01E Diffusion Flux

Equivalence with water flowing through the pipe

•Think of the number of molecules of water flowing through a pipe per unit cross section of the pipe.

This is the flux, call it J in units of N m^{-2} s^{-1}.

The cross section of the pipe is A in m^2

Therefore the total number of molecules flow through the pipe are JA N s^{-1}

Volume of each molecule is Ω in units of m^3

Therefore, the volumetric mass flowing through the pipe is $\phi = JA\Omega$ m^3s^{-1}.

The driving force is the pressure gradient i.e. $\frac{dp}{dx}$

From elementary fluid mechanics,

$$J\Omega = \frac{1}{\eta}\frac{d(p\Omega^{2/3})}{dx}$$

The relationship between the viscosity, η, and the coefficient of diffusion of water molecules is given by the Stokes Einstein Equation

$$\eta = \frac{k_B T}{6\pi\Omega^{1/3}D}$$

$$\Delta\mu = p\Omega$$

Therefore, generally,

$$j\Omega = \frac{1}{\eta}\frac{d(p\Omega^{2/3})}{dx}$$

$$j = \frac{1}{\Omega}\frac{6\pi\Omega^{1/3}D}{k_B T}\frac{d(p\Omega^{2/3})}{dx} = 6\pi\frac{D}{\Omega k_B T}\frac{d(p\Omega)}{dx}$$

J= (diffusion coefficient terms)*(driving force)

General diffusion equation for solid state diffusion is given by

$$\boxed{j = \frac{D}{\Omega k_B T}\frac{d\Delta\mu}{dx}} \qquad (1)$$

D: m^2s^{-1}

Omega: m^3

T: K

k_B: J K^{-1}atom^{-1}

$\Delta\mu$: J*

x: m

Upon insertion of these units into Eq. (1) we have the following for the Right Hand Side:

$$\frac{m^2}{s}\,\frac{1}{m^3 JK^{-1}atom^{-1}K}\,\frac{J}{m} = \frac{m^2}{s}\frac{1}{m^3 JK^{-1}atom^{-1}K}\frac{J}{m} = \qquad atoms\, m^{-2}s^{-1}$$

The physical meaning of flux is number of atoms $m^{-2}s^{-1}$

Remember that atoms can be replaced by molecules

*(Note: $\Delta\mu$ is the chemical potential of the species, which was shown to be equal to $\sigma\Omega$, which has units of energy, i.e. J)