

Montogue

Quiz HT109

DIFFUSION MASS TRANSFER

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■ Problems

■ Problem 1.1

Using the Hirschfelder et al. equation, evaluate the diffusion coefficient of methane in air at 25°C and atmospheric pressure.

- A) $D_{AB} = 0.0981 \text{ cm}^2/\text{s}$
- B) $D_{AB} = 0.216 \text{ cm}^2/\text{s}$
- C) $D_{AB} = 0.472 \text{ cm}^2/\text{s}$
- D) $D_{AB} = 0.681 \text{ cm}^2/\text{s}$

■ Problem 1.2

Answer, without using the Hirschfelder equation again: what would the diffusion coefficient be if the temperature were doubled and the pressure were increased by 50%?

■ Problem 1.3

Repeat the calculations of Part 1 using the Fuller-Schettler-Giddings correlation.

■ Problem 2.1

Using the Hirschfelder et al. equation, determine the diffusion coefficient of hydrogen sulfide in oxygen at 25°C and a pressure of 0.1 atm.

- A) $D_{AB} = 0.349 \text{ cm}^2/\text{s}$
- B) $D_{AB} = 0.683 \text{ cm}^2/\text{s}$
- C) $D_{AB} = 1.10 \text{ cm}^2/\text{s}$
- D) $D_{AB} = 1.63 \text{ cm}^2/\text{s}$

■ Problem 2.2

Answer, without using the Hirschfelder equation again: what would the diffusion coefficient be if the temperature were doubled and the pressure were decreased by 40%?

■ Problem 2.3

Repeat the calculations of Part 1 using the Fuller-Schettler-Giddings correlation.

Problem 3 (Modified from Benítez, 2009)

Estimate the effective diffusivity of hydrogen in ethane in a porous solid with an average pore size of 300 nm, 40% porosity, and tortuosity of 2.0. The gas mixture is at a pressure of 12 atm and a temperature of 393 K. For this system, the ordinary diffusion coefficient is given by $D_{AB} = 0.85/P$, where D_{AB} is in cm^2/s and P is in atm. For a mixture of hydrogen and ethane, the collision diameter is $\sigma_{AB} = 3.64 \text{ \AA}$. Take $P^{\text{sat}} = 1.71 \text{ kPa}$ as the saturation pressure of water at 15°C , $\nu = 1.52 \times 10^{-5} \text{ m}^2/\text{s}$ as the kinematic viscosity of air and $D_{AB} = 2.42 \times 10^{-5} \text{ m}^2/\text{s}$ as the mass diffusivity of water vapor in air.

- A) $D_{AB,\text{eff}} = 0.0113 \text{ cm}^2/\text{s}$
- B) $D_{AB,\text{eff}} = 0.0676 \text{ cm}^2/\text{s}$
- C) $D_{AB,\text{eff}} = 0.120 \text{ cm}^2/\text{s}$
- D) $D_{AB,\text{eff}} = 0.277 \text{ cm}^2/\text{s}$

Problem 4 (Modified from Benítez, 2009)

A mixture of fluorine gas (F_2 , component A) and chlorine gas (Cl_2 , component B) diffuses through the pores of a 2.5-mm-thick piece of unglazed porcelain at a total pressure of 0.08 atm and a temperature of 323 K. The average pore diameter is $0.45 \mu\text{m}$, the porosity is 32%, and the tortuosity is 4.0. Estimate the diffusion fluxes of both components when the mole fractions of F_2 are 80 and 20% on either side of the porcelain. The collision diameter of a mixture of F_2 and Cl_2 is $\sigma_{AB} = 3.431 \text{ \AA}$, and the binary diffusivity at the abovementioned conditions is $D_{AB} = 1.62 \text{ cm}^2/\text{s}$.

- A) $|\dot{N}_A| = 7.62 \times 10^{-4} \text{ mol}/\text{m}^2 \cdot \text{s}$ and $|\dot{N}_B| = 5.58 \times 10^{-4} \text{ mol}/\text{m}^2 \cdot \text{s}$
- B) $|\dot{N}_A| = 7.62 \times 10^{-4} \text{ mol}/\text{m}^2 \cdot \text{s}$ and $|\dot{N}_B| = 1.99 \times 10^{-3} \text{ mol}/\text{m}^2 \cdot \text{s}$
- C) $|\dot{N}_A| = 2.72 \times 10^{-3} \text{ mol}/\text{m}^2 \cdot \text{s}$ and $|\dot{N}_B| = 5.58 \times 10^{-4} \text{ mol}/\text{m}^2 \cdot \text{s}$
- D) $|\dot{N}_A| = 2.72 \times 10^{-3} \text{ mol}/\text{m}^2 \cdot \text{s}$ and $|\dot{N}_B| = 1.99 \times 10^{-3} \text{ mol}/\text{m}^2 \cdot \text{s}$

Problem 5

Using the method outlined in the Appendix, calculate the diffusion coefficient of uranium dioxide dust particles in atmospheric air at 298 K ($\mu = 1.86 \times 10^{-5} \text{ kg}/\text{m} \cdot \text{s}$, $\rho = 1.18 \text{ kg}/\text{m}^3$) for a particle equivalent volume diameter of $0.02 \mu\text{m}$.

- A) $D_p = 5.33 \times 10^{-5} \text{ cm}^2/\text{s}$
- B) $D_p = 1.08 \times 10^{-4} \text{ cm}^2/\text{s}$
- C) $D_p = 7.71 \times 10^{-4} \text{ cm}^2/\text{s}$
- D) $D_p = 1.08 \times 10^{-3} \text{ cm}^2/\text{s}$

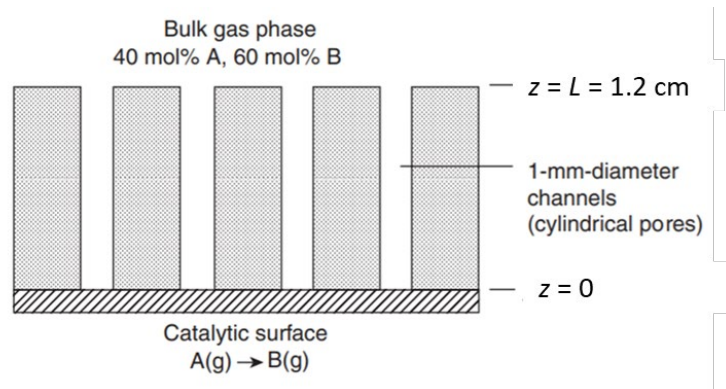
Problem 6

Hydrogen gas is maintained at pressures of 5 bar and 1 bar on opposite sides of a 2-mm-thick membrane. The binary diffusion coefficient of hydrogen in the plastic is $9.5 \times 10^{-8} \text{ m}^2/\text{s}$ and the solubility of hydrogen in the membrane is $0.0015 \text{ kg} \cdot \text{mol}/\text{m}^3 \cdot \text{bar}$. Calculate, under uniform conditions and 25°C , the molar diffusion flux of hydrogen through the membrane.

- A) $N_{\text{H}_2} = 2.76 \times 10^{-8} \text{ kg} \cdot \text{mole}/\text{s} \cdot \text{m}^2$
- B) $N_{\text{H}_2} = 5.62 \times 10^{-8} \text{ kg} \cdot \text{mole}/\text{s} \cdot \text{m}^2$
- C) $N_{\text{H}_2} = 2.85 \times 10^{-7} \text{ kg} \cdot \text{mole}/\text{s} \cdot \text{m}^2$
- D) $N_{\text{H}_2} = 8.14 \times 10^{-7} \text{ kg} \cdot \text{mole}/\text{s} \cdot \text{m}^2$

■ Problem 7.1 (Welty et al., 2008, w/ permission)

Consider the process shown in the figure below. A slab contains parallel linear channels running through a nonporous slab of thickness 1.2 cm. The gas space over the slab contains a mixture of A and B maintained at a constant composition. Gas-phase species A diffuses down a straight, 1.0-mm-diameter channel. At the base of the slab is a catalytic surface that promotes the isomerization reaction $A_{(g)} \rightarrow B_{(g)}$. This reaction occurs very rapidly so that the production of B is diffusion limited. The quiescent gas space in the channel consists of only species A and B. The process is isothermal at 100°C and isobaric at 2.0 atm total system pressure. The bulk composition over the slab is maintained at 40 mol% A and 60 mol% B. The molecular mass of species A and its isomer B is 58 g/mol. The binary gas-phase molecular diffusion coefficient of species A in species B is 0.1 cm²/s at 25°C and 1 atm. What is a reasonable estimate for the molecular flux of species B in species A under the conditions of the operation?



