Mass Transfer Operations - I

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Diffusion Mass Transfer - II

Lecture – 07

Gas Phase Diffusion Coefficient prediction and liquid phase diffusion coefficient measurement and prediction

Welcome to the 7'th lecture on Mass Transfer Operation. In this module, we are discussing on Diffusion Mass Transfer.

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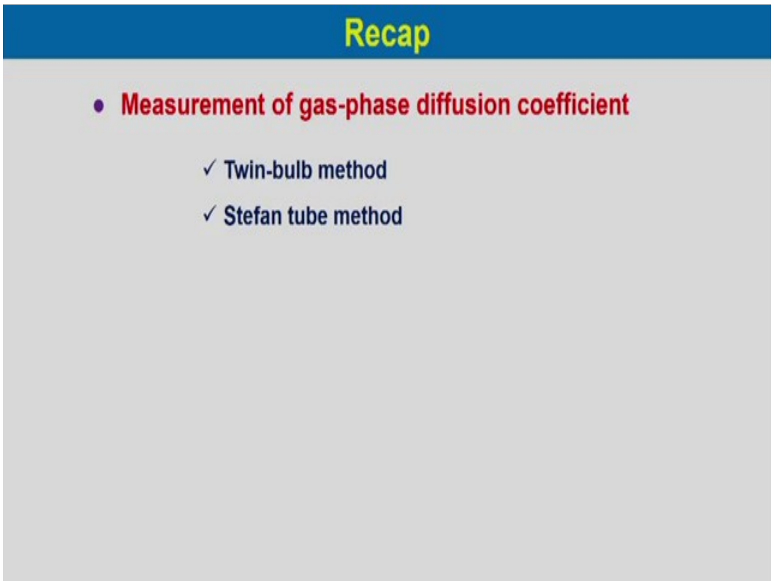

Recap

- Measurement of gas-phase diffusion coefficient
  - ✓ Twin-bulb method
  - ✓ Stefan tube method

So, before going to the lecture let us have small recap on our previous lecture. In our previous lecture, we have discussed measurement of gas phase diffusion coefficient and under this experimental measurement of the diffusion coefficient we have considered 2 methods. The first method is Twin-bulb method and we have considered counter current diffusion for 2 components using the twin bulb method and we have solved certain problems on this method.

The second method we have considered is Stefan tube method, where we considered the diffusion of a component through non diffusing B. In this lecture we will consider 3 cases one is gas phase diffusion coefficient predictions, then we will consider liquid phase diffusion coefficient measurements and then third case we will consider the liquid phase diffusion coefficient prediction.

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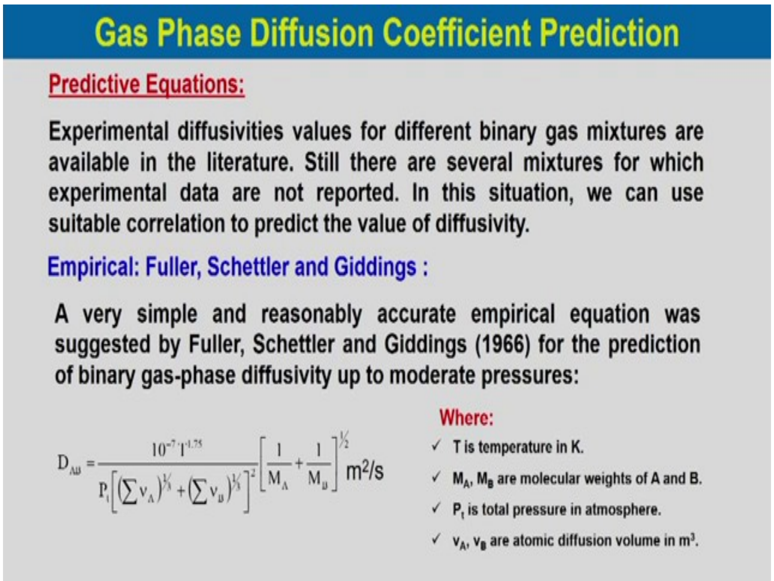

Gas Phase Diffusion Coefficient Prediction

Predictive Equations:

Experimental diffusivities values for different binary gas mixtures are available in the literature. Still there are several mixtures for which experimental data are not reported. In this situation, we can use suitable correlation to predict the value of diffusivity.

Empirical: Fuller, Schettler and Giddings :

A very simple and reasonably accurate empirical equation was suggested by Fuller, Schettler and Giddings (1966) for the prediction of binary gas-phase diffusivity up to moderate pressures:

$$D_{AB} = \frac{10^{-7} T^{1.75}}{P_t\left[\left(\sum v_A\right)^{1/3} + \left(\sum v_B\right)^{1/3}\right]^2}\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} \text{ m}^2/\text{s}$$

Where:

- ✓ T is temperature in K.
- ✓ M_A, M_B are molecular weights of A and B.
- ✓ P_t is total pressure in atmosphere.
- ✓ v_A, v_B are atomic diffusion volume in m^3.

The first one is gas phase diffusion coefficient prediction. Predictive equations basically in many situations we have experimental diffusivities values for binary gas mixtures and that are available in the literature, but still there are several mixtures for which experimental data are not reported. So, in this situation we can use suitable correlation to predict the value of diffusivity. These which values the predictive equations which are obtained from the predictive equation is based on some relations which is developed for different system based on the variation of the temperature pressure of the systems or the molecular weight of the components or their molecular volumes, so based on that these equations the predictive equations are proposed.

One of the empirical relations is Fuller equations. So, a very simple and reasonably accurate empirical equations which was proposed by Fuller et al in 1966 for the prediction of binary gas phase diffusivity which is up to moderate pressure which is D AB would be equal to 10 to the power minus 7 T to the power 1.75 divided by Pt total pressure and then multiplied by summation over VA to the power 1 3rd plus summation over VB to the power one-third whole square into 1 by MA plus 1 by MB to the power half metre square per second. D AB is the diffusion coefficient of component A into component B mutual diffusivities, where T is the temperature in Kelvin MA and MB are the molecular weights of component A and B, Pt is the total pressure in atmosphere and VA VB are the atomic diffusion volumes that is in metre cube.

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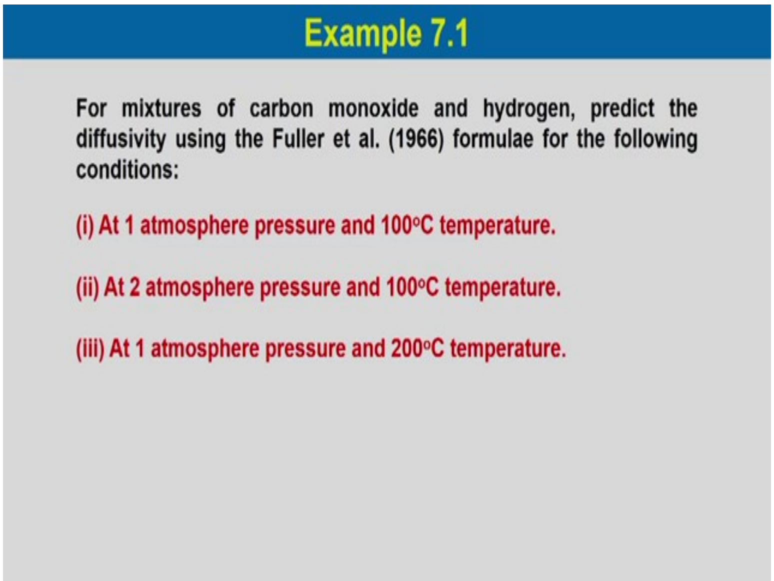

Example 7.1

For mixtures of carbon monoxide and hydrogen, predict the diffusivity using the Fuller et al. (1966) formulae for the following conditions:

(i) At 1 atmosphere pressure and 100°C temperature.

