Hw1: 24.4, 24.5, 24.8, 24.10

24.4

24.4.

$$\vec{N}_A = -cD_{AB}\nabla y_A + y_A[\vec{N}_A + \vec{N}_B]$$

Multiply each term by M_A and treat c as a constant.

$$\vec{N}_A M_A = -D_{AB}\nabla(c_A M_A) + y_A[\vec{N}_A + \vec{N}_B]M_A$$

$$w_A = \frac{y_A M_A}{y_A M_A + y_B M_B} = \frac{y_A M_A}{M_{ave}}$$

$$\therefore y_A M_A = w_A M_{ave}$$

$$\vec{n}_A = -D_{AB}\nabla\rho_A + w_A M_{ave}\underbrace{[\vec{N}_A + \vec{N}_B]}_{\vec{n}_A + \vec{n}_B}$$

With constant ρ

$$\vec{n}_A = -D_{AB}\rho\nabla w_A + w_A[\vec{n}_A + \vec{n}_B]$$

b) constant c

$$\vec{N}_A = -D_{AB}\nabla c_A + \frac{c_A}{c}[c_A\vec{v}_A + c_B\vec{v}_B]$$

$$c_A\vec{v}_A = -D_{AB}\nabla c_A + c_A\vec{v}$$

$$c_A(\vec{v}_A - \vec{v}) = \vec{J}_A = -D_{AB}\nabla c_A$$

c) Using results obtained in (a)

$$\vec{n}_A = -D_{AB}\rho\nabla w_A + w_A[\vec{n}_A + \vec{n}_B]$$

$$\rho_A\vec{v}_A = -D_{AB}\rho\nabla w_A + \frac{\rho_A}{\rho}[\rho_A\vec{v}_A + \rho_B\vec{v}_B]$$

$$= -D_{AB}\rho\nabla w_A + \rho_A\vec{v}$$

$$\rho_A(\vec{v}_A - \vec{v}) = \vec{j}_A = -\rho D_{AB}\nabla w_A$$

24.5

a) $N_{Az} = -cD_{AB}\frac{dy_A}{dz} + y_A[N_{Az} + N_{Bz}]$

\+ $N_{Bz} = -cD_{BA}\frac{dy_B}{dz} + y_B[N_{Az} + N_{Bz}]$

Add

$N_{Az} + N_{Bz} = -cD_{AB}\frac{dy_A}{dz} - cD_{BA}\frac{dy_B}{dz} + (y_A + y_B)(N_{Az} + N_{Bz})$ (1.0)

$0 = -cD_{AB}\frac{dy_A}{dz} - cD_{BA}\frac{dy_B}{dz}$

or $D_{AB}\frac{dy_A}{dz} = -D_{BA}\frac{dy_B}{dz}$

Since $y_A + y_B = 1.0$; $\frac{dy_A}{dz} = -\frac{dy_B}{dz}$

$\therefore \underline{D_{AB} = D_{BA}}$

b) $\vec{J}_A + \vec{J}_B = -cD_{AB}\frac{dy_A}{dz} - cD_{BA}\frac{dy_B}{dz}$

But $D_{AB} = D_{BA}$ and $\frac{dy_A}{dz} = -\frac{dy_B}{dz}$

$\therefore \vec{J}_A + \vec{J}_B = -cD_{AB}\frac{dy_A}{dz} + cD_{AB}\frac{dy_A}{dz} = \underline{0}$

c) $\vec{N}_A + \vec{N}_B = -cD_{AB}\frac{dy_A}{dz} + y_A[\vec{N}_A + \vec{N}_B]$

$-cD_{BA}\frac{dy_B}{dz} + y_B[\vec{N}_A + \vec{N}_B]$

$= -cD_{AB}\frac{dy_A}{dz} + cD_{AB}\frac{dy_B}{dz}$

$+ (y_A + y_B)[\vec{N}_A + \vec{N}_B]$

$= (1)[\vec{N}_A + \vec{N}_B] = \underline{c\left[\frac{\vec{N}_A + \vec{N}_B}{c}\right]}$

