MODULE 2: DIFFUSION

LECTURE NO. 2

2.2 STEADY STATE MOLECULAR DIFFUSION IN FLUIDS UNDER STAGNANT AND LAMINAR FLOW CONDITIONS

2.2.1 Steady state diffusion through a constant area

Steady state diffusion through a stagnant gas film

Assume steady state diffusion in the Z direction without any chemical reaction in a binary gaseous mixture of species A and B. For one dimensional diffusion of species A, the Equation of molar flux can be written as

\[ N_A = -CD_{AB} \frac{dy_A}{dZ} + y_A(N_A + N_B) \quad (2.11) \]

Separating the variables in Equation (2.11), it can be expressed as

\[ \frac{-dy_A}{N_A - y_A(N_A + N_B)} = \frac{dZ}{CD_{AB}} \quad (2.12) \]

For the gaseous mixture, at constant pressure and temperature C and D_{AB} are constant, independent of position and composition. Also all the molar fluxes are constant in Equation (2.12). Therefore the Equation (2.12) can be integrated between two boundary conditions as follows:

at \[ Z = Z_1, \quad y_A = y_{A1} \]

at \[ Z = Z_2, \quad y_A = y_{A2} \]

where 1 indicates the start of the diffusion path and 2 indicates the end of the diffusion path. After integration with the above boundary conditions the Equation for diffusion for the said condition can be expressed as

\[ N_A = \frac{N_A}{(N_A + N_B)} \frac{CD_{AB}}{Z_2 - Z_1} \ln \left[ \frac{N_A}{(N_A + N_B)} - y_{A2} \right] - \left[ \frac{N_A}{(N_A + N_B)} - y_{A1} \right] \quad (2.13) \]
For steady state one dimensional diffusion of A through non-diffusing B, \( N_B = 0 \) and \( N_A \) = constant. Therefore, \( \frac{N_A}{(N_A + N_B)} = 1 \). Hence Equation (2.13) becomes

\[
N_A = \frac{CD_{AB}}{Z_2 - Z_1} \ln \left[ \frac{1 - y_{A_2}}{1 - y_{A_1}} \right] \tag{2.14}
\]

Since for an ideal gas \( C = \frac{p}{RT} \) and for mixture of ideal gases \( y_A = \frac{P_A}{P} \), the Equation (2.14) can be expressed in terms of partial pressures as

\[
N_A = \frac{PD_{AB}}{(Z_2 - Z_1)RT} \ln \left[ \frac{P - P_{A_2}}{P - P_{A_1}} \right] \tag{2.15}
\]

Where \( P \) is the total pressure and \( p_{A_1} \) and \( p_{A_2} \) are the partial pressures of A at point 1 and 2 respectively. For diffusion under turbulent conditions, the flux is usually calculated based on linear driving force. For this purpose the Equation (2.13) can be manipulated to rewrite it in terms of a linear driving force. Since for the binary gas mixture of total pressure \( P \), \( P - p_{A_1} = p_{B_1} \); \( P - p_{A_2} = p_{B_2} \);

\[
p_{A_1} - p_{A_2} = p_{B_2} - p_{B_1} \]

Then the Equation (2.15) can be written as

\[
N_A = \frac{PD_{AB}}{(Z_2 - Z_1)RT} \ln \left[ \frac{p_{A_1} - p_{A_2}}{p_{B_2} - p_{B_1}} \right] \ln \left[ \frac{p_{B_1}}{p_{B_2}} \right] \tag{2.16}
\]

Or

\[
N_A = \frac{PD_{AB}}{(Z_2 - Z_1)RTp_{B,M}} (p_{A_1} - p_{A_2}) \tag{2.17}
\]

Where \( p_{B,M} \) is called logarithmic mean partial pressure of species B which is defined as

\[
p_{B,M} = \frac{p_{B_1} - p_{B_2}}{\ln \left( \frac{p_{B_1}}{p_{B_2}} \right)} \tag{2.18}
\]

A schematic concentration profile for diffusion A through stagnant B is shown in Figure 2.1. The component A diffuses by concentration gradient, \( -\frac{dy_A}{dZ} \). Here flux is inversely proportional to the distance through which diffusion occurs and the
concentration of the stagnant gas \( p_{B,M} \) because with increase in \( Z \) and \( p_{B,M} \), resistance increases and flux decreases.

\[
p_A = p_A^0 + p_B^0
\]

\[
0.0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0
0.0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1.0
p_B^0
p_A^0 \quad p_B^1
p_A^1
p = p_A + p_B
\]

Distance, \( Z \) (cm)

\[\text{Figure 2.1: Partial pressure distribution of } A \text{ in non-diffusing } B\]

2.2.2 Steady state equimolar counter diffusion:

This is the case for the diffusion of two ideal gases, where an equal number of moles of the gases diffusing counter-current to each other. In this case \( N_B = -N_A \) = constant and \( N_A + N_B = 0 \). The molar flux Equation (Equation (2.11)) at steady state can then be written as

\[
N_A = - \frac{D_{AB} P}{RT} \frac{dy_A}{dZ}
\]  
(2.19)

Integrating the Equation (2.19) with the boundary conditions: at \( Z = Z_1 \), \( y_A = y_{A1} \); at \( Z = Z_2 \), \( y_A = y_{A2} \), the Equation of molar diffusion for steady-state equimolar counter diffusion can be represented as
It may be noted here also that molar latent heats of vaporization of \( A \) and \( B \) are equal. So, \( \Delta H_A^V = \Delta H_B^V \), where, \( \Delta H_A^V \) and \( \Delta H_B^V \) are molar latent heats of vaporization of \( A \) and \( B \), respectively. The concentration profile in terms of partial pressure is shown in Figure 2.2.

\[
N_A = \frac{D_{AB} P}{RT (Z_2 - Z_1)} (y_A - y_{A_1})
\]
\[
= \frac{D_{AB}}{RT (Z_2 - Z_1)} (P_A - P_{A_1})
\]

(2.20)

Figure 2.2: Equimolar counter diffusion of \( A \) and \( B \): Partial pressure distribution with position
2.2.3 Non-equimolar counter diffusion

In some practical cases, A and B molecules diffuse in opposite directions at different molar velocities [1]. Let carbon monoxide is generated from the reaction between hot char and oxygen. The stoichiometry is as follows:

\[ 2C + O_2(A) \leftrightarrow 2CO(B) \quad (2.21) \]

When one mole oxygen molecule diffuses towards char, two moles carbon monoxide molecules diffuse in opposite direction. Here, \( N_A = -N_B / 2 \) and molar latent heats of vaporization are not equal. Hence,

\[ N_A \Delta H_A^V = -N_B \Delta H_B^V \quad (2.22) \]