EXAMPLE 8

A pure nitrogen carrier gas flows parallel to the 0.6 m^2 surface of a liquid acetone in an open tank. The acetone temperature is maintained at 290 K. If the average mass-transfer coefficient, k_c, for the mass transfer of acetone into the nitrogen stream is 0.0324 m/s, determine the total rate of acetone release in units of kg.mol/s.

The total molar rate of acetone transfer from the liquid to the gas phase can be evaluated by

$$W_A = N_A A = k_c A(c_{As} - c_{A\infty})$$

The mass transfer area is specified as 0.6 m^2. At 290 K, acetone exerts a vapor pressure of 161 mmHg or 2.148×10^4 Pa. Therefore, the concentration of acetone in the gas phase at the acetone surface is

$$c_{As} = \frac{P_A}{RT} = \frac{2.148 \times 10^4 \text{ Pa}}{\left(8.314 \frac{\text{Pa} \times \text{m}^3}{\text{kg mol} \times \text{K}}\right)(290 \text{ K})} = 8.91 \frac{\text{kg mol}}{\text{m}^3}$$

and the concentration of acetone in the nitrogen carrier gas is near zero because the molar flowrate of the carrier gas is in a large excess relative to the rate of acetone transfer. Thus

$$W_A = k_c A(c_{As} - c_{A\infty}) = \left(0.0324 \frac{\text{m}}{\text{s}}\right)(0.6 \text{ m}^2)\left(8.91 \frac{\text{kg.mol}}{\text{m}^3} - 0\right) = 0.1732 \frac{\text{kg.mol}}{\text{s}}$$

24.4 CLOSURE

In this chapter, the two modes of mass transport, molecular and convective mass transfer, have been introduced. As diffusion of mass involves a multicomponent mixture, fundamental relations were presented for concentrations and velocities of the individual species as well as for the mixture. The molecular transport property, D_{AB}, the diffusion coefficient or mass diffusivity in gas, liquid, and solid systems, has been discussed and correlating equations presented.

The rate equations for the mass transfer of species A in a binary mixture are as follows:

molecular mass transfer:

$\mathbf{J}_A = -cD_{AB} \nabla y_A$	molar flux relative to the molar-average velocity
$\mathbf{j}_A = -\rho D_{AB} \nabla \omega_A$	mass flux relative to the mass-average velocity
$\mathbf{N}_A = -cD_{AB} \nabla y_A + y_A(\mathbf{N}_A + \mathbf{N}_B)$	molar flux relative to fixed spatial coordinates
$\mathbf{n}_A = -\rho D_{AB} \nabla \omega_A + \omega_A(\mathbf{n}_A + \mathbf{n}_B)$	mass flux relative to fixed spatial coordinates

convective mass transfer:

$N_A = k_c \, \Delta c_A$

PROBLEMS

24.1 Liquified natural gas, LNG, is to be shipped from the Alaskan Kenai Peninsula by an ocean carrier to processing plant on Yaquina Bay, Oregon. The molar composition of the commercial LNG is

methane, CH_4	93.5 mol %
ethane, C_2H_6	4.6%
Propane, C_3H_8	1.2%
Carbon dioxide, CO_2	0.7%

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.

24.2 In the manufacture of microelectronic devices, a thin film of solid silicon (Si) is uniformly deposited on a wafer surface by the chemical decomposition of silane (SiH_4) in the presence of H_2 gas. If the gas composition is maintained at 40 mol % SiH_4 and 60 mol % H_2, determine

a. the weight fraction of these species;

b. the average molecular weight of the gas mixture;

c. the molar concentration, c_A, of SiH_4 if the feed gas is maintained at 900 K and a system pressure of 60 torr.

24.3 Air is contained in a 30 m^3 container at 400 K and 1.013×10^5 Pa. Determine the following properties of the gas mixture:

a. mole fraction of O_2;

b. volume fraction of O_2;

c. weight of the mixture;

d. mass density of O_2;

e. mass density of N_2;

f. mass density of the air;

g. mass density of the air;

h. average molecular weight of the gas mixture.

24.4 Starting with Fick's equation for the diffusion of A through a binary mixture of species A and B as given by $N_{Az} = -cD_{AB}\frac{dy_A}{dz} + y_A(N_{Az} + N_{Bz})$ and Fick's equation for the diffusion of B through the same binary mixture given by $N_{Bz} = -cD_{BA}\frac{dy_B}{dz} + y_B(N_{Bz} + N_{Az})$, prove the two gas diffusivities, D_{AB} and D_{BA}, are equal. Does the Hirshfelder equation for gas evaluating gas diffusivities verify this same equality?

