Dynamics and collisions of anisotropic particles settling in turbulence: application to cloud microphysics

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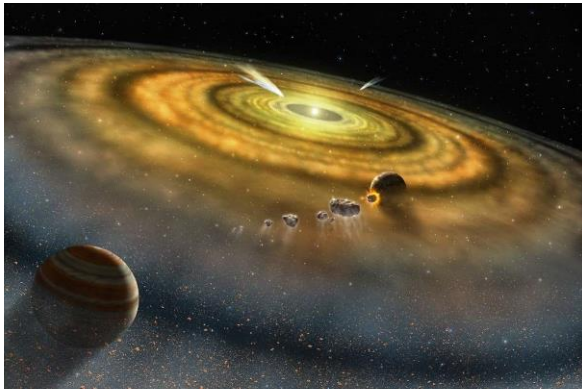
Introduction



Particles in turbulence

(solid inclusions, drops, bubbles)

Turbulent transport of small (d < η) inclusions

Lagrangian description of particles motion by a force balance:

$$m_p \frac{d\mathbf{V}}{dt} = m_p\mathbf{g} + m_f\left(\frac{D\mathbf{U}}{Dt} - \mathbf{g}\right) + \mathbf{F_P}$$

$\mathbf{F_P}$ (force due to the particle) = ???

Turbulent transport of small (d < η) inclusions

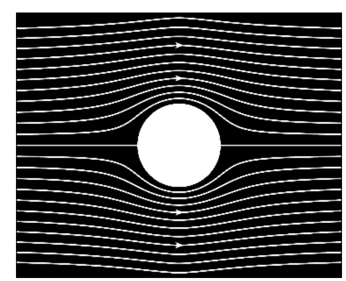
Basset-Boussinesq-Oseen equation (spherical solid particle)

Boussinesq , C. R. Acad. Sci. Paris 1885; *Basset,1888*
(revisited by *Gatignol, J. Mech. Theor. Appl. 1983*; *Maxey & Riley, PoF 1983*)

$$m_p \frac{d\mathbf{v}_p}{dt} = m_f \frac{D\mathbf{u}}{Dt} + 6\pi r \mu_f (\mathbf{u} - \mathbf{v}_p) + \frac{1}{2} m_f \left(\frac{D\mathbf{u}}{Dt} - \frac{d\mathbf{v}_p}{dt} \right)$$
$$+ 6r^2 (\pi \mu_f \rho_f)^{1/2} \int_0^t \frac{d(\mathbf{u} - \mathbf{v}_p)/d\tau}{(t-\tau)^{1/2}} d\tau + (m_p - m_f)\mathbf{g}$$

= Fluid acceleration + Stokes drag + Added mass + History force + Buoyancy

Expression derived assuming a Stokes flow
at the particle scale: $Re_p = 2r|u-v|/\nu << 1$!!!

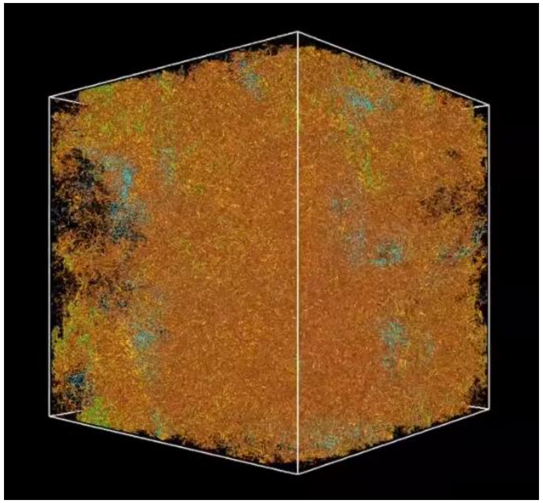


Turbulent transport of small ($d < \eta$) inclusions

In the limit of small, spherical, very dense particles, $\rho_p/\rho_f >> 1$

(e.g., sand in air, water droplets in air, …)

$$m_p \frac{d\mathbf{v}_p}{dt} = 6\pi r \mu_f (\mathbf{u} - \mathbf{v}_p) + m_p \mathbf{g} \quad \longrightarrow \quad \frac{d\mathbf{v}_p'}{dt} = \frac{\mathbf{u}' - \mathbf{v}_p'}{St} + \mathbf{g}'$$



Ireland & Collins

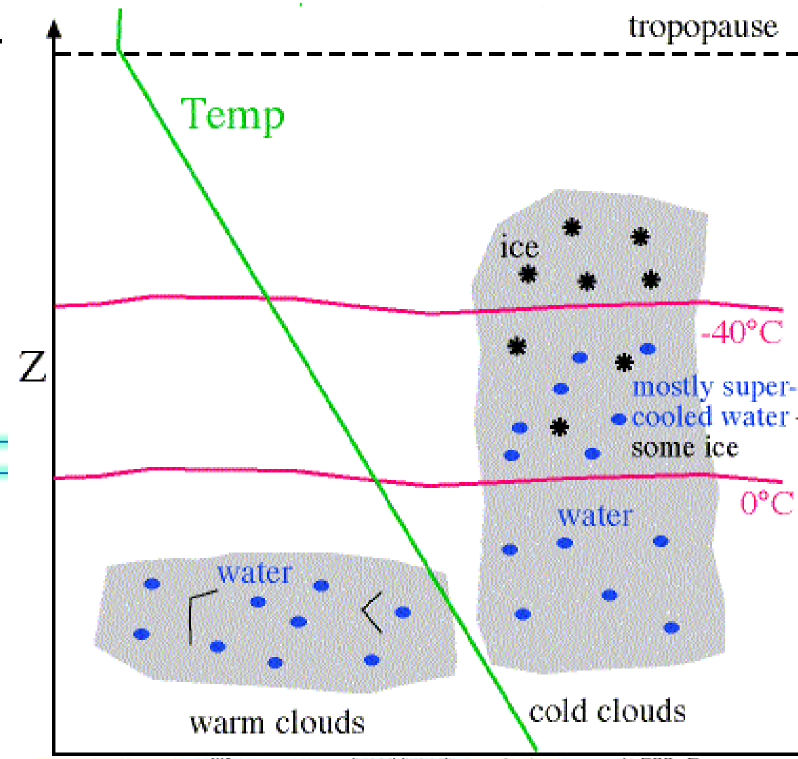
$$St = \frac{2r^2}{9\nu\tau_\eta}\frac{\rho_p}{\rho_f} = \tau_p / \tau_\eta$$

