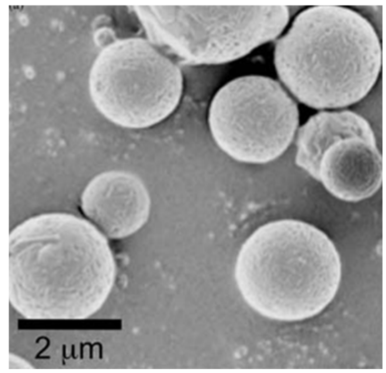
Chapter 4
Properties of aerosol particles

- Calculation of the properties of aerosol particles.
- Aerosol dynamics.
- Aerosol particle statistics



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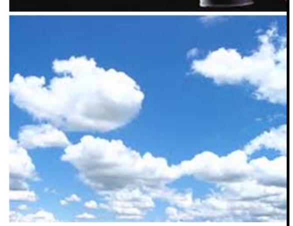
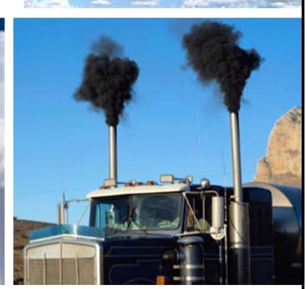
Aerosol /Particulate Matter



- An aerosol is a mixture of solid particles and/or liquid droplets suspended in a gas.

- The gas phase can be air or another gas



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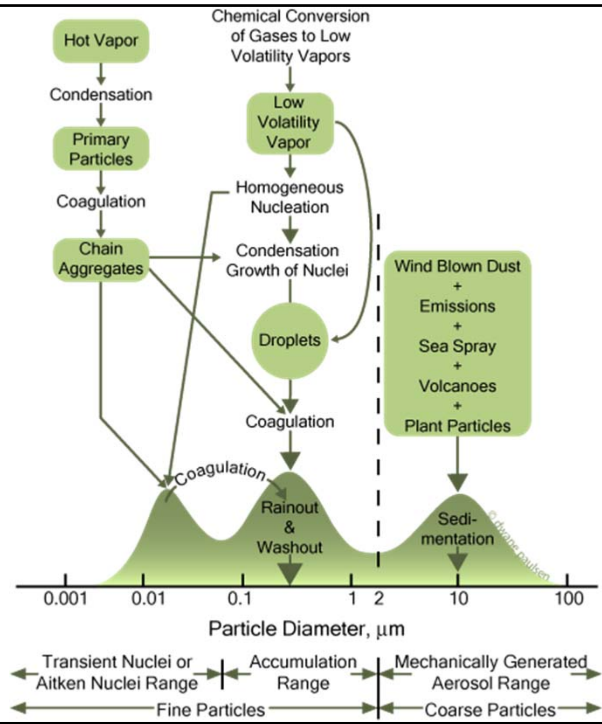

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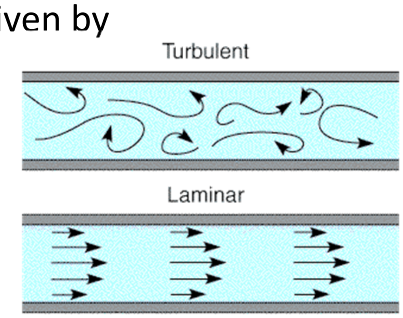
Fluid Reynolds Number

- Reynolds number of fluids in motion has been introduced in fluid mechanics.
- It quantifies the relative importance of inertial forces (ρV) and viscous forces (μ/D) for a flow.
- Mathematically it is given by

$$\mathrm{Re} = \frac{\rho V D}{\mu}$$



For bulk fluids
- Laminar: Re<2000
- Turbulent: Re>4000

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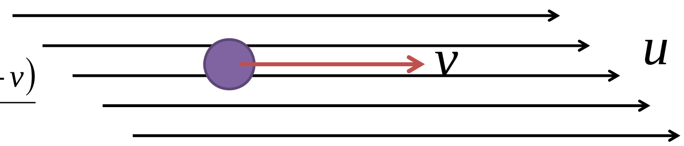
Particle Reynolds Number

$$\mathrm{Re}_p = \frac{\rho_g d_p (u - v)}{\mu}$$



- Flow around the moving particle could be laminar although the bulk air flow is turbulent
- When v=0 → Fluid dynamics!
- Viscosity of air:

  μ = *1.81 x10*$^{-5}$ *Pa.s*

Flow Regime around a particle

1. Stokes: $Re_p<1$
2. Transient: $1<Re_p<5$
3. Turbulent: $5<Re_p<1000$
4. Newton's: $Re_p>1000$

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Most flow around a particle is in Stokes regime

Example: Particle diameter = 10 μm, *relative velocity* = 1 m/s; air μ = *1.81 x10*$^{-5}$ *Pa.s*

$$\mathrm{Re}_p = \frac{\rho_g d_p (u - v)}{\mu} \qquad = \frac{1.2\times10^{-5}\times1}{1.81\times10^{-5}} < 1$$

