Particle Transport, Deposition and Removal

Mass Diffusion

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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 → $D = \frac{kTC_c}{3\pi\mu d}$

Mass Diffusivity

Table of Particle Mass Diffusivity

d (μm)	D (cm^2/s)
10^{-2}	5.24×10^{-4}
10^{-1}	6.82×10^{-6}
1	2.74×10^{-7}
10	2.38×10^{-8}

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Mean Square Displacement → $\overline{s^2} = 2Dt$

Brownian Motion of Rotation → $\overline{\theta^2} = \frac{2kT}{\pi\mu d^3} t$

Particle Fluctuation Energy: $\frac{1}{2} m\overline{u^2} = \frac{3}{2} kT$, $\sqrt{\overline{u^2}} = \sqrt{3kT/m}$

Concentration in gravitational field: $C = C_0 \exp\{-\frac{mg(x-x_0)}{kT}\}$

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

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

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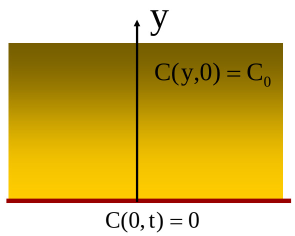
$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial y^2}$$



Similarity Variable

$$\eta = \frac{y}{\sqrt{4Dt}}$$

$$\frac{\partial c}{\partial y} = \frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial y} = \frac{\partial c}{\partial \eta}\frac{1}{\sqrt{4Dt}}$$

$$\frac{\partial^2 c}{\partial y^2} = \frac{\partial^2 c}{\partial \eta^2}\frac{1}{4Dt}$$

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$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial \eta}\frac{\partial \eta}{\partial t} = \frac{\partial c}{\partial \eta}\frac{-y}{2t\sqrt{4Dt}} = -\frac{\partial c}{\partial \eta}\frac{\eta}{2t}$$

Similarity Equation

$\frac{d^2 c}{d\eta^2} + 2\eta\frac{dc}{d\eta} = 0$ → $\ln(\frac{dc}{d\eta}) = -\eta^2 + \ln A$

$\frac{dc}{d\eta} = Ae^{-\eta^2}$ → $c = A\int_0^{\eta} e^{-\eta_1^2} d\eta_1 + B$

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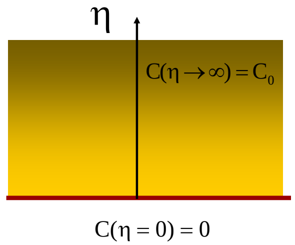
$$C(y,t) = C_0 \,\mathrm{erf}\,(y/\sqrt{4Dt})$$



$$\mathrm{erf}\,(\xi) = \frac{2}{\sqrt{\pi}} \int_0^{\xi} e^{-\xi^2} d\xi$$

$$\mathrm{erf}\,(0) = 0$$

$$\mathrm{erf}\,(\infty) = 1$$

Particle Diffusion to a Wall

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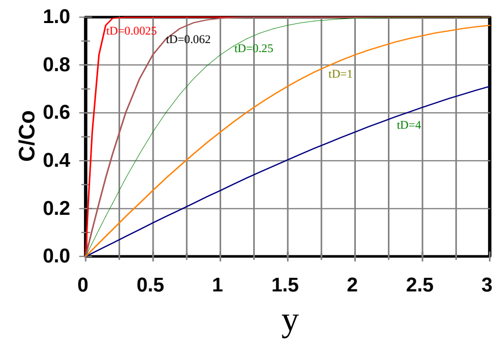

Variation of concentration profile with time.

Particle Diffusion to a Wall

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Diffusion Velocity → $$u_D = \frac{J}{C_0} = \sqrt{\frac{D}{\pi t}} = \frac{D}{\delta_c}$$

Diffusion Boundary Layer → $$\delta_c = \sqrt{\pi D t}$$

Diffusion Force → $$F_d = 3\pi\mu d u_D / C_c$$

Particle Diffusion to a Wall

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Number Deposited in Time dt → $$dN = J dt = C_0 \sqrt{\frac{D}{\pi t}} dt$$

Total Deposited in Time Interval (0,t) → $$N = C_0 \sqrt{\frac{4Dt}{\pi}}$$

Tube Deposition

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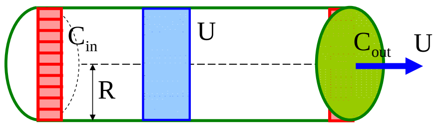

$$N = C_0\sqrt{\frac{4Dt}{\pi}} \quad \xrightarrow{t = L/u} \quad N = C_{in}\sqrt{\frac{4DL}{\pi u}}$$