Stokes number

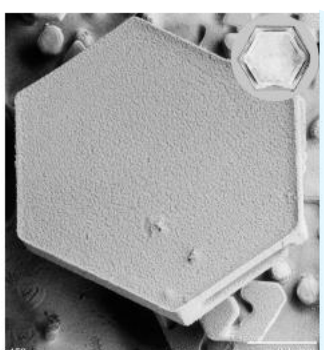
- St<<1: particle ~ fluid tracer
- St ↑: particle inertia ↑

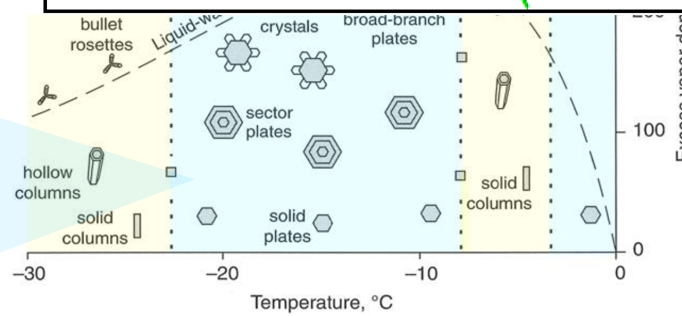
Ice particles in cold clouds

- Cold clouds (top < 0°C) contain ice particles.



- For $-20\,^{\circ}\mathrm{C} \lesssim T \lesssim -10\,^{\circ}\mathrm{C}$, these particles are shaped like plates.

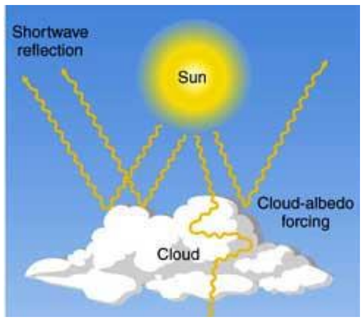




W. Brune (after Lamb and Verlinde)

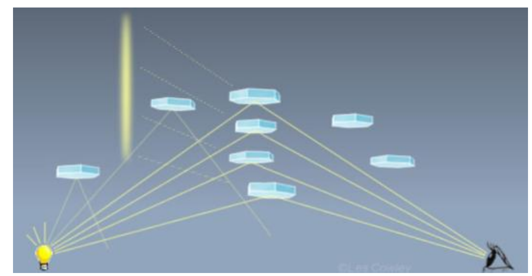
Settling, orientation, collisions and aggregation of particles in cold clouds

- Ice crystals orientation
  → EM waves (light) reflexion, albedo

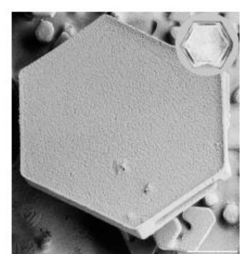


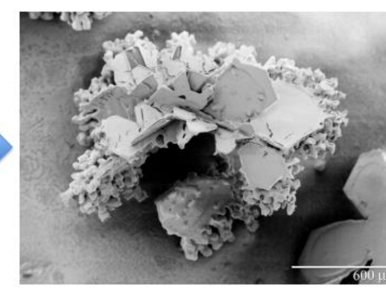
See also *Bréon & Dubrulle, JAS 2004*.

https://www.atoptics.co.uk/halo/lpil.htm



- Collision and aggregation of ice crystals
  → formation of graupels



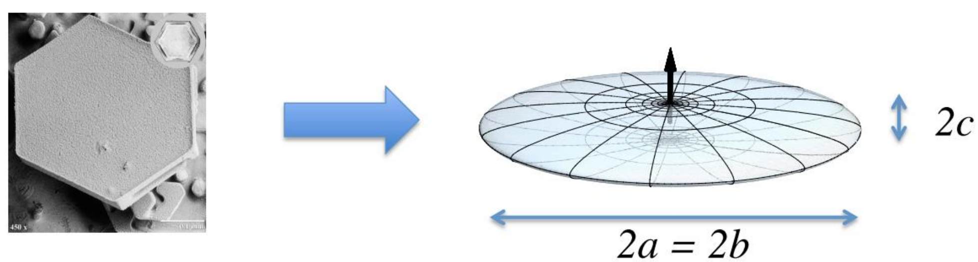


Electron and confocal microscopy laboratory, US Agriculture Research Center

Purpose of the study

- Determination of the crystals orientation and settling velocity, and of their collision rate, in turbulent conditions and with gravity.
  Direct numerical simulation of an idealized system.

- Assume that the crystal is a thin oblate ellipsoid of revolution (spheroid): $c \ll b=a$.



$\beta \equiv a/c$

- Small ($a < \eta$), heavy ($\rho_p \gg \rho_f$) and spheroidal particle.

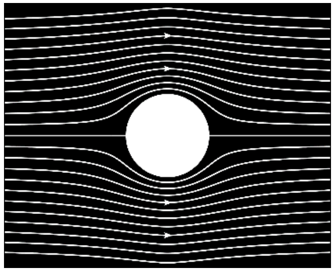
- Equation of motion ? Force and torque acting on the spheroid ?

Equations of motion of the spheroids:
the role of fluid inertia

Equations of motion of the spheroids

- Translational and rotational dynamics of spheroidal particles in turbulence:
  For particles ≠ fluid tracers, need to write equations of motion

  m_p d**v**/dt = **hydrodynamic force** + buoyancy
  I_p dω/dt = **hydrodynamic torque**



- Using Stokes approximation: hydrodynamic force = Stokes force
  hydrodynamic torque = Jeffery's torque

For a spherical object: $\mathbf{F}_{Stokes} = 6\pi r \mu_f (\mathbf{u} - \mathbf{v}_p)$

First effect of fluid inertia:

$$\mathbf{F}_{Oseen} = \mathbf{F}_{Stokes} \times \left(1 + \frac{3Re_p}{16}\right) \sim \mathbf{F}_{Stokes} \text{ if } Re_p \ll 1$$ (in practice if r << η)

Translational motion (Stokes)

$$\frac{\mathrm{d}\boldsymbol{r}_C}{\mathrm{d}t} = \boldsymbol{v}_C,$$

$$\frac{\mathrm{d}\boldsymbol{v}_C}{\mathrm{d}t} = \frac{\nu\rho_f}{m_C}\boldsymbol{R}^{-1}\hat{\boldsymbol{K}}\boldsymbol{R}\cdot[\boldsymbol{u}(\boldsymbol{r}_C,t)-\boldsymbol{v}_C]+\boldsymbol{g}$$

