CHAPTER FOUR

4.1 **a.** <u>Continuous, Transient</u>

b. Input – Output = Accumulation
No reactions ⇒ Generation = 0, Consumption = 0

$$6.00\frac{\text{kg}}{\text{s}} - 3.00\frac{\text{kg}}{\text{s}} = \frac{dn}{dt} \Rightarrow \underline{\underline{\frac{dn}{dt} = 3.00\frac{\text{kg}}{\text{s}}}}$$

c.

$$t = \frac{1.00\,\text{m}^3}{} \left| \frac{1000\,\text{kg}}{1\,\text{m}^3} \right| \frac{1\,\text{s}}{3.00\,\text{kg}} = \underline{\underline{333\ \text{s}}}$$

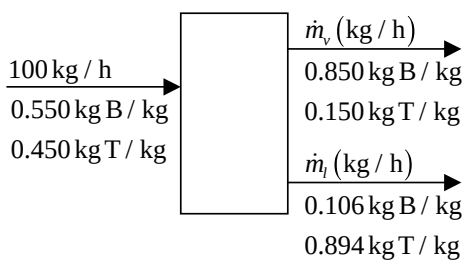
4.2 **a.** <u>Continuous, Steady State</u>

b. $k = 0 \Rightarrow \underline{\underline{\text{C}_\text{A} = \text{C}_\text{A0}}}$ $\qquad k = \infty \Rightarrow \underline{\underline{\text{C}_\text{A} = 0}}$

c. Input – Output – Consumption = 0
Steady state ⇒ Accumulation = 0
A is a reactant ⇒ Generation = 0

$$\dot{V}\left(\frac{\text{m}^3}{\text{s}}\right)C_{A0}\left(\frac{\text{mol}}{\text{m}^3}\right) = \dot{V}\left(\frac{\text{m}^3}{\text{s}}\right)C_A\left(\frac{\text{mol}}{\text{m}^3}\right) + kVC_A\left(\frac{\text{mol}}{\text{s}}\right) \Rightarrow \underline{\underline{C_A = \frac{C_{A0}}{1 + \frac{kV}{\dot{V}}}}}$$

4.3 **a.**



Input – Output = 0
Steady state ⇒ Accumulation = 0
No reaction ⇒ Generation = 0, Consumption = 0

(1) Total Mass Balance: $100.0\ \text{kg/h} = \dot{m}_v + \dot{m}_l$

(2) Benzene Balance: $[0.550 \times 100.0]\ \text{kg B/h} = 0.850\dot{m}_v + 0.106\dot{m}_l$

Solve (1) & (2) simultaneously ⇒ $\underline{\underline{\dot{m}_v = 59.7\ \text{kg/h},\ \dot{m}_l = 40.3\ \text{kg/h}}}$

b. The flow chart is identical to that of (a), except that mass flow rates (kg/h) are replaced by masses (kg). The balance equations are also identical (initial input = final output).

c. Possible explanations ⇒ a chemical reaction is taking place, the process is not at steady state, the feed composition is incorrect, the flow rates are not what they are supposed to be, other species are in the feed stream, measurement errors.

4.4 **b.** $n\,(\text{mol})$ $\longrightarrow$

$0.500\ \text{mol N}_2/\text{mol}$

$0.500\ \text{mol CH}_4/\text{mol}$

$$\frac{0.500n\left(\text{mol N}_2\right)}{}\left|\frac{28\ \text{g N}_2}{\text{mol N}_2}\right|\frac{1\ \text{kg}}{1000\ \text{g}} = \underline{\underline{0.014n\left(\text{kg N}_2\right)}}$$

c. $100.0\ \text{g/s}$ $\longrightarrow$

$x_E\left(\text{g C}_2\text{H}_6/\text{g}\right)$

$x_P\left(\text{g C}_3\text{H}_8/\text{g}\right)$

$x_B\left(\text{g C}_4\text{H}_{10}/\text{g}\right)$

$$\dot{n}_E = \frac{100x_E\left(\text{g C}_2\text{H}_6\right)}{\text{s}}\left|\frac{1\ \text{lb}_\text{m}}{453.593\text{g}}\right|\frac{\text{lb - mole C}_2\text{H}_6}{30\,\text{lb}_\text{m}\ \text{C}_2\text{H}_6}\left|\frac{3600\ \text{s}}{\text{h}}\right.$$

$$= \underline{\underline{26.45x_E\left(\text{lb - mole C}_2\text{H}_6\ /\ \text{h}\right)}}$$

d. $\dot{n}_1\left(\text{lb - mole H}_2\text{O/s}\right)$ $\longrightarrow$

$$\left\{\begin{array}{l}\dot{n}_2\left(\text{lb - mole DA/s}\right)\\ \quad 0.21\ \text{lb - mole O}_2/\text{lb - mole DA}\\ \quad 0.79\ \text{lb - mole N}_2/\text{lb - mole DA}\end{array}\right\}$$

$$\dot{n}_{\text{O}_2} = \underline{\underline{0.21\dot{n}_2\left(\text{lb-mole O}_2\ /\ \text{s}\right)}}$$

$$x_{\text{H}_2\text{O}} = \underline{\underline{\frac{\dot{n}_1}{\dot{n}_1+\dot{n}_2}\left(\frac{\text{lb-mole H}_2\text{O}}{\text{lb-mole}}\right)}}$$

$$x_{\text{O}_2} = \underline{\underline{\frac{0.21\dot{n}_2}{\dot{n}_1+\dot{n}_2}\left(\frac{\text{lb-mole O}_2}{\text{lb-mole}}\right)}}$$

e. $n\left(\text{mol}\right)$ $\longrightarrow$

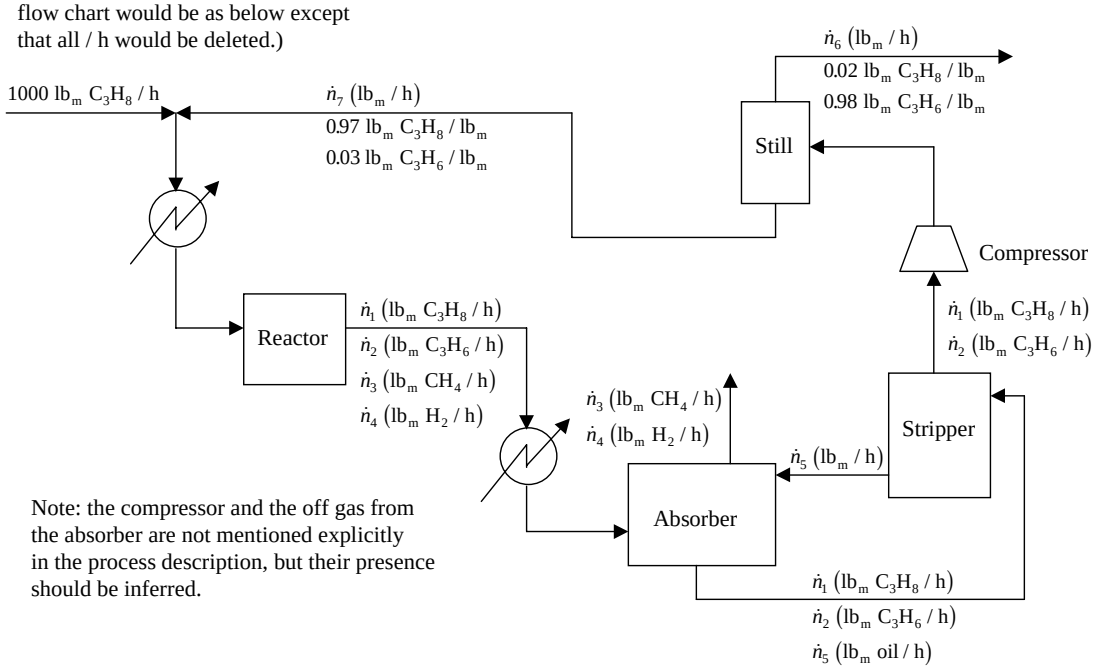
$0.400\ \text{mol NO/mol}$

$y_{\text{NO}_2}\left(\text{mol NO}_2/\text{mol}\right)$

$0.600 - y_{\text{NO}_2}\left(\text{mol N}_2\text{O}_4/\text{mol}\right)$

$$n_{\text{N}_2\text{O}_4} = n\left[0.600 - y_{\text{NO}_2}\right]\left(\text{mol N}_2\text{O}_4\right)$$

4.5 **a.** <u>Basis</u>: 1000 lb_m C_3H_8 / h fresh feed
(Could also take 1 h operation as basis - flow chart would be as below except that all / h would be deleted.)



Note: the compressor and the off gas from the absorber are not mentioned explicitly in the process description, but their presence should be inferred.

4.5 (cont'd)

b. Overall objective: To produce C_3H_6 from C_3H_8.
Preheater function: Raise temperature of the reactants to raise the reaction rate.
Reactor function: Convert C_3H_8 to C_3H_6.
Absorption tower function: Separate the C_3H_8 and C_3H_6 in the reactor effluent from the other components.
Stripping tower function: Recover the C_3H_8 and C_3H_6 from the solvent.
Distillation column function: Separate the C_3H_5 from the C_3H_8.

4.6 **a.** 3 independent balances (one for each species)

b. 7 unknowns ($\dot{m}_1, \dot{m}_3, \dot{m}_5, x_2, y_2, y_4, z_4$)
– 3 balances
– 2 mole fraction summations
2 unknowns must be specified

c. $y_2 = 1 - x_2$

A Balance: $5300x_2\left(\frac{\text{kg A}}{\text{h}}\right) = \left[\dot{m}_3 + (1200)(0.70)\right]\left(\frac{\text{kg A}}{\text{h}}\right)$

Overall Balance: $\left[\dot{m}_1 + 5300\right]\left(\frac{\text{kg}}{\text{h}}\right) = \left[\dot{m}_3 + 1200 + \dot{m}_5\right]\left(\frac{\text{kg}}{\text{h}}\right)$

B Balance: $\left[0.03\dot{m}_1 + 5300x_2\right]\left(\frac{\text{kg B}}{\text{h}}\right) = \left[1200y_4 + 0.60\dot{m}_5\right]\left(\frac{\text{kg B}}{\text{h}}\right)$

$z_4 = 1 - 0.70 - y_4$

4.7 **a.** 3 independent balances (one for each species)

b.

Water Balance: $\frac{400\,g}{\text{min}}\left|\frac{0.885\,\text{g H}_2\text{O}}{\text{g}} = \frac{\dot{m}_R\,(g)}{(\text{min})}\right|\frac{0.995\,\text{g H}_2\text{O}}{\text{g}} \Rightarrow \dot{m}_R = 356\,\text{g/min}$

Acetic Acid Balance: $\left[(400)(0.115)\right]\left(\frac{\text{g CH}_3\text{OOH}}{\text{min}}\right) = \left[0.005\dot{m}_R + 0.096\dot{m}_E\right]\left(\frac{\text{g CH}_3\text{OOH}}{\text{min}}\right)$

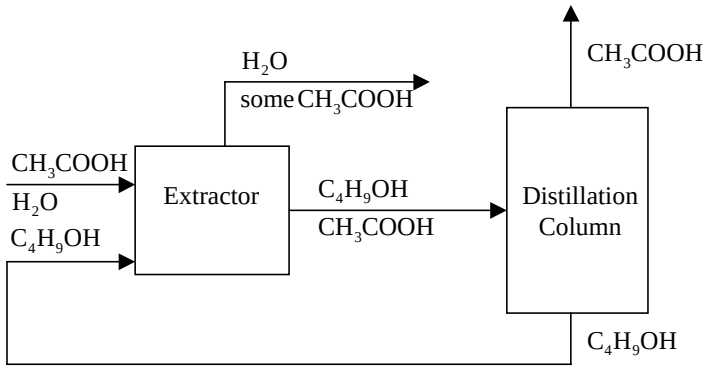
$\Rightarrow \dot{m}_E = 461\,\text{g/min}$

Overall Balance: $\left[\dot{m}_C + 400\right]\left(\frac{\text{g}}{\text{min}}\right) = \left[\dot{m}_R + \dot{m}_E\right]\left(\frac{\text{g}}{\text{min}}\right) \Rightarrow \dot{m}_C = 417\,\text{g/min}$

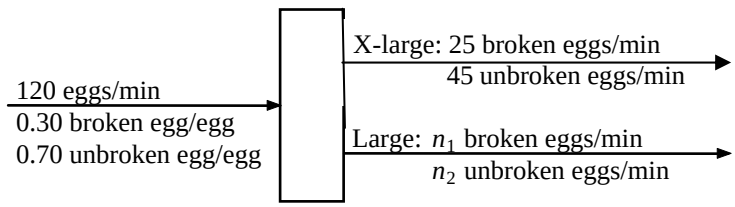
c. $\left[(0.115)(400) - (0.005)(356)\right]\left(\frac{\text{g}}{\text{min}}\right) = \left[(0.096)(461)\right]\left(\frac{\text{g}}{\text{min}}\right) \Rightarrow 44\,\text{g/min} = 44\,\text{g/min}$

4.7 (cont'd)

d.



4.8 **a.**



b. $120 = 25 + 45 + n_1 + n_2 \ (\text{eggs/min}) \Rightarrow \underline{\underline{n_1 + n_2 = 50}}$

$\underline{\underline{(0.30)(120) = 25 + n_1}}$

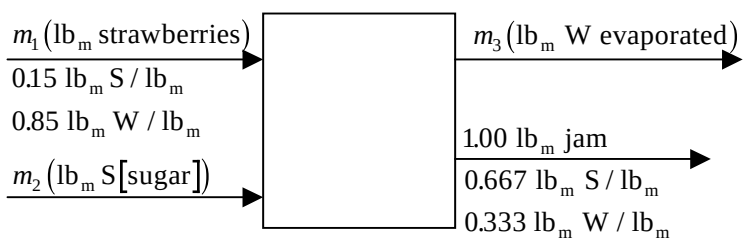
$\Rightarrow \underline{\underline{n_1 = 11}}$, $\underline{\underline{n_2 = 39}}$

c. $n_1 + n_2 = \underline{\underline{50 \text{ large eggs/min}}}$

n_1 large eggs broken/50 large eggs $= (11/50) = \underline{\underline{0.22}}$

d. 22% of the large eggs (right hand) and $(25/70) \Rightarrow 36\%$ of the extra-large eggs (left hand) are broken. Since it does not require much strength to break an egg, the left hand is probably poorly controlled (rather than strong) relative to the right. Therefore, Fred is <u>right-handed</u>.

4.9 **a.**



b. 3 unknowns (m_1, m_2, m_3)

– 2 balances

<u>– 1 feed ratio</u>

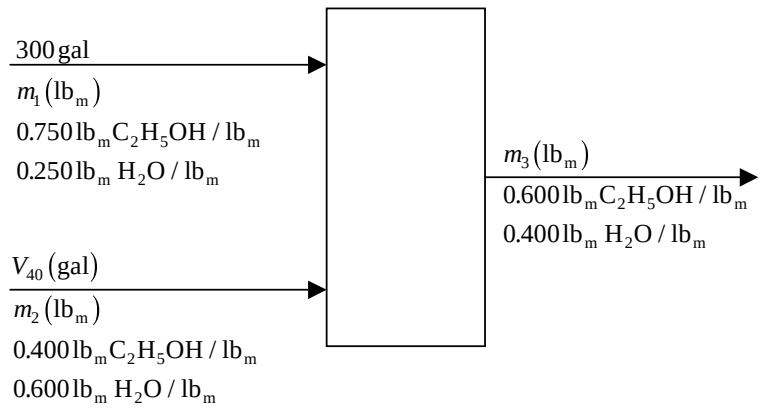
0 DF

c. Feed ratio: $m_1 / m_2 = 45/55$ (1)

S balance: $0.15m_1 + m_2 = 0.667$ (2)

Solve simultaneously $\Rightarrow$ $m_1 = \underline{\underline{0.49 \text{ lb}_m \text{ strawberries}}}$, $m_2 = 0.59 \text{ lb}_m$ sugar

4.10 **a.**



4 unknowns (m_1, m_2, V_{40}, m_3)
– 2 balances
– 2 specific gravities
0 DF

b.

$$m_1 = \frac{300\,\text{gal}}{} \left| \frac{1\,\text{ft}^3}{7.4805\,\text{gal}} \right| \frac{0.877 \times 62.4\,\text{lb}_\text{m}}{\text{ft}^3} = 2195\,\text{lb}_\text{m}$$

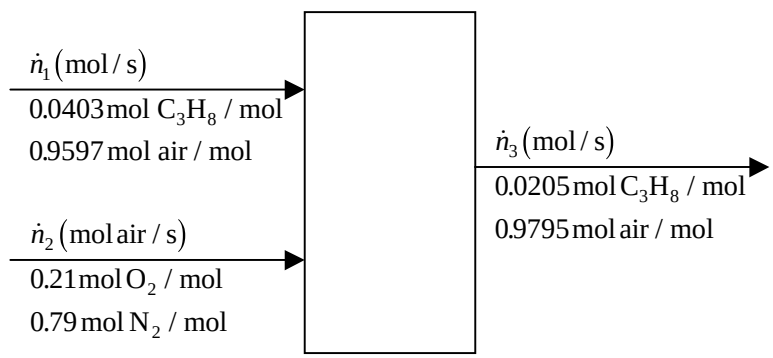
Overall balance: $m_1 + m_2 = m_3$ (1)

C_2H_5OH balance: $0.750 m_1 + 0.400 m_2 = 0.600 m_3$ (2)

Solve (1) & (2) simultaneously $\Rightarrow m_2 = 1646\,\text{lb}_\text{m}, m_3 = 3841\,\text{lb}_\text{m}$

$$V_{40} = \frac{1646\,\text{lb}_\text{m}}{} \left| \frac{\text{ft}^3}{0.952 \times 62.4\,\text{lb}_\text{m}} \right| \frac{7.4805\,\text{gal}}{1\,\text{ft}^3} = \underline{\underline{207\,\text{gal}}}$$

4.11 **a.**



3 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_3$)
– 2 balances
1 DF

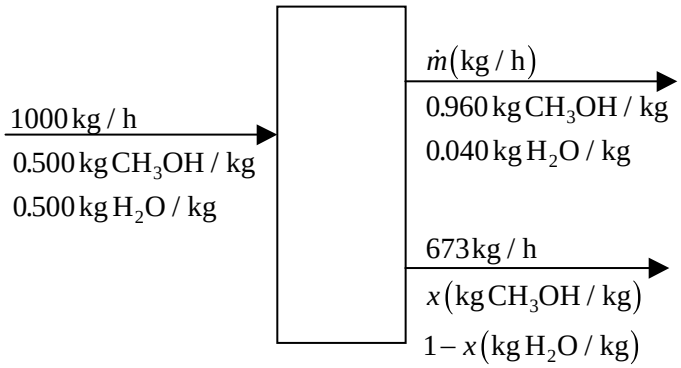
b. Propane feed rate: $0.0403\dot{n}_1 = 150 \Rightarrow \dot{n}_1 = 3722\,(\text{mol/s})$

Propane balance: $0.0403\dot{n}_1 = 0.0205\dot{n}_3 \Rightarrow \dot{n}_3 = 7317\,(\text{mol/s})$

Overall balance: $3722 + \dot{n}_2 = 7317 \Rightarrow \underline{\underline{\dot{n}_2 = 3600\,(\text{mol/s})}}$

c. $\geqq$. The dilution rate should be greater than the value calculated to ensure that ignition is not possible even if the fuel feed rate increases slightly.

4.12 **a.**



2 unknowns ($\dot{m}, x$)
– 2 balances
0 DF

b. Overall balance: $1000 = \dot{m} + 673 \Rightarrow \dot{m} = 327\,\text{kg / h}$

Methanol balance: $0.500(1000) = 0.960(327) + x(673) \Rightarrow \underline{\underline{x = 0.276\,\text{kg CH}_3\text{OH / kg}}}$

Molar flow rates of methanol and water:

$$\frac{673\,\text{kg}}{\text{h}}\left|\frac{0.276\,\text{kg CH}_3\text{OH}}{\text{kg}}\right|\frac{1000\,\text{g}}{\text{kg}}\left|\frac{\text{mol CH}_3\text{OH}}{32.0\,\text{g CH}_3\text{OH}}\right. = \underline{\underline{5.80\times10^3\,\text{mol CH}_3\text{OH / h}}}$$

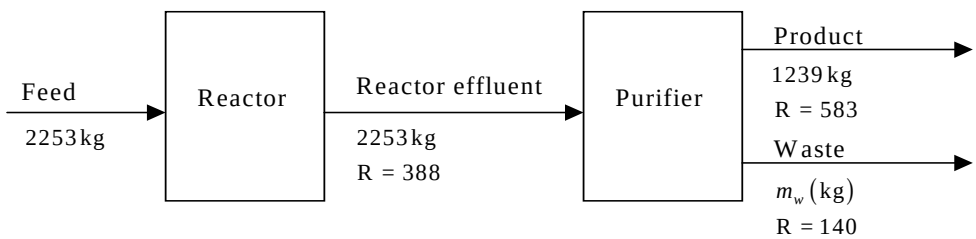
$$\frac{673\,\text{kg}}{\text{h}}\left|\frac{0.724\,\text{kg H}_2\text{O}}{\text{kg}}\right|\frac{1000\,\text{g}}{\text{kg}}\left|\frac{\text{mol H}_2\text{O}}{18\,\text{g H}_2\text{O}}\right. = \underline{\underline{2.71\times10^4\,\text{mol H}_2\text{O / h}}}$$

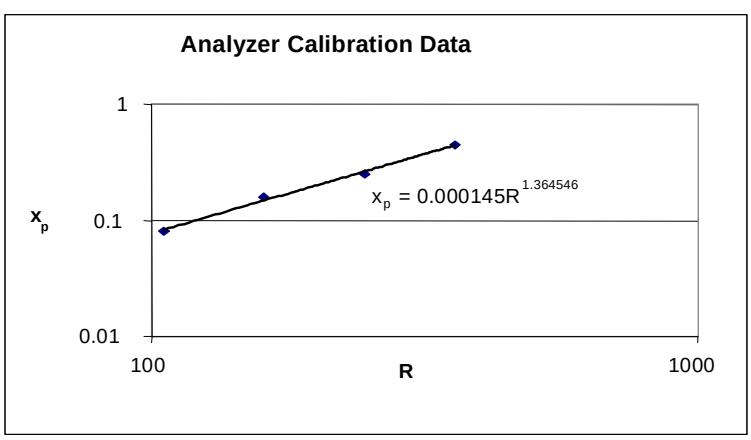
Mole fraction of Methanol:

$$\frac{5.80\times10^3}{5.80\times10^3 + 2.71\times10^4} = \underline{\underline{0.176\,\text{mol CH}_3\text{OH / mol}}}$$

c. Analyzer is wrong, flow rates are wrong, impurities in the feed, a reaction is taking place, the system is not at steady state.

4.13 **a.**





4.13 (cont'd)

b. Effluent: $x_p = 0.000145(388)^{1.3645} = \underline{\underline{0.494\,\text{kg P / kg}}}$

Product: $x_p = 0.000145(583)^{1.3645} = \underline{\underline{0.861\,\text{kg P / kg}}}$

Waste: $x_p = 0.000145(140)^{1.3645} = \underline{\underline{0.123\,\text{kg P / kg}}}$

$$\underline{\text{Efficiency}} = \frac{0.861(1239)}{0.494(2253)} \times 100\% = \underline{\underline{95.8\%}}$$

c. Mass balance on purifier: $2253 = 1239 + m_w \Rightarrow m_w = 1014\,\text{kg}$

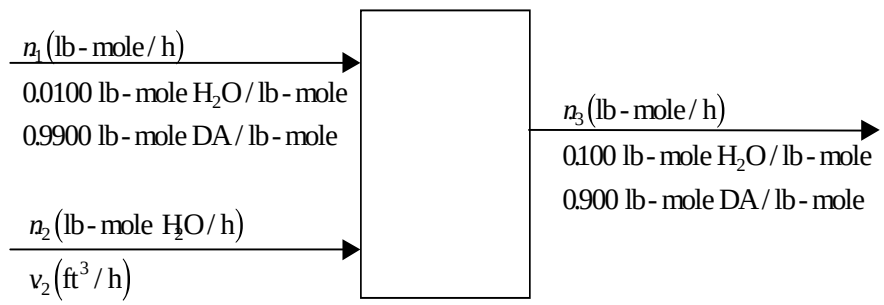
P balance on purifier:

Input: $(0.494\ \text{kg P / kg})(2253\ \text{kg}) = 1113\ \text{kg P}$

Output: $(0.861\ \text{kg P / kg})(1239\ \text{kg}) + (0.123\ \text{kg P / kg})(1014\ \text{kg}) = 1192\ \text{kg P}$

The P balance does not close. Analyzer readings are wrong; impure feed; extrapolation beyond analyzer calibration data is risky -- recalibrate; get data for R > 583; not at steady state; additional reaction occurs in purifier; normal data scatter.

4.14 a.



4 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{v}$) – 2 balances – 1 density – 1 meter reading = 0 DF

Assume linear relationship: $\dot{v} = aR + b$

Slope: $a = \dfrac{\dot{v}_2 - \dot{v}_1}{R_2 - R_1} = \dfrac{96.9 - 40.0}{50 - 15} = 1.626$

Intercept: $b = \dot{v}_a - aR_1 = 40.0 - 1.626(15) = 15.61$

$\dot{v}_2 = 1.626(95) + 15.61 = 170\left(\text{ft}^3 / \text{h}\right)$

$$\dot{n}_2 = \frac{170\ \text{ft}^3}{\text{h}} \left| \frac{62.4\ \text{lb}_\text{m}}{\text{ft}^3} \right| \frac{\text{lb - mol}}{18.0\ \text{lb}_\text{m}} = 589\left(\text{lb - moles H}_2\text{O / h}\right)$$

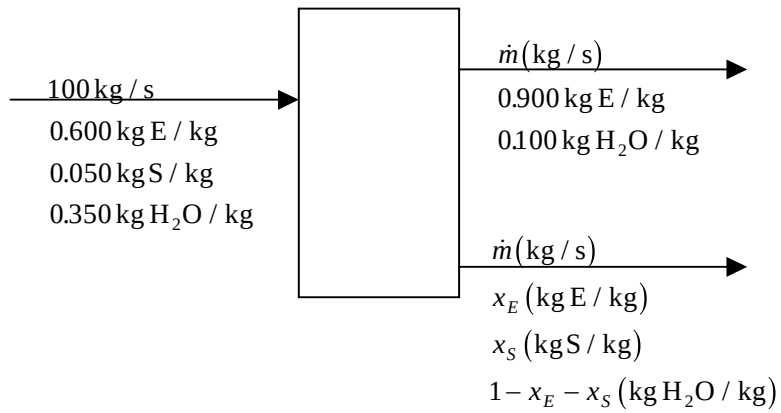
DA balance: $0.9900\dot{n}_1 = 0.900\dot{n}_3$ (1)

Overall balance: $\dot{n}_1 + \dot{n}_2 = \dot{n}_3$ (2)

Solve (1) & (2) simultaneously $\Rightarrow \dot{n}_1 = 5890$ lb - moles / h, $\underline{\underline{\dot{n}_3 = 6480\ \text{lb - moles / h}}}$

b. Bad calibration data, not at steady state, leaks, 7% value is wrong, $\dot{v}$ – R relationship is not linear, extrapolation of analyzer correlation leads to error.

