**Mass Transfer**

**Reference:**

1. Separation Process Principles, Chemical and Biochemical Operations, by J. D. Seader, Ernest J. Henley, and D. Keith Roper, 2011.
2. Mass Transfer Operation by Robert E. Treybal, 1980.

***Diffusion***

  **Introduction:** The term mass transfer is used to denote the transference of a component in a mixture from a region where its concentration is high to a region where the concentration is lower. Mass transfer process can take place in a gas or vapor or in a liquid, and it can result from the random velocities of the molecules (*molecular diffusion*)or from the circulating or eddy currents present in a turbulent fluid (*eddy diffusion*)*.*

Convective mass transfer in flowing fluid (Molecular+eddy diffusion)

**Molecular Diffusion:** The basic equations of diffusion are

\* = -*DAB* Fick’s first law (steady state)

 = -*DAB*

\* = *D*AB  Fick’s second law (unsteady state in one dimension)

Where:

: mole flux of A in medium B i.e. rate of mass transfer per unit area (kmol/m2s)

*DAB*: Diffusivity (Diffusion coefficient) of A in medium B (m2/s) {depends on components of the mixture, and affected by temperature and pressure}

*CA*: concentration of A (Kmol/m3)

*y*: distance of transfer (m)

*a*: area across which mass transfer occurs (m2)

: Concentration gradient or change in concentration of A with distance

**The general basic equation of transfer is:**

Total transfer = transfer by diffusion + transfer by bulk flow

For transfer of component A in medium B:  *= NA* + *UFCA*

Bulk flow velocity, *UF* = = 

 → = -*D*AB + *xA* (*+*) , 

 Diffusion transfer Bulk flow transfer

Where *xA*: mole fraction of A

  **Two modes of diffusion:**

1. Counter diffusion, e.g. catalytic reaction, distillation ..etc (special case but general is equimolar counter diffusion).

2- Diffusion through stagnant layer, e.g. absorption, liq-liq extraction, evaporation ..etc

 Note:

 = -*D*AB +  (*+*) ,  = (For gases)

 *C*A = *dC*A =  (also for gases)

 

 Or  , since *CA* = *xACT* → *dCA = CTdxA*

**Equimolar counter diffusion:**

We start with general mass transfer equation

   *xA*1 y = 0

Catalyst surface

Since equimolar i.e. *= -* 

  *xA2 y = δ*

 → 

  =*CT* (*xA1 - xA2*) =  (*CA*1 – *CA*2)

Or for gases the mole flux can be writing: =  (*PA*1 – *PA*2)

 **Diffusion through stagnant layer:**

Boundary layer

A = O2

B = N2

H2O

Liq film=δ

*Bubble*

 Again, ,

Since through stagnant layer i.e= 0

 → (1 *– xA*) *= -CT DAB *

 → 

= *CT* 

**Diffusivity (Diffusion coefficient) in gases:**

 *DAB*= 4.3×10-4 *T*1.5  (m2/s)

*T* = Temp. (K),

*P* = total Press. (N/m2),

*M* = molecular weight,

*V* = molar volume (m3/Kmol)

 **Diffusivity (Diffusion coefficient) in liquids**

  (m2/s) {for small solutes with VM ≤ 0.50 m3/Kmol}

  (m2/s) {for larger solutes with VM > 0.50 m3/Kmol}

*µL* = viscosity of solvent B (Kg/m.s), *VM* =molar volume of solute A (m3/Kmol), *ML*= molecular weight of solvent, *λ* = association parameter, a measure of interactions among molecules of the solvent, *MA* = molecular weight of solute A

**Relation of diffusivity with temperature and pressure:** 

**Ex:** Estimate the diffusivity of the protein lysozyme in water at 25oC. The molecular weight of lysozyme is 14,100 and the viscosity of water at 25oC is 0.001 kg/m s.

Solution: = 

 = 1.16×10-10 m2/s

**Multicomponent Diffusion:**

 

 Where: *DAm*is the diffusioncoefficient of A in the mixture.