- In air pollution, we deal with particle with even smaller sizes and aerosol particle tends to follow air under normal condition

$$Re_p \propto d_p \text{ and } v \rightarrow u$$

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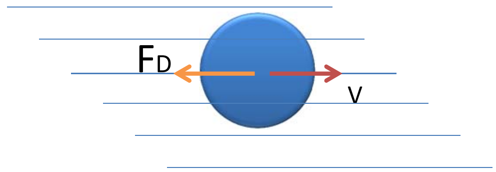
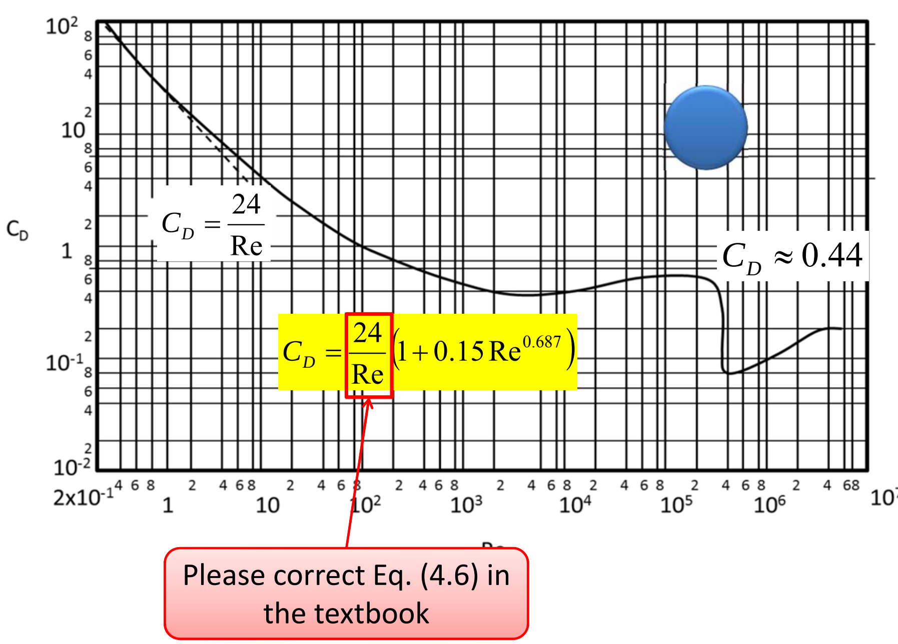
Newton's Resistance Law

From Fluid Dynamics

$$F_D = C_D\left(\rho_g \frac{\pi}{8} d_p^2 v^2\right)$$

C_D is the drag coefficient





Slipping Effect and Cunningham Correction Factor

- An important assumption of Stokes' law is that there is no slipping between the gas and the rigid particles.
- However, when the particle is getting smaller and smaller, approaching the mean free path of the gas molecules, this assumption is no longer valid.

$$F_D = \frac{3\pi\mu |u - v| d_p}{C_c}$$

C_c ← Cunningham correction factor

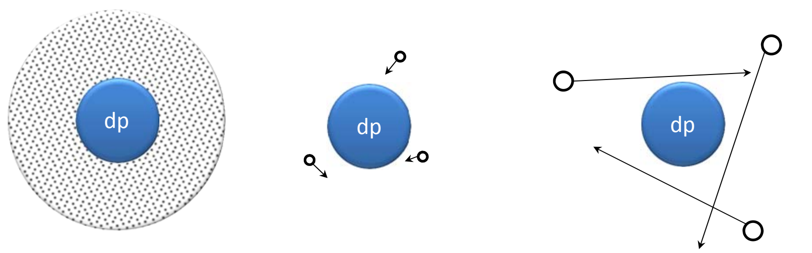
Slipping Effect

- An important assumption of Stokes' law is that there is no slipping between the gas and the rigid particles.
- However, when the particle is getting smaller and smaller, approaching the mean free path of the gas molecules, this assumption is no longer valid.
- **Introducing the Knudsen Number**

$$Kn = \lambda / \left(\frac{d_p}{2}\right) = 2\lambda / d_p$$

λ = mean free path of the gas

The Knudsen Number $Kn = 2\lambda/d_p$



Continuum regime Kn<<1 (large particles)	Transition regime	Non continuum regime Kn>>1

Aerosol Particle in Stokes Regime

For $Re_p<1$ $\quad C_D = \frac{24}{Re_p} \longleftarrow Re_p = \frac{\rho_g |v-u| d_p}{\mu}$

$$C_D = \frac{24\mu}{\rho_g |u-v| d_p}$$

$$\downarrow$$

$$F_D = C_D \rho_g \frac{\pi}{8} d_p^2 v^2$$

$$\Rightarrow \quad \boxed{F_D = 3\pi\mu d_p |u-v|}$$

Cunningham correction factor

- The drag force is reduced by the slipping effect:

$$F_D = \frac{3\pi\mu |u - v| d_p}{C_c}$$

$$C_c = 1 + Kn\left[1.142 + 0.558exp\left(-\frac{0.999}{Kn}\right)\right]$$

$$Kn = 2\lambda/d_p$$

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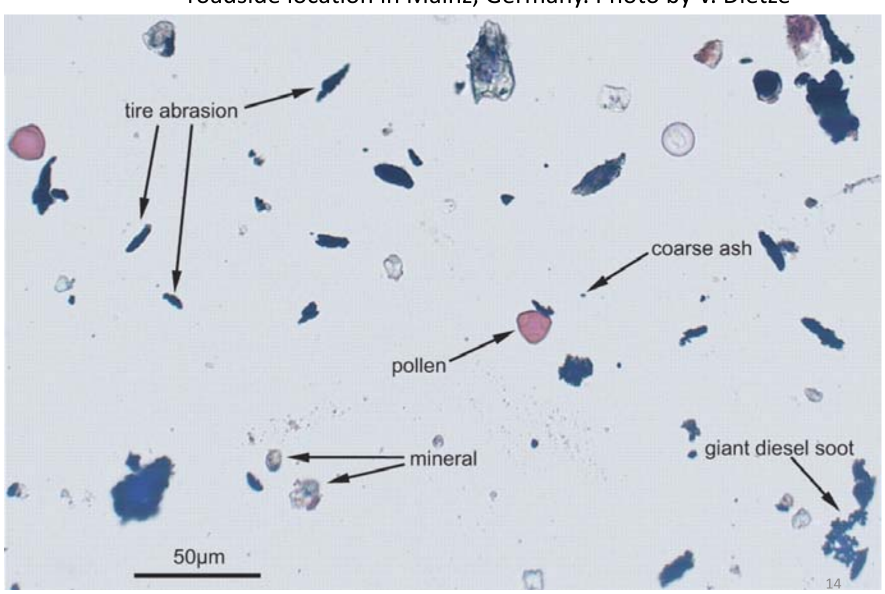
Shape factor

