Estimation of Diffusivity Using the Wilke–Chang Equation — CHE324 :PhD Problem University of Alabama

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Problem 4

Estimate the diffusivity of acetic acid in a dilute solution of acetone at 313 K using the Wilke–Chang equation. The following data are provided:

- Temperature, $T = 313\,\mathrm{K}$

- Viscosity of acetone, $\mu = 0.264\,\mathrm{cP}$

- Molecular weight of solute (acetic acid), $M_A = 60.05\,\mathrm{g/mol}$

- Density of acetic acid, $\rho_A = 1.05\,\mathrm{g/cm}^3$

- Molecular weight of solvent (acetone), $M_B = 58.08\,\mathrm{g/mol}$

- Association parameter for acetone, $\phi = 1$

Solution

We use the **Wilke–Chang equation**:

$$D_{AB} = \frac{7.4 \times 10^{-8} \cdot (\phi M_B)^{1/2} \cdot T}{\mu \cdot V_A^{0.6}}$$

where:

- D_{AB} is the diffusivity in cm^2/s

- ϕ is the association parameter of the solvent

- M_B is the molecular weight of the solvent (g/mol)

- μ is the viscosity in centipoise (cP)

- V_A is the molar volume of solute at normal boiling point (cm^3/mol)

Step 1: Estimate the molar volume of acetic acid:

$$V_A = \frac{M_A}{\rho_A} = \frac{60.05}{1.05} \approx 57.19 \, \text{cm}^3/\text{mol}$$

Step 2: Plug into the Wilke–Chang equation:

$$D_{AB} = \frac{7.4 \times 10^{-8} \cdot \sqrt{58.08} \cdot 313}{0.264 \cdot (57.19)^{0.6}}$$

Compute intermediate values:

$$\sqrt{58.08} \approx 7.622, \quad (57.19)^{0.6} \approx 13.85$$

$$D_{AB} = \frac{7.4 \times 10^{-8} \cdot 7.622 \cdot 313}{0.264 \cdot 13.85}$$

$$= \frac{1.7644 \times 10^{-4}}{3.655} \approx 4.827 \times 10^{-5} \, \text{cm}^2/\text{s}$$

Final Answer

$$\boxed{D_{AB} \approx 4.83 \times 10^{-5} \, \text{cm}^2/\text{s}}$$