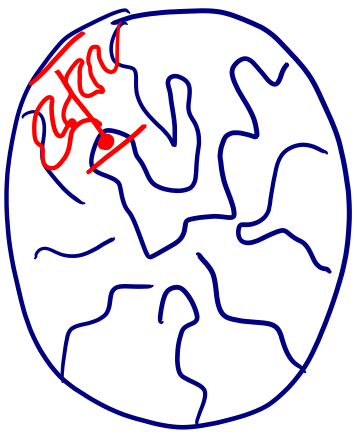
effective diffusivity

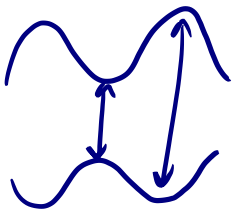
$$D_e = \frac{D_{AB}\,\phi_p\,\sigma_c}{\tau}$$



D_{AB} = gas phase diffusion

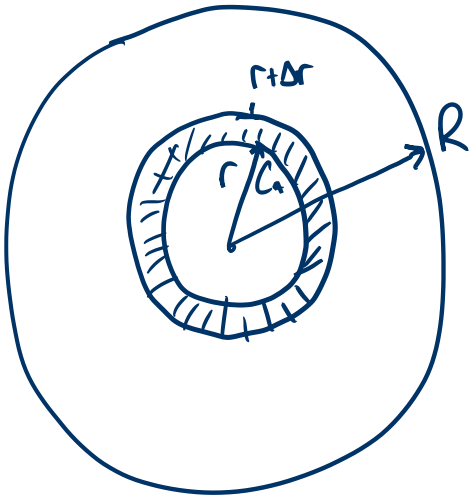
ϕ_p = porosity $\quad \frac{\text{void volume}}{\text{total volume}} \quad (0, 1)$

σ_c = constriction factor $\quad (0, 1)$



$W_{Ar} = \frac{\text{molar flux}}{\frac{\text{mol}}{\text{cm}^2 \cdot \text{s}}}$

τ = tortuosity = $\frac{\text{actual distance traveled}}{\text{shortest distance between 2 pts}}$



C_{As} at $r+\Delta r$

at r: $W_{Ar} * 4\pi r^2\big|_r$

$W_{Ar} * 4\pi r^2\big|_{r+\Delta r}$

$r_{Agen} = r_A' \cdot \rho_c \times 4\pi r^2 \Delta r$

- r_A': rate per mass catalyst
- ρ_c: mass catalyst / vol
- $4\pi r^2 \Delta r$: Volume

$$\Rightarrow \boxed{\frac{d(W_{Ar} \cdot r^2)}{dr} - r_A' \rho_c r^2 = 0}$$

$$W_{Ar} = -D_e \frac{dC_A}{dr}$$ for dilute concentrations

$$\frac{d^2C_A}{dr^2} + \frac{2}{r}\frac{dC_A}{dr} - \frac{k_n}{D_e} C_A^n = 0$$ where $r_A = -k_n C_A^n$

Boundary value problem

At $r = R \quad C_A = C_{AS}$

$r = 0 \quad \frac{dC_A}{dr} = 0$ or C_A is finite at $r = 0$

let $W_A = \frac{dC_A}{dr}$

then $\frac{dW_A}{dr} = \frac{d^2C_A}{dr^2}$

$$\frac{dW_A}{dr} = -\frac{2}{r} W_A + \frac{k_n}{D_e} C_A^n$$

$$\frac{dC_A}{dr} = W_A$$

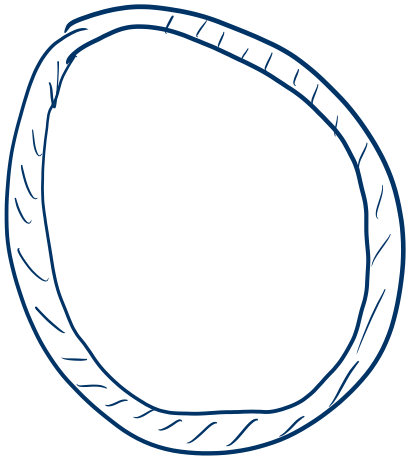
$D_e = 0.1 \ cm^2/s$

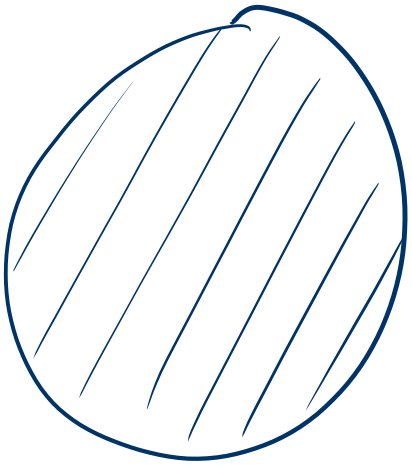
$R = 0.5 \ cm$

$k = 6.4 \ 1/s$

$C_{AS} = 0.2 \ \frac{mol}{L}$

1st order reaction in a spherical particle





internal diffusion

PBR

$$\frac{dF_A}{dW} = r_A$$

$$\frac{dF_A}{dW} = \eta\, r_A$$

η ↑ effectiveness factor