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

Tube Deposition

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Concentration Ratio →

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

Detailed Analysis →

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

$$\phi = \frac{DL}{uR^2}$$

Convective Diffusion to a Flat Plate

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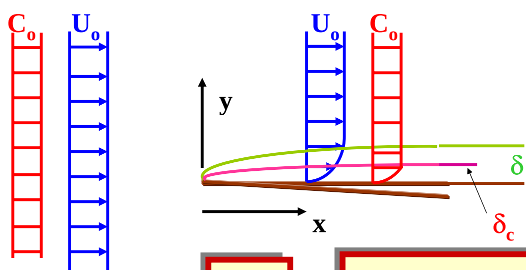

$y = 0$ $\quad u = v = c = 0$

$y \to \infty$ $\quad u = U_0, c = c_0$

Convective Diffusion to a Flat Plate

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Momentum →

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\frac{\partial^2 u}{\partial y^2}$$

Mass →

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

Concentration →

$$u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = D\frac{\partial^2 c}{\partial y^2}$$

Flat Plate - Similarity Variables

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$$\eta = y\sqrt{\frac{U_0}{\nu x}}$$

$$\frac{u}{U_0} = f'(\eta)$$

$$\psi = \sqrt{\nu U_o x}\, f(\eta)$$

$$c = c(\eta)$$

Momentum/Mass

$$ff'' + 2f''' = 0$$

Blasius Equation

Concentration

$$c'' + \frac{1}{2} S_c f c' = 0$$

$$S_c = \frac{\nu}{D}$$

Flat Plate - Similarity Variables

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Boundary Conditions

$$f(0) = f'(0) = 0 \qquad f'(\infty) = 1$$

$$c(0) = 0 \qquad c(\infty) = c_0$$

Blasius Solution

$$\delta = 5\sqrt{\frac{\nu x}{U_0}} \qquad f''(0) = \gamma = 0.332$$

Near the Plate

$$f \simeq \frac{\gamma}{2}\eta^2 + \ldots$$

Concentration Profile

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$$C = \frac{C_0 \int_0^{\eta} \exp(-\gamma_1 s_c z^3) dz}{\int_0^{\infty} \exp(-\gamma_1 s_c z^3) dz}$$

$$\gamma_1 = \frac{\gamma}{12}$$

$$\frac{c}{c_0} = \frac{\sqrt[3]{\gamma_1 s_c}}{0.89} \int_0^{\eta} [\exp(-\gamma_1 s_c z^3)] dz$$

Concentration Profile

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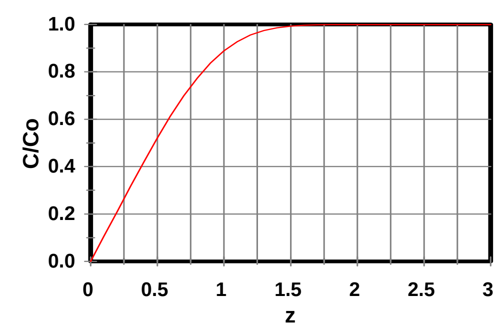

Diffusion to a Flat Plate

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$$J = D\left[\frac{\partial c}{\partial y}\right]_{y=0} = Dc_0 \frac{\sqrt[3]{(\gamma_1 s_c)}}{0.89}\sqrt{\frac{U_0}{vx}} = 0.34 Dc_0 \sqrt[3]{s_c}\sqrt{\frac{U_0}{vx}}$$

Diffusion Boundary Layer

$$\delta_c = \frac{Dc_0}{J} \approx \frac{3}{\sqrt[3]{s_c}}\sqrt{\frac{vx}{U_0}} \approx \frac{0.6\delta}{\sqrt[3]{s_c}}$$

Total Diffusion

$$I = \int_0^L J dx = 0.68 Dc_0 \sqrt[3]{s_c}\sqrt{R_{eL}}$$

$$R_{eL} = \frac{U_0 L}{\nu}$$

Diffusion in a Tube Flow

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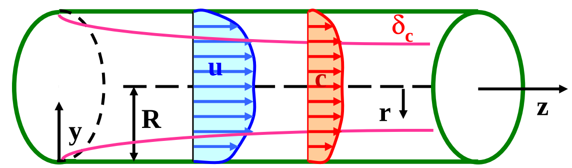