- A) $N_B = 7.43 \times 10^{-7}$ g·mol/cm²·s
- B) $N_B = 1.52 \times 10^{-6}$ g·mol/cm²·s
- C) $N_B = 8.67 \times 10^{-6}$ g·mol/cm²·s
- D) $N_B = 3.06 \times 10^{-5}$ g·mol/cm²·s

■ Problem 7.2

If the total production rate, W_A , is 0.01 mol B/min, what is the required number of 1.0-mm-diameter channels necessary to accomplish this production rate?

- A) $n = 9850$ channels
- B) $n = 14,000$ channels
- C) $n = 20,500$ channels
- D) $n = 26,200$ channels

■ Problem 8

Air is contained in a tire tube of surface area 0.75 m² and wall thickness 12 mm. The pressure of air drops from 2 bar to 1.2 bar over the course of a week. The solubility of air in the rubber is 0.08 m³ of air per m³ of rubber at 1 bar. Determine the diffusivity of air in rubber at the operating temperature of 298 K if the volume of air in the tube is 0.03 m³.

- A) $D_{AB} = 5.14 \times 10^{-9}$ m²/s
- B) $D_{AB} = 2.13 \times 10^{-8}$ m²/s
- C) $D_{AB} = 7.75 \times 10^{-8}$ m²/s
- D) $D_{AB} = 2.13 \times 10^{-7}$ m²/s

Problem 9

Helium gas at 25°C and 3.6 atm flows through a rubber tubing of 10 mm inside radius and 20 mm outside radius. The binary diffusion coefficient of helium is $1.1 \times 10^{-8} \text{ m}^2/\text{s}$ and the solubility of helium is 0.04 m³ of helium per m³ of rubber at 3.6 atm. If the gas constant for helium is 4200 J/kg·K and the concentration of helium at the outer surface of tubing is negligible, calculate the diffusion mass transfer rate of hydrogen per meter length of rubber tubing.

- A) $\dot{m}' = 4.13 \times 10^{-9} \text{ kg/s}\cdot\text{m}$
- B) $\dot{m}' = 8.76 \times 10^{-9} \text{ kg/s}\cdot\text{m}$
- C) $\dot{m}' = 4.41 \times 10^{-8} \text{ kg/s}\cdot\text{m}$
- D) $\dot{m}' = 8.80 \times 10^{-8} \text{ kg/s}\cdot\text{m}$

Problem 10

Calculate the time required for the sublimation of 1 g of naphthalene from a naphthalene ball of mass 2 g suspended in a large volume of stagnant air at 50°C and 1.013 bar pressure. Diffusivity of naphthalene in air under the given conditions is $7.15 \times 10^{-6} \text{ m}^2/\text{s}$, its density is 1130 kg/m³, and its sublimation pressure at 50°C is 0.87 mmHg. The molecular mass of naphthalene is 128.

- A) $t' = 12.0 \text{ h}$
- B) $t' = 55.4 \text{ h}$
- C) $t' = 103 \text{ h}$
- D) $t' = 187 \text{ h}$

Problem 11 (Çengel & Ghajar, 2015, w/ permission)

You probably have noticed that balloons inflated with helium gas rise in the air the first day during a party but they fall down the next day and act like ordinary balloon filled with air. This is because the helium in the balloon slowly leaks out through the wall while air leaks by diffusion. Consider a balloon that is made of 0.1-mm-thick soft rubber and has a diameter of 15 cm when inflated. The pressure and temperature inside the balloon are initially at 110 kPa and 25°C. The permeability of rubber to helium is $9.4 \times 10^{-13} \text{ kmol/m}\cdot\text{s}\cdot\text{bar}$. Find an equation for the variation of pressure in the balloon with time as a result of mass transfer, then determine the time it takes for the pressure in the balloon to drop from 110 to 100 kPa.

- A) $t' = 55 \text{ min}$
- B) $t' = 2.83 \text{ h}$
- C) $t' = 4.62 \text{ h}$
- D) $t' = 6.35 \text{ h}$

■ Problem 12.1 (Welty et al., 2008, w/ permission)

A tank with its top open to the atmosphere contains liquid methanol (MeOH, molar mass 32 g/mol) at the bottom of the tank. The tank is maintained at 30°C. The diameter of the cylindrical tank is 1.0 m, the total height of the tank is 3.0 m, and the liquid level at the bottom of the tank is maintained at 0.5 m. The gas space inside the tank is stagnant and the MeOH vapors are immediately dispersed once they exit the tank. At 30°C, the vapor pressure exerted by liquid MeOH is 215 mmHg and at 40°C the MeOH vapor pressure is 265 mmHg. The mass diffusivity of methanol in air at 30°C is 0.166 cm²/s. We are concerned that this open tank might be emitting a considerable amount of MeOH vapor. What is the emission rate of MeOH vapor from the tank in units of kg MeOH/day when the tank is at a temperature of 30°C? State all assumptions and boundary conditions.

- A) $\Delta \dot{m}_A = 76.5$ g MeOH/day
- B) $\Delta \dot{m}_A = 288$ g MeOH/day
- C) $\Delta \dot{m}_A = 485$ g MeOH/day
- D) $\Delta \dot{m}_A = 965$ g MeOH/day

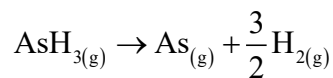
■ Problem 12.2

Repeat the previous problem for a temperature of 40°C.

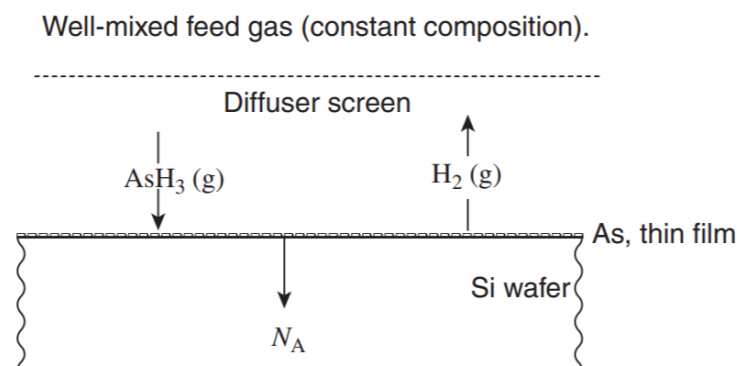
- A) $\Delta \dot{m}_A = 1260$ g MeOH/day
- B) $\Delta \dot{m}_A = 1880$ g MeOH/day
- C) $\Delta \dot{m}_A = 2350$ g MeOH/day
- D) $\Delta \dot{m}_A = 2940$ g MeOH/day

■ Problem 13.1 (Welty et al., 2008, w/ permission)

Microelectronic devices are fabricated by forming many layers of thin films into a silicon wafer. For example, thin films of arsenic as a common dopant of silicon are commonly deposited onto silicon by chemical vapor deposition, or CVD, of arsine (AsH₃) vapor onto the surface of the wafer. The chemical reaction for this CVD process is



It is proposed to allow this process to take place at a pressure of 303.9 Pa and a temperature of 600°C. In many CVD reactors, the gas phased over the film is not mixed. Furthermore, at high temperatures, the surface reaction is very rapid. Consequently, the molecular diffusion of AsH₃ vapor to the surface often controls the rate of As_(s) formation. Consider the very simplified CVD reactor illustrated below. A mixture of arsine and hydrogen gas continuously flows into the reactor. The mixture contains 20 mol% arsine. A diffuser provides a quiescent gas space over the growing As film. The distance from the diffuser to the film surface is 6.0 cm. The gas mixture may be assumed to behave as an ideal gas. The molecular mass of arsenic, As, is 75 g/mol. The Lennard-Jones parameters for AsH₃ are $\sigma_A = 4.08$ Å and $\epsilon_A/\kappa = 207.6$.



- A) $D_{AB} = 88.5$ cm²/s
- B) $D_{AB} = 390$ cm²/s
- C) $D_{AB} = 676$ cm²/s
- D) $D_{AB} = 1230$ cm²/s

■ Problem 13.2

The diameter of the wafer is 15 cm. Estimate the initial deposition rate of arsenic onto the surface of the wafer, in units of grams of As per minute.

- A) $\dot{m}_A = 0.851$ g/min
- B) $\dot{m}_A = 1.30$ g/min
- C) $\dot{m}_A = 2.25$ g/min
- D) $\dot{m}_A = 3.73$ g/min

■ Problem 14

One of the applications of Fick's second law is the calculation of the carbon depth obtained during the carburization of steel. For example, consider the gas carburization of type 1020 steel at 900°C. The steel has a nominal carbon content of 0.15%, and the carbon content at the surface is 1.19%. The diffusion coefficient of carbon in air is $D_{900} = 1.1 \times 10^{-11}$ m²/s. Determine the time necessary to increase the carbon content to 0.45% at a distance of 0.5 mm below the surface.

