Atmospheric Aerosol Physics, Physical Measurements, and Sampling

Definitions & Mechanical Properties

São Paulo School of Advanced Science on Atmospheric Aerosols: properties, measurements, modeling, and effects on climate and health

Member of Leibniz Leibniz Association

ECAC European Center for Aerosol Calibration

WCCAP World Calibration Centre for Aerosol Physics

TROPOS Leibniz Institute for Tropospheric Research

Definitions

General Definitions

Definition of an aerosol

Solid and /or liquid particles suspended in a gas

Coarse Particles

Particles	>1 µm in diameter

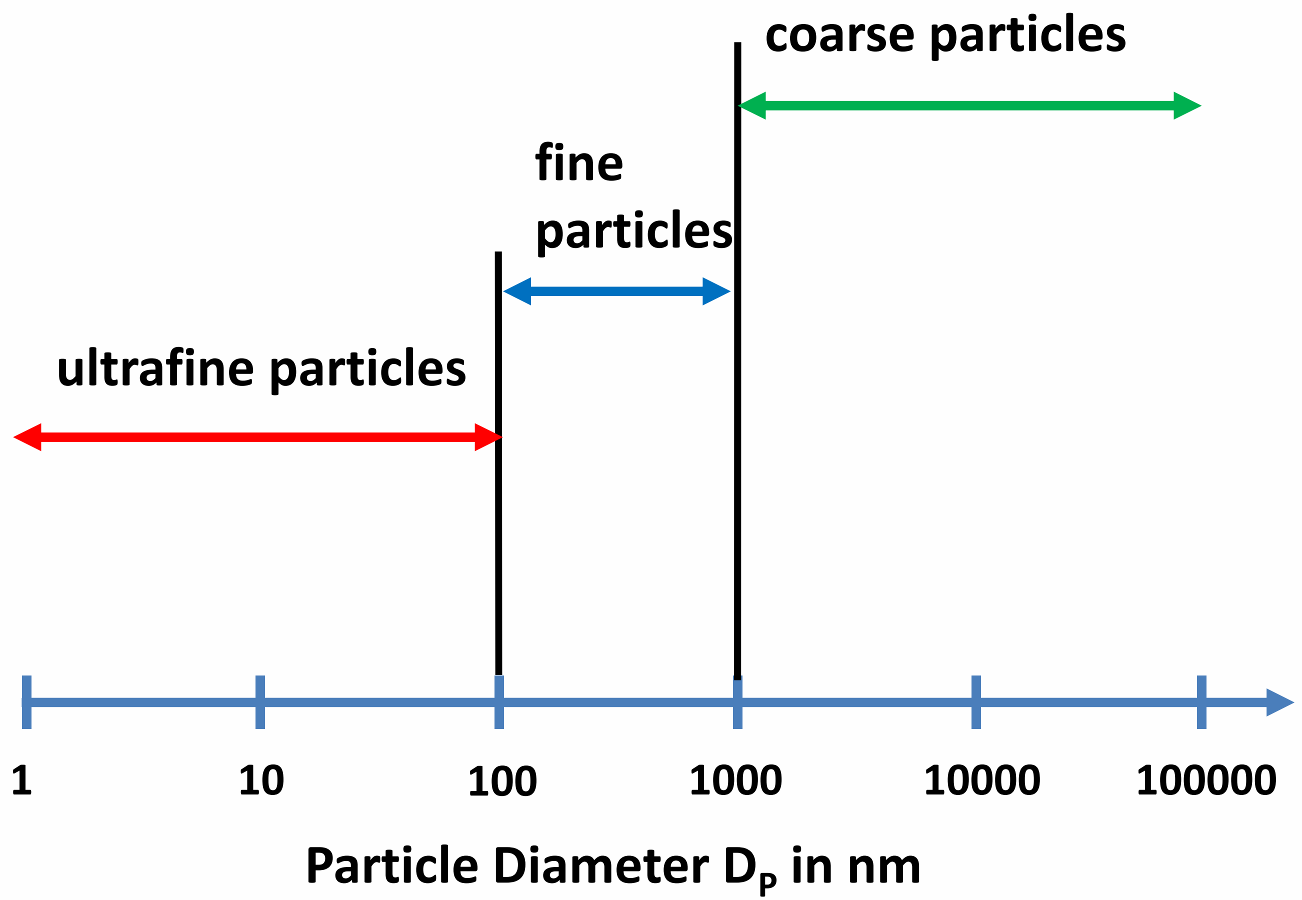
Fine Particles

Particles	<1 µm in diameter
Accumulation mode range	100-1000 nm

Ultrafine Particles

Particles	< 100 nm in diameter
Aitken mode range	10-100 nm
Nucleation mode range	1-10 nm

Particle Size Ranges



Particle Size

Definition	1 nm < D_P< 100 µm
	10^{-9} m < D_P< 10^{-4} m

Micro-Range	Macro-Range
1 nm particle	0.1 mm tip of a needle
350 nm particle	3.5 cm ping-pong ball
2.5 µm particle	25 cm soccer ball
100 µm particle	10 m balloon

Shape & Concentrations

Particle Shape

Aerosol particles are normally non-spherical.

