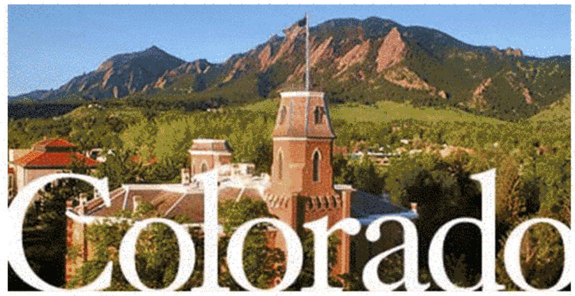
Segregation and Non-equipartition Phenomena in Hard-Sphere Mixtures



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Segregation in Collision-Dominated Flows

Hunt (1996): theory
- Thermal segregation (→ temperature gradient; no external forces)

Jenkins, Louge, and Arnarson (1998, 2000) : theory, simulations, and experiments
- Thermal segregation

Jenkins and Yoon (2002): theory
- External-force segregation (no granular temperature gradient)

Luding (2000): simulation
- Thermal segregation

Hrenya (2004): simulation
- Thermal segregation: continuous PSD

Marconi (2004): simulation
- Segregation in clustering, homogeneous cooling system

Note 1: **Theoretical contributions based on kinetic theories with equipartition assumption**
Note 2: **Comparison between theory and experiments (or simulation) performed for low mass ratios**

exception: **Brey** (last Friday's seminar!): theory
- Thermal segregation

Non-equipartition

Experiments

- **Gollub** (1999), **Wildman/Parker** (2002), **Menon** (2002)

Theory

- **Garzo/Dufty** (1999), **Barrat/Trizac** (2002), **Montanero/Garzo** (2003)

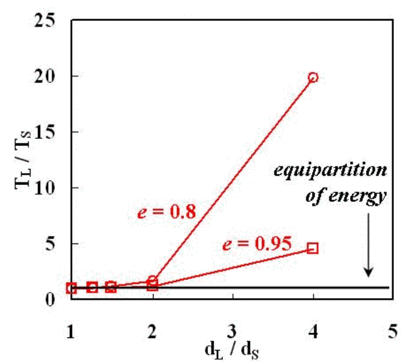
Simulation

- **Hrenya** (2002), **Luding** (2003)

Questions: **What is the impact of Non-equipartition on segregation? Is it important in practical systems?**

Motivation: **Single-temp. theory vs. multi-temp. theory**

Approach: **Compare theory (can turn equipartition on/off) to simulation (or experiment)**



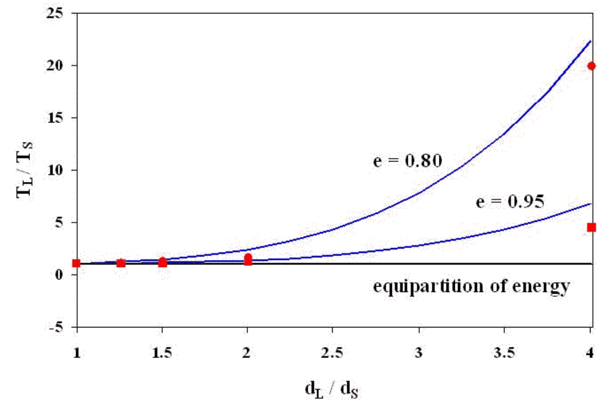
Clelland and Hrenya (PRE 2002)

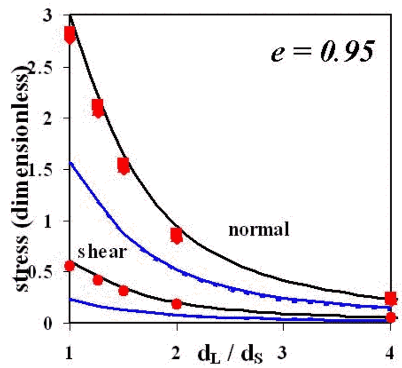
Kinetic theory for binary mixtures

Researchers	*Single-particle velocity distribution*	*Energy distribution*
Jenkins and Mancini (1987)	Maxwellian	*non*-equipartition ←
Jenkins and Mancini (1989)	*non*-Maxwellian	equipartition
Zamankhan (1995)	*non*-Maxwellian	equipartition
Arnarson and Willits (1998) Willits and Arnarson (1999)	*non*-Maxwellian	equipartition
Garzó and Dufty (2002) *(dilute systems only)*	*non*-Maxwellian	*non*-equipartition
		new

