Mass Transfer Operations - I Prof. Bishnupada Mandal Department of Chemical Engineering Indian Institute of Technology, Guwahati

Diffusion Mass Transfer Lecture – 04 Steady State Molecular Diffusion in fluids under stagnant and laminar flow conditions

Welcome to the 4th lecture on Mass Transfer Operations. In this lecture, we will discuss the diffusion mass transfer in particular to the Steady State Molecular Diffusion under stagnant and laminar flow conditions. Before going to the lecture let us have small recap on the previous lecture. In the previous lecture we have considered the Fick's law of diffusions and we have considered study state diffusion and unsteady state diffusion.

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Recap , Fick's first Law , Fick's 2nd Law

In study sate diffusion we discuss the Fick's first law and the second case we have discussed the Fick's second law which is applicable for unsteady state diffusion.

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Steady State Molecular Diffusion in Fluids Under Stagnant and Laminar Flow Conditions		
Steady state diffusion through a constant area :		
 Assume steady state diffusion in the x-direction without any chemical reaction in a binary gaseous mixture of species A and B. 		
For one dimensional diffusion of species A, molar flux:		
$N_{A} = -CD_{AB} \frac{dy_{A}}{dx} + y_{A}N$ Where N = $N_{A} + N_{B}$		
 Separating the variables in equation (a), it can be expressed as: 		
$\frac{-dy_A}{N_A - y_A N} = \frac{dx}{CD_{AB}}$		

Now, steady state molecular diffusion in fluids under stagnant and laminar flow conditions. Steady state diffusion through a constant area if we consider and then we assume that steady state diffusion in the x direction without any chemical reactions in a binary gaseous mixture of species A and B for one dimensional diffusions of species A.

We know the molar flux equations N A is equal to minus C D A B d y A d x plus y A N this is N is the total mole molar flux is equal to N A plus N B. Now, separating the variables in this equations this equation can be expressed as minus d y A divided by N A minus y A N is equal to d x by C D A B so this is equation b.

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Now, for the gaseous mixture at constant pressure and temperature the concentration and diffusion coefficient D A B are constant and independent of position and composition also all the molar fluxes are constant in equation b, equation b is minus d y A divided by N A minus y A N is equal to d x C D A B.

Therefore, the equation b can be integrated between the 2 boundary conditions which is given as follows at x is equal to $x \ 1 \ y \ A$ would be equal to $y \ A \ 1$, $y \ A$ is the mole fractions of component A in the gas phase. At x is equal to $x \ 2 \ y \ A$ would be equal to $y \ A \ 2$, $y \ A \ 2$ is the mole fractions of component 2 in the gas phase. So, 1 indicates the start of diffusion path and 2 indicates the end of the diffusion path.

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Now, if we integrate equation b with the above boundary conditions we can get integral y A 1 to y A 2 minus d y A divided by N A minus y A N is equal to integral x 1 x 2 d x C D A B. Let N A minus y A N would be equal to Z. So, from here we can write minus d y A N would be equal to d Z and minus d y would be equal to d Z by N.

So, substituting the values in the above equations minus d y A it would be integral Z 1 to Z 2 d Z by N Z would be equal to integral x 1 to x 2 d x C D A B. So, since N A minus y A N is Z. So, it is Z and minus d y A over here which is substituted by d Z by N. So, it becomes integral Z 1 to Z 2 d Z by N into Z is equal to integral x 1 to x 2 d x by C D A B.

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Steady State Molecular Diffusion Through a Constant Area
$\int_{Z_1}^{Z_2} \frac{dZ}{NZ} = \int_{x_1}^{x_2} \frac{dx}{CD_{AB}} \text{Or,} \qquad \frac{1}{N} (\ln Z_2 - \ln Z_1) = \frac{1}{CD_{AB}} (x_2 - x_1)$
$\implies \ln\left(\frac{Z_2}{Z_1}\right) = \frac{N}{CD_{AB}}(x_2 - x_1)$
$\implies \ln\left(\frac{N_A - y_{A_2}N}{N_A - y_{A_1}N}\right) = \frac{N}{CD_{AB}}(x_2 - x_1)$
$\implies \ln\left[\frac{N\left(\frac{N_A}{N}-y_{A_2}\right)}{N\left(\frac{N_A}{N}-y_{A_1}\right)}\right] = \frac{N}{CD_{AB}}(x_2-x_1)$
> Multiplying both sides with N_A in above equation,