However, particles are often assumed to be spheres for a simpler description and use (equivalent diameter).

Aerosol particles with extreme shapes should not be described as spherical particles.

Examples for non-spherical particles

- Asbestos fibers
- Chain agglomerates

Examples for "spherical particles"

- Droplets
- Fly ash particles
- Inorganic salt particles (crystals)
- Compact particles

Particle Concentrations

- The particle number concentration is described by the parameter N.
- It is defined by the number of particles per volume unit, and given in #/cm$^{3.}$

Other concentrations:

- Particle surface area concentration — S [$\mu m^2/cm^3$]
- Particle volume concentration — V [$\mu m^3/cm^3$]
- Particle mass concentration — M [$\mu g/m^3$]

- The mass concentration can be calculated from the volume concentration and the particle density $\rho_{P.}$
- The particle density is given in [g/cm^3].

Reynolds Numbers

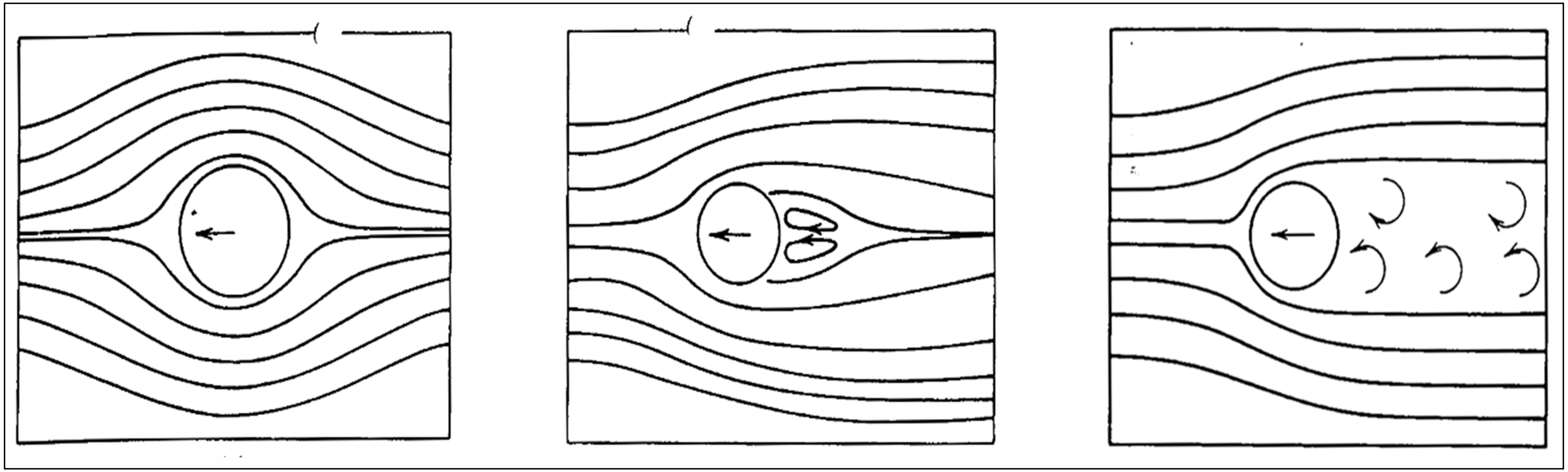
Particle Reynolds Number

The Particle-Reynolds-Number is an important quantity for the characterization of the mechanical properties of aerosol particles.