(ii) At 2 atmosphere pressure and 100°C temperature.

(iii) At 1 atmosphere pressure and 200°C temperature.

Now, let us take an example to calculate that diffusion coefficient for mixtures of carbon monoxide and hydrogen, we need to predict the divisibility using Fuller et al 1966 formula for the following conditions. At 1 atmosphere pressure and 100 degree centigrade temperature the second case is at 2 atmosphere pressure and 100 degree centigrade temperature that means the temperature kept constant and pressure is doubled.

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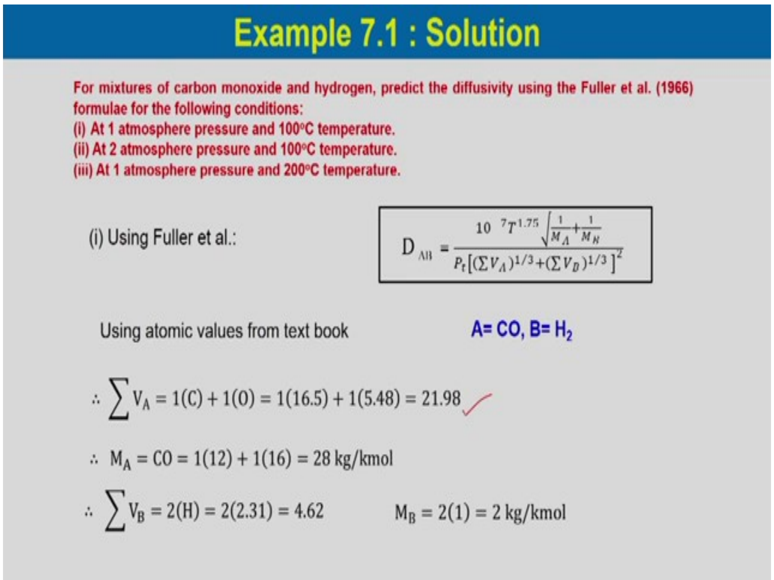

Example 7.1 : Solution

For mixtures of carbon monoxide and hydrogen, predict the diffusivity using the Fuller et al. (1966) formulae for the following conditions:
(i) At 1 atmosphere pressure and 100°C temperature.
(ii) At 2 atmosphere pressure and 100°C temperature.
(iii) At 1 atmosphere pressure and 200°C temperature.

(i) Using Fuller et al.:

$$\boxed{D_{AB} = \frac{10^{\ 7} T^{1.75}\sqrt{\frac{1}{M_A}+\frac{1}{M_B}}}{P_t\left[(\Sigma V_A)^{1/3}+(\Sigma V_B)^{1/3}\right]^2}}$$

Using atomic values from text book

A= CO, B= H_2

$$\therefore \sum V_A = 1(C) + 1(0) = 1(16.5) + 1(5.48) = 21.98 \checkmark$$

$$\therefore M_A = CO = 1(12) + 1(16) = 28 \text{ kg/kmol}$$

$$\therefore \sum V_B = 2(H) = 2(2.31) = 4.62 \qquad M_B = 2(1) = 2 \text{ kg/kmol}$$

In the third case is at 1 atmosphere pressure and at 200 degree centigrade temperature, in this case compare to the first problem the pressure remains constant and temperature is doubled. Now let us solve this. So, Fuller equations you know D AB would be equal to 10 to the power minus 7 T to the power 1.5 into root over 1 by MA plus 1 by MB whole divided by Pt whole into summation over VA to the power 1 3rd plus VB to the power one-third whole square. Now using no values from the textbook we can calculate or the data would be given consider component A is carbon monoxide and component B is hydrogen.

So, if we wanted to calculate summation over VA which is carbon monoxide would be equal to 1 into the volume of carbon plus 1 into the atomic volume of oxygen. So, it would be equal to 1 into 16.5 plus 1 into 5.48 so it would be equal to 21.98. So, the molar volume is calculated for component A and its molecular weight MA is equal to CO component CO would be equal to 1 into 12 molecular weight of carbon plus 1 into molecular weight of oxygen 16 which is 28 kg per kmol. Similarly, for component B we can calculate summation over VB would be equal to 2H which is hydrogen would be equal to 2 into 2.31 would be equal to 4.62 and the molecular weight of hydrogen would be MB would be equal to 2 into 1 is equal to 2 kg per kmol.

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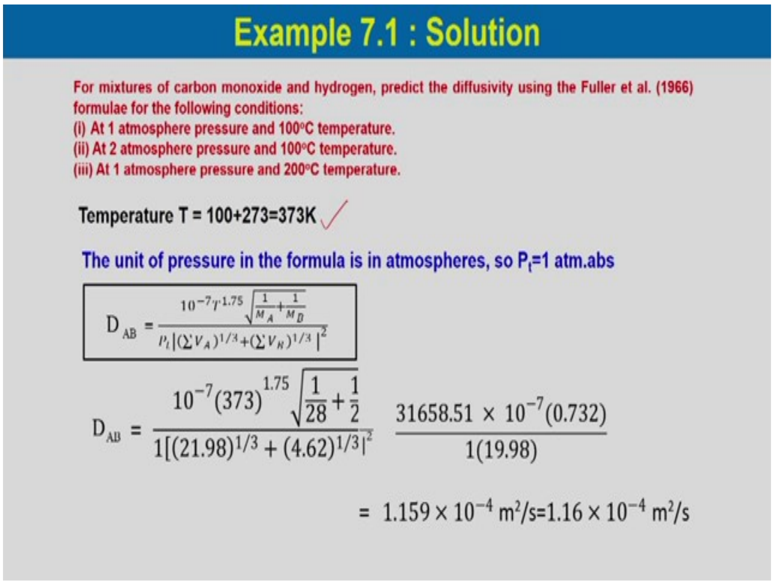

Example 7.1 : Solution

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(i) At 1 atmosphere pressure and 100°C temperature.
(ii) At 2 atmosphere pressure and 100°C temperature.
(iii) At 1 atmosphere pressure and 200°C temperature.

Temperature T = 100+273=373K ✓

The unit of pressure in the formula is in atmospheres, so P_t=1 atm.abs

$$\boxed{D_{AB} = \frac{10^{-7}T^{1.75}\sqrt{\frac{1}{M_A}+\frac{1}{M_B}}}{P_t|(\sum V_A)^{1/3}+(\sum V_B)^{1/3}|^2}}$$

$$D_{AB} = \frac{10^{-7}(373)^{1.75}\sqrt{\frac{1}{28}+\frac{1}{2}}}{1[(21.98)^{1/3}+(4.62)^{1/3}|^2} \quad \frac{31658.51 \times 10^{-7}(0.732)}{1(19.98)}$$

$$= 1.159 \times 10^{-4}\ m^2/s = 1.16 \times 10^{-4}\ m^2/s$$

Now, temperature is given for problem 1 a temperature is 100 degree centigrade. So, we can just add 273 to get Kelvin in terms of Kelvin T would be equal to 100 plus 273 would be equal to 373 Kelvin. So, temperature is calculated and the unit of pressure in the formula is in atmosphere, so Pt would be equal to 1 atmosphere absolute.