$= c\left[\frac{c_A\vec{v}_A + c_B\vec{v}_B}{c}\right] = \underline{c\vec{V}}$

24.8

Hirschfelder

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

$T = 673\ K$; $T^{3/2} = (673)^{3/2} = 17{,}459$

$P = 2.0\ atm$

$M_A = M_B = 58$; $\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} = 0.1857$

	ϵ_i	σ_i
iso-b	313	5.341
n-b	410	4.997

$$\sigma_{AB} = \frac{5.341 + 4.997}{2} = 5.169$$

$$\sigma_{AB}^2 = 26.718$$

$$\frac{\epsilon_{AB}}{K} = \sqrt{(313)(410)} = 358.2$$

$$\frac{TK}{\epsilon_{AB}} = \frac{673}{358.2} = 1.88 \text{ ; } \Omega_D = 1.098$$

$$D_{AB} = \frac{0.001858\,(17{,}459)(0.1857)}{(2)(26.718)(1.098)} = 0.103\ \frac{cm^2}{s}$$

Fuller-Schettler & Giddings

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

$T^{1.75} = (673)^{1.75} = 88{,}925$

$(\Sigma v_A) = (\Sigma v_B) = [4(16.5) + 10(1.98)] = 85.8$

$[(\Sigma v_A)^{1/3} + (\Sigma v_B)^{1/3}]^2 = [4.404 + 4.404]^2$

$= 77.58$

$$D_{AB} = \frac{10^{-3}(88{,}925)(0.1857)}{(2)(77.58)} = 0.106\ \frac{cm^2}{s}$$

24.10

24.10

	MW	ϵ_i/K	σ_i
$SiCl_4$	169.89	358	5.08
H_2	2.016	33.3	2.968

$T^{3/2} = (1073)^{3/2} = 35,148$

$P = 1 atm$

$\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} = \left[\frac{1}{169.89} + \frac{1}{2.016}\right]^{1/2} = 0.7085$

$\sigma_{AB} = \frac{\sigma_A + \sigma_B}{2} = \frac{5.08 + 2.968}{2} = 4.024$

$\sigma_{AB}^2 = 16.193$

$\frac{\epsilon_{AB}}{K} = \sqrt{(358)(33.3)} = 109.19$

$\frac{TK}{\epsilon_{AB}} = \frac{1073}{109.19} = 9.83 ; \Omega_D = 0.7446$

$D_{SiH_4-H_2} = \frac{0.001858(35,148)(0.7085)}{(1)(16.193)(0.7446)}$

$= 3.837 \ cm^2/s$

b)

	MW	ϵ_i/K	σ_i
$SiCl_4$	169.89	358	5.08
HCl	36.46	360	3.305

$T^{3/2} = 35,148$

$\left[\frac{1}{M_A} + \frac{1}{M_B}\right]^{1/2} = \left[\frac{1}{169.89} + \frac{1}{36.46}\right]^{1/2} = 0.182$

$\sigma_{AB} = \frac{5.08 + 3.305}{2} = 4.193$

$\sigma_{AB}^2 = 17.58$

$\frac{\epsilon_{AB}}{K} = \sqrt{(358)(360)} = 359$

$\frac{TK}{\epsilon_{AB}} = \frac{1073}{359} = 2.99 ; \Omega_D = 0.9586$

$D_{SiCl_4-HCl} = \frac{0.001858(35,148)(0.182)}{(1)(17.58)(0.9586)}$

$= 0.705 \ cm^2/s$

Gas mixture

$y_{SiH_4} = 0.40$ $\quad y'_{H_2} = \frac{0.40}{0.60} = 0.667$

$y_{H_2} = 0.40$

$y_{HCl} = 0.20$ $\quad y'_{HCl} = \frac{0.20}{0.60} = 0.333$

$$D_{SiCl_4\text{-}mix} = \frac{1}{\frac{y'_{H_2}}{D_{SiCl_4\text{-}H_2}} + \frac{y'_{HCl}}{D_{SiCl_4\text{-}HCl}}}$$

$$= \frac{1}{\frac{0.667}{3.837} + \frac{0.333}{0.705}} = 1.547 \frac{cm^2}{s}$$