MASS TRANSFER CO-EFFICIENT

We consider a fluid layer of stagnant film of thickness δ around the solid particle. It is also considered that all the resistance to mass transfer is limited at this film and the properties, i.e., concentration, temperature etc. are the same at the outer edge of the film as the bulk fluid.

Curvature effect is neglected. So one dimensional diffusion equation will be solved.

For either dilute solution or EMCD, the mass flux at a single point can be written as,

$W_{A(p)} = \frac{D_{AB}}{\delta^{\sim}} (C_{Ab} - C_{As})$, where $W_{A(p)}$ is the flux at a specific point or portion on the sphere. Now, the ratio of diffusivity to the layer thickness is the mass transfer co-efficient $k_{c.}$

CONTD..

Therefore, $\dfrac{D_{AB}}{\delta^{\sim}} = k_c^{\sim}$,

where $k_c^{\sim}$ is the local mass transfer coefficient at a particular point.

Integration for the whole surface area of the catalyst pellet gives the average mass transfer co-efficient for the area A,

$$k_c = \int k_c^{\sim} \frac{dA}{A}$$

Average molar flux from the bulk fluid to the surface is,

$$W_A = k_c(C_{Ab} - C_{As})$$

As for heat transfer, we have the equation,

$$q_r = h(T_0 - T_s) \qquad h \text{ is heat transfer coefficient}$$

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Nusselt number and Reynold's number are defined as,

$$Nu = \frac{hd}{k_t} \quad \text{and} \quad Re = \frac{du\rho}{\mu}$$

d is particle size/diameter and k_t thermal conductivity

Prandlt number is defined as,

$$P_r = \frac{C_p\mu}{k_t} = \frac{\mu}{\rho} \cdot \left(\frac{\rho C_p}{k_t}\right) = \frac{\gamma}{\alpha_t} = \frac{Kinematic\ viscosity}{Thermal\ diffusivity}$$

$$= \frac{Momentum\ diffusivity}{Thermal\ diffusivity} \frac{(m^2/s)}{(m^2/s)}$$

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The relation between Nusselt number, Prandlt number and Reynold's number is,

$$Nu = 2 + 0.6\ Re^{\frac{1}{2}}.Pr^{\frac{1}{3}}$$

For stagnant film, $Re = 0,\ \ Nu = 2$

For higher Reynold's number, in which boundary layer is laminar,

$$Nu = 0.6\ Re^{\frac{1}{2}}.Pr^{\frac{1}{3}}$$

To draw the analogy between heat and mass transfer, we can write,

$$Nu \rightarrow Sherwood\ number\ (Sh)$$
$$Pr \rightarrow Schmidt\ number\ (Sc)$$

$$\therefore Sh = \frac{k_c d}{D_{AB}} = \frac{(m/s).m}{m^2/s} = \text{dimensionless and } Nu = \frac{hd}{k_t}$$

$\therefore$ Therefore, it can be said that

h is analogous to k_c and k_t is analogous to D_{AB}

$q_z = h(T - T_s)$

$W_{AZ} = k_c(C_A - C_{As})$

Again, $P_r = \frac{\gamma}{\alpha_t}$ and $Sc = \frac{\gamma}{D_{AB}} = \frac{m^2/s}{m^2/s} = \text{dimensionless}$

$\therefore \alpha_t$ is analogous to D_{AB}

Therefore, the correlation between Schmidt no and Sherwood no is written as,

$$Sh = 2 + 0.6 \, Re^{\frac{1}{2}}.Sc^{\frac{1}{3}}$$

This relationship refers to Frossling correlation

MASS TRANSFER TO A SINGLE PARTICLE

There are two limiting cases for reaction with diffusion:

➢The reaction is so rapid that the rate of diffusion to the surface limits the reaction rate

➢The reaction is so slow compared to the rate of diffusion that almost no concentration gradient exists between the bulk and the surface, and reaction is limiting step

Rapid reaction on a catalyst surface:

Problem: *Calculate the mass flux of reactant A to a single catalyst pellet, 1 cm in diameter, suspended in a large body of liquid. The reactant is present in dilute conc. and the reaction is instantaneous on the catalyst surface (i.e, C_{AS}=0). The bulk conc.of reactant=1 M and liquid velocity= 0.1 m/s. The kinematic viscosity= 0.5 centistoke(1 cs= 10^{-6} m²/s) and liquid diffusivity of A is 10^{-10} m²/s.*

For dilute conc., $W_A = k_c(C_{Ab} - C_{As})$----(1)

