Lecture 3 Airborne Particulate Matter
Particulate Matter

HUMAN HAIR
50-70 μm (microns) in diameter

PM$_{2.5}$
Combustion particles, organic compounds, metals, etc.
< 2.5 μm (microns) in diameter

PM$_{10}$
Dust, pollen, mold, etc.
< 10 μm (microns) in diameter

90 μm (microns) in diameter
FINE BEACH SAND

Figure 1.1 Examples of aerosol particle size ranges.
Early developments

  \[ F_d = 3\pi \mu Ud \]
- Knudt and Warburg (1875) – observation of gas non-continuum effect on drag force.
- Ebenezer Cunningham (1910) – slip correction equation for drag force.
  \[ C = 1 + \frac{2\lambda}{d} \cdot (A_1 + A_2 \cdot e^{-\frac{A_3 d}{\lambda}}) \]
- Robert A. Millikan (1910) – experimental verification of the Cunningham slip correction equation.
- Albert Einstein (1905) - Brownian motion
  \[ \frac{r^2(t)}{m_p} t = \frac{2k_B T e^{-\frac{A_3 d}{\lambda}}}{3\pi \mu D_p} \]
- Gustav Mie (1908) – Scattering of electromagnetic waves by a homogeneous sphere
"On the movement of small particles suspended in a stationary liquid demanded by the molecular-kinetic theory of heat"

Ferner fanden wir in §4 für den Mittelwert der Verschiebungen der Teilchen in Richtung der X-Achse in der Zeit $t$:

$$\lambda = \sqrt{2Dt}.$$

Durch Eliminieren von $D$ erhalten wir:

$$\lambda = \sqrt{T}\sqrt{\frac{RT}{6\pi kP}}.$$  

Diese Gleichung läßt erkennen, wie $\lambda$ von $T$, $k$ und $P$ abhängen muß.

Wir wollen berechnen, wie groß $\lambda$ für eine Sekunde ist, wenn $N$ gemäß den Resultaten der kinetischen Gastheorie $3 \times 10^{28}$ gesetzt wird; es sei als Flüssigkeit Wasser von $17^\circ C$ gewählt ($k = 1,35 \times 10^{-2}$) und der Teilchendurchmesser sei $0,001$ mm. Man erhält:

$$\lambda = 8 \times 10^{-5} \text{cm} = 0,8 \text{Mikron}.$$
Brownian diffusion

Equation of diffusion

Consider the particle diffusion flux $J$ in each direction for the elemental volume, the rate of change of particle number concentration due to diffusion can be derived:

$$\frac{dn}{dt} = - \left( \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z} \right) = \nabla \cdot \mathbf{J}$$

Applying the Fick's first law:

$$J_x = -D \frac{\partial n}{\partial x} \quad J_y = -D \frac{\partial n}{\partial y} \quad J_z = -D \frac{\partial n}{\partial z}$$

We can derive the equation of diffusion:

$$\frac{dn}{dt} = D \left( \frac{\partial^2 n}{\partial x^2} + \frac{\partial^2 n}{\partial y^2} + \frac{\partial^2 n}{\partial z^2} \right) = D \nabla^2 n$$

(D: diffusion coefficient, or diffusivity, m$^2$/s)
Consider particle transport in one dimension (infinite in both +x and –x directions), with all particles initially located on an infinitesimally thin plane at x=0 with a concentration of $N_0$ (# of particles/m2):

$$\frac{dn}{dt} = D \frac{\partial^2 n}{\partial x^2}$$

B.C.: $n(-\infty, t) = 0, n(\infty, t)=0$

I.C.: $n(x, 0) = 0$ except at $x=0$

The solution is:

$$n(x, t) = \frac{N_0}{2\sqrt{\pi Dt}} \exp\left(\frac{-x^2}{4Dt}\right)$$

The mean square displacement of the particles is:

$$\bar{x}^2 = \frac{1}{N_0} \int_{-\infty}^{\infty} x^2 n(x, t) dx = 2Dt$$

Einstein derived that, for Brownian motion:

$$D = \frac{kT}{3\pi \mu d_p} \quad \bar{x}^2 = \frac{2kTt}{3\pi \mu d_p}$$

$k$ is the Boltzmann constant (1.38e-23 m$^2$kg/s$^2$K)

This equation applies for particles with $dp >>$ mean free path of gas.
Friction coefficient ($f$)

