Lecture 38: Conditions at the Interface

The Lecture Contains:

- **Boundary Conditions**
- **Stationary Media with Specified Surface Concentrations**

◀❚❚ Previous   Next ❚❚▶

Boundary Conditions

The first condition corresponds to a situation for which the species concentration at the surface is maintained at a constant value. Expressing this condition on a molar basis for the surface , $x = 0$, we have.

$$x_A(0,t) = x_{A,W} \qquad \text{(9.30)}$$

The second condition corresponds to constant species $j_{a,w}^*$ at the surface and using **Fick's law, equation (9.2)** may be expressed as.

$$-CD_{AB}\frac{\partial x_A}{\partial x}\bigg|_{x=0} = j_{A,W}^* \qquad \text{(9.31)}$$

A special case of this condition corresponds to the impermeable surface for which

$$\frac{\partial x_A}{\partial x}\bigg|_{x=0} = 0$$

In applying **equation (9.30)** , we are often interested in knowing the concentration of species **A** in a liquid or a solid **(species B)** at the interface with a gas containing species **A**. If species **A** is only weakly soluble in a liquid, species **B**, Henry's law may be used to relate the mole fraction of **A** in the liquid to the partial pressure of **A** in the gas phase outside the liquid
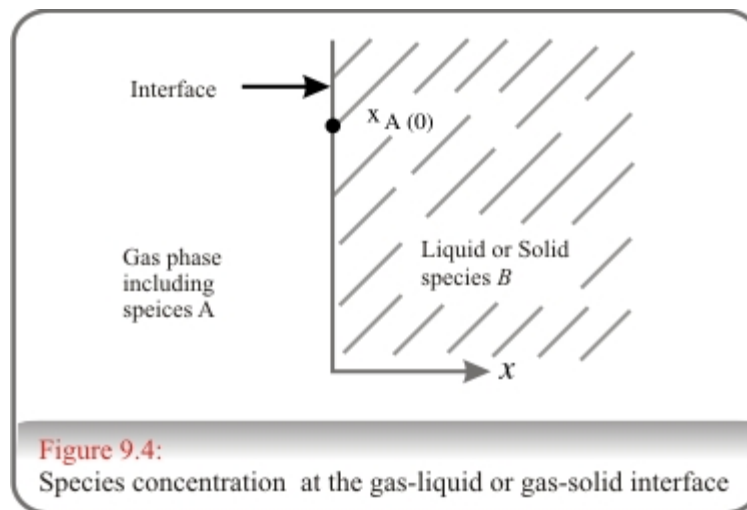
$$x_A(0) = p_A/H \qquad \text{(9.32)}$$

The coeffiecient **H** is known as Henry's constant. **H** depends on temperature, its pressure dependence may generally be neglected for values of p upto 5 bars.

Figure 9.4:
Species concentration at the gas-liquid or gas-solid interface

Conditions at a gas-solid interface may also be determined if the gas, species A, dissolves in the solid, species B, and a homogeneous solution is formed. Treating the solid as a uniform substance, the concentration of the gas in the solid at the interface may be obtained through use of a property known as solubility S. It is defined by the expression.

$$C_A(0) = S p_A \qquad (9.33)$$

Where p_A is the partial pressure of the gas adjoining the interface.

◀▌▌ Previous   Next ▌▌▶

Module 9: Mass Transfer
Lecture 38: Conditions at the Interface

The molar concentration of **A** in the solid at interface, $c_A(0)$, is in units of kilomoles of **A** per cubic meter of solid, in which case the units of **S** must be kilomoles of **A** per cubic meter of solid per bar partial pressure of **A**.

Gas	Solid	T(k)	S (k mol/m^{3}bar)
O_2	Rubber	298	3.12×10^{-3}
N_2	**Rubber**	**298**	1.56×10^{-3}
Co_2	Rubber	298	40.15×10^{-3}
He	SiO_2	**298**	0.45×10^{-3}

Previous   Next

Stationary Media with Specified Surface Concentrations

Consider one-dimensional diffusion of species A through a planar medium of A and B. For steady-state conditions with no homogeneous chemical reactions, the molar form of the species diusion equation reduces to

$$\frac{d}{dx}\left(CD_{AB}\frac{dx_A}{dx}\right) = 0 \qquad\qquad \textbf{(9.34)}$$

The solution: **(the flux distribution)**

$$x_A(x) = \left(x_{A,W2} - x_{A,W1}\right)\frac{x}{L} + x_{A,W1} \qquad\qquad \textbf{(9.35)}$$