Laminar Flow

$$u = u_0\left(1 - \frac{r^2}{R^2}\right)$$

$$y = R - r$$

$$u \simeq u_0 \frac{2y}{R} + \ldots$$

Diffusion in a Tube Flow

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Diffusion Equation

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

Boundary Condition

$y = 0$ $c = 0$

$y \to \infty$ $c = c_0$

$$\eta = \sqrt[3]{\frac{u_0}{DR}}\frac{y}{\sqrt[3]{x}}$$

Similarity Variable

$$c'' + \frac{2}{3}\eta^2 c' = 0$$

Solution for Diffusion in a Tube Flow

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Concentration Profile

$$c = \frac{c_0 \int_0^{\eta} \exp\{\frac{-2}{9}\eta_1^3\} d\eta_1}{\int_0^{\infty} \exp\{\frac{-2}{9}\eta_1^3\} d\eta_1}$$

Wall Flux

$$J = D\left[\frac{\partial c}{\partial y}\right]_{y=0} = \frac{\frac{Dc_0}{\sqrt[3]{x}}\sqrt[3]{\frac{u_0}{DR}}}{\int_0^{\infty}\exp(-\frac{2}{9}\eta_1^3) d\eta_1}$$

$$J = 0.67 c_0 D \sqrt[3]{\frac{u_0}{DRx}}$$

Solution for Diffusion in a Tube Flow

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Total Flux

$$I = 2\pi R\int_0^L J dx = 2.01\pi c_0 D R\sqrt[3]{\frac{u_0 L^2}{DR}}$$

Diffusion Boundary layer

$$\delta_c = \frac{Dc_0}{J} = \frac{\sqrt[3]{R^2 x}}{0.67 s_c^{1/3} R_{eR}^{1/3}} = \frac{1}{0.67}\sqrt[3]{\frac{R^2 x}{s_c R_{eR}}}$$

$$R_{e_R} = \frac{u_0 R}{\nu}$$

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Taylor Diffusion

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

Neglecting Axial Diffusion

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

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

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Taylor Diffusion

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For $\left[\frac{\partial c}{\partial r}\right]_R = 0$ $\quad \frac{\partial c}{\partial t} \approx 0$

Moving Frame $\quad \frac{\partial c}{\partial x} = \text{const} = \frac{\partial \bar{c}}{\partial x}$

Diffusion In Moving Frame

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

Solution

$$c = c_o + \frac{UR^2}{4D}\frac{\partial \bar{c}}{\partial x}\left(\frac{r^2}{R^2} - \frac{1}{2}\frac{r^4}{R^4}\right)$$

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Taylor Diffusion

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$$c_o = [c]_{r=0}$$

$$\bar{c} = \frac{1}{A}\int_A c\,dA = \frac{1}{\pi R^2}\int_0^R 2\pi r c\,dr = \frac{2}{R^2}\int_0^R c r\,dr$$

Concentration

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

Total Flux

$$Q_c = 2\pi\int_0^R c(u - U) r\,dr = -(\pi R^2)\frac{R^2 U^2}{48D}\frac{\partial \bar{c}}{\partial x}$$

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Taylor Diffusion

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Flux Per Unit Area → $J = \frac{Q}{\pi R^2} = -\left(\frac{R^2U^2}{48D}\right)\frac{\partial \bar{c}}{\partial x}$

Effective (Taylor) Diffusivity → $D_{eff} = \frac{R^2U^2}{48D}$

$\frac{\partial \bar{c}}{\partial x} \neq \text{const.}$ → $\frac{\partial \bar{c}}{\partial t} = -\frac{\partial}{\partial x}J = D_{eff}\frac{\partial^2 \bar{c}}{\partial x^2}$

Range of Validity $\frac{L}{R} >> P_e >> 14$ $P_e = \frac{2UR}{D} = R_eS_c$

Taylor Diffusion

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$t = 0$ → $c = \frac{N}{\pi R^2}\delta(x)$

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

Taylor Diffusion

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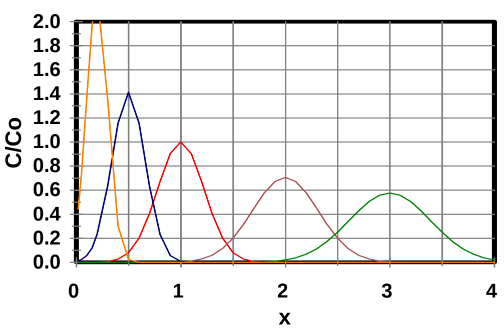

Variations of concentration along the tube at different times.

Summary

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