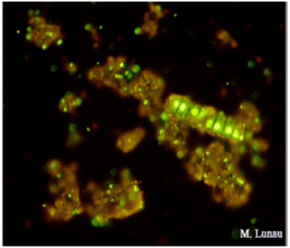
Aggregation and fragmentation dynamics of aerosols in synthetic turbulence

Ksenia Guseva, Ulrike Feudel

ICBM, University of Oldenburg

PARTICLES IN A FLOW

- Rain drops in clouds
- Marine aggregates (carbon cycle)
- Industrial colloids
- Formation of planets

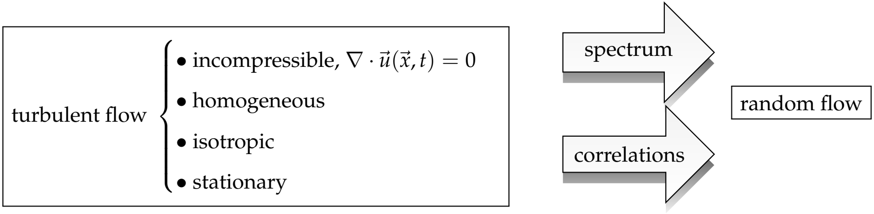


Outline

- Model
  - Flow field – Random flow
  - Inertial particles
  - Interacting particles in a flow field (aggregation and fragmentation)
- Results
  - Steady state – balance between aggregation ad fragmentation
  - Influence of the flow field

Random flow

mimicking turbulence at the dissipative scale



- Random fourrier modes (Kraichnan)
- Stochastic differential equation

Random flow

Ornstein-Uhlembeck process

$$\vec{u} = \nabla \times \psi(\vec{r})\vec{n_z} = \begin{bmatrix} \partial_y \psi \\ -\partial_x \psi \end{bmatrix}$$

with

$$\vec{k} = \frac{2\pi}{L} \begin{bmatrix} n_x \\ n_y \end{bmatrix}$$

(wave number),

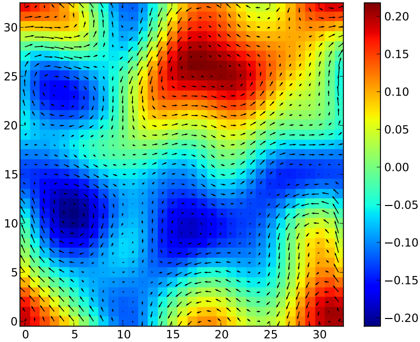
$$\psi(r,t) = u_0 \frac{\sqrt{\pi}\lambda^2}{L} \sum_{\vec{k}} \xi_k e^{\left(i\vec{k}\cdot\vec{r} - \frac{\lambda^2 k^2}{4}\right)}$$

Kraichnan energy spectrum:
$E(k) \sim k^3 e^{-\lambda^2 k^2}$

$$\xi_k(t+dt) = \xi_k(t)\left(1 - \frac{dt}{\tau}\right) + \sqrt{\frac{2dt}{\tau}} dw_k$$

- u_0 – mean velocity,
- λ – correlation length,
- $\frac{\lambda}{u_0} = \tau_e$ – eddy turnover time,
- τ – correlation time,
- w_k – Gaussian noise.

Random flow



- Gaussian statistics
- single length scale
- Kubo number

$$Ku = \frac{u_0 \tau}{\lambda}$$

$Ku < 1$ – stirring (nonlinear regime)

$Ku > 1$ – persistence of coherent structures

$Ku \sim 1$ – “turbulence”

Particle advection

- Tracers $\rightarrow$ $v_p = u_f$: "point like"

  Follow the flow filed exactly, behave as part of it.

- Inertial particles:

  Do not follow the flow field exactly, because of:

$$\text{Size and Density} \begin{cases} \text{Aerosol, } \rho_p > \rho_f \text{(falls)} \\ \text{Bubbles, } \rho_p < \rho_f \text{(rises)} \end{cases}$$

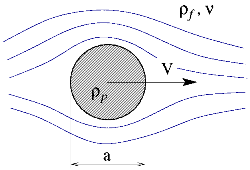
There are additional (aerodynamic or hydrodynamic) forces which act on inertial particles, they have to be included

Forces exerted on the particle

Newton's law

Assumptions and approximations:

- spherical particles (shape is very important);
- viscous fluid;
- small $Re_p = \frac{a(u - v_p)}{\nu}$.



$$F_{tot} = F_{\text{drag}} + F_{\text{added mass}} + F_{\text{gravity}} + F_{\text{history}}$$