From $N'' = -CD_{AB}\nabla x_A$, we get
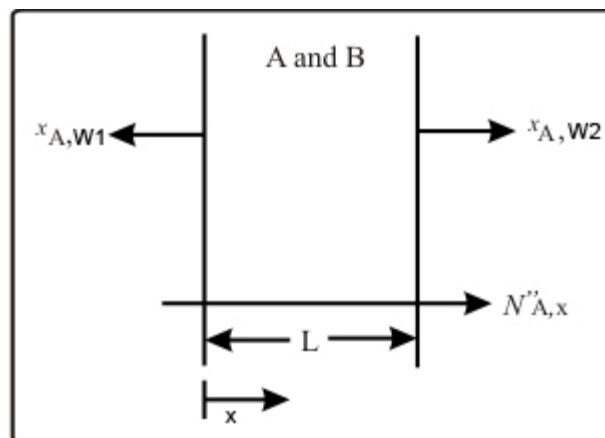
Figure 9.5: Mass transfer in a stationary planar medium

$$N''_{A,x} = -CD_{AB}\frac{x_{A,W2} - x_{A,W1}}{L} \qquad\qquad \textbf{(9.36)}$$

Multiplying by the surface area **A** and substituting $x_A = C_A/C,$ the molar rate is then.

$$N_{A,x} = \frac{D_{AB}\,A}{L}\left(C_{A,w1} - C_{A,w2}\right) \qquad\qquad \textbf{(9.37)}$$

◀‖ Previous   Next ‖▶

From the earlier expression, we can define a resistance to species transfer by diffusion in a planar medium as.

$$R_{m,diff} = \frac{C_{A,w1} - C_{A,w2}}{N_{Ax}} = \frac{L}{D_{AB}A} \qquad (9.38)$$

Similarly for diffusion in the radial direction in a cylindrical medium we have to solve.

$$\frac{d}{dr}\left(rCD_{AB}\frac{dx_A}{dr}\right) = 0 \qquad (9.39)$$

Flux Distribution: Can be obtained after integrating the above eqaution.

$$x_A(r) = \frac{x_{A,W1} - x_{A,W2}}{\ln r_1/r_2}\ln\left(\frac{r}{r_2}\right) + x_{A,W2}$$

$$R_{m,diff} = \frac{\ln(r_2/r_1)}{2\pi L D_{AB}} \qquad (9.40)$$

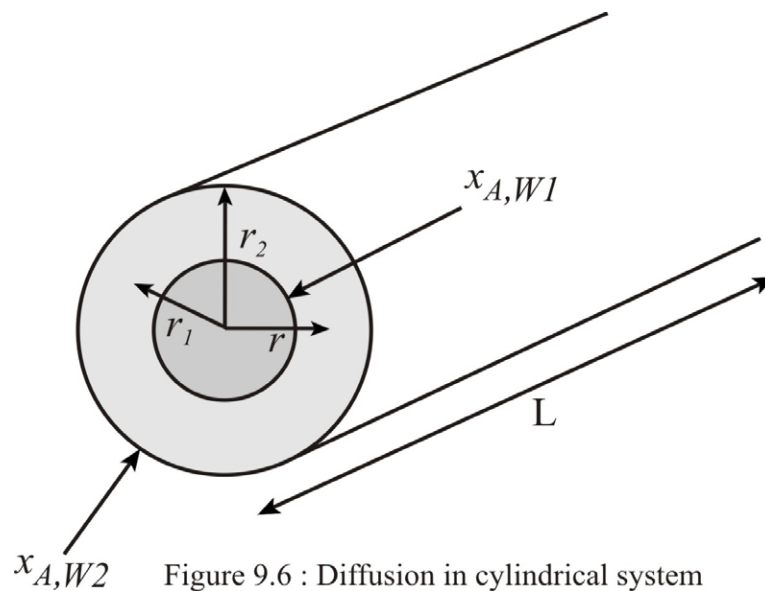$$N_{A,r} = \frac{C_{A,w1} - C_{A,W2}}{R_{m,diff}}$$

$x_{A,W2}$ Figure 9.6 : Diffusion in cylindrical system

Previous   Next

Module 9: Mass Transfer

Lecture 38: Conditions at the Interface

Problem:

Previous   Next

Stationary Media with Catalytic Surface Reactions

Many mass transfer problems involve specification of species flux, rather than the species concentration, at the surface.

A catalytic surface is placed in a gas stream for the purpose of promoting a heterogeneous chemical reaction involving species **A**. Assume that the reaction results in the production of species A at a rate given by $\dot{N}_A''$, which is defined as the molar rate of production of species A per unit surface area of the catalyst.