Transmitted-light microscope image of airborne particles collected over a period of 7 days with a passive sampler at a roadside location in Mainz, Germany. Photo by V. Dietze



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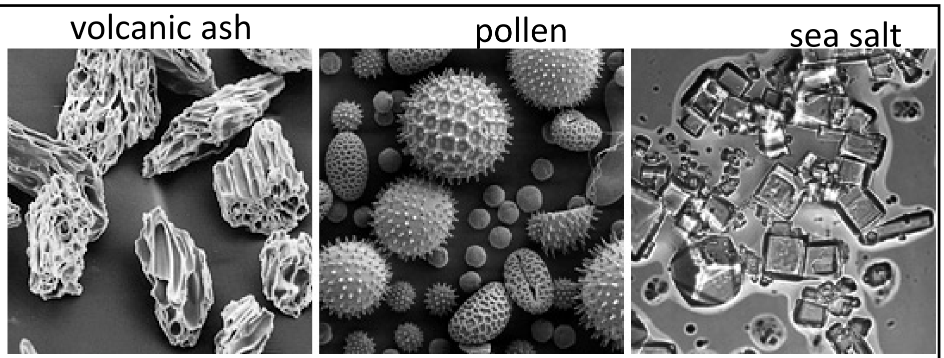
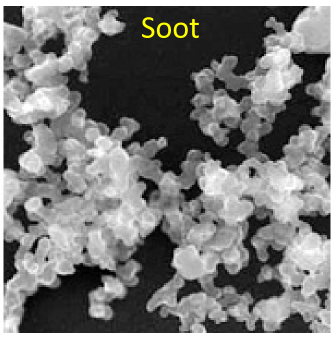
Bernard Grobéty, Reto Gieré, Volker Dietze, and Peter Stille, 2010, Airborne Particles in the Urban Environment, *ELEMENTS*, VOL. 6, PP. 229–234





These SEM images show the wide variety of aerosol shapes.

http://earthobservatory.nasa.gov/Features/Aerosols/

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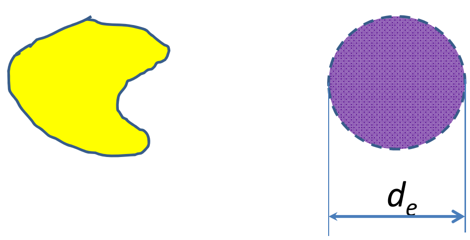
Equivalent Volume Diameter, d_e

- Equivalent volume diameter is the diameter of a sphere having the same volume as that of the irregular particle.



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Shape factor (Optional)

$$S_f = \frac{F_D}{3\pi\mu v d_e} \qquad F_D = 3\pi\mu v d_e S_f$$

Shape	Dynamic shape factor			
		Axial ratio		
		2	5	10
Geometric shapes				
Sphere	1.00			
Cube (e.g. Ocean salt)	1.08			
Cylinder				
Vertical axis		1.01	1.06	1.20
Horizontal axis		1.14	1.34	1.58
Orientation averaged		1.09	1.23	1.43
Straight chain		1.10	1.35	1.68
Compact cluster				
Three spheres	1.15			
Four spheres	1.17			
Dust particles				
Bituminous coal	1.05-1.11			
Quartz	1.36			
Sand	1.57			
Talc	1.88			

$S_f \geq 1$

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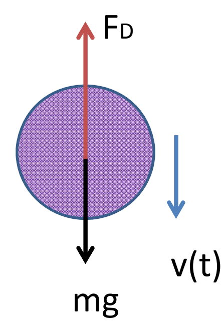
Aerosol Dynamics

- Consider a <u>spherical</u> particle released in still air



$$mg - F_D = ma = m\frac{dv}{dt}$$

$$\Rightarrow \quad mg - \frac{3\pi\mu d_p v}{C_c} = m\frac{dv}{dt}$$

$$\left(\frac{mgC_c}{3\pi\mu d_p}\right) - v = \left(\frac{mC_c}{3\pi\mu d_p}\right)\frac{dv}{dt}$$

$$\left(\frac{mgC_c}{3\pi\mu d_p}\right) - v = \left(\frac{mC_c}{3\pi\mu d_p}\right)\frac{dv}{dt}$$

Initial condition:
v=0 @ t=0

$$volume = \frac{1}{6}\pi d_p^3$$

$$\left(\frac{3\pi\mu\, d_p}{mC_c}\right)\int_0^t dt = -\int_0^{v(t)} \frac{dv(t)}{\left[v(t) - \left(\frac{mgC_c}{3\pi\mu d_p}\right)\right]}$$

$$\left(\frac{3\pi\mu\, d_p}{mC_c}\right)t = \ln\left(\frac{mgC_c}{3\pi\mu d_p}\right) - \ln\left[v(t) - \left(\frac{mgC_c}{3\pi\mu d_p}\right)\right]$$

$$\frac{t}{\left(\frac{\rho_p d_p^2 C_c}{18\mu}\right)} = \ln\left[\frac{\rho_p d^2 g C_c}{18\mu}\right] - \ln\left[\frac{\rho_p d^2 g C_c}{18\mu} - v(t)\right] = \ln\left(\frac{\frac{\rho_p d^2 g C_c}{18\mu}}{\frac{\rho_p d^2 g C_c}{18\mu} - v(t)}\right)$$

$$-\frac{t}{\left(\frac{\rho_p d_p^2 C_c}{18\mu}\right)} = \ln\left(\frac{\frac{\rho_p d^2 g C_c}{18\mu} - v(t)}{\frac{\rho_p d^2 g C_c}{18\mu}}\right)$$