$$\mathrm{Re}_{\mathrm{P}} = \frac{\rho_{\mathrm{G}} u_{\mathrm{P}} D_{\mathrm{P}}}{\eta}$$

- It characterizes the flow around an aerosol particle.
- Equal Particle-Reynolds-Numbers imply the same pattern of stream lines in the vicinity of particles with different size and in different gases.
- It is the most important property for the determination of the drag force a gas exerts on a suspended particle.

Flow around a sphere



Laminar flow, Re = 0.1 Turbulent flow, Re ≈ 2 Turbulent flow, Re ≈ 250

Hinds: Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles

Flow-Reynolds-Number

The Flow-Reynolds-Number depends mainly on the flow rate and the tube diameter

$$\mathrm{Re}_{\mathrm{flow}} = \frac{\rho_{\mathrm{gas}} \cdot \overline{u}_{\mathrm{flow}} \cdot D_{\mathrm{pipe}}}{\eta}$$

ρ_{gas} … gas density

u_{flow} … flow velocity

D_{pipe} … tube diameter

η … dynamic viscosity

Forces & Stokes Law

External Forces

External forces on a particles will result in a macroscopically directed particle motion.

Examples for external forces:

- Gravitational force

$$\vec{F}_{\mathrm{g}} = \frac{\pi}{6} D_{\mathrm{P}}^3 \cdot \rho_{\mathrm{P}} \cdot \vec{g} \cdot \left(1 - \frac{\rho_{\mathrm{G}}}{\rho_{\mathrm{P}}}\right)$$

- Electrical force

$$\vec{F}_{\mathrm{e}} = n_{\mathrm{e}} \cdot \mathrm{e} \cdot \vec{E}$$

- Thermophoresis

$$\vec{F}_{\mathrm{th}} = -\frac{3 \cdot \pi \cdot \eta^2 \cdot D_{\mathrm{P}} \cdot K_{\mathrm{th}}}{\rho_{\mathrm{G}}} \cdot \frac{\nabla T}{T}$$