- A) $t' = 36$ min
- B) $t' = 1.05$ h
- C) $t' = 2.81$ h
- D) $t' = 4.02$ h

■ Problem 15 (Çengel & Ghajar, 2015, w/ permission)

A pond with an initial oxygen content of zero is to be oxygenated by forming a tent over the water surface and filling the tent with oxygen gas at 25°C and 130 kPa. Determine the mole fraction of oxygen at a depth of 1 cm from the surface after 2 days. The diffusion coefficient of oxygen in water at 25°C is $D_{AB} = 2.4 \times 10^{-9}$ m²/s. Henry's constant for oxygen dissolved in water at 300 K is $H = 43,600$ bar, and the saturation pressure of water at 25°C is 3.17 kPa.

- A) $y_{O_2} = 6.86 \times 10^{-6}$
- B) $y_{O_2} = 2.12 \times 10^{-5}$
- C) $y_{O_2} = 7.84 \times 10^{-5}$
- D) $y_{O_2} = 3.12 \times 10^{-4}$

■ Problem 16.1 (Çengel & Ghajar, 2015, w/ permission)

A steel part whose initial carbon content is 0.12 percent by mass is to be case-hardened in a furnace at 1150 K by exposing it to a carburizing gas. The diffusion coefficient of carbon in steel is strongly temperature dependent, and at the surface temperature it is given to be $D_{AB} = 7.2 \times 10^{-12}$ m²/s. Also, the mass fraction of carbon at the exposed surface of the steel part is maintained at 0.011 by the carbon-rich environment in the furnace. If the hardening process is to continue until the mass fraction of carbon at a depth of 0.7 mm is raised to 0.32 percent, determine how long the part should be held in the furnace.

- A) $t' = 53$ min
- B) $t' = 2.96$ h
- C) $t' = 5.83$ h
- D) $t' = 7.22$ h

■ Problem 16.2

How long would the part have to be held in the furnace for a temperature of 500 K, at which the diffusion coefficient of carbon in steel is $D_{AB} = 2.1 \times 10^{-20}$ m²/s?

- A) $t' = 10.7$ h
- B) $t' = 20.6$ h
- C) $t' = 104$ h
- D) $t' = \text{More than } 200$ h

Additional Information

Equations

Eq. 1 → Hirschfelder et al. equation for mass diffusivity

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

where D_{AB} is the binary mass diffusivity in cm^2/s , T is temperature in K, M_A and M_B are the molar masses of components A and B respectively, P is pressure in atm, σ_{AB} is the collision diameter in angstroms, and Ω_D is the collision integral (Table 3).

Eq. 2 → Fuller-Schettler-Giddings equation for mass diffusivity

$$D_{AB} = \frac{10^{-3}T^{1.75} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \left[(\Sigma v)_A^{1/3} + (\Sigma v)_B^{1/3} \right]^2}$$

where D_{AB} is the binary mass diffusivity in cm^2/s , T is temperature in K, M_A and M_B are the molar masses of components A and B respectively, P is pressure in atm, and $(\Sigma v)_A$ and $(\Sigma v)_B$ are the sum of diffusion-volume increments for components A and B (Table 4), respectively.

Eq. 3 → Mean free path

$$\lambda = \frac{\kappa T}{\sqrt{2}\pi\sigma_{AB}^2 P}$$

where $\kappa = 1.38 \times 10^{-23}$ J/K is the Boltzmann constant, T is temperature, σ_{AB} is collision diameter, and P is pressure.

Eq. 4 → Knudsen number

$$\text{Kn} = \frac{\lambda}{d}$$

where λ is the mean free path of diffusing molecules and d is pore diameter. The Knudsen number dictates the prevailing mode of diffusion through a pore in accordance with the following table.

Range	Characteristic
$\text{Kn} < 0.05$	Ordinary molecular diffusion dominates
$0.05 < \text{Kn} < 5.0$	Both Knudsen and molecular diffusion are important
$\text{Kn} > 5.0$	Knudsen diffusion dominates

Eq. 5 → Effective diffusivity in porous media

$$D_{\text{eff}} = \frac{\varepsilon D}{\tau}$$

where D is the corresponding diffusivity (molecular or Knudsen) in a nonporous medium, ε is porosity, and τ is tortuosity.

Eq. 6 → Knudsen diffusivity

$$D_{\text{Kn}} = \frac{d}{3} \left(\frac{8RT}{\pi M} \right)^{1/2}$$

where d is pore diameter, R is the gas constant, T is temperature, and M is molar mass.

Eq. 7 → Molar flux when both molecular diffusion and Knudsen diffusion are relevant

$$N_A = \Psi_A \frac{PD_{AB,\text{eff}}}{RTL} \ln \left[\frac{\Psi_A \left(1 + \frac{D_{AB,\text{eff}}}{D_{\text{Kn},A,\text{eff}}} \right) - y_{A,2}}{\Psi_A \left(1 + \frac{D_{AB,\text{eff}}}{D_{\text{Kn},A,\text{eff}}} \right) - y_{A,1}} \right]$$

where Ψ_A is the molar flux fraction of component A, P is pressure, $D_{AB,eff}$ is the effective binary mass diffusivity, $D_{Kn,A,eff}$ is the effective Knudsen diffusivity, y_A is the molar fraction of component A, R is the gas constant, T is temperature, and L is pore length. The molar flux fraction Ψ_A is defined as

$$\Psi_A = \frac{N_A}{N_A + N_B}$$

Eq. 8 → *Graham's law*

$$\sum N_i \sqrt{M_i} = 0$$

where N_i and M_i the molar flux and molar mass of mixture component i , respectively.

Eq. 9 → *Steady state diffusion through a plain membrane*

$$N = \frac{D_{AB}(C_1 - C_2)}{L}$$

where D_{AB} is mass diffusivity, C are concentrations, and L is the membrane thickness.

Eq. 10 → *Steady state diffusion through a stagnant gas film*

$$N_A = \frac{D_{AB}P}{RTL} \ln \left(\frac{P - P_{A,\infty}}{P - P_{A,0}} \right)$$

where D_{AB} is mass diffusivity, P is system pressure, $P_{A,\infty}$ is the partial pressure of component A in the surrounding medium, $P_{A,0}$ is the partial pressure of component A in the reference initial level, T is temperature, and L is film thickness.

Eq. 11 → *Diffusive evaporation of a spherical droplet*

$$r_{s,0}^2 - r_s'^2 = \frac{2D_{AB}PM_A t'}{RT\rho_A} \ln \left(\frac{P - P_{A,\infty}}{P - P_{A,s}} \right)$$

where $r_{s,0}$ is the initial particle radius, r_s is the particle radius at time t , D_{AB} is mass diffusivity, P is pressure, M_A is the molar mass of the droplet material, P is the system pressure, $P_{A,\infty}$ is the partial pressure of A in the free stream medium, $P_{A,s}$ is the partial pressure of A at the surface, R is the gas constant, T is temperature, and ρ_A is the density of the droplet material.

Eq. 12 → *Transient diffusion in a semi-infinite stationary medium*

$$\frac{C_A(x,t) - C_{A,i}}{C_{A,s} - C_{A,i}} = \operatorname{erfc} \left(\frac{x}{2\sqrt{D_{AB}t}} \right)$$

where $C_{A,i}$ is the initial concentration of component A in time $t = 0$, $C_{A,s}$ is the concentration at the inner side of the exposed surface of the medium, x is the distance from the surface, D_{AB} is mass diffusivity, and t is time. erfc denotes the complementary error function.

Appendix: Microhydrodynamics of small particles (Ghiaasiaan, 2018)

Ghiaasiaan recommends the following procedure to estimate the particle diffusion coefficient of particles suspended in a quiescent medium.

Step 1: Compute the mean free path with the relation

$$\lambda_p = \nu \left(\frac{\pi M}{2R_u T} \right)^{1/2}$$

where ν is kinematic viscosity, M is molar mass, R_u is the gas constant, and T is temperature.

Step 2: If the particles are not perfectly spherical, compute the equivalent volume diameter d_p with the relation

$$d_{p,e} = \left(\frac{6V_p}{\pi} \right)^{1/3}$$

where V_p is the volume of the particle.

Step 3: Using the results of the two previous steps, determine the Knudsen number,

$$Kn_p = \frac{\lambda_p}{d_{p,e}}$$

Step 4: Using the Knudsen number, compute Cunningham's correction factor C_C ,

$$C_C = 1 + 2Kn_p \left[1.257 + 0.4 \exp\left(-\frac{0.55}{Kn_p}\right) \right]$$

Step 5: Compute the particle friction coefficient f , which is given by

$$f = \frac{3\pi\mu d_{p,e}\chi}{C_C}$$

where μ is the viscosity of the quiescent medium and χ is the so-called dynamic shape factor, which accounts for non-spherical particle geometries and can be read from Table 1.