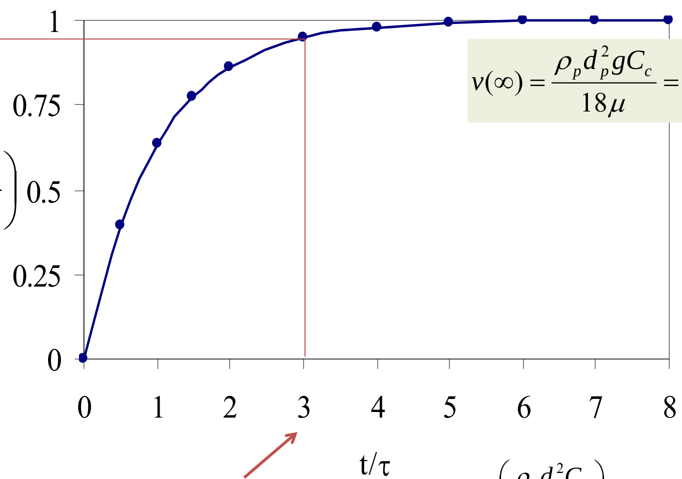
$$v(t) = \frac{\rho_p d_p^2 g C_c}{18\mu}\left\{1 - \exp\left[-\frac{t}{\left(\frac{\rho_p d_p^2 C_c}{18\mu}\right)}\right]\right\} \Rightarrow v(t\to\infty) = \frac{\rho_p d_p^2 g C_c}{18\mu} = v_{TS}$$

$$\tau = \left(\frac{\rho_p d_p^2 C_c}{18\mu}\right) \Rightarrow \frac{v(t)}{v_{TS}} = 1 - \exp\left(-\frac{t}{\tau}\right)$$

Terminal Settling Velocity

95%

$$\frac{v(t)}{v_{TS}} = 1 - \exp\left(-\frac{t}{\tau}\right)$$



$$v(\infty) = \frac{\rho_p d_p^2 g C_c}{18\mu} = v_{TS}$$

- Acceleration time
- Relaxation time

$$\tau = \left(\frac{\rho_p d_p^2 C_c}{18\mu}\right)$$

Example 4.1

- *Consider a spherical glass bead with a diameter of 30 μm and density of 2500 kg/m³ is released from rest in still air.*
  1. *How long it will take to reach its terminal velocity?*
  2. *What is its terminal velocity*

Solution: *Given d_p=30 μm, ρ_p = 2500 kg/m³, and μ = 1.81 x10⁻⁵ Pa.s*

$$Kn = 2\lambda/d_p = 2 \times \frac{0.066\ \mu m}{30\ \mu m} = 0.0044$$

$$C_c = 1 + Kn\left[1.142 + 0.558\exp\left(-\frac{0.999}{Kn}\right)\right]$$

$$= 1 + 0.0044\left[1.142 + 0.558exp\left(-\frac{0.999}{0.044}\right)\right] = 1.0055$$

$$\tau = \frac{\rho_p d_p^2 C_c}{18\mu} = \frac{2500 \times (30\times10^{-6})^2 \times 1.055}{18 \times 1.81 \times 10^{-5}} = 0.0073\ s$$

$$t = 3\tau = 3 \times 0.0073\ s = 0.0219\ s \qquad v_{TS} = \tau g = 0.0715\ \ m/s$$

Comments

- Aerosol particle reaches its terminal settling velocity almost instantaneously
- The terminal settling speed is very low.

Table 4.1

d_p(μm)	$0.95v_{TS}$ **(m/s)**	$t = 3\tau$ **(s)**
0.01	0.0000001	0.0000000
0.1	0.0000008	0.0000003
1	0.0000331	0.0000107
10	0.0028980	0.0009329

Example

- *Scientific research results indicated the total average size distribution of the droplets by coughing was 0.58-5.42 micron, and 82% of droplet nuclei centered in 0.74-2.12 micrometer*
- *A spherical droplet released by coughing with a diameter of 5 μm and density of 1000 kg/m^3 being released the mouth horizontally in still air.*
- *If the mouth is about 1.5 m above the floor when she coughed, how long would it take for the 5-μm droplet to settle down to the floor in calm air.*

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Solution

Given $d_p = 5\ \mu m$, $\rho_p = 1000\ kg/m^3$, and $\mu = 1.81 \times 10^{-5}$ Pa.s,