Newton's Law

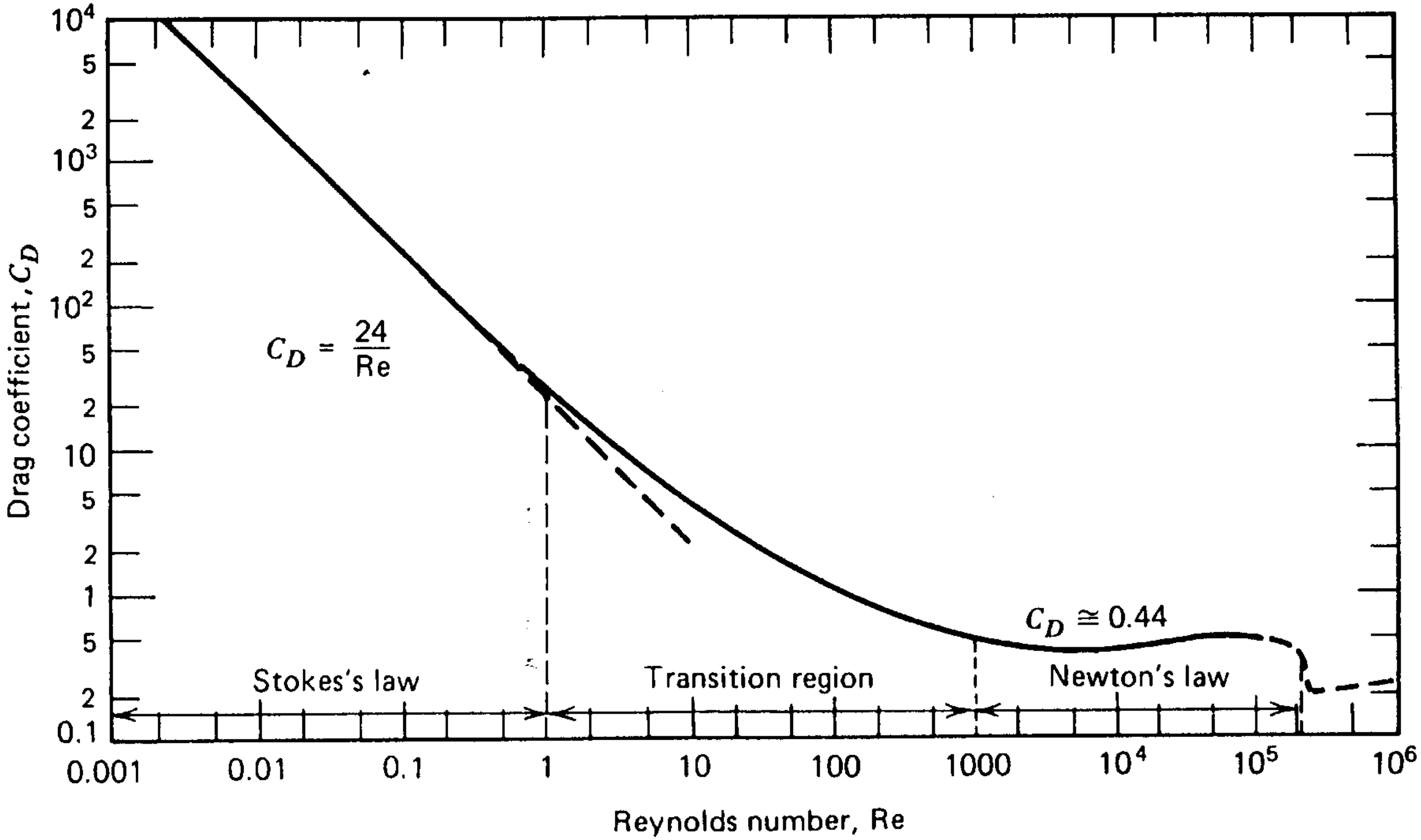
Newton's Law describes the drag force as stagnant gas exerts on a moving body, e.g. a sphere.

$$F_D = \frac{\pi}{8} \cdot \rho_G \cdot u_P^2 \cdot C_D \cdot D_P^2$$

- This general equation is applicable over a wide range of Reynolds-Numbers ($Re = 10^3 - 10^5$).
- In this regime, the drag coefficient C_D is nearly constant.
- For Reynolds-Numbers Re < 1000, the drag coefficient is a function of Reynolds-Number.

$$C_D = \frac{24}{Re}\left(1 + \frac{Re^{2/3}}{6}\right)$$

- In the regime 3 < Re < 400, the introduced error is less than 2 % and up to Re = 1000 less than 10 %.



Drag coefficient versus Reynolds number for spheres

Figure: Hinds: Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles

Stokes' Law

Most particle movement takes place at low Particle-Reynolds-Numbers, as both, the flow velocity and the particle diameter are usually small.

Stokes' Law is a special solution of the momentum, i.e. the Navier-Stokes-equation.

Therefore, the following assumptions are made:

- incompressible flow
- steady state
- gas velocity equal to zero at the particle surface (no slip boundary)

The drag coefficient can be determined applying Newton's Law:

$$C_D = \frac{24}{\mathrm{Re}}$$

The drag force results in:

$$\vec{F}_D = 3\pi \cdot \eta \cdot \vec{u}_P \cdot D_P$$

The temperature dependency of the viscosity can be described as follows:

$$\eta = \eta_0 \left(\frac{T}{T_0}\right)^{3/2} \left(\frac{T_0 + 110.4\mathrm{K}}{T + 110.4\mathrm{K}}\right)$$

Cunningham Correction Factor

For particle diameters D_P < 10000 nm, the gas velocity at the particle surface is not equal to zero, which results in a reduced drag force.