- $\hat{\boldsymbol{K}}$: anisotropic resistance tensor, expressed in the eigenframe of the particle
- **R** : rotation matrix (laboratory frame → particle eigenframe)
- **u**: fluid velocity
  $\mathbf{v}_C$: particle velocity

Rotational motion (Stokes)

- **Angular momentum:** *(Jeffery, 1922)*

$$\frac{d}{dt}\begin{pmatrix}\Omega_x\\ \Omega_y\\ \Omega_z\end{pmatrix} = \begin{pmatrix}\Omega_y\Omega_z\frac{\beta^2-1}{1+\beta^2}\\ \Omega_z\Omega_x\frac{1-\beta^2}{1+\beta^2}\\ 0\end{pmatrix} + 20\frac{\rho_f}{\rho_p}\frac{\nu}{a^2}\begin{pmatrix}\frac{1}{\alpha_0+\beta^2\gamma_0} & 0 & 0\\ 0 & \frac{1}{\alpha_0+\beta^2\gamma_0} & 0\\ 0 & 0 & \frac{1}{2\alpha_0}\end{pmatrix}\begin{pmatrix}\frac{1-\beta^2}{1+\beta^2}\hat{S}_{yz}+(\hat{\Omega}_{zy}-\Omega_x)\\ \frac{\beta^2-1}{1+\beta^2}\hat{S}_{xz}+(\hat{\Omega}_{xz}-\Omega_y)\\ (\hat{\Omega}_{yx}-\Omega_z)\end{pmatrix}$$

Ω : angular velocity of the particle (in its reference frame !)

$$\mathrm{A}_{ij} = \partial_j u_i$$

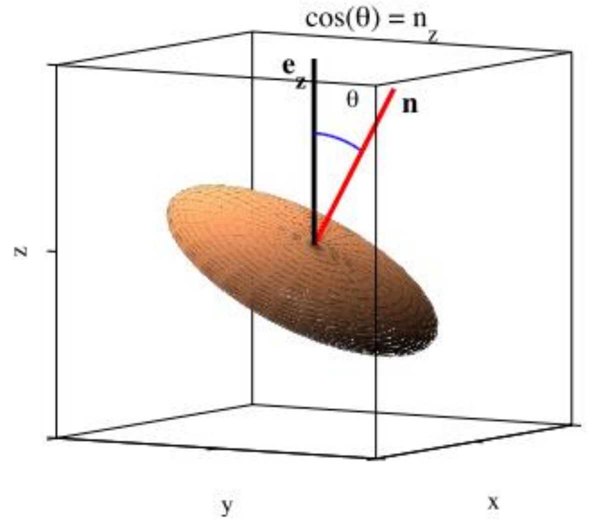
$$\hat{\mathbf{A}} = \mathbf{R}\mathbf{A}\mathbf{R}^{-1},$$
$$\hat{\mathbf{S}} = \frac{1}{2}(\hat{\mathbf{A}}+\hat{\mathbf{A}}^t),$$
$$\hat{\mathbf{\Omega}} = \frac{1}{2}(\hat{\mathbf{A}}-\hat{\mathbf{A}}^t)$$

- **Orientation of the spheroid:**

$$d\mathbf{R}/dt = \mathbf{\Omega}\,.\,\mathbf{R}$$

Orientation statistics

- ***n* =** normal vector to the axisymmetry plane of the crystal;
- $\boldsymbol{g} = -g\,\boldsymbol{e}_z$ ($\boldsymbol{e}_z$ points upwards).

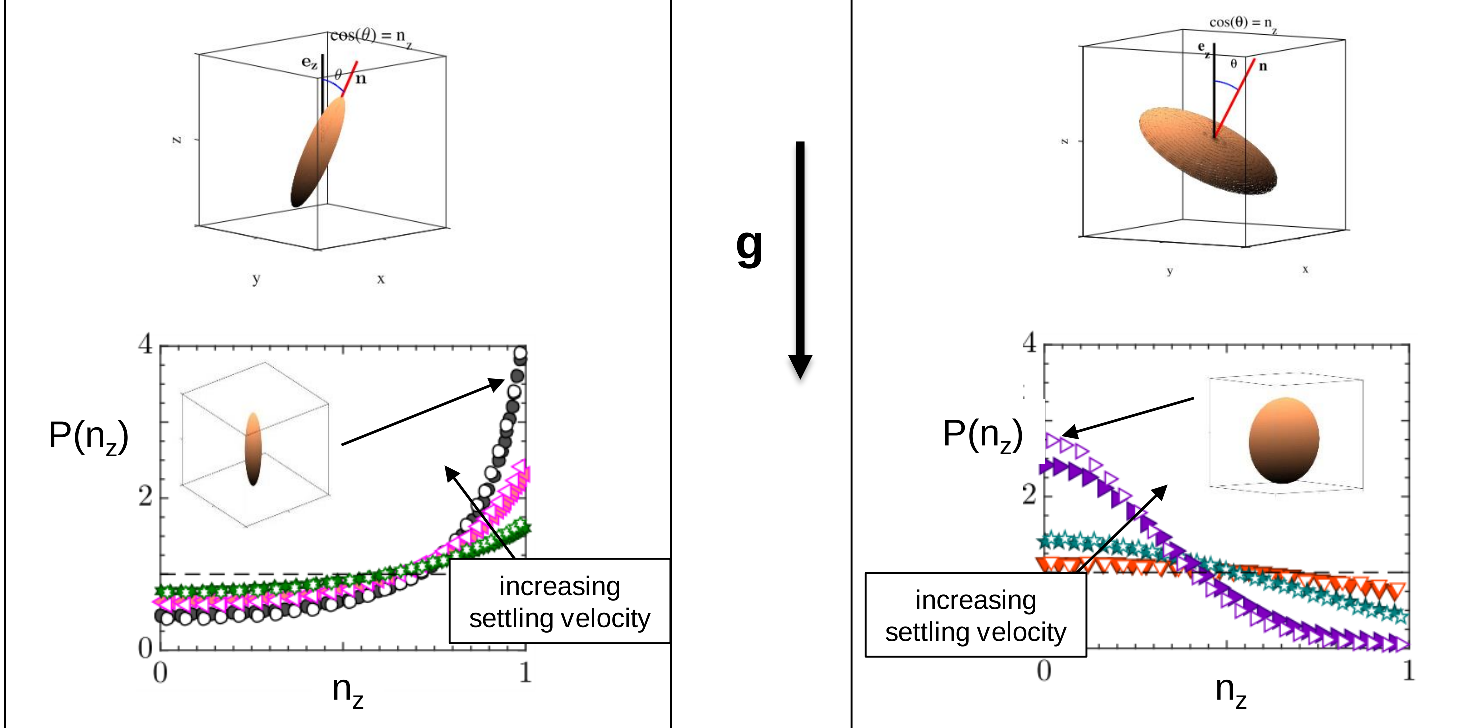


Settling of spheroids in a turbulent flow:
orientation distribution calculated numerically using **Stokes torque**