Equations of motion

Inertial particles – Maxey-Rilay equations

$$\frac{d\vec{V}}{dt} = \underbrace{\frac{1}{St}(\vec{u} - \vec{V})}_{\text{Stokes drag}} + \underbrace{\beta \frac{D\vec{u}}{Dt}}_{\text{Pressure term}} - \underbrace{\sqrt{\frac{9St}{\beta 2\pi}} \int_0^t \frac{\frac{d(\vec{V}-\vec{u})}{dt}}{\sqrt{t-\tau}} d\tau}_{\text{History (Basset)}}$$

$$St = \frac{r^2}{3\nu\beta}\frac{1}{\tau_f}$$

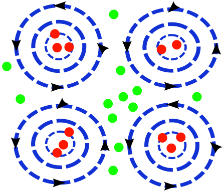
$$\beta = \frac{3\rho_f}{\rho_f + 2\rho_p} \begin{cases} \beta < 1 & \text{aerosols} \\ \beta > 1 & \text{bubbles} \end{cases}$$

- r — particle radius
- ν — kinetic viscosity
- τ_f — time scale of the flow
- ρ_p — particle density
- ρ_f — fluid density

Effects of inertia

Preferential concentration – centrifugal effect

- Aerosols avoid the regions of high vorticity (green dots)
- Bubbles are trapped by the regions of high vorticity (red dots)



Caustics

- Particles with very different velocities close to each other in space
- Increase of the collision rates

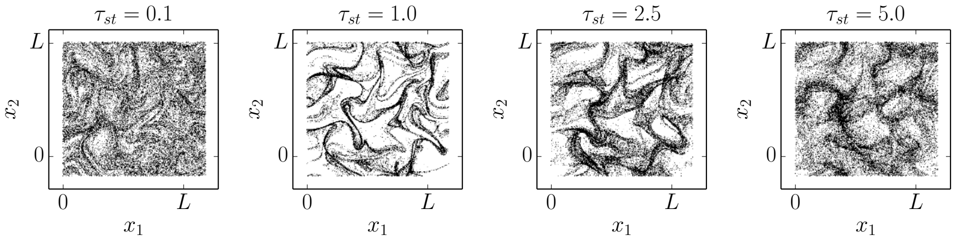
STOKES NUMBER

ASYMPTOTICS

$\boxed{St \to 0}$

$\vec{u}(\vec{x},t) \sim \vec{v}_p$ and the particle becomes a tracer.

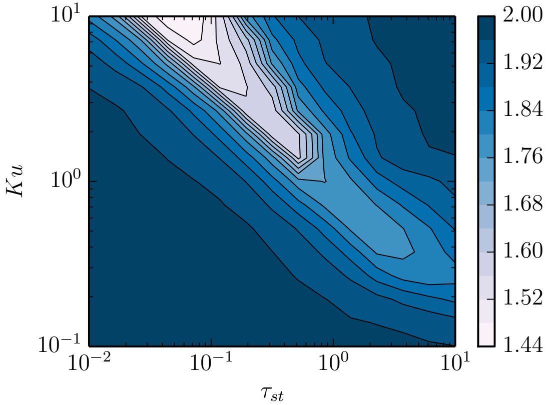
$\boxed{St \to \infty}$



Ergodic vs non-ergodic clustering

Effects of the flow

Capacity dimension, D_0 of the spatial distribution of particles.



$Ku < 1$

particles experience the velocity field as noise signal

$Ku > 1$

aerosols expelled from persistent coherent structure

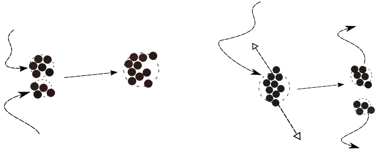
Aggregation and fragmentation dynamics

Steady-state size distribution

Advection $\longrightarrow$ Aggregation $\longrightarrow$ Fragmentation

α_i – size class, composed by i unit particles

α_1	α_2	α_3	α_4	α_5	$\cdots$	α_n



Aggregation:

$$\alpha_i + \alpha_j \rightarrow \alpha_{i+j}$$

- All particle collisions result in aggregation

Fragmentation:

$$\alpha_{i+j} \rightarrow \alpha_i + \alpha_j$$

- Due to forces in the flow
- Binary (two fragments)
- Cascade of fragmentation events

Fragmentation

Critical shear

Particles break when the shear forces of the flow exceed the binding forces.