Step 6: Determine the particle diffusion coefficient with the relation

$$D_p = \frac{\kappa T}{f}$$

where $\kappa = 1.38 \times 10^{-23}$ is the Boltzmann constant and T is temperature. The particle Schmidt number $Sc_p = \nu/D_p$ may also be useful.

Table 1 Dynamic shape factors for some particle geometries

Particle shape	Dynamic shape factor χ
Sphere	1.0
Cube, averaged over all orientations	1.08
Cylinder, averaged over all directions	1.10 for $L/D = 2$ 1.35 for $L/D = 5$ 1.68 for $L/D = 10$
<i>Dust</i>	
Bituminous coal	1.05 – 1.11
Quartz	1.36 - 1.82
Sand	1.57
UO ₂	1.28
ThO ₂	0.99
<i>Compact sphere clusters</i>	
Double spheres	1.10
Three spheres	1.15
Four spheres	1.17

Table 2 Lennard-Jones potential parameters for selected compounds

<i>Compound</i>	σ (Å)	ϵ/k (K)	<i>Compound</i>	σ (Å)	ϵ/k (K)
He	2.551	10.22	Air	3.711	78.6
CCl ₄	5.947	322.7	CHCl ₃	5.389	340.2
CH ₃ Cl	4.182	350.0	CH ₃ OH	3.626	481.8
CH ₄	3.758	148.6	CS ₂	4.483	467.0
C ₂ H ₄	4.163	224.7	C ₂ H ₆	4.443	215.7
C ₂ H ₅ Cl	4.898	300.0	C ₂ H ₅ OH	4.530	362.6
Propylene	4.678	298.9	Acetone	4.600	560.2
<i>n</i> -Butane	4.687	531.4	Di-ethyl ether	5.678	313.8
<i>n</i> -Hexane	5.949	399.3	Cl ₂	4.217	316.0
Ethyl acetate	5.205	521.3	HCl	3.339	344.7
HBr	3.353	449.0	H ₂	2.827	59.7
H ₂ O	2.641	809.1	H ₂ S	3.623	301.1
NH ₃	2.900	558.3	NO	3.492	116.7
N ₂	3.798	71.4	O ₂	3.467	106.7
SO ₂	4.112	335.4	Benzene	5.349	412.3

Table 3 Numerical values of the collision integral Ω_D

kT/ϵ	Ω_D	kT/ϵ	Ω_D	kT/ϵ	Ω_D
0.30	2.662	0.95	1.476	1.90	1.094
0.35	2.476	1.00	1.439	2.00	1.075
0.40	2.318	1.05	1.406	2.5	0.9996
0.45	2.184	1.10	1.375	3.0	0.949
0.50	2.066	1.15	1.346	3.5	0.912
0.55	1.966	1.20	1.320	4.0	0.8836
0.60	1.877	1.25	1.296	4.5	0.861
0.65	1.798	1.30	1.273	5.0	0.8422
0.70	1.729	1.40	1.233	7.0	0.7896
0.75	1.667	1.50	1.198	10.0	0.7424
0.80	1.612	1.60	1.167	30	0.6232
0.85	1.562	1.70	1.140	50	0.5756
0.90	1.517	1.80	1.116	70	0.5464

Table 4 Atomic and diffusion volumes

C	16.5	H ₂	7.07	CO ₂	26.9
H	2.31	He	2.88	N ₂ O	35.9
O	5.48	N ₂	17.9	NH ₃	14.9
N	5.69	O ₂	16.6	H ₂ O	12.7
Cl	19.5	Air	20.1	Cl ₂	37.7
S	17.0	Ar	16.1	SO ₂	41.1
Aromatic ring	-20.2	Kr	22.8		
Heterocyclic ring	-20.2	CO	18.9		

Table 5 The complementary error function

η	erfc (η)	η	erfc (η)	η	erfc (η)	η	erfc (η)	η	erfc (η)	η	erfc (η)
0.00	1.00000	0.38	0.5910	0.76	0.2825	1.14	0.1069	1.52	0.03159	1.90	0.00721
0.02	0.9774	0.40	0.5716	0.78	0.2700	1.16	0.10090	1.54	0.02941	1.92	0.00662
0.04	0.9549	0.42	0.5525	0.80	0.2579	1.18	0.09516	1.56	0.02737	1.94	0.00608
0.06	0.9324	0.44	0.5338	0.82	0.2462	1.20	0.08969	1.58	0.02545	1.96	0.00557
0.08	0.9099	0.46	0.5153	0.84	0.2349	1.22	0.08447	1.60	0.02365	1.98	0.00511
0.10	0.8875	0.48	0.4973	0.86	0.2239	1.24	0.07950	1.62	0.02196	2.00	0.00468
0.12	0.8652	0.50	0.4795	0.88	0.2133	1.26	0.07476	1.64	0.02038	2.10	0.00298
0.14	0.8431	0.52	0.4621	0.90	0.2031	1.28	0.07027	1.66	0.01890	2.20	0.00186
0.16	0.8210	0.54	0.4451	0.92	0.1932	1.30	0.06599	1.68	0.01751	2.30	0.00114
0.18	0.7991	0.56	0.4284	0.94	0.1837	1.32	0.06194	1.70	0.01612	2.40	0.00069
0.20	0.7773	0.58	0.4121	0.96	0.1746	1.34	0.05809	1.72	0.01500	2.50	0.00041
0.22	0.7557	0.60	0.3961	0.98	0.1658	1.36	0.05444	1.74	0.01387	2.60	0.00024
0.24	0.7343	0.62	0.3806	1.00	0.1573	1.38	0.05098	1.76	0.01281	2.70	0.00013
0.26	0.7131	0.64	0.3654	1.02	0.1492	1.40	0.04772	1.78	0.01183	2.80	0.00008
0.28	0.6921	0.66	0.3506	1.04	0.1413	1.42	0.04462	1.80	0.01091	2.90	0.00004
0.30	0.6714	0.68	0.3362	1.06	0.1339	1.44	0.04170	1.82	0.01006	3.00	0.00002
0.32	0.6509	0.70	0.3222	1.08	0.1267	1.46	0.03895	1.84	0.00926	3.20	0.00001
0.34	0.6306	0.72	0.3086	1.10	0.1198	1.48	0.03635	1.86	0.00853	3.40	0.00000
0.36	0.6107	0.74	0.2953	1.12	0.1132	1.50	0.03390	1.88	0.00784	3.60	0.00000

Solutions

P.1 Solution

Part 1: From Table 2, we read $\sigma_A = 3.711 \text{ \AA}$ and $\varepsilon_A/k = 78.6 \text{ K}$ for air and $\sigma_B = 3.758 \text{ \AA}$ and $\varepsilon_B/k = 148.6 \text{ K}$ for methane. We proceed to compute the collision diameter σ_{AB} ,

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{3.711 + 3.758}{2} = 3.735 \text{ \AA}$$

and ε_{AB}/k ,

$$\varepsilon_{AB}/k = \sqrt{(\varepsilon_A/k)(\varepsilon_B/k)} = \sqrt{78.6 \times 148.6} = 108.1 \text{ K}$$

From the latter result, we write

$$\frac{\varepsilon_{AB}}{kT} = \frac{108.1}{298} = 0.363$$

$$\therefore \frac{kT}{\varepsilon_{AB}} = 2.75$$

Interpolating from Table 3, the collision integral is found to be $\Omega_D = 0.9743$. Substituting in the Hirschfelder et al. equation brings to

$$D_{AB} = \frac{0.001858 T^{3/2} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \sigma_{AB}^2 \Omega_D} = \frac{0.001858 \times 298^{3/2} \times \left(\frac{1}{29} + \frac{1}{16} \right)^{1/2}}{1.0 \times 3.758^2 \times 0.9743} = \boxed{0.216 \text{ cm}^2/\text{s}}$$

◆ The correct answer is **B**.