$$Kn = 2\lambda/d_p = 2 \times \frac{0.066\ \mu m}{5\ \mu m} = 0.0264$$

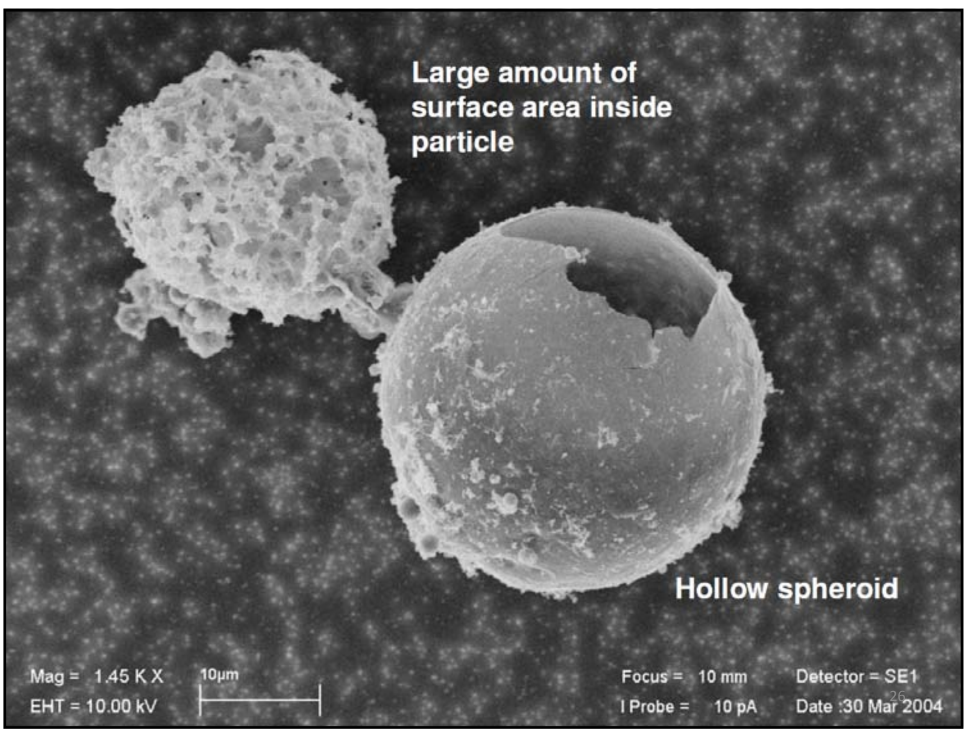
$$C_c = 1 + Kn\left[1.257 + 0.40 exp\left(-\frac{1.10}{Kn}\right)\right] = 1.033 \quad for\ 0.001 < Kn < 100$$

$$t = 3\tau = 3\left(\frac{\rho_p d_p^2 C_c}{18\mu}\right) = 3\left(\frac{1000 \times (5 \times 10^{-6})^2 \times 1.0333}{18 \times 1.81 \times 10^{-5}}\right) = 0.00024\ s$$

$$v_{TS} = g\tau = \frac{\rho_p d_p^{\,2} g C_c}{18\mu} = \frac{1000 \times (5 \times 10^{-6})^2 \times 9.81 \times 1.033}{18 \times 1.81 \times 10^{-5}} = 0.000753 \text{ m/s}$$

$$\Delta t = \frac{H}{V_{TS}} = \frac{1.5\text{m}}{0.000753\text{ m/s}} = 1992 \text{ s} \approx 33 \text{ min}$$

Comment: Could be slower for smaller droplets



Aerodynamic Diameter, d_a

- The aerodynamic diameter, d_a is an equivalent diameter that finds wide applications in aerosol studies.
- It is defined as the diameter of the spherical particle with a standard density of 1,000 kg/m^3 that has the same gravitational settling velocity as the particle when they are both present in the same gravitational field.

$$v_{TS} = \frac{\rho_p d_e^2 g C_c}{18 \mu S_f} = \frac{\rho_0 d_a^2 g C_c}{18 \mu}$$

ρ_0 =1000 kg/m^3

NOTE: Cc in both sides of the equations shall be based on d_e rather than d_a, because the slipping effect is a geometric factor

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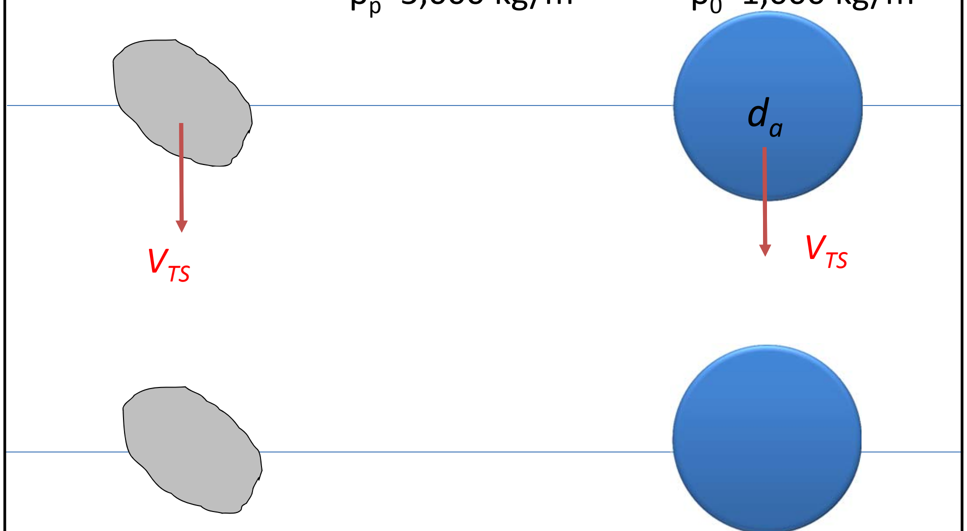
Real particle
ρ_p=5,000 kg/m^3

Equivalent diameter d_e
ρ_p=5,000 kg/m^3

Spherical particle
ρ_0=1,000 kg/m^3



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Example

- *Estimate the aerodynamic diameter for a steel particle with geometric equivalent diameter d_e = 10 µm and a density of ρ_p = 8000 kg/m³.*

Solution

Assume particle is spherical so that shape factor, S_f=1

$$d_a = d_e\left(\frac{\rho_p}{\rho_0 S_f}\right)^{1/2} = 10\times10^{-6}\left(\frac{8000}{1000\times1}\right)^{\frac{1}{2}} = 2.83\times10^{-5}\ m = 28.3\ \mu m$$