4.15 **a.**



3 unknowns ($\dot{m}, x_E, x_S$)
– 3 balances
0 DF

b. Overall balance: $100 = 2\dot{m} \Rightarrow \dot{m} = 50.0\,(\text{kg / s})$

S balance: $0.050(100) = x_S(50) \Rightarrow \underline{\underline{x_S = 0.100\,(\text{kg S / kg})}}$

E balance: $0.600(100) = 0.900(50) + x_E(50) \Rightarrow x_E = 0.300\,\text{kg E / kg}$

$$\frac{\text{kg E in bottom stream}}{\text{kg E in feed}} = \frac{0.300(50)}{0.600(100)} = \underline{\underline{0.25\,\frac{\text{kg E in bottom stream}}{\text{kg E in feed}}}}$$

c. $x = aR^b \Rightarrow \ln(x) = \ln(a) + b\ln(R)$

$$b = \frac{\ln(x_2 / x_1)}{\ln(R_2 / R_1)} = \frac{\ln(0.400 / 0.100)}{\ln(38/15)} = 1.491$$

$$\ln(a) = \ln(x_1) - b\ln(R_1) = \ln(0.100) - 1.491\ln(15) = -6.340 \Rightarrow a = 1.764 \times 10^{-3}$$

$$\underline{\underline{x = 1.764 \times 10^{-3} R^{1.491}}}$$

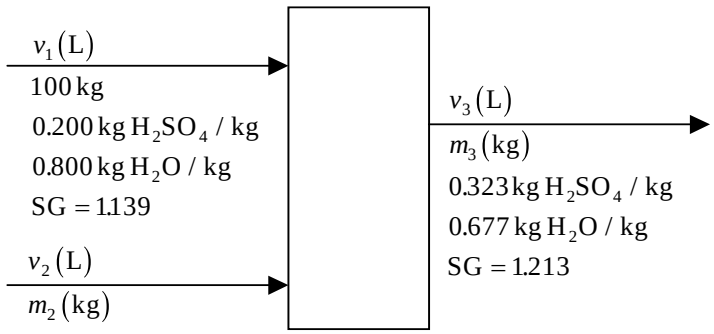
$$R = \left(\frac{x}{a}\right)^{\frac{1}{b}} = \left(\frac{0.900}{1.764 \times 10^{-3}}\right)^{\frac{1}{1.491}} = \underline{\underline{65.5}}$$

d. Device not calibrated – recalibrate. Calibration curve deviates from linearity at high mass fractions – measure against known standard. Impurities in the stream – analyze a sample. Mixture is not all liquid – check sample. Calibration data are temperature dependent – check calibration at various temperatures. System is not at steady state – take more measurements. Scatter in data – take more measurements.

4.16 **a.**

$$\frac{4.00\,\text{mol}\,H_2SO_4}{\text{L of solution}}\left|\frac{0.098\,\text{kg}\,H_2SO_4}{\text{mol}\,H_2SO_4}\right|\frac{\text{L of solution}}{1.213\,\text{kg solution}} = \underline{\underline{0.323\left(\text{kg}\,H_2SO_4/\text{kg solution}\right)}}$$

b.



5 unknowns (v_1, v_2, v_3, m_2, m_3)
– 2 balances
– 3 specific gravities
0 DF

$$\left.\begin{array}{l}\underline{\text{Overall mass balance}}:\ 100 + m_2 = m_3 \\ \underline{\text{Water balance}}:\ 0.800(100) + 0.400m_2 = 0.677m_3\end{array}\right\} \Rightarrow \begin{array}{l} m_2 = 44.4\,\text{kg} \\ m_3 = 144\,\text{kg}\end{array}$$

$$v_1 = \frac{100\,\text{kg}}{}\left|\frac{\text{L}}{1.139\,\text{kg}}\right. = 87.80\,\text{L 20\% solution}$$

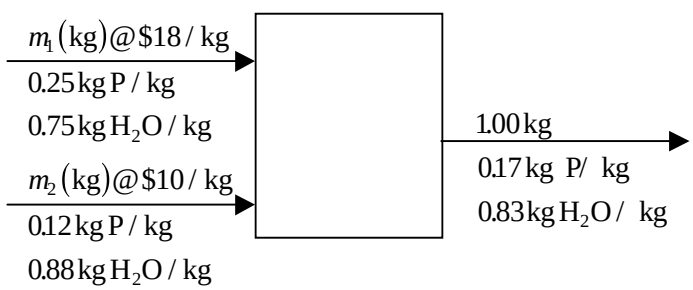
$$v_2 = \frac{44.4\,\text{kg}}{}\left|\frac{\text{L}}{1.498\,\text{kg}}\right. = 29.64\,\text{L 60\% solution}$$

$$\frac{v_1}{v_2} = \frac{87.80}{29.64} = \underline{\underline{2.96\,\frac{\text{L 20\% solution}}{\text{L 60\% solution}}}}$$

c.

$$\frac{1250\,\text{kg P}}{\text{h}}\left|\frac{44.4\,\text{kg 60\% solution}}{144\,\text{kg P}}\right|\frac{\text{L}}{1.498\,\text{kg solution}} = \underline{\underline{257\,\text{L/h}}}$$

4.17



$\underline{\text{Overall balance}}$: $m_1 + m_2 = 1.00$ (1)

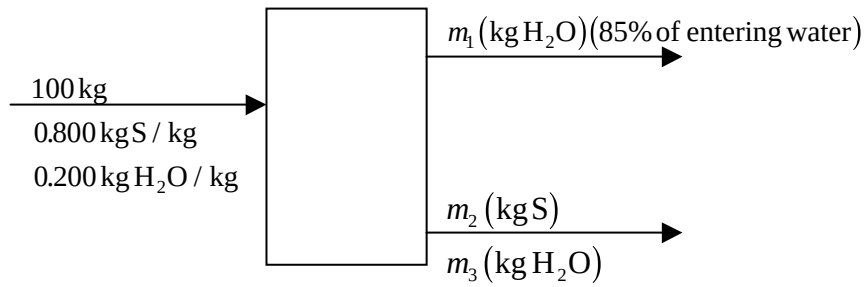
$\underline{\text{Pigment balance}}$: $0.25m_1 + 0.12m_2 = 0.17(1.00)$ (2)

Solve (1) and (2) simultaneously $\Rightarrow m_1 = 0.385\,\text{kg 25\% paint}, m_2 = 0.615\,\text{kg 12\% paint}$

$\underline{\text{Cost of blend}}$: $0.385(\$18.00) + 0.615(\$10.00) = \$13.08\,\text{per kg}$

$\underline{\text{Selling price}}$: $1.10(\$13.08) = \underline{\underline{\$14.39\,\text{per kg}}}$

4.18 **a.**



<u>85% drying</u>: $m_1 = 0.850(0.200)(100) = 17.0\,\text{kg H}_2\text{O}$

<u>Sugar balance</u>: $m_2 = 0.800(100) = 80.0\,\text{kg S}$

<u>Overall balance</u>: $100 = 17 + 80 + m_3 \Rightarrow m_3 = 3\,\text{kg H}_2\text{O}$

$$x_w = \frac{3\text{ kg H}_2\text{O}}{(3+80)\text{ kg}} = \underline{\underline{0.0361\text{ kg H}_2\text{O / kg}}}$$

$$\frac{m_1}{m_2+m_3} = \frac{17\text{ kg H}_2\text{O}}{(80+3)\text{ kg}} = \underline{\underline{0.205\text{ kg H}_2\text{O / kg wet sugar}}}$$

b.

$$\frac{1000\text{ tons wet sugar}}{\text{day}}\left|\frac{3\text{ tons H}_2\text{O}}{100\text{ tons wet sugar}}\right. = \underline{\underline{30\text{ tons H}_2\text{O / day}}}$$

$$\frac{1000\text{ tons WS}}{\text{day}}\left|\frac{0.800\text{ tons DS}}{\text{ton WS}}\right|\frac{2000\text{ lb}_\text{m}}{\text{ton}}\left|\frac{\$0.15}{\text{lb}_\text{m}}\right|\frac{365\text{ days}}{\text{year}} = \underline{\underline{\$8.8\times10^7\text{ per year}}}$$

c.

$$\bar{x}_w = \frac{1}{10}\left(x_{w1} + x_{w2} + \ldots + x_{w10}\right) = 0.0504\text{ kg H}_2\text{O / kg}$$

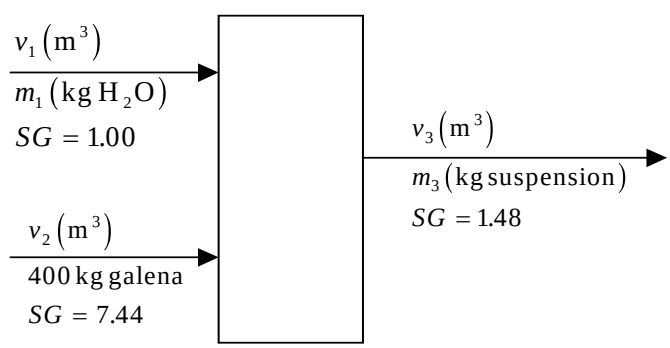
$$\text{SD} = \sqrt{\frac{1}{9}\left[\left(x_{w1}-\bar{x}_w\right)^2 + \ldots + \left(x_{w10}-\bar{x}_w\right)^2\right]} = 0.00181\text{ kg H}_2\text{O / kg}$$

$$\text{Endpoints} = 0.0504 \pm 3(0.00181)$$

$$\underline{\underline{\text{Lower limit} = 0.0450}},\ \underline{\underline{\text{Upper limit} = 0.0558}}$$

d. The evaporator is probably not working according to design specifications since $x_w = 0.0361 < 0.0450$.

4.19 **a.**



5 unknowns (v_1, v_2, v_3, m_1, m_3)
– 1 mass balance
– 1 volume balance
<u>– 3 specific gravities</u>
0 DF

<u>Total mass balance</u>: $m_1 + 400 = m_3$ (1)

4.19 (cont'd)

<u>Assume volume additivity</u>: $\dfrac{m_1(\text{kg})}{}\left|\dfrac{\text{m}^3}{1000\,\text{kg}}\right. + \dfrac{400\,\text{kg}}{}\left|\dfrac{\text{m}^3}{7440\,\text{kg}}\right. = \dfrac{m_3(\text{kg})}{}\left|\dfrac{\text{m}^3}{1480\,\text{kg}}\right.$ (2)

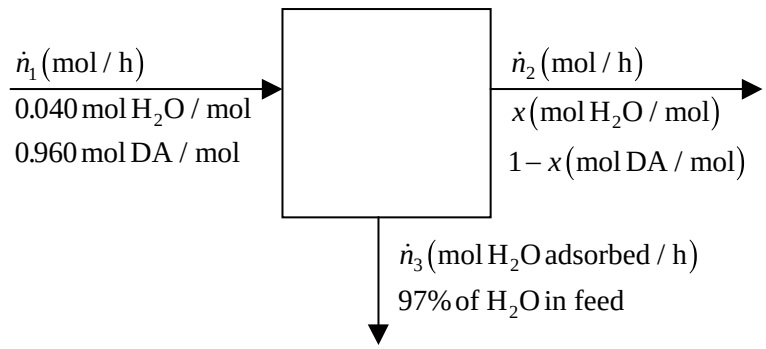
Solve (1) and (2) simultaneously $\Rightarrow m_1 = 668\,\text{kg H}_2\text{O}, m_3 = 1068\,\text{kg suspension}$

$v_1 = \dfrac{668\,\text{kg}}{}\left|\dfrac{\text{m}^3}{1000\,\text{kg}}\right. = \underline{\underline{0.668\,\text{m}^3\text{ water fed to tank}}}$

b. Specific gravity of coal < 1.48 < Specific gravity of slate

c. The suspension begins to settle. Stir the suspension. 1.00 < Specific gravity of coal < 1.48

4.20 a.



<u>Adsorption rate</u>: $\dot{n}_3 = \dfrac{(3.54-3.40)\,\text{kg}}{5\text{ h}}\left|\dfrac{\text{mol H}_2\text{O}}{0.0180\,\text{kg H}_2\text{O}}\right. = 1.556\,\text{mol H}_2\text{O / h}$

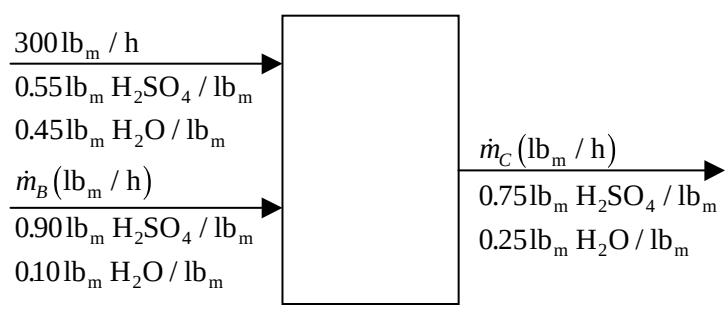
<u>97% adsorbed</u>: $1.56 = 0.97(0.04\dot{n}_1) \Rightarrow \dot{n}_1 = \underline{\underline{40.1\,\text{mol / h}}}$

<u>Total mole balance</u>: $\dot{n}_1 = \dot{n}_2 + \dot{n}_3 \Rightarrow \dot{n}_2 = 40.1 - 1.556 = 38.54\,\text{mol / h}$

<u>Water balance</u>: $0.040(40.1) = 1.556 + x(38.54) \Rightarrow x = \underline{\underline{1.2\times10^{-3}\,(\text{mol H}_2\text{O/mol})}}$

b. The calcium chloride pellets have reached their saturation limit. Eventually the mole fraction will reach that of the inlet stream, i.e. 4%.

4.21 a.



<u>Overall balance</u>: $300 + \dot{m}_B = \dot{m}_C$ (1)

<u>H_2SO_4 balance</u>: $0.55(300) + 0.90\dot{m}_B = 0.75\dot{m}_C$ (2)

Solve (1) and (2) simultaneously $\Rightarrow \dot{m}_B = \underline{\underline{400\,\text{lb}_\text{m}\text{ / h}}}, \dot{m}_C = \underline{\underline{700\,\text{lb}_\text{m}\text{ / h}}}$

4.21 (cont'd)

b.

$$\dot{m}_A - 150 = \frac{500-150}{70-25}(R_A - 25) \Rightarrow \underline{\underline{\dot{m}_A = 7.78R_A - 44.4}}$$

$$\dot{m}_B - 200 = \frac{800-200}{60-20}(R_B - 20) \Rightarrow \underline{\underline{\dot{m}_B = 15.0R_B - 100}}$$

$$\ln x - \ln 20 = \frac{\ln 100 - \ln 20}{10-4}(R_x - 4) \Rightarrow \ln x = 0.2682R_x + 1.923 \Rightarrow \underline{\underline{x = 6.841e^{0.2682R_x}}}$$

$$m_A = 300 \Rightarrow R_A = \frac{300+44.4}{7.78} = \underline{\underline{44.3}}, m_B = 400 \Rightarrow R_B = \frac{400+100}{15.0} = \underline{\underline{33.3}},$$

$$x = 55\% \Rightarrow R_x = \frac{1}{0.268}\ln\left(\frac{55}{6.841}\right) = \underline{\underline{7.78}}$$

c. Overall balance: $\dot{m}_A + \dot{m}_B = \dot{m}_C$

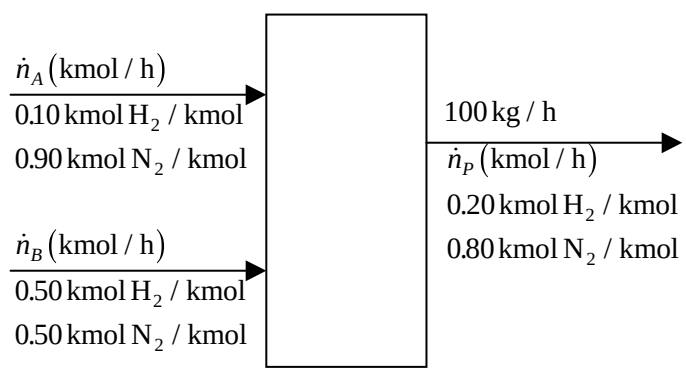
H_2SO_4 balance: $0.01x\dot{m}_A + 0.90\dot{m}_B = 0.75\dot{m}_C = 0.75(\dot{m}_A + \dot{m}_B) \Rightarrow \dot{m}_B = \dfrac{(0.75-0.01x)\dot{m}_A}{0.15}$

$$\Rightarrow 15.0R_B - 100 = \frac{\left[0.75 - 0.01\left(6.841e^{0.2682R_x}\right)\right](7.78R_A - 44.4)}{0.15}$$

$$\Rightarrow \underline{\underline{R_B = \left(2.59 - 0.236e^{0.2682R_x}\right)R_A + 1.35e^{0.2682R_x} - 8.13}}$$

Check: $R_A = 44.3, R_x = 7.78 \Rightarrow R_B = \left(2.59 - 0.236e^{0.2682(7.78)}\right)44.3 + 1.35e^{0.2682(7.78)} - 8.13 = 33.3$

4.22 a.



$$\overline{\text{MW}} = 0.20(2.016) + 0.80(28.012) = 22.813 \text{ kg / kmol}$$

$$\Rightarrow \dot{n}_P = \frac{100\text{ kg}}{\text{h}}\left|\frac{\text{kmol}}{22.813\text{ kg}}\right. = 4.38 \text{ kmol / h}$$

Overall balance: $\dot{n}_A + \dot{n}_B = 4.38$ (1)

H_2 balance: $0.10\dot{n}_A + 0.50\dot{n}_B = 0.20(4.38)$ (2)

Solve (1) and (2) simultaneously $\Rightarrow \dot{n}_A = \underline{\underline{3.29 \text{ kmol / h}}}$, $\dot{n}_B = \underline{\underline{1.10 \text{ kmol / h}}}$

4.22 (cont'd)

b. $\dot{n}_P = \dfrac{\dot{m}_P}{22.813}$

<u>Overall balance</u>: $\dot{n}_A + \dot{n}_B = \dfrac{\dot{m}_P}{22.813}$

<u>H_2 balance</u>: $x_A \dot{n}_A + x_B \dot{n}_B = \dfrac{x_P \dot{m}_P}{22.813}$

$$\Rightarrow \quad \underline{\underline{\dot{n}_A = \frac{\dot{m}_P}{22.813}\frac{(x_B - x_P)}{(x_B - x_A)}}} \qquad \underline{\underline{\dot{n}_B = \frac{\dot{m}_P}{22.813}\frac{(x_P - x_A)}{(x_B - x_A)}}}$$

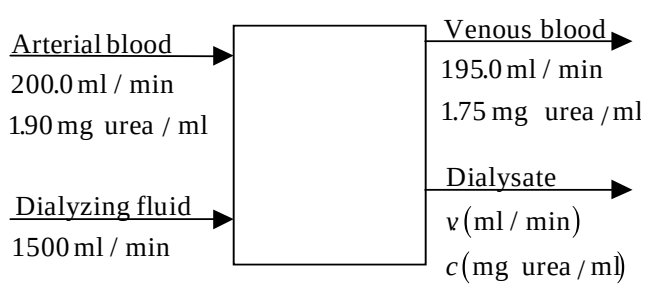
c.

Trial	X_A	X_B	X_P	m_P	n_A	n_B
1	0.10	0.50	0.10	100	4.38	0.00
2	0.10	0.50	0.20	100	3.29	1.10
3	0.10	0.50	0.30	100	2.19	2.19
4	0.10	0.50	0.40	100	1.10	3.29
5	0.10	0.50	0.50	100	0.00	4.38
6	**0.10**	**0.50**	**0.60**	**100**	**-1.10**	**5.48**
7	0.10	0.50	0.10	250	10.96	0.00
8	0.10	0.50	0.20	250	8.22	2.74
9	0.10	0.50	0.30	250	5.48	5.48
10	0.10	0.50	0.40	250	2.74	8.22
11	0.10	0.50	0.50	250	0.00	10.96
12	**0.10**	**0.50**	**0.60**	**250**	**-2.74**	**13.70**

The results of trials 6 and 12 are impossible since the flow rates are negative. You cannot blend a 10% H_2 mixture with a 50% H_2 mixture and obtain a 60% H_2 mixture.

d. Results are the same as in part c.

4.23



a. <u>Water removal rate</u>: $200.0 - 195.0 = \underline{\underline{5.0 \text{ ml / min}}}$

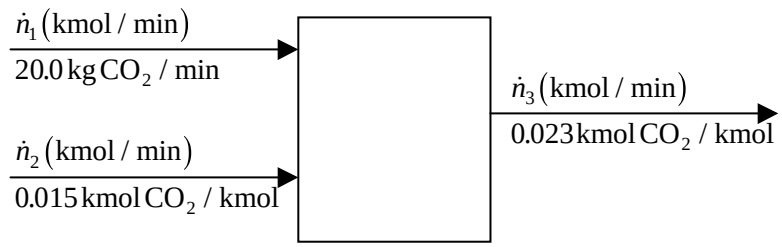
<u>Urea removal rate</u>: $1.90(200.0) - 1.75(195.0) = \underline{\underline{38.8 \text{ mg urea / min}}}$

b. $\dot{v} = 1500 + 5.0 = 1505 \text{ ml / min}$

$$c = \frac{38.8 \text{ mg urea/min}}{1505 \text{ ml/min}} = \underline{\underline{0.0258 \text{ mg urea/ml}}}$$

c. $$\frac{(2.7 - 1.1) \text{ mg removed}}{\text{ml}} \left| \frac{1 \text{ min}}{38.8 \text{ mg removed}} \right| \frac{10^3 \text{ ml}}{1 \text{ L}} \left| 5.0 \text{ L} \right. = \underline{\underline{206 \text{ min}}} \text{ (3.4 h)}$$

4.24 **a.**



$$\dot{n}_1 = \frac{20.0\,\text{kg CO}_2}{\text{min}}\left|\frac{\text{kmol}}{44.0\,\text{kg CO}_2}\right. = 0.455\ \text{kmol CO}_2\ /\ \text{min}$$

<u>Overall balance</u>: $0.455 + \dot{n}_2 = \dot{n}_3$ (1)

<u>CO_2 balance</u>: $0.455 + 0.015\dot{n}_2 = 0.023\dot{n}_3$ (2)

Solve (1) and (2) simultaneously $\Rightarrow \dot{n}_2 = \underline{\underline{55.6\ \text{kmol / min}}}, \dot{n}_3 = 56.1\ \text{kmol / min}$

b.

$$u = \frac{150\,\text{m}}{18\,\text{s}} = \underline{\underline{8.33\ \text{m / s}}}$$

$$A = \frac{1}{4}\pi D^2 = \frac{56.1\,\text{kmol}}{\text{min}}\left|\frac{\text{m}^3}{0.123\,\text{kmol}}\right|\frac{1\,\text{min}}{60\,\text{s}}\left|\frac{\text{s}}{8.33\,\text{m}}\right. \Rightarrow D = \underline{\underline{1.08\ \text{m}}}$$

4.25

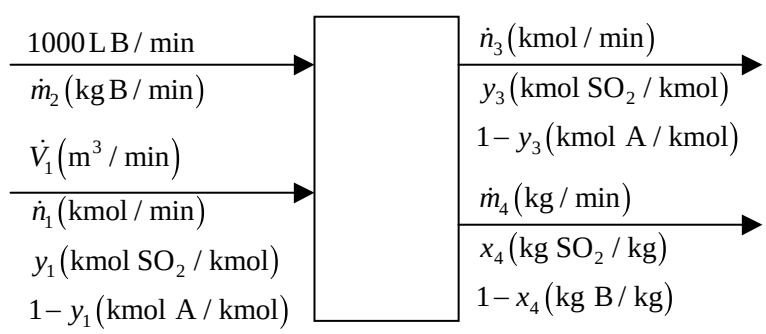
<u>Spectrophotometer calibration</u>: $C = kA \xRightarrow[\substack{A=0.9\\C=3}]{} C\ (\mu\text{g / L}) = 3.333A$

<u>Dye concentration</u>: $A = 0.18 \Rightarrow C = (3.333)(0.18) = 0.600\ \mu\text{g / L}$

$$\underline{\text{Dye injected}} = \frac{0.60\ \text{cm}^3}{}\left|\frac{1\ \text{L}}{10^3\ \text{cm}^3}\right|\frac{5.0\ \text{mg}}{1\ \text{L}}\left|\frac{10^3\ \mu\text{g}}{1\ \text{mg}}\right. = 3.0\ \mu\text{g}$$

$$\Rightarrow (3.0\ \mu\text{g})/V(\text{L}) = 0.600\ \mu\text{g / L} \Rightarrow \underline{\underline{V = 5.0\ \text{L}}}$$

4.26 **a.**



4.26 (cont'd)

8 unknowns ($\dot{n}_1, \dot{n}_3, \dot{v}_1, \dot{m}_2, \dot{m}_4, x_4, y_1, y_3$)
– 3 material balances
– 2 analyzer readings
– 1 meter reading
– 1 gas density formula
– 1 specific gravity
0 DF

b. Orifice meter calibration:

A log plot of $\dot{V}$ vs. h is a line through the points $(h_1 = 100, \dot{V}_1 = 142)$ and $(h_2 = 400, \dot{V}_2 = 290)$.

$$\ln \dot{V} = b \ln h + \ln a \Rightarrow \dot{V} = a h^b$$

$$b = \frac{\ln(\dot{V}_2/\dot{V}_1)}{\ln(h_2/h_1)} = \frac{\ln(290/142)}{\ln(400/100)} = 0.515$$

$$\ln a = \ln \dot{V}_1 - b \ln h_1 = \ln(142) - 0.515 \ln 100 = 2.58 \Rightarrow a = e^{2.58} = 13.2 \Rightarrow \underline{\underline{\dot{V} = 13.2 h^{0.515}}}$$

Analyzer calibration:

$$\ln y = bR + \ln a \Rightarrow y = a e^{bR}$$

$$\left.\begin{aligned} b &= \frac{\ln(y_2/y_1)}{R_2 - R_1} = \frac{\ln(0.1107/0.00166)}{90 - 20} = 0.0600 \\ \ln a &= \ln y_1 - bR_1 = \ln(0.00166) - 0.0600(20) = -7.60 \\ &\Downarrow \\ a &= 5.00 \times 10^{-4} \end{aligned}\right\} \Rightarrow \underline{\underline{y = 5.00 \times 10^{-4} e^{0.0600R}}}$$

c.

$$h_1 = 210 \text{ mm} \Rightarrow \dot{V}_1 = 13.2(210)^{0.515} = 207.3 \text{ m}^3/\text{min}$$

$$\rho_{\text{feed gas}} = \frac{(12.2)[(150 + 14.7)/14.7](\text{atm})}{[(75 + 460)/1.8](\text{K})} = 0.460 \text{ mol / L} = 0.460 \text{ kmol / m}^3$$

$$\Downarrow$$

$$\dot{n}_1 = \frac{207.3 \text{ m}^3}{\text{min}} \left| \frac{0.460 \text{ kmol}}{\text{m}^3} \right. = 95.34 \text{ kmol/min}$$

$$R_1 = 82.4 \Rightarrow y_1 = 5.00 \times 10^{-4} \exp(0.0600 \times 82.4) = 0.0702 \text{ kmol SO}_2/\text{kmol}$$

$$R_3 = 11.6 \Rightarrow y_3 = 5.00 \times 10^{-4} \exp(0.0600 \times 11.6) = 0.00100 \text{ kmol SO}_2/\text{kmol}$$

$$\dot{m}_2 = \frac{1000 \text{ L B}}{\text{min}} \left| \frac{1.30 \text{ kg}}{\text{L B}} \right. = 1300 \text{ kg / min}$$

4.26 (cont'd)

A balance: $(1-0.0702)(95.34)=(1-0.00100)n_3 \Rightarrow n_3 = 88.7 \text{ kmol/min}$

SO_2 balance: $(0.0702)(95.34)(64.0 \text{ kg/kmol}) = (0.00100)(88.7)(64) + \dot{m}_4 x_4$ (1)

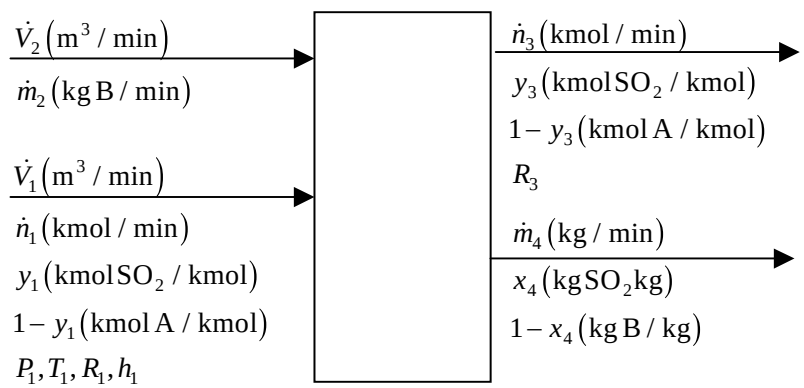
B balance: $1300 = \dot{m}_4(1-x_4)$ (2)

Solve (1) and (2) simultaneously $\Rightarrow \dot{m}_4 = 1723 \text{ kg/min}$, x_4 = 0.245 kg SO_2 absorbed / kg

SO_2 removed $= \dot{m}_4 x_4 =$ 422 kg SO_2 / min

d. Decreasing the bubble size increases the bubble surface-to-volume ratio, which results in a higher rate of transfer of SO_2 from the gas to the liquid phase.

4.27 **a.**



b. 14 unknowns ($\dot{n}_1, \dot{V}_1, y_1, P_1, T_1, R_1, h_1, \dot{V}_2, \dot{m}_2, \dot{n}_3, y_3, R_3, \dot{m}_4, x_4$)

– 3 material balances

– 3 analyzer and orifice meter readings

– 1 gas density formula (relates $\dot{n}_1$ and $\dot{V}_1$)

– 1 specific gravity (relates $\dot{m}_2$ and $\dot{V}_2$)

6 DF

A balance: $(1-y_1)\dot{n}_1 = (1-y_3)\dot{n}_3$ (1)

SO_2 balance: $y_1\dot{n}_1 = y_3\dot{n}_3 + \dfrac{x_4\dot{m}_4}{64 \text{ kg SO}_2/\text{kmol}}$ (2)

B balance: $\dot{m}_2 = (1-x_4)\dot{m}_4$ (3)

Calibration formulas: $y_1 = 5.00\times10^{-4} e^{0.060 R_1}$ (4)

$y_3 = 5.00\times10^{-4} e^{0.060 R_3}$ (5)

$\dot{V}_1 = 13.2 h_1^{0.515}$ (6)

Gas density formula: $\dot{n}_1 = \dfrac{12.2\left[(P_1+14.7)/14.7\right]}{\left[(T_1+460)/1.8\right]}\dot{V}_1$ (7)

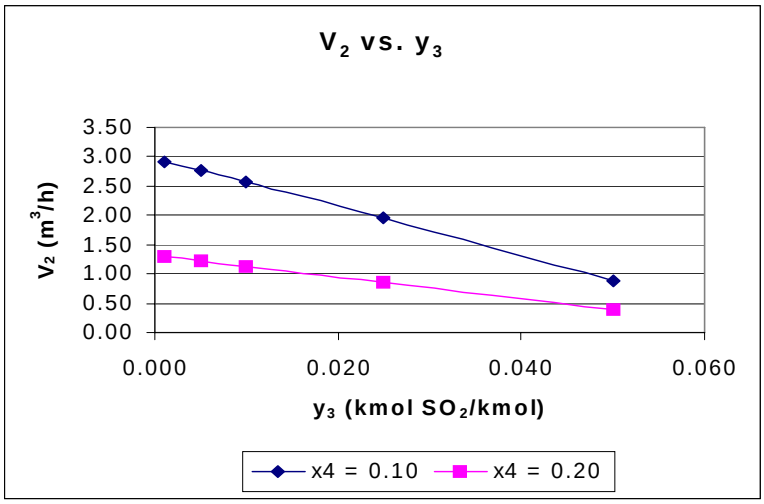
Liquid specific gravity: $SG = 1.30 \Rightarrow \dot{V}_2 = \dfrac{\dot{m}_2\,(\text{kg})}{\text{h}}\left|\dfrac{\text{m}^3}{1300 \text{ kg}}\right.$ (8)

4.27 (cont'd)

c.

T_1	75	°F	y_1	0.07	kmol SO_2/kmol
P_1	150	psig	V_1	207	m3/h
h_1	210	torr	n_1	95.26	kmol/h
R_1	82.4				

Trial	x_4 (kg SO_2/kg)	y_3 (kmol SO_2/kmol)	V_2 (m_3/h)	n_3 (kmol/h)	m_4 (kg/h)	m_2 (kg/h)
1	0.10	0.050	0.89	93.25	1283.45	1155.11
2	0.10	0.025	1.95	90.86	2813.72	2532.35
3	0.10	0.010	2.56	89.48	3694.78	3325.31
4	0.10	0.005	2.76	89.03	3982.57	3584.31
5	0.10	0.001	2.92	88.68	4210.72	3789.65
6	0.20	0.050	0.39	93.25	641.73	513.38
7	0.20	0.025	0.87	90.86	1406.86	1125.49
8	0.20	0.010	1.14	89.48	1847.39	1477.91
9	0.20	0.005	1.23	89.03	1991.28	1593.03
10	0.20	0.001	1.30	88.68	2105.36	1684.29



For a given SO_2 feed rate removing more SO_2 (lower y_3) requires a higher solvent feed rate ($\dot{V}_2$).

For a given SO_2 removal rate (y_3), a higher solvent feed rate ($\dot{V}_2$) tends to a more dilute SO_2 solution at the outlet (lower x_4).

d. Answers are the same as in part c.

4.28 Maximum balances: Overall - 3, Unit 1 - 2; Unit 2 - 3; Mixing point - 3

Overall mass balance $\Rightarrow \dot{m}_3$

Mass balance - Unit 1 $\Rightarrow \dot{m}_1$

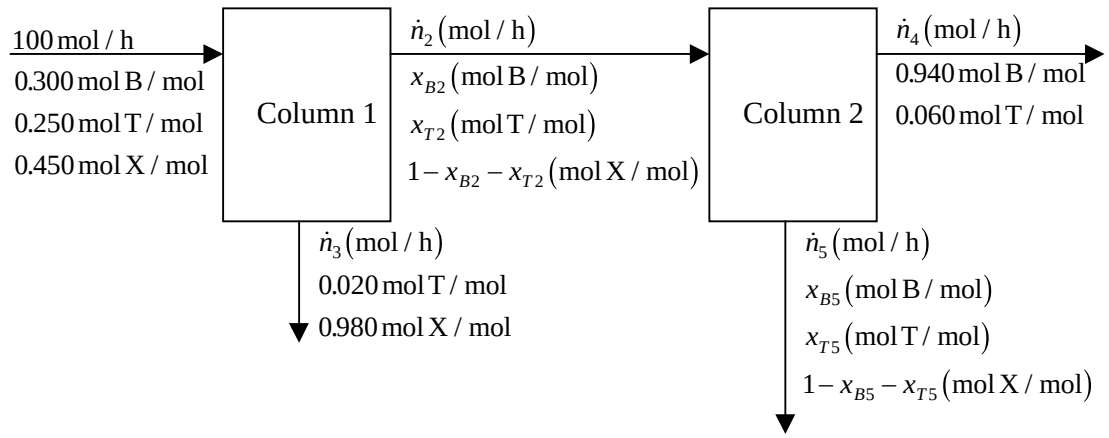
A balance - Unit 1 $\Rightarrow x_1$

Mass balance - mixing point $\Rightarrow \dot{m}_2$

A balance - mixing point $\Rightarrow x_2$

C balance - mixing point $\Rightarrow y_2$

4.29 **a.**



<u>Column 1</u>
4 unknowns ($\dot{n}_2, \dot{n}_3, x_{B2}, x_{T2}$)
–3 balances
<u>– 1 recovery of X in bot. (96%)</u>
0 DF

<u>Column 2</u>:
4 unknowns ($\dot{n}_3, \dot{n}_4, \dot{n}_5, y_x$)
– 3 balances
<u>– 1 recovery of B in top (97%)</u>
0 DF

<u>Column 1</u>

<u>96% X recovery</u>: $0.96(0.450)(100) = 0.98\underline{\underline{\dot{n}_3}}$ (1)

<u>Total mole balance</u>: $100 = \underline{\underline{\dot{n}_2}} + \dot{n}_3$ (2)

<u>B balance</u>: $0.300(100) = \underline{\underline{x_{B2}}}\dot{n}_2$ (3)

<u>T balance</u>: $0.250(100) = \underline{\underline{x_{T2}}}\dot{n}_2 + 0.020\dot{n}_3$ (4)

<u>Column 2</u>

<u>97% B recovery</u>: $0.97x_{B2}\dot{n}_2 = 0.940\underline{\underline{\dot{n}_4}}$ (5)

<u>Total mole balance</u>: $\dot{n}_2 = \dot{n}_4 + \underline{\underline{\dot{n}_5}}$ (6)

<u>B balance</u>: $x_{B2}\dot{n}_2 = 0.940\dot{n}_4 + \underline{\underline{x_{B5}}}\dot{n}_5$ (7)

<u>T balance</u>: $x_{T2}\dot{n}_2 = 0.060\dot{n}_4 + \underline{\underline{x_{T5}}}\dot{n}_5$ (8)

b. $(1) \Rightarrow \dot{n}_3 = 44.1$ mol / h $\quad (2) \Rightarrow \dot{n}_2 = 55.9$ mol / h

$(3) \Rightarrow x_{B2} = 0.536$ mol B / mol $\quad (4) \Rightarrow x_{T2} = 0.431$ mol T / mol

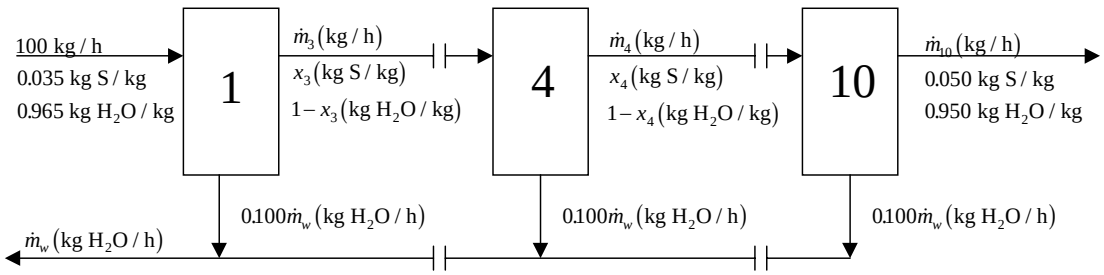
$(5) \Rightarrow \dot{n}_4 = 30.95$ mol / h $\quad (6) \Rightarrow \dot{n}_5 = 24.96$ mol / h

$(7) \Rightarrow x_{B5} = 0.036$ mol B / mol $\quad (8) \Rightarrow x_{T5} = 0.892$ mol T / mol

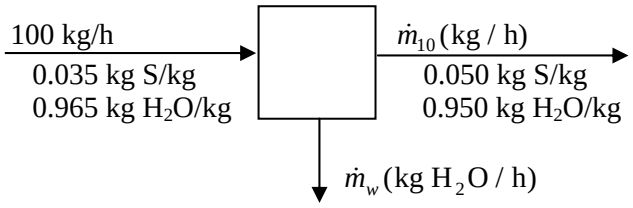
Overall benzene recovery: $\dfrac{0.940(30.95)}{0.300(100)} \times 100\% = \underline{\underline{97\%}}$

Overall toluene recovery: $\dfrac{0.892(24.96)}{0.250(100)} \times 100 = \underline{\underline{89\%}}$

4.30 **a.**



b. Overall process

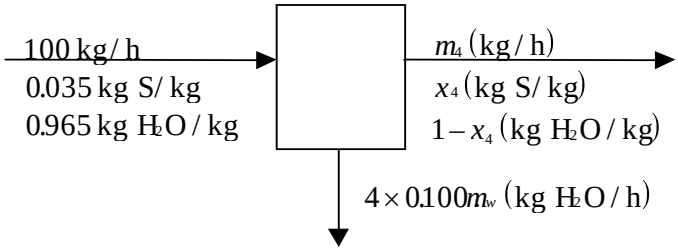


Salt balance: $0.035(100) = 0.050\dot{m}_{10}$

Overall balance: $100 = \dot{m}_w + \dot{m}_{10}$

H_2O yield: $Y_w = \dfrac{\dot{m}_w\,(\text{kg H}_2\text{O recovered})}{96.5\,(\text{kg H}_2\text{O in fresh feed})}$

First 4 evaporators



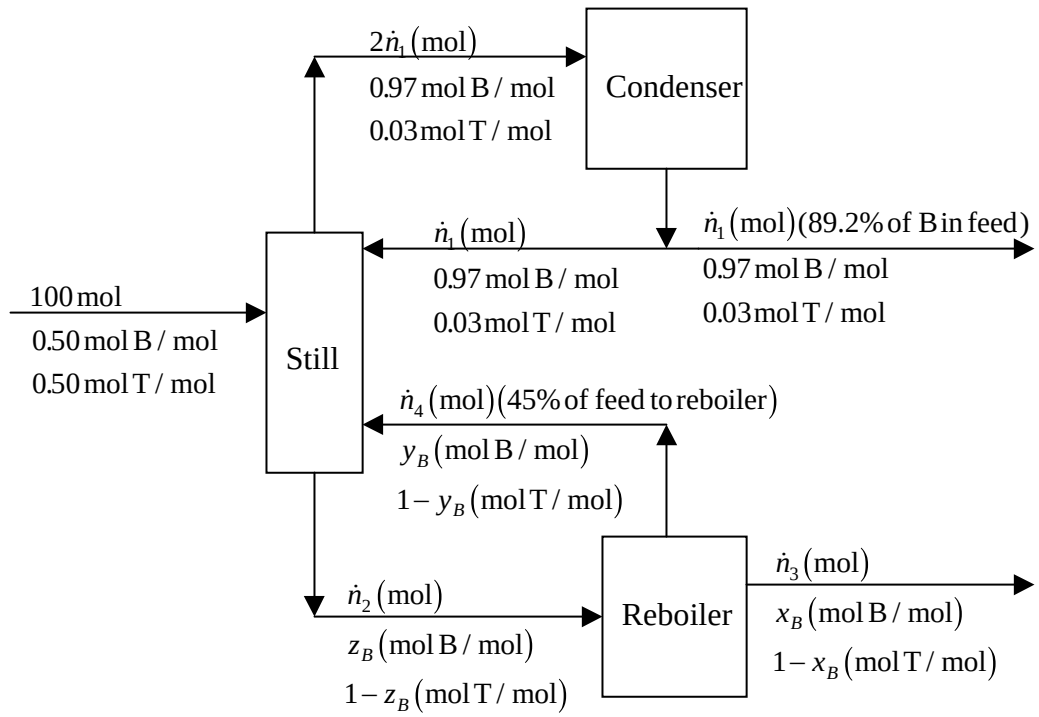
Overall balance: $100 = 4(0.100)\dot{m}_w + \dot{m}_4$

Salt balance: $0.035(100) = x_4\dot{m}_4$

c. $Y_w = 0.31$

$x_4 = 0.0398$

4.31 a.



Overall process: 3 unknowns ($\dot{n}_1, \dot{n}_3, x_B$)
– 2 balances
– 1 relationship (89.2% recovery)
0 DF

Still: 5 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_4, y_B, z_B$)
– 2 balances
3 DF

Condenser: 1 unknown ($\dot{n}_1$)
– 0 balances
1 DF

Reboiler: 6 unknowns ($\dot{n}_2, \dot{n}_3, \dot{n}_4, x_B, y_B, z_B$)
– 2 balances
– 2 relationships (2.25 ratio & 45% vapor)
3 DF

Begin with overall process.

b. Overall process

89.2% recovery: $0.892(0.50)(100) = 0.97\underline{\underline{\dot{n}_1}}$

Overall balance: $100 = \dot{n}_1 + \underline{\underline{\dot{n}_3}}$

B balance: $0.50(100) = 0.97\dot{n}_1 + \underline{\underline{x_B}}\dot{n}_3$

Reboiler

Composition relationship: $\dfrac{\underline{\underline{y_B}} / (1 - \underline{\underline{y_B}})}{x_B / (1 - x_B)} = 2.25$

Percent vaporized: $\underline{\underline{\dot{n}_4}} = 0.45\underline{\underline{\dot{n}_2}}$ (1)

Mole balance: $\underline{\underline{\dot{n}_2}} = \dot{n}_3 + \underline{\underline{\dot{n}_4}}$ (2)

(Solve (1) and (2) simultaneously.)

B balance: $\underline{\underline{z_B}}\dot{n}_2 = x_B\dot{n}_3 + y_B\dot{n}_4$

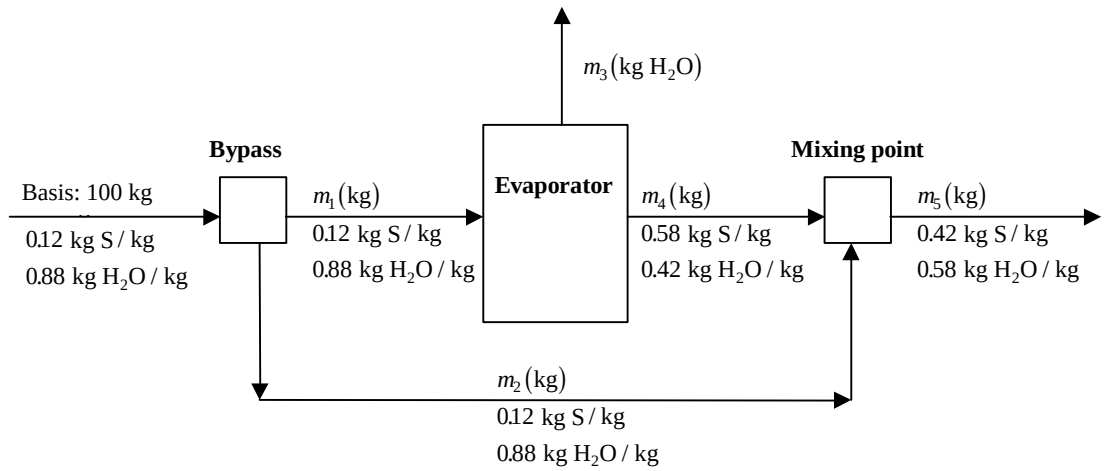
4.31 (cont'd)

c. B fraction in bottoms: $x_B = \underline{\underline{0.100 \text{ mol B / mol}}}$

Moles of overhead: $\dot{n}_1 = \underline{\underline{46.0 \text{ mol}}}$ Moles of bottoms: $\dot{n}_3 = \underline{\underline{54.0 \text{ mol}}}$

Recovery of toluene: $\dfrac{(1-x_B)\dot{n}_3}{0.50(100)} \times 100\% = \dfrac{(1-0.10)(54.02)}{0.50(100)} \times 100\% = \underline{\underline{97\%}}$

4.32 a.



Overall process: 2 unknowns (m_3, m_5)
– 2 balances
0 DF

Bypass: 2 unknowns (m_1, m_2)
– 1 independent balance
1 DF

Evaporator: 3 unknowns (m_1, m_3, m_4)
– 2 balances
1 DF

Mixing point: 3 unknowns (m_2, m_4, m_5)
– 2 balances
1 DF

Overall S balance: $0.12(100) = 0.42\underline{\underline{m_5}}$

Overall mass balance: $100 = \underline{\underline{m_3}} + m_5$

Mixing point mass balance: $\underline{\underline{m_4}} + \underline{\underline{m_2}} = m_5$ (1)

Mixing point S balance: $0.58\underline{\underline{m_4}} + 0.12\underline{\underline{m_2}} = 0.42m_5$ (2)

Solve (1) and (2) simultaneously

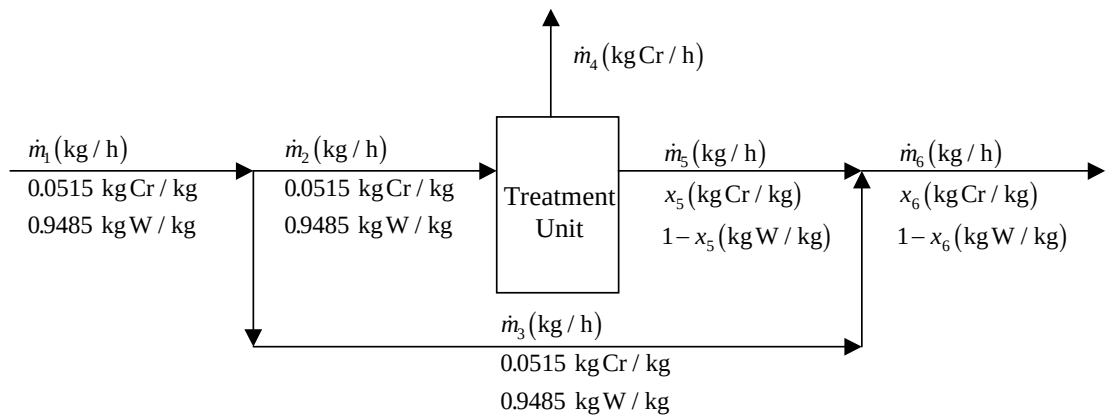
Bypass mass balance: $100 = \underline{\underline{m_1}} + m_2$

b. $m_1 = 90.05$ kg, $m_2 = 9.95$ kg, $m_3 = 71.4$ kg, $m_4 = 18.65$ kg, $m_5 = \underline{\underline{28.6 \text{ kg product}}}$

Bypass fraction: $\dfrac{m_2}{100} = \underline{\underline{0.095}}$

c. Over-evaporating could degrade the juice; additional evaporation could be uneconomical; a stream consisting of 90% solids could be hard to transport.

4.33 **a.**



b. $\dot{m}_1 = 6000 \text{ kg / h} \Rightarrow \dot{m}_2 = 4500 \text{ kg / h (maximum allowed value)}$

<u>Bypass point mass balance</u>: $\dot{m}_3 = 6000 - 4500 = 1500 \text{ kg / h}$

<u>95% Cr removal</u>: $\dot{m}_4 = 0.95(0.0515)(4500) = 220.2 \text{ kg Cr / h}$

<u>Mass balance on treatment unit</u>: $\dot{m}_5 = 4500 - 220.2 = 4279.8 \text{ kg / h}$

<u>Cr balance on treatment unit</u>: $x_5 = \dfrac{0.0515(4500) - 220.2}{4779.8} = 0.002707 \text{ kg Cr / kg}$

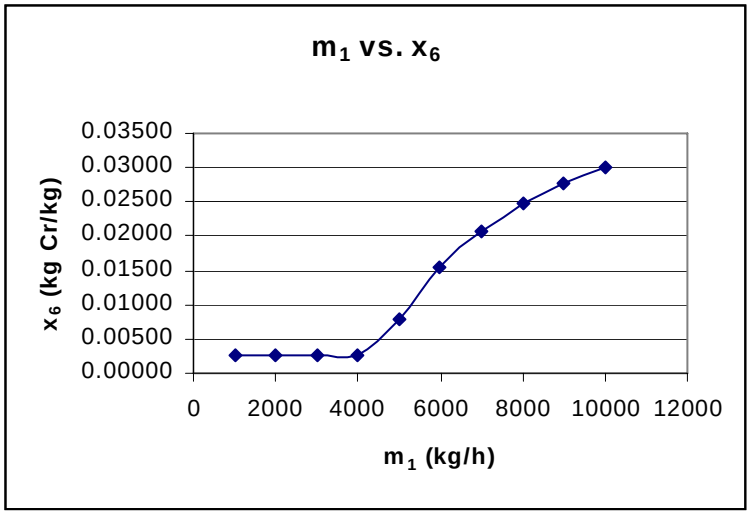
<u>Mixing point mass balance</u>: $\dot{m}_6 = 1500 + 4279.8 = \underline{\underline{5779.8 \text{ kg / h}}}$

<u>Mixing point Cr balance</u>: $x_6 = \dfrac{0.0515(1500) + 0.0002707(4279.8)}{5779.8} = \underline{\underline{0.0154 \text{ kg Cr / kg}}}$

c.