So, if we substitute the values which we have calculated for no temperature molecular weight of component A and component B total pressure and then the molecular volume of component A and component B in this Fuller equations, we can able to calculate the value is for D AB. So, which would be equal to 1.159 into 10 to the power minus 4 metre square per second; so this is the diffusivity of gaseous component.

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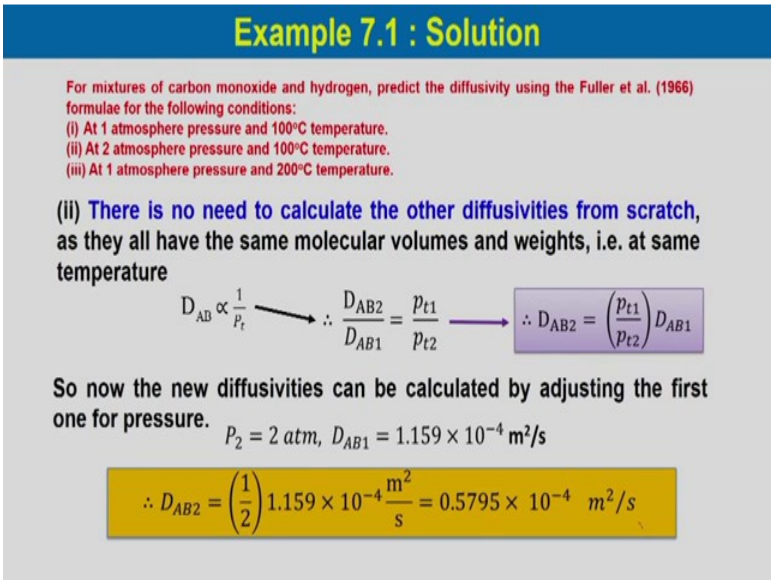

Example 7.1 : Solution

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(i) At 1 atmosphere pressure and 100°C temperature.
(ii) At 2 atmosphere pressure and 100°C temperature.
(iii) At 1 atmosphere pressure and 200°C temperature.

(ii) There is no need to calculate the other diffusivities from scratch, as they all have the same molecular volumes and weights, i.e. at same temperature

$$D_{AB} \propto \frac{1}{P_t} \longrightarrow \therefore \frac{D_{AB2}}{D_{AB1}} = \frac{p_{t1}}{p_{t2}} \longrightarrow \boxed{\therefore D_{AB2} = \left(\frac{p_{t1}}{p_{t2}}\right) D_{AB1}}$$

So now the new diffusivities can be calculated by adjusting the first one for pressure. $P_2 = 2\,atm,\ D_{AB1} = 1.159 \times 10^{-4}\ \mathrm{m^2/s}$

$$\boxed{\therefore D_{AB2} = \left(\frac{1}{2}\right) 1.159 \times 10^{-4} \frac{\mathrm{m^2}}{\mathrm{s}} = 0.5795 \times 10^{-4}\ m^2/s}$$

Now, for the second problem when we change the pressure from 1 atmosphere to 2 atmosphere keeping the temperature constant at 100 degree centigrade, we need not to calculate from the scratch. If we know the relations between the diffusivity and the pressure we can have the data at 1 atmosphere pressure and 100 degree centigrade, since their molecular volume and weights are same and at the same temperature we can use the formula D AB proportional to 1 by Pt.

So, if we use that formula we can write D AB 2 by D AB 1 would be equal to Pt 1 by Pt 2. So, D AB 1 is the diffusivity which is calculated at a particular temperature and pressure that is at temperature t 1 and then pressure p 1 and then the D AB 2 is at the same temperature and pressure at Pt 2.

So, D AB 2 would be equal to Pt 1 by Pt 2 into D AB 1. So, if we substitute diffusivities using the first one then we can get p 2 is 2 atmosphere and D AB 1 would be equal to 1.159 into 10 to the power minus 4 metre square per second. Now if we substitute that it would be half into 1.159 into 10 to the power minus 4 metre square per second, which would be 0.5795 into 10 to the power minus 4 metre square per second.

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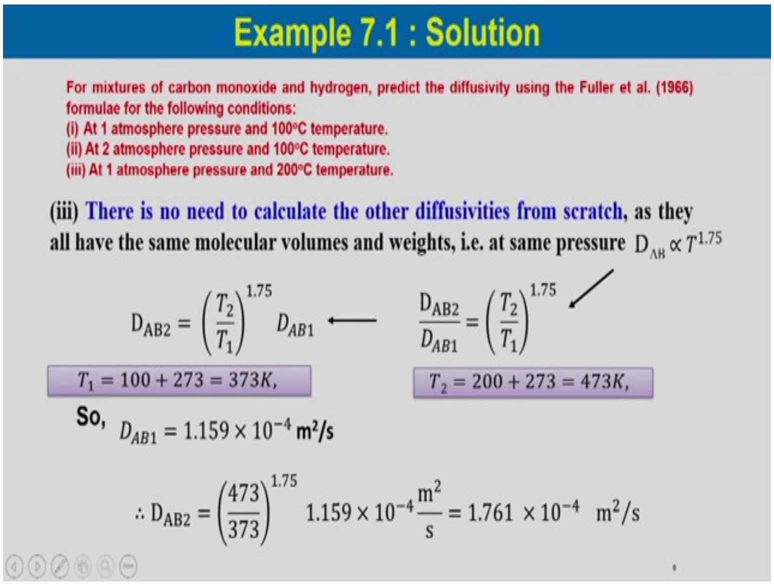

Example 7.1 : Solution

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(i) At 1 atmosphere pressure and 100°C temperature.
(ii) At 2 atmosphere pressure and 100°C temperature.
(iii) At 1 atmosphere pressure and 200°C temperature.

(iii) There is no need to calculate the other diffusivities from scratch, as they all have the same molecular volumes and weights, i.e. at same pressure $D_{AB} \propto T^{1.75}$

$$D_{AB2} = \left(\frac{T_2}{T_1}\right)^{1.75} D_{AB1} \longleftarrow \frac{D_{AB2}}{D_{AB1}} = \left(\frac{T_2}{T_1}\right)^{1.75}$$

$T_1 = 100 + 273 = 373K,$

$T_2 = 200 + 273 = 473K,$

So, $D_{AB1} = 1.159 \times 10^{-4}$ m²/s

$$\therefore D_{AB2} = \left(\frac{473}{373}\right)^{1.75} 1.159 \times 10^{-4} \frac{\text{m}^2}{\text{s}} = 1.761 \times 10^{-4} \ \text{m}^2/\text{s}$$

Now, in case of the third problem which is at 1 atmosphere pressure and 200 degree centigrade temperature in this case the pressure remain constant and but the temperature is doubled. So, in this case as well we need to use the temperature correlations between the diffusivity and then we can calculate from the first one. So, that is why there is no need to calculate the other diffusivities from scratch as they all have the same molecular volumes and weights and that is at same pressure, we can write D AB proportional to T to the power 1.75. So, we can write D AB 2 by D AB 1 would be equal to T2 by T1 to the power 1.75.

Now, if we substitute the values T2 and T1 and then D AB 1 we can get D AB 2. So, which is T1 is 273 Kelvin and T2 is 200 is 473 Kelvin. Now if we substitute D AB 1 already we have calculated 1.159 into 10 to the power minus 4 metre square per second, we can calculate D AB 2 would be equal to 1.761 into 10 to the power minus 4 metre square per second.

