Mass transfer within Phases

How can we predict the rate of mass transfer?

We can predict the rate of mass transfer by using the following equations:

1. Fick's law (microscopic approach)

$$J_A = - D_{AB} \frac{dC_A}{dz}$$

good for diffusion dominated problems

2. Mass transfer coefficient equation (macroscopic approach)

$$N_A = - k \Delta C_A$$

where **k is known as the mass transfer coefficient**

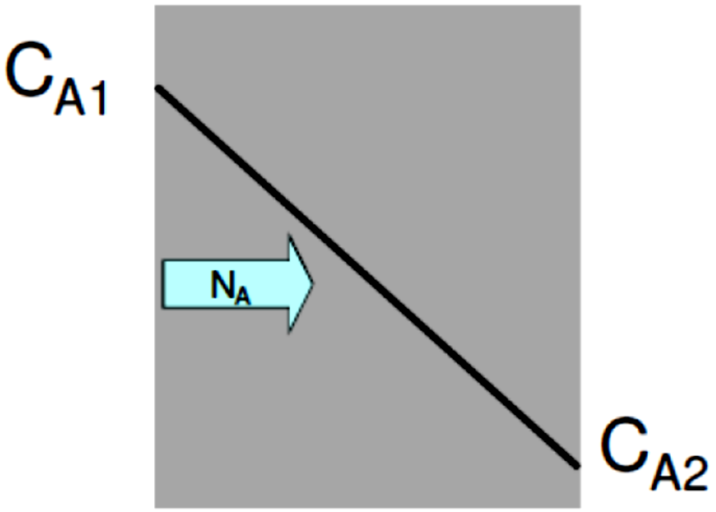
good for convection dominated problems

Mass Transfer Coefficient Method; liquid phase mass transfer

$$N_A = k_c \, \Delta C_A = k_c \, (C_{A1} - C_{A2}) \qquad (1)$$

For mass transfer in liquids:

k_c is the liquid-phase mass-transfer coefficient.



What is the unit of k_c?

Mass Transfer Coefficient Method; gas-phase mass transfer

$$\therefore \ N_A = k_c \, \Delta C_A = k_c \, (C_{A1} - C_{A2}) \qquad (1)$$

Using the following relationships between concentrations and partial pressures:

$$C_{A1} = p_{A1} / RT; \qquad C_{A2} = p_{A2} / RT$$

Equation (1) can be written as

$$N_A = k_c \, (p_{A1} - p_{A2}) / RT = k_p \, (p_{A1} - p_{A2}) \qquad (2)$$

where $k_p = k_c / RT$ (3)

k_p is a gas-phase mass-transfer coefficient based on a partial-pressure driving force.

What is the unit of k_p?

Mass Transfer through phases & Applications

- In general, mass Transfer can take place at different phases.
- Mass transfer between phases across the interface is of great interest in separation processes:
  - gas/liquid interface
  - liquid/liquid interface
- Such interfaces are found in the following applications:
  - absorption
  - distillation
  - extraction

Models for mass transfer coefficients and Mass Transfer between phases

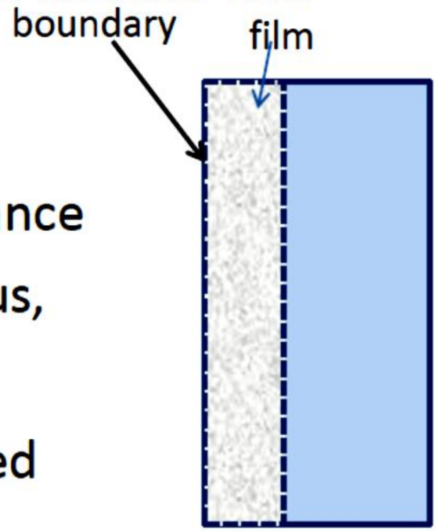
- Theoretical models used to describe mass transfer between a fluids through an interface are:
  - Film Theory
  - Penetration Theory
  - Boundary layer theory