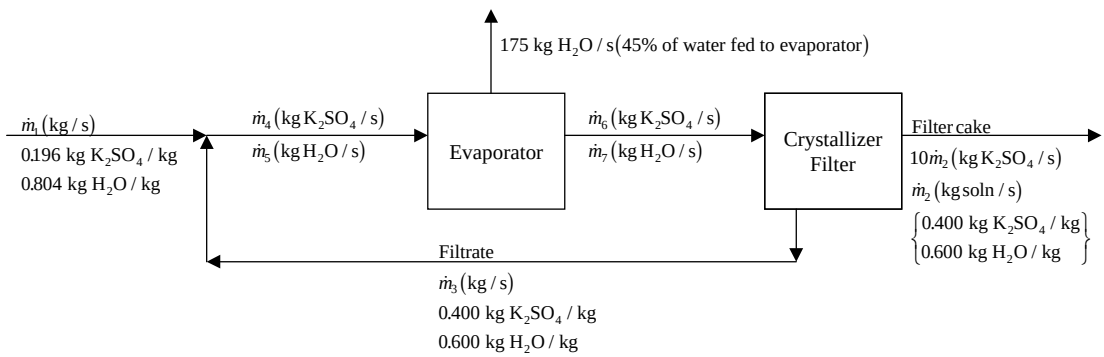
m_1 (kg/h)	m_2 (kg/h)	m_3 (kg/h)	m_4 (kg/h)	m_5 (kg/h)	x_5	m_6 (kg/h)	x_6
1000	1000	0	48.9	951	0.00271	951	0.00271
2000	2000	0	97.9	1902	0.00271	1902	0.00271
3000	3000	0	147	2853	0.00271	2853	0.00271
4000	4000	0	196	3804	0.00271	3804	0.00271
5000	4500	500	220	4280	0.00271	4780	0.00781
6000	4500	1500	220	4280	0.00271	5780	0.0154
7000	4500	2500	220	4280	0.00271	6780	0.0207
8000	4500	3500	220	4280	0.00271	7780	0.0247
9000	4500	4500	220	4280	0.00271	8780	0.0277
10000	4500	5500	220	4280	0.00271	9780	0.0301

4.33 (cont'd)



d. Cost of additional capacity – installation and maintenance, revenue from additional recovered Cr, anticipated wastewater production in coming years, capacity of waste lagoon, regulatory limits on Cr emissions.

4.34 a.



Let K = K_2SO_4, W = H_2 <u>Basis</u>: 175 kg W evaporated/s

<u>Overall process</u>: 2 unknowns ($\dot{m}_1, \dot{m}_2$)
<u>- 2 balances</u>
0 DF

<u>Mixing point</u>: 4 unknowns ($\dot{m}_1, \dot{m}_3, \dot{m}_4, \dot{m}_5$)
<u>- 2 balances</u>
2 DF

<u>Evaporator</u>: 4 unknowns ($\dot{m}_4, \dot{m}_5, \dot{m}_6, \dot{m}_7$)
<u>– 2 balances</u>
<u>– 1 percent evaporation</u>
1 DF

<u>Crystallizer</u>: 4 unknowns ($\dot{m}_2, \dot{m}_3, \dot{m}_6, \dot{m}_7$)
<u>– 2 balances</u>
2 DF

<u>Strategy</u>: Overall balances $\Rightarrow \dot{m}_1, \dot{m}_2$
% evaporation $\Rightarrow \dot{m}_5$
Balances around mixing point $\Rightarrow \dot{m}_3, \dot{m}_4$
Balances around evaporator $\Rightarrow \dot{m}_6, \dot{m}_7$

} verify that each chosen subsystem involves no more than two unknown variables

4.34 (cont'd)

$$\left.\begin{array}{ll}\underline{\text{Overall mass balance:}} & \underline{\underline{\dot{m}_1}} = 175 + 10\underline{\underline{\dot{m}_2}} + \underline{\underline{\dot{m}_2}} \\ \underline{\text{Overall K balance:}} & 0.196\underline{\underline{\dot{m}_1}} = 10\underline{\underline{\dot{m}_2}} + 0.400\underline{\underline{\dot{m}_2}}\end{array}\right\}$$

$$\underline{\text{Production rate of crystals}} = \underline{\underline{10\dot{m}_2}}$$

$$\underline{\text{45\% evaporation:}}\ \ 175 \text{ kg evaporated/min} = 0.450\underline{\underline{\dot{m}_5}}$$

$$\underline{\text{W balance around mixing point:}}\ \ 0.804\dot{m}_1 + 0.600\underline{\underline{\dot{m}_3}} = \dot{m}_5$$

$$\underline{\text{Mass balance around mixing point:}}\ \ \dot{m}_1 + \dot{m}_3 = \underline{\underline{\dot{m}_4}} + \dot{m}_5$$

$$\underline{\text{K balance around evaporator:}}\ \ \underline{\underline{\dot{m}_6}} = \dot{m}_4$$

$$\underline{\text{W balance around evaporator:}}\ \ \dot{m}_5 = 175 + \underline{\underline{\dot{m}_7}}$$

$$\underline{\text{Mole fraction of K in stream entering evaporator}} = \underline{\underline{\frac{\dot{m}_4}{\dot{m}_4 + \dot{m}_5}}}$$

b. $\underline{\text{Fresh feed rate}}$: $\dot{m}_1 = \underline{\underline{221 \text{ kg/s}}}$

$$\underline{\text{Production rate of crystals}} = 10\dot{m}_2 = \underline{\underline{41.6 \text{ kg K(s)/s}}}$$

$$\underline{\text{Recycle ratio:}}\ \ \frac{\dot{m}_3(\text{kg recycle/s})}{\dot{m}_1(\text{kg fresh feed/s})} = \frac{352.3}{220.8} = \underline{\underline{1.60 \frac{\text{kg recycle}}{\text{kg fresh feed}}}}$$

c. Scale to 75% of capacity.

$$\underline{\text{Flow rate of stream entering evaporator}} = 0.75(398 \text{ kg/s}) = \underline{\underline{299 \text{ kg/s}}}$$

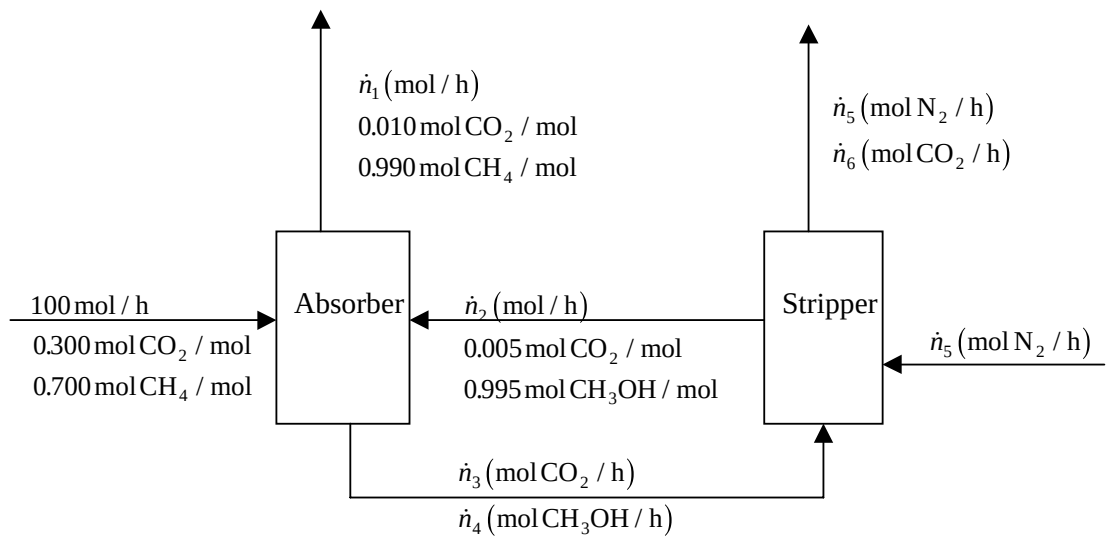
$$\underline{\underline{46.3\% \text{ K},\ 53.7\% \text{ W}}}$$

d. $\underline{\underline{\text{Drying}}}$. Principal costs are likely to be the heating cost for the evaporator and the dryer and the cooling cost for the crystallizer.

4.35 **a.** Overall objective: Separate components of a CH_4-CO_2 mixture, recover CH_4, and discharge CO_2 to the atmosphere.
Absorber function: Separates CO_2 from CH_4.
Stripper function: Removes dissolved CO_2 from CH_3OH so that the latter can be reused.

b. The top streams are liquids while the bottom streams are gases. The liquids are heavier than the gases so the liquids fall through the columns and the gases rise.

c.



Overall: 3 unknowns ($\dot{n}_1, \dot{n}_5, \dot{n}_6$)
– 2 balances
1 DF

Absorber: 4 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4$)
– 3 balances
1 DF

Stripper: 4 unknowns ($\dot{n}_2, \dot{n}_3, \dot{n}_4, \dot{n}_5$)
– 2 balances
– 1 percent removal (90%)
1 DF

Overall CH_4 balance: $[(0.700)(100)](\text{mol } CH_4 / \text{h}) = 0.990\underline{\underline{\dot{n}_1}}$

Overall mole balance: $100(\text{mol / h}) = \dot{n}_1 + \underline{\underline{\dot{n}_6}}$

Percent CO_2 stripped: $0.90\underline{\underline{\dot{n}_3}} = \dot{n}_6$

Stripper CO_2 balance: $\dot{n}_3 = \dot{n}_6 + 0.005\underline{\underline{\dot{n}_2}}$

Stripper CH_3OH balance: $\underline{\underline{\dot{n}_4}} = 0.995\dot{n}_2$

d. $\dot{n}_1 = 70.71 \text{ mol / h}, \dot{n}_2 = 651.0 \text{ mol / h}, \dot{n}_3 = 32.55 \text{ mol } CO_2 \text{ / h}, \dot{n}_4 = 647.7 \text{ mol } CH_3OH \text{ / h},$
$\dot{n}_6 = 29.29 \text{ mol } CO_2 \text{ / h}$

Fractional CO_2 absorption: $f_{CO_2} = \dfrac{30.0 - 0.010\dot{n}_1}{30.0} = \underline{\underline{0.976 \text{ mol } CO_2 \text{ absorbed / mol fed}}}$

4.35 (cont'd)

Total molar flow rate of liquid feed to stripper and mole fraction of CO_2:

$$\dot{n}_3 + \dot{n}_4 = \underline{\underline{680\,\text{mol / h}}},\ x_3 = \frac{\dot{n}_3}{\dot{n}_3 + \dot{n}_4} = \underline{\underline{0.0478\,\text{mol CO}_2\text{ / mol}}}$$

e. Scale up to 1000 kg/h (=10^6 g/h) of product gas:

$$\overline{\text{MW}_1} = 0.01(44\text{ g CO}_2\text{ / mol}) + 0.99(16\text{ g CH}_4\text{ / mol}) = 16.28\text{ g / mol}$$

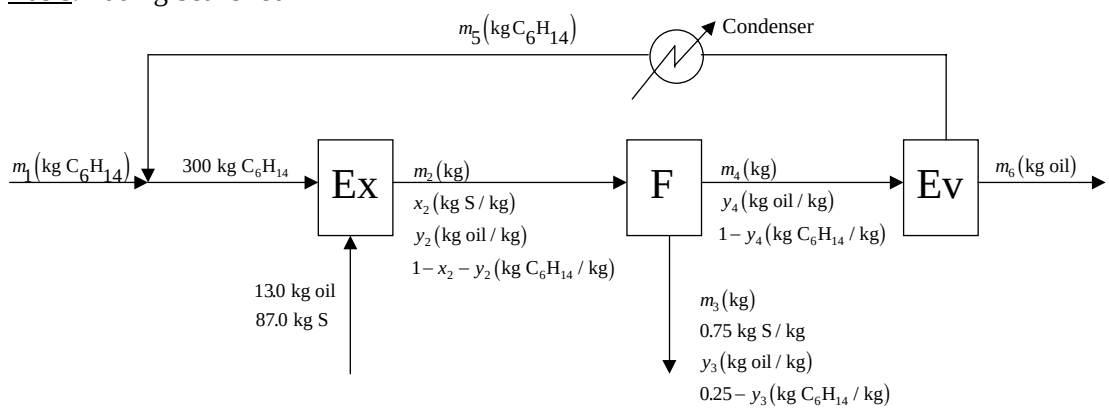
$$(\dot{n}_1)_{new} = (1.0\times10^6\text{ g / h})(16.28\text{ g / mol}) = 6.142\times10^4\text{ mol / h}$$

$$(\dot{n}_{\text{feed}})_{new} = (100\text{ mol / h})\left[(6.142\times10^4\text{ mol / h}) / (70.71\text{ mol / h})\right] = \underline{\underline{8.69\times10^4\text{ mol / h}}}$$

f. $T_a < T_s$ The higher temperature in the stripper will help drive off the gas.
$P_a > P_s$ The higher pressure in the absorber will help dissolve the gas in the liquid.

g. The methanol must have a high solubility for CO_2, a low solubility for CH_4, and a low volatility at the stripper temperature.

4.36 a. Basis: 100 kg beans fed



Overall: 4 unknowns (m_1, m_3, m_6, y_3)
– 3 balances
1 DF

Extractor: 3 unknowns (m_2, x_2, y_2)
– 3 balances
0 DF

Mixing Pt: 2 unknowns (m_1, m_5)
– 1 balance
1 DF

Evaporator: 4 unknowns (m_4, m_5, m_6, y_4)
– 2 balances
2 DF

Filter: 7 unknowns ($m_2, m_3, m_4, x_2, y_2, y_3, y_4$)
– 3 balances
– 1 oil/hexane ratio
3 DF

Start with extractor (0 degrees of freedom)

Extractor mass balance: $[300 + 87.0 + 13.0]$ kg = $\underline{\underline{m_2}}$

4.36 (cont'd)

Extractor S balance: 87.0 kg S = $\underline{\underline{x_2}}m_2$

Extractor oil balance: 13.0 kg oil = $\underline{\underline{y_2}}m_2$

Filter S balance: 87.0 kg S = $0.75\underline{\underline{m_3}}$

Filter mass balance: $m_2\,(\text{kg}) = m_3 + \underline{\underline{m_4}}$ Oil / hexane ratio in filter cake:

$$\frac{\underline{\underline{y_3}}}{0.25 - \underline{\underline{y_3}}} = \frac{y_2}{1 - x_2 - y_2}$$

Filter oil balance: 13.0 kg oil = $y_3 m_3 + \underline{\underline{y_4}}m_4$

Evaporator hexane balance: $(1 - y_4)m_4 = \underline{\underline{m_5}}$

Mixing pt. Hexane balance: $\underline{\underline{m_1}} + m_5 = 300$ kg C_6H_{14}

Evaporator oil balance: $y_4 m_4 = \underline{\underline{m_6}}$

b.

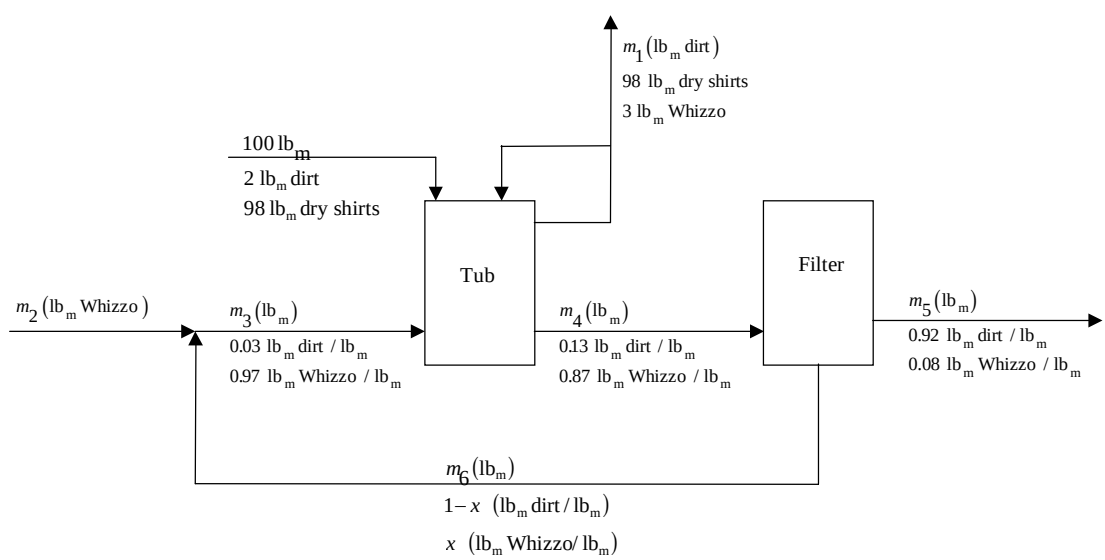
$$\underline{\text{Yield}} = \frac{m_6}{100} = \frac{11.8 \text{ kg oil}}{100 \text{ kg beans fed}} = \underline{\underline{0.118\,(\text{kg oil / kg beans fed})}}$$

$$\underline{\text{Fresh hexane feed}} = \frac{m_1}{100} = \frac{28 \text{ kg } C_6H_{14}}{100 \text{ kg beans fed}} = \underline{\underline{0.28\,(\text{kg } C_6H_{14} \text{ / kg beans fed})}}$$

$$\text{Recycle ratio} = \frac{m_5}{m_1} = \frac{272 \text{ kg } C_6H_{14} \text{ recycled}}{28 \text{ kg } C_6H_{14} \text{ fed}} = \underline{\underline{9.71\,(\text{kg } C_6H_{14} \text{ recycled / kg } C_6H_{14} \text{ fed})}}$$

c. Lower heating cost for the evaporator and lower cooling cost for the condenser.

4.37



Strategy

95% dirt removal $\Rightarrow m_1$ (= 5% of the dirt entering)

Overall balances: 2 allowed (we have implicitly used a clean shirt balance in labeling the chart) $\Rightarrow m_2, m_5$ (solves Part (a))

4.37 (cont'd)

Balances around the mixing point involve 3 unknowns (m_3, m_6, x), as do balances around the filter (m_4, m_6, x), but the tub only involves 2 (m_3, m_4) and 2 balances are allowed for each subsystem. Balances around tub $\Rightarrow m_3, m_4$

Balances around mixing point $\Rightarrow m_6, x$ (solves Part (b))

a. <u>95% dirt removal</u>: $m_1 = (0.05)(2.0) = 0.10 \text{ lb}_\text{m}$ dirt

<u>Overall dirt balance</u>: $2.0 = 0.10 + (0.92)m_5 \Rightarrow m_5 = 2.065 \text{ lb}_\text{m}$ dirt

<u>Overall Whizzo balance</u>: $m_2 = [3 + (0.08)(2.065)](\text{lb}_\text{m} \text{ Whizzo}) = \underline{\underline{3.17 \text{ lb}_\text{m} \text{ Whizzo}}}$

b. <u>Tub dirt balance</u>: $2 + 0.03m_3 = 0.10 + 0.13m_4$ (1)

<u>Tub Whizzo balance</u>: $0.97m_3 = 3 + 0.87m_4$ (2)

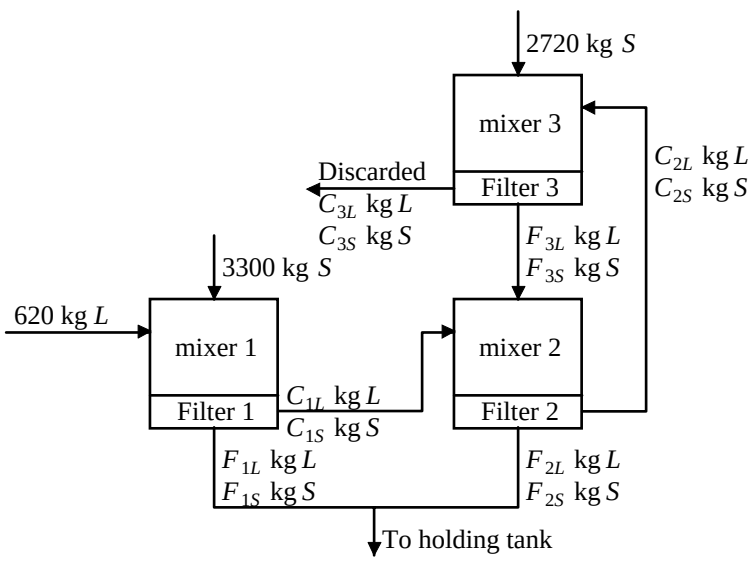
Solve (1) & (2) simultaneously $\Rightarrow m_3 = 20.4 \text{ lb}_\text{m}, m_4 = 19.3 \text{ lb}_\text{m}$

<u>Mixing pt. mass balance</u>: $3.17 + m_6 = 20.4 \text{ lb}_\text{m} \Rightarrow m_6 = 17.3 \text{ lb}_\text{m}$

<u>Mixing pt. Whizzo balance</u>:

$3.17 + x(17.3) = (0.97)(20.4) \Rightarrow x = 0.961 \text{ lb}_\text{m}$ Whizzo/lb_m $\Rightarrow$ <u>96% Whizzo, 4% dirt</u>

4.38 a.



mixer/filter 1:	$0.01(620) = F_{1L} \Rightarrow$	$F_{1L} = 6.2$ kg L
balance:	$620 = 6.2 + C_{1L} \Rightarrow$	$C_{1L} = 613.8$ kg L
mixer/filter 2:	$0.01(613.8 + F_{3L}) = F_{2L}$	$F_{2L} = 6.2$ kg L
balance:	$613.8 + F_{3L} = F_{2L} + C_{3L} \Rightarrow$	$C_{2L} = 613.7$ kg L
mixer/filter 3:	$0.01C_{2L} = F_{3L}$	$F_{3L} = 6.1$ kg L
balance:	$613.7 = 6.1 + C_{3L} \Rightarrow$	$C_{3L} = 607.6$ kg L

4.38 (cont'd)

Solvent

m/f 1: $0.15(3300) = C_{1S} \Rightarrow \quad C_{1S} = 495 \text{ kg S}$

balance: $3300 = 495 + F_{1S} \Rightarrow \quad F_{1S} = 2805 \text{ kg S}$

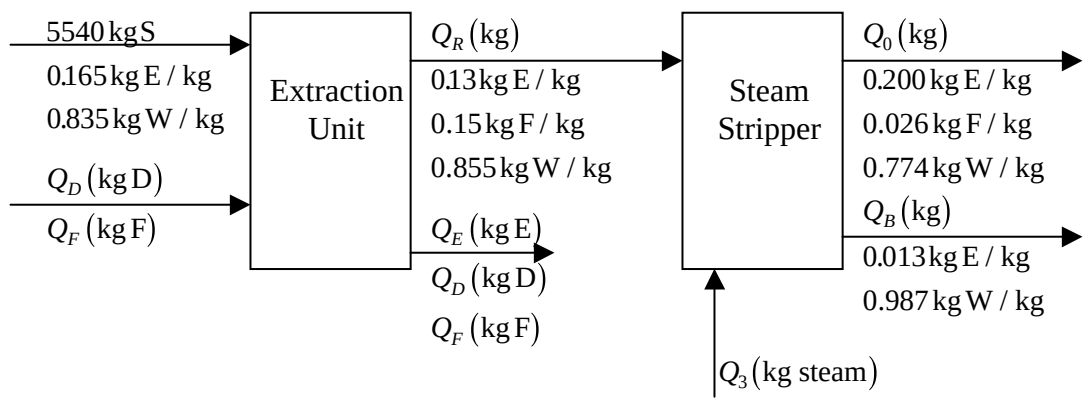
$$\left.\begin{array}{ll} \text{m/f 2:} & 0.15(495 + F_{3S}) = C_{2S} \\ \text{balance:} & 495 + F_{3S} = C_{2S} + F_{2S} \\ \text{m/f 3:} & 0.15(2720 + C_{2S}) = C_{3S} \\ \text{balance:} & 2720 + C_{2S} = F_{3S} + C_{3S} \end{array}\right\} \Rightarrow \begin{array}{l} C_{2S} = 482.6 \text{ kg S} \\ F_{2S} = 2734.6 \text{ kg S} \\ C_{3S} = 480.4 \text{ kg S} \\ F_{3S} = 2722.2 \text{ kg S} \end{array}$$

Holding Tank Contents

$6.2 + 6.2 = \underline{\underline{12.4 \text{ kg leaf}}}$

$2805 + 2734.6 = \underline{\underline{5540 \text{ kg solvent}}}$

b.



Mass of D in Product: $\dfrac{1 \text{ kg D}}{1000 \text{ kg leaf}} \Big| \dfrac{620 \text{ kg leaf}}{} = \underline{\underline{0.62 \text{ kg D} = Q_D}}$

Water balance around extraction unit: $0.835(5540) = 0.855Q_R \Rightarrow Q_R = 5410 \text{ kg}$

Ethanol balance around extraction unit:

$0.165(5540) = 0.13(5410) + Q_E \Rightarrow \underline{\underline{Q_E = 211 \text{ kg}}}$ (ethanol in extract)

c. F balance around stripper

$0.015(5410) = 0.026Q_0 \Rightarrow \underline{\underline{Q_0 = 3121 \text{ kg}}}$ (mass of stripper overhead product)

E balance around stripper

$0.13(5410) = 0.200(3121) + 0.013Q_B \Rightarrow \underline{\underline{Q_B = 6085 \text{ kg}}}$ (mass of stripper bottom product)

W balance around stripper

$0.855(5410) + Q_S = 0.774(3121) + 0.987(6085) \Rightarrow \underline{\underline{Q_S = 3796 \text{ kg steam fed to stripper}}}$

4.39 **a.** $C_2H_2 + 2H_2 \rightarrow C_2H_6$

$\underline{\underline{2 \text{ mol } H_2 \text{ react / mol } C_2H_2 \text{ react}}}$

$\underline{\underline{0.5 \text{ kmol } C_2H_6 \text{ formed / kmol } H_2 \text{ react}}}$

4.39 (cont'd)

b. $\dfrac{n_{H_2}}{n_{C_2H_2}} = 1.5 < 2.0 \Rightarrow \underline{\underline{H_2 \text{ is limiting reactant}}}$

$1.5 \text{ mol } H_2 \text{ fed} \Rightarrow 1.0 \text{ mol } C_2H_2 \text{ fed} \Rightarrow 0.75 \text{ mol } C_2H_2 \text{ required (theoretical)}$

$$\% \text{ excess } C_2H_2 = \frac{1.0 \text{ mol fed} - 0.75 \text{ mol required}}{0.75 \text{ mol required}} \times 100\% = \underline{\underline{33.3\%}}$$

c. $$\frac{4\times10^6 \text{ tonnes } C_2H_6}{\text{yr}}\left|\frac{1 \text{ yr}}{300 \text{ days}}\right|\frac{1 \text{ day}}{24 \text{ h}}\left|\frac{1 \text{ h}}{3600 \text{ s}}\right|\frac{1000 \text{ kg}}{\text{tonne}}\left|\frac{1 \text{ kmol } C_2H_6}{30.0 \text{ kg } C_2H_6}\right|\frac{2 \text{ kmol } H_2}{1 \text{ kmol } C_2H_6}\left|\frac{2.00 \text{ kg } H_2}{1 \text{ kmol } H_2}\right.$$

$= 20.6 \text{ kg } H_2 / \text{s}$

d. The extra cost will be involved in separating the product from the excess reactant.

4.40 **a.** $4\,NH_3 + 5\,O_2 \rightarrow 4\,NO + 6\,H_2O$

$$\frac{5 \text{ lb-mole } O_2 \text{ react}}{4 \text{ lb-mole NO formed}} = \underline{\underline{1.25 \text{ lb-mole } O_2 \text{ react / lb-mole NO formed}}}$$

b. $$\left(n_{O_2}\right)_{\text{theoretical}} = \frac{100 \text{ kmol } NH_3}{\text{h}}\left|\frac{5 \text{ kmol } O_2}{4 \text{ kmol } NH_3}\right. = 125 \text{ kmol } O_2$$

$40\% \text{ excess } O_2 \Rightarrow \left(n_{O_2}\right)_{\text{fed}} = 1.40(125 \text{ kmol } O_2) = \underline{\underline{175 \text{ kmol } O_2}}$

c. $(50.0 \text{ kg } NH_3)(1 \text{ kmol } NH_3 / 17 \text{ kg } NH_3) = 2.94 \text{ kmol } NH_3$

$(100.0 \text{ kg } O_2)(1 \text{ kmol } O_2 / 32 \text{ kg } O_2) = 3.125 \text{ kmol } O_2$

$$\left(\frac{n_{O_2}}{n_{NH_3}}\right)_{\text{fed}} = \frac{3.125}{2.94} = 1.06 < \left(\frac{n_{O_2}}{n_{NH_3}}\right)_{\text{stoich}} = \frac{5}{4} = 1.25$$

$\Rightarrow \underline{\underline{O_2 \text{ is the limiting reactant}}}$

<u>Required NH_3</u>: $$\frac{3.125 \text{ kmol } O_2}{}\left|\frac{4 \text{ kmol } NH_3}{5 \text{ kmol } O_2}\right. = 2.50 \text{ kmol } NH_3$$

$$\underline{\%\text{excess } NH_3} = \frac{2.94 - 2.50}{2.50} \times 100\% = \underline{\underline{17.6\% \text{ excess } NH_3}}$$

<u>Extent of reaction</u>: $n_{O_2} = \left(n_{O_2}\right)_0 - \nu_{O_2}\xi \Rightarrow 0 = 3.125 - (-5)\xi \Rightarrow \xi = 0.625 \text{ kmol} = \underline{\underline{625 \text{ mol}}}$

<u>Mass of NO</u>: $$\frac{3.125 \text{ kmol } O_2}{}\left|\frac{4 \text{ kmol NO}}{5 \text{ kmol } O_2}\right|\frac{30.0 \text{ kg NO}}{1 \text{ kmol NO}} = \underline{\underline{75.0 \text{ kg NO}}}$$

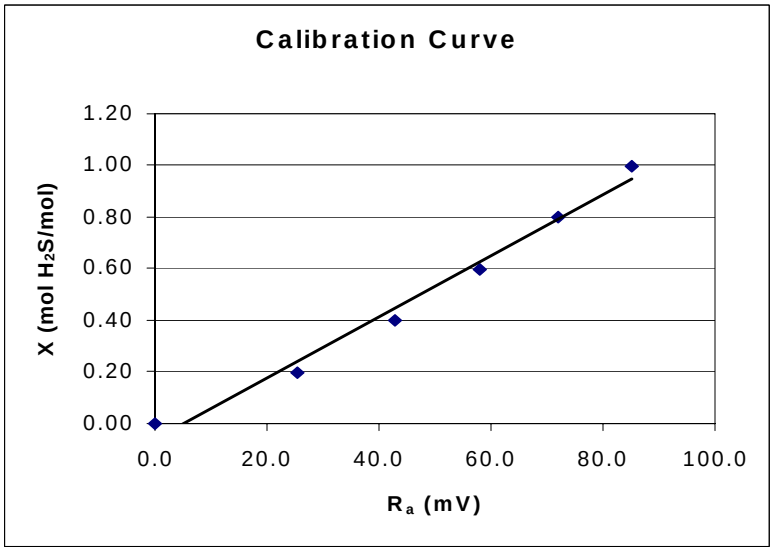
4.41 **a.** By adding the feeds in stoichometric proportion, all of the H_2S and SO_2 would be consumed. Automation provides for faster and more accurate response to fluctuations in the feed stream, reducing the risk of release of H_2S and SO_2. It also may reduce labor costs.

4.41 (cont'd)

b.

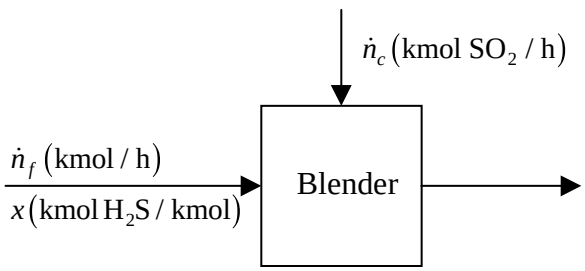
$$\dot{n}_c = \frac{3.00\times10^2\ \text{kmol}}{\text{h}}\left|\frac{0.85\ \text{kmol}\ H_2S}{\text{kmol}}\right|\frac{1\ \text{kmol}\ SO_2}{2\ \text{kmol}\ H_2S} = \underline{\underline{127.5\,\text{kmol}\,SO_2\ /\ \text{h}}}$$

c.



$$\underline{\underline{X = 0.0199R_a - 0.0605}}$$

d.



<u>Flowmeter calibration</u>: $\left.\begin{array}{r}\dot{n}_f = aR_f \\ \dot{n}_f = 100\,\text{kmol/h}, R_f = 15\,\text{mV}\end{array}\right\}\dot{n}_f = \frac{20}{3}R_f$

<u>Control valve calibration</u>: $\left.\begin{array}{r}\dot{n}_c = 25.0\,\text{kmol/h}, R_c = 10.0\,\text{mV} \\ \dot{n}_c = 60.0\,\text{kmol/h}, R_c = 25.0\,\text{mV}\end{array}\right\}\dot{n}_c = \frac{7}{3}R_c + \frac{5}{3}$

<u>Stoichiometric feed</u>: $\dot{n}_c = \frac{1}{2}\dot{n}_f x \Rightarrow \frac{7}{3}R_c + \frac{5}{3} = \frac{1}{2}\left(\frac{20}{3}R_f\right)(0.0119R_a - 0.0605)$

$$\Rightarrow \underline{\underline{R_c = \frac{10}{7}R_f(0.0119R_a - 0.0605) - \frac{5}{7}}}$$

$$\dot{n}_f = 3.00\times10^2\ \text{kmol/h} \Rightarrow R_f = \frac{3}{20}\dot{n}_f = 45\,\text{mV}$$

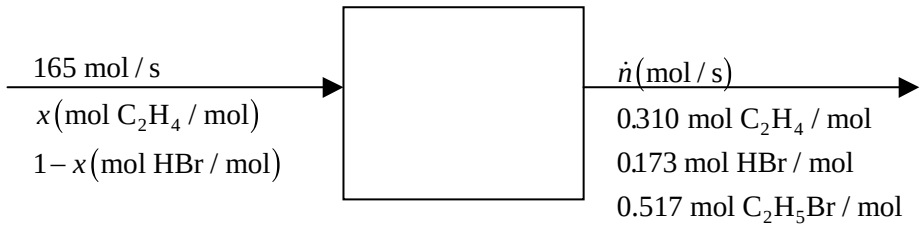
4.41 (cont'd)

$$R_c = \frac{10}{7}(45)\left[(0.0119)(76.5) - 0.0605\right] - \frac{5}{7} = 53.9\ \text{mV}$$

$$\Rightarrow \dot{n}_c = \frac{7}{3}(53.9) + \frac{5}{3} = 127.4\ \text{kmol / h}$$

e. Faulty sensors, computer problems, analyzer calibration not linear, extrapolation beyond range of calibration data, system had not reached steady state yet.

4.42



$$C_2H_4 + HBr \rightarrow C_2H_5Br$$

<u>C balance</u>: $\frac{165\,\text{mol}}{\text{s}}\left|\frac{x\,(\text{mol}\,C_2H_4)}{\text{mol}}\right|\frac{2\,\text{mol C}}{\text{mol}\,C_2H_4} = \dot{n}(0.310)(2) + \dot{n}(0.517)(2)$ (1)

<u>Br balance</u>: $165(1-x)(1) = \dot{n}(0.173)(1) + \dot{n}(0.517)(1)$ (2)

(Note: An atomic H balance can be obtained as 2*(Eq. 2) + (Eq. 1) and so is not independent)

Solve (1) and (2) simultaneously $\Rightarrow \dot{n} = 108.77\,\text{mol / s},\ x = 0.545\,\text{mol}\,C_2H_4\ /\ \text{mol}$

$\Rightarrow (1-x) = 0.455\,\text{mol HBr / mol}$

Since the C_2H_4/HBr feed ratio (0.545/0.455) is greater than the stoichiometric ration (=1), <u>HBr is the limiting reactant</u> .

$$(\dot{n}_{HBr})_{fed} = (165\,\text{mol / s})(0.455\,\text{mol HBr / mol}) = 75.08\,\text{mol HBr}$$

<u>Fractional conversion of HBr</u> $= \frac{75.08 - (0.173)(108.8)}{75.08} = \underline{\underline{0.749\ \text{mol HBr react/mol fed}}}$

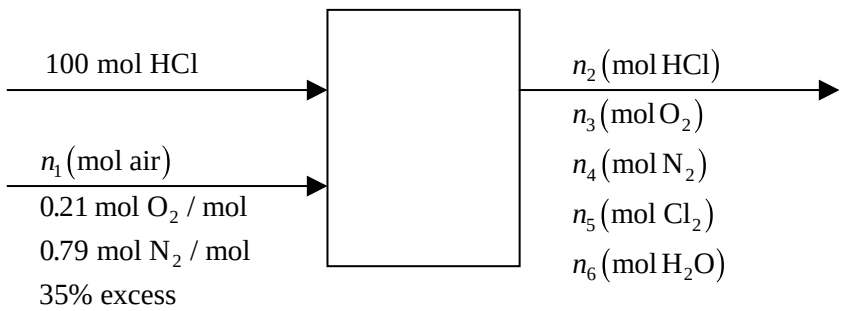
$$(\dot{n}_{C_2H_4})_{stoich} = 75.08\,\text{mol}\,C_2H_4$$

$$(\dot{n}_{C_2H_4})_{fed} = (165\,\text{mol/s})(0.545\,\text{mol}\,C_2H_4/\text{mol}) = 89.93\,\text{mol}\,C_2H_4$$

<u>% excess of C_2H_4</u> $= \frac{89.93 - 75.08}{75.08} = \underline{\underline{19.8\%}}$

<u>Extent of reaction</u>: $\dot{n}_{C_2H_5Br} = (\dot{n}_{C_2H_5Br})_0 + \nu_{C_2H_5Br}\xi \Rightarrow (108.8)(0.517) = 0 + (1)\xi \Rightarrow \underline{\underline{\xi = 56.2\,\text{mol/s}}}$

4.43 **a.** $2HCl + \frac{1}{2}O_2 \rightarrow Cl_2 + H_2O$ Basis: 100 mol HCl fed to reactor



$$(O_2)_{stoic} = \frac{100 \text{ mol HCl}}{} \left| \frac{0.5 \text{ mol } O_2}{2 \text{ mol HCl}} \right. = 25 \text{ mol } O_2$$

35% excess air: $0.21 n_1 (\text{mol } O_2 \text{ fed}) = 1.35 \times 25 \Rightarrow n_1 = 160.7 \text{ mol air fed}$

85% conversion $\Rightarrow$ 85 mol HCl react $\Rightarrow n_2 = 15$ mol HCl

$$n_5 = \frac{85 \text{ mol HCl react}}{} \left| \frac{1 \text{ mol } Cl_2}{2 \text{ mol HCl}} \right. = 42.5 \text{ mol } Cl_2$$

$n_6 = (85)(1/2) = 42.5 \text{ mol } H_2O$

N_2 balance: $(160.7)(0.79) = n_4 \Rightarrow n_4 = 127 \text{ mol } N_2$

O balance:

$$\frac{(160.7)(0.21) \text{ mol } O_2}{} \left| \frac{2 \text{ mol O}}{1 \text{ mol } O_2} \right. = 2n_3 + \frac{42.5 \text{ mol } H_2O}{} \left| \frac{1 \text{ mol O}}{1 \text{ mol } H_2O} \right. \Rightarrow n_3 = 12.5 \text{ mol } O_2$$

Total moles:

$$\sum_{j=2}^{5} n_j = 239.5 \text{ mol} \Rightarrow \frac{15 \text{ mol HCl}}{239.5 \text{ mol}} = \underline{\underline{0.063 \ \frac{\text{mol HCl}}{\text{mol}}}}, \ \underline{\underline{0.052 \ \frac{\text{mol } O_2}{\text{mol}}}}, \ \underline{\underline{0.530 \ \frac{\text{mol } N_2}{\text{mol}}}},$$

$$\underline{\underline{0.177 \ \frac{\text{mol } Cl_2}{\text{mol}}}}, \ \underline{\underline{0.177 \ \frac{\text{mol } H_2O}{\text{mol}}}}$$

b. As before, $n_1 = 160.7$ mol air fed, $n_2 = \underline{\underline{15 \text{ mol HCl}}}$

$2HCl + \frac{1}{2}O_2 \rightarrow Cl_2 + H_2O$

$n_i = (n_i)_0 + \nu_i \xi$

$\Downarrow$

HCl: $15 = 100 - 2\xi \Rightarrow \xi = 42.5$ mol

4.43 (cont'd)

$\underline{O_2}$: $n_3 = 0.21(160.7) - \frac{1}{2}\xi = \underline{\underline{12.5 \text{ mol } O_2}}$

$\underline{N_2}$: $n_4 = 0.79(160.7) = \underline{\underline{127 \text{ mol } N_2}}$

$\underline{Cl_2}$: $n_5 = \xi = \underline{\underline{42.5 \text{ mol } Cl_2}}$

$\underline{H_2O}$: $n_6 = \xi = \underline{\underline{42.5 \text{ mol } H_2O}}$

These molar quantities are the same as in part (a), so the mole fractions would also be the same.

c. Use of pure O_2 would eliminate the need for an extra process to remove the N_2 from the product gas, but O_2 costs much more than air. The cheaper process will be the process of choice.

4.44

$$FeTiO_3 + 2H_2SO_4 \rightarrow (TiO)SO_4 + FeSO_4 + 2H_2O$$
$$Fe_2O_3 + 3H_2SO_4 \rightarrow Fe_2(SO_4)_3 + 3H_2O$$
$$(TiO)SO_4 + 2H_2O \rightarrow H_2TiO_3(s) + H_2SO_4$$
$$H_2TiO_3(s) \rightarrow TiO_2(s) + H_2O$$

<u>Basis</u>: 1000 kg TiO_2 produced

$$\frac{1000 \text{ kg } TiO_2}{} \left| \frac{\text{kmol } TiO_2}{79.90 \text{ kg } TiO_2} \right| \frac{1 \text{ kmol } FeTiO_3}{1 \text{ kmol } TiO_2} = 12.52 \text{ kmol } FeTiO_3 \text{ decomposes}$$

$$\frac{12.52 \text{ kmol } FeTiO_3 \text{ dec.}}{} \left| \frac{1 \text{ kmol } FeTiO_3 \text{ feed}}{0.89 \text{ kmol } FeTiO_3 \text{ dec.}} \right. = 14.06 \text{ kmol } FeTiO_3 \text{ fed}$$

$$\frac{14.06 \text{ kmol } FeTiO_3}{} \left| \frac{1 \text{ kmol Ti}}{1 \text{ kmol } FeTiO_3} \right| \frac{47.90 \text{ kg Ti}}{\text{kmol Ti}} = 673.5 \text{ kg Ti fed}$$

$$673.5 \text{ kg Ti} / M(\text{kg ore}) = 0.243 \Rightarrow M = \underline{\underline{2772 \text{ kg ore fed}}}$$

Ore is made up entirely of 14.06 kmol $FeTiO_3$ + $n(\text{kmol } Fe_2O_3)$ (<u>Assumption!</u>)

$$n = 2772 \text{ kg ore} - \frac{14.06 \text{ kmol } FeTiO_3}{} \left| \frac{151.74 \text{ kg } FeTiO_3}{\text{kmol } FeTiO_3} \right. = 638.1 \text{ kg } Fe_2O_3$$

$$\frac{638.1 \text{ kg } Fe_2O_3}{} \left| \frac{\text{kmol } Fe_2O_3}{159.69 \text{ kg } Fe_2O_3} \right. = 4.00 \text{ kmol } Fe_2O_3$$

$$\frac{14.06 \text{ kmol } FeTiO_3}{} \left| \frac{2 \text{ kmol } H_2SO_4}{1 \text{ kmol } FeTiO_3} \right. + \frac{4.00 \text{ kmol } FeTiO_3}{} \left| \frac{3 \text{ kmol } H_2SO_4}{1 \text{ kmol } Fe_2O_3} \right. = 40.12 \text{ kmol } H_2SO_4$$

<u>50% excess</u>: $1.5(40.12 \text{ kmol } H_2SO_4) = 60.18 \text{ kmol } H_2SO_4$ fed

<u>Mass of 80% solution</u>: $\frac{60.18 \text{ kmol } H_2SO_4}{} \left| \frac{98.08 \text{ kg } H_2SO_4}{1 \text{ kmol } H_2SO_4} \right. = 5902.4 \text{ kg } H_2SO_4$

$$5902.4 \text{ kg } H_2SO_4 / M_a(\text{kg soln}) = 0.80 \Rightarrow M_a = \underline{\underline{7380 \text{ kg 80\% } H_2SO_4 \text{ feed}}}$$

4.45 **a.** Plot C (log scale) vs. R (linear scale) on semilog paper, get straight line through

$$\left(R_1 = 10,\ C_1 = 0.30\ \text{g/m}^3\right) \text{ and } \left(R_2 = 48,\ C_2 = 2.67\ \text{g/m}^3\right)$$

$$\ln C = bR + \ln a \Leftrightarrow C = ae^{br}$$

$$b = \frac{\ln(2.67/0.30)}{48-10} = 0.0575\ ,\quad \ln a = \ln(2.67) - 0.0575(48) = -1.78 \Rightarrow a = e^{-1.78} = 0.169$$

$$\Rightarrow\ C = 0.169e^{0.0575R}$$

$$C\left(\text{g/m}^3\right) = \frac{C'(\text{lb}_\text{m})}{\text{ft}^3}\left|\frac{453.6\ \text{g}}{1\ \text{lb}_\text{m}}\right|\frac{35.31\ \text{ft}^3}{1\ \text{m}^3} = 16{,}020C'$$

$$\Downarrow$$

$$16{,}020C' = 0.169e^{0.0575R} \Rightarrow \underline{\underline{C'\left(\text{lb}_\text{m}\ \text{SO}_2/\text{ft}^3\right) = 1.055\times10^{-5}e^{0.0575R}}}$$

b.

$$\frac{\left(2867\ \text{ft}^3/\text{s}\right)\left(60\ \text{s/min}\right)}{1250\ \text{lb}_\text{m}/\text{min}} = \underline{\underline{138\ \text{ft}^3/\text{lb}_\text{m}\ \text{coal}}}$$

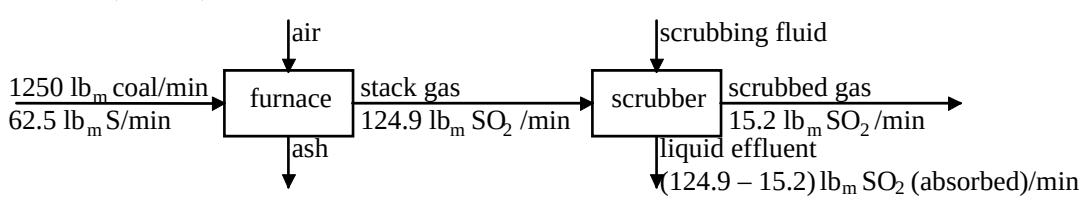
$$R = 37 \Rightarrow C'\left(\text{lb}_\text{m}\ \text{SO}_2/\text{ft}^3\right) = 1.055\times10^{-5}e^{(0.0575)(37)} = 8.86\times10^{-5}\ \text{lb}_\text{m}\ \text{SO}_2/\text{ft}^3$$

$$\frac{8.86\times10^{-5}\ \text{lb}_\text{m}\ \text{SO}_2}{\text{ft}^3}\left|\frac{138\ \text{ft}^3}{1\ \text{lb}_\text{m}\ \text{coal}}\right. = 0.012 < 0.018\frac{\text{lb}_\text{m}\ \text{SO}_2}{\text{lb}_\text{m}\ \text{coal}}\ \ \underline{\underline{\text{compliance achieved}}}$$

c. $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$

$$\frac{1250\ \text{lb}_\text{m}\ \text{coal}}{\text{min}}\left|\frac{0.05\ \text{lb}_\text{m}\ \text{S}}{1\ \text{lb}_\text{m}\ \text{coal}}\right|\frac{64.06\ \text{lb}_\text{m}\ \text{SO}_2}{32.06\ \text{lb}_\text{m}\ \text{S}} = 124.9\ \text{lb}_\text{m}\ \text{SO}_2\ \text{generated/min}$$

$$\frac{2867\ \text{ft}^3}{\text{s}}\left|\frac{60\ \text{s}}{1\ \text{min}}\right|\frac{8.86\times10^{-5}\ \text{lb}_\text{m}\ \text{SO}_2}{\text{ft}^3} = 15.2\ \text{lb}_\text{m}\ \text{SO}_2/\text{min}\ \text{in scrubbed gas}$$



$$\underline{\%\ \text{removal}} = \frac{(124.9 - 15.2)\ \text{lb}_\text{m}\ \text{SO}_2\ \text{scrubbed/min}}{124.9\ \text{lb}_\text{m}\ \text{SO}_2\ \text{fed to scrubber/min}}\times100\% = \underline{\underline{88\%}}$$

d. The regulation was avoided by diluting the stack gas with fresh air before it exited from the stack. The new regulation prevents this since the mass of SO_2 emitted per mass of coal burned is independent of the flow rate of air in the stack.