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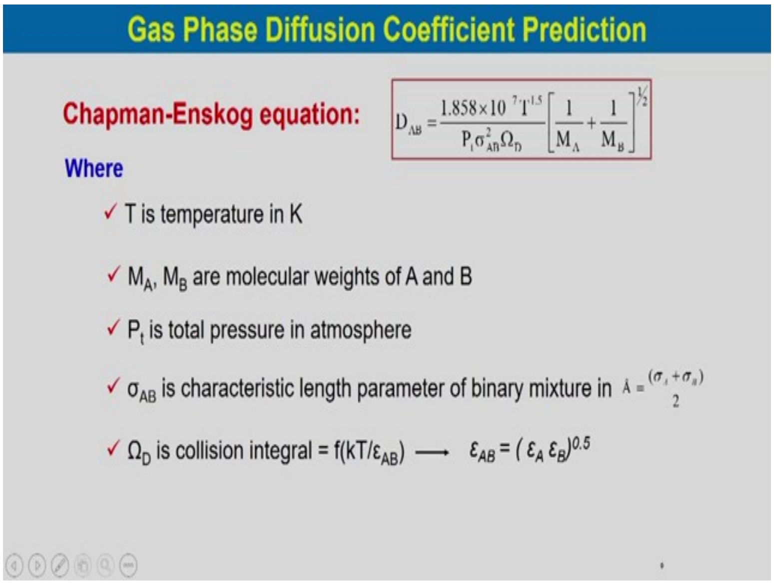

Gas Phase Diffusion Coefficient Prediction

Chapman-Enskog equation: $D_{AB} = \frac{1.858\times10^{-7}T^{1.5}}{P_t\sigma_{AB}^2\Omega_D}\left[\frac{1}{M_A}+\frac{1}{M_B}\right]^{1/2}$

Where

- ✓ T is temperature in K
- ✓ M_A, M_B are molecular weights of A and B
- ✓ P_t is total pressure in atmosphere
- ✓ σ_{AB} is characteristic length parameter of binary mixture in Å $= \frac{(\sigma_A+\sigma_B)}{2}$
- ✓ Ω_D is collision integral = $f(kT/\varepsilon_{AB}) \longrightarrow \varepsilon_{AB} = (\varepsilon_A\,\varepsilon_B)^{0.5}$

Now, we will discuss the gas phase diffusion coefficient prediction. Chapman equation in this equation basically D AB is equal to 1.858 into 10 to the power minus 7 T to the power 1.5 divided by Pt sigma AB square zeta D into 1 by MA plus 1 by MB to the power half. In this case T is the temperature in Kelvin MA and MB are molecular weights of A and B, Pt is the total pressure in atmosphere, sigma AB is the characteristics length parameter of a binary mixture in angstrom which is sigma A plus sigma B by 2, theta D is collision integral is equal to function of KT divided by epsilon AB. So, this is we can write from here it is epsilon A epsilon B to the power 0.5.

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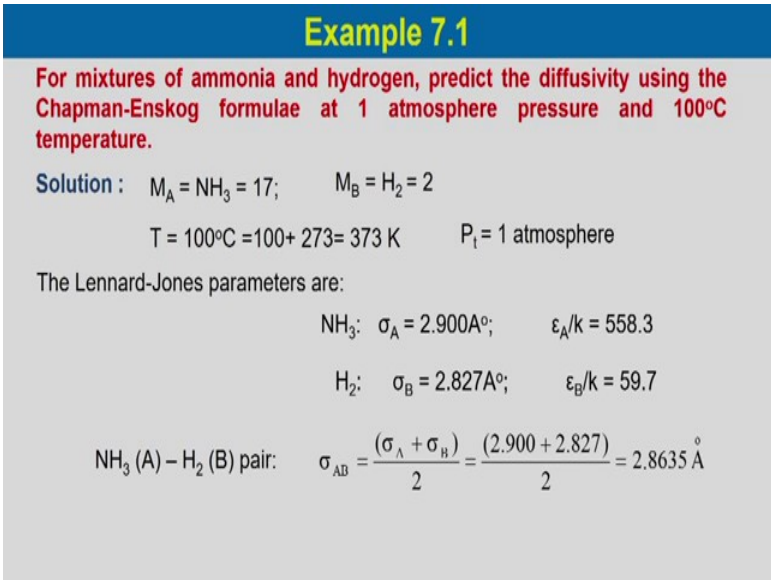

Example 7.1

For mixtures of ammonia and hydrogen, predict the diffusivity using the Chapman-Enskog formulae at 1 atmosphere pressure and 100°C temperature.

Solution : $M_A = NH_3 = 17$; $M_B = H_2 = 2$

$T = 100°C = 100 + 273 = 373$ K $P_t = 1$ atmosphere

The Lennard-Jones parameters are:

NH_3: $\sigma_A = 2.900$A°; $\varepsilon_A/k = 558.3$

H_2: $\sigma_B = 2.827$A°; $\varepsilon_B/k = 59.7$

NH_3 (A) – H_2 (B) pair: $\sigma_{AB} = \frac{(\sigma_A+\sigma_B)}{2} = \frac{(2.900+2.827)}{2} = 2.8635\,\text{Å}$

Now, for mixture of ammonia and hydrogen predict the diffusivity using the Chapman formula at 1 atmosphere pressure and 100 degree centigrade temperature.

So, MA is the molecular weight of ammonia we can write 17 and MB is hydrogen so molecular weight is 2 temperature is 100 degree centigrade. So, which is equal to 373 Kelvin pressure is 1 atmosphere total pressure.

The Lennard Jones parameter are given for ammonia sigma is equal to 2.9 angstrom and epsilon A by K would be equal to 558.3 sigma B is 2.87 angstrom and epsilon B by K would be equal to 59.7. So, now for ammonia hydrogen pair we can calculate sigma AB would be equal to sigma A plus sigma B by 2 would be equal to 2.900 plus 2.827 divided by 2 which would be equal to 2.8635 angstrom.

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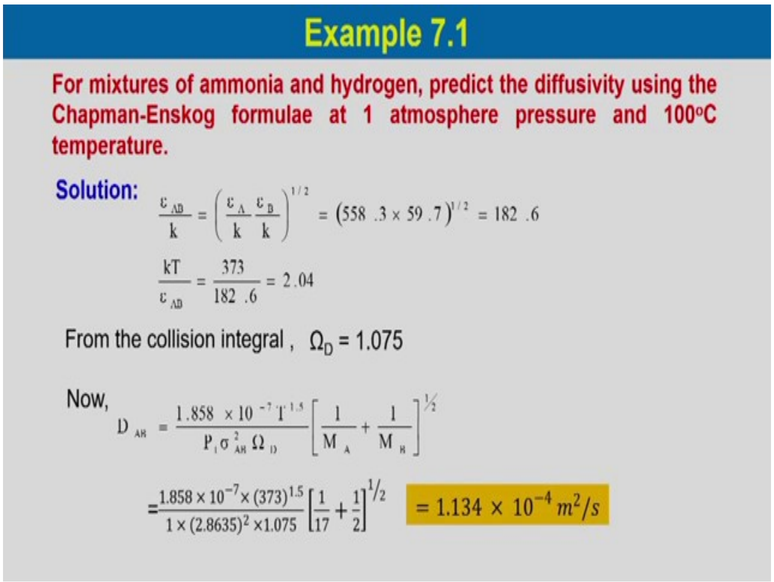

Example 7.1

For mixtures of ammonia and hydrogen, predict the diffusivity using the Chapman-Enskog formulae at 1 atmosphere pressure and 100°C temperature.