24.5 Starting with the Fick's equation for the diffusion of A through a binary mixture of components A and B

$$\mathbf{N}_A = -cD_{AB}\nabla y_A + y_A(\mathbf{N}_A + \mathbf{N}_B)$$

derive the following relations, stating the assumptions made in the derivations:

a. $\mathbf{n}_A = -D_{AB}\nabla\rho_A + w_A(\mathbf{n}_A + \mathbf{n}_B)$

b. $\mathbf{J}_A = -D_{AB}\nabla c_A$

24.6 Starting with Fick's equation for the diffusion of A through a binary mixture of A and B, prove

a. $\mathbf{N}_A + \mathbf{N}_B = c\mathbf{V}$;

b. $\mathbf{n}_A + \mathbf{n}_B = \rho\mathbf{v}$

c. $\mathbf{j}_A + \mathbf{j}_B = 0$.

24.7 Stefan and Maxwell explained the diffusion of A through B in terms of the driving force dc_A, the resistances that must overcome the molecular mass transfer, and a proportionality constant, β. The following equation expresses mathematically the resistances for an isothermal, isobaric gaseous system:

$$-dc_A = \beta\frac{\rho_A}{M_A}\frac{\rho_B}{M_B}(v_{Az} - v_{Bz})dz$$

Wilke[33] extended this theory to a multicomponent gas mixture. The appropriate form of the Maxwell-type equation was assumed to be

$$-\frac{dc_A}{dz} = \beta_{AB}\frac{\rho_A}{M_A}\frac{\rho_B}{M_B}(v_{Az} - v_{Bz}) + \beta_{AC}\frac{\rho_A}{M_A}\frac{\rho_C}{M_C}(v_{Az} - v_{Cz}) + \beta_{AD}\frac{\rho_A}{M_A}\frac{\rho_D}{M_D}(v_{Az} - v_{Dz}) + \cdots$$

Using this relation, verify equation (24-49).

[33] C. Wilke, *Chem. Eng. Prog.*, **46**, 95 (1950).

24.8 Determine the value of the following gas diffusivites using the Hirschfelder equation:

a. carbon dioxide/air at 310 K and 1.5×10^5 Pa

b. ethanol/air at 325 K and 2.0×10^5 Pa

c. carbon monoxide/air at 310 K and 1.5×10^5 Pa

d. carbon tetrachloride/air at 298 K and 1.913×10^5 Pa

24.9 The isomerization of *n*-butane to *iso*-butane is carried out on a catalyst surface at 2.0 atm and 400°C. What is the gas-phase molecular diffusion coefficient of *n*-butane in *iso*-butane? Compare values obtained from both the Hirschfelder and Fuller–Schettler–Giddings equations.

24.10 Determine the diffusivity of methane in air using (a) the Hirschfelder equation and (b) the Wilke equation for a gas mixture. The air is at 373 K and 1.5×10^5 *Pa*.

24.11 An absorption tower is proposed to remove selectively ammonia from an exhaust gas stream. Estimate the diffusivity of ammonia in air at 1.013×10^5 Pa and 373 K using the Brokaw equation (24-43). The dipole moment for ammonia is 1.46 debye. Compare the evaluated value with the experimental value reported in Appendix Table J.1.

24.12 Highly purified tetrachlorosilane ($SiCl_4$) gas is reacted with hydrogen gas (H_2) to produce electronic-grade polycrystalline silicon at 800°C and 1.5×10^5 Pa according to the equction:

$$SiCl_4(g) + 2H_2(g) \rightarrow Si(s) + 4HCl(g).$$

There are concerns that the reaction experiences diffusional limitations at the growing Si solid surface. Estimate the molecular diffusion coefficient for (a) $SiCl_4$ in H_2 and (b) $SiCl_4$ in a gas phase mixture containing 40 mol % $SiCl_4$, 40 mol % H_2, and 20 mol % HCl. The Lennard–Jones parameters for $SiCl_4$ (species A) are $\varepsilon_A/\kappa = 358$ K, $\sigma_A = 5.08$ Å

24.13 An absorption tower has been proposed to remove selectively two pollutants, hydrogen sulfide (H_2S) and sulfur 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 sulfide in the gas mixture at 350 K and 1.013×10^5 Pa. The critical temperature (T_C) of H_2S is 373.2 K and the critical volume (V_C) of H_2S is 98.5 cm^3/mol.