4.46 **a.** A + B $\rightleftharpoons$ C + D

$$\left.\begin{aligned} n_A &= n_{A_0} - \xi \\ n_B &= n_{B_0} - \xi \\ n_C &= n_{C_0} + \xi \\ n_D &= n_{D_0} + \xi \\ n_I &= n_{I_0} \\ \text{Total } n_T &= \sum n_i \end{aligned}\right\} \Longrightarrow \begin{aligned} y_A &= \left(n_{A_0} - \xi\right)/n_T \\ y_B &= \left(n_{B_0} - \xi\right)/n_T \\ y_C &= \left(n_{C_0} + \xi\right)/n_T \\ y_D &= \left(n_{D_0} + \xi\right)/n_T \end{aligned}$$

At equilibrium: $\dfrac{y_C y_D}{y_A y_B} = \dfrac{(n_{C0} + \xi_c)(n_{D0} + \xi_c)}{(n_{A0} - \xi_c)(n_{B0} - \xi_c)} = 4.87$ (n_T's cancel)

$$3.87\xi_c^2 - \left(n_{C0} + n_{D0} + 4.87(n_{A0} + n_{B0})\right)\xi_c - \left(n_{C0}n_{D0} - 4.87 n_{A0}n_{B0}\right) = 0$$

$$[a\xi_c^2 + b\xi_c + c = 0]$$

$$\therefore \xi_c = \frac{1}{2a}\left(-b \pm \sqrt{b^2 - 4ac}\right) \text{ where } \begin{aligned} a &= 3.87 \\ b &= -\left[n_{C0} + n_{D0} + 4.87(n_{A0} + n_{B0})\right] \\ c &= -\left[n_{C0}n_{D0} - 4.87 n_{A0}n_{B0}\right] \end{aligned}$$

b. Basis: 1 mol A feed $\quad n_{A0} = 1 \quad n_{B0} = 1 \quad n_{C0} = n_{D0} = n_{I0} = 0$

Constants: $a = 3.87 \quad b = -9.74 \quad c = 4.87$

$$\xi_e = \frac{1}{2(3.87)}\left(9.74 \pm \sqrt{(9.74)^2 - 4(3.87)(4.87)}\right) \Rightarrow \xi_{e1} = 0.688$$

$\left(\xi_{e2} = 1.83 \text{ is also a solution but leads to a negative conversion}\right)$

Fractional conversion: $X_A(= X_B) = \dfrac{n_{A0} - n_A}{n_{A0}} = \dfrac{\xi_{e1}}{n_{A0}} = \underline{\underline{0.688}}$

c. $n_{B0} = 80, n_{C0} = n_{D0} = n_{J0} = 0$

$$n_C = 70 = n_{C0} + \xi_c \xRightarrow{n_{C0} = 0} \xi_c = 70 \text{ mol}$$

$$n_A = n_{A0} - \xi_c = n_{A0} - 70 \text{ mol}$$

$$n_B = n_{B0} - \xi_c = 80 - 70 = 10 \text{ mol}$$

$$n_C = n_{C0} + \xi_c = 70 \text{ mol}$$

$$n_D = n_{D0} + \xi_c = 70 \text{ mol}$$

$$4.87 = \frac{y_C y_D}{y_A y_B} = \frac{n_C n_D}{n_A n_B} \Rightarrow \frac{(70)(70)}{(n_{A0} - 70)(10)} = 4.87 \Rightarrow \underline{\underline{n_{A0} = 170.6 \text{ mol methanol fed}}}$$

4.46 (cont'd)

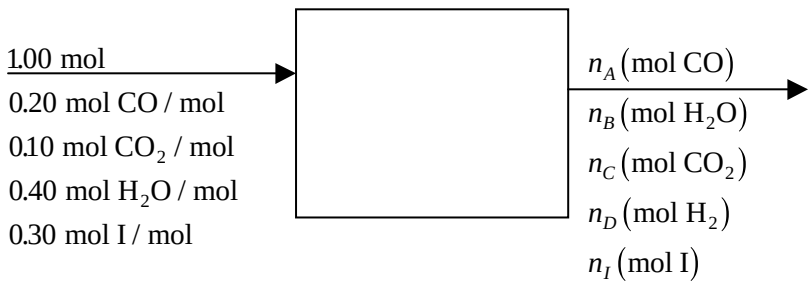
$$\underline{\text{Product gas}}\quad \left.\begin{aligned} n_A &= 170.6 - 70 = 100.6 \text{ mol} \\ n_B &= 10 \text{ mol} \\ n_C &= 70 \text{ mol} \\ n_D &= 70 \text{ mol} \end{aligned}\right\} \Rightarrow \begin{aligned} &\underline{\underline{y_A = 0.401 \text{ mol } CH_3OH/\text{mol}}} \\ &\underline{\underline{y_B = 0.040 \text{ mol } CH_3COOH/\text{mol}}} \\ &\underline{\underline{y_C = 0.279 \text{ mol } CH_3COOCH_3/\text{mol}}} \\ &\underline{\underline{y_D = 0.279 \text{ mol } H_2O/\text{mol}}} \end{aligned}$$

$$n_{total} = 250.6 \text{ mol}$$

d. Cost of reactants, selling price for product, market for product, rate of reaction, need for heating or cooling, and many other items.

4.47 **a.** $CO + H_2O \longleftrightarrow CO_2 + H_2$

(A) (B) (C) (D)



<u>Degree of freedom analysis</u>: 6 unknowns ($n_A, n_B, n_C, n_D, n_I, \xi$)

– 4 expressions for $n_i(\xi)$

– 1 balance on I

– 1 equilibrium relationship

0 DF

b. Since two moles are prodcued for every two moles that react,

$$(n_{\text{total}})_{\text{out}} = (n_{\text{total}})_{\text{in}} = \underline{\underline{1.00(\text{mol})}}$$

$$n_A = 0.20 - \xi \qquad (1)$$

$$n_B = 0.40 - \xi \qquad (2)$$

$$n_C = 0.10 + \xi \qquad (3)$$

$$n_D = \xi \qquad (4)$$

$$\underline{n_I = 0.30} \qquad (5)$$

$$n_{tot} = 1.00 \text{ mol}$$

At equilibrium: $\dfrac{y_C y_D}{y_A y_B} = \dfrac{n_C n_D}{n_A n_B} = \dfrac{(0.10+\xi)(\xi)}{(0.20-\xi)(0.40-\xi)} = 0.0247 \exp\left(\dfrac{4020}{1123}\right) \Rightarrow \xi = 0.110 \text{ mol}$

$$y_D = n_D = \xi = \underline{\underline{0.110(\text{mol } H_2 / \text{mol})}}$$

c. The reaction has not reached equilibrium yet.

4.47 (cont'd)

d.

T (K)	x (CO)	x (H_2O)	x (CO_2)	Keq	Keq (Goal Seek)	Extent of Reaction	y (H_2)
1223	0.5	0.5	0	0.6610	0.6610	0.2242	0.224
1123	0.5	0.5	0	0.8858	0.8856	0.2424	0.242
1023	0.5	0.5	0	1.2569	1.2569	0.2643	0.264
923	0.5	0.5	0	1.9240	1.9242	0.2905	0.291
823	0.5	0.5	0	3.2662	3.2661	0.3219	0.322
723	0.5	0.5	0	6.4187	6.4188	0.3585	0.358
623	0.5	0.5	0	15.6692	15.6692	0.3992	0.399
673	0.5	0.5	0	9.7017	9.7011	0.3785	0.378
698	0.5	0.5	0	7.8331	7.8331	0.3684	0.368
688	0.5	0.5	0	8.5171	8.5177	0.3724	0.372
1123	0.2	0.4	0.1	0.8858	0.8863	0.1101	0.110
1123	0.4	0.2	0.1	0.8858	0.8857	0.1100	0.110
1123	0.3	0.3	0	0.8858	0.8856	0.1454	0.145
1123	0.5	0.4	0	0.8858	0.8867	0.2156	0.216

The lower the temperature, the higher the extent of reaction. An equimolar feed ratio of carbon monoxide and water also maximizes the extent of reaction.

4.48 a. $\mathrm{A} + 2\mathrm{B} \rightarrow \mathrm{C}$

$$\ln K_e = \ln A_0 + E/T(K)$$

$$E = \frac{\ln(K_{e1}/K_{e2})}{1/T_1 - 1/T_2} = \frac{\ln(10.5/2.316\times10^{-4})}{1/373 - 1/573} = 11458$$

$$\ln A_0 = \ln K_{e1} - 11458/T_1 = \ln 10.5 - 11458/373 = -28.37 \Rightarrow A_0 = 4.79\times10^{-13}$$

$$K_e = \underline{\underline{4.79\times10^{-13}\exp(11458/T(K))\ \mathrm{atm}^{-2}}} \Rightarrow \underline{\underline{K_e(450K) = 0.0548\ \mathrm{atm}^{-1}}}$$

b.

$$\left.\begin{aligned} n_A &= n_{A0} - \xi \\ n_B &= n_{B0} - 2\xi \\ n_C &= n_{C0} + \xi \\ \hline n_T &= n_{T0} - 2\xi \end{aligned}\right\} \Rightarrow \begin{aligned} y_A &= (n_{A0} - \xi)/(n_{T0} - 2\xi) \\ y_B &= (n_{B0} - 2\xi)/(n_{T0} - 2\xi) \\ y_C &= (n_{C0} + \xi)/(n_{T0} - 2\xi) \\ \hline &(n_{T0} = n_{A0} + n_{B0} + n_{C0}) \end{aligned}$$

At equilibrium,

$$\frac{y_C}{y_A y_B^2}\frac{1}{P^2} = \underline{\underline{\frac{(n_{C0}+\xi_e)(n_{T0}-2\xi_e)^2}{(n_{A0}-\xi_e)(n_{B0}-2\xi_e)^2}\frac{1}{P^2}}} = K_e(T)$$ (substitute for $K_e(T)$ from Part a.)

c. <u>Basis</u>: 1 mol A (CO)

$$n_{A0} = 1 \quad n_{B0} = 1 \quad n_{C0} = 0 \Rightarrow n_{T0} = 2,\ P = 2\ \mathrm{atm},\ T = 423\mathrm{K}$$

$$\frac{\xi_e(2-2\xi_e)^2}{(1-\xi_e)(1-2\xi_e)^2}\frac{1}{4\ \mathrm{atm}^2} = K_e(423) = 0.278\ \mathrm{atm}^{-2} \Rightarrow \xi_e^2 - \xi_e + 0.1317 = 0$$

4.48 (cont'd)

(For this particular set of initial conditions, we get a quadratic equation. In general, the equation will be cubic.)

$\xi_e = 0.156$, ~~0.847~~ Reject the second solution, since it leads to a negative n_B.

$$y_A = (1-0.156)/(2-2(0.156)) \Rightarrow \underline{\underline{y_A = 0.500}}$$

$$y_B = (1-2(0.156))/(2-2(0.156)) \Rightarrow \underline{\underline{y_B = 0.408}}$$

$$y_C = (0+0.156)/(2-2(0.156)) \Rightarrow \underline{\underline{y_C = 0.092}}$$

Fractional Conversion of CO $(A) = \dfrac{n_{A0} - n_A}{n_{A0}} = \dfrac{\xi}{n_{A0}} = \underline{\underline{0.156 \text{ mol } A \text{ reacted / mol } A \text{ feed}}}$

d. Use the equations from part b.

i) Fractional conversion decreases with increasing fraction of CO.
ii) Fractional conversion decreases with increasing fraction of CH_3OH.
iii) Fractional conversion decreases with increasing temperature.
iv) Fractional conversion increases with increasing pressure.

```
      REAL TRU, A, E, YA0, YC0, T, P, KE, P2KE, C0, C1, C2, C3, EK, EKPI,
     *        FN, FDN, NT, CON, YA, YB, YC
      INTEGER NIT, INMAX
      TAU = 0.0001
      INMAX = 10
      A = 4.79E–13
      E = 11458.
      READ (5, *) YA0, YB0, YC0, T, P
      KE = A * EXP(E/T)
      P2KE = P*P*KE
      C0 = YC0 – P2KE * YA0 * YB0 * YB0
      C1 = 1. – 4. * YC0 + P2KE * YB0 * (YB0 + 4. * YA0)
      C2 = 4. * (YC0 –1. – P2KE * (YA0 + YB0))
      C3 = 4. * (1. + P2KE)
      EK = 0.0          (Assume an initial value ξe = 0.0)
      NIT = 0
    1 FN = C0 + EK * (C1 + EK * (C2 + EK * C3))   FDN = C1 + EK * (2. * C2 +
      EK * 3. * C3)   EKPI = EK - FN/FDN   NIT = NIT + 1   IF (NIT.EQ.INMAX)
      GOTO 4   IF (ABS((EKPI – EK)/EKPI).LT.TAU) GOTO 2   EK =
      EKPI   GOTO 1
    2 NT = 1. – 2. * EKPI
      YA = (YA0 – EKPI)/NT
      YB = (YB0 – 2. + EKPI)/NT
      YC = (YC0 + EKPI)/NT
```

4.48 (cont'd)

```
      CON = EKPI/YA0   WRITE (6, 3) YA, YB, YC, CON   STOP
4     WRITE (6, 5) INMAX, EKPI
3     FORMAT ('  YA    YB    YC    CON', 1, 4(F6.3, 1X))   FORMAT ('DID NOT
      CONVERGE IN', I3, 'ITERATIONS',/,
  *                 'CURRENT VALUE = ', F6.3)   END
  $   DATA   0.5      0.5       0.0       423.     2.
```

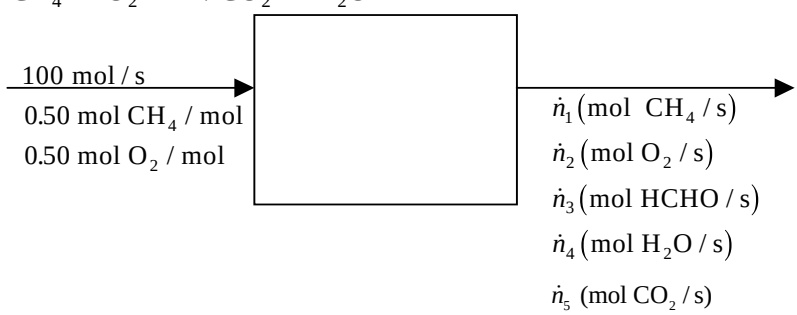
RESULTS: <u>YA = 0.500, YB = 0.408, YC = 0.092, CON = 0.156</u>

Note: This will only find one root — there are two others that can only be found by choosing different initial values of ξ_a

4.49 **a.**

$$CH_4 + O_2 \longrightarrow HCHO + H_2O \qquad (1)$$

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O \qquad (2)$$



7 unknowns ($\dot{n}_1, \dot{n}_2, \dot{n}_3, \dot{n}_4, \dot{n}_5, \dot{\xi}_1, \dot{\xi}_2$)

$-$5 equations for $\dot{n}_i\left(\dot{\xi}_1, \dot{\xi}_2\right)$

2 DF

b.

$$\dot{n}_1 = 50 - \dot{\xi}_1 - \dot{\xi}_2 \qquad (1)$$

$$\dot{n}_2 = 50 - \dot{\xi}_1 - 2\dot{\xi}_2 \qquad (2)$$

$$\dot{n}_3 = \dot{\xi}_1 \qquad (3)$$

$$\dot{n}_4 = \dot{\xi}_1 + 2\dot{\xi}_2 \qquad (4)$$

$$\dot{n}_5 = \dot{\xi}_2 \qquad (5)$$

c.

<u>Fractional conversion</u>: $\dfrac{(50 - \dot{n}_1)}{50} = 0.900 \Rightarrow \dot{n}_1 = 5.00\,\text{mol}\,CH_4\,/\,s$

<u>Fractional yield</u>: $\dfrac{\dot{n}_3}{50} = 0.855 \Rightarrow \dot{n}_3 = 42.75\,\text{mol}\,HCHO\,/\,s$

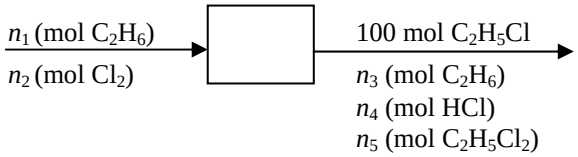
$$\left.\begin{array}{l} \text{Equation 3} \Rightarrow \xi_1 = 42.75 \\ \text{Equation 1} \Rightarrow \xi_2 = 2.25 \\ \text{Equation 2} \Rightarrow \dot{n}_2 = 2.75 \\ \text{Equation 4} \Rightarrow \dot{n}_4 = 47.25 \\ \text{Equation 5} \Rightarrow \dot{n}_5 = 2.25 \end{array}\right\} \Rightarrow \begin{array}{l} y_{CH_4} = \underline{\underline{0.0500\,\text{mol}\,CH_4\,/\,\text{mol}}} \\ y_{O_2} = \underline{\underline{0.0275\,\text{mol}\,O_2\,/\,\text{mol}}} \\ y_{HCHO} = \underline{\underline{0.4275\,\text{mol}\,HCHO\,/\,\text{mol}}} \\ y_{H_2O} = \underline{\underline{0.4725\,\text{mol}\,H_2O\,/\,\text{mol}}} \\ y_{CO_2} = \underline{\underline{0.0225\,\text{mol}\,CO_2\,/\,\text{mol}}} \end{array}$$

<u>Selectivity</u>: $[(42.75\,\text{mol HCHO/s})/(2.25\,\text{mol}\,CO_2\text{/s}) = \underline{\underline{19.0\,\text{mol HCHO/mol}\,CO_2}}$

4.50 **a.** <u>Design for low conversion and feed ethane in excess.</u> Low conversion and excess ethane make the second reaction unlikely.

b. $C_2H_6 + Cl_2 \rightarrow C_2H_5Cl + HCl$, $C_2H_5Cl + Cl_2 \rightarrow C_2H_4Cl_2 + HCl$

<u>Basis</u>: 100 mol C_2H_5Cl produced



5 unknowns
<u>–3 atomic balances</u>
2 D.F.

c. <u>Selectivity:</u> $100 \text{ mol } C_2H_5Cl = 14n_5 \text{ (mol } C_2H_4Cl_2) \Rightarrow n_5 = 7.143 \text{ mol } C_2H_4Cl_2$

<u>15% conversion:</u> $(1-0.15)n_1 = n_3$

<u>C balance:</u> $2n_1 = 2(100) + 2n_3 + 2(7.143)$

$\Rightarrow$ $n_1 = 714.3 \text{ mol } C_2H_6$ in, $n_3 = 114.3 \text{ mol } C_2H_6$ out

<u>H balance</u>: $6(714.3) = 5(100) + 6(114.3) + n_4 + 4(7.143) \Rightarrow n_4 = 607.1 \text{ mol HCl}$

<u>Cl balance:</u> $2n_2 = 100 + 607.1 + 2(7.143) \Rightarrow n_2 = 114.3 \text{ mol } Cl_2$

<u>Feed Ratio</u>: $114.3 \text{ mol } Cl_2 \,/\, 714.3 \text{ mol } C_2H_6 = \underline{\underline{0.16 \text{ mol } Cl_2 \,/\, \text{mol } C_2H_6}}$

<u>Maximum possible amount of C_2H_5Cl</u>:

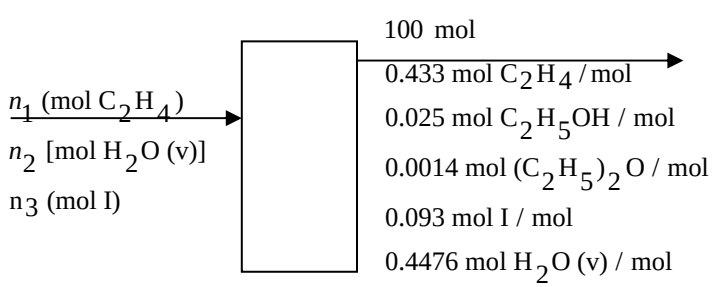
$$n_{max} = \frac{114.3 \text{ mol } Cl_2}{} \left| \frac{1 \text{ mol } C_2H_5Cl}{1 \text{ mol } Cl_2} \right. = 114.3 \text{ mol } C_2H_5Cl$$

<u>Fractional yield of C_2H_5Cl</u>: $\dfrac{n_{C_2H_5Cl}}{n_{max}} = \dfrac{100 \text{ mol}}{114.3 \text{ mol}} = 0.875$

d. Some of the $C_2H_4Cl_2$ is further chlorinated in an undesired side reaction:
$C_2H_5Cl_2 + Cl_2 \rightarrow C_2H_4Cl_3 + HCl$

4.51 **a.** $C_2H_4 + H_2O \rightarrow C_2H_5OH$, $2\ C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O$

<u>Basis</u>: 100 mol effluent gas



3 unknowns
-2 independent atomic balances
-1 I balance
<u>0 D.F.</u>

(1) C balance: $2n_1 = 100(2*0.433 + 2*0.025 + 4*0.0014)$

(2) H balance: $4n_1 + 2n_2 = 100(4*0.433 + 6*0.025 + 10*0.0014 + 2*0.4476)$

(3) O balance: $n_2 = 100(0.025 + 0.0014 + 0.4476)$

Note; *Eq.* (1)$*2 +$ Eq. (3)$*2 =$ Eq. (2) $\Rightarrow$2 independent atomic balances

(4) I balance: $n_3 = 9.3$

4.51 (cont'd)

b.

$$\left.\begin{array}{l}(1)\ \Rightarrow\ n_1 = 46.08 \text{ mol } C_2H_6 \\ (3)\ \Rightarrow n_2 = 47.4 \text{ mol } H_2O \\ (4)\ \Rightarrow n_3 = 9.3 \text{ mol I}\end{array}\right\} \Rightarrow \underline{\underline{\text{Reactor feed contains } 44.8\%\ C_2H_6,\ 46.1\%\ H_2O,\ 9.1\%\ \text{I}}}$$

<u>% conversion of C_2H_4</u>: $\dfrac{46.08 - 43.3}{46.08} \times 100\% = \underline{\underline{6.0\%}}$

If all C_2H_4 were converted and the second reaction did not occur, $\left(n_{C_2H_5OH}\right)_{\max} = 46.08$ mol

$\Rightarrow$ <u>Fractional Yield of C_2H_5OH</u>: $n_{C_2H_5OH} / \left(n_{C_2H_5OH}\right)_{\max} = (2.5 / 46.08) = \underline{\underline{0.054}}$

<u>Selectivity of C_2H_5OH to $(C_2H_5)_2O$</u>:

$$\frac{2.5 \text{ mol } C_2H_5OH}{0.14 \text{ mol } (C_2H_5)_2O} = \underline{\underline{17.9 \text{ mol } C_2H_5OH / \text{ mol } (C_2H_5)_2O}}$$

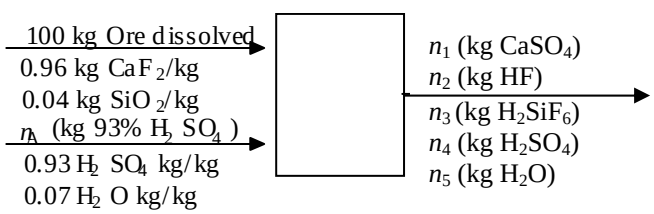
c. Keep conversion low to prevent C_2H_5OH from being in reactor long enough to form significant amounts of $(C_2H_5)_2O$. Separate and recycle unreacted C_2H_4.

4.52

$$CaF_2(s) + H_2SO_4(l) \rightarrow CaSO_4(s) + 2HF(g)$$

$$\frac{1 \text{ metric ton acid}}{} \left| \frac{1000 \text{ kg acid}}{1 \text{ metric ton acid}} \right| \frac{0.60 \text{ kg HF}}{1 \text{ kg acid}} = 600 \text{ kg HF}$$

<u>Basis: 100 kg Ore dissolved (not fed)</u>



<u>Atomic balance - Si:</u>

$$\frac{0.04(100) \text{ kg } SiO_2}{} \left| \frac{28.1 \text{ kg Si}}{60.1 \text{ kg } SiO_2} \right. = \frac{n_3 \text{ (kg } H_2SiF_6)}{} \left| \frac{28.1 \text{ kg Si}}{144.1 \text{ kg } H_2SiF_6} \right. \Rightarrow n_3 = 9.59 \text{ kg } H_2SiF_6$$

<u>Atomic balance - F:</u>

$$\frac{0.96(100) \text{ kg } CaF_2}{} \left| \frac{38.0 \text{ kg F}}{78.1 \text{ kg } CaF_2} \right. = \frac{n_2 \text{ (kg HF)}}{} \left| \frac{19.0 \text{ kg F}}{20.0 \text{ kg HF}} \right.$$

$$+ \frac{9.59 \text{ kg } H_2SiF_6}{} \left| \frac{114.0 \text{ kg F}}{144.1 \text{ kg } H_2SiF_6} \right. \Rightarrow n_2 = 41.2 \text{ kg HF}$$

$$\frac{600 \text{ kg HF}}{} \left| \frac{100 \text{ kg ore diss.}}{41.2 \text{ kg HF}} \right| \frac{1 \text{ kg ore feed}}{0.95 \text{ kg ore diss.}} = \underline{\underline{1533 \text{ kg ore}}}$$

4.53 **a.** $C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl$

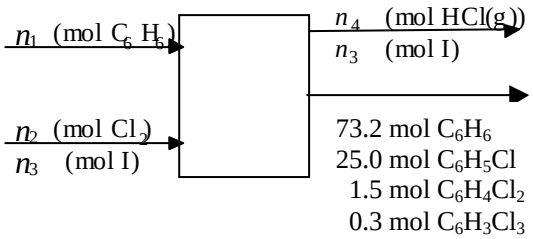
$C_6H_5Cl + Cl_2 \rightarrow C_6H_4Cl_2 + HCl$

$C_6H_4Cl_2 + Cl_2 \rightarrow C_6H_3Cl_3 + HCl$

Convert output wt% to mol%: Basis 100 g output

species	g	Mol. Wt.	mol	mol %
C_6H_6	65.0	78.11	0.832	73.2
C_6H_5Cl	32.0	112.56	0.284	25.0
$C_6H_4Cl_2$	2.5	147.01	0.017	1.5
$C_6H_3Cl_3$	0.5	181.46	0.003	0.3
			total 1.136	

<u>Basis: 100 mol output</u>



4 unknowns
-3 atomic balances
-1 wt% Cl_2 in feed
0 D.F.

b. <u>C balance:</u> $6n_1 = 6(73.2 + 25.0 + 1.5 + 0.3) \Rightarrow n_1 = 100 \text{ mol } C_6H_6$

<u>H balance:</u> $6(100) = 6(73.2) + 5(25.0) + 4(1.5) + 3(0.3) + n_4 \Rightarrow n_4 = 28.9 \text{ mol HCl}$

<u>Cl balance:</u> $2n_2 = 28.9 + 25.0 + 2(1.5) + 3(0.3) \Rightarrow n_2 = 28.9 \text{ mol } Cl_2$

<u>Theoretical C_6H_6</u> $= 28.9 \text{ mol } Cl_2 \left(1 \text{ mol } C_6H_6 / 1 \text{ mol } Cl_2\right) = 28.9 \text{ mol } C_6H_6$

<u>Excess C_6H_6</u>: $(100 - 28.9)/28.9 \times 100\% = \underline{\underline{246\% \text{ excess } C_6H_6}}$

<u>Fractional Conversion:</u> $(100 - 73.2)/100 = \underline{\underline{0.268 \text{ mol } C_6H_6 \text{ react/mol fed}}}$

<u>Yield:</u> $(25.0 \text{ mol } C_6H_5Cl)/(28.9 \text{ mol } C_6H_5Cl \text{ maximum}) = \underline{\underline{0.865}}$

$$\left.\begin{array}{l} \underline{\text{Gas feed:}} \quad \dfrac{28.9 \text{ mol } Cl_2}{} \left| \dfrac{70.91 \text{ g } Cl_2}{\text{mole } Cl_2} \right| \dfrac{1 \text{ g gas}}{0.98 \text{ g } Cl_2} = 2091 \text{ g gas} \\ \underline{\text{Liquid feed:}} \quad (100 \text{ mol } C_6H_6)\left(\dfrac{78.11 \text{ g } C_6H_6}{\text{mol } C_6H_6}\right) = 7811 \text{ g liquid} \end{array}\right\} \Rightarrow 0.268 \frac{\text{g gas}}{\text{g liquid}}$$

c. Low conversion $\Rightarrow$ low residence time in reactor $\Rightarrow$ lower chance of 2nd and 3rd reactions occurring. Large excess of $C_6H_6 \Rightarrow Cl_2$ much more likely to encounter C_6H_6 than substituted $C_6H_6 \Rightarrow$ higher selectivity.

d. Dissolve in water to produce hydrochloric acid.

e. Reagent grade costs <u>much</u> more. Use only if impurities in technical grade mixture affect the reaction rate or desired product yield.