- Integration of the resulting set of equations for particles suspended in a turbulent flow (*Gustavsson et al, 2014*; *Siewert et al, 2014a,b*; *Gustavsson et al, 2017*; *Jucha et al, 2018*; *Naso et al, 2018*):

If W_s (settling velocity) > U_0 (fluid velocity), the orientation distribution is biased ("vertical"):

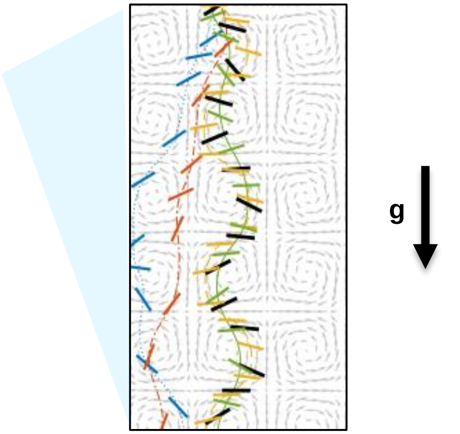
Prolate (rod-like): | Oblate (disk-like):



Fluid-inertia effect

First effect of fluid inertia on the rotational motion of settling spheroids

- Experimental results:
  - * *Lopez & Guazzelli, PRF 2017*: rods in a 2D laminar flow
    → "horizontal" settling
  - * *Kramel, PhD 2017*: rods in turbulence
    → "horizontal" settling
  - * *Roy et al, JFM 2019*; *Cabrera et al, 2021*: rods in quiescent fluid
    → "horizontal" settling



Results opposite to those obtained by DNS in turbulent flows using Stokes approximation !

- Fluid inertia correction on rotational motion of spheroids recently derived for arbitrary aspect ratios (*Dabade et al, JFM 2015*).

  Problem: fluid-inertia torque ~ Stokes torque !!!

  This inertial correction → "horizontal" settling.

- Determine the conditions under which fluid inertia can be neglected for the angular dynamics of spheroids settling in turbulence.

Angular motion of spheroids

Hydrodynamic torque: $\hat{\mathbf{T}} = \hat{\mathbf{T}}_{St} + \hat{\mathbf{T}}_I$

"Stokes" contribution
(*Jeffery, 1922*)

Contribution due to fluid inertia
for a particle moving steadily
in a homogeneous flow
(*Dabade et al, 2015*)

- NB: Fluid inertia can also induce corrections due to shear (*Candelier, Mehlig & Magnaudet, JFM 2019*) and unsteadiness.

- Estimate the ratio $|\hat{\mathbf{T}}_I|/|\hat{\mathbf{T}}_{St}|$:

  * $|\hat{\mathbf{T}}_I|/|\hat{\mathbf{T}}_{St}| \ll 1$: Stokes expected to dominate ("vertical" settling if $W_s > U_0$)

  * $|\hat{\mathbf{T}}_I|/|\hat{\mathbf{T}}_{St}| \gg 1$: inertia expected to dominate ("horizontal" settling if $W_s > U_0$)

Evaluation of the ratio $|\mathbf{T}_{St}|/|\mathbf{T}_I|$

- For very flat disks (aspect ratio β << 1) and for thin rods (5 ≤ β ≤ 100), it can be shown that:

$$|\hat{\mathbf{T}}_I|/|\hat{\mathbf{T}}_{St}| \sim \boxed{\mathscr{R} \equiv \left(\frac{W_s}{U_0}\right)^2 Re_f^{1/2}}$$

$Re_f = U_0 L/\nu$: large scale Reynolds number of the flow

- Therefore, in the high Re_f regime, the fluid-inertia torque can be neglected (i.e., $\mathscr{R}$ can be small) only if W_s/U_0 is small
  → orientation distribution nearly uniform

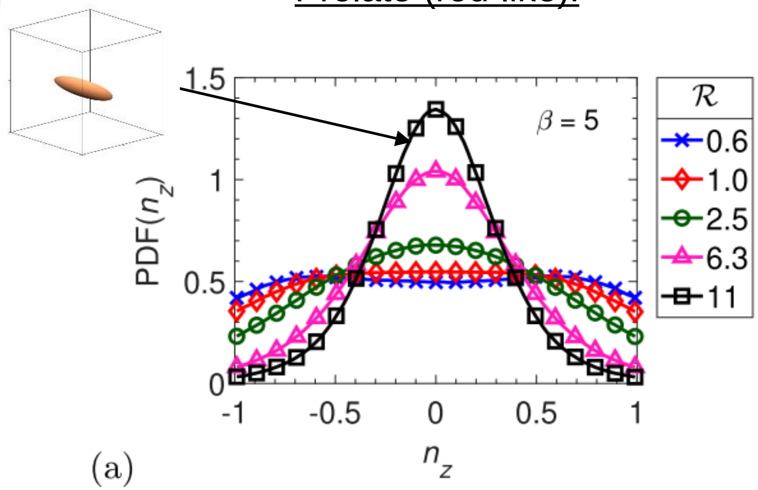
- The Stokes contribution can be neglected ($\mathscr{R} \gg 1$) simultaneously with a large ratio W_s/U_0
  → biased "horizontal" distribution

- **Therefore the orientation bias obtained in numerical works which neglect the fluid-inertia torque (biased "vertical" distribution) cannot be observed at large Re_f !!!**

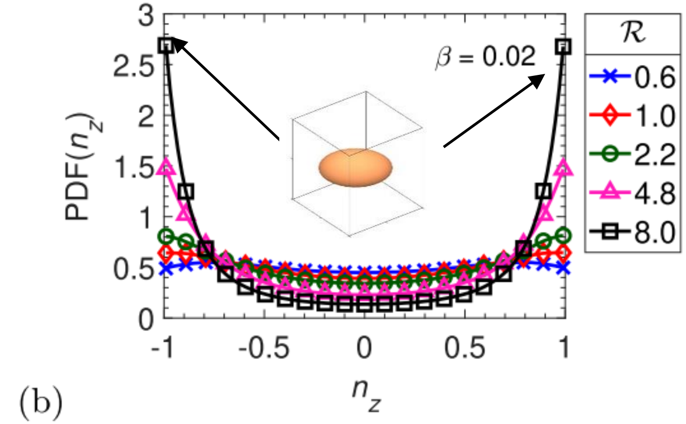
Sheikh, Gustavsson, Lopez, Lévêque, Mehlig, Pumir & Naso, JFM 2020

Numerical results in homogeneous and isotropic turbulence

Prolate (rod-like):



Oblate (disk-like):



- Transition from a uniform to a biased "horizontal" distribution observed at increasing $\mathscr{R}$.
- Biased "vertical" distribution never observed.
- Analysis seems to be valid for any β.