Here, $C_{As}=0$ and $C_{Ab}= 1 \text{mol/dm}^3 = 10^3 \text{mol/m}^3$

Now, k_c can be calculated from the Frossling correlation,

$$Sh = \frac{k_c d}{D_{AB}} = 2 + 0.6\ Re^{\frac{1}{2}}.Sc^{\frac{1}{3}}$$

Now, $Re = \dfrac{du\rho}{\mu} = \dfrac{du}{\gamma} = \dfrac{0.01 \times 0.1}{0.5 \times 10^{-6}} = 2000$

$Sc = \dfrac{\gamma}{D_{AB}} = \dfrac{0.5 \times 10^{-6}}{10^{-10}} = 5000$

$Sh = 2 + 0.6\ (2000)^{\frac{1}{2}}(5000)^{\frac{1}{3}} = 460.7$

$k_c = \dfrac{D_{AB}Sh}{d} = \dfrac{10^{-10}}{0.01}\text{x } 460.7 = 4.61\text{x } 10^{-6} \text{ m/s}$

Substituting k_c and C_{Ab} in eq (1),

W_A= 4.61x 10^{-6}x 10^3

   = 4.61x10^{-3}mol/m^2.s

A general case is considered, $A \rightarrow B$

The reaction is taking place on the surface of a solid sphere. Let us consider the surface reaction follows a Langmuir-Hinshelwood single site mechanism

$$-r_A' = \frac{k_r C_{As}}{1+ K_A C_A + K_B C_B}$$

At high temperature, adsorption is very low,

Hence, $K_A C_A + K_B C_B << 1$

$\therefore -r_A' = k_r C_{As}$

Now, the boundary conditions are,

At the surface, $W_A = -r_A'$ and at boundary layer, $W_A = k_c(C_{Ab} - C_{As})$

$\therefore W_A = k_c(C_{Ab} - C_{As}) = -r_A' = k_r C_{As}$ ------(2)

It is difficult to measure C_{As}, hence, it can be written from eq (2),

$$C_{As} = \frac{k_c C_A}{k_r + k_c}$$

The rate of the reaction on the surface becomes,

$$W_A = -r'_A = \frac{k_c k_r}{k_r + k_c} . C_A = k_{eff} . C_A$$

Where, k_{eff} is effective transport coefficient

Rapid reaction:

When the rate of the mass transfer from the surface limits the overall rate of reaction, then,

$$k_r \gg k_c, \quad \therefore \frac{k_c}{k_r} \ll 1.$$

Therefore, $-r'_A = \dfrac{k_c C_A}{1 + {k_c}/{k_r}} \approx k_c C_A$

To increase the rate of the reaction, we either have to increase k_c or C_A or both.

Now, for gas phase catalytic reaction and for most liquids, Sc no is large enough, so that we can neglect '2' in Frossling correlation equation.

Therefore, the equation becomes,

$$Sh = 0.6 \ Re^{\frac{1}{2}}.Sc^{\frac{1}{3}}$$

Now,
$$\frac{k_c d}{D_{AB}} = 0.6 \ \left(\frac{du}{\gamma}\right)^{\frac{1}{2}} (\frac{\gamma}{D_{AB}})^{\frac{1}{3}}$$

$$k_c = 0.6 \frac{D_{AB}}{d} \left(\frac{du}{\gamma}\right)^{\frac{1}{2}} (\frac{\gamma}{D_{AB}})^{\frac{1}{3}}$$

$$= 0.6 \ (\frac{D_{AB}^{2/3}}{\gamma^{1/6}}) \cdot (\frac{u^{1/2}}{d^{1/2}})$$

(term 1) (term 2)

➤ Term 1 is a function of temperature and pressure only. Diffusivity increases with increase in the temperature for both gas and liquid. Kinematic viscosity γ increases with temperature ($\gamma \ \alpha \ T^{3/2}$) for gases and decreases exponentially with temperature for liquids.

➤ Term 2 is a function of flow of gas and particle size of catalyst. Thus, to increase k_c as well as rate of the reaction, either flow past the solid particle is to be increased or particle size should be decreased.

Slow reaction: Here the rate constant is smaller compared to the mass transfer coefficient.

$$k_r << k_c, \qquad \text{and} \qquad -r'_A = \frac{k_r C_A}{1 + {k_r}/{k_c}} \approx k_r C_A$$

It should be noticed that here, the specific reaction rate, $-r'_A$ is not dependent on the velocity of the fluid and also on the particle size.

The figure shows the variation of reaction rate with particle size and velocity.

At low velocity, the mass transfer boundary layer thickness is large and diffusion limits the reaction. As the velocity past the solid particle increases, the boundary layer thickness decreases and the mass transfer across the boundary layer can not limit the reaction.