• For a rigid sphere that moves through a fluid at constant velocity $U$, and the Reynolds number $Re << 1$, the friction coefficient $f$, can be calculated using the Stokes equation

$$F = fU, \quad f = 3\pi\mu d_p \quad R_e = \frac{\rho_f d_p U}{\mu_f}$$

The particle must be many diameters away from any surfaces and much larger than the mean free path of the gas molecules, $\lambda$

$$\lambda = \frac{\mu}{\rho} \sqrt{\frac{\pi m_1}{2kT}}$$

- $m_1$: molecular mass of the gas molecule (~4.817x10^{-26} kg)
- $k$: Boltzmann constant (1.38x10^{-23} m^2 kg/s^2 K)
- $T$: temperature (K)
- $\mu$: dynamic viscosity (18.37x10^{-6} Ns/m^2)
- $\rho$: density (1.225 kg/m^3)
Friction coefficient \( (f) \)

- When \( dp \ll \lambda \)

\[
f = \frac{2}{3} d_p^2 \rho \left( \frac{2\pi k T}{m_1} \right)^{1/2} \left( 1 + \frac{\pi \alpha}{8} \right)
\]

- \( m_1 \): molecular mass of the gas molecule (~4.817x10\(^{-26}\) kg)
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- \( \rho \): density (1.225 kg/m\(^3\))
- \( \alpha \): accommodation coefficient (~0.9)

Note that in this range, the friction coefficient increases quadratically with particle diameter.
Friction coefficient ($f$)

- The Cunningham slip correction ($C_c$) can be used to correct the friction coefficient for the Stokes equation so that it can be applied for the entire particle size range

\[ F = fU, \quad f = \frac{3\pi\mu d_p}{C_c} \]

\[ C_c = 1 + \frac{2\lambda}{d_p} \left[ 1.257 + 0.4 \exp\left(-\frac{0.55d_p}{\lambda}\right) \right] \]

Define Knudsen number, $K_n = \frac{2\lambda}{d_p}$

<table>
<thead>
<tr>
<th>Kn</th>
<th>Cc (air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>1.01</td>
</tr>
<tr>
<td>0.1</td>
<td>1.12</td>
</tr>
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<td>1</td>
<td>2.39</td>
</tr>
<tr>
<td>10</td>
<td>16.77</td>
</tr>
</tbody>
</table>
Migration of particles in an external force field

• Gravitational field and settling velocity

\[ F = f v_t \]
\[ F = \frac{\pi d_p^3}{6} (\rho_p - \rho_f) g \]
\[ f = \frac{3\pi \mu d_p}{C_c} \]
\[ v_t = \frac{\rho_p g d_p^2 C_c}{18 \mu} \left(1 - \frac{\rho_f}{\rho_p}\right) \]

• Electric field

\[ F = f v_t \]
\[ F = q E \]
\[ f = \frac{3\pi \mu d_p}{C_c} \]
\[ v_t = \left(\frac{q C_c}{3\pi \mu d_p}\right) E = Z E \]

Z: electrical mobility
Relaxation time

• Time scale to reach terminal velocity

Newton’s second law: F=ma
and the definition of acceleration: a=dv/dt

\[ m \frac{dv}{dt} = mg - \frac{3\pi \mu d_p}{C_c} v \]

v=0 when t=0

Solution:

\[ v = \tau g \left( 1 - e^{-t/\tau} \right) \]

\[ \tau = \frac{\rho_p d_p^2 C_c}{18 \mu} \]

is called the relaxation time
Stop distance

How far could a particle travel through a stagnant layer of air before its velocity goes to zero?

\[
\frac{m \, dv}{dt} = - \frac{3 \pi \mu d_p}{C_c} v
\]

\(v = v_0\) when \(t = 0\)

Solution:

\[v = v_0 e^{-t/\tau}\]

\[
\frac{dS}{dt} = v = v_0 e^{-t/\tau}
\]

\(S = 0\) when \(t = 0\)

Solution: (integrate from \(t = 0\) to \(t = \infty\))

\[S = v_0 \tau\]

Stokes number:

\[S_t = \frac{v_0 \tau}{L}\]

\(L\) is the length scale of the problem.
Mass transfer between gas and particles – (1) condensation/evaporation

Consider a large particle (Kn<<1) made of pure species A in the air that also contains vapor molecules of A. Particle growth or evaporation depends on the direction of the net flux of vapor molecules relative to the particle.

Let the radius of the particle be \( r_p \), and \( r \) be the radial distance from the center of the particle, the steady state diffusion of gas A to the surface of the particle is

\[
\frac{\partial C}{\partial t} = - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 J \right) = - \left( \frac{\partial J}{\partial r} + \frac{2J}{r} \right)
\]

Applying Fick’s first law, \( J = -D_g \frac{\partial C}{\partial r} \)

\[
\frac{\partial C}{\partial t} = - \left( \frac{\partial J}{\partial r} + \frac{2J}{r} \right) = D_g \left( \frac{\partial^2 C}{\partial r^2} + \frac{2 \partial C}{r \partial r} \right)
\]

I.C.: \( C(r,0) = C_\infty \)
B.C.: \( C(\infty,t)=C_\infty \)
\( C(r_p,t)=C_s \)