Quick assessment of theories

	velocity distribution	energy distribution
● MD data	-----	------
—— Arnarson-Willits (1998)	non-Maxwellian	equipartition
—— Jenkins-Mancini (1987)	Maxwellian	non-equipartition
- - - Jenkins-Mancini (1987)	Maxwellian	equipartition





$\phi = 0.3$

$\phi_L / \phi_S = 1$

Clelland and Hrenya (PRE, 2002)

Galvin, Dahl, and Hrenya (JFM, 2005)

Kinetic theory: species segregation

Diffusion velocity equation

Previous efforts - Hsiau and Hunt, 1996; Arnarson and Jenkins, 2000

$$\overline{v_1} - \overline{v_2} = -D_{12}\left(\frac{n^2}{n_1 n_2}\right)\left\{\begin{aligned}&\frac{\rho_1\rho_2}{\rho n T}\left[\frac{1}{\rho_1}\nabla P_1 - \frac{1}{\rho_2}\nabla P_2 - \frac{\overline{F_1}}{m_1} + \frac{\overline{F_2}}{m_2}\right] - \frac{K_{12}}{n}\left(\frac{m_2 - m_1}{m_{12}}\right)\frac{1}{T}\nabla T\\ &-\frac{K_{12}}{n}\left[\frac{1}{n_1}\nabla n_1 - \frac{1}{n_2}\nabla n_2\right]\end{aligned}\right\}$$

Key assumption : equipartition of energy

P_i : functions of n_i, T

Kinetic theory: species segregation

Diffusion velocity equation

Current effort - non-equipartition theory of Jenkins and Mancini, 1987

$$\overline{v_1}-\overline{v_2}=-D_{12}\left(\frac{n^2}{n_1 n_2}\right)\left\{\begin{array}{l}\dfrac{\rho_1\rho_2}{\rho n T}\left[\dfrac{1}{\rho_1}\nabla P_1-\dfrac{1}{\rho_2}\nabla P_2-\dfrac{\overline{F_1}}{m_1}+\dfrac{\overline{F_2}}{m_2}\right]-\dfrac{K_{12}}{n}\left(\dfrac{m_2-m_1}{m_{12}}\right)\dfrac{1}{T}\nabla T\\ -\dfrac{K_{12}}{n}\left[\dfrac{1}{n_1}\nabla n_1-\dfrac{1}{n_2}\nabla n_2\right]+\dfrac{\rho_1\rho_2}{\rho n T}\left(\dfrac{1}{\rho_1}\boxed{\nabla P_{1,new}}-\dfrac{1}{\rho_2}\boxed{\nabla P_{2,new}}\right)\end{array}\right\}$$

Non-equipartition effects

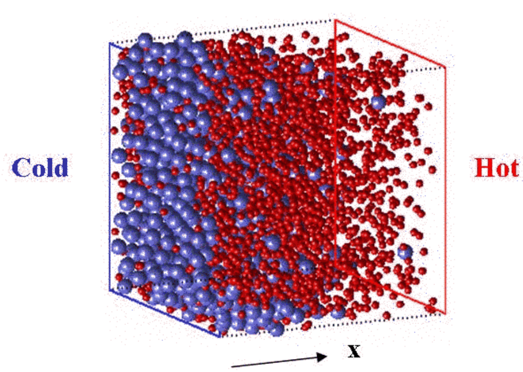
- Species temperature gradients

P_i : functions of n_i, T

$P_{i,new}$: functions of n_i, T_i

Approach: Simulation

Basic Idea: *use profiles from simulation to evaluate relative magnitude of terms impacting segregation*



System description
- No mean flow
- No external forces
- Temperature gradient (walls of unequal, constant temperature)

Algorithm
- Inelastic, frictionless particles
- Hard particle/overlap

Data collection
- Spatial-temporal averaging
- Variables reported as function of x/L

Are non-equipartition effects important?