4.54 **a.** $2CO_2 \Leftrightarrow 2CO + O_2$ $\qquad$ $2A \Leftrightarrow 2B + C$

$O_2 + N_2 \Leftrightarrow 2NO$ $\qquad$ $C + D \Leftrightarrow 2E$

$$\begin{aligned}
n_A &= n_{A0} - 2\xi_{e1} & y_A &= (n_{A0} - 2\xi_{e1})/(n_{T0} + \xi_{e1}) \\
n_B &= n_{B0} + 2\xi_{e2} & y_B &= (n_{B0} + 2\xi_{e1})/(n_{T0} + \xi_{e1}) \\
n_C &= n_{C0} + \xi_{e1} - \xi_{e2} \Rightarrow & y_C &= (n_{C0} + \xi_{e1} - \xi_{e2})/(n_{T0} + \xi_{e1}) \\
n_D &= n_{D0} - \xi_{e2} & y_D &= (n_{D0} - 1\xi_{e2})/(n_{T0} + \xi_{e1}) \\
n_E &= n_{E0} + 2\xi_{e2} & y_E &= (n_{E0} + 2\xi_{e2})/(n_{T0} + \xi_{e1})
\end{aligned}$$

$n_{total} = n_{T0} + \xi_{e1}$ $\qquad$ $(n_{T0} = n_{A0} + n_{B0} + n_{C0} + n_{D0} + n_{E0})$

<u>Equilibrium at 3000K and 1 atm</u>

$$\frac{y_B^2 y_C}{y_A^2} = \frac{(n_{B0} + 2\xi_{e1})^2 (n_{C0} + \xi_{e1} - \xi_{e2})}{(n_{A0} - 2\xi_{e1})^2 (n_{T0} + \xi_{e1})} = 0.1071$$

$$\frac{y_E^2}{y_C y_D} = \frac{(n_{E0} + 2\xi_{e2})^2}{(n_{A0} + \xi_{e1} - \xi_{e2})(n_{D0} - \xi_{e2})} = 0.01493$$

$\Downarrow$

$$\left.\begin{aligned}
f_1 &= 0.1071(n_{A0} - 2\xi_{e1})^2 (n_{T0} + \xi_{e1}) - (n_{B0} + 2\xi_{e1})^2 (n_{C0} + \xi_{e1} - \xi_{e2}) = 0 \\
f_2 &= 0.01493(n_{C0} + \xi_{e1} - \xi_{e2})(n_{D0} - \xi_{e2}) - (n_{E0} + 2\xi_{e2})^2 = 0
\end{aligned}\right\} \text{Defines functions } f_1(\xi_1, \xi_2) \text{ and } f_2(\xi_1, \xi_2)$$

b. Given all n_{io}'s, solve above equations for ξ_{e1} and $\xi_{e2} \Rightarrow n_A, n_B, n_C, n_D, n_E \Rightarrow y_A, y_B, y_C, y_D, y_E$

c. $n_{A0} = n_{C0} = n_{D0} = 0.333$, $n_{B0} = n_{E0} = 0 \Rightarrow \xi_{e1} = 0.0593$, $\xi_{e2} = 0.0208$

$\Rightarrow$ $\underline{y_A = 0.2027}$, $\underline{y_B = 0.1120}$, $\underline{y_C = 0.3510}$, $\underline{y_D = 0.2950}$, $\underline{y_E = 0.0393}$

d.

$$\begin{aligned}
a_{11}d_1 + a_{12}d_2 &= -f_1 & a_{21}d_1 + a_{22}d_2 &= -f_2 \\
d_1 &= \frac{a_{12}f_2 - a_{22}f_1}{a_{11}a_{22} - a_{12}a_{21}} & d_2 &= \frac{a_{21}f_1 - a_{11}f_2}{a_{11}a_{22} - a_{12}a_{21}} \\
(\xi_{e1})_{new} &= \xi_{e1} + d_1 & (\xi_{e2})_{new} &= \xi_{e1} + d_2
\end{aligned}$$

(Solution given following program listing.)

```
.          IMPLICIT REAL * 4(N)
           WRITE (6, 1)
 1         FORMAT('1', 30X, 'SOLUTION TO PROBLEM 4.57'///)
30         READ (5, *) NA0, NB0, NC0, ND0, NE0
           IF (NA0.LT.0.0)STOP
           WRITE (6, 2) NA0, NB0, NC0, ND0, NE0
```

4.54 (cont'd)

```
 2    FORMAT('0', 15X, 'NA0, NB0, NC0, ND0, NE0 *', 5F6.2/)
      NTO = NA0 + NB0 + NC0 + ND0 + NE0
      NMAX = 10
      X1 = 0.1
      X2 = 0.1
      DO 100 J = 1, NMAX
      NA = NA0 – X1 – X1
      NB = NB0 + X1 + X1
      NC = NC0 + X1 – X2
      ND = ND0 – X2
      NE = NE0 + X2 + X2
      NAS = NA ** 2
      NBS = NB ** 2
      NES = NE ** 2
      NT = NT0 + X1
      F1 = 0.1071 * NAS * NT – NBS * NC
      F2 = 0.01493 * NC * ND – NES
      A11 = –0.4284 * NA * NT * 0.1071 * NAS – 4.0 * NB * NC – NBS
      A12 = NBS
      A21 = 0.01493 * ND
       A22 = –0.01493 * (NC + ND) – 4.0 * NE
      DEN = A11 * A22 – A12 * A21
      D1 = (A12 * F2 – A22 * F1)/DEN
      D2 = (A21 * F1 – A11 * F2)/DEN
      X1C = X1 + D1
      X2C = X2 + D2
      WRITE (6, 3) J, X1, X2, X1C, X2C
 3    FORMAT(20X, 'ITER *', I3, 3X, 'X1A, X2A =', 2F10.5, 6X, 'X1C, X2C =', * 2F10.5)
      IF (ABS(D1/X1C).LT.1.0E–5.AND.ABS(D2/X2C).LT.1.0E–5) GOTO 120
      X1 = X1C
      X2 = X2C
100   CONTINUE
      WRITE (6, 4) NMAX
 4    FORMAT('0', 10X, 'PROGRAM DID NOT CONVERGE IN', I2, 'ITERATIONS'/)
      STOP
120   YA = NA/NT
      YB = NB/NT
      YC = NC/NT
      YD = ND/NT
      YE = NE/NT
      WRITE (6, 5) YA, YB, YC, YD, YE
    5 FORMAT ('0', 15X, 'YA, YB, YC, YD, YE =', 1P5E14.4///)
      GOTO 30
      END
      $DATA
      0.3333   0.00   0.3333   0.3333   0.0
      0.50     0.0    0.0      0.50     0.0
      0.20     0.20   0.20     0.20     0.20
```

SOLUTION TO PROBLEM 4.54

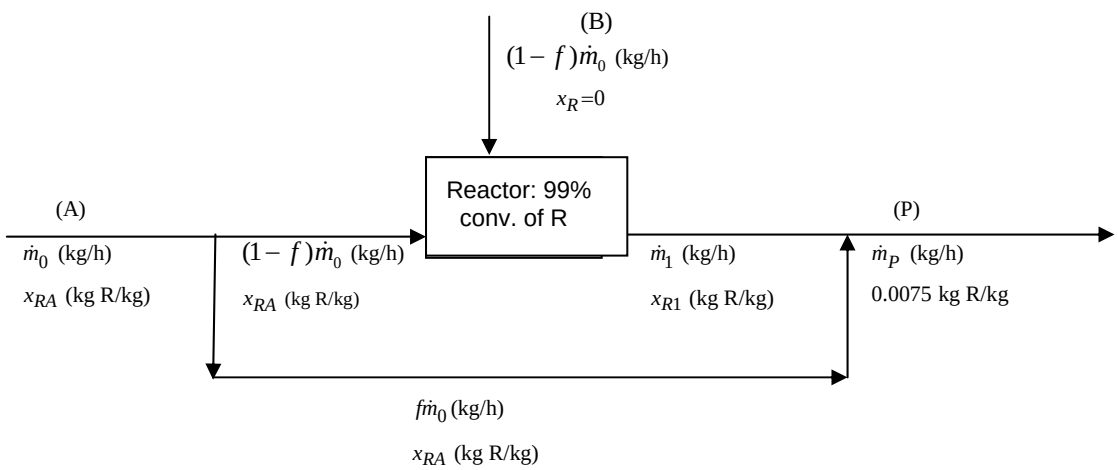
```
NA0, NB0, NC0, ND0, NE0 = 0.33   0.00    0.33    0.33    0.00
ITER = 1   X1A, X2A = 0.10000    0.10000          X1C, X2C = 0.06418      0.05181
ITER = 2   X1A, X2A = 0.06418    0.05181          X1C, X2C = 0.05969      0.02986
ITER = 3   X1A, X2A = 0.05969    0.02486          X1C, X2C = 0.05937      0.02213
```

4.54 (cont'd)

```
ITER = 4   X1A, X2A = 0.05437    0.02213          X1C, X2C = 0.05931       0.02086
ITER = 5   X1A, X2A = 0.05931    0.02086          X1C, X2C = 0.05930       0.02083
ITER = 6   X1A, X2A = 0.05930    0.02083          X1C, X2C = 0.05930       0.02083
YA, YB, YC, YD, YE =        2.0270E – 01    1.1197E – 01    3.5100E – 01
                            2.9501E – 01    3.9319E – 02
```

```
NA0, NB0, NC0, ND0, NE0 = 0.20   0.20   0.20   0.20   0.20
ITER = 1   X1A, X2A = 0.10000                 0.10000   X1C, X2C = 0.00012      0.00037
  ↓
ITER = 7   X1A, X2A = –0.02244                –0.08339  X1C, X2C = –0.02244     –0.08339
YA, YB, YC, YD, YE=         2.5051E – 01    1.5868E – 01    2.6693E – 01
                            2.8989E – 01    3.3991E – 02
```

4.55 a.



<u>Mass balance on reactor</u>: $2(1-f)\dot{m}_0 = \dot{m}_1$ (1)

<u>99% conversion of R</u>: $\dot{m}_1 x_{R1} = 0.01(1-f)\dot{m}_0 x_{RA}$ (2)

<u>Mass balance on mixing point</u>: $\dot{m}_1 + f\dot{m}_0 = \dot{m}_P$ (3)

<u>R balance on mixing point</u>: $\dot{m}_1 x_{R1} + f\dot{m}_0 x_{RA} = 0.0075\dot{m}_P$ (4)

The system has 6 unknowns $(\dot{m}_0, x_{RA}, f, \dot{m}_1, x_{R1}, \dot{m}_P)$ and four independent equations relating them, so there must be two degrees of freedom.

b.

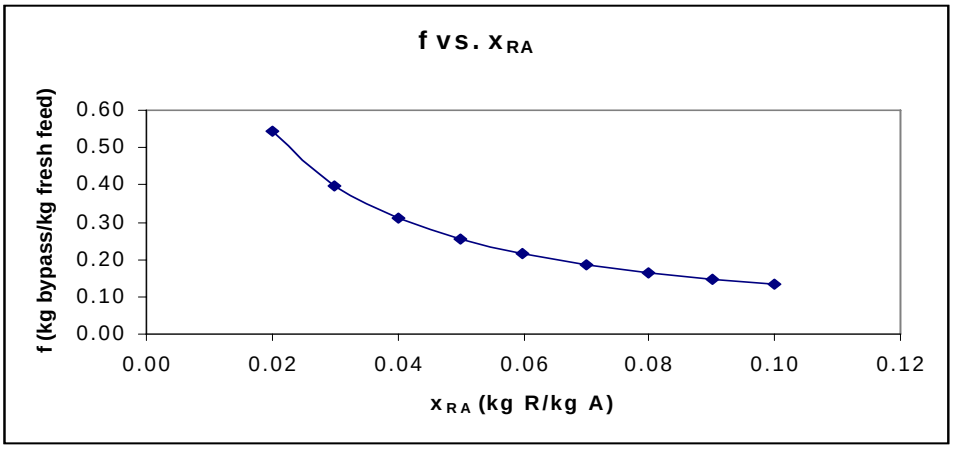
$$\left.\begin{aligned} &2(1-f)\dot{m}_0 = \dot{m}_1 \\ &\dot{m}_1 x_{R1} = 0.01(1-f)\dot{m}_0 x_{RA} \\ &\dot{m}_1 + f\dot{m}_0 = \dot{m}_P \\ &\dot{m}_1 x_{R1} + f\dot{m}_0 x_{RA} = 0.0075\dot{m}_P \\ &\dot{m}_P = 4850 \\ &x_{RA} = 0.0500 \end{aligned}\right\} \xrightarrow{\text{E-Z Solve}} \begin{aligned} &\dot{m}_0 = 2780 \text{ kg/h} \\ &f = 0.254 \text{ kg bypassed/kg fresh feed} \end{aligned}$$

4.55 (cont'd)

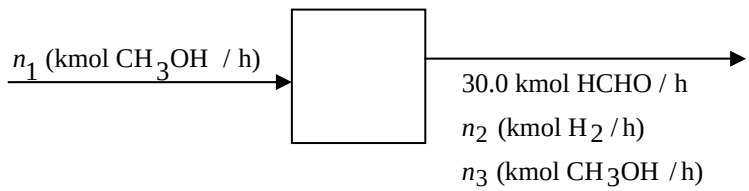
c.

m_P	x_{RA}	m_{A0}	m_{B0}	f
4850	0.02	3327	1523	0.54
4850	0.03	3022	1828	0.40
4850	0.04	2870	1980	0.31
4850	0.05	2778	2072	0.25
4850	0.06	2717	2133	0.21
4850	0.07	2674	2176	0.19
4850	0.08	2641	2209	0.16
4850	0.09	2616	2234	0.15
4850	0.10	2596	2254	0.13

m_P	x_{RA}	m_{A0}	m_{B0}	f
2450	0.02	1663	762	0.54
2450	0.03	1511	914	0.40
2450	0.04	1435	990	0.31
2450	0.05	1389	1036	0.25
2450	0.06	1359	1066	0.22
2450	0.07	1337	1088	0.19
2450	0.08	1321	1104	0.16
2450	0.09	1308	1117	0.15
2450	0.10	1298	1127	0.13

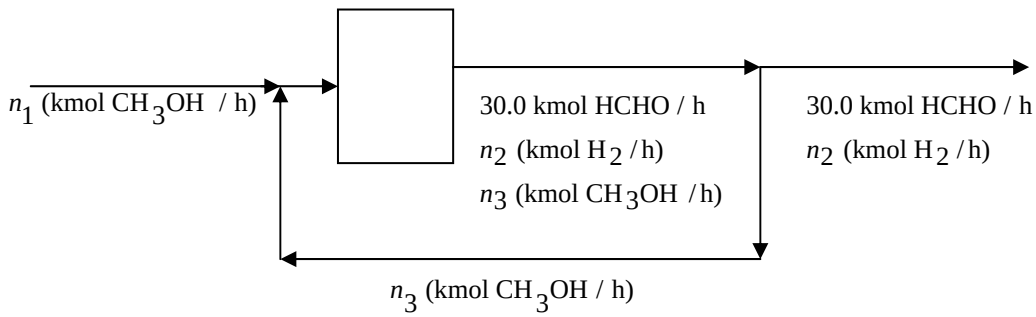


4.56 **a.** $\dfrac{900 \text{ kg HCHO}}{h} \left| \dfrac{1 \text{ kmol HCHO}}{30.03 \text{ kg HCHO}} \right. = 30.0 \text{ kmol HCHO / h}$



<u>% conversion</u>: $\dfrac{30.0}{n_1} = 0.60 \Rightarrow \underline{\underline{n_1 = 50.0 \text{ kmol } CH_3OH \text{ / h}}}$

b.



<u>Overall C balance</u>: n_1 (1) = 30.0 (1) $\Rightarrow$ n_1 = 30.0 kmol CH_3OH/h (fresh feed)

<u>Single pass conversion</u>: $\dfrac{30.0}{n_1 + n_3} = 0.60 \Rightarrow \underline{\underline{n_3 = 20.0 \text{ kmol } CH_3OH \text{ / h}}}$

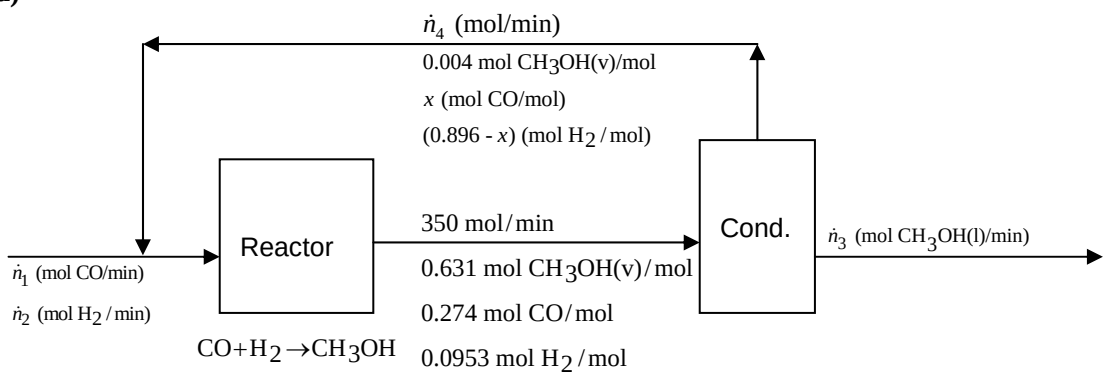
$n_1 + n_3$ = <u>50.0 kmol CH_3OH fed to reactor/h</u>

c. Increased x_{sp} will (1) require a larger reactor and so will increase the cost of the reactor and (2) lower the quantities of unreacted methanol and so will decrease the cost of the separation. The plot would resemble a concave upward parabola with a minimum around x_{sp} = 60%.

4.57 **a.** <u>Convert effluent composition to molar basis</u>. <u>Basis</u>: 100 g effluent:

$$\left.\begin{array}{l} \dfrac{10.6 \text{ g } H_2}{} \left| \dfrac{1 \text{ mol } H_2}{2.01 \text{ g } H_2} \right. = 5.25 \text{ mol } H_2 \\ \dfrac{64.0 \text{ g CO}}{} \left| \dfrac{1 \text{ mol CO}}{28.01 \text{ g CO}} \right. = 2.28 \text{ mol CO} \\ \dfrac{25.4 \text{ g } CH_3OH}{} \left| \dfrac{1 \text{ mol } CH_3OH}{32.04 \text{ g } CH_3OH} \right. \\ \quad = 0.793 \text{ mol } CH_3OH \end{array}\right\} \Rightarrow \begin{array}{r} H_2\text{: } 0.631 \text{ mol } H_2 \text{ / mol} \\ \text{CO: } 0.274 \text{ mol CO / mol} \\ CH_3OH\text{: } 0.0953 \text{ mol } CH_3OH \text{ / mol} \end{array}$$

4.57 (cont'd)



<u>Condenser</u>

3 unknowns $(\dot{n}_3, \dot{n}_4, x)$

–<u>3 balances</u>

0 degrees of freedom

<u>Overall process</u>

2 unknowns $(\dot{n}_1, \dot{n}_2)$

–<u>2 independent atomic balances</u>

0 degrees of freedom

<u>Balances around condenser</u>

$$\left.\begin{array}{r} \text{CO: } 350 * 0.274 = \dot{n}_4 * x \\ \text{H}_2: \ 350 * 0.631 = \dot{n}_4 * (0.996 - x) \\ \text{CH}_3\text{OH}: \ 350 * 0.0953 = \dot{n}_3 + 0.004 * \dot{n}_4 \end{array}\right\} \Rightarrow \begin{array}{c} \underline{\underline{\dot{n}_3 = 32.1 \text{ mol } CH_3OH(l)/\text{min}}} \\ \dot{n}_4 = 318.7 \text{ mol recycle/min} \\ x = .301 \text{ molCO/mol} \end{array}$$

<u>Overall balances</u>

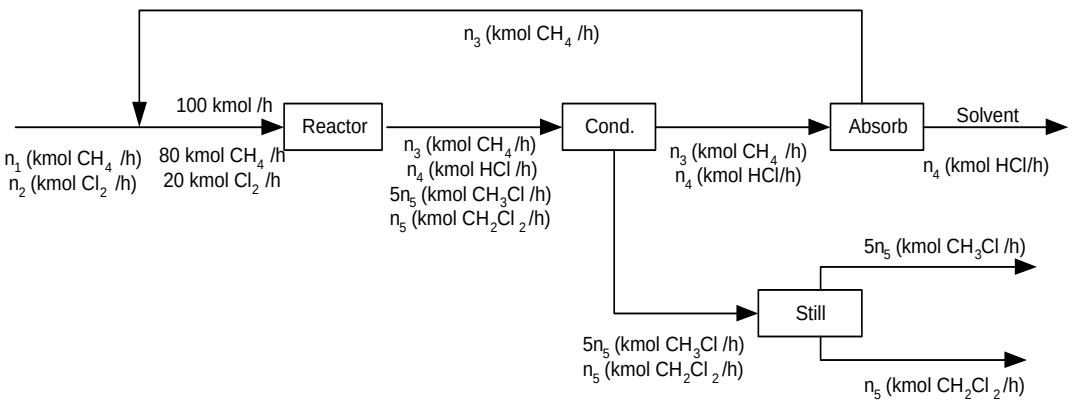
$$\left.\begin{array}{r} \text{C: } \dot{n}_1 = \dot{n}_3 \\ \text{H: } 2\dot{n}_2 = 4\dot{n}_3 \end{array}\right\} \Rightarrow \begin{array}{c} \underline{\underline{\dot{n}_1 = 32.08 \text{ mol/min CO in feed}}} \\ \underline{\underline{\dot{n}_2 = 64.16 \text{ mol/min } H_2 \text{ in feed}}} \end{array}$$

<u>Single pass conversion of CO:</u> $\dfrac{(32.08 + 318.72 * 0.3009) - 350 * 0.274}{(32.08 + 318.72 * 0.3009)} \times 100\% = \underline{\underline{25.07\%}}$

<u>Overall conversion of CO:</u> $\dfrac{32.08 - 0}{32.08} \times 100\% = \underline{\underline{100\%}}$

b.
- Reactor conditions or feed rates drifting. (Recalibrate measurement instruments.)
- Impurities in feed. (Re-analyze feed.)
- Leak in methanol outlet pipe before flowmeter. (Check for it.)