Solution:

$$\frac{\varepsilon_{AB}}{k} = \left(\frac{\varepsilon_A}{k}\frac{\varepsilon_B}{k}\right)^{1/2} = (558.3 \times 59.7)^{1/2} = 182.6$$

$$\frac{kT}{\varepsilon_{AB}} = \frac{373}{182.6} = 2.04$$

From the collision integral , $\Omega_D = 1.075$

Now,

$$D_{AB} = \frac{1.858 \times 10^{-7} T^{1.5}}{P_t \sigma_{AB}^2 \Omega_D}\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2}$$

$$= \frac{1.858 \times 10^{-7} \times (373)^{1.5}}{1 \times (2.8635)^2 \times 1.075}\left[\frac{1}{17} + \frac{1}{2}\right]^{1/2} \quad = 1.134 \times 10^{-4}\, m^2/s$$

Now, epsilon AB by K would be equal to epsilon A by K into epsilon B by K to the power half, if we substitute the values we will get it is 182.6, KT by epsilon A we can then calculate 373 divided by 182.6 which would be equal to 2.04. Now collision integral would be equal to 1.075, so if we substitute the parameters in this equation Chapman equation we can obtain the diffusion coefficient as 1.134 into 10 to the power minus 4 metre square per second.

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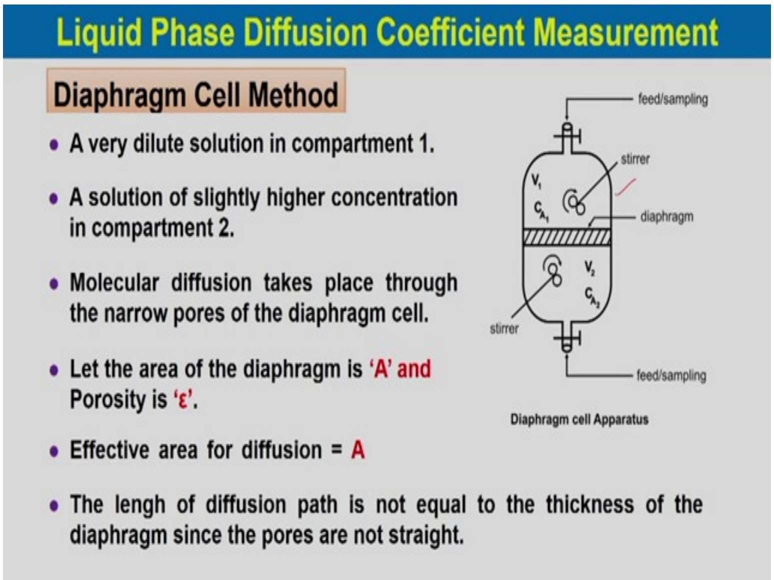

Liquid Phase Diffusion Coefficient Measurement

Diaphragm Cell Method

- A very dilute solution in compartment 1.
- A solution of slightly higher concentration in compartment 2.
- Molecular diffusion takes place through the narrow pores of the diaphragm cell.
- Let the area of the diaphragm is 'A' and Porosity is 'ε'.
- Effective area for diffusion = A
- The lengh of diffusion path is not equal to the thickness of the diaphragm since the pores are not straight.

Diaphragm cell Apparatus

Now, we will discuss the, another topic liquid phase diffusion coefficient measurements. The first method which we will discuss is the Diaphragm Cell Method that is how we measure the diffusion coefficient in the liquid phase. A very dilute solution is taken in compartment 1, so the top part of this (Refer Time: 16:48) is compartment 1 and a very dilute solution are taken over here.

A solution of slightly higher concentration in compartment 2 molecular diffusion takes place through the narrow pores of the diaphragm cell, so there is a diaphragm at the middle from through his the molecular diffusion takes place of the components. Let the area of the diaphragm is A and the porosity is epsilon the effective area for diffusion is A, the length of diffusion path is not equal to the thickness of the diaphragm since the pores are not straight.

So, basically if we take a diaphram from the path of the diffusion or the pores inside the diaphragm are not a straight channel it is a tortuous channel and the length that is why which should not be equal to the thickness of the diaphragm.

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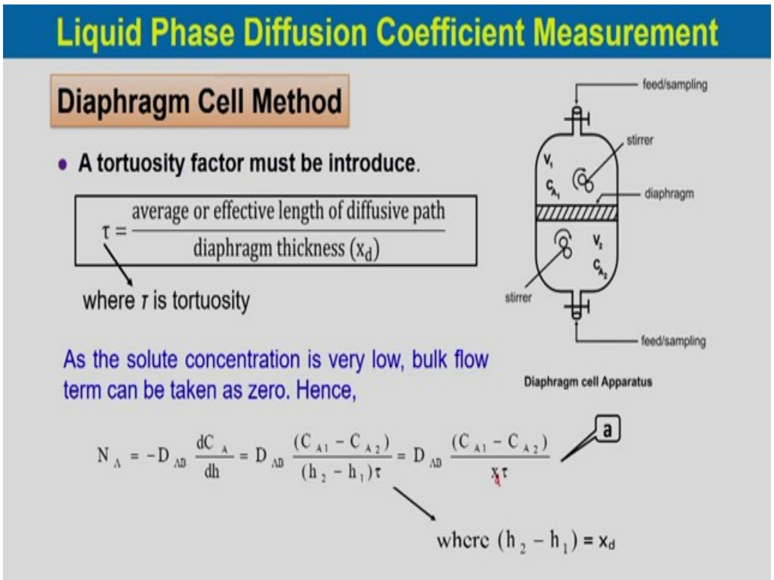

Liquid Phase Diffusion Coefficient Measurement

Diaphragm Cell Method

- A tortuosity factor must be introduce.

$$\boxed{\tau = \frac{\text{average or effective length of diffusive path}}{\text{diaphragm thickness } (x_d)}}$$

where τ is tortuosity

As the solute concentration is very low, bulk flow term can be taken as zero. Hence,

$$N_A = -D_{AB}\frac{dC_A}{dh} = D_{AB}\frac{(C_{A1} - C_{A2})}{(h_2 - h_1)\tau} = D_{AB}\frac{(C_{A1} - C_{A2})}{x_d\tau} \quad \boxed{a}$$

where $(h_2 - h_1) = x_d$

Diaphragm cell Apparatus

So, a tortuosity factor must be introduced in this, so to calculate that tau tortuosity factor would be equal to average or effective length of diffusive path divided by the diaphragm thickness, so tau is the tortuosity. As the solute concentration is very low bulk flow term can be taken as 0 and hence we can write Na would be equal to that is the flux of component a would be equal to minus D AB dC A dh which would be equal to D AB into the concentration gradient C A1 minus C A2 divided by h 2 minus h 1 into tau, we can write this would be equal to D AB C A1minus C A2 divided by X d into tau, where h 2 minus h 1 is X d let call this equation as equation a.

