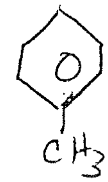
**3.9** GAS DIFFUSIVITY




$N_2$ (A) in Toluene (B)

@ 25°C (298 K)

@ 3 atm

Chapman-Enskog

$$D_{AB} = D_{BA} = \frac{0.00143\, T^{1.75}}{P\, M_{AB}^{1/2} \left[ (\Sigma_v)_A^{1/3} + (\Sigma_v)_B^{1/3} \right]^2}$$

T in K

P in atm $\Rightarrow$ $D_{AB}$ in $\frac{cm^2}{s}$

$M_A = 28$ g/mol

$M_B = 92$ g/mol

$$M_{AB} = \frac{2}{\frac{1}{28} + \frac{1}{92}}$$

$$\boxed{M_{AB} = 42.93 \text{ g/mol}}$$

from Table 3.1:

$(\Sigma_v)_A = 18.5$

$(\Sigma_v)_B = 7(15.9) + 8(2.31) - 18.31 = 111.47$

$$D_{AB} = \frac{0.00143\,(298)^{1.75}}{(3)(42.93)^{1/2}\left[18.5^{1/3} + 111.47^{1/3}\right]^2} \Rightarrow \boxed{D_{AB} = 0.028 \frac{cm^2}{s}}$$

3.11 $CCl_4$ @ 25°C (298K)

@ Methanol (Solvent)

<u>Wilke-Chang Equation:</u>

$$D_{AB} = \frac{7.4\times10^{-8}\,(\Phi_B M_B)^{1/2}\,T}{\mu_B\, V_A^{0.6}}$$

Methanol:

$\Phi_B = 1.9$

$M_B = 32\,g/mol$

$T = 298K$

$\mu_B = 0.55\,cP$ (McCabe et al., App. 9)

$V_A = 4\cdot(21.6) + 14.8 = 101.2\times10^{-3}\,\frac{m^3}{kmol}$

$\Rightarrow V_A = 101.2\,\frac{cm^3}{mol}$

$$D_{AB} = \frac{(7.4\times10^{-8})\,[(1.9)(32)]^{1/2}\,(298)}{(0.55)(101.2)^{0.6}} = 1.96\times10^{-5}\,\frac{cm^2}{s}$$

<u>Experimental:</u> $1.69\times10^{-5}\,\Big|\,\frac{298}{288} = 1.75\times10^{-5}\,\frac{cm^2}{s}$

$\Rightarrow$ 11.4% greater than experimental

(b) Ethanol

$\Phi_B = 1.5$ $\quad$ $\mu_B = 1.1\ cP$ (McCabe et al, App. 9)

$M_B = 46\ g/mol$ $\quad$ $V_A = 101.2\ \frac{cm^3}{mol}$

$T = 298\ K$

$$D_{AB} = \frac{(7.4 \times 10^{-8})\left[(1.5)(46)\right]^{1/2}(298)}{(1.1)(101.2)^{0.6}} = 1.04 \times 10^{-5}\ \frac{cm^2}{s}$$

Experimental: $1.50 \times 10^{-5}\ \frac{cm^2}{s}$

$\Rightarrow$ 30.7% less than experimental

(c) Benzene

$\Phi_B = 1.0$ $\quad$ $\mu_B = 0.6\ cP$ (McCabe et al, App. 9)

$M_B = 78\ g/mol$ $\quad$ $V_A = 101.2\ \frac{cm^3}{mol}$

$T = 298\ K$

$$D_{AB} = \frac{(7.4 \times 10^{-8})\left[(1.0)(78)\right]^{1/2}(298)}{(0.6)(101.2)^{0.6}} = 2.03 \times 10^{-5}\ \frac{cm^2}{s}$$

Experimental: $1.92 \times 10^{-5}\ \frac{cm^2}{s}$

$\Rightarrow$ 5.7% greater than experimental

(d) n-hexane

$\Phi_B = 1.0$

$M_B = 86$ g/mol

$T = 298$K

$\mu_B = 0.31$ cP (McCabe et al, App. 9)

$V_A = 101.2 \frac{cm^3}{mol}$

$$D_{AB} = \frac{(7.4\times10^{-8})\left[(1.0)(86)\right]^{1/2}(298)}{(0.31)(101.2)^{0.6}} = 4.13\times10^{-5}\frac{cm^2}{s}$$

Experimental: $3.70\times10^{-5}\frac{cm^2}{s}$

$\Rightarrow$ 11.6% greater than experimental

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HAYDUK-MINHAS TECHNIQUE:

$$(D_{AB})_\infty = \frac{1.55\times10^{-8}\, T^{1.29}\left(P_B^{0.5}/P_A^{0.42}\right)}{\mu_B^{0.92}\, V_B^{0.23}}$$

(a) Methanol

$T = 298$K

$\mu_B = 0.55$ cP

$P_B = 88.8$

$V_B = 37 \frac{cm^3}{mol}$

$P_A = 9 + 4(55.2) = 229.8$

$(D_{AB})_\infty = 1.75\times10^{-5}\frac{cm^2}{s}$ $\Rightarrow$ matches exp. well

(b) Ethanol

$T = 298\ K$ $\mu_B = 1.1\ cP$

$\varphi_B = 125.3$ $V_B = 59.2\ \frac{cm^3}{mol}$

$\varphi_A = 229.8$

$$(D_{AB})_\infty = 0.985 \times 10^{-5}\ \frac{cm^2}{s}$$ ⇒ 50% off exp.

(c) Benzene

$T = 298K$ $\mu_B = 0.6\ cP$

$\varphi_B = 205.3$ $V_B = 96\ \frac{cm^3}{mol}$

$\varphi_A = 229.8$

$$(D_{AB})_\infty = 1.97 \times 10^{-5}\ \frac{cm^2}{s}$$ ⇒ almost right on

(d) n-hexane

$T = 298\ K$ $\mu_B = 0.31\ cP$

$\varphi_B = 271$ $V_B = 140.6\ \frac{cm^3}{mol}$

$\varphi_A = 229.8$

$$(D_{AB})_\infty = 3.81 \times 10^{-5}\ \frac{cm^2}{s}$$ ⇒ Closer to exp. than Wilke-Chang