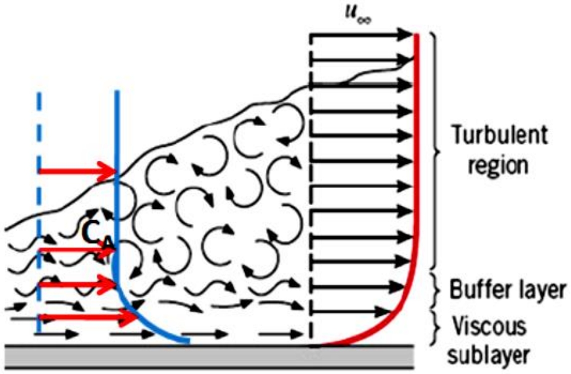
Film Theory

- This theory assumes the presence of a fictitious laminar film next to the boundary.
- This film, where only molecular diffusion is assumed to be occurring, has the same resistance to mass transfer as actually exists in the viscous, transition, and turbulent core regions.
- The actual mass transfer coefficient k_c' is related to the film thickness δ_f by

$$J_A^* = k_c'(c_{A1} - c_{A2}) = \frac{D_{AB}}{\delta_f}(c_{A1} - c_{A2})$$

$$k_c' = \frac{D_{AB}}{\delta_f}$$





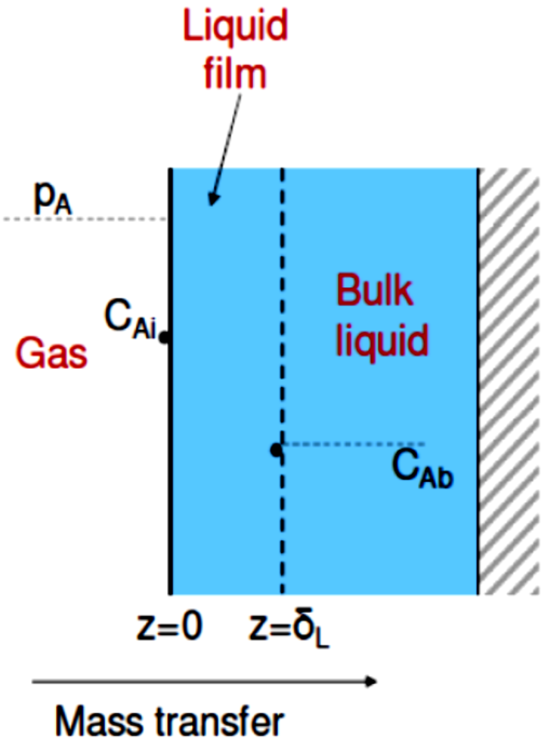
Film Theory

- Entire resistance to mass transfer in a given turbulent phase is in a thin, stagnant region of that phase at the interface, called a film.
- For the system shown,

  gas A diffuses

  into nonvolatile liquid B.

In reality, there may be mass transfer resistances in both liquid and gas phases. So we need to add a gas film in which gas is stagnant.