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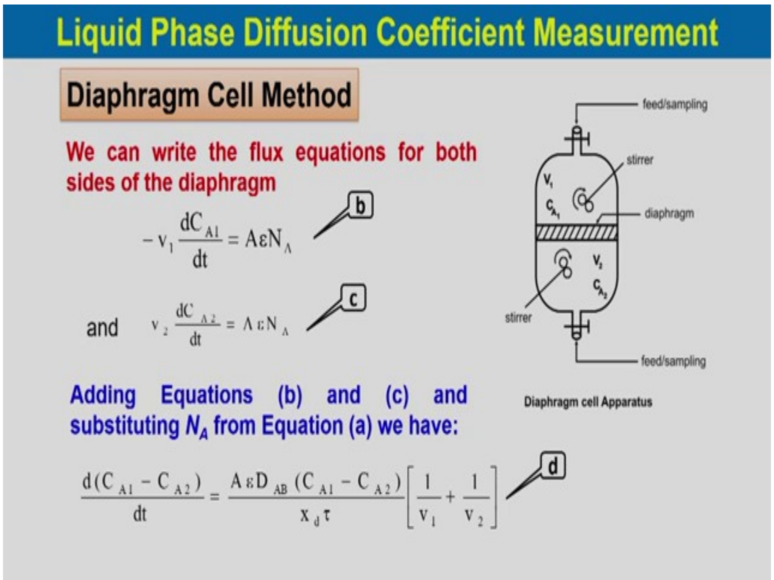

Liquid Phase Diffusion Coefficient Measurement

Diaphragm Cell Method

We can write the flux equations for both sides of the diaphragm

$$-v_1\frac{dC_{A1}}{dt} = A\varepsilon N_A \quad \boxed{b}$$

and $$v_2\frac{dC_{A2}}{dt} = A\varepsilon N_A \quad \boxed{c}$$

Adding Equations (b) and (c) and substituting N_A from Equation (a) we have:

$$\frac{d(C_{A1} - C_{A2})}{dt} = \frac{A\varepsilon D_{AB}(C_{A1} - C_{A2})}{x_d\tau}\left[\frac{1}{v_1} + \frac{1}{v_2}\right] \quad \boxed{d}$$

Diaphragm cell Apparatus

We can write the flux equation for both sides of the diaphragm as follows, for cell 1 it is minus v 1 dC A1 divided by dt would be equal to A into epsilon NA this is equation b. Now for compartment 2 we can write it is volume is v 2 which would be v 2 into dC A2 dt would be equal to A epsilon NB this is for this is we can call equation c. Now if we add both equation a and b and c and then if we substitute Na from the earlier equations equation a then we can obtain the following equations, dC A1 minus dC A2 divided by dt would be equal to A epsilon D AB C A1 minus C A2 divided by X d tau whole into 1 by VA 1 plus 1 by VA 2 this is equation d.

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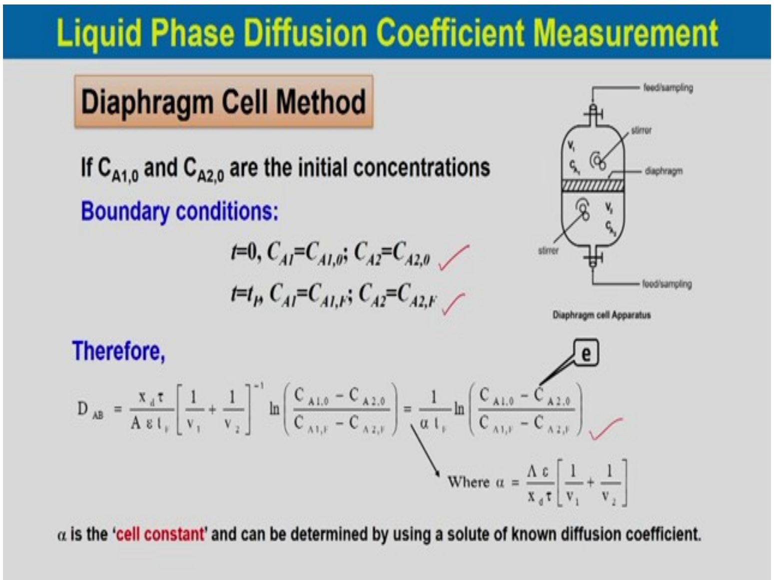

Liquid Phase Diffusion Coefficient Measurement

Diaphragm Cell Method

If $C_{A1,0}$ and $C_{A2,0}$ are the initial concentrations

Boundary conditions:

$t=0,\ C_{A1}=C_{A1,0};\ C_{A2}=C_{A2,0}$ ✓

$t=t_F,\ C_{A1}=C_{A1,F};\ C_{A2}=C_{A2,F}$ ✓

Diaphragm cell Apparatus

Therefore,

$$D_{AB}=\frac{x_d\tau}{A\varepsilon t_F}\left[\frac{1}{V_1}+\frac{1}{V_2}\right]^{-1}\ln\left(\frac{C_{A1,0}-C_{A2,0}}{C_{A1,F}-C_{A2,F}}\right)=\frac{1}{\alpha t_F}\ln\left(\frac{C_{A1,0}-C_{A2,0}}{C_{A1,F}-C_{A2,F}}\right) \quad \boxed{e} \ ✓$$

$$\text{Where } \alpha=\frac{A\varepsilon}{x_d\tau}\left[\frac{1}{V_1}+\frac{1}{V_2}\right]$$

α is the '**cell constant**' and can be determined by using a solute of known diffusion coefficient.

Now, if C A1 0 and C A2 0 are the initial concentration, then we can write the boundary conditions for this at t is equal to 0 C A 1 would be C A naught and C A2 would be C A2 naught, at t is equal to tf C A1 would be C A1 F and C A2 would C A2 F. So, these are the 2 boundary conditions we will obtain at time is equal to 0 and time is equal to tf.

So, using these 2 boundary condition if we integrate equation d as we have derived before we will obtain equation e like this, D AB would be equal to X d tau by A epsilon tf whole into 1 by v 1 plus 1 by v 2 inverse into ln C A1 naught minus C A 2 naught divided by C A 1 F minus A 2 F. So, we can simplify this is equal to 1 by alpha tf ln C A 1 naught minus C A 2 naught divided by C A 1 F minus C A 2 F. So, this is the final equations where alpha is equal to A epsilon divided by Xd tau into one by v 1 plus 1 by v

2. So, alpha is the cell constant and can be determined by using a solute of non diffusion coefficient.

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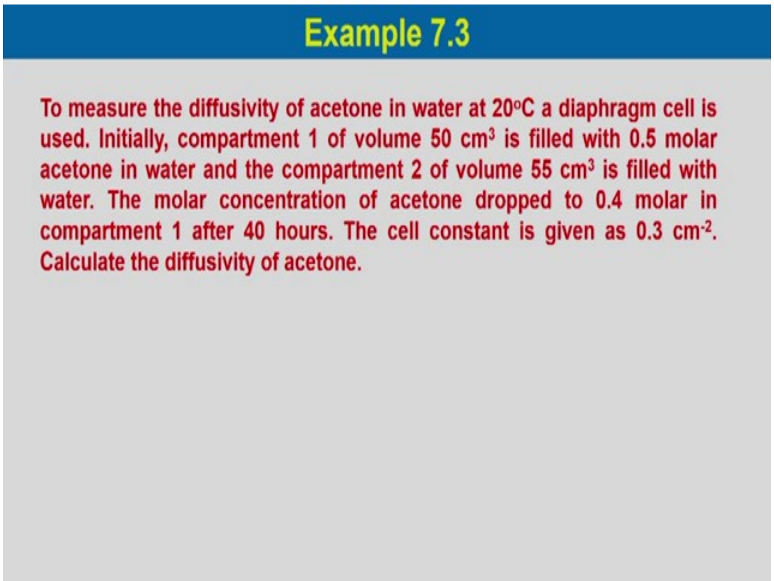

Example 7.3

To measure the diffusivity of acetone in water at 20°C a diaphragm cell is used. Initially, compartment 1 of volume 50 cm^3 is filled with 0.5 molar acetone in water and the compartment 2 of volume 55 cm^3 is filled with water. The molar concentration of acetone dropped to 0.4 molar in compartment 1 after 40 hours. The cell constant is given as 0.3 cm^{-2}. Calculate the diffusivity of acetone.