Settling and collisions of ice crystals

Settling, orientation and collisions of ice crystals: numerical setup

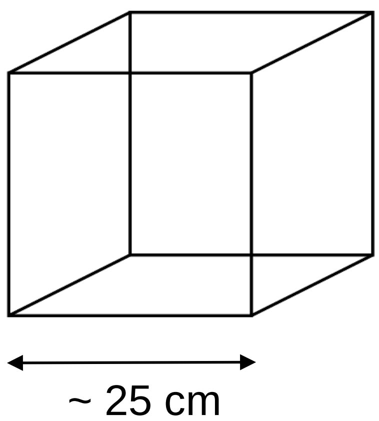
- Generation of an idealized stationary, homogeneous and isotropic turbulent flow in a cubic box with periodic boundary conditions (pseudo-spectral method).

$$\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\frac{\nabla p}{\rho_f} + \nu\nabla^2\mathbf{u} + \mathbf{f},$$

$$\nabla\cdot\mathbf{u} = 0,$$

- 3 values of R_λ (or ε) considered:

Flow	I	II	III
ε (cm^2/s^3)	0.976	15.62	246.4
Re_λ	55.8	94.6	151.2
τ_K (s)	0.341	0.085	0.021
T_L (s)	1.96	0.70	0.26
u_{rms} (cm/s)	2.18	5.72	14.4
N	384	768	1576



Physical parameters

- Simulations designed for representing at best realistic situations in cloud conditions. Physical parameters at $T = -20\,°\mathrm{C}$ (*Pruppacher & Klett, 1997*).

- Parameters common to all runs:

Fluid			Ice crystals		Gravity
ρ_f (g cm^{-3})	ν (cm^2 s^{-1})	μ (g cm^{-1} s^{-1})	ρ_i (g cm^{-3})	a (µm)	g (cm s^{-2})
1.413×10^{-3}	0.1132	1.599×10^{-4}	0.9194	150	981

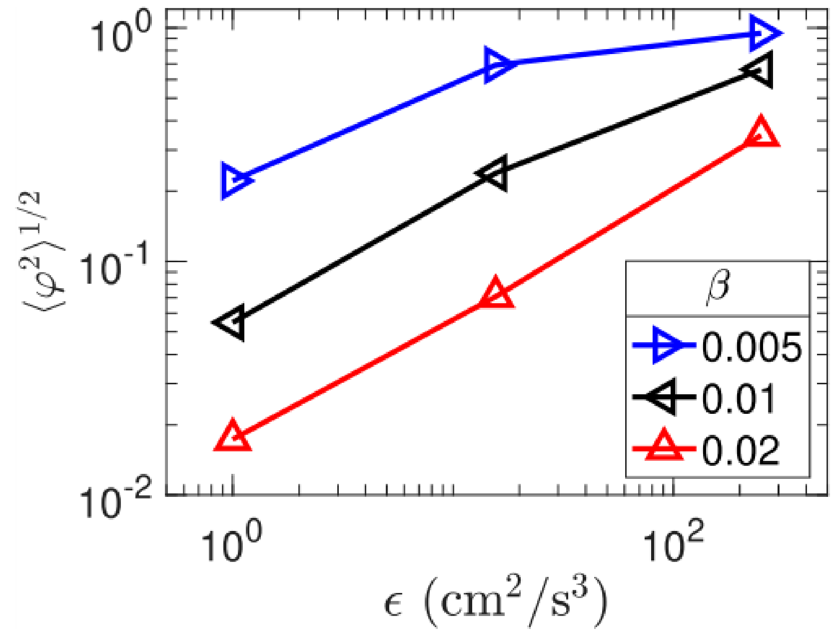
TABLE 1. Values of the physical parameters common to all runs. The fluid is moist air, whose volumetric mass, kinematic and dynamic viscosities are ρ_f, ν and μ, respectively. The density of the water droplets is ρ_l. The ellipsoidal ice crystals have a volumetric mass ρ_i and a semi-major axis a. The gravitational acceleration is denoted g.

Physical parameters

Runs	Flows	β	N_c	T_{run} (s)	$\langle U_s \rangle$ (cm/s)	St	Sv
1	I	0.005	100^3	98	1.84	$8.4\,10^{-3}$	4.89
2	I	0.01	100^3	112	3.08	$1.7\,10^{-2}$	9.78
3	I	0.02	70^3	126	5.48	$3.4\,10^{-2}$	19.6
4	II	0.005	100^3	24	2.12	$3.4\,10^{-2}$	2.44
5	II	0.01	70^3	30	3.50	$6.8\,10^{-2}$	4.89
6	II	0.02	70^3	36	5.78	0.135	9.78
7	II	0.05	70^3	31.5	11.5	0.338	24.5
8	III	0.005	100^3	5.28	2.4	0.134	1.23
9	III	0.01	100^3	5.28	4.5	0.268	2.45
10	III	0.02	100^3	5.28	7.4	0.536	4.91

w or w/o gravity.