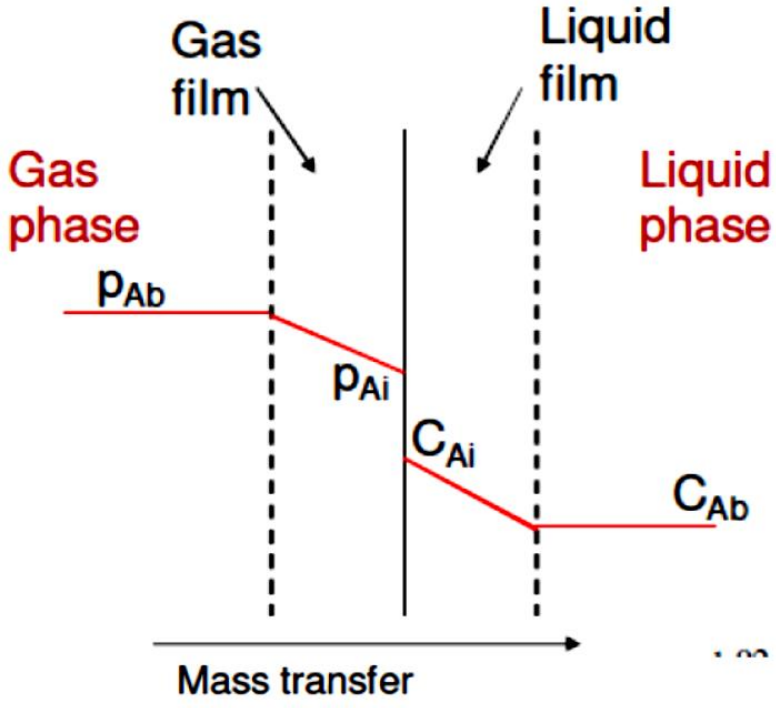


Two film Theory

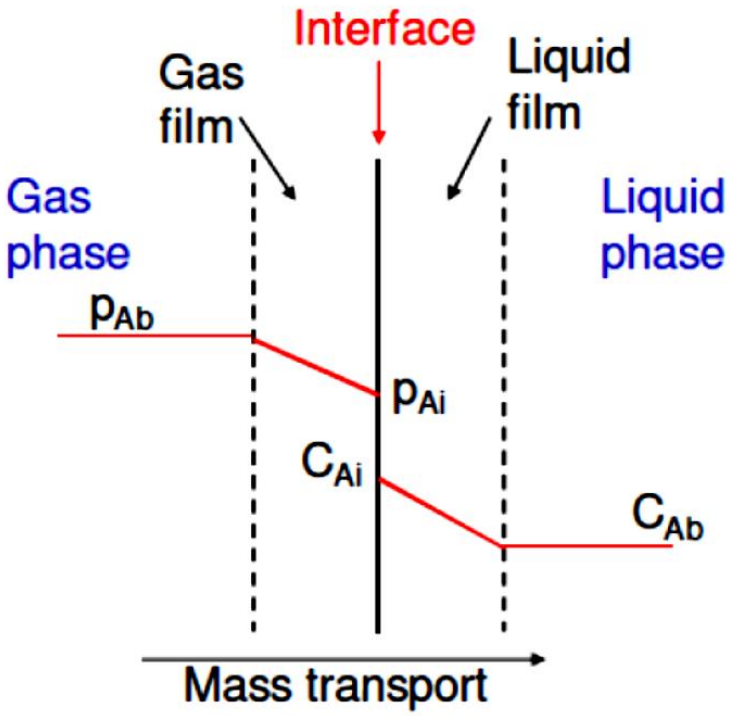
There are two stagnant films (on either side of the fluid-fluid interface).

Each film presents a resistance to mass transfer.

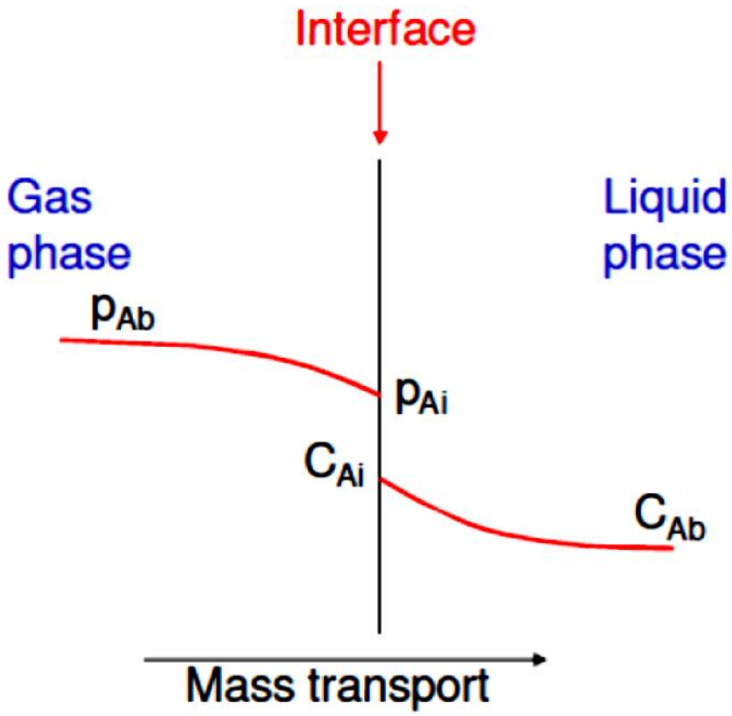
Concentrations in the two fluid at the interface are assumed to be in phase equilibrium.



Two film Theory



Concentration gradients for the film theory



More realistic concentration gradients

Two Film Theory applied at steady state

Mass transfer in the gas phase:

$$N_A = k_p \, (p_{Ab} - p_{Ai}) \qquad (2)$$

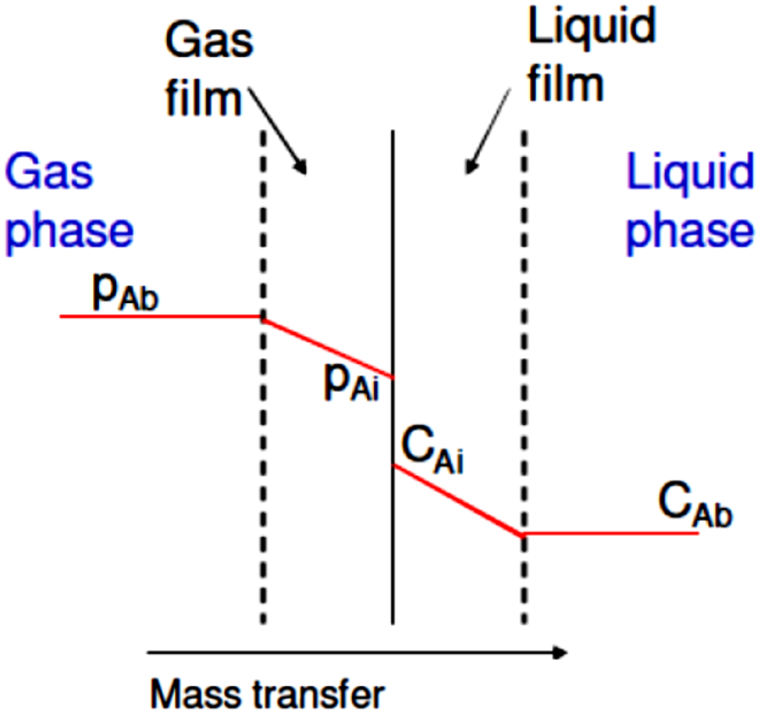
Mass transfer in the liquid phase:

$$N_A = k_c \, (C_{Ai} - C_{Ab}) \qquad (1)$$

Phase equilibrium is assumed at the gas-liquid interface.

Applying Henry's law,

$$p_{Ai} = H_A \, C_{Ai} \qquad (3)$$

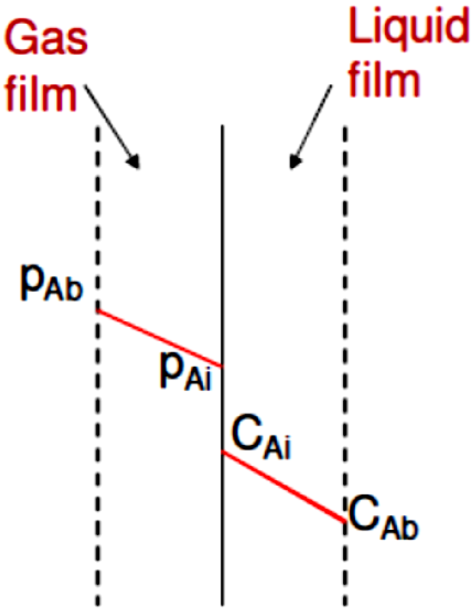


Henry's Law

$p_{Ai} = H_A C_{Ai}$ at equilibrium,

where H_A is **Henry's constant for A**

Note that p_{Ai} is the gas phase pressure and C_{Ai} is the liquid phase concentration.

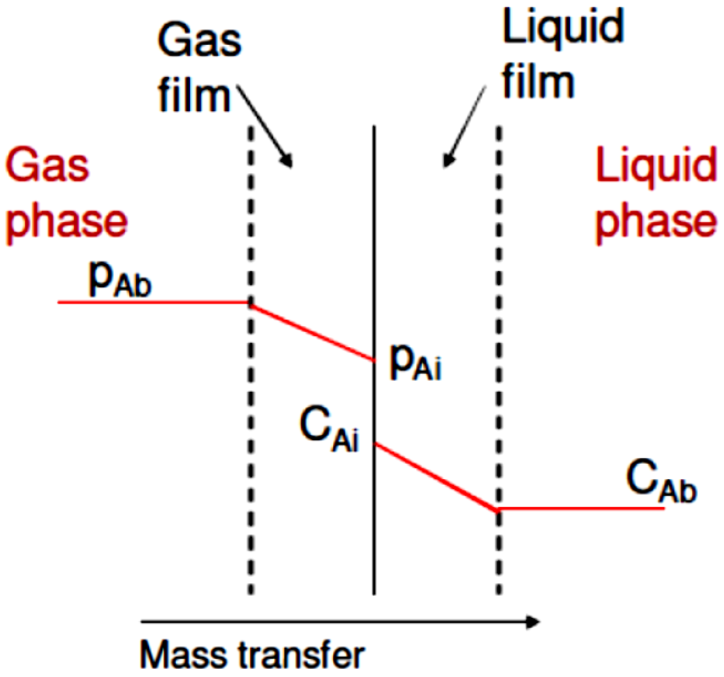


Two Film Theory applied at steady state

We know the bulk concentration and bulk partial pressure.

Usually, we do not know the interface concentration and the interface partial pressure.

Therefore, we eliminate p_{Ai} and C_{Ai} from equations (1), (2) and (3) by combining them.



Two Film Theory applied at steady state

From (2): $$p_{Ai} = p_{Ab} - \frac{N_A}{k_p} \qquad (4)$$

From (1): $$C_{Ai} = C_{Ab} + \frac{N_A}{k_c} \qquad (5)$$

Substituting the above in (3) and rearranging:

$$\boxed{N_A = \frac{p_{Ab} - H_A\, C_{Ab}}{H_A / k_c + 1 / k_p} \qquad \text{——} \qquad (6)}$$

The above expression is based on gas-phase and liquid-phase mass transfer coefficients.

Let us now introduce <u>overall</u> gas-phase and <u>overall</u> liquid-phase mass transfer coefficients.

Introducing overall gas-phase mass transfer coefficient:

Let’s start from (6):

Introduce the following imaginary gas-phase partial pressure:

$$p_A^* \equiv H_A C_{Ab} \qquad\qquad (7)$$

where p_A^* is a partial pressure that would have been in equilibrium with the concentration of A in the bulk liquid.

Introduce an overall gas-phase mass-transfer coefficient (K_G) as

$$\frac{1}{K_G} \equiv \frac{1}{k_p} + \frac{H_A}{k_c} \qquad \text{———} \qquad (8)$$

Combining (6), (7) and (8):

$$\mathbf{N_A = K_G\,(p_{Ab} - p_A^*)} \qquad\qquad (9)$$

Introducing overall liquid-phase mass transfer coefficient:

Once again, let's start from (6).

Introduce the following imaginary liquid-phase concentration:

$$p_{Ab} \equiv H_A C_A^* \qquad (10)$$

where C_A^* is a concentration that would have been in equilibrium with the partial pressure of A in the bulk gas.

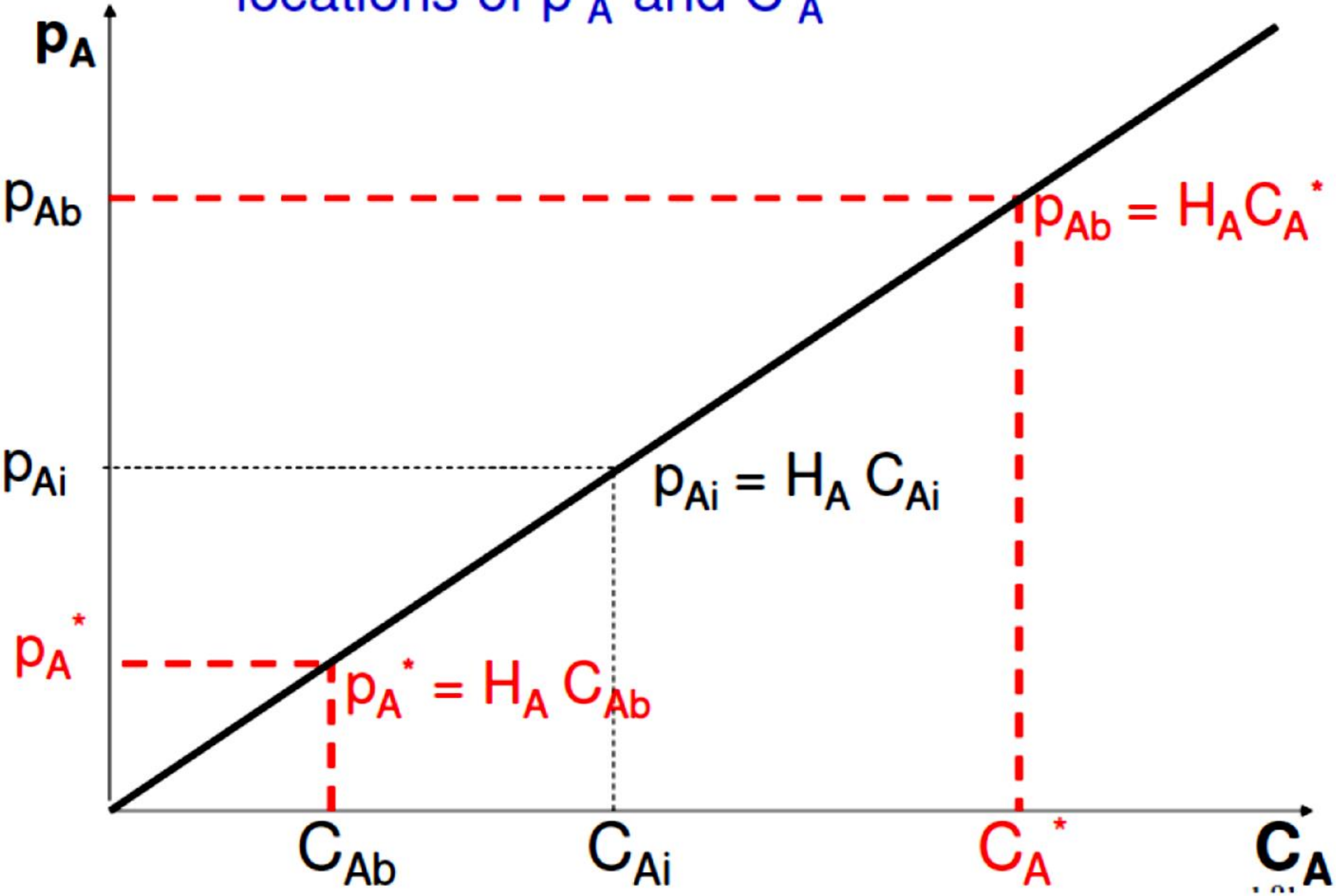
Introduce an overall liquid-phase mass-transfer coefficient (K_L) as

$$\frac{1}{K_L} \equiv \frac{1}{H_A k_p} + \frac{1}{k_c} \qquad (11)$$

Combining (6), (10) and (11):

$$\mathbf{N_A = K_L (C_A^* - C_{Ab})} \qquad (12)$$

Gas-Liquid Equilibrium Partitioning Curve showing the locations of p^*_A and C^*_A



Summary

$$N_A = K_L (C_A^* - C_{Ab}) \qquad (12)$$

$$= K_G (p_{Ab} - p_A^*) \qquad (9)$$

where

$$C_A^* = p_{Ab} / H_A \qquad (10)$$

$$p_A^* = H_A C_{Ab} \qquad (7)$$

$$\frac{1}{K_G} = \frac{H_A}{K_L} = \frac{1}{k_p} + \frac{H_A}{k_c} \qquad \text{(8 and 11)}$$

Summary

Two Film Theory applied at steady-state

$$N_A = \underset{(2)}{k_p\,(p_{Ab} - p_{Ai})} = \underset{(1)}{k_c\,(C_{Ai} - C_{Ab})} = \underset{(9)}{K_G\,(p_{Ab} - p_A^*)} = \underset{(12)}{K_L\,(C_A^* - C_{Ab})}$$

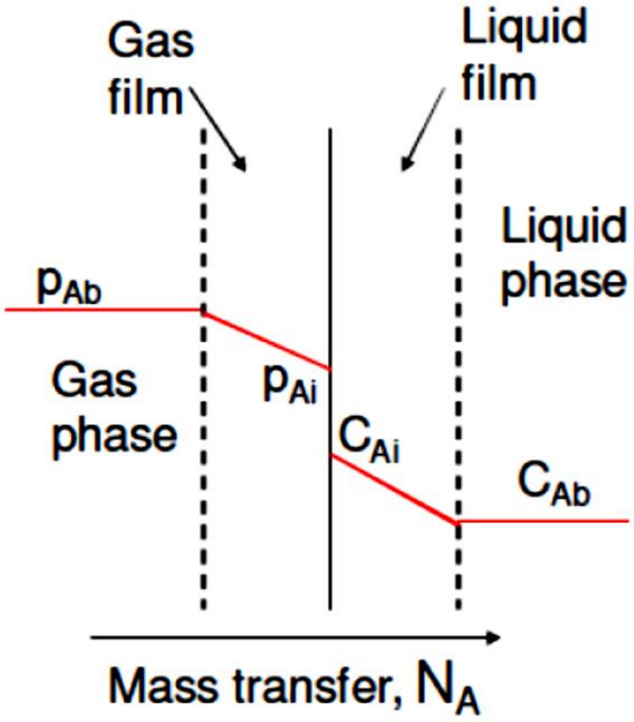
$$p_{Ai} = H_A\,C_{Ai} \qquad (3)$$

$$p_{Ab} = H_A\,C_A^* \qquad (10)$$

$$p_A^* = H_A\,C_{Ab} \qquad (7)$$

$$\frac{1}{K_G} = \frac{H_A}{K_L} = \frac{1}{k_p} + \frac{H_A}{k_c}$$

(8 and 11)



Gas & Liquid-side Resistances in Interfacial Mass Transfer

$$\frac{1}{K_G} = \frac{1}{k_p} + \frac{H}{k_c}$$

f_G = fraction of gas-side resistance

$$= \frac{1/k_p}{1/K_G} = \frac{1/k_p}{1/k_p + H/k_c} = \frac{k_c}{k_c + H\,k_p}$$

$$\frac{1}{K_L} = \frac{1}{H\,k_p} + \frac{1}{k_c}$$

f_L = fraction of liquid-side resistance

$$= \frac{1/k_c}{1/K_L} = \frac{1/k_c}{1/Hk_p + 1/k_c} = \frac{k_p}{k_p + k_c/H}$$

Notes

- If $f_G > f_L$ use the overall gas-side mass transfer coefficient and the overall gas-side driving force.
- If $f_L > f_G$ use the overall liquid-side mass transfer coefficient and the overall liquid-side driving force.