This effect is accounted for by the **Cunningham correction factor**

$$C_\mathrm{C} = 1 + \frac{\lambda}{D_\mathrm{P}}\left(2.514 + 0.8 \cdot \exp\left(-0.55 \frac{D_\mathrm{P}}{\lambda}\right)\right)$$

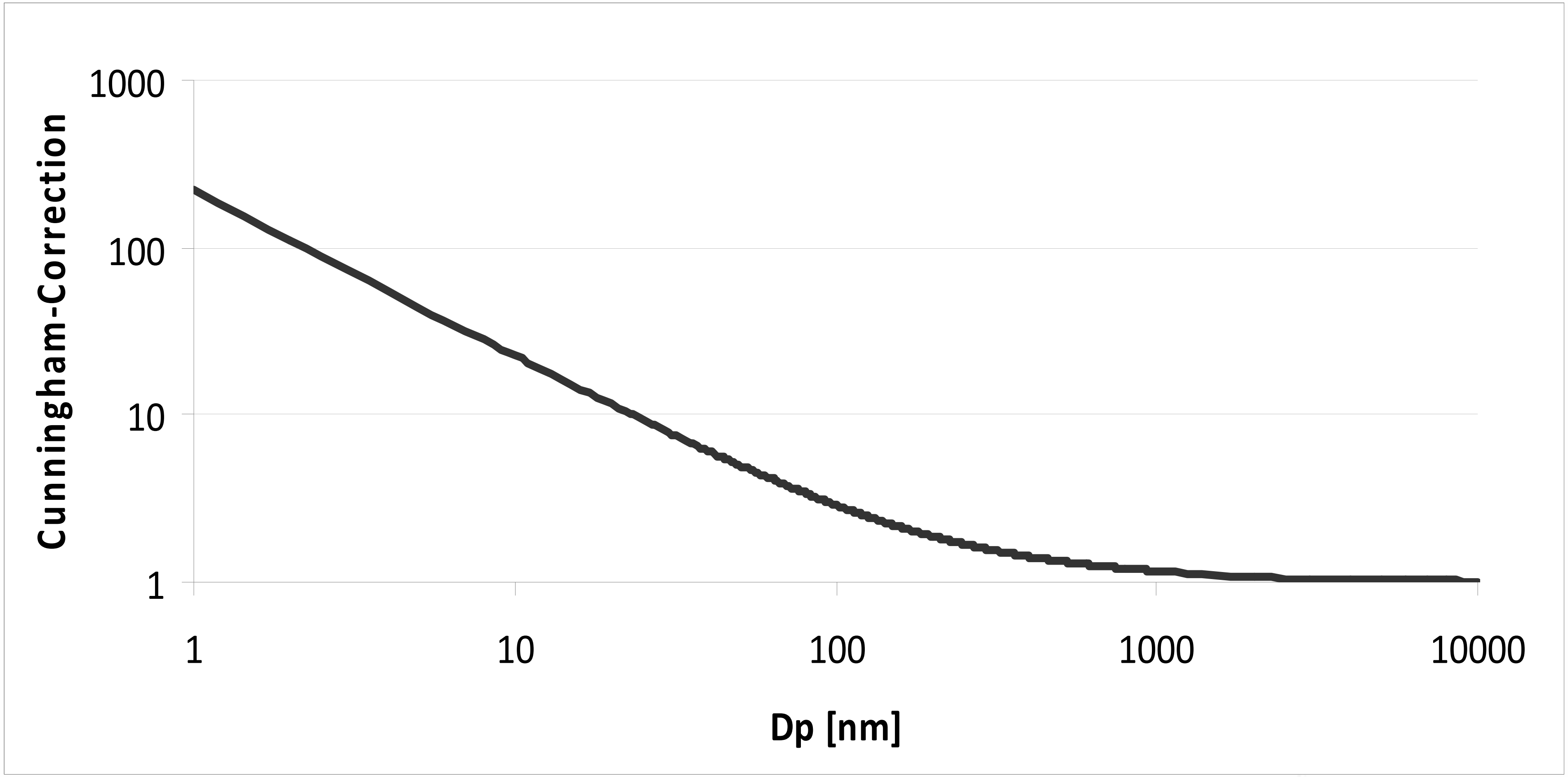
The **drag force** then becomes:

$$\vec{F}_\mathrm{D} = \frac{3\pi \cdot \eta \cdot \vec{u}_\mathrm{P} \cdot D_\mathrm{P}}{C_\mathrm{C}}$$

The Cunningham correction factor was determined empirically via the determination of the settling velocity of particles with known size and density.

For the pressure & temperature dependency of the Cunningham correction factor, the mean free path has to be corrected according to:

$$\lambda = \lambda_0 \left(\frac{T}{T_0}\right)^2 \left(\frac{p_0}{p}\right)\left(\frac{T_0 + 110.4\mathrm{K}}{T + 110.4\mathrm{K}}\right)$$



Cunningham correction factor as function of particle size

Mobility & Settling

Mechanical Mobility

The **drag force** on a particle in an uniform motion results in:

$$\vec{F}_{\mathrm{D}} = \frac{3\pi \cdot \eta \cdot \vec{u}_{\mathrm{P}} \cdot D_{\mathrm{P}}}{C_{\mathrm{C}}}$$

In Stokes' Law the drag force is directly proportional to the relative velocity between the particle and the gas. This fact can be used to introduce the **mechanical mobility** *B* :

$$B = \frac{\vec{u}_{\mathrm{P}}}{\vec{F}_{\mathrm{D}}} = \frac{C_{\mathrm{C}}}{3\pi \cdot \eta \cdot D_{\mathrm{P}}}$$

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Sedimentation Velocity

An important application of Stokes' law is the determination of the **sedimentation velocity** u_s of aerosol particles. In this case, the drag forces F_D is equal to the gravitational force F_G acting on the particle.

$$\vec{F}_D = \vec{F}_G$$

$$\frac{3\pi \cdot \eta \cdot \vec{u}_s \cdot D_P}{C_C} = \frac{\pi \cdot \rho_P \cdot D_P^3 \cdot \vec{g}}{6}(1 - \frac{\rho_G}{\rho_P})$$

If the gas density is small compared to the particle density, the sedimentation velocity u_s can be calculated as follows:

$$\vec{u}_s = \frac{\rho_P D_P^2 C_C \vec{g}}{18\eta}$$

Settling velocity	
density = 1	
Dp (nm)	Us (m/s)
1	6,67E-09
10	6,82E-08
100	8,73E-07
1000	3,49E-05
10000	3,03E-03
100000	2,99E-01

Non-Spherical Particles

Non-Spherical Particles

The equations presented up to now are based on the assumption of a spherical particle shape.

Liquid droplets are spherical, but most of the aerosol particles are non-spherical.

The actual form (cubes, fibers, agglomerates) of a particle however affects the drag force and consequently e.g. the sedimentation velocity.

This is accounted for by introducing a **dynamic shape factor** into Stokes' Law:

$$\vec{F}_{\mathrm{D}} = \frac{3\pi \cdot \eta \cdot \vec{u}_{\mathrm{P}} \cdot D_{\mathrm{P,ve}}}{C_{\mathrm{C}}} \cdot \chi$$

The resulting mechanical mobility and sedimentation velocity are:

$$B = \frac{\vec{u}_{\mathrm{P}}}{\vec{F}_{\mathrm{D}}} = \frac{C_{\mathrm{C}}}{3\pi \cdot \eta \cdot D_{\mathrm{P,\,Ve}} \cdot \chi}$$

$$\vec{u}_{s} = \frac{\rho_{\mathrm{P}} \cdot D_{\mathrm{P,Ve}}^{2} \cdot C_{\mathrm{C}} \cdot \vec{g}}{18\eta \cdot \chi}$$

