficult for complex systems (e.g., polydisperse)</td>
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<td>• frictional effects</td>
<td>Example: For rapid granular flows, several theories exist for mixtures with discrete number of species though no theories for continuous size distributions are available</td>
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<td>• cohesive (attractive) forces</td>
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Nonetheless, constitutive relations (or models) are still required to describe particle-particle contacts, gas-solid drag, etc., however, number of required constitutive relations is fewer than for Eulerian approach.
### Pros/Cons (con’t)

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<td><strong>3) Disadvantage:</strong> Physical insight &amp; system design is often more challenging</td>
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<tr>
<td>- for design and optimization, parameters too large for trial-and-error approach</td>
<td>- examination of governing equations and order-of-magnitude analysis allows for identification of important physical mechanisms</td>
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<td>- can use to observed trends, but difficult to identify source of trends</td>
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**Analogy:** DEM models vs. continuum models  
numerical solutions vs. analytical solutions to equations
**DEM vs. Continuum Modeling?**

**Bottom Line:** Due to tradeoffs, both DEM and continuum models will continue to play a complementary role in modeling particulate systems.

For example, DEM models, along with experiments, provide a good testbed for continuum models assuming DEM systems are small enough to be computationally efficient and large enough for good averaging.
DEM Models: Particle Contact

before contact

\( \omega_1 \) \hspace{1cm} \omega_2 \hspace{1cm} \rightarrow \hspace{1cm} \rightarrow \hspace{1cm} \rightarrow \hspace{1cm} \text{at contact} \hspace{1cm} \text{deformation (often small) occurs at contact!} \hspace{1cm} \text{after contact} \hspace{1cm} \nu_1' = ? \hspace{1cm} \nu_2' = ? \hspace{1cm} \omega_1' = ? \hspace{1cm} \omega_2' = ?

Q: In the context of MD simulations, is it important to accurately model particle deformation, or is its outcome (i.e., post-collision velocities) all that matters?

A: It depends!

Scenario 1: Dense collection of particles with enduring, multiple contacts

deformation theory important, since stress transmission during contact (e.g., “stress chain” across particles) impacts flow behavior

Scenario 2: Not-so-dense system with \(~\) instantaneous, binary collisions

deformation dynamics negligible
DEM: Hard sphere

- Details of deformation are not modeled
  - Pro: computationally efficient (relatively)
  - Con: limited to “rapid” (not-so-dense) flows
- Equations for collision resolution are determined via
  - Conservation of overall momentum (translational + rotational)
  - Definition of energy dissipation (e.g., via restitution coefficient $e$)

**Normal direction (along line of particle centers):**

\[
\begin{align*}
mc'_1 &= mc_1 - J = mc_1 - \frac{m}{2}(1+e)(k \cdot c_{12})k \\
mc'_2 &= mc_2 + J = mc_2 + \frac{m}{2}(1+e)(k \cdot c_{12})k
\end{align*}
\]

where:
- $c$ = pre-collision vel.
- $c'$ = post-collision vel.
- $J$ = impulse (amount of momentum exchanged from 1 to 2)
- $c_{12} = c_1 - c_2$ (relative velocity)
- $e$ = restitution coefficient: $k \cdot c'_{12} = -e (k \cdot c_{12})$

**Tangential direction: analogous treatment = f (friction coefficient $\mu$, etc.)**

- Input Parameters: $e, \mu, ...$ (physical quantities that are directly measurable)
- Output Parameters: post-collisional velocities
**DEM: Soft-sphere**

- Details of deformation (integration of force) are modeled
  - Pro: applicable to dense flows as well
  - Con: computationally inefficient (relatively)
- Many force models available (Kruggel-Emden *et al*, 2007 and 2008)
  For example, spring-dashpot-slider model:

  ![Spring-Dashpot-Slider Model](image)

  - **Input Parameters:** $c_n$, $c_s$, $k_n$, $k_s$ (*not physical or directly measurable*)
  - **Output Parameters:** deformation details (force, velocities etc) and post-collisional velocities & collision duration
  - **Approach:** can choose $c_n$ and $k_n$ to match measured $e$ and collision time,
    *but particles typically made artificially soft (longer collision time)* to reduce CPU time
    (Stevens & Hrenya, 2005)
Continuum : Polydisperse Balance Equations

