

Cheatsheet: Pre-midterm Mass Transfer

1D Equation. Other forms see below

Flux Equation (Solving N_A)

$$N_A = \underbrace{-c_T D_{AB} \frac{dx_A}{dz}}_{\text{Diffusive } J_{Az}^*} + \underbrace{x_A(N_A + N_B)}_{\text{Convective } c_A v_m}$$

Solutions **Gas, Steady State (Gen=Acc=0)**

General solution

$$N_A = \frac{c_T D_{AB}}{(z_2 - z_1)} \frac{N_A}{N_A + N_B} \ln \left[\frac{N_A - x_{A2}(N_A + N_B)}{N_A - x_{A1}(N_A + N_B)} \right]$$

Suitable: boundary of heterogeneous reaction

Special case 1: EMCD

$$N_A = \frac{D_{AB}}{(z_2 - z_1)} (c_{A1} - c_{A2})$$

Special case 2: Through stagnant B

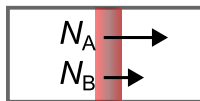
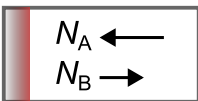
$$N_A = \frac{c_T D_{AB}}{(z_2 - z_1)} \ln \left(\frac{1 - x_{A2}}{1 - x_{A1}} \right)$$

Use log-mean format

$$N_A = \frac{D_{AB}}{RT(z_2 - z_1)} \frac{p_T}{p_{Bm}} (p_{A1} - p_{A2})$$

Special case 3: reactive coupling

Use general solution, need N_A/N_B ratio & sign



Stoichiometry



Magnitude ratio

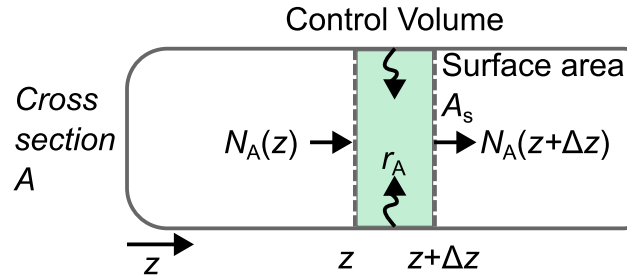
$$N_A/m = N_B/n$$

sign: determined from boundary condition

Mass Balance Equation

$$[\text{In}] - [\text{Out}] + [\text{Gen}] = [\text{Acc}]$$

$$N_A(z)A(z) - N_A(z+\Delta z)A(z+\Delta z) + r_A A_s(\Delta z) = dc_A/dt$$



Diffusivity D_{AB}

Gas: Kinetic theory

$$D_{AB} = \frac{1}{3} \bar{u} \lambda_{A,B}$$

Gas: Chapman-Enskog

$$D_{AB} = \frac{1.8583 \times 10^{-7} T^{3/2}}{p_T \sigma_{AB}^2 \Omega_{D,AB}} \left(\frac{1}{m_A} + \frac{1}{m_B} \right)^{1/2} \propto \frac{T^{3/2}}{p_T} \left(\frac{1}{m_A} + \frac{1}{m_B} \right)^{1/2}$$

Gas: Fuller method

$$D_{AB} = \frac{1.0 \times 10^{-7} T^{1.75}}{p_T [(\sum \nu_A)^{1/3} + (\sum \nu_B)^{1/3}]^2} \left(\frac{1}{m_A} + \frac{1}{m_B} \right)^{1/2} \propto \frac{T^{1.75}}{p_T}$$

Liq: Stokes-Einstein (Mw > 1000)

$$D_{AB} = \frac{9.96 \times 10^{-16} T}{\eta V_A^{0.333}}$$

Liq: Wilke-Chang (278 K ~ 313 K)

$$D_{AB} = \frac{1.173 \times 10^{-16} (\phi_{MB})^{1/2} T}{\eta_B V_A^{0.6}}$$

Inhom. Solid: effective

$$D_{AB,eff} = \frac{\varepsilon}{\tau} D_{AB}$$

Liquid / solid common case (like stagnant B)

$$N_A = \frac{D_{AB} c_{A,av}}{(z_2 - z_1)} \frac{(x_{A1} - x_{A2})}{x_{B,m}} \quad x_{B,m} = \frac{x_{B2} - x_{B1}}{\ln(x_{B2}/x_{B1})}$$

Solid case $x_{Bm} \sim 1$

Liq. dilute case $x_{Bm} \sim (x_{B1} + x_{B2})/2$

Generation term / orthogonal M.T.

Coefficient - driving force form

Example: (details see review after mid-term)

$$r_A = k(c_{A,s} - c_A)$$

Coeff Driving force

Unit m/s Concentration diff

Unsteady state $dc_A/dt \neq 0$

1D uniform cross sectional area (remove Δz)

$$\frac{\partial c_A}{\partial t} = - \frac{\partial N_A(z)}{\partial z} \Big|_z + r_A$$

1D

$$\nabla^2 c = \frac{\partial^2 c}{\partial z^2}$$

$$\nabla c = \frac{\partial c}{\partial z}$$

3D general term

$$\frac{\partial c_A}{\partial t} = r_A - \frac{\partial N_{Ax}}{\partial x} - \frac{\partial N_{Ay}}{\partial y} - \frac{\partial N_{Az}}{\partial z} = r_A - \nabla \cdot \vec{N}_A$$

Most used form: incompressible liquid

$$\frac{\partial c_A}{\partial t} = D_{AB} \nabla^2 c_A - \vec{v}_m \cdot \nabla c_A + r_A$$

likely diffusion can be ignored

Varying cross section problem

N_A can vary! Steady state use $\bar{N}_A = N_A(z)A(z)$

Gen = 0. Spherical case (stagnant B)

$$\frac{\bar{N}_A}{4\pi} \left(\frac{1}{r_1} - \frac{1}{r_2} \right) = \frac{D_{AB} p_T}{RT} \ln \left(\frac{p_T - p_{A2}}{p_T - p_{A1}} \right)$$

Gen = 0. Spherical case (far field stagnant B)

$$N_{A1} = \frac{D_{AB} p_T}{RT p_{Bm}} (p_{A1} - p_{A2})$$