Part 2: From the Chapman-Enskog model, it can be seen that the diffusion coefficient is proportional to temperature to the 3/2 power and linear-inversely proportional to pressure. Accordingly, if the temperature were $T_2 = 2 \times T_1 = 2 \times 298 = 596 \text{ K}$ and the pressure were $P_2 = 1.5 \times P_1 = 1.5 \times 1.0 = 1.5 \text{ atm}$, the ensuing diffusion coefficient would be

$$\frac{D_2}{D_1} = \left(\frac{T_2}{T_1} \right)^{3/2} \left(\frac{P_1}{P_2} \right) \rightarrow D_2 = D_1 \left(\frac{T_2}{T_1} \right)^{3/2} \left(\frac{P_1}{P_2} \right)$$

$$\therefore D_2 = 0.216 \times 2^{3/2} \times 1.5^{-1} = \boxed{0.407 \text{ cm}^2/\text{s}}$$

Part 3: The Fuller-Schettler-Giddings correlation is

$$D_{AB} = \frac{10^{-3} T^{1.75} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \left[(\Sigma v)_A^{1/3} + (\Sigma v)_B^{1/3} \right]^2}$$

Referring to Table 4, we read $v_A = 20.1$ for air; as for methane, which has one carbon atom and four hydrogen atoms, we have

$$(\Sigma v)_B = v_C + 4v_H = 16.5 + 4 \times 2.31 = 25.74$$

Substituting in the FSG correlation gives

$$D_{AB} = \frac{10^{-3} \times 298^{1.75} \times \left(\frac{1}{29} + \frac{1}{16} \right)^{1/2}}{1.0 \times (25.74^{1/3} + 20.1^{1/3})^2} = \boxed{0.207 \text{ cm}^2/\text{s}}$$

P.2 | Solution

Part 1: From Table 2, we read $\sigma_A = 3.467 \text{ \AA}$ and $\varepsilon_A/k = 106.7 \text{ K}$ for oxygen and $\sigma_B = 3.623$ and $\varepsilon_B/k = 301.1 \text{ K}$ for hydrogen sulfide. We proceed to compute the collision diameter σ_{AB} ,

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{3.467 + 3.623}{2} = 3.545 \text{ \AA}$$

and ε_{AB}/k ,

$$\varepsilon_{AB}/k = \sqrt{(\varepsilon_A/k)(\varepsilon_B/k)} = \sqrt{106.7 \times 301.1} = 179.2 \text{ K}$$

From the latter result, we write

$$\frac{\varepsilon_{AB}}{kT} = \frac{179.2}{298} = 0.601$$

$$\therefore \frac{kT}{\varepsilon_{AB}} = 1.66$$

Interpolating from Table 3, the collision integral is found to be $\Omega_D = 1.151$. Substituting in the Hirschfelder et al. equation brings to

$$D_{AB} = \frac{0.001858 T^{3/2} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \sigma_{AB}^2 \Omega_D} = \frac{0.001858 \times 298^{3/2} \times \left(\frac{1}{32} + \frac{1}{34} \right)^{1/2}}{0.1 \times 3.545^2 \times 1.151} = \boxed{1.63 \text{ cm}^2/\text{s}}$$

♦ The correct answer is **D**.

Part 2: If the temperature were $T_2 = 0.5 \times T_1 = 0.5 \times 298 = 149 \text{ K}$ and the pressure were $P_2 = 0.60 \times P_1 = 0.6 \times 0.1 = 0.06 \text{ atm}$, the ensuing diffusion coefficient would be

$$\frac{D_2}{D_1} = \left(\frac{T_2}{T_1} \right)^{3/2} \left(\frac{P_1}{P_2} \right) \rightarrow D_2 = D_1 \left(\frac{T_2}{T_1} \right)^{3/2} \left(\frac{P_1}{P_2} \right)$$

$$\therefore D_2 = 1.63 \times 0.5^{3/2} \times 0.6^{-1} = \boxed{0.960 \text{ cm}^2/\text{s}}$$

Part 3: The FSG correlation is

$$D_{AB} = \frac{10^{-3} T^{1.75} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P \left[(\Sigma v)_A^{1/3} + (\Sigma v)_B^{1/3} \right]^2}$$

In view of the values given in Table 4, the diffusion volume of gaseous oxygen is $v_A = 16.6$. The diffusion volume for hydrogen sulfide, which has one sulfur atom and two hydrogen atoms, is

$$(\Sigma v)_B = v_S + 2v_H = 17.0 + 4 \times 2.31 = 26.24$$

Substituting in the FSG equation yields

$$D_{AB} = \frac{10^{-3} \times 298^{1.75} \times \left(\frac{1}{32} + \frac{1}{34} \right)^{1/2}}{0.1 \times (16.6^{1/3} + 26.24^{1/3})^2} = \boxed{1.73 \text{ cm}^2/\text{s}}$$

P.3 Solution

To begin, we compute the mean free path λ ,

$$\lambda = \frac{\kappa T}{\sqrt{2} \pi \sigma_{AB}^2 P} = \frac{(1.38 \times 10^{-23}) \times 393}{\sqrt{2} \times \pi \times (3.64 \times 10^{-10})^2 \times (12 \times 10^5)} = 7.68 \text{ nm}$$

The Knudsen number $\text{Kn} = 7.68/300 = 0.026$, which is less than 0.05 and hence indicates that diffusion inside the pores occurs solely by ordinary molecular diffusion. At a pressure of 12 atm, $D_{AB} = 0.85/12 = 0.0708 \text{ cm}^2/\text{s}$. Substituting this quantity into equation 5, along with the fractional porosity $\varepsilon = 0.4$ and the tortuosity $\tau = 2.5$, yields

$$D_{AB,\text{eff}} = \frac{\varepsilon D_{AB}}{\tau} = \frac{0.4 \times 0.0708}{2.5} = \boxed{0.0113 \text{ cm}^2/\text{s}}$$

♦ The correct answer is **A**.

P.4 Solution

To begin, we compute the mean free path λ ,

$$\lambda = \frac{\kappa T}{\sqrt{2} \pi \sigma_{AB}^2 P} = \frac{(1.38 \times 10^{-23}) \times 323}{\sqrt{2} \times \pi \times (3.431 \times 10^{-10})^2 \times (0.08 \times 10^5)} = 1.06 \text{ } \mu\text{m}$$

The Knudsen number is $\text{Kn} = 1.06/0.45 = 2.36$; since $0.02 < \text{Kn} < 5.0$, both molecular and Knudsen diffusion are important and the molar flux should be determined with equation 7. The molar fluxes of components A and B are related by Graham's law (equation 8),

$$\sum N_i \sqrt{M_i} = 0$$

which becomes, in the present case,

$$\frac{N_B}{N_A} = -\sqrt{\frac{M_A}{M_B}} = -\sqrt{\frac{38}{71}} = -0.732 \quad (\text{I})$$

so that the molar flux fraction Ψ_A can be computed as

$$\Psi_A = \frac{N_A}{N_A + N_B} = \frac{1}{1 + \frac{N_B}{N_A}} = \frac{1}{1 - 0.732} = 3.73$$

Given the porosity $\varepsilon = 0.32$ and the tortuosity $\tau = 4.0$, the effective binary diffusivity is calculated as

$$D_{AB,\text{eff}} = \frac{\varepsilon D_{AB}}{\tau} = \frac{0.32 \times 1.62}{4.0} = 0.130 \text{ cm}^2/\text{s}$$

The Knudsen diffusivity of component A (fluorine), in turn, is given by equation 6,

$$D_{Kn,A} = \frac{d}{3} \left(\frac{8RT}{\pi M} \right)^{1/2} = \frac{0.45}{3} \times \left(\frac{8 \times 0.8314 \times 323}{\pi \times 38} \right)^{1/2} = 0.636 \text{ cm}^2/\text{s}$$

and corresponds to an effective diffusivity $D_{Kn,A,\text{eff}}$ such that

$$D_{Kn,A,\text{eff}} = \frac{\varepsilon D_{Kn,A}}{\tau} = \frac{0.32 \times 0.636}{4.0} = 0.0509 \text{ cm}^2/\text{s}$$

Accordingly, we have the ratio $D_{AB,\text{eff}}/D_{Kn,A,\text{eff}} = 0.130/0.0509 = 2.55$. Substituting this and other variables into equation 7 gives

$$N_A = \Psi_A \frac{PD_{AB,\text{eff}}}{RTL} \ln \left[\frac{\Psi_A \left(1 + \frac{D_{AB,\text{eff}}}{D_{Kn,\text{eff}}} \right) - y_{A,2}}{\Psi_A \left(1 + \frac{D_{Kn,\text{eff}}}{D_{AB,\text{eff}}} \right) - y_{A,1}} \right]$$

$$\therefore N_A = 3.73 \times \frac{(0.08 \times 10^5) \times (0.130 \times 10^{-4})}{8.314 \times 323 \times (2.5 \times 10^{-3})} \ln \left[\frac{3.73 \times (1 + 2.55) - 0.2}{3.73 \times (1 + 2.55) - 0.8} \right] = \boxed{2.72 \times 10^{-3} \text{ mol/m}^2 \cdot \text{s}}$$

Substituting N_A into equation (I), we ultimately obtain

$$N_B = -0.732 N_A = -0.732 \times 2.72 \times 10^{-3} = \boxed{-1.99 \times 10^{-3} \text{ mol/m}^2 \cdot \text{s}}$$

♦ The correct answer is **D**.

