

Assignment MT1-2023-1

Section =1

(Based on lecture notes)

Note: 1) Use the notations used in the class whenever necessary
2) Assume Binary mixture
3) Extract and use necessary data from literature and data tables.

Q.1) Define

1. Mass average velocity
2. Molar average velocity
3. n_i and j
4. N , I and J

Q.2) Write the statement of Fick's Law and Express in mathematical terms.
Express Fick's law in terms of other fluxes.

Q.3) What is diffusivity? What are the factors which affect the diffusivity?
What is the unit of diffusivity?

Q.4) Proof $D_{AB}=D_{BA}$ (For ideal gas)

Q.5) State Ernst Einstein Equation.

Q.6) Write the equations for the following correlations to estimate gas phase diffusivity

- (1) Chapman - Enskog correlation based on KT
- (2) Fuller correlation

Q.7) Write the equations for following correlations to estimate liquid phase diffusivity

1. Stokes Einstein equation

2. Wilke Chang Equation

Q.8) Provide the relationship to estimate the gas mixture diffusivity from binary diffusivity

Q.9) Describe (1) Knudsen (pore) diffusivity (2) Knudsen number (3) values of Knudsen number for Knudsen diffusivity to occur.

Q.10) What is surface diffusivity?

Section-2

(Based on the work out problems in the textbook)

1. From book: Principle of mass transfer by B.K.Dutta Ex.2.1 Page no.10

Section=3

(Unsolved problems)

Q1. Liquified natural gas, LNG, is to be shipped from the Alaskan Kenai Peninsula by

an ocean carrier to the processing plant in Yaquina Bay, Oregon. The molar composition of the commercial LNG is

Methane, CH_4 93.5 mol %

Ethane, C_2H_6 4.6% mol %

Propane, C_3H_8 1.2% mol%

Carbon dioxide, CO_2 0.7% mol%

Determine

a. the weight fraction of ethane.

b. the average molecular weight of the LNG mixture.

- c. the density of the gas mixture when heated to 207 K and at 1.4×10^5 Pa.
- d. the partial pressure of methane when the total pressure is 1.4×10^5 Pa.
- e. the mass fraction of carbon dioxide in parts per million by weight.

Q2. Evaluate the diffusion coefficient of carbon disulfide in the air at 20°C and atmospheric pressure by Chapman-Enskog relation.

Q3. Re-evaluate the diffusion coefficient of carbon disulfide in the air at 208°C and atmospheric pressure using the Fuller, Schettler, and Giddings equation and compare the new value with the one reported in question 2. Explain intuitively the reason behind difference in the results from these relations.

Q4. In the manufacture of conductive contacts of photovoltaic materials, a thin film of solid tungsten is used as a conductive layer due its good thermal conductivity for electrical materials. The tungsten is uniformly deposited on a conductive surface by molecular epitaxy process of tungsten hexafluoride (WF_6) in presence of hydrogen gas. If the gas composition is maintained at 40 mol % WF_6 and 10 mol % H_2 and 50 mol% N_2 , determine:

- a. Calculate the Diffusivity of WF_6 in hydrogen (cm^2/s) through hirschfelder spotz relation of tungsten hexafluoride through the gas mixture at 400°C and a system pressure of 20 bar and the effective diffusivity through the gas mixture if WF_6 has a diffusivity of $0.0157 \text{ cm}^2/\text{s}$ in nitrogen.
- b. Calculate the same at 440°C and 17 bar.
- c. What is the significance of the lennard-jones parameters and are empirical correlations always valid for calculation of diffusivity, if not why not and what assumptions are made?

(Assume required constants and use atmospheric conditions if not specified)

	(σ)	ϵ/k (400°C)	ϵ/k (440°C)
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WF ₆	4.02 Å	200 K	180 K
Carrier gas (H ₂)	3.1 Å	206.1 K	195 K

Q5. Calculate the diffusivity of ethylbenzene (EB) into the water at 293K. The viscosity of water at this temperature is 1 cP and the density of ethylbenzene at normal boiling temperature is 0.761 gm/cc by Wilke Chang correlation. solute molar volume for EB is 139.5 cm³/mol. (Assume required constants and use atmospheric conditions if not specified)

(a) Compare with the experimental value of $D_{AB} = 0.81 \times 10^{-5} \text{ cm}^2/\text{sec}$ and find the deviation.

(b) Estimate the diffusivity of EB at an elevated temperature of 393 K and viscosity of 0.5 cP using the temperature-diffusivity relations.

(c) Which factor prominently affects the diffusivity in liquids and which operations in everyday life show its significance? Comment on the diffusion of NaCl crystals in water and does ionic mobility play a role in diffusion.

Q6. Diffusion of CO₂ is to be carried out through a porous membrane. The porous membrane has been characterized by scattered pore diameter sizes ranging from 0.5 nm to 9 nm in an inert nitrogen atmosphere. The conditions for the entire system are maintained at 300K and thrice the atmospheric pressure. (Assume required constants and use atmospheric conditions if not specified)

(a) Calculate the diffusivity of CO₂ with following data: Lennard-jones constants of CO₂-N₂ mixture are $(\sigma_{\text{CO}_2\text{-N}_2}) = 0.3636$, $(\epsilon/k) = 101.48 \text{ K}$

- (b) Estimate the pore diffusivity in the two extreme pore ranges and the effective diffusivity of the system.
- (c) Comment about the porous media diffusion parameters and whether they are dependent on pressure why, why not.

Q7. For the Hydrogenation of ethylene Nickel catalyst has a mean pore diameter of 100 Å.

- (a) Calculate the diffusivity of hydrogen by Chapman-Enskog relation for this catalyst in hydrogen-ethane mixture temperature 100° C, pressure 10 atm.
- (b) Calculate the diffusivity of hydrogen by Chapman-Enskog relation in the bulk medium over the catalyst surface with the following compositions 40% hydrogen, 40 % Ethylene, and 20% ethane.

Q8. For the mixture of carbon monoxide and Hydrogen, predict the diffusivity using fuller empirical relation for the following condition

- 1 atm pressure 100° C temperature.
- 2 atm pressure 100° C temperature.
- 1 atm pressure 200° C temperature.

Q9. Estimate the diffusivity of Acetone in water at 30° C and 60°C by Wilke-Chang relation.

	Molar Vol
carbon	0.0148
hydrogen	0.0037
oxygen	0.0074

Molar volume at the Normal Boiling Point (v)

Viscosity of water are 0.8007×10^{-3} (pa.s) and 0.4688×10^{-3} (pa.s) at 30°C and 60°C respectively

Q10. An absorption tower has been proposed to remove selectively two pollutants, hydrogen sulphide (H_2S) and Sulphur dioxide (SO_2), from an exhaust gas stream containing-

H_2S 3 vol %

SO_2 5 vol %

N_2 92 vol %

Estimate the diffusivity of hydrogen sulphide in the gas mixture at 350 K and 1.013×10^5 Pa.