Such a reaction enhances surface concentration of **A,** and in order to maintain steady state conditions it is necessary that the rate of species transfer from the surface, $N_{A,x}''$ must be equal to the surface reaction rate.

$$N_{A,x}''(0) = \dot{N}_A''$$
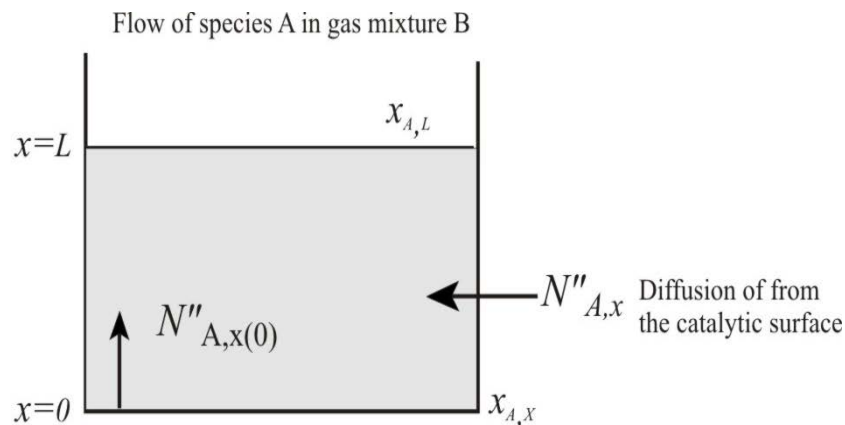
(9.41)

Flow of species A in gas mixture B

Figure 9.7: One-dimensional diffusion with heterogenous catalysis

It is assumed that the transfer occurs exclusively by diffusion. It is also assumed that the species A leaves the surface as result of one dimensional transfer through a thin film of thickness L and that no reactions occur within the film itself. The mole fraction of A at x = L , $x_{A,L}$, corresponds to conditions in the mainstream of the mixture and it is known. Representing the remaining species of the mixture as a single species **B** and assuming the medium to be stationary, we get the governing equation,

$$\frac{d}{dx}\left(CD_{AB}\frac{dx_A}{dx}\right) = 0 \qquad\qquad \textbf{(9.42)}$$

Where D_{AB} is the binary diffusion coefficient for A in B and B is a multicomponent mixture.

◀‖ Previous   Next ‖▶

Assuming **C** and D_{AB} to be constant, **equation (9.42)** may be solved subject to the condtions that

$$x_A(L) = x_{A,L}$$

and

$$N''_{A,x}(0) = -CD_{AB} \left. \frac{dx_A}{dx} \right|_{x=0} = \dot{N}''_A \qquad \textbf{(9.43)}$$

For a catalytic surface, N''_A depends on $C_A(0)$ surface concentration. For a first order reaction **(that results in a species consumption at the surface)**.

$$\dot{N}''_A = -k''_1 C_A(0) \qquad \textbf{(9.44)}$$

where, $k''_1 \, (m/s)$ is the reaction rate constant. **Accordingly (9.43)** reduces to

$$-D_{AB} \frac{dx_A}{dx}\big|_{x=0} = -k''_1 x_A(0) \qquad \textbf{(9.45)}$$

◀▌▌Previous   Next▐▌▶

Solving (9.42), we get a linear distribution of mole fraction

$$\frac{x_A(x)}{x_A(L)} = \frac{1 + (xk_1''/D_{AB})}{1 + (Lk_1''/D_{AB})} = \frac{x_A(x)}{x_{A,L}} \qquad \textbf{(9.46)}$$

At the catalytic surface this reduces to

$$\frac{x_A(0)}{x_{A,L}} = \frac{1}{1 + (Lk_1''/D_{AB})} \qquad \textbf{(9.47)}$$

and the **molar flux** is .

$$N_A''(0) = -CD_{AB} \left.\frac{dx_A}{dx}\right|_{x=0} = -k_1'' C x_A(0)$$

or

$$N_A''(0) = -\frac{k_1'' C x_{A,L}}{1 + (Lk_1''/D_{AB})} \qquad \textbf{(9.48)}$$

The negative sign implies that the mass is transferred to the surface . Two limiting cases are very important :

1. $k_1'' \to 0$, $(Lk_1''/D_{AB}) << 1$, and equations (9.47) and (9.48) reduce to

$$\frac{x_{Ax}}{x_{A,L}} \approx 1 \text{ and } N_A''(0) = -k_1'' C x_{A,L}$$

This process is REACTION LIMITED

2. $k_1'' \to 0$, $(Lk_1''/D_{AB}) >> 1$, and equations (9.47) and (9.48) reduce to

$$x_{Ax} \approx 0 \text{ and } N_A''(0) = -k_1'' C x_{A,L}$$

This process is DIFFUSION LIMITED