Now, integral Z 1 to Z 2 d Z by N Z equal to integral x 1 to x 2 d x C D A B can be written as 1 by N into ln Z 2 minus ln Z 1 is equal to 1 by C D A B into x 2 minus x 1 and from that if we rearrange it would be ln Z 2 by Z 1 is equal to N by C D A B x 2 minus x 1. Now, if we substitute Z at Z 1 and Z 2 then it would be ln N A minus y A 2 N divided by N A minus y A 1 N would be equal to N by C D A B x 2 minus x 1.

So, it would be ln N N A by N minus y A 2 divided by N into N A by N minus y A 1. If we just multiply both numerator and the denominator by N it would be like this the left hand side equation and the right hand side equations should be N A by C C D A B x 2 minus x 1 Now, if we multiply both sides with N A in this equation.



We will obtain N A would be equal to N A by N into C D A B by x 2 minus x 1 ln N A by N minus y A 2 divided by N A by N minus y A 1. Therefore, after integration with the boundary conditions the equation for diffusion for the said conditions can be expressed as this relations. So, N A would be equal to N A by N C D A B by x 2 minus x 1 ln N A by N minus y A 2 divided by N A by N minus y A 1.

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Now, steady state diffusion through non diffusing B, for steady state one dimensional diffusion of A through non diffusing B N B would be equal to 0 and N A would be equal

to constant. Therefore, the N A by N would be equal to N A by N A plus N B would be equal to 0. Since N B is equal to 0. So, N A by N A plus N B would be equal to N A by N A would be equal to 1. Hence equation c becomes N A is equal to C D A B x 2 minus x 1 ln 1 minus y A 2 by 1 minus y A 1.

For an ideal gas we can write concentration would be equal to total pressure Pt divided by RT R is the universal gas constant and T is any temperature. For mixture of ideal gases the mole fractions y A in the gas phase can be expressed as the partial pressure of that component divided by the total pressure. The equation d can be expressed in terms of the partial pressures as follows; N A would be equal to D A B Pt divided by x 2 minus x 1 RT ln Pt minus P A 2 divide by Pt minus P A 1. Where Pt is the total pressure P A 1 and P A 2 are the partial pressures of A at point 1 and 2 respectively.

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For diffusion under turbulent conditions the flux is usually calculated based on linear driving force for this purpose the equation e can be manipulated to rewrite in terms of a linear driving force. Since for binary gas mixture of total pressure Pt we can write Pt is equal to P A plus P B. P A and P B are the partial pressure of component A and component B. So, that we can write Pt minus P A 2 would be equal to P B 2 and Pt minus P A 1 would be equal to P B 1.

Hence, we can write P A 1 minus P A 2 would be equal to P B 2 minus P A 1. Then the equation e can be written as N A would be equal to D A B Pt divided by RT x 2 minus x

1 in to P A 1 minus P A 2 divided by P B 2 minus P B 1 into ln P B 2 by P B 1. So, we can rearrange this relation as N A would be equal to D A B Pt by RT x 2 minus x 1 P B LM into P A 1 minus P A 2.

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In this relation P B LM is the logarithmic mean of partial pressure of species B which is defined as P B LM is equal to P B 2 minus P B 1 divided by ln P B 2 by P B 1. The component A diffuses by concentration gradients the gradient is minus d y A d x. Here flux is inversely proportional to the distance through which the diffusion occurs and the concentration of the stagnant gas that is in terms of the logarithmic mean of partial pressures of species B. Because with increase in x and P B LM resistance increases and flux decreases.

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This change of concentration or the partial pressure can be expressed in terms of the simple profiles which is shown over here y axis p A or p B in terms of say atmosphere and x axis is the distance may be represented by z. So, which varies from 0 0.2 0.4 0.6 0.8 and 1.0 and this partial pressure can vary from.