Crystal settling: orientation statistics

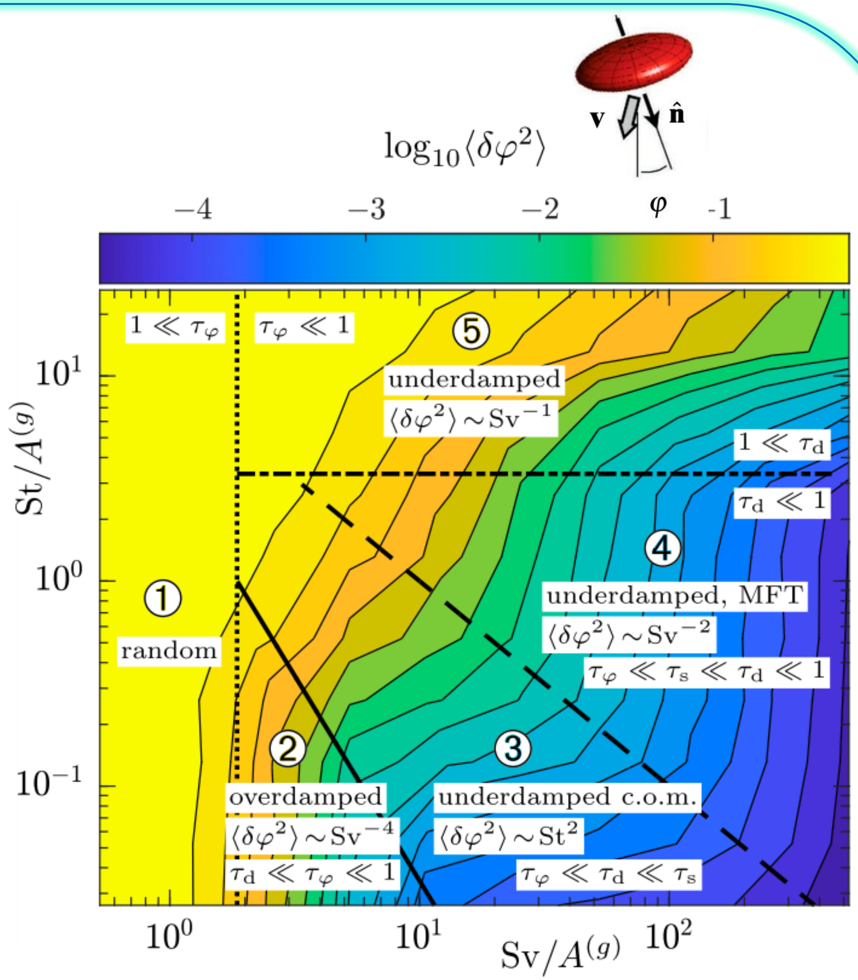


Broader orientation distribution at high ε (turbulence)
and small β (particle inertia).

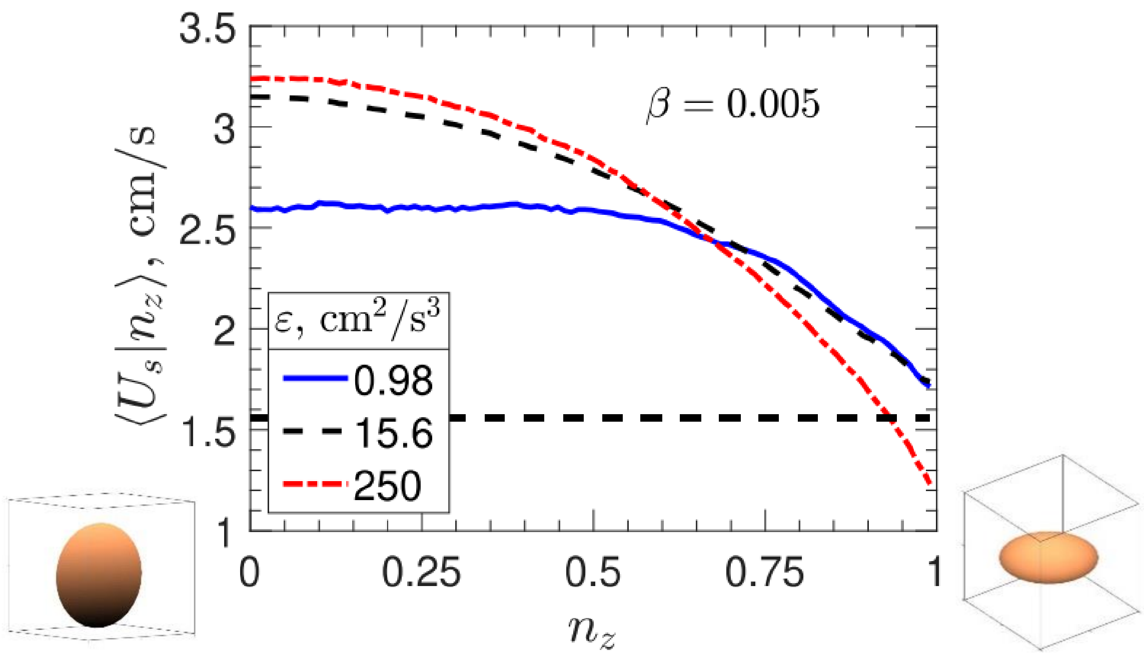
Parameter space for the orientation distribution

Theoretical modeling and numerical statistical model for orientation statistics as a function of β, St = τ_p / τ_η (Stokes number) and Sv = $g\tau_p / u_\eta$ (settling number).

Gustavsson, Sheikh, Naso, Pumir & Mehlig, J. Atm. Sci. 2021



Settling velocity conditioned on orientation



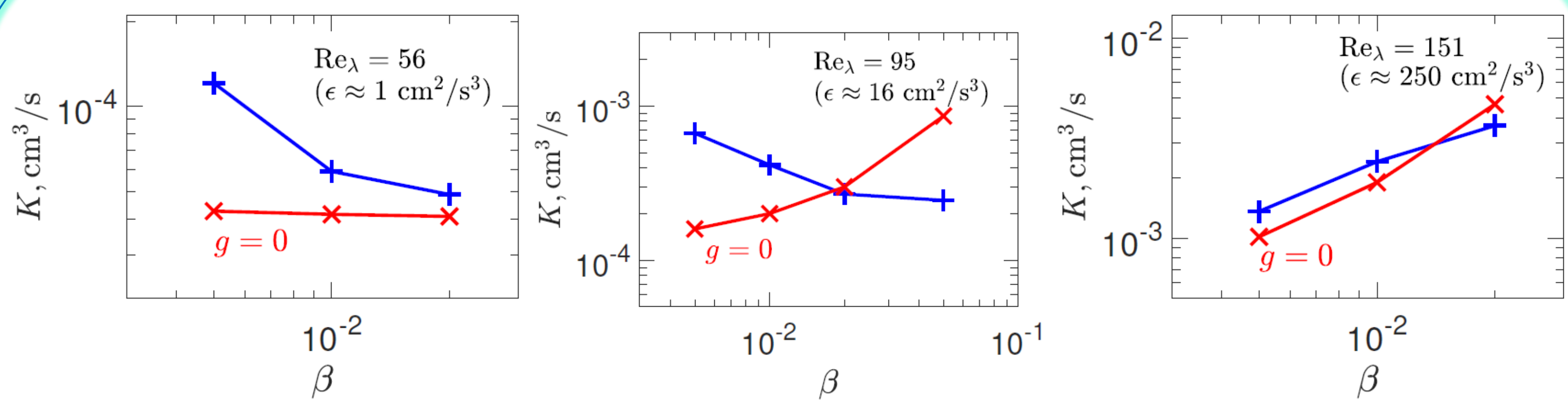
Two particles very close to each other may have a significant velocity difference, provided that they have different orientations → consequences for the collision rate…