Now, let us take an example to measure the diffusivity of acetone in water at 20 degree centigrade a diaphragm cell is used, initially compartment one of volume 50 centimetre cube is filled with 0.5 molar acetone in water and the compartment 2 of volume 55 centimetre cube is filled with water. The molar concentration of acetone dropped 2.5 molar in compartment one after 40 hours, the cell constant is given as 0.3 per centimetre square now we need to calculate the diffusivity of acetone.

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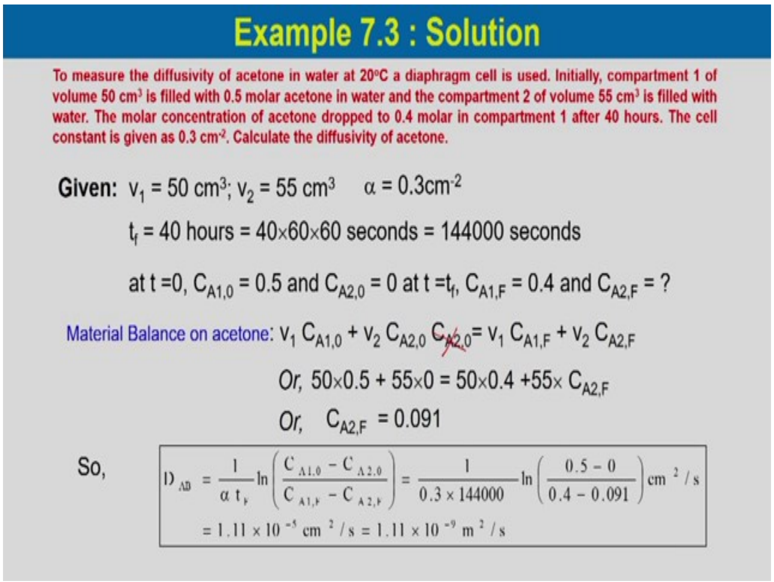

Example 7.3 : Solution

To measure the diffusivity of acetone in water at 20°C a diaphragm cell is used. Initially, compartment 1 of volume 50 cm^3 is filled with 0.5 molar acetone in water and the compartment 2 of volume 55 cm^3 is filled with water. The molar concentration of acetone dropped to 0.4 molar in compartment 1 after 40 hours. The cell constant is given as 0.3 cm^{-2}. Calculate the diffusivity of acetone.

Given: $v_1 = 50\ cm^3;\ v_2 = 55\ cm^3 \quad \alpha = 0.3 cm^{-2}$

$t_f = 40$ hours $= 40 \times 60 \times 60$ seconds $= 144000$ seconds

at $t = 0$, $C_{A1,0} = 0.5$ and $C_{A2,0} = 0$ at $t = t_f$, $C_{A1,F} = 0.4$ and $C_{A2,F} = ?$

Material Balance on acetone: $v_1 C_{A1,0} + v_2 C_{A2,0} \cancel{C_{A2,0}} = v_1 C_{A1,F} + v_2 C_{A2,F}$

Or, $50 \times 0.5 + 55 \times 0 = 50 \times 0.4 + 55 \times C_{A2,F}$

Or, $C_{A2,F} = 0.091$

So,

$$\boxed{\begin{aligned} D_{AB} &= \frac{1}{\alpha t_F} \ln\left(\frac{C_{A1,0} - C_{A2,0}}{C_{A1,F} - C_{A2,F}}\right) = \frac{1}{0.3 \times 144000} \ln\left(\frac{0.5 - 0}{0.4 - 0.091}\right) cm^2/s \\ &= 1.11 \times 10^{-5}\ cm^2/s = 1.11 \times 10^{-9}\ m^2/s \end{aligned}}$$

So, the data which are given V1 50 centimetre cube V2 55 centimetre cube then alpha cell constant is 0.3 per centimetre square, then time of operations is tf which is forty hours we can calculate in terms of second. So, it is 144000 seconds at t is equal to 0 C A 1 naught is given is equal to 0.5 and C A 2 naught is equal to 0 at t is equal to tf C A 1 F is equal to 0.4 and C A 2 F we need to find out. The C A 2 naught equal to 0 at t is equal to 0 because, the water in one side is pure water and it does not contain any acetone. So, C A 2 naught at t is equal to 0 is equal which is equal to 0.

Now if we do the material balance on acetone we can write V1 C A1 naught plus V2 C A 2 naught would be equal to V1 C A 1 F plus V2 C A 2 F. So, if we substitute the values from the no data which are given we can calculate C AF C A 2 F which is equal to 0.091. Now all other values are know if we substitute over here in this equation D AB would be equal to 1 by alpha t F ln C A C A naught C A 1 naught minus C A 2 naught divided by C A 1 F minus C A 2 F. So, if we substitute those values it would be equal to 1.11 into 10 to the power minus 9 metre square per second.

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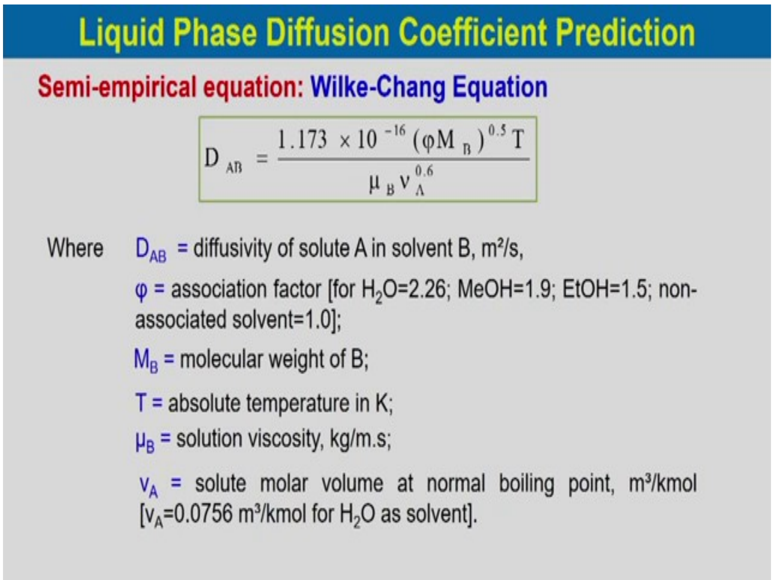

Liquid Phase Diffusion Coefficient Prediction

Semi-empirical equation: Wilke-Chang Equation

$$D_{AB} = \frac{1.173 \times 10^{-16} (\varphi M_B)^{0.5} T}{\mu_B v_A^{0.6}}$$

Where D_{AB} = diffusivity of solute A in solvent B, m²/s,

φ = association factor [for H_2O=2.26; MeOH=1.9; EtOH=1.5; non-associated solvent=1.0];

M_B = molecular weight of B;

T = absolute temperature in K;

μ_B = solution viscosity, kg/m.s;

v_A = solute molar volume at normal boiling point, m³/kmol [v_A=0.0756 m³/kmol for H_2O as solvent].