So, this is the variation of concentration of p A 2 to p A 1 and the concentration variation of p B can be expressed p B 1. So, Pt is the total pressure which is equal to partial pressure of A plus partial pressure of B this is the variation of p A and this is the variation of partial pressure of component B. So, A is diffusing through this directions. So, this is the partial pressure distribution of A in non diffusing B.

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Example 1 : Solution			
Solution: Assume ideal gas Let air = B	$\rm CO_2$ is diffusing through non diffusing air under steady state conditions at a total pressure of 1 atmosphere and temperature 300K. The partial pressure of CO_2 is 20kPa at one point and 5kPa at other point. The distance between the points is 5cm. Calculate the flux of CO_2. Given that at 300K and at 1 atm, $\rm D_{CO2-air}=2~x~10^{-5}~m^2/s.$		
$N_{CO_2} = \frac{D_{CO_2 - air}}{RT(x_2 - x_1)}$	$\frac{1}{D} \times \frac{P_t}{P_{BLM}} \left(P_{CO_{2,1}} - P_{CO_{2,2}} \right)$		
Given that D_{CO_2-air} =	= 2 x 10 ⁻⁵ m²/s at 300K and 1 atm .		
P = 1 atm = 101.3	kPa = 1.013 × 10 ⁵ Pa		
T= 300 K, $x_2 - x_1$	$= 5 \ cm = 0.05 m,$		
$p_{CO_{2,1}} = 20 \ kPa =$	20,000 <i>Pa</i> $P_{B,1} = P_t - P_{CO_{2,1}} = (101.3 - 20) kPa = 81.3 kPa$		
$p_{CO_{2,2}} = 5 \ kPa = 5$ $R = 8314 \ Pa \ m^3/l$	$P_{B,2} = P_t - P_{CO_{2,2}} = (101.3 - 5) kPa = 96.3 kPa$ accord K		

Now, let us take an example carbon dioxide is diffusing through non diffusing air under steady state conditions at a total pressure of one atmosphere and temperature of 300 Kelvin. The partial pressure of carbon dioxide is 20 kilo Pascal at one point and 5 kilo Pascal at other point the distance between the points is 5 centimeter. We need to calculate the flux of carbon dioxide given that at 300 Kelvin at and at 1 atmosphere pressure the diffusion coefficient of carbon dioxide in air is equal to 2 into 10 to the power minus 5 meter square per second.

Now, let us solve this we assume that it is ideal gas let air B the component B. So, we can write N CO 2 would be equal to D CO 2 air divided by RT in into x 2 minus x 1 into Pt by P B L M into partial pressure of CO 2 at 1 and partial pressure minus partial pressure of CO 2 at 2. So, this is D CO 2 air is given 2 into 10 to the power minus 5 meter square per second at 300 Kelvin and 1 atmosphere pressure so that these data is given.

Now, P is the total pressure which is 1 atmosphere and if we just convert into kilo Pascal it would be 101.3 kilo Pascal which is equal to 1.01 into 10 to the power 5 Pascal. Now temperature is 300 Kelvin which is given x 2 minus x 1 the distance of diffusion is 5 centimeter. If we convert to meter it would be point 0.5 0.05 meter and then partial pressure of carbon dioxide at 0.1 is given 20 kilo Pascal which is 20000 Pascal partial

pressure of carbon dioxide at 0.2 is 5 kilo Pascal which is 5000 Pascal and R is given as 8314 Pascal meter cube per kilo mole Kelvin.

So, P B 1 would be equal to Pt minus P carbon dioxide at point 1 which would be equal to 101.3 minus 20 kilo Pascal which is around 81.3 kilo Pascal. And P B 2 you can calculate Pt minus P CO 2 at point 2 which is equal to 101.3 minus 5 kilo Pascal which is 96.3 kilo Pascal.