Collision kernel

$$N_c = \frac{1}{2} K \times \frac{N^2}{V} \times T$$

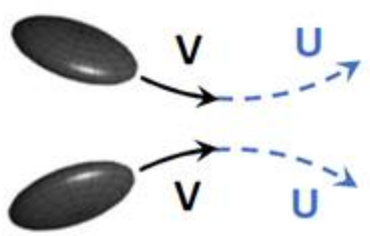
N_c: number of collisions.
K: collision kernel.
N: number of particles.
V: volume of the domain.
T: simulation time.

Pumir & Wilkinson, ARCMP 2016



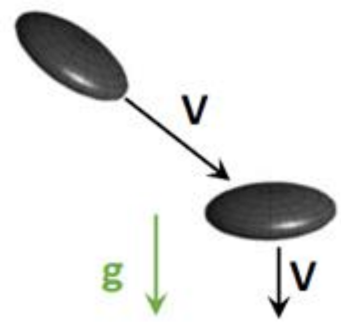
- Without gravity, K increases with β and ε (particle inertia), ~ spheres.
- Behavior less trivial in the presence of gravity.

Collision mechanisms for settling anisotropic particles



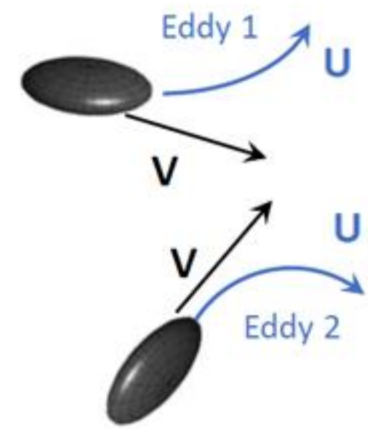
Turbulence: tracer particles brought together by velocity gradients.

Saffman & Turner, JFM 1956



Differential settling: faster spheroids fall on slower ones.

Jucha et al, PRF 2018



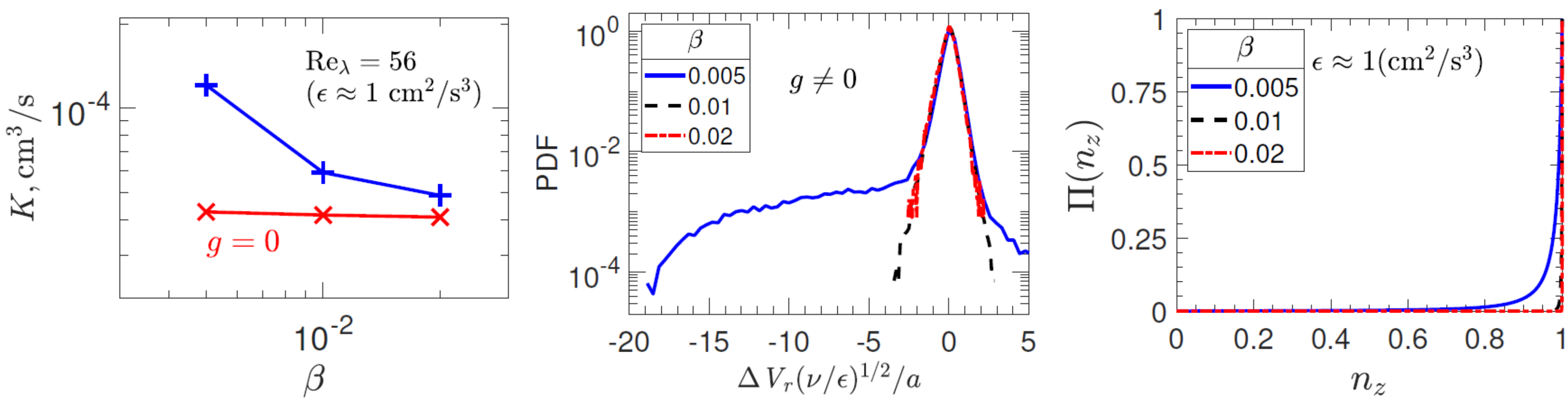
Particle inertia: particles from different locations collide due to the « sling effect ».

Falkovich & Pumir, JAS 2007

Collision kernel

ε = 1 cm^2/s^3; Re$_\lambda$ = 56 (St < 0.04)

$$\Delta V_r = (\mathbf{V_2} - \mathbf{V_1}) \cdot \frac{\mathbf{r_2} - \mathbf{r_1}}{|\mathbf{r_2} - \mathbf{r_1}|}$$