**Basis:** Analogy with Kinetic Theory of Gases (“rapid” flows only)

**Approach:** Statistical mechanical description based on Enskog (kinetic) eqn.

**Mass Balance** \((N \) balances for \(N\) species)

\[
\frac{Dn_i}{Dt} + n_i \nabla \cdot \mathbf{U} + \frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i} = 0
\]

**Momentum Balance** \((1\) balance)

\[
\rho \frac{DU}{Dt} + \nabla \cdot \mathbf{\sigma} = \sum_{i=1}^{N} n_i \mathbf{F}_i
\]

**Granular Energy Balance** \((1\) balance)

\[
\frac{3}{2} n \frac{DT}{Dt} - \frac{3}{2} T \sum_{i=1}^{N} \frac{1}{m_i} \nabla \cdot \mathbf{j}_{0i} = -\nabla \cdot \mathbf{q} + \mathbf{\sigma} : \nabla \mathbf{U} - \frac{3}{2} nT \zeta + \sum_{i=1}^{N} \frac{1}{m_i} \mathbf{F}_i \cdot \mathbf{j}_{0i}
\]

Garzó, Dufty & Hrenya (PRE, 2007)
Garzó, Hrenya & Dufty (PRE, 2007)
Continuum Modeling: Constitutive Relations

Mass flux

\[ j_{0i} = -\sum_{j=1}^{N} \frac{m_i m_j n_j}{\rho} D_{ij} \nabla \ln n_j - \rho D_i^T \nabla \ln T - \sum_{j=1}^{N} D_{ij}^F F_j \]

Driving forces for segregation on RHS!

Stress tensor

\[ \sigma_{\alpha\beta} = p\delta_{\alpha\beta} - \eta \left( \frac{\partial U_\beta}{\partial r_\alpha} + \frac{\partial U_\alpha}{\partial r_\beta} - \frac{2}{3} \delta_{\alpha\beta} \nabla \cdot U \right) - \kappa \delta_{\alpha\beta} \nabla \cdot U \]

Heat flux

\[ q = -\sum_{i=1}^{N} \sum_{j=1}^{N} T^2 D_{q,ij} \nabla \ln n_j + L_{ij} F_j - T\lambda \nabla \ln T \]

Cooling Rate

\[ \zeta = \zeta^{(0)} + \zeta_U \nabla \cdot U \]

Garzó, Dufty & Hrenya (PRE, 2007)
Garzó, Hrenya & Dufty (PRE, 2007)
Continuum Model: Relation to previous theories…

Garzó, Dufty & Hrenya (PRE, 2007)
Garzó, Hrenya & Dufty (PRE, 2007)

See also review of polydisperse models in chapter by Hrenya in book (2011):
Computational Gas-Solids Flows and Reacting Systems: Theory, Methods and Practice

Robustness

- Dilute to moderately dense (based on RET)
- Non-Maxwellian
- Non-equipartition
- No restrictions on $e$ (HCS = zeroth order solution
- Low $Kn$ assumption (CE expansion)

Computational Considerations

- Current Theory: $n_i$, $U$, and $T$ ($s + 2$ governing equations)
- Previous Theories: $n_i$, $U_i$, and $T_i$ ($3s$ governing equations)
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Types of Polydispersity: Binary vs. Continuous

Binary Mixtures: much previous research (expt, theory & simulation)
Continuous PSD: little previous research (expt, theory & simulation)
Do binary and continuous PSD’s behave differently?

Somewhat surprisingly, yes!

For example, consider axial segregation in bubbling fluidized beds…

In binary mixtures, monotonic behavior (segregation $\uparrow$ as size disparity $\uparrow$)

In continuous PSD’s, non-monotonic variation with distribution width

$S_{\text{cont}} = 1 \rightarrow$ perfect segregation

$S_{\text{cont}} = 0 \rightarrow$ perfect mixing
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Case Study: Lunar Regolith Ejection

Spraying of Lunar Soil upon Landing/Launches
- reduced visibility for crew
- “sandblasting” of not-so-nearby Surveyor
  (1-2 km/s = 2000-5000 mph!)
  (160-180 m = 2 football fields!)
- interference with later landings/launches

Future Ramifications: Moon Outpost (beginning 2019) Design
Case Study: Basics

Focus: Predicting Lunar Erosion Rates
- Role of Collisions
- Polydispersity

“State of the Art” Approach: Single-particle trajectory
- Inherent assumption: *no* inter-particle collisions

If collisions are important…
- Erosion rate will be impacted
- Species segregation (de-mixing) will be impacted

Q: Is DEM or continuum more appropriate? Which would you use?
Case Study: Challenges of DEM

DEM (soft-sphere): extremely wide size distribution →
very small time steps needed to integrate deformation of smallest particles

In literature, largest size ratio simulated via DEM is only \( O(10) \)!
Case Study: Challenges of Continuum Model

Continuum Model: derived for discrete number of particle sizes \( \rightarrow \) how to model a continuous PSD using \( s \) discrete particles sizes?