P.5 | Solution

From Table 1, we read a dynamic shape factor $\chi = 1.28$. The molecular mean free path is determined as

$$\lambda_{\text{mol}} = v \left(\frac{\pi M}{2RT} \right)^{1/2} = \left(\frac{1.86 \times 10^{-5}}{1.18} \right) \times \left(\frac{\pi \times 29}{2 \times 8314 \times 298} \right)^{1/2} = 6.76 \times 10^{-8} \text{ m}$$

The Knudsen number follows as

$$Kn_p = \frac{\lambda_{\text{mol}}}{d_p} = \frac{6.76 \times 10^{-8}}{0.02 \times 10^{-6}} = 3.38$$

Cunningham's correction factor is determined next,

$$C_C = 1 + 2Kn_p \left[1.257 + 0.4 \exp \left(-\frac{0.55}{Kn_p} \right) \right]$$

$$\therefore C_C = 1 + 2 \times 3.38 \times \left[1.257 + 0.4 \exp \left(-\frac{0.55}{3.38} \right) \right] = 11.8$$

The particle friction coefficient is then

$$f = \frac{3\pi\mu d_p \chi}{C_C} = \frac{3\pi \times (1.86 \times 10^{-5}) \times (0.02 \times 10^{-6}) \times 1.28}{11.8} = 3.80 \times 10^{-13} \text{ N} \cdot \text{s/m}$$

We proceed to determine the particle diffusion coefficient,

$$D_p = \frac{\kappa T}{f} = \frac{(1.381 \times 10^{-23}) \times 298}{3.80 \times 10^{-13}} = 1.08 \times 10^{-8} \text{ m}^2/\text{s}$$

$$D_p = 1.08 \times 10^{-4} \text{ cm}^2/\text{s}$$

We can also determine the particle Schmidt number,

$$Sc_p = \frac{\nu}{D_p} = \frac{(\mu/\rho)}{D_p} = \frac{(1.86 \times 10^{-5})/1.18}{1.08 \times 10^{-8}} = 1460$$

We can easily extend these calculations for other particle diameters. Results for $d_p = 0.2 \mu\text{m}$ and $d_p = 2 \mu\text{m}$ are listed in the following table.

d_p (μm)	λ_{mol} (m)	Kn_p	C_c	f (N-s/m)	D_p (cm^2/s)	Sc_p
0.02	6.76E-08	3.38	11.8	3.805E-13	1.08E-04	1457
0.2	6.76E-08	0.34	1.9	2.358E-11	1.75E-06	90329
2	6.76E-08	0.03	1.1	4.136E-10	9.95E-08	1584212

◆ The correct answer is **B**.

P.6 | Solution

The molar concentration, the total pressure (P) and the solubility (s) of the diffusing gas are related by $C = s \times P$. Accordingly, the molar concentrations of hydrogen at the opposite faces of the plastic membrane are $C_{H_2,1} = 0.0015 \times 5.0 = 0.0075 \text{ kg-mole/m}^3$ and $C_{H_2,2} = 0.0015 \times 1.0 = 0.0015 \text{ kg-mole/m}^3$. The molar diffusion flux of hydrogen through the membrane follows from Fick's law (equation 9),

$$N_{H_2} = \frac{D_{AB}(C_{H_2,1} - C_{H_2,2})}{L} = \frac{(9.5 \times 10^{-8}) \times (0.0075 - 0.0015)}{2 \times 10^{-3}} = \boxed{2.85 \times 10^{-7} \text{ kg} \cdot \text{mole/s} \cdot \text{m}^2}$$

◆ The correct answer is **C**.

P.7 | Solution

Part 1: The process in question can be modeled as a 1-D, steady-state diffusion, so that

$$\dot{N}_A = -\dot{N}_B = \frac{CD_{AB}}{L}(y_{A,1} - y_{A,2})$$

The molar fractions are $y_{A,1}(0) = 0.4$ and $y_{A,2}(0.012) = 0$. The concentration of gas A follows from the ideal gas law,

$$C = \frac{P}{RT} = \frac{2}{82.06 \times 373} = 6.53 \times 10^{-5} \text{ mol/cm}^3$$

We were given the diffusivity $D_{AB} = 0.1 \text{ cm}^2/\text{s}$ at 298 K and 1 atm; this can be easily adapted to $T = 373 \text{ K}$ and $P = 2 \text{ atm}$,

$$D_{AB} = 0.1 \times \left(\frac{373}{298}\right)^{3/2} \times \left(\frac{1.0}{2.0}\right) = 0.07 \text{ cm}^2/\text{s}$$

The molar flux is then

$$\dot{N}_B = -\dot{N}_A = \frac{(6.53 \times 10^{-5}) \times 0.07}{1.2} \times (0.4 - 0) = \boxed{1.52 \times 10^{-6} \text{ g} \cdot \text{mol/cm}^2 \cdot \text{s}}$$

◆ The correct answer is **B**.

Part 2: The molar flow rate and the molar flux are related by

$$W_A = N_A \times S$$

where $W_A = 0.01 \text{ mol/min} = 1.67 \times 10^{-4} \text{ mol/s}$ and S is the surface area. Thus,

$$W_A = N_A \times S \rightarrow 1.67 \times 10^{-4} = (1.52 \times 10^{-6}) \times S$$

$$\therefore S = 110 \text{ cm}^2$$

The area per channel is $\pi \times 0.1^2/4 = 0.00785 \text{ cm}^2$, and the total number of channels follows as

$$n = \frac{110}{0.00785} = \boxed{14,000 \text{ channels}}$$

◆ The correct answer is **B**.

P.8 | Solution

The initial mass of air in the tube is

$$m_0 = \frac{P_0 V}{RT} = \frac{(2.0 \times 10^5) \times 0.03}{287 \times 298} = 0.0702 \text{ kg}$$

while the final mass is

$$m_1 = \frac{P_1 V}{RT} = \frac{(1.2 \times 10^5) \times 0.03}{287 \times 298} = 0.0421 \text{ kg}$$

This means that the mass of air escaped during the week is $m_{\text{air}} = 0.0702 - 0.0421 = 0.0281 \text{ kg}$, and the mass flux of escaped air follows as

$$\dot{m}'' = \frac{m_{\text{air}}}{\text{Time elapsed} \times \text{Area}} = \frac{0.0281}{(7 \times 24 \times 3600) \times 0.75} = 6.19 \times 10^{-8} \text{ kg/m}^2 \cdot \text{s}$$

The solubility of air should be evaluated at the mean operating pressure of $(2.0 + 1.2)/2 = 1.6 \text{ bar}$, so that $s = 0.08 \times 1.6 = 0.128 \text{ m}^3/\text{m}^3$ of rubber. The air that escapes to the atmosphere will be at a pressure of 1 bar and its solubility will remain at $0.08 \text{ m}^3/\text{m}^3$ rubber as given in the problem statement. We can now determine the mass concentration at the inner surface of the tube,

$$C_{\text{air},1} = \frac{P_1 V_1}{RT_1} = \frac{(1.6 \times 10^5) \times 0.128}{287 \times 298} = 0.239 \text{ kg/m}^3$$

and at the outer surface,

$$C_{\text{air},2} = \frac{P_2 V_2}{RT_2} = \frac{(1.01 \times 10^5) \times 0.08}{287 \times 298} = 0.0945 \text{ kg/m}^3$$

Appealing to Fick's law, we ultimately have

$$\dot{m}'' = \frac{D_{AB} (C_{\text{air},1} - C_{\text{air},2})}{L} \rightarrow 6.19 \times 10^{-8} = \frac{D_{AB} \times (0.239 - 0.0945)}{0.012}$$

$$\therefore \boxed{D_{AB} = 5.14 \times 10^{-9} \text{ m}^2/\text{s}}$$

◆ The correct answer is **A**.

P.9 | Solution

The solubility of hydrogen at a pressure of 3.6 atm is $s = 0.04 \times 3.6 = 0.144 \text{ m}^3/\text{m}^3$ rubber tubing = volume of helium in m^3/m^3 rubber. The concentration of helium at the inner surface of the pipe is determined as

$$C_{\text{He},1} = \frac{PV}{RT} = \frac{(3.6 \times 10^5) \times 0.144}{4200 \times 298} = 0.0414 \text{ kg/m}^3 \text{ rubber tubing}$$

The concentration at the outer surface of the pipe, in turn, is $C_{\text{He},2} = 0$. The log-mean area A_m for a cylindrical geometry such as the present one is

$$A_m = \frac{2\pi L(r_2 - r_1)}{\ln(r_2/r_1)} = \frac{2\pi \times 1.0 \times (20 \times 10^{-3} - 10 \times 10^{-3})}{\ln(20/10)} = 0.0906 \text{ m}^2$$

Finally, the mass transfer rate through the cylinder is calculated as

$$\dot{m}' = \frac{D_{AB}(C_{\text{He},1} - C_{\text{He},2})}{\Delta x} A_m = \frac{(1.1 \times 10^{-8}) \times (0.0414 - 0)}{(0.02 - 0.01)} \times 0.0906 = \boxed{4.13 \times 10^{-9} \text{ kg/s} \cdot \text{m}}$$

♦ The correct answer is **A**.

