ChE 333 Transport Phenomena III, fundamentals of Mass Transfer
Studio Worksheet #2 - Diffusion coefficient

NAME____

Studio Section	**Studio 12:00-12:50**	**Studio 13:00-13:50**	**Studio 14:00-14:50**	**Studio 15:00-15:50**

Instructions: Open book, notes, and homework. Make sure to write your name and studio on any additional sheet of paper with your solution. Show your calculation, algebraic setup, and make sure to include units. Please turn in your studio at the end of class.

Problem 1. A new gas separation process is being developed to separate ethylene (C_2H_4) from a gas mixture which contain ethylene and small amounts of carbon dioxide (CO_2), and carbon monoxide (CO). The separation process is operated at 2.0 atm and 77 °C (350 K). As part of the process analysis, the gas phase diffusion coefficient of CO gas in ethylene is needed. The amounts of CO_2 is so small that it can be ignored for the analysis of CO gas diffusion in ethylene.

From Appendix K, Table K.2, the Lennard-Jones constants for ethylene are σ_B = 4.232 Å, and ε_B/κ = 205 K and the measured diffusion coefficient for the CO-C_2H_4 binary pair is D_{AB} = 0.151 cm^2/sec at 1.0 atm and 273 K

(a) Using the Hirschfelder correlations calculate the diffusion coefficient for CO-C_2H_4 binary pair at 1.0 atm and 273 K and compare to the experimental value, discuss.

$$D_{AB} = \frac{0.001858\ T^{3/2}\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2}}{P\,\sigma_{AB}^2\,\Omega_D}$$

given T = 273 K; P = 2 atm; M_A = 28 gr/mol; M_B = 28 gr/mol

lookup

	σ_A	ϵ_A/k
CO	3.59	110 K
C_2H_4	4.232	205 K

$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = 3.911$ Å

$\epsilon_{AB}/k = \sqrt{(\epsilon_A/k)(\epsilon_B/k)} = 150.17$ K

$$T/\epsilon_{AB}/k = \frac{273\text{ K}}{150.17\text{ K}} = 1.33$$

lookup $\Omega_D = 1.267$

plug into Hirschfelder eqn. $\boxed{D_{AB} = 0.116\ cm^2/s}$

slightly lower than experimental value

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(b) For the CO-C_2H_4 binary pair, estimate the gas phase binary diffusion coefficient by the Hirschfelder correlations at the process conditions (2.0 atm and 77 ºC (350 K)) and compare that to the extrapolation of the measured diffusion coefficient to the same conditions. How much would it change if you assumed $\Omega_D(T_1) \simeq \Omega_D(T_2)$

same as above but

$$T/\varepsilon_{AB}/k = \frac{350\,K}{150.17\,K} = 2.33$$

$$\Omega_D(T) = 1.0218$$

plugging into Hirschfelder: $\boxed{D_{AB} = 0.104\ cm^2/s}$

using the experimental value

$$D_{AB}(T_2, P_2) = D(T_1, P_1)\left(\frac{P_1}{P_2}\right)\left(\frac{T_2}{T_1}\right)^{3/2}\frac{\Omega_D(T_1)}{\Omega_D(T_2)}$$

$$D_{AB}(T_2, P_2) = 0.151\left(\frac{2}{2}\right)\left(\frac{350}{273}\right)^{3/2}\frac{1.267}{1.0218} = \boxed{0.09\ cm^2/s}$$

if assume $\dfrac{\Omega_D(T_1)}{\Omega_D(T_2)} = 1$

$$\boxed{D_{AB}(T_2, P_2) = 0.109\ cm^2/s}$$

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(c) The Fuller-Schettler-Giddings correlation is often used when the Lennard-Jones parameters for the Hirschfelder are not available. The Fuller-Schettler-Gibbings correlation is shown below, were v_i is the diffusion volume from table 24-3 (see below). Use this correlation to determine the diffusion coefficient for the CO-C_2H_4 binary pair at the process conditions, how does it compare to value you found in part B.

Atomic and Structure Diffusion-Volume Increments, v_i			
C	16.5	Cl	19.5
H	1.98	S	17.0
O	5.48	Aromatic Ring	−20.2
N	5.69	Heterocyclic Ring	−20.2

Diffusion Volumes for Simple Molecules, v					
H_2	7.07	Ar	16.1	H_2O	12.7
D_2	6.70	Kr	22.8	$C(Cl_2)(F_2)$	114.8
He	2.88	CO	18.9	SF_6	69.7
N_2	17.9	CO_2	26.9	Cl_2	37.7
O_2	16.6	N_2O	35.9	Br_2	67.2
Air	20.1	NH_3	14.9	SO_2	41.1

$$D_{AB} = \frac{0.001\, T^{1.75}\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2}}{P\left[\left(\sum v_i\right)_A^{1/3}+\left(\sum v_i\right)_B^{1/3}\right]^2} \qquad (24\text{-}42)$$

$$D_{AB} = \frac{0.001\, T^{1.75}\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2}}{P\left[\left(\Sigma v_i\right)_A^{1/3}+\left(\Sigma v_i\right)_B^{1/3}\right]^2}$$

from table $V_A = 18.9$; $V_B = 2(16.5) + 4(1.98) = 40.92$

for $P = 2\text{ atm}$; $T = 273\text{K}$; $\boxed{D_{AB} = 0.131\ \text{cm}^2/\text{s}}$

$P = 2\text{ atm}$; $T = 350\text{K}$; $\boxed{D_{AB} = 0.101\ \text{cm}^2/\text{s}}$

(d) How much do the estimates of the diffusion coefficient vary with different methods and how do the compare to the experimental value ?