***Comment**: For a particle with this great density, its aerodynamic particle diameter is much greater than its geometric equivalent diameter.*

Stokes Number, Stk

- The Stokes number is defined as the ratio of the stopping distance of a particle to a characteristic dimension of the obstacle

$$Stk = \frac{\tau u_0}{d_c} = \frac{\rho_p d_p^2 C_c u_0}{18\mu d_c}$$

- The characteristic dimension d_c can be defined differently for different applications
- Note that in calculation of Cc it shall be based on geometric diameter

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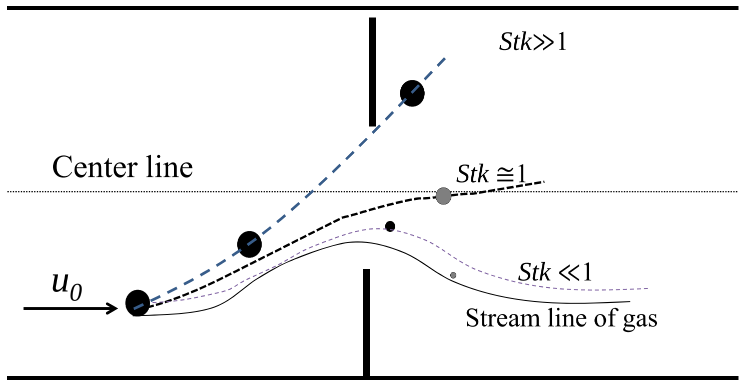
Stokes number indicates particle inertia

$$Stk = \frac{\tau u_0}{d_c} = \frac{\rho_p d_p^2 C_c u_0}{18\mu d_c}$$



Example *Estimate the Stokes number of a 1-μm particle with the density of 8000 kg/m³ in an air flowing at 1 m/s perpendicular to a cylinder of diameter 10 cm, assuming standard conditions.*

Given d_e = 1 μm, U_o =1m/s, d_c = 10 cm, ρ_p = 8000 kg/m³

- $Kn = 2\lambda/d_p = 2\lambda/d_e = 2 \times 0.066/1 = 0.132$
- $C_c = 1 + Kn\left[1.257 + 0.40exp\left(-\frac{1.10}{Kn}\right)\right]$ $\quad 0.001 < Kn < 100$
- $C_c = 1 + 0.132\left[1.257 + 0.40exp\left(-\frac{1.10}{0.132}\right)\right] = 1.166$

$$Stk = \frac{\rho_p d_p^2 C_c u_0}{18\mu d_c} = \frac{8000 \times (1 \times 10^{-6})^2 \times 1.166 \times 1}{18 \times 1.81 \times 10^{-5} \times 0.1} = 2.86 \times 10^{-4}$$

The geometric diameter is used in determining the Knudsen number because Kn is a geometric ratio rather than an aerodynamic property.

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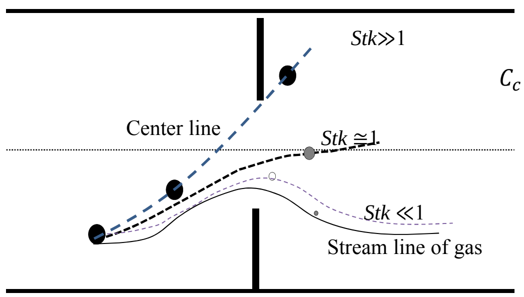
How to separate this particle from the air

Stokes number indicates particle inertia

$$\lambda = \frac{1}{\sqrt{2}\pi N_a}\frac{RT}{Pd^2}$$



$$Kn = 2\lambda/d_p$$

$$C_c = 1 + Kn\left[1.257 + 0.40exp\left(-\frac{1.10}{Kn}\right)\right]$$

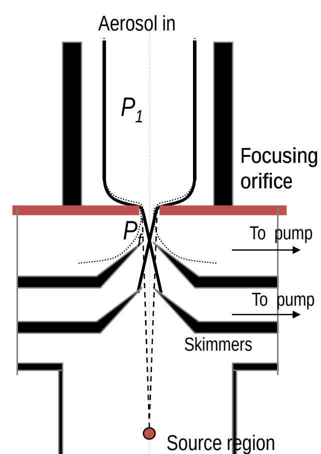
$$Stk = \frac{\tau U_0}{d_c} = \frac{\rho_p d_p^2 C_c U_0}{18\mu d_c}$$

$$\mu = \frac{2\sqrt{mkT}}{3\pi^{3/2}d^2}$$

Aerodynamic particle focusing (APF)

(Graduate students only)

- ❑ Particle beam formed when aerosol passes through an orifice into an evacuated chamber
- ❑ Particle beam has a diameter due to Brownian motion
- ❑ Optimum focused particle d_p^* is a function of Stk_f=1-2, by
  - ■ variable orifice geometry: **impractical**
  - ■ variable upstream pressure (→ particle mean free path) (3 mm orifice is to keep gas flow continuum at very low pressure)
- ❑ Various focusing devices to enhance transmission efficiency for smaller particles (<10 nm)

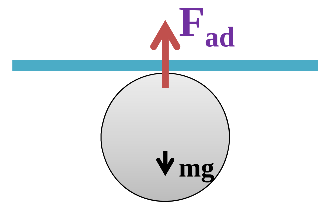


$$d_p^* = \sqrt{(1.66\lambda)^2 + (d_p^m)^2} - 1.66\lambda$$

$$d_p^m = \frac{18\mu Stk_f}{\rho_p v_f} \qquad \lambda_f = \lambda_0 \frac{p_0}{p_f}\frac{T_f}{T_0}$$

Aerosol-surface adhesion

- Unlike gas molecules, most aerosol particles, attach firmly to surfaces they come in contact with.



