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Example 2.2

Using the equation of Wilke and Chang, determine the diffusivity at low concentration for the following diffusing pairs at 25°C and compare the results with experimental values: (a) methanol–water, and (b) ethanol–water.

A solute
B water

Solution:

$$T = 298 \qquad \xi_B = 2.6 \qquad M_B = 18$$

From Appendix A,

$$\mu \simeq \mu_B(25°C) = 0.89 \text{ cP (mPa·s)}$$

From Table 2-1,

$$V_A(\text{methanol}) = 0.0148 + 4(0.0037) + 0.0074 = 0.037$$

$$V_A(\text{ethanol}) = 2(0.0148) + 6(0.0037) + 0.0074 = 0.0592$$

Substituting into the Wilke–Chang equation gives

Methanol–water:

$$D^\circ_{AB} = \frac{(1.17 \times 10^{-13})[(2.6)(18)]^{1/2}(298)}{(0.037)^{0.6}(0.89)} = 1.94 \times 10^{-9} \text{ m}^2/\text{s}$$

Ethanol–water:

$$D^\circ_{AB} = \frac{(1.17 \times 10^{-13})[(2.6)(18)]^{1/2}(298)}{(0.0592)^{0.6}(0.89)} = 1.46 \times 10^{-9} \text{ m}^2/\text{s}$$

Experimental diffusivities obtained from Perry and Chilton's *Chemical Engineers' Handbook* (1963) are 1.6×10^{-9} m²/s for methanol–water and 1.28×10^{-9} m²/s for ethanol–water.

Table 2-1:

Carbon 14.8×10^{-3} m³/kg atom

Hydrogen: 3.7×10^{-3} "

Methanol: CH_4O

Oxygen: 7.4×10^{-3} m³/kg atom

Ethanol $[CH_3]_2O$

B solvent water, A solute Methanol or ethanol

Example 2.3

Determine the diffusivity of ethanol in benzene at 30°C using the equation of Wilke and Chang and the equation of Sitaraman et al. Convert the diffusivity to 15°C and compare the result with the experimental value given in Table 2-6.

Solution:

$$T = 303\ \text{K} \qquad \xi_B = 1 \qquad M_B = 78$$

From the *Chemical Engineers' Handbook,*

$$\Delta H_A = 85.52 \times 10^4\ \text{J/kg} \qquad \Delta H_B = 43.33 \times 10^4\ \text{J/kg}$$

From Table 2-1,

$$V_A = 2(0.0148) + 6(0.0037) + 0.0074 = 0.0592$$

From Appendix A,

$$\mu_B(30°\text{C}) = 0.56\ \text{cP} \qquad \mu_B(15°\text{C}) = 0.70\ \text{cP}$$

Substituting into the Wilke–Chang equation yields

$$D^\circ_{AB} = \frac{(1.17 \times 10^{-13})(78)^{1/2}(303)}{(0.0592)^{0.6}(0.56)} = 3.06 \times 10^{-9}\ \text{m}^2/\text{s}$$

Substituting into the equation of Sitaraman et al. gives us

$$D^\circ_{AB} = 16.79 \times 10^{-14}\left[\frac{(78)^{1/2}(43.33 \times 10^4)^{1/3}(303)}{(0.56)(0.0592)^{1/2}(85.52 \times 10^4)^{0.3}}\right]^{0.93}$$

$$= 2.04 \times 10^{-9}\ \text{m}^2/\text{s}$$

Convert to 15°C using the equation of Wilke and Chang:

$$\frac{D^\circ_{AB_2}\mu_2}{T_2} = \frac{D^\circ_{AB_1}\mu_1}{T_1}$$

$$D_{AB} = \frac{288}{303}\left(\frac{0.56}{0.7}\right)(3.06 \times 10^{-9}) = 2.33 \times 10^{-9}\ \text{m}^2/\text{s}$$

The experimental value at 15°C is 2.25×10^{-9} m²/s. If the experimental value given in Table 2-6 is corrected to 30°C by using the Wilke–Chang equation, then at 30°C, $D^\circ_{AB} = 2.96 \times 10^{-9}$ m²/s. This compares favorably with the value predicted by the Wilke–Chang equation.

A ... solute, B ... solvent

Sitaraman et al's eq:

$$D^\circ_{AB} = 16.79 \times 10^{-14}\left(\frac{M_B^{1/2}\,\Delta H_B^{1/3}\,T}{\mu_B\,V_A^{1/2}\,\Delta H_A^{0.3}}\right)^{0.93}$$

ΔH.. latent heats of vaporization at normal boiling points in J/kg

μ... viscosity of solvent in centipoise (mPa·s)