$\phi = 0.2$

$e = 0.9$

$\phi_{heavy} / \phi_{light} = 4$

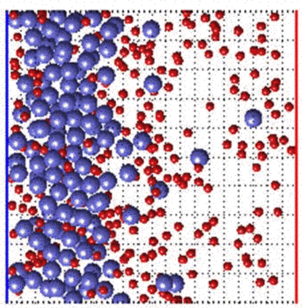
$\rho_{heavy} / \rho_{light} = 2$

$d_{heavy} / d_{light} = 2$

$T_{hot} / T_{cold} = 10$

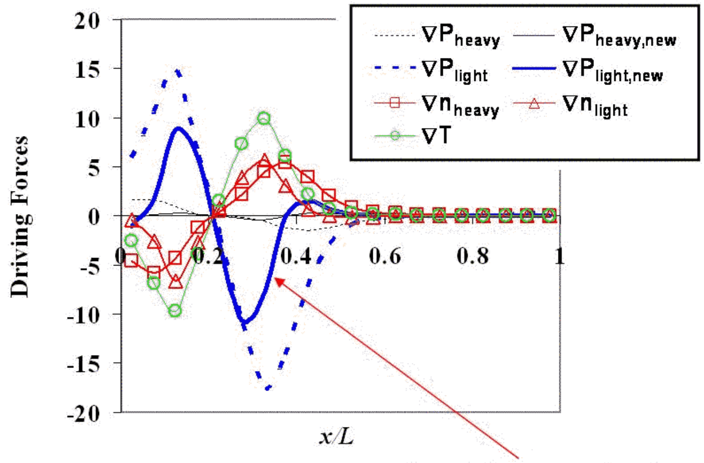
Snapshot of xy-plane

Cold



Hot

x



non-equipartition contribution

Non-equipartition effects are of similar magnitude to other terms

Galvin, Dahl, and Hrenya (JFM, 2005)

An interesting observation…

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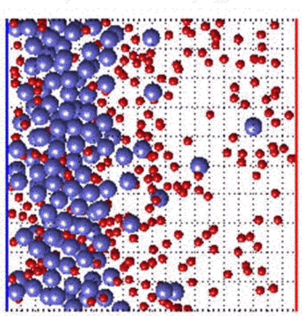
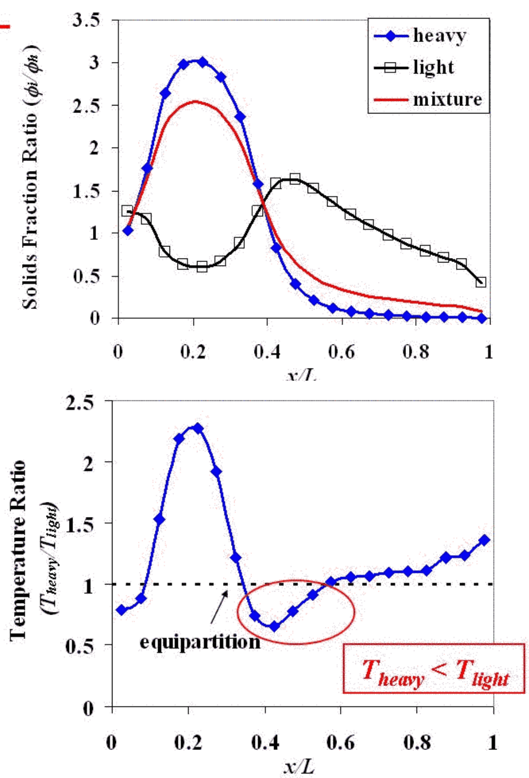