 *xi* is the mole fraction of component *i* in the miture

**Diffusion of solute through porous solid (e.g. diffusion through membrane)**

The equation of un-hindered diffusion of a solute through a porous solid (e.g. transport of NaCl through a microfiltration membrane):



*ε =* porosity of the medium (-)

*τ =* tortuosity of the medium (-) reflects the length of the average pore compared to the membrane thickness.



 *Lp* = effective pore length

The equation of hindered diffusion of a solute through a porous solid (e.g. transport of albumin through an ultrafiltration membrane):



*Deff* = effective hindered diffusivity (m2/s)

*Deff* = *D  , ds =*  solute diameter (m) , *dp* = pore diameter (m)

**Ex:** Glucose is diffusing at 25oC in water within a porous medium having a porosity of 0.5, tortuosity of 1.8 and average pore diameter of 8.6×10-3 microns. Determine the steady state flux of glucose between two points within the medium separated by a distance of 1 mm and having concentrations 1.51 g/1 and 1.5 g/1 respectively. Molecular weight of glucose = 180, size of glucose = 8.6×10-4 microns.

Solution:  ……(\*)

=4.96×10-10 m2/s

*Deff* = *D * = 4.96×10-10 = 3.25×10-10 m2/s

So from Eq. (\*) = = 5.02×10-12 kmol/m2s

**Convective mass transfer:**  It is observed in the flowing fluids. If the flow of liquid is laminar, the transfer of solute would be by molecular diffusion. If the flow were turbulent, mass transfer would take place by a combination of molecular diffusion and eddy diffusion.

*JA* = -(*D + E*)  ,

*JA* = mole flux in case of convective transfer (kmol/m2s) , *E* = eddy diffusivity (m2/s)

Also *JA* = *kA*∆*cA* , *kA* = mass transfer coefficient (m/s)

**Ex:** An aqueous solution of human immunoglobulin G at 4oC is being pumped through a tube having a diameter of 1 mm. The mass transfer coefficient for the protein in the radial direction was found to be 1×10-6 m/s. Comment on this value vis-a-vis the diffusivity of the protein. Estimate the eddy diffusivity of the flowing system. Molecular weight of immunoglobulin G = 155000.

Solution: = = 4.85×10-11 m2/s

The length of diffusion is radius of the tube = 0.5 mm. If the solute transport is due to diffusion alone, then:

*kA* = = = 9.69×10-8 m/s < 1×10-6

So there is eddy diffusion involved in the solute transport:

*kA* = 

→ *E = kAr – D =* (1×10-6×0.5×10-3) - 4.85×10-11 = 4.52×10-10 m2/s

**An experiment to measure the diffusivity of vapors in air**

y yo

 This is a case of diffusion through stagnant layer

  ……(1)

Also  ……(2)

 Equating (1) & (2)

 → 

 

→ = + 

**Ex:** The diffusivity of the vapor of a volatile liquid in air can be conveniently determined by Winkelmann's method in which liquid is contained in a narrow diameter vertical tube, maintained at a constant temperature, and an air stream is passed over the top of the tube sufficiently rapidly to ensure that the partial pressure of the vapor there remains approximately zero. On the assumption that the vapor is transferred from the surface of the liquid to the air stream by molecular diffusion alone, calculate the diffusivity of carbon tetrachloride vapor in air at 321 K and atmospheric pressure from the experimental data given in Table below:

|  |  |  |  |
| --- | --- | --- | --- |
| Time from commencement of experiment (ks) | Liquid level (mm) | Time from commencement of experiment (ks) | Liquid level (mm) |
| 0.0 | 0.0 | 117.5 | 54.7 |
| 1.6 | 2.5 | 168.6 | 67 |
| 11.1 | 12.9 | 199.7 | 73.8 |
| 27.4 | 23.2 | 289.3 | 90.3 |
| 80.2 | 43.9 | 383.1 | 104.8 |

The vapor pressure of carbon tetrachloride at 321 K is 37.6 kN/m2 and the density of the liquid is

1540 kg/m3. The kilogram molecular volume may be taken as 22.4 m3/kmol (at 0oC and 1 atm). Mw = 154.

Solution: this is a diffusion through stagnant layer: