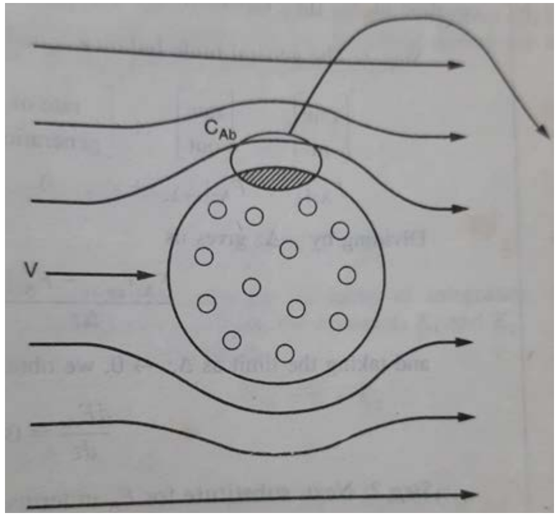
DIFFUSION THROUGH A FILM TO A CATALYST PARTICLE

Species A, which is present in dilute concentrations, is diffusing at steady state from the bulk fluid through a stagnant film of B of thickness δ to the external surface of the catalyst.



The concentration of A at the external boundary is C_{Ab} and at the external catalyst surface is C_{As}, with $C_{Ab} > C_{As}$. As the thickness of the hypothetical stagnant film next to the surface is small with regard to the diameter of the catalyst particle, hence the curvature is neglected. The diffusion is considered to occur in rectilinear coordinates.

DETERMINATION OF THE CONCENTRATION PROFILE AND FLUX OF A IN THE SURFACE

Mole balance of A,

Rate in – rate out + rate of formation = rate of accumulation

If F_{Az} is the molar flow rate at z and F_{Az+dz} is the molar flow rate at $z + dz$,

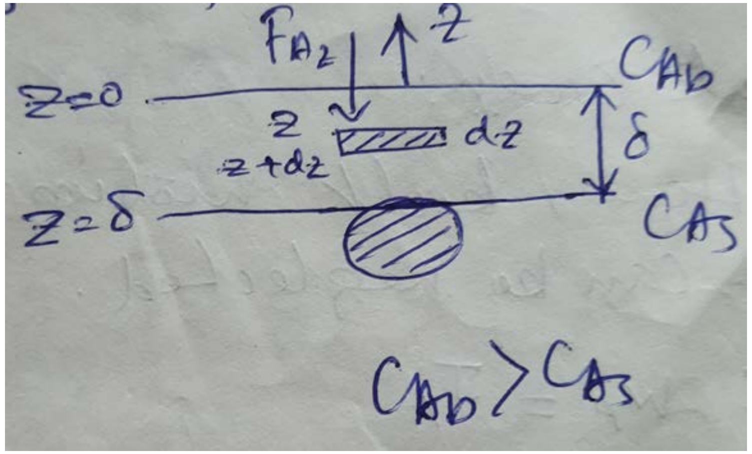
$F_{Az} - F_{Az+dz}$ +0 = 0

Diving by dz, we get, $\frac{F_{Az} - F_{Az+dz}}{dz}$ =0,

Taking limit dz → 0, $\frac{dF_{Az}}{dz}$ =0

If A_c is the area of section dz, $F_{Az} = W_{Az}.\, A_c$

$\frac{dW_{Az}}{dz}$ = 0, as A_c is constant.



We have considered dilute solution and z direction only.

$$\therefore W_A = -D_{AB}\frac{dC_A}{dz}$$

$$\frac{dW_A}{dz} = -D_{AB}\frac{dC_A^2}{dz^2}$$

Now, $\frac{dC_A^2}{dz^2}$ =0 as, $\frac{dW_A}{dz}$= 0

$\therefore \frac{dC_A}{dz}= k_1$ and $C_A= k_1 z + k_2$ where, k_1 and k_2 are integration constants

Now, applying boundary conditions to evaluate the constants,

At $z = 0, C_A= C_{Ab}$, $\therefore\ k_2= C_{Ab}$

And at $z = \delta, C_A= C_{As}$,

$C_{As}= k_1\delta + k_2$ or, $C_{As}= k_1\delta + C_{Ab}$

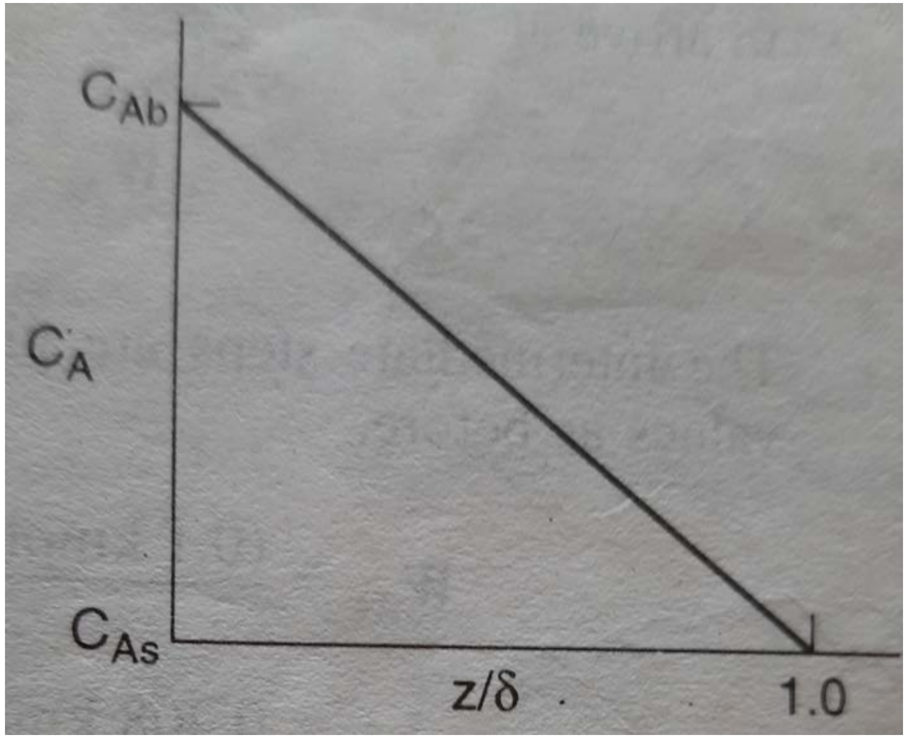
$$\therefore k_1= \frac{C_{As}-C_{Ab}}{\delta}$$

Putting the values of k_1 and k_2,

$C_A = \frac{C_{As}-C_{Ab}}{\delta}. z + C_{Ab},$ $C_A = (C_{As} - C_{Ab}).\frac{z}{\delta} + C_{Ab}$

$\frac{C_A-C_{Ab}}{C_{As}-C_{Ab}} = \frac{z}{\delta}$

The concentration profile of A is obtained by plotting C_A against $\frac{z}{\delta}$. It is a straight line with a negative slope, as $(C_{As} - C_{Ab})$ is negative. $C_{Ab} > C_{As}$, concentration of A in the bulk is greater than that on the catalyst surface due to diffusional resistance.



Determination of molar flux of A diffusing through the stagnant film, dilute solution and EMCD:

1. For dilute solution and EMCD, the flux is given as,

$W_A = -D_{AB}\frac{dC_A}{dz}$ ------(1)

Previously we obtained, $C_A = (C_{As} - C_{Ab}).\frac{z}{\delta} + C_{Ab},$

Putting C_A in (1),

$W_A = -D_{AB}\frac{d[C_{Ab}+(C_{As}-C_{Ab}).\frac{z}{\delta}]}{dz} = D_{AB}\frac{(C_{Ab}-C_{As})}{\delta}$

In terms of mole fraction, $W_A = \frac{D_{AB}}{\delta}(y_{Ab} - y_{As})C_{T_0},$

where C_{T_0}=total mole

If, D_{AB}= 10^{-6}m^2/s, C_{T_0}= 0.1 mol/m^3, δ=10^{-6}m, y_{Ab}=0.9 and $y_{As}(y_{A\delta})$= 0.2, then,