P.10 | Solution

The initial volume of the ball, which has 2 g mass at the beginning of the process, is

$$m = \rho \forall_0 \rightarrow \forall_0 = \frac{m}{\rho} = \frac{2}{1.13} = 1.77 \text{ cm}^3$$

This corresponds to a radius $r_{s,0} = 0.750 \text{ cm}$. The final mass of the ball is $2 - 1 = 1 \text{ g}$, which corresponds to a volume of $1/1.13 = 0.885 \text{ cm}^3$ and a radius $r_s = 0.596 \text{ cm}$. Other parameters include the diffusivity $D_{AB} = 0.0715 \text{ cm}^2/\text{s}$, pressure $P = 1.013 \text{ bar}$, temperature $T = 323 \text{ K}$, molar mass of naphthalene $M_A = 128 \text{ g/mol}$, the partial pressure of naphthalene in bulk air $P_{A,\infty} = 0$, and the sublimation pressure of naphthalene at the temperature in question $P_{A,s} = 0.87 \text{ mmHg} = 0.00115 \text{ bar}$. We proceed to substitute these data into equation 11,

$$r_{s,0}^2 - r_s'^2 = \frac{2D_{AB}PM_A t'}{RT\rho_A} \ln\left(\frac{P - P_{A,\infty}}{P - P_{A,s}}\right)$$

$$\therefore 0.750^2 - 0.596^2 = \frac{2 \times 0.0715 \times 1.013 \times 128 \times t'}{83.14 \times 323 \times 1.13} \ln\left(\frac{1.013 - 0}{1.013 - 0.00115}\right)$$

$$\therefore \boxed{t' = 103 \text{ h}}$$

♦ The correct answer is **C**.

Note

Solving equation 11 for t with $r_s' = 0$, we could just as well compute the time required for complete evaporation of the drop,

$$t' = \frac{RT\rho_A r_{s,0}^2}{2D_{AB}PM_A \ln\left[\frac{P - P_{A,\infty}}{P - P_{A,s}}\right]}$$

$$\therefore t' = \frac{83.14 \times 323 \times 1.13 \times 0.75^2}{2 \times 0.0715 \times 1.013 \times 128 \times \ln\left[\frac{1.013 - 0}{1.013 - 0.00115}\right]} = 225 \text{ h}$$

The droplet should require about 225 hours, or about 9.4 days, to evaporate completely.

P.11 | Solution

We can consider the total molar concentration to be constant and the balloon to be a stationary medium since there is no diffusion of rubber molecules and the concentration of helium in the balloon is very low. The partial pressure of helium in the air is negligible. Since the balloon is filled with pure helium gas at 110 kPa, the initial partial pressure of helium in the balloon is 110 kPa. When permeability data is available, the molar flow rate of a gas through a solid wall of thickness L under steady one-dimensional conditions can be determined with the relation

$$\dot{N}_{\text{diff,A,wall}} = \Pi_{AB} A \frac{P_{A,1} - P_{A,2}}{L} = \Pi_{AB} A \frac{P}{L}$$

where Π_{AB} is permeability and $P_{A,1}$ and $P_{A,2}$ are the partial pressures of helium in the two sides of the wall. Noting that the amount of helium in the balloon can be expressed as $N = PV/RT$ and taking the temperature and volume to be constants, we derive to obtain

$$N = \frac{PV}{RT} \rightarrow \frac{dN}{dt} = \frac{V}{RT} \frac{dP}{dt}$$

$$\therefore \frac{dP}{dt} = \frac{RT}{V} \frac{dN}{dt}$$

Conservation of mass dictates that the mass flow rate of helium from the balloon should be equal to the rate of change of mass inside the balloon; that is,

$$\frac{dN}{dt} = \dot{N}_{\text{diff,A,wall}} = -\Pi_{AB} A \frac{P}{L}$$

Combining the two previous equations and separating variables, we have

$$\frac{dP}{dt} = \frac{RT}{V} \frac{dN}{dt} = \frac{RT}{V} \times \left(-\Pi_{AB} A \frac{P}{L} \right) = -\frac{RT\Pi_{AB}AP}{VL}$$

$$\therefore \frac{dP}{P} = -\frac{RT\Pi_{AB}A}{VL} dt$$

Integrating, we get

$$\frac{dP}{P} = -\frac{RT\Pi_{AB}A}{VL} dt \rightarrow \ln\left(\frac{P}{P_0}\right) = -\frac{RT\Pi_{AB}A}{VL} t$$

where P_0 is the initial pressure. Resolving the logarithm, we have

$$P = P_0 \exp\left(-\frac{RT\Pi_{AB}A}{VL} t\right)$$

For a sphere, the ratio of surface area to volume is

$$\frac{A}{V} = \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = \frac{3}{r}$$

so that

$$P = P_0 \exp\left(-\frac{3RT\Pi_{AB}}{rL} t\right)$$

We have established an expression that relates the pressure inside the balloon to time. Lastly, the time required for the pressure inside the balloon to drop from $P_0 = 110$ kPa to $P = 100$ kPa is

$$100 = 110 \times \exp\left[-\frac{3 \times 0.08314 \times 298 \times (9.4 \times 10^{-13})}{0.075 \times (0.1 \times 10^{-3})} \times t'\right]$$

$$\therefore 100 = 110 \times \exp\left[-9.32 \times 10^{-6} \times t'\right]$$

$$t' = 10,200 \text{ sec} = \boxed{2.83 \text{ h}}$$

The balloon will lose 10 kPa of pressure within about 2 hours and 50 minutes.

♦ The correct answer is **B**.

P.12 | Solution

Part 1: The molar flux is given by equation 10,

$$N_A = \frac{D_{AB}P}{RTL} \ln\left(\frac{P - P_{A,\infty}}{P - P_{A,0}}\right)$$

Here, the reference pressure $P = P_{\text{atm}} = 101.3$ kPa, $P_{A,\infty} = P_{\text{atm}}$, and $P_{A,0} = 215$ mmHg = 28.7 kPa. The mass diffusivity is converted as $D_{AB} = 1.66 \times 10^{-5}$ m²/s. Substituting these and other variables in the equation above, we get

$$N_A = \frac{D_{AB}P}{RTL} \ln\left(\frac{P - P_{A,\infty}}{P - P_{A,0}}\right) = \frac{(1.66 \times 10^{-5}) \times 101.3}{8.314 \times 303 \times 0.5} \ln\left(\frac{101.3 - 0}{101.3 - 28.7}\right) = 4.45 \times 10^{-7} \frac{\text{kmol}}{\text{m}^2 \cdot \text{sec}}$$

$$\therefore N_A = 4.45 \times 10^{-4} \frac{\text{mol}}{\text{m}^2 \cdot \text{sec}}$$

The cross-sectional area of the cylinder is $A = \pi \times 1.0^2/4 = 0.785$ m². The rate of emission follows as

$$W_A = N_A A = (4.45 \times 10^{-4}) \times 0.785 = 3.49 \times 10^{-4} \text{ mol/sec}$$

The amount of methanol that evaporates over the course of a day follows as

$$\Delta m_A = 3.49 \times 10^{-4} \frac{\text{mol}}{\text{sec}} \times 86,400 \frac{\text{sec}}{\text{day}} \times 32 \frac{\text{g}}{\text{mol}} = \boxed{965 \text{ g MeOH/day}}$$

♦ The correct answer is **D**.

Part 2: Recalling that $D_{AB} \propto T^{3/2}$, we first update the diffusion coefficient,

$$D_{AB} = 0.166 \times \left(\frac{313}{303}\right)^{3/2} = 0.174 \text{ cm}^2/\text{sec}$$

In addition, we now have $P_{A,0} = 265$ mmHg = 35.3 kPa. Substituting into equation 10 gives

$$N_A = \frac{(1.74 \times 10^{-5}) \times 101.3}{8.314 \times 313 \times 0.5} \ln\left(\frac{101.3 - 0}{101.3 - 35.3}\right) = 5.80 \times 10^{-7} \frac{\text{kmol}}{\text{m}^2 \cdot \text{sec}}$$

$$\therefore N_A = 5.80 \times 10^{-4} \frac{\text{mol}}{\text{m}^2 \cdot \text{sec}}$$

This corresponds to a rate of emission $W_A = (5.80 \times 10^{-4}) \times 0.785 = 4.55 \times 10^{-4}$ mol/sec. The amount of methanol that evaporates per day is then

$$W_A = 4.55 \times 10^{-3} \frac{\text{mol}}{\text{sec}} \times 86,400 \frac{\text{sec}}{\text{day}} \times 32 \frac{\text{g}}{\text{mol}} = \boxed{1260 \text{ g MeOH/day}}$$

That is, increasing the temperature from 30 to 40°C will cause the rate of evaporation of methanol to increase by about 30 percent.