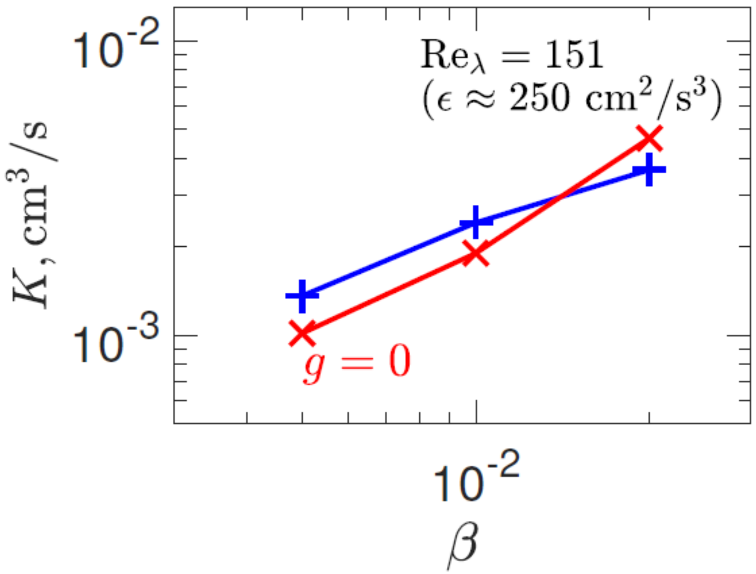


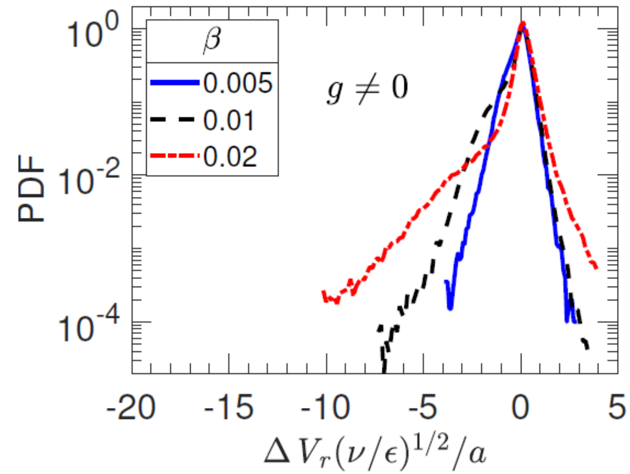
(A) $\epsilon = 0.98$ cm^2/s^3

- Saffman-Turner (K ~ 3.10^{-5} cm^3/s; Δv_r ~ a / τ_η) for $\beta \geq 0.01$.
- When g ≠ 0, differential settling for β = 0.005.

Collision kernel

ε = 246 cm²/s³; Re$_\lambda$ = 150 (St = 0.1-0.6)

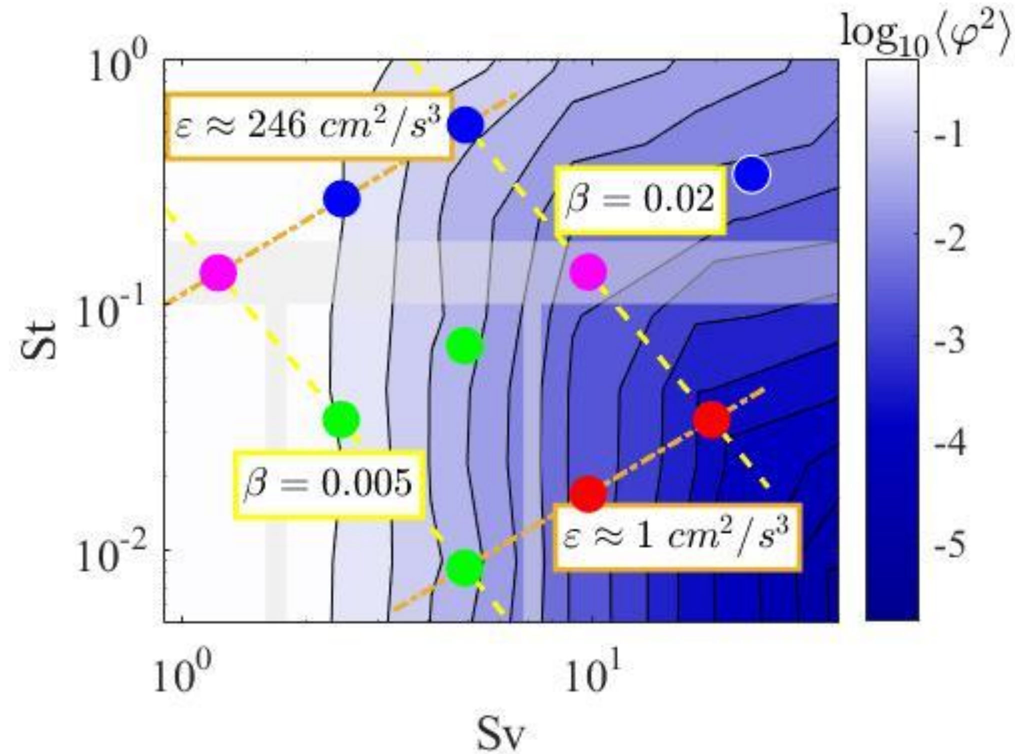




(c) $\epsilon = 250$ cm²/s³

- Saffman-Turner ($\Delta v_r \sim a / \tau_\eta$) for β = 0.005.
- Inertial effects (St ~ 0.6) for $\beta \geq$ 0.01.

Collision regimes in the (Sv, St) plane



St = τ_p / τ_η (Stokes number)
Sv = $g\tau_p / u_\eta$ (settling number)

Red: Saffman-Turner
Green: differential settling
Blue: inertial effects

Summary - Discussion

Take-home message (rotational motion of settling spheroids):

- In a turbulent flow, heavy spheroids can only settle either with a random orientation or preferentially horizontally. Neglecting the fluid-inertia torque may lead to wrong results !
- In laminar flows (not shown here), the three orientation regimes can be observed (uniform distribution, "vertical", "horizontal"). The limit $Re_f \to 0$ requires some care.
- Our estimates were derived for very flat disks (aspect ratio $\beta << 1$) and for thin rods ($5 \leq \beta \leq 100$), but our numerical results show that they are also relevant for moderate values of β.

Take-home message (orientation, settling and collisions of ice crystals in clouds):

- Our results improve the predictions of orientation fluctuations of earlier works (*Cho et al, J. Atmos. Soc. 1981*; *Klett, J. Atmos. Sci. 1995*), and are consistent with real observations.
- The settling velocity of ice-crystals strongly depends on their orientation.
- The resulting differential settling can play a crucial role in the collisions process. Collisions driven by three mechanisms: fluid velocity gradients, differential settling, effects of particle inertia.

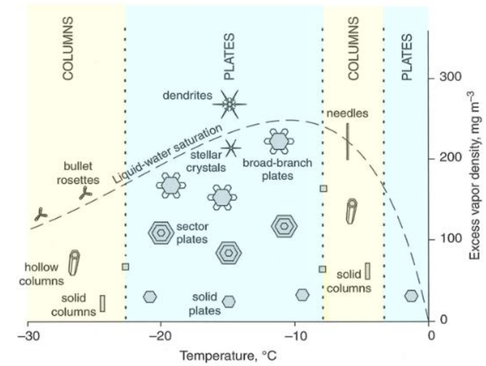
Conclusion

Limitations of the present approach:

- “One-way coupling”.
- “Ghost collision” approximation.

- Simplified crystal geometry, homogeneous mass density.

- Equations of motion valid for small Re_p.
  Effects of shear and unsteadiness neglected.



W. Brune (after Lamb and Verlinde)

Perspectives:

- Prolate spheroids ($-10\,^{\circ}\mathrm{C} \lesssim T \lesssim -5\,^{\circ}\mathrm{C}$).

- Investigating further the collision mechanisms when particle inertia is dominant.

- Collisions between ice crystals and supercooled water droplets
  coexisting in mixed phase clouds.