Mass Diffusion

Outline

- Diffusivity
- Diffusion Equation
- Diffusion to a Wall
- Deposition Velocity, Diffusion Boundary Layer, Diffusion Force
- Diffusion to a Flat Plate
- Diffusion in Tube
- Taylor Diffusion

Brownian Diffusion and Fick's Law

Fick's Law

\[ J = -D \frac{dc}{dx} \]

Diffusion Equation

\[ \frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = D \nabla^2 c \]

Diffusivity

\[ D = \frac{kTc_\infty}{3\pi\eta d} \]

Mass Diffusivity

Table of Particle Mass Diffusivity

<table>
<thead>
<tr>
<th>d (\mu m)</th>
<th>D (cm²/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10⁻²</td>
<td>5.24 × 10⁻⁴</td>
</tr>
<tr>
<td>10⁻¹</td>
<td>6.82 × 10⁻⁶</td>
</tr>
<tr>
<td>1</td>
<td>2.74 × 10⁻⁷</td>
</tr>
<tr>
<td>10</td>
<td>2.38 × 10⁻⁸</td>
</tr>
</tbody>
</table>
Particle Diffusion

Mean Square Displacement
\[ \overline{s^2} = 2Dt \]

Brownian Motion of Rotation
\[ \overline{\theta^2} = \frac{2kT}{\pi \mu d^2} t \]

Particle Fluctuation Energy
\[ \frac{1}{2} m \overline{u^2} = \frac{3}{2} kT \]
\[ \overline{u^2} = \sqrt{3kT/m} \]

Concentration in gravitational field
\[ C = C_0 \exp \left\{ -\frac{mg(x-x_0)}{kT} \right\} \]

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Particle Diffusion

Effect of Particle Mass
\[ s^2 = 2Dt \left[ 1 - \tau(1 - e^{-t/\tau}) / t \right] \]

Particle Mean Free Path
\[ \lambda_\alpha \approx \tau \sqrt{8kT / \pi m} \]

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Particle Diffusion to a Wall

Similarity Variable
\[ \eta = \frac{y}{\sqrt{4Dt}} \]
\[ \overline{c} = \frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial y^2} \]
\[ C(0,t) = 0 \]
\[ C(0,t) = C_0 \]

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Particle Diffusion to a Wall

Similarity Equation
\[ \frac{d^2c}{dn^2} + 2\eta \frac{dc}{dn} = 0 \]
\[ \ln \left( \frac{dc}{dn} \right) = -\eta^2 + \ln A \]
\[ c = A \int_{n_0}^n e^{-\eta^2} dn_1 + B \]

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Particle Diffusion to a Wall

\[ C(y, t) = C_0 \text{erf} \left( \frac{y}{\sqrt{4Dt}} \right) \]

\[ C(\eta = 0) = 0 \]

\[ \text{erf} (\xi) = \frac{2}{\sqrt{\pi}} \int_0^\xi e^{-z^2} \, dz \]

\[ \text{erf} (0) = 0 \quad \text{erf} (\infty) = 1 \]

\[ \delta_c = \sqrt{\pi Dt} \]

\[ F_d = 3\pi \mu u_D / C_c \]

\[ \frac{\partial C}{\partial t} = \frac{J}{C_0} = \sqrt{\frac{D}{\pi t}} = \frac{D}{\delta_c} \]

\[ dN = J dt = C_0 \sqrt{\frac{D}{\pi t}} dt \]

\[ N = C_0 \sqrt{\frac{4D t}{\pi}} \]
**Tube Deposition**

\[ \frac{N}{L/u} = C_0 \sqrt{\frac{4Dt}{\pi}} \]
\[ N = C_{in} \sqrt{\frac{4DL}{\pi u}} \]

\[ C_{out} - C_{in} = -N \frac{2R\pi L}{\pi R^2 L} \]

**Concentration Ratio**

\[ \frac{C_{out}}{C_{in}} = 1 - \frac{4}{\sqrt{\pi}} \sqrt{\frac{DL}{uR^2}} \]

\[ \phi = \frac{DL}{uR^2} \]

**Detailed Analysis**

\[ \frac{C_{out}}{C_{in}} = 1 - 2.56\phi^{2/3} + 1.2\phi + 0.177\phi^{4/3} \]

**Convective Diffusion to a Flat Plate**

**Momentum**

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \]

**Mass**

\[ \frac{\partial u}{\partial x} + \frac{\partial c}{\partial y} = 0 \]

**Concentration**

\[ \frac{\partial c}{\partial x} + \frac{\partial c}{\partial y} = D \frac{\partial^2 c}{\partial y^2} \]

\[ y = 0 \quad u = v = c = 0 \]

\[ y \rightarrow \infty \quad u = U_0 \quad c = c_0 \]
**Flat Plate - Similarity Variables**

\[ \eta = y \frac{U_0}{v_x} \]

\[ u = f'(\eta) \]

\[ \psi = \sqrt{vU_0} x f(\eta) \]

\[ c = c(\eta) \]

\[ f f'' + 2 f''' = 0 \]

\[ c'' + \frac{1}{2} S \eta c' = 0 \]

\[ s_x = \frac{\eta}{D} \]

**Boundary Conditions**

\[ f(0) = f'(0) = 0 \]

\[ f'(\infty) = 1 \]

\[ c(0) = 0 \]

\[ c(\infty) = c_0 \]

**Blasius Solution**

\[ \delta = 5 \sqrt{\frac{v_x}{U_0}} \]

\[ f''(0) = \gamma = 0.332 \]

**Near the Plate**

\[ f \sim \frac{\gamma}{2} \eta^2 + \ldots \]