Now we will discuss the liquid phase diffusion coefficient prediction, there is a semi empirical relations which is proposed by Wilke-Chang Equations and this is the diffusion coefficient is related with 1.0 which is equal to 1.173 into 10 to the power minus s16 into phi B phi into MB to the power 0.5 into T divided by mu B VA to the power 0.6.

So, it depends on these no properties of component A and B and the temperature, D AB is the diffusivity of solute A in solvent B which is in metre square per second, phi is the association factor for water it is 2.26 and for methanol it is 1.9 for ethanol it is 1.5 and for non associated solvent it is 1, MB is the molecular weight of component B T is the absolute temperature in Kelvin, mu B is the solution viscosity which is in kg per metre second, VA is the solute molar volume at normal boiling point which is in metre cube per kmol VA is equal to 0.0756 meter cube per kmol for water as solvent.

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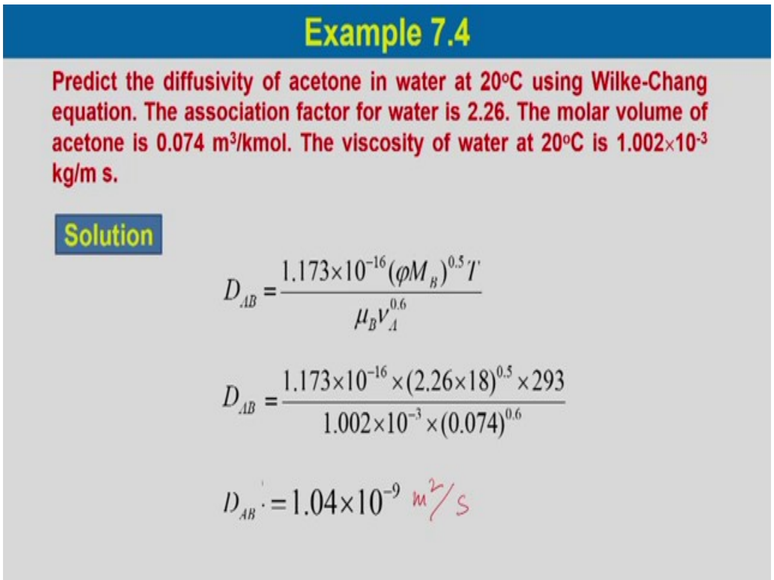

Example 7.4

Predict the diffusivity of acetone in water at 20°C using Wilke-Chang equation. The association factor for water is 2.26. The molar volume of acetone is 0.074 m³/kmol. The viscosity of water at 20°C is 1.002×10⁻³ kg/m s.

Solution

$$D_{AB} = \frac{1.173\times10^{-16}(\varphi M_B)^{0.5}T}{\mu_B V_A^{0.6}}$$

$$D_{AB} = \frac{1.173\times10^{-16}\times(2.26\times18)^{0.5}\times293}{1.002\times10^{-3}\times(0.074)^{0.6}}$$

$$D_{AB} = 1.04\times10^{-9}\ m^2/s$$

Now, let us take an example predict the diffusivity of acetone in water at 20 degree centigrade using Wilke-Chang equation, the association factor for water is 22.26. The molar volume of acetone is 0.074 metre cube per k mole the viscosity of water at twenty degree centigrade is 1.002 into 10 to the power minus 3 kg per metre second. The equations is known to us the Wilke-Chang equation, now the data which are given if you substitute over here we will obtain the diffusivity of acetone in water D AB would be equal to 1.04 into 10 to the power minus 9 metre square per second.

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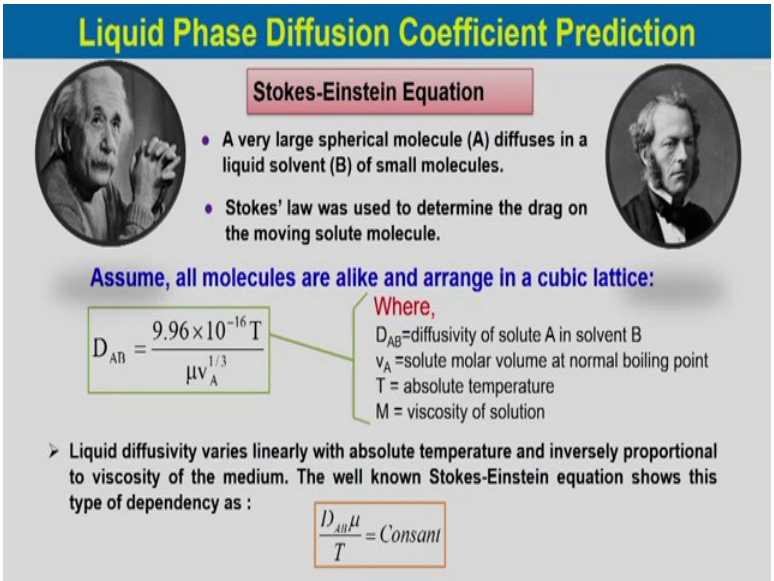

Liquid Phase Diffusion Coefficient Prediction

Stokes-Einstein Equation

- A very large spherical molecule (A) diffuses in a liquid solvent (B) of small molecules.
- Stokes' law was used to determine the drag on the moving solute molecule.

Assume, all molecules are alike and arrange in a cubic lattice:

$$D_{AB} = \frac{9.96\times10^{-16}T}{\mu V_A^{1/3}}$$

Where,

D_{AB}=diffusivity of solute A in solvent B

V_A =solute molar volume at normal boiling point

T = absolute temperature

M = viscosity of solution

- Liquid diffusivity varies linearly with absolute temperature and inversely proportional to viscosity of the medium. The well known Stokes-Einstein equation shows this type of dependency as :

$$\frac{D_{AB}\mu}{T} = Consant$$

Now, there is another equations is known as the Stokes Einstein Equation, a very large spherical molecule A diffuses in liquid solvent B of small molecules, in this case the stokes law was used to determine the track on the moving solute molecules. So, we assume all molecules are alike and arrange in a cubic lattice. So, the diffusivity D AB is given as 9.96 into 10 to the power minus 16 T divided by mu VA to the power one third. In this case D AB is the difficulty of solute A in solvent B VA is the solute molar volume at normal boiling point, T is the absolute temperature, M is the viscosity of solution. So, liquid viscosity varies linearly with absolute temperature we can see D AB has a linear proportional which is proportional to T directly proportional to T and it is inversely proportional to the viscosity of the solution or of the medium.

So, the well known Stokes equation shows this type of dependency as D AB mu by T is constant. So, if you just substitute because the molecular volume of component is constant, so if we multiply D AB into mu divide by the temperature which would be constant. So, this is all about the diffusion coefficient in the liquid phase prediction, there are many more liquid phase diffusion coefficient measurements equations which are not covered.

So, please refer to the different note text and reference books which are proposed to study in particular (Refer Time: 31:18) and B K Dutta's book and also Treyball's book (Refer Time: 31:22) for more further studies. Thank you very much for hearing this lecture and in the next lecture we will consider multiphase diffusion coefficient.