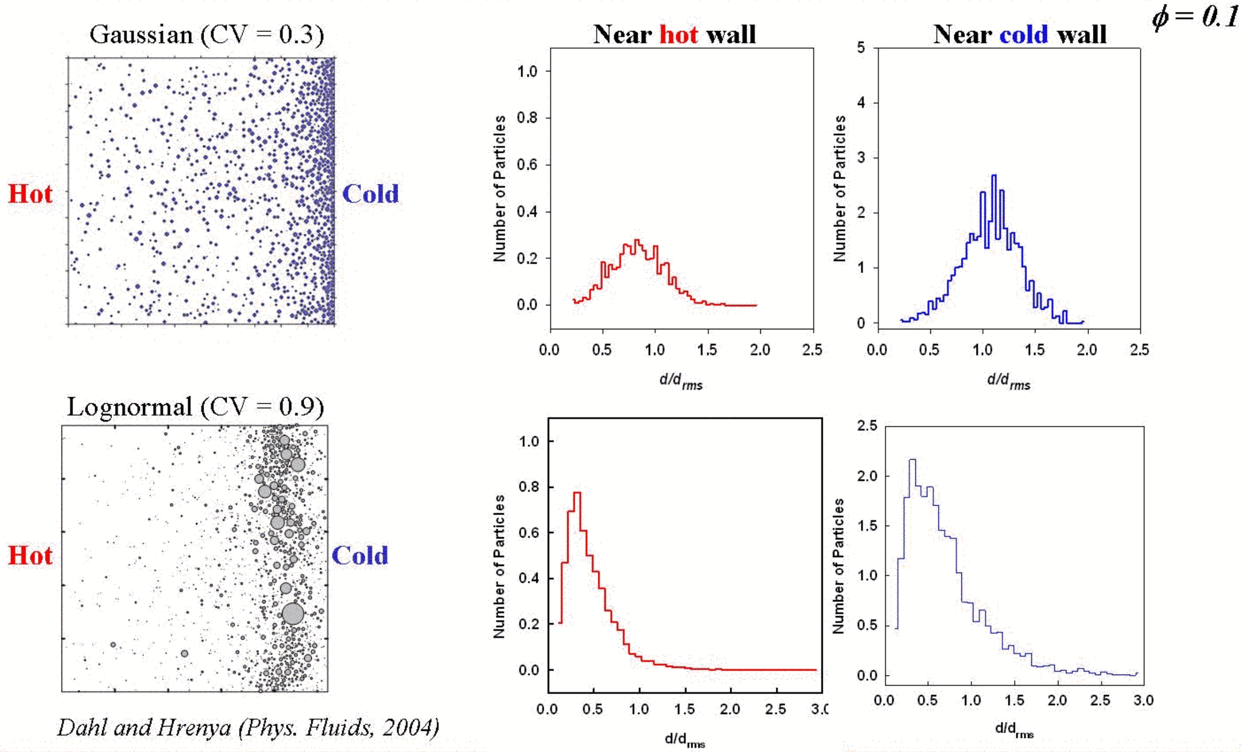
Hot

x



Galvin, Dahl, and Hrenya (JFM, 2005)

Another interesting observation: continuous PSD



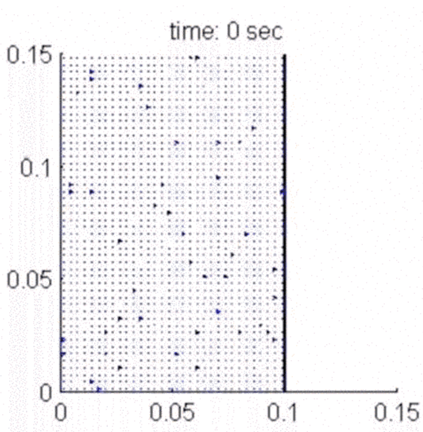
Dahl and Hrenya (Phys. Fluids, 2004)

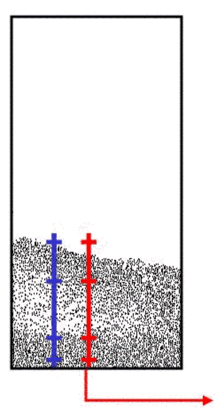
***Local* size distributions have same form as *overall* distribution, even in presence of size segregation**

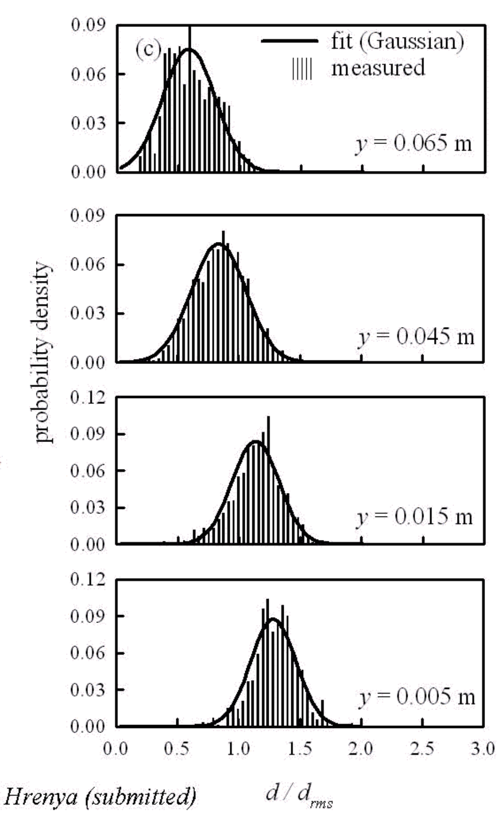
Robustness of local PSD behavior?

Fluidized Bed Simulation (2D)

Gaussian
$e = 0.95$
$N = 5000$
$\mu_f = 0.15$
$\mu_{wf} = 0$
$u_f = 1.0$ m/s
$\sigma/d_{ave} = 0.3$







Dahl and Hrenya (submitted)

Summary

Binary Mixtures

- Non-equipartition effects on segregation appear important in some systems
  - Question/Issue: Is this important in practical systems?

- MD indicates that $T_{heavy} < T_{light}$ in some regions
  - Question/Issue: Can experiments verify it? Does kinetic theory predict it? What is the responsible mechanism?

Continuous Size Distributions

- The form of *local* size distribution mimics form of *overall* size distribution for range of systems
  - Question/Issue: Can this be used to simplify theoretical descriptions of these flows?