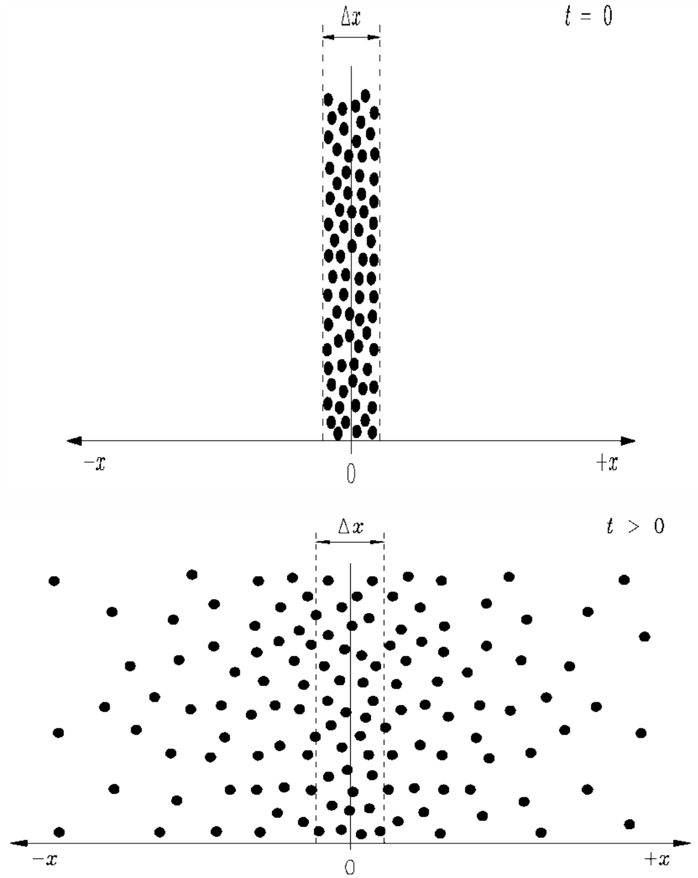
Shape factors

Shape	Dynamic Shape Factor
Sphere	1.00
Cube	1.08
Cluster chain of 4 spheres	1.32
Quartz	1.36
Sand	1.57

Table: Numbers taken from Hinds: Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles

Diffusion

Brownian Motion of Aerosol Particles



Hinds: Aerosol Technology: Properties, Behavior, and Measurement of Airborne Particles

Particle Diffusion

- The particle diffusion results from interactions between particles and gas molecules.
- Due to the impulse exchange molecules and particles, the Brownian motion of the molecules is transferred to the particles.
- The resulting particle motion is then called Brownian particle motion.
- A measure of the Brownian particle motion is the particle diffusion coefficient *D*.
- The Brownian particle motion is macroscopically non-directional.

$$\boxed{D = k \cdot T \cdot B}$$

Stokes Number & Relaxation Time

Stokes Number & Relaxation Time

The Stokes number characterizes the particle inertia in a flow

$$\mathrm{Stk} = \frac{\tau \cdot u_0}{D_{\mathrm{pipe}}}$$

with

$$\tau = \frac{\rho_{\mathrm{P}} \cdot D_{\mathrm{P}}^2 \cdot C_{\mathrm{C}}}{18\eta}$$

τ	… relaxation time
u_0	… wind velocity
D_{pipe}	… tube diameter

The Stokes Number is the ratio between the particle stopping distance to characteristic dimensions of the flow profile.

Example

Particle diameter nm	Relaxation time s	Stopping distance m	Stokes number
10	6,95E-09	9,23E-09	2,31E-06
100	8,90E-08	1,18E-07	2,95E-05
1000	3,56E-06	4,72E-06	1,18E-03
10000	3,09E-04	4,11E-04	1,03E-01
100000	3,05E-02	4,04E-02	1,01E+01
Density: ρ_P	2000 kg/m^3		
Tube diameter: D_t	0.004 m		
Tube velocity: u_t	1.33 m/s		
	(5 l/min in ¼” tube)		