♦ The correct answer is **A**.

P.13 | Solution

Part 1: For hydrogen gas, we read $\sigma_B = 2.827$ Å and $\varepsilon_B/\kappa = 59.7$ K (Table 2). The collision diameter and ε_{AB}/κ are respectively determined as

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{4.08 + 2.827}{2} = 3.454 \text{ Å} \rightarrow \sigma_{AB}^2 = 11.93$$

$$\frac{\varepsilon_{AB}}{\kappa} = \sqrt{(\varepsilon_A/\kappa)(\varepsilon_B/\kappa)} = \sqrt{207.6 \times 59.7} = 111.3$$

$$\therefore \frac{kT}{\varepsilon_{AB}} = \frac{T}{(\varepsilon_{AB}/k)} = \frac{873}{111.3} = 7.84$$

Interpolating from Table 3, the collision integral $\Omega_D = 0.776$. Substituting in equation 1 gives

$$D_{AB} = \frac{0.001858T^{3/2} \left(\frac{1}{M_A} + \frac{1}{M_B} \right)^{1/2}}{P\sigma_{AB}^2\Omega_D} = \frac{0.001858 \times 873^{1.5} \times \left[\frac{1}{2} + \frac{1}{(75+3)} \right]^{1/2}}{\left[303.9 / (1.01 \times 10^5) \right] \times 11.93 \times 0.776} = \boxed{1230 \text{ cm}^2/\text{s}}$$

◆ The correct answer is **D**.

Part 2: The molar flux is given by equation 10, here written in terms of concentrations,

$$N_A = \frac{CD_{AB}}{L} \ln \left(\frac{1+y_{A,0}}{1+y_{A,S}} \right)$$

The concentration of AsH₃ is given by

$$C = \frac{P}{RT} = \frac{303.9 / (1.01 \times 10^5)}{82.06 \times 873} = 4.20 \times 10^{-8} \text{ mol/cm}^3$$

so that N_A is calculated as

$$N_A = \frac{(4.20 \times 10^{-8}) \times 1230}{6.0} \ln \left(\frac{1+0.2}{1+0} \right) = 1.57 \times 10^{-6} \text{ mol/cm}^2 \cdot \text{s}$$

Given the surface area of the wafer $S = \pi \times 15^2/4 = 177 \text{ cm}^2$ and the molar mass of arsine $M = 78 \text{ g/mol}$, the deposition rate of arsenic is found as

$$\dot{m}_A = N_A S = (1.57 \times 10^{-6}) \times 177 \times 78 \times 60 = \boxed{1.30 \text{ g/min}}$$

◆ The correct answer is **B**.

P.14 **Solution**

This problem is an example of transient mass diffusion in a semi-infinite stationary medium. This system can be modeled with equation 12, namely

$$\frac{C_x - C_0}{C_s - C_0} = \text{erfc} \left(\frac{x}{2\sqrt{D_{AB}t}} \right)$$

Here, C_s is the surface concentration of gas diffusing into the surface, C_0 is the initial concentration of the element in the solid, x is the distance from the surface, C_x is the concentration at a distance x from the surface, D_{AB} is the diffusion coefficient, and t is time. In the case in point, $C_s = 1.19\%$, $C_0 = 0.15\%$, $C_x = 0.45\%$, $x = 0.5 \times 10^{-3} \text{ m}$, and $D = 1.1 \times 10^{-11} \text{ m}^2/\text{s}$. Substituting in the formula above yields

$$\frac{C_x - C_0}{C_s - C_0} = \text{erfc} \left(\frac{x}{2\sqrt{D_{AB}t}} \right) = \frac{0.45 - 0.15}{1.19 - 0.15} = 0.288$$

Referring to Table 5, we see that the value of η for which $\text{erfc } \eta = 0.288$ is about 0.751. Thus,

$$\begin{aligned} \eta &= \frac{x}{2\sqrt{D_{AB}t}} = 0.751 \\ \therefore \frac{0.5 \times 10^{-3}}{2 \times \sqrt{(1.1 \times 10^{-11}) \times t'}} &= 0.751 \\ \therefore t' &= 10,100 \text{ sec} = \boxed{2.81 \text{ h}} \end{aligned}$$

The desired concentration of carbon will be achieved within a period of 2 hours and 49 minutes.

◆ The correct answer is **C**.

P.15 | Solution

The vapor pressure in the tent is the saturation pressure of water at 25°C since the oxygen in the tent is saturated, and thus the partial pressure of oxygen in the tank is

$$P_{O_2} = P - P_v = 130 - 3.17 = 126.83 \text{ kPa}$$

Then, the mole fraction of oxygen in the water at the pond surface becomes

$$y_{O_2, \text{liquid side}}(0) = \frac{P_{O_2, \text{gas side}}(0)}{H} = \frac{1.2683 \text{ bar}}{43,600 \text{ bar}} = 2.91 \times 10^{-5}$$

The molar concentration of oxygen at a depth of 1 cm from the surface after 2 days can be determined with equation 12, namely

$$\frac{y_{O_2} - y_{O_2,i}}{y_{O_2,s} - y_{O_2,i}} = \text{erfc}\left(\frac{x}{2\sqrt{D_{AB}t}}\right)$$

$$\therefore \frac{y_{O_2} - 0}{2.91 \times 10^{-5} - 0} = \text{erfc}\left(\frac{0.02}{2\sqrt{(2.4 \times 10^{-9}) \times (2 \times 86,400)}}\right) = 0.728$$

$$\therefore y_{O_2} = 0.728 \times (2.91 \times 10^{-5}) = \boxed{2.12 \times 10^{-5}}$$

That is, there will be 21 moles of oxygen per million at a depth of 1 cm from the surface within 2 days.

♦ The correct answer is **B**.

P.16 | Solution

Part 1: Much like Problems 14 and 15, the problem at hand is one of transient mass transfer in a semi-infinite medium. The pertinent equation is

$$\frac{w_A(x,t) - w_{A,i}}{w_{A,s} - w_{A,i}} = \text{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\therefore \frac{0.0032 - 0.0012}{0.011 - 0.0012} = \text{erfc}\left(\frac{0.7 \times 10^{-3}}{2\sqrt{(7.2 \times 10^{-12}) \times t}}\right) = 0.204$$

The value of Z such that $\text{erf}(Z) = 0.204$ is read as 0.90 from Table 5, with the result that

$$t' = \frac{x^2}{4D_{AB} \times 0.9^2} = \frac{(0.7 \times 10^{-3})^2}{4 \times (7.2 \times 10^{-12}) \times 0.9^2} = 21,000 \text{ s} = \boxed{5.83 \text{ h}}$$

♦ The correct answer is **C**.

Part 2: The solution remains unchanged up until the point where we established that $Z = 0.90$. The only difference is that, when computing t , we use $D_{AB} = 2.1 \times 10^{-20} \text{ m}^2/\text{s}$ as the diffusion coefficient for a furnace temperature of 500 K. Indeed,

$$t = \frac{x^2}{4D_{AB} \times 0.9^2} = \frac{(0.7 \times 10^{-3})^2}{4 \times (2.1 \times 10^{-20}) \times 0.9^2} = 7.20 \times 10^{12} \text{ s}$$

This equates to nearly 230,000 years (!) and indicates that the desired level of hardening cannot be practically achieved with a furnace temperature of 500 K. The process must be carried out at a higher temperature so as to increase the diffusion coefficient D_{AB} and thereby reduce t .

♦ The correct answer is **D**.

Answer Summary

Problem 1	1.1	B
	1.2	Open-ended pb.
	1.3	Open-ended pb.
Problem 2	2.1	D
	2.2	Open-ended pb.
	2.3	Open-ended pb.
Problem 3		A
Problem 4		D
Problem 5		B
Problem 6		C
Problem 7	7.1	B
	7.2	B
Problem 8		A
Problem 9		A
Problem 10		C
Problem 11		B
Problem 12	12.1	D
	12.2	A
Problem 13	13.1	D
	13.2	B
Problem 14		C
Problem 15		B
Problem 16	16.1	C
	16.2	D

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