W_A= 0.07 Kmol/m^2.s

2. For stagnant film,

Mole flux is, $W_A = -D_{AB}\frac{dC_A}{dz} + y_A W_A$, (as W_B=0 and B_A=$y_A W_A$)

$$W_A(y_A - 1) = D_{AB}\frac{dC_A}{dz} = D_{AB}.C.\frac{dy_A}{dz}$$

Or, $W_A \int_0^{\delta} dz = D_{AB}.C \int_{y_{Ab}}^{y_{A\delta}} \frac{dy_A}{(y_A - 1)}$

Boundary conditions are,

When, $z = \delta,\ y_A = y_{A\delta}(y_{As})$

And when $z = 0,\ y_A = y_{Ab}$

$$\therefore W_A.\delta = D_{AB}.C\ ln\frac{1-y_{A\delta}}{1-y_{Ab}}$$

Putting the previous values of the quantities, W_A= 0.208 Kmol/m^2.s

Hence, the flux through stagnant film is greater than that for dilute solution or EMCD.

Now, the above equations can be written in terms of mole fractions as,

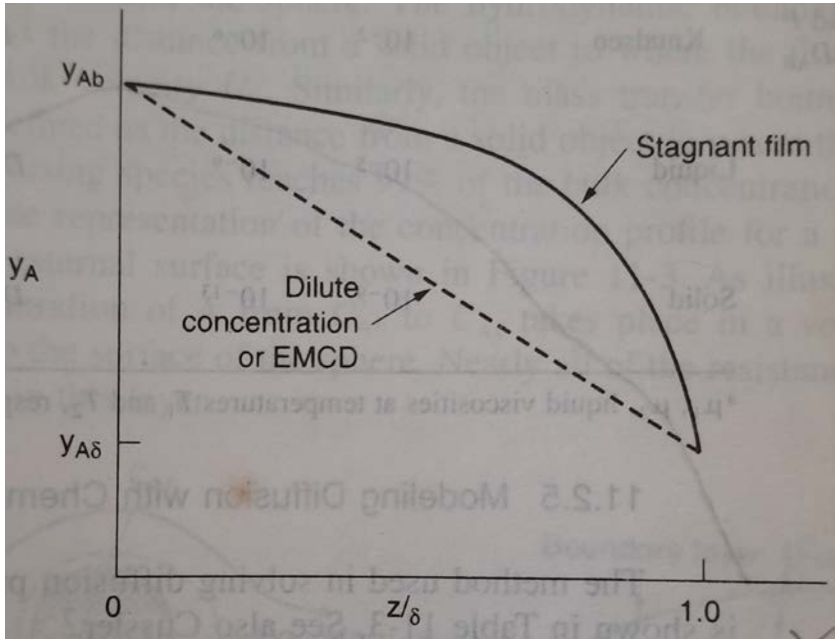
For dilute solution or EMCD,

$$y_A = y_{Ab} - (y_{Ab} - y_{A\delta})\frac{z}{\delta}$$

And for stagnant film,

$$y_A = 1 - (1 - y_{Ab})\left(\frac{1-y_{A\delta}}{1-y_{Ab}}\right)^{\frac{z}{\delta}}$$

The concentration profile is as shown in the figure.



EXTERNAL RESISTANCE TO MASS TRANSFER

To discuss about the diffusion of reactants from bulk fluid to external surface of the catalyst, we will focus our attention on the flow past a single catalyst pellet.

- Reaction takes place only on the catalyst and not in the fluid surrounding it. The fluid velocity in the vicinity of the spherical pellet will vary with the position around the sphere.
- The hydrodynamic boundary layer is usually defined as the distance from a solid object to where the fluid velocity is 99% of the bulk velocity.
- Similarly the mass transfer boundary layer thickness δ is defined as distance from a solid object to where the concentration of the diffusing species reaches 99% of the bulk concentration.

CONTD...

The representation of the concentration profile for a reactant A diffusing to the external surface is shown in figure. The change in concentration of A from $C_{Ab}$to C_{As} takes place in a very narrow fluid layer next to the surface of the sphere. Nearly all of the resistance to mass transfer is found in this layer.