**Q1:** What *method* do we choose to find \( d \)'s and \( \nu_i \)'s for given \( \nu \)?

**A1:** matching of \( 2s \) moments

**Q2:** What *value* of ‘\( s \)’ is required for “accurate” representation of continuous PSD? (tradeoff: accuracy vs. CPU time)

**A2:** “collapsing” of continuum transport coefficients from GHD polydisperse theory  
 (*Garzo, Hrenya & Dufty, PRE, 2007*)

*Murray & Hrenya (in preparation)*
Continuum Model: Approximating the Continuous PSD

\[ w_j \]

\[ w_4 = 0.001 \]

\[ f_n (\text{microns}^{-1}) \]

\[ d (\text{microns}) \]
Continuum Model: Determining Number of Species

Lognormal Parameters: $d_{ave} = 894$ microns, $\sigma/d_{ave} = 30\%$
Overall Volume Fraction: $\phi = 0.1$

Zeroth-Order Cooling Rate (time$^{-1}$)

Coefficient of Restitution ($e$)

Murray & Hrenya (in preparation)
Lognormal Distribution

Conclusion: $\sigma/\mu \rightarrow$ Generally $s$

Murray & Hrenya (in preparation)
Conclusions:

• The curves for GHD predictions using $s = 1$ decrease with increasing $\sigma/d_{ave}$.

• GHD predictions using $s = 3$ agree qualitatively and quantitatively with MD data for the entire parameter space evaluated.

Murray & Hrenya (in preparation)
Q: Which would you use – DEM or continuum?

**Bottom:** settled layer
- Soft-sphere DEM

**Middle:** “collisional” layer?
- Continuum model with DEM testbed

**Top:** “above” collisions?
- Single-trajectory calculations
System Description

6 m
Computational Model: Discrete Particles

Particle-Plume Coupling

• *one-way* (particles do not impact gas, but gas impacts particles)

Particles: Discrete Element Method (DEM)

• Plume forces: *lift and drag* via Loth (*AIAA J.*, 2008) expressions for lunar conditions (*isolated sphere*)
• Contact forces: *soft-sphere* model (inelastic, frictional spheres w/ sustained contacts)

Plume

• CFD simulations (no particles) for lunar conditions

Multiphase CFD Solver

• MFIX (DOE NETL)
**MFIX Computational Domain**

**Periodic BC’s:** $x$ and $z$ direction, gravity $-y$ direction

**Anchoring & Erosion Planes:** dynamic adjustment to maintain constant distance from surface

**Base Case:**
- Monodisperse: $d = 0.1$ cm, 800 particles
- Domain size: $L_x = 1$ cm, $L_z = 0.5$ cm
- Initial Settled-bed Height: $\sim 1.4$ cm
- Anchoring Plane Height: bed height $- 4d$
- Erosion Plane Height: bed height $+ d$
Results: Cumulative Erosion

Observations (before depletion)

1) Average erosion rate (=slope) is \( \sim \) constant

2) Negative erosion (sedimentation) is present \( \Rightarrow \) collisions!!

3) Kinks on the plot: clustering instabilities?
Results: Fractional Collision Number

Observations

- Maximum fractional collision (contacts) = 0.1
- 20% of the particles in the collisional layer are engaging in a collision
Results: Relation between Collision-Erosion

Observations

- Following an increase in the collision number there is a decrease in the erosion (and vice versa)
- Collisions cause negative erosion (sedimentation)
Case Study: Summary

Current Work

• *Particle collisions are important qualitatively* (negative erosion/sedimentation) *and quantitatively* (up to 20% of particles)

Next Steps...

• DEM model: continuous PSD (e.g., lognormal distribution)
• Continuum theory
  • validate with DEM simulations (narrow distributions)
  • apply to wider distributions than possible with DEM