Aerodynamic diameter (μm)	Force (N)	
	Adhesion	Gravity
0.1	10^{-8}	5×10^{-18}
1	10^{-7}	5×10^{-15}
10	10^{-6}	5×10^{-12}
100	10^{-5}	5×10^{-9}

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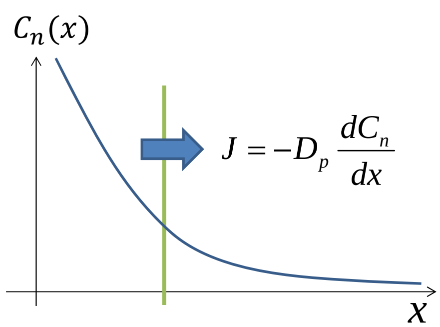
Aerosol diffusion in air

- J=flux of particles, expressed in terms of the number of particles per unit time,
- D_p=diffusivity of the particles in the gas, and
- dC_n/dx=gradient in number concentration of particles.



$$D_p = \frac{kTC_c}{3\pi\mu d_p}$$

The particle diffusion coefficient has a unit of m^2/s and it increases with temperature but decreases with particle diameter and the viscosity of the gas stream.

Aerosol particle size distribution

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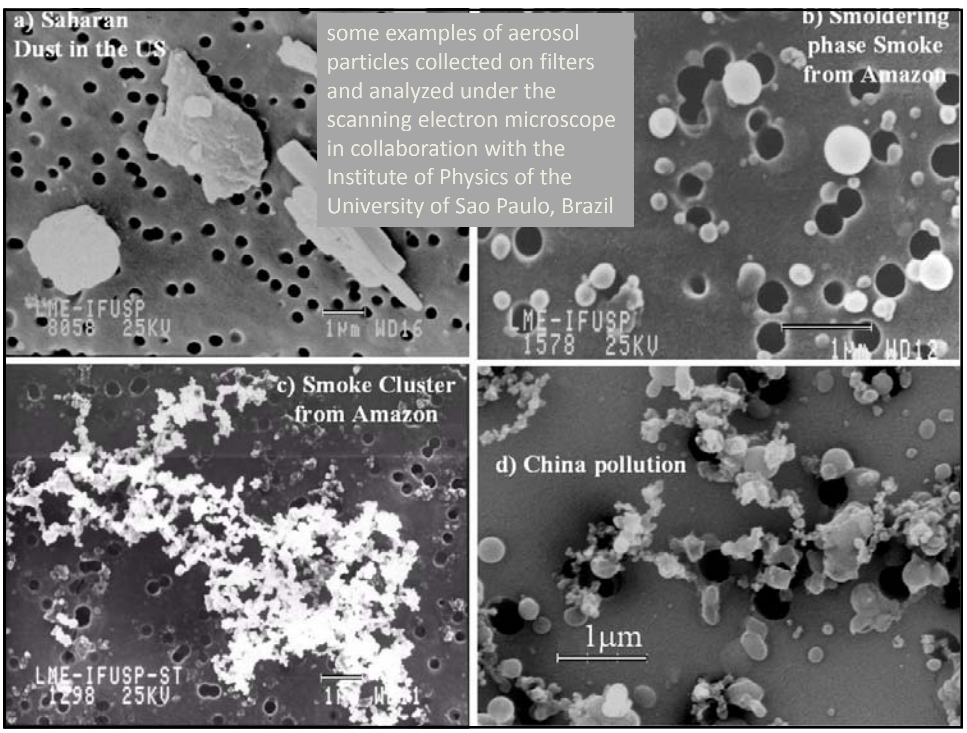
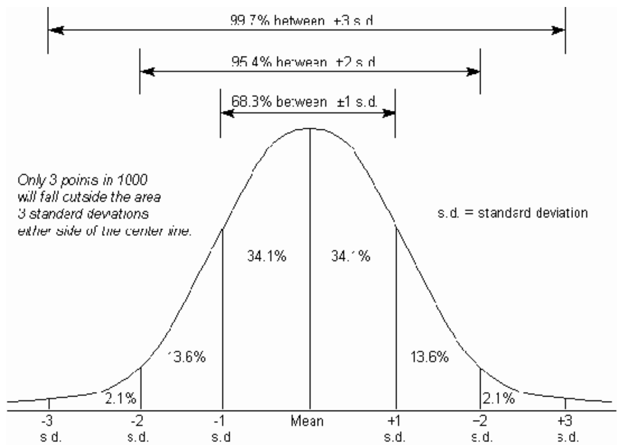


Normal Distribution



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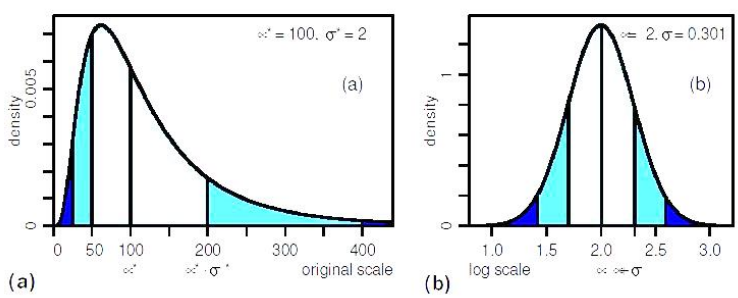
Log-normal distribution



$$df = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) dx$$

$$df = \frac{1}{\sqrt{2\pi}\ln\sigma_g} \exp\left(-\frac{(\ln d_p - \ln CMD)^2}{2(\ln\sigma_g)^2}\right) d(\ln d_p)$$