4.58 **a.** Basis: 100 kmol reactor feed/hr



Overall process: 4 unknowns (n_1, n_2, n_4, n_5) -3 balances = 1 D.F.
Mixing Point: 3 unknowns (n_1, n_2, n_3) -2 balances = 1 D.F.
Reactor: 3 unknowns (n_3, n_4, n_5) -3 balances = 0 D.F.
Condenser: 3 unknowns (n_3, n_4, n_5) -0 balances = 3 D.F.
Absorption column: 2 unknowns (n_3, n_4) -0 balances = 2 D.F.
Distillation Column: 2 unknowns (n_4, n_5) -0 balances = 2 D.F.
Atomic balances around reactor:

$$\left.\begin{array}{l} 1)\ \text{C balance}:\ 80 = n_3 + 5n_5 + n_5 \\ 2)\ \text{H balance}: 320 = 4n_3 + n_4 + 15n_5 + 2n_5 \\ 3)\ \text{Cl balance}: 40 = n_4 + 5n_5 + 2n_5 \end{array}\right\} \Rightarrow \text{Solve for } n_3, n_4, n_5$$

CH_4 balance around mixing point: $n_1 = (80 - n_3)$ Solve for n_1

Cl_2 balance: $n_2 = 20$

b. For a basis of 100 kmol/h into reactor

n_1 = 17.1 kmol CH_4/h
n_2 = 20.0 kmol Cl_2/h
n_3 = 62.9 kmol CH_4/h
n_4 = 20.0 kmol HCl/h
$5n_5$ = 14.5 kmol CH_3Cl/h

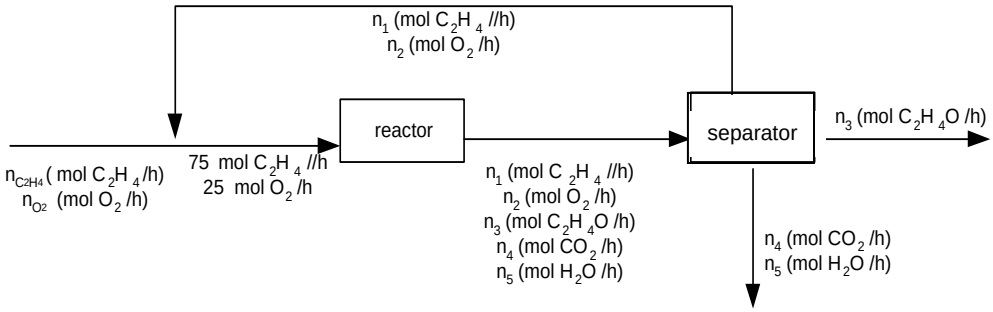
c. (1000 kg CH_3Cl/h)(1 kmol/50.49 kg) = 19.81 kmol CH_3Cl/h

Scale factor = $\dfrac{19.81\ \text{kmol CH}_3\text{Cl/h}}{14.5\ \text{kmol CH}_3\text{Cl/h}} = 1.366$

Fresh feed: $\left.\begin{array}{l} n_1 = (17.1)(1.366) = 23.3\ \text{kmol CH}_4\text{/h} \\ n_2 = (20.0)(1.366) = 27.3\ \text{kmol Cl}_2\text{/h} \end{array}\right\} \Rightarrow \begin{array}{c} n_{tot} = 50.6\ \text{kmol/h} \\ 46.0\ \text{mol\% CH}_4,\ 54.0\ \text{mole\% Cl}_2 \end{array}$

Recycle: n_3 = (62.9)(1.366) = 85.9 kmol CH_4 recycled/h

4.59 **a.** Basis: 100 mol fed to reactor/h ⇒ 25 mol O_2/h, 75 mol C_2H_4/h



<u>Reactor</u>

5 unknowns (n_1 - n_5)

-3 atomic balances

-1 - % yield

-<u>1 - % conversion</u>

0 D.F.

<u>Strategy</u>: 1. Solve balances around reactor to find n_1- n_5

2. Solve balances around mixing point to find n_{O2}, n_{C2H4}

(1) % Conversion ⇒ n_1 = .800 * 75

(2) % yield: $(.200)(75)\ \text{mol}\ C_2H_4 \times \dfrac{90\ \text{mol}\ C_2H_4O}{100\ \text{mol}\ C_2H_4} = n_3$ (production rate of C_2H_4O)

(3) C balance (reactor): 150 = 2 n_1 + 2 n_3 + n_4

(4) H balance (reactor): 300 = 4 n_1 + 4 n_3 + 2 n_5

(5) O balance (reactor): 50 = 2 n_2 + n_3 + 2 n_4 + n_5

(6) O_2 balance (mix pt): n_{O2} = 25 – n_2

(7) C_2H_4 balance (mix pt): n_{C2H4} = 75 – n_1

<u>Overall conversion of C_2H_4</u>: 100%

b.

n_1 = 60.0 mol C_2H_4/h

n_2 = 13.75 mol O_2 /h

n_3 = <u>13.5 mol C_2H_4O/h</u>

n_4 = 3.00 mol CO_2/h

n_5 = 3.00 mol H_2O/h

n_{O2} = <u>11.25 mol O_2/h</u>

n_{C2H4} = <u>15.0 mol C_2H_4/h</u>

<u>100% conversion of C_2H_4</u>

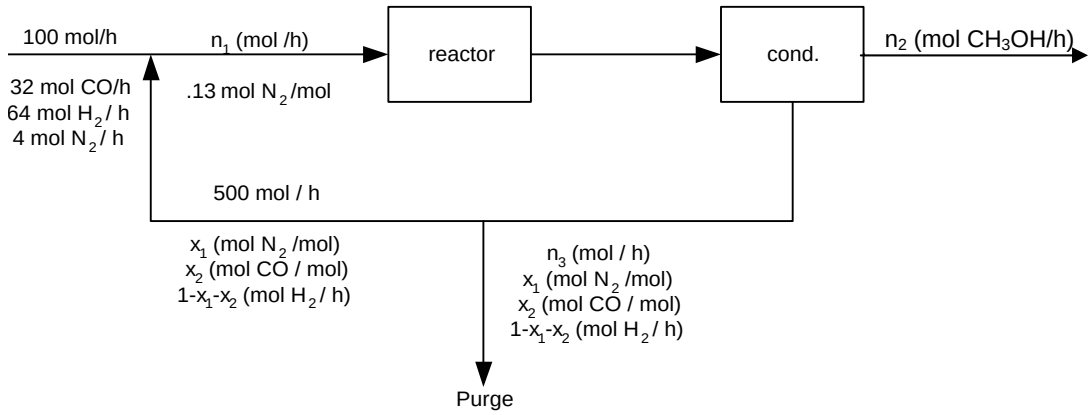
c.

$$\underline{\text{Scale factor}} = \frac{2000\ \text{lbm}\ C_2H_4O}{\text{h}}\left|\frac{1\ \text{lb - mole}\ C_2H_4O}{44.05\ \text{lbm}\ C_2H_4O}\right|\frac{\text{h}}{13.5\ \text{mol}\ C_2H_4O} = 3.363\frac{\text{lb}-\text{mol/h}}{\text{mol/h}}$$

n_{C2H4} = (3.363)(15.0) = <u>50.4 lb-mol C_2H_4/h</u>

n_{O2} = (3.363)(11.25) = <u>37.8 lb-mol O_2/h</u>

4.60 **a.** Basis: 100 mol feed/h. Put dots above all *n*'s in flow chart.



Mixing point balances:

total: (100) + 500 = $\dot{n}_1$ $\Rightarrow$ $\dot{n}_1$ = 600 mol/h

N_2: 4 + x_1 * 500 = .13 * 600 $\Rightarrow$ x_1 = 0.148 mol N_2/mol

Overall system balances:

N_2: 4 = .148 * $\dot{n}_3$ $\Rightarrow$ $\dot{n}_3$ = 27 mol/h

$$\left.\begin{array}{l}\text{Atomic C: } 32 = \dot{n}_2 + x_2*27 \\ \text{Atomic H: } 2*64 = 4*24.3 + 2*(1-0.148-x_2)*27\end{array}\right\} \Rightarrow \begin{array}{l}\dot{n}_2 = 24.3 \text{ mol } CH_3OH/h \\ x_2 = 0.284 \text{ mol CO/mol}\end{array}$$

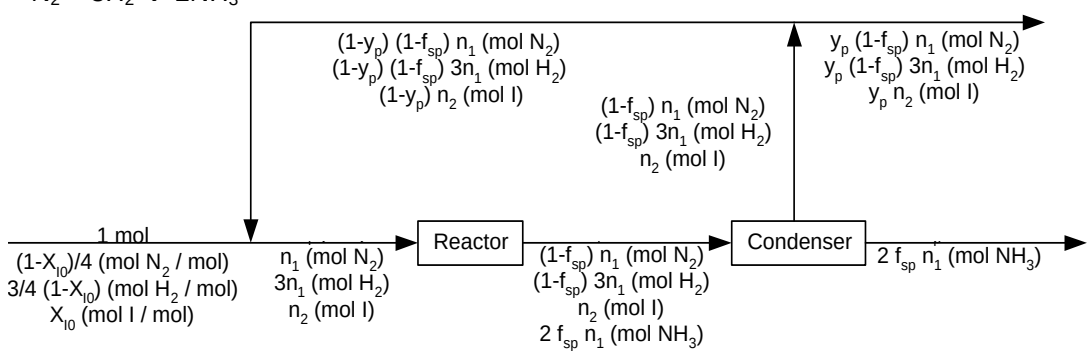
Overall CO conversion: 100*[32-0.284(27)]/32 = 76%

Single pass CO conversion: 24.3/ (32+.284*500) = 14%

b. Recycle: To recover unconsumed CO and H_2 and get a better overall conversion.

Purge: to prevent buildup of N_2.

4.61 **a.** $N_2 + 3H_2 \rightarrow 2NH_3$



4.61 (cont'd)

At mixing point:

N_2: $(1-X_{I0})/4 + (1-y_p)(1-f_{sp})\, n_1 = n_1$

I: $X_{I0} + (1-y_p)\, n_2 = n_2$

Total moles fed to reactor: $n_r = 4n_1 + n_2$

Moles of NH_3 produced: $n_p = 2f_{sp}n_1$

Overall N_2 conversion: $\dfrac{(1-X_{I0})/4 - y_p(1-f_{sp})n_1}{(1-X_{I0})/4} \times 100\%$

b. $X_{I0} = 0.01$ $f_{sp} = 0.20$ $y_p = 0.10$

$n_1 = 0.884$ mol N_2

$n_2 = 0.1$ mol I

n_r = 3.636 mol fed

n_p = 0.3536 mol NH_3 produced

N_2 conversion = 71.4%

c. Recycle: recover and reuse unconsumed reactants.

Purge: avoid accumulation of I in the system.

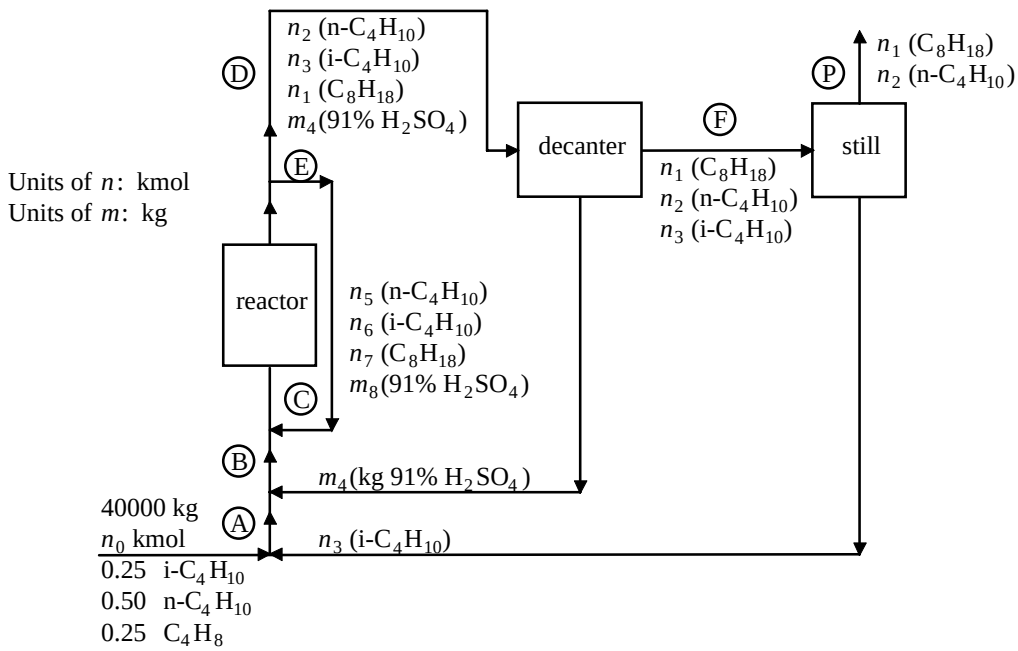
d. Increasing X_{I0} results in increasing n_r, decreasing n_p, and has no effect on f_{ov}. Increasing f_{sp} results in decreasing n_r, increasing n_p, and increasing f_{ov}.

Increasing y_p results in decreasing n_r, decreasing n_p, and decreasing f_{ov}.

Optimal values would result in a low value of n_r and f_{sp}, and a high value of n_p, this would give the highest profit.

X_{I0}	f_{sp}	y_p	n_r	n_p	f_{ov}
0.01	0.20	0.10	3.636	0.354	71.4%
0.05	0.20	0.10	3.893	0.339	71.4%
0.10	0.20	0.10	4.214	0.321	71.4%
0.01	0.30	0.10	2.776	0.401	81.1%
0.01	0.40	0.10	2.252	0.430	87.0%
0.01	0.50	0.10	1.900	0.450	90.9%
0.10	0.20	0.20	3.000	0.250	55.6%
0.10	0.20	0.30	2.379	0.205	45.5%
0.10	0.20	0.40	1.981	0.173	38.5%

4.62 **a.** $i\text{-}C_4H_{10} + C_4H_8 = C_8H_{18}$ <u>Basis</u>: 1-hour operation



<u>Calculate moles of feed</u>

$$\overline{M} = 0.25M_{\text{L-C}_4\text{H}_{10}} + 0.50M_{\text{n-C}_4\text{H}_{10}} + 0.25M_{\text{C}_4\text{H}_8} = (0.75)(58.12) + (0.25)(56.10)$$
$$= 57.6 \text{ kg/kmol}$$
$$n_0 = (40000 \text{ kg})(1 \text{ kmol}/57.6 \text{ kg}) = 694 \text{ kmol}$$

<u>Overall n - C_4H_{10} balance:</u> $n_2 = (0.50)(694) = \underline{\underline{347 \text{ kmol n - C}_4\text{H}_{10} \text{ in product}}}$

<u>C_8H_{18} balance:</u>

$$n_1 = \frac{(0.25)(694) \text{ kmol C}_4\text{H}_8 \text{ react}}{} \left| \frac{1 \text{ mol C}_8\text{H}_{18}}{1 \text{ mol C}_4\text{H}_8} \right. = \underline{\underline{173.5 \text{ kmol C}_8\text{H}_8 \text{ in product}}}$$

<u>At (A)</u>, 5 mol $i\text{-}C_4H_{10}$/1 mole C_4H_8 $\Rightarrow n(\text{mol } i\text{-C}_4\text{H}_{10})_A = \underbrace{(5)(0.25)(694)}_{\text{moles C}_4\text{H}_8 \text{ at A=173.5}} = 867.5 \text{ kmol}$ (i-C_4H_{10} at (A) and (B))

Note: $n(\text{mol C}_4\text{H}_8) = 173.5$ at (A), (B) and (C) and in feed

<u>$i\text{-}C_4H_{10}$ balance around first mixing point</u> $\Rightarrow (0.25)(694) + n_3 = 867.5$

$$\Rightarrow n_3 = \underline{\underline{694 \text{ kmol } i\text{-C}_4\text{H}_{10} \text{ recycled from still}}}$$

At C, 200 mol $i\text{-}C_4H_{10}$/mol C_4H_8

$$\Rightarrow n(\text{mol } i\text{-C}_4\text{H}_{10})_C = (200)(173.5) = 34{,}700 \text{ kmol } i\text{-C}_4\text{H}_{10}$$

4.62 (cont'd)

$\underline{i\text{-}C_4H_{10} \text{ balance around second mixing point}} \Rightarrow 867.5 + n_6 = 34{,}700$

$$\Rightarrow n_6 = \underline{\underline{33{,}800 \text{ kmol } C_4H_{10} \text{ in recycle E}}}$$

<u>Recycle E</u>: Since Streams (D) and (E) have the same composition,

$$\frac{n_5\ (\text{moles n-}C_4H_{10})_E}{n_2\ (\text{moles n-}C_4H_{10})_D} = \frac{n_6\ (\text{moles } i\text{-}C_4H_{10})_E}{n_3\ (\text{moles } i\text{-}C_4H_{10})_D} \Rightarrow n_5 = \underline{\underline{16{,}900 \text{ kmol n-}C_4H_{10}}}$$

$$\frac{n_7\ (\text{moles } C_8H_{18})_E}{n_1\ (\text{moles } C_8H_{18})_D} = \frac{n_6}{n_3} \Rightarrow n_7 = \underline{\underline{8460 \text{ kmol } C_4H_{18}}}$$

<u>Hydrocarbons entering reactor:</u>

$$\left[(347 + 16900)(\text{kmol n-}C_4H_{10})\right]\left(58.12\ \frac{\text{kg}}{\text{kmol}}\right)$$
$$+\left[(867.5 + 33800)(\text{kmol } i\text{-}C_4H_{10})\right]\left(58.12\ \frac{\text{kg}}{\text{kmol}}\right) + \left[173.5 \text{ kmol } C_4H_8\right]\left(56.10\ \frac{\text{kg}}{\text{kmol}}\right)$$
$$+\left[8460 \text{ kmol } C_8H_{18}\right]\left(114.22\ \frac{\text{kg}}{\text{kmol}}\right) = 4.00 \times 10^6 \text{ kg}.$$

$$\frac{\underline{H_2SO_4 \text{ solution entering reactor}}}{\underline{(\text{and leaving reactor})}} = \frac{4.00 \times 10^6 \text{ kg HC}}{} \left| \frac{2 \text{ kg } H_2SO_4(\text{aq})}{1 \text{ kg HC}} \right.$$
$$= 8.00 \times 10^6 \text{ kg } H_2SO_4(\text{aq})$$

$$\frac{m_8(H_2SO_4 \text{ in recycle})}{8.00 \times 10^6 (H_2SO_4 \text{ leaving reactor})} = \frac{n_5(\text{n-}C_4H_{10} \text{ in recycle})}{n_2 + n_5(\text{n-}C_4H_{10} \text{ leaving reactor})}$$

$$\Rightarrow m_8 = 7.84 \times 10^6 \text{ kg } H_2SO_4(\text{aq}) \text{ in recycle E}$$

$m_4 = H_2SO_4$ entering reactor $- H_2SO_4$ in E

$= 1.6 \times 10^5$ kg $H_2SO_4(\text{aq})$ recycled from decanter

$$\Rightarrow \left[(1.6 \times 10^5)(0.91)\text{kg } H_2SO_4\right](1 \text{ kmol}/98.08 \text{ kg}) = 1480 \text{ kmol } H_2SO_4 \text{ in recycle}$$

$$\left[(1.6 \times 10^5)(0.09)\text{kg } H_2O\right](1 \text{ kmol}/18.02 \text{ kg}) = 799 \text{ kmol } H_2O \text{ from decanter}$$

<u>Summary:</u> (Change amounts to flow rates)

<u>Product: 173.5 kmol C_8H_{18}/h, 347 kmol n-C_4H_{10}/h</u>

<u>Recycle from still: 694 kmol i-C_4H_{10}/h</u>

<u>Acid recycle: 1480 kmol H_2SO_4/h, 799 kmol H_2O/h</u>

<u>Recycle E: 16,900 kmol n-C_4H_{10}/h, 33,800 kmol L-C_4H_{10}/h, 8460 kmol C_8H_{18}/h,</u>

<u>7.84×10^6 kg/h 91% $H_2SO_4 \Rightarrow 72{,}740$ kmol H_2SO_4/h, 39,150 kmol H_2O/h</u>

4.63 **a.** <u>A balance on *i*th tank</u> (input = output + consumption)

$$\dot{v}(\text{L/min})C_{A,\,i-1}(\text{mol/L}) = \dot{v}C_{Ai} + kC_{Ai}C_{Bi}(\text{mol/liter}\cdot\text{min})V(\text{L})$$

$$\Downarrow \div \dot{v},\ \text{note } V/\dot{v} = \tau$$

$$\underline{\underline{C_{A,\,i-1} = C_{Ai} + k\tau C_{Ai}C_{Bi}}}$$

<u>B balance</u>. By analogy, $C_{B,\,i-1} = C_{Bi} + k\tau C_{Ai}C_{Bi}$

Subtract equations $\Rightarrow C_{Bi} - C_{Ai} = C_{B,\,i-1} - C_{A,\,i-1} \underset{\substack{\uparrow \\ \text{from balances on} \\ (i-1)^{\text{st}}\ \text{tank}}}{=} C_{B,\,i-2} - C_{A,\,i-2} = \ldots = C_{B0} - C_{A0}$

b. $C_{Bi} - C_{Ai} = C_{B0} - C_{A0} \Rightarrow C_{Bi} = C_{Ai} + C_{B0} - C_{A0}$. Substitute in A balance from part (a).

$C_{A,\,i-1} = C_{Ai} + k\tau C_{Ai}\left[C_{Ai} + (C_{B0} - C_{A0})\right]$. Collect terms in C_{Ai}^2, C_{Ai}^1, C_{Ai}^0.

$C_{Ai}^2[k\tau] + C_{AL}\left[1 + k\tau(C_{B0} - C_{A0})\right] - C_{A,\,i-1} = 0$

$\Rightarrow \alpha C_{AL}^2 + \beta C_{AL} + \gamma = 0$ where $\alpha = k\tau, \beta = 1 + k\tau(C_{B0} - C_{A0}), \gamma = -C_{A,\,i-1}$

<u>Solution</u>: $C_{Ai} = \dfrac{-\beta + \sqrt{\beta^2 - 4\alpha\gamma}}{2\alpha}$ (Only + rather than ±: since αγ is negative and the negative solution would yield a negative concentration.)

c.

		N	gamma	CA(N)	xA(N)
k =	36.2	1	-5.670E-02	2.791E-02	0.5077
v =	5000	2	-2.791E-02	1.512E-02	0.7333
V =	2000	3	-1.512E-02	8.631E-03	0.8478
CA0 =	0.0567	4	-8.631E-03	5.076E-03	0.9105
CB0 =	0.1000	5	-5.076E-03	3.038E-03	0.9464
alpha =	14.48	6	-3.038E-03	1.837E-03	0.9676
beta =	1.6270	7	-1.837E-03	1.118E-03	0.9803
		8	-1.118E-03	6.830E-04	0.9880
		9	-6.830E-04	4.182E-04	0.9926
		10	-4.182E-04	2.565E-04	0.9955
		11	-2.565E-04	1.574E-04	0.9972
		12	-1.574E-04	9.667E-05	0.9983
		13	-9.667E-05	5.939E-05	0.9990
		14	-5.939E-05	3.649E-05	0.9994

($x_{\min} = 0.50$, $N = 1$), ($x_{\min} = 0.80$, $N = 3$), ($x_{\min} = 0.90$, $N = 4$), ($x_{\min} = 0.95$, $N = 6$), ($x_{\min} = 0.99$, $N = 9$), ($x_{\min} = 0.999$, $N = 13$).

As $x_{\min} \to 1$, the required number of tanks and hence the process cost becomes infinite.

d. (i) k increases $\Rightarrow$ N decreases (faster reaction $\Rightarrow$ fewer tanks)

(ii) $\dot{v}$ increases $\Rightarrow$ N increases (faster throughput $\Rightarrow$ less time spent in reactor $\Rightarrow$ lower conversion per reactor)

(iii) V increases $\Rightarrow$ N decreases (larger reactor $\Rightarrow$ more time spent in reactor $\Rightarrow$ higher conversion per reactor)

4.64 **a.** Basis: 1000 g gas

Species	m (g)	MW	n (mol)	**mole % (wet)**	**mole % (dry)**
C_3H_8	800	44.09	18.145	**77.2%**	**87.5%**
C_4H_{10}	150	58.12	2.581	**11.0%**	**12.5%**
H_2O	50	18.02	2.775	**11.8%**	
Total	1000		23.501	**100%**	**100%**

Total moles = 23.50 mol, Total moles (dry) = 20.74 mol

Ratio: 2.775 / 20.726 = $\underline{\underline{0.134 \text{ mol } H_2O \ / \ \text{mol dry gas}}}$

b. $C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$, $C_4H_{10} + 13/2\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$

Theoretical O_2:

$$\underline{C_3H_8}: \frac{100 \text{ kg gas}}{\text{h}} \left| \frac{80 \text{ kg } C_3H_8}{100 \text{ kg gas}} \right| \frac{1 \text{ kmol } C_3H_8}{44.09 \text{ kg } C_3H_8} \left\| \frac{5 \text{ kmol } O_2}{1 \text{ kmol } C_3H_8} \right. = 9.07 \text{ kmol } O_2 \ / \ \text{h}$$

$$\underline{C_4H_{10}}: \frac{100 \text{ kg gas}}{\text{h}} \left| \frac{15 \text{ kg } C_4H_{10}}{100 \text{ kg gas}} \right| \frac{1 \text{ kmol } C_4H_{10}}{58.12 \text{ kg } C_4H_{10}} \left| \frac{6.5 \text{ kmol } O_2}{1 \text{ kmol } C_4H_{10}} \right. = 1.68 \text{ kmol } O_2 \ / \ \text{h}$$

Total: (9.07 + 1.68) kmol O_2/h = 10.75 kmol O_2/h

$$\text{Air feed rate}: \frac{10.75 \text{ kmol } O_2}{\text{h}} \left| \frac{1 \text{ kmol Air}}{.21 \text{ kmol } O_2} \right| \frac{1.3 \text{ kmol air fed}}{1 \text{ kmol air required}} = \underline{\underline{66.5 \text{ kmol air / h}}}$$

The answer does not change for incomplete combustion

4.65

$$\frac{5 \text{ L } C_6H_{14}}{} \left| \frac{0.659 \text{ kg } C_6H_{14}}{\text{L } C_6H_{14}} \right| \frac{1000 \text{ mol } C_6H_{14}}{86 \text{ kg } C_6H_{14}} = 38.3 \text{ mol } C_6H_{14}$$

$$\frac{4 \text{ L } C_7H_{16}}{} \left| \frac{0.684 \text{ kg } C_7H_{16}}{\text{L } C_7H_{16}} \right| \frac{1000 \text{ mol } C_7H_{16}}{100 \text{ kg } C_7H_{16}} = 27.36 \text{ mol } C_7H_{16}$$

$C_6H_{14} + 19/2\ O_2 \rightarrow 6\ CO_2 + 7\ H_2O$ $\qquad$ $C_6H_{14} + 13/2\ O_2 \rightarrow 6\ CO + 7\ H_2O$

$C_7H_{16} + 11\ O_2 \rightarrow 7\ CO_2 + 8\ H_2O$ $\qquad$ $C_7H_{16} + 15/2\ O_2 \rightarrow 7\ CO + 8\ H_2O$

Theoretical oxygen:

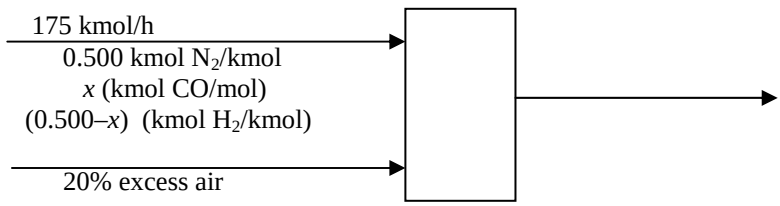
$$\frac{38.3 \text{ mol } C_6H_{14}}{} \left| \frac{9.5 \text{ mol } O_2}{\text{mol } C_6H_{14}} \right. + \frac{27.36 \text{ mol } C_7H_{16}}{} \left| \frac{11 \text{ mol } O_2}{\text{mol } C_7H_{16}} \right. = 665 \text{ mol } O_2 \text{ required}$$

O_2 fed: (4000 mol air)(.21 mol O_2 / mol air) = 840 mol O_2 fed

$$\text{Percent excess air}: \frac{840 - 665}{665} \times 100\% = \underline{\underline{26.3\% \text{ excess air}}}$$

4.66

$$CO + \frac{1}{2}O_2 \rightarrow CO_2 \qquad H_2 + \frac{1}{2}O_2 \rightarrow H_2O$$



Note: Since CO and H_2 each require 0.5 mol O_2 / mol fuel for complete combustion, we can calculate the air feed rate without determining x_{CO}. We include its calculation for illustrative purposes.

A plot of x vs. R on log paper is a straight line through the points $(R_1 = 10.0, x_1 = 0.05)$ and $(R_2 = 99.7, x_2 = 1.0)$.

$$\ln x = b \ln R + \ln a \qquad b = \ln(1.0/0.05)/\ln(99.7/10.0) = 1.303$$

$$\Updownarrow \qquad \ln a = \ln(1.0) - 1.303\ln(99.7) = -6.00 \quad \Rightarrow \underline{\underline{x = 2.49 \times 10^{-3} R^{1.303}}}$