**Concentration Profile**

\[ C = \frac{C_0}{\int_0^\infty \exp(-\gamma \eta S_c z^3) dz} \]

\[ \gamma_1 = \frac{\gamma}{12} \]

\[ c = \frac{3 \sqrt{\gamma_1 S_c}}{0.89 \int_0^\infty \exp(-\gamma_1 S_c z^3) dz} \]
**Diffusion to a Flat Plate**

\[ J = D \left[ \frac{\partial c}{\partial y} \right]_{y=0} = Dc_0 \frac{\sqrt{y \delta_x}}{U_0} \left( \frac{U_0}{v_x} \right) \]

**Boundary Layer**

\[ \delta_x = \frac{Dc_0 \approx \frac{3}{J} \sqrt{\frac{v_x}{U_0}} \approx 0.6\delta} \]

**Total Diffusion**

\[ I = \int_0^1 J dx = 0.68Dc_0 \frac{\sqrt{R_d}}{\sqrt{R_d}} \]

\[ \frac{R_d}{U_0} = \frac{L}{v} \]

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**Diffusion in a Tube Flow**

- **Laminar Flow**
  \[ u = u_0 (1 - \frac{r^2}{R^2}) \]
  \[ y = R - r \]

- **Wall Flux**
  \[ J = \frac{Dc_0}{\frac{DX}{v_x}} \int_0^{\frac{2}{9} \eta^3} \exp \left\{ -\frac{2}{9} \eta^3 \right\} d\eta \]

\[ J = 0.67c_0D \frac{\sqrt{D_0}}{\sqrt{v_x}} \]

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**Solution for Diffusion in a Tube Flow**

- **Concentration Profile**
  \[ c = \frac{1}{\frac{\eta}{\frac{\eta^3}{d\eta}}} \int_0^{\frac{2}{9} \eta^3} \exp \left\{ -\frac{2}{9} \eta^3 \right\} d\eta \]

\[ c = 0 \]

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**Diffusion Equation**

\[ \frac{2u_0}{R} \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial y^2} \]

**Boundary Condition**

- \( y = 0 \) \( c = 0 \)
- \( y \rightarrow \infty \) \( c = c_0 \)

**Similarity Variable**

\[ \eta = \sqrt{\frac{u_0}{DR} \frac{y}{\sqrt{x}}} \]

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**Wall Flux**

\[ c' + \frac{2}{3} \eta^2 c' = 0 \]
**Solution for Diffusion in a Tube Flow**

**Total Flux**

\[ I = 2\pi R \int_0^L Jdx = 2.01 \pi c_0 DR \frac{u_0 L^2}{DR} \]

**Diffusion Boundary layer**

\[ \delta_e = \frac{Dc_o}{J} = \frac{0.67 s_{c} \sqrt{R^2 x}}{s_{c} R \sqrt{R^2 x}^{1/3}} = \frac{1}{0.67} \] \[ R_s = \frac{u_0 R}{v} \]

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**Taylor Diffusion**

\[ \frac{\partial c}{\partial t} + u(r) \frac{\partial c}{\partial x} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial x^2} \right) \]

**Neglecting Axial Diffusion**

\[ u(r) = 2U \left( 1 - \frac{r^2}{R^2} \right) \]

\[ \frac{\partial c}{\partial t} + U(1 - \frac{2r^2}{R^2}) \frac{\partial c}{\partial x} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \]

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**For Moving Frame**

\[ \frac{\partial c}{\partial t} \approx 0 \]

\[ \frac{\partial c}{\partial x} = \text{const} \]

\[ U(1 - \frac{2r^2}{R^2}) \frac{\partial c}{\partial x} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} \right) \]

**Solution**

\[ c = c_0 + \frac{U R^2}{4D} \frac{\partial c}{\partial x} \left( \frac{r^2}{R^2} - \frac{1}{2} \frac{r^4}{R^4} \right) \]

**Concentration**

\[ c = c + \frac{R^2 U}{4D} \frac{\partial c}{\partial x} \left( -\frac{1}{3} + \frac{r^2}{R^2} - \frac{1}{2} \frac{r^4}{R^4} \right) \]

**Total Flux**

\[ Q_c = 2\pi \int_0^R c(u - U) rdr = -\frac{(\pi R^2)^2 U^2}{48D} \frac{\partial c}{\partial x} \]
The Flux Per Unit Area is given by:

\[ J = \frac{Q}{\pi R^2} = -\left(\frac{R^2 U^2}{48D}\right) \frac{\partial c}{\partial x} \]

The Effective (Taylor) Diffusivity is defined as:

\[ D_{\text{eff}} = \frac{R^2 U^2}{48D} \]

The partial derivative of concentration with respect to time and position is given by:

\[ \frac{\partial c}{\partial t} = -\frac{\partial}{\partial x} J = D_{\text{eff}} \frac{\partial^2 c}{\partial x^2} \]

The Range of Validity is given by:

\[ \frac{L}{R} \gg P_e > 14 \]

\[ P_e = \frac{2UR}{D} = R_S \]

At \( t = 0 \), the concentration is:

\[ c = \frac{N}{\pi R^2} \delta(x) \]

The concentration at any time \( t \) is given by:

\[ c = \frac{1}{2} \frac{N}{\pi R^2} \frac{1}{\sqrt{\pi D_{\text{eff}} t}} \exp\left\{ -\frac{(x - Ut)^2}{4D_{\text{eff}} t} \right\} \]

**Summary**

- Mass diffusion decreases with size
- Diffusion Boundary Layer is generally smaller than momentum boundary layer
- Convective diffusion in a tube
- Taylor diffusion in a tube

Variations of concentration along the tube at different times.