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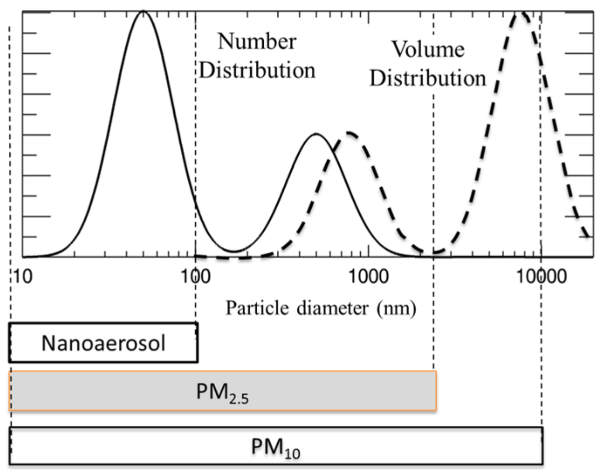
Actual aerosol size distribution in the atmosphere

- Based on number, surface area and volume (mass).

1. Can you match them with the figures?
2. Any comments on the regulation over $PM_{2.5}$ and PM_{10}?



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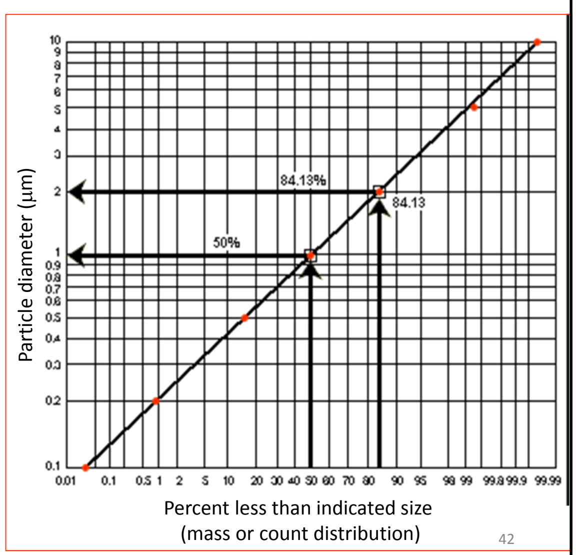
Log-probability graphs for cumulative distribution

- A practical application of log-normal distribution
- Download it from website

$$\sigma_g = \frac{d_{84\%}}{d_{50\%}} = \frac{d_{50\%}}{d_{16\%}} = \left(\frac{d_{84\%}}{d_{16\%}}\right)^{1/2}$$

- σ_g is the same for count and mass distribution



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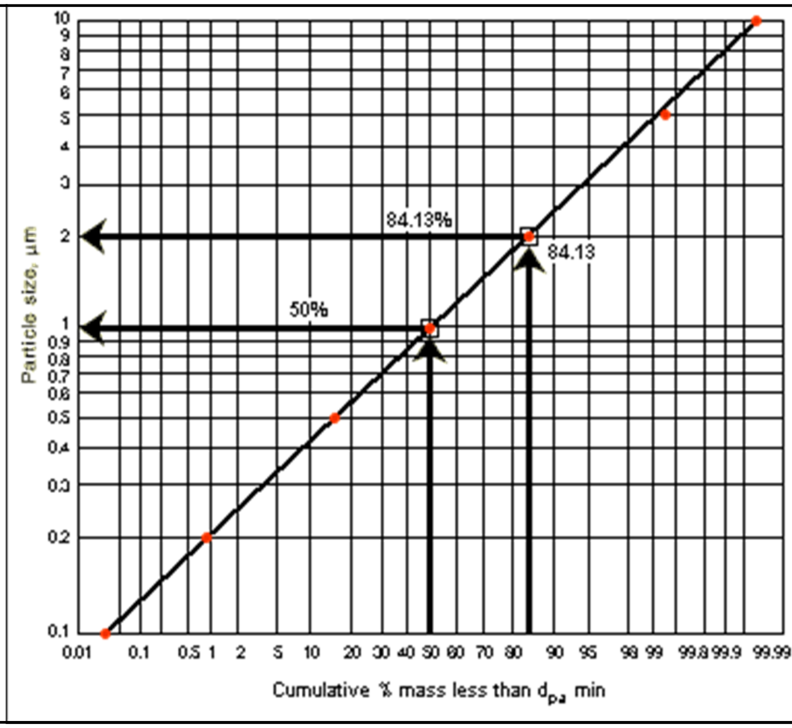

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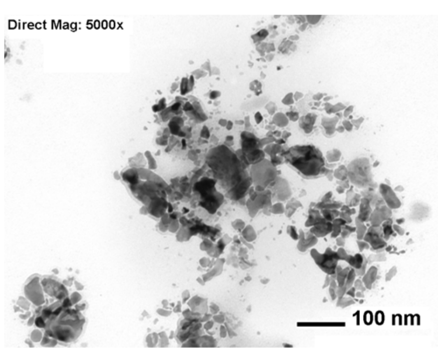
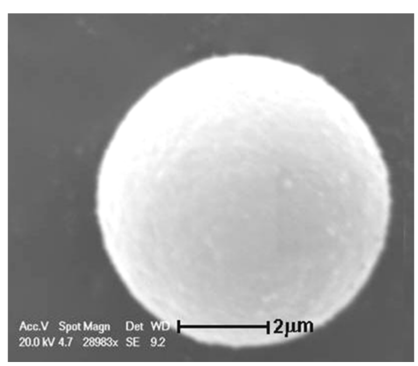
Size distribution change by coagulation

- When the particle comes in contact with another particle, both particles adhere to each other and the process is referred to as **coagulation**.





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Discussion

- Do particles of different sizes from the same materials have the same density?

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