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i}\right)$$

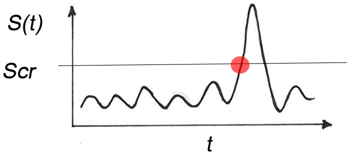
$$S = (2S_{ij}S_{ji})^{1/2}$$

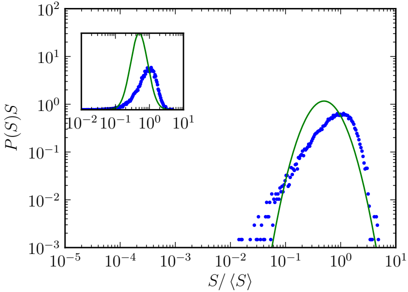
$$\boxed{S_{crit} = \gamma \alpha_i^{-1/3}}$$

α_i – particle size class

γ – binding strength

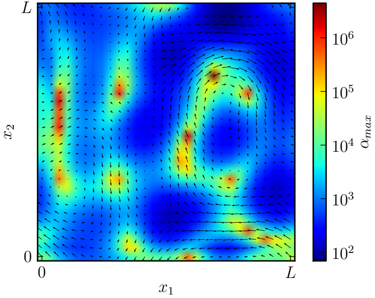
$$\boxed{\text{If } S_{flow}(\mathbf{X}) > S_{crit} \rightarrow \text{break.}}$$

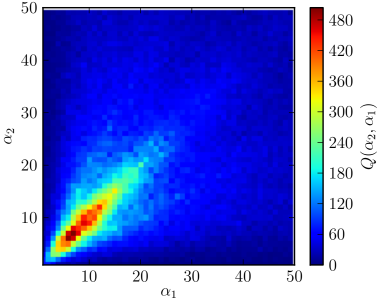




Location of events

Shear forces of the flow

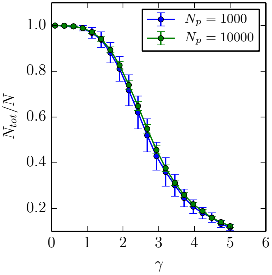




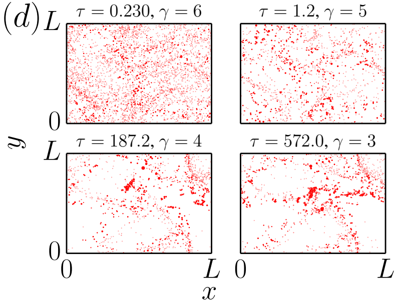
aggregate sizes:
- binding strength γ
- correlation time τ_f:
  - preferential concentration $\longrightarrow$ aggregation
  - changes of $S_{cr}(\alpha, x_1, x_2, t)$ $\longrightarrow$ fragmentation

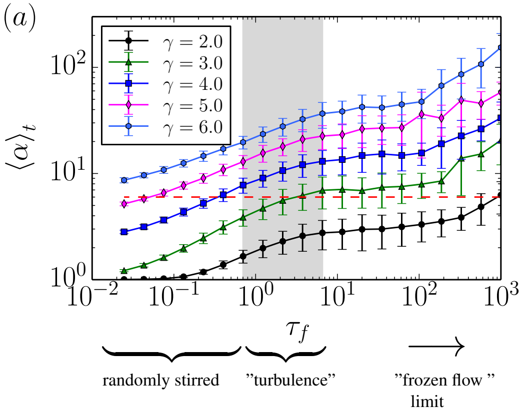
Aggregates size distributions

Binding strength (γ) and time scale of the flow (τ)

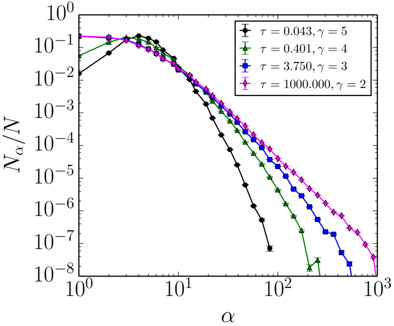


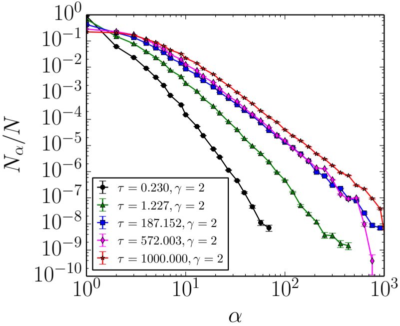
$$\tau_f \begin{cases} \text{preferential concentration} \longrightarrow \text{aggregation} \\ \text{changes of the shear forces} \longrightarrow \text{fragmentation} \end{cases}$$





SIZE DISTRIBUTIONS





aggregate sizes $\begin{cases} \text{small } Ku \\ \text{large } Ku \longrightarrow \text{"frozen flow" limit – broad distributions} \end{cases}$

CONCLUSIONS

- Importance of the fragmentation rates
- The fragmentation rate depends on the flow properties, Ku
- For $Ku \sim 1$, the fragmentation results from the interplay of the sampling of coherent flow structures and of the local changes of the flow
- The fragmentation by local forces in the flow segregates the particles by sizes, increasing the collision rates between similar particles