Hines et. al.

Example 2.1

Estimate the diffusion coefficient for the hydrogen–ammonia system at 25°C and 1 atm pressure. Use the collision integrals to find the diffusivity at 85°C. Compare the results with experimental values.

Solution:

$$P = 1 \text{ atm}$$

$$T = 298 \text{ K}$$

$$M_A = 2 \qquad M_B = 17$$

From Table 2-3,

$$\sigma_A = 2.827 \times 10^{-10} \text{ m} \qquad \frac{\epsilon_A}{k} = 59.7 \text{ K}$$

$$\sigma_B = 2.900 \times 10^{-10} \text{ m} \qquad \frac{\epsilon_B}{k} = 558.3 \text{ K}$$

$$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{2.827 \times 10^{-10} + 2.900 \times 10^{-10}}{2} = 2.8635 \times 10^{-10} \text{ m}$$

$$\frac{\epsilon_{AB}}{k} = \left(\frac{\epsilon_A}{k} \times \frac{\epsilon_B}{k}\right)^{1/2} = [(59.7)(558.3)]^{1/2} = 182.57 \text{ K}$$

$$\frac{kT}{\epsilon_{AB}} = \frac{298}{182.57} = 1.632$$

From Table 2-4,

$$\Omega_D = 1.158$$

$$\frac{1}{M_A} + \frac{1}{M_B} = \frac{1}{2} + \frac{1}{17} = 0.5588$$

From Eq. (2-8),

$$D_{AB} = \frac{1.858 \times 10^{-27} T^{3/2}}{P\sigma_{AB}^2 \Omega_D}\left(\frac{1}{M_A} + \frac{1}{M_B}\right)^{1/2}$$

$$= \frac{1.85 \times 10^{-27}(298)^{3/2}}{1(2.8635 \times 10^{-10})^2(1.158)}(0.5588)^{1/2}$$

$$= 7.52 \times 10^{-5} \text{ m}^2/\text{s}$$

Temperature correction:

$$D_{AB,T_2} = D_{AB,T_1}\left(\frac{T_2}{T_1}\right)^{3/2} \frac{\Omega_{T_1}}{\Omega_{T_2}}$$

$$\frac{kT_2}{\epsilon_{AB}} = \frac{358}{182.57} = 1.961$$

Table 2-4 gives

$$\Omega_D = 1.082$$

$$D_{AB,T_2} = 7.52 \times 10^{-5}\left(\frac{358}{298}\right)^{3/2}\frac{1.158}{1.082}$$

$$= 1.06 \times 10^{-4} \text{ m}^2/\text{s}$$

From Table 2-5 the experimental values at 25 and 85°C are 7.83×10^{-5} m²/s and 1.093×10^{-4} m²/s, respectively.