Using DNS to Understand Aerosol Dynamics

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Direct Numerical Simulations of Microstructures

Aerosols
- Dispersion
- Turbulence modulation
- Coagulation

Droplets*
- Breakup
- Coalescence

Polymer Molecules
- Orientation
- Stretch
- Drag Reduction

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Outline

- Background on aerosols
- Direct numerical simulations (DNS)
- Numerical Results
- Theory
- Experiments
- Summary
Examples

DuPont TiO$_2$ Process

Cloud Condensation Nuclei (CCN)

Buoyancy

R. Shaw, ARFM 2003
Turbulent clustering

Aerosol particles in a turbulent flow field cluster outside of vortices due to a centrifugal effect, sometimes referred to as “preferential concentration.”

Maxey (1987)
Squires & Eaton (1991)
Wang & Maxey (1993)
Snapshot of particle clustering in DNS

Snapshot from a DNS (St=1 and $R_{\lambda} = 54$). The **green tubes** are vortex tubes where fluid circulates rapidly and the **white** shows where the particle concentration is greater than 10 times the mean.

How does this affect coalescence rates?
Direct numerical simulation

\[ \nabla \cdot \mathbf{u} = 0 \]

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{\nabla p}{\rho} = \nu \nabla^2 \mathbf{u} + \mathbf{F} \]
Particle update

\[
\begin{align*}
\frac{dx_p^{(i)}}{dt} &= \mathbf{v}_p^{(i)} \\
\frac{dv_p^{(i)}}{dt} &= \left[ \mathbf{u}(x_p^{(i)}, t) - \mathbf{v}_p^{(i)} \right] \frac{\tau_p^{(i)}}{\tau_p^{(i)}} + \sum_{j \neq i} F^{(ij)} \\
\tau_p^{(i)} &= \frac{1}{18} \frac{\rho_p}{\rho} \left( \frac{d}{\eta} \right)^2
\end{align*}
\]

Stokes drag

Collisions
(neighborhood search)
Particle-particle interactions

Elastic Rebound:

Coalescence:

Interpenetration:
Parameters

Flow:
\[ U' \] turbulence intensity
\[ \varepsilon \] dissipation rate
\[ \nu \] kinematic viscosity

Particles:
\[ d \] diameter
\[ \rho_p \] density
\[ n \] loading

\[ R_\lambda = \sqrt{\frac{15}{\nu \varepsilon}} U'^2 \]

\[ St = \frac{\tau_p}{\tau_\eta} \] Stokes number
\[ \frac{d}{\eta} \] size parameter
\[ \Phi \] volumetric loading
**Parameter Ranges**

<table>
<thead>
<tr>
<th>System</th>
<th>$R_\lambda$</th>
<th>$St$</th>
<th>$d/\eta$</th>
<th>$\Phi$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clouds</td>
<td>$10^4$</td>
<td>$10^{-4} - 10^{-1}$</td>
<td>$10^{-2} - 10^{-3}$</td>
<td>$&lt; 10^{-6}$</td>
</tr>
<tr>
<td>DNS</td>
<td>$50 - 160^*$</td>
<td>$10^{-2} - 1$</td>
<td>$10^{-2} - 10^{-1}$</td>
<td>$&lt; 10^{-5}$</td>
</tr>
<tr>
<td>Exp't</td>
<td>$10^2 - 10^3$</td>
<td>$&gt; 10^{-3}$</td>
<td>$10^{-2} - 10^{-1}$</td>
<td>$&lt; 10^{-5}$</td>
</tr>
</tbody>
</table>

- We are not able to simulate **atmospheric Reynolds numbers**
- It’s therefore critical that we understand the importance of this parameter (from experiments, theory, etc.)

* High end DNS is $4096^3$, corresponding to $R_\lambda \sim 1000$
  Gotoh & Fukayama (2001)
Limiting theories for collision

Saffman and Turner (1956)
Zero Stokes number:

\[ N_c = \frac{1}{2} n^2 d^3 \left( \frac{8\pi \epsilon}{15 \nu} \right)^{1/2} \]

Abrahamson (1975)
Infinite Stokes number:

\[ N_c = \frac{1}{2} n^2 d^2 \left( \frac{16\pi \frac{v^2}{p}}{3} \right)^{1/2} \]

Brunk, Koch & Lion (1998)
Wang, Wexler and Zhou (1998)

Reade & Collins (1998)

\( n \) number density
\( \frac{v^2}{p} \) particle kinetic energy
Collision vs Stokes number

Sundaram & Collins (1997)
Evolution of size distribution

Reade & Collins JFM (2000)
General collision formula

\[ N_c = \pi d_{ij}^2 n_i n_j g_{ij}(d_{ij}) \int_{-\infty}^{0} (-w) P_{ij}(w | d_{ij}) \, dw \]

\[ d_{ij} = \frac{(d_i + d_j)}{2} \]

\[ g_{ij}(r) = \text{radial distribution function (RDF)} \]

\[ w = \text{relative velocity} \]

\[ P(w | r) = \text{PDF of relative velocity} \]

RDF corrects for preferential concentration
(dominant effect at low Stokes numbers)

Sundaram & Collins (1997)
Wang, Wexler and Zhou (1998)
RDF \( g(r) \equiv \frac{\text{# pairs}}{\text{expected # pairs}} \)

Parametric Dependence
- volume fraction
- Stokes number
- size parameter
- Reynolds number

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Stokes number dependence

- Graph showing RDF (Redistribution Function) vs. St (Stokes number)
- Different symbols and colors represent different Reynolds numbers:
  - Re = 82.5 (red diamonds)
  - Re = 69.7 (blue triangles)
  - Re = 54.5 (green diamonds)
  - Re = 37.1 (black circles)

- Images labeled (a) to (f) with St values 0.0, 0.2, 0.7, 1.0, 2.0, and 4.0 respectively.
Bi-disperse St dependence

Suppression of off-diagonal collisions broadens the distribution
Size parameter

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Physics of clustering

Maxey (1987)

Frame moving with a test particle

Rotation

Strain

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Recent Theoretical Developments

  - relative velocity clustering effect

- **Falkovich, Fouxon and Stepanov (2002)**
  - clustering effect in clouds

- **Zaichik & Alipchenkov (2003)**
  - relative velocity clustering

- **Chun, Koch, Ahluwalia & Collins (2003)**
  - clustering \((St \ll 1)\)
  
  \[
g\left(\frac{r}{\eta}\right) = c_0 \left(\frac{\eta}{r}\right)^{c_1}
\]

\[
c_0 \left(R_\lambda, St, \Phi\right)
\]

\[
c_1 \left(R_\lambda, St, \Phi\right)
\]

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\[
\frac{\partial g}{\partial t} = -\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 A \frac{\partial g}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 B r^2 \frac{\partial g}{\partial r} \right]
\]

\[
A = \frac{St}{3 \tau_\eta} \left( \langle S^2 \rangle_p - \langle R^2 \rangle_p \right)
\]

\[
\frac{\Delta \langle S^2 \rangle_p}{St} = \left[ \frac{\sigma_\varepsilon^2}{\varepsilon^2} T_{\varepsilon\varepsilon} - \frac{\rho_{\varepsilon\varepsilon} \sigma_\varepsilon \sigma_\zeta}{\varepsilon^2} T_{\varepsilon\zeta} \right], \quad \frac{\Delta \langle R^2 \rangle_p}{St} = \left[ \frac{\rho_{\varepsilon\varepsilon} \sigma_\varepsilon \sigma_\zeta}{\varepsilon^2} T_{\varepsilon\zeta} - \frac{\sigma_\zeta^2}{\varepsilon^2} T_{\zeta\zeta} \right]
\]

**Steady State**

\[
g(r) = c_0 \left( \frac{\eta}{r} \right)^{c_1}
\]

\[
c_1 = \frac{A}{B} = 6.6 \text{ St}^2
\]

\[
c_1 = 3.6 \text{ St} \left( \langle S^2 \rangle_p - \langle R^2 \rangle_p \right)
\]
Chun et al. (2003) Bidisperse

- Fluid accelerations give rise to relative diffusion

\[ g_{AB}(r) = c_0 \left[ \frac{\eta^2}{r^2 + r_c^2} \right]^{c_1/2} \]

\[ r_c = B' \left| St_A - St_B \right| \eta \]

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Reynolds Number Dependence

\[ c_1 = 3.6 \text{ St } \left( \frac{S^2}{R^2} \right)_p - \left( \frac{R^2}{S^2} \right)_p \]
Experimental 3D Particle Imaging
Professor Hui Meng

Why 3D?

- Cover a Broader Range of $R_\lambda$
- Validate DNS and Theory

Holtzer & Collins (2002)
Preliminary Results

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Particle Tracking
Eberhard Bodenschatz and Zellman Warhaft

Wind Tunnel
(active grid)

- Track droplets
  - Multiple (4) cameras
  - High speed (above 50,000 fps)
  - Integral time and length scales
- Measure accelerations
  - Compare with DNS
  - Test theoretical predictions

Droplets
10 - 50 microns

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Summary

- **Particle clustering in turbulent flows**
  - Increases collision frequency 1-2 orders of magnitude
  - Strongly favors like collisions; broadens particle size distribution

- **Theoretical predictions for RDF**
  - Stokes number dependence
  - Size parameter
  - Reynolds number dependence remains in dispute (key for cloud physics)

- **Experiments**
  - Validate DNS and theory
  - Increase the range of Reynolds numbers

- **Enabling Technologies**
  - 3D imaging essential
  - Holographic imaging (RDF at an instant)
  - High-Speed Stereoscopic Tracking (Lagrangian statistics)

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DNS has continuously guided theoretical and experimental work

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Future Work

- High-resolution DNS (JC.001)
  - Effect of shear flow
  - Hydrodynamic interactions
- Extend theory to coalescing system
- Experimental measurements
  - HPIV at an instant
  - Lagrangian statistics