Predictive Equations for the Gas-phase diffusivity

- Empirical equation: Fuller, Schettler & Giddings (1966)

$$D_{AB} = \frac{1.0133\times10^{-7}\,T^{1.75}}{P\left[(\Sigma v)_A^{1/3} + (\Sigma v)_B^{1/3}\right]^2}\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} \ m^2/s$$

• Ficks law for liquids
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Σv_A = Diffusion volume of component A [Ex:

M_A, M_B = Molecular weights of A & B, resp.

P = total pressure, in bar

T = temp in K

Molecular diffusion in liquids:

- Liquids are closely packed than gases & hence diffuse slowly. $D \sim (0.5-2)\times10^{-5}\ cm^2/s$
- Fick's law of diffusion is applicable for liquids as well

For liquids: $N_A = (N_A + N_B)\,x_A - D_{AB}\left(\frac{\rho}{M}\right)_{av}\frac{dx_A}{dz}$; $x_A = C_A/C$

$(\rho/M)_{av}$ = Average molar conc. of the Liquid

ρ = Density

M = Molecular weight

For gases: $N_A = (N_A+N_B)\frac{C_A}{C} - D_{AB}\,C\,\frac{dx_A}{dz}$

Fluxes for the following cases, discussed earlier, can be derived similarly for liquids also:

(a) Diffusion of A through non-diffusing B: $N_A = \frac{D_{AB}(\rho/M)_{av}(x_{A0} - x_{Al})}{l\,x_{BM}}$; $x_{BM} = \frac{x_{Bl} - x_{B0}}{\ln(x_{Bl}/x_{B0})}$

(b) Equimolar counter diffusion of A & B: $N_A = \frac{D_{AB}(\rho/M)_{av}(x_{A0} - x_{Al})}{l}$

Liquid-phase diffusivity:

Empirical correlation, Wilke-Chang equation (1955)

$$D^{\circ}_{AB} = \frac{1.173\times10^{-16}(\phi M_B)^{1/2}\,T}{\mu\, v_A^{0.6}} \Rightarrow$$

$D_{AB} \propto \frac{1}{\mu}$

$\propto 1/v_A^{0.6}$ [Larger molecules have lower diffusivity]

$\propto T$

D°_{AB} = Diffusivity of solute A in solvent B @ infinite dilution

M_B = molecular weight of B

ϕ = Association factor for the Solvent

T = temp, K

μ = Solution viscosity

v_A = Solute molar volume @ normal boiling point.