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So, this P B 1 and P B 2 are calculated, now if we calculate P B L M log mean partial pressure difference P B 2 minus P B 1 divided by ln P B 2 by P B 1 it would be equal to 96.3 minus 81.3 divided by ln to 96.3 divided by 181.3 kilo Pascal which is 88.59 kilo Pascal and which is equal to 88590 Pascal.

Now, we can calculate the flux NCO 2 would be equal to 2 into 10 to the power 5 meter square per second into 1.013 into 10 to the power 5 Pascal divided by 8314 Pascal meter cube per kilo mole Kelvin into 300 Kelvin is the temperature. And then distance is point not 5 meter into 88590 Pascal and the pressure differential is 20000 minus 5000 Pascal. So, it will lead to 2.75 into 10 to the power minus 6 kilo mole per meter square second.

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Now, 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 currently to each other. In this case N B would be equal to minus N A which is equal to constant. And so from this we can write N A plus N B is equal to 0. Now the molar flux in equation a at steady state can be written as this is equation 1 N A is equal to minus C D A B d y d x plus y A N and N A plus N B is equal to N which is 0. So, if we substitute that N is 0 we will get N A is equal to minus C D A B d y A d x.

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$$N_{A} = \frac{D_{AB}P_{t}}{RT(x_{2} - x_{1})} (y_{A_{1}} - y_{A_{2}})$$
$$= \frac{D_{AB}}{RT(x_{2} - x_{1})} (p_{A_{1}} - p_{A_{2}})$$

Now, for ideal gas the concentration is equal to total pressure Pt divided by RT where R is the universal gas constant and T is the temperature. So, we can write N A would be equal to minus d A B P t by RT into d y A d x. Now if we integrate this relation with the boundary conditions at x would be equal to x 1 and y A would be equal to y A 1 and x is equal to x 2 y A would be equal to y A 2.

The equation of molar diffusion for steady state equimolar counter diffusion can be represented as N A would be equal to D A B Pt by RT x 2 minus x 1 y A 1 minus y A 2. So, from here if we rearrange it would be D A B by RT x 2 minus x 1 into partial pressure of P A 1 minus partial pressure of component 2 at point 2 is P A 2.

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Now, let us consider another examples carbon dioxide is diffusing at steady state through a straight tube of 0.5 meter long with an inside diameter of point not 5 meter containing nitrogen at 300 Kelvin and 1 atmosphere pressure. The partial pressure of carbon dioxide at one end is 15 kilo Pascal and 5 kilo Pascal at the other end given that at 300 Kelvin and one atmosphere pressure the diffusion coefficient is 4 into 10 to the power minus 5 meter square per second. Now, we need to calculate the following for the steady state equimolar counter diffusion the molar flow rate of carbon dioxide and the molar flow rate of nitrogen and we need to see whether they are equal or not.

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Example 2 : Solution	
Assume ideal gas in equimolar counter diffusion for CO ₂ flux:	
$N_{CO_2} = \frac{D_{CO_2 - N_2}}{RT(x_2 - x_1)} (p_{CO_2, 1} - p_{CO_2, 2})$	
$D_{CO_2 - N_2} = 4 \times 10^{-5} m^2 / s$	
$P_t = 1 \text{ atm} = 101.3 \text{ kPa} = 1.013 \times 10^5 \text{ fz}$	
T= 300 K, $x_2 - x_1 = 0.5m$	
$p_{CO_{2,1}} = 15 \ kPa = 15,000 \ Pa$	
$p_{CO_{2,2}} = 5 \ kPa = 5,000 \ Pa$	
$R = 8314 Pam^3 / kmol K$	

So, we assume the ideal gas in equimolar counter diffusion for CO2. So, the flux for CO 2 we can write N CO 2 would be equal to D CO 2 N 2 divided by RT x 2 minus x 1 P CO 2 at 1 minus D CO 2 at 2. So, the value which are given DCO 2 N 2 would be equal to 4 into 10 to the power minus 5 meter square per second. Pt is the total pressure 1 atmosphere which is equal to 101.3 kilo Pascal which is equal to 1013 into 10 to the power 5 Pascal.

T is the temperature is 300 Kelvin and x 2 minus x 1 is the distance of diffusion which is 0.5 meter partial pressure of CO 2 at one is 15 kilo Pascal which is 15000 Pascal and partial pressure of CO 2 at 0.2 is 5 kilo Pascal which is 5000 Pascal R is known 8314 Pascal meter cube per kilo mole Kelvin.

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So, N CO 2 if we substitute this parameters we will get 4 into 10 to the power minus 5 divided by 8314 into 300 into 0.5 into the partial pressure difference 15000 minus 5000. So, it will lead to 3.21 into 10 to the power minus 7 kilo mole per meter square second.

Now, the molar flow rate of carbon dioxide is equal to NCO 2 into the area A is the cross sectional area of the tube. So, given that internal diameter of the tube is D i which is 0.05 meter. So, cross sectional area of the tube A is equal to pi D i square by 4 which is equal to pi by 4 into 0.05 square which is equal to 1.96 into 10 to the power minus 3 meter square.

Now molar flow rate of carbon dioxide we can calculate which is equal to 3.21 into 10 to the power minus 7 kilo mole per meter square second which we have calculated flux into the cross sectional area 1.96 into 10 to the power minus 3 meter square which will give 6.29 into 10 to the power minus 10 kilo mole per second.

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Example 2 : Solution (ii) $N_{N_2} = \frac{D_{CO_2-N_2}}{RT(x_2-x_1)} (p_{N_2,1} - p_{N_2,2})$ Given $P_{N_2,1} = P_t - p_{CO_{2,1}} = (101.3 - 15)kPa = 86.3kPa = 86300 \text{ Pa}$ $P_{N_2,2} = P_t - p_{CO_{2,2}} = (101.3 - 5)kPa = 96.3kPa = 96300 \text{ Pa}$ We know that for equimolar counter diffusion in ideal gases $D_{CO2-N_2} = D_{N_2-CO2}$ Or, $\frac{4 \times 10^{-5}}{8314 \times 300 \times 0.5} (86300 - 96300) = \frac{0.4}{1247100} = -3.21 \times 10^{-7} \frac{kmol}{m^2 s}$ $\therefore Molar flow rate of N_2 = -3.21 \times 10^{-7} \frac{kmol}{m^2 s} \times 1.96 \times 10^{-3} m^2 = -6.29 \times 10^{-10} \frac{kmol}{s}$

Now, let us calculate for nitrogen using the similar equations it is CO 2 N 2 by RT x 2 minus x 1 into the partial pressure of N 2 at 1 minus partial pressure of N 2 at 0.2. So, the data for P N 2 1 is P t minus P CO 2 at 1 which is equal to 101.3 minus 15 kilo Pascal. So, which is around 83.3 kilo Pascal so which is 86300 Pascal P N 2 at 2 is equal to Pt minus P CO 2 at 2 which is equal to 101.3 minus 5 kilo Pascal which is equal to 96.3 kilo Pascal which is equal to 96300 Pascal.

So, P N 2 at 1 and P N 2 at 2 is known now we know that for equimolar counter diffusion the diffusion coefficient of D CO 2 n 2 would be equal to DN 2 CO 2. Now if we substitute that we will obtain the flux is 3 minus 3.21 into 10 to the power minus 7 kilo mole per meter square second. So, the molar flow rate we can calculate using similar way minus 321 into 10 to the power minus 7 kilo mole per meter square second into 1.96 into 10 to the power minus 3 meter square which would be equal to minus 6.29 into 10 to the power minus 10 kilo mole per meter square second. So, this proves that the mutual diffusivities for the flux for both the components for equimolar counter diffusions are same.

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For non equimolar counter diffusion in many situation A and B molecules diffuse in opposite directions at different molar velocities like let us consider the following reactions. We can consider 2 A plus B is equal to 2 C. So, in this case when one mole of B diffuses towards A and two moles of A diffuse in opposite direction we can write N A is equal to minus N B by 2. So, from these we can calculate the flux of different components using this relations. So, thank you for hearing this lectures and in the next lecture we will discuss on the diffusion mass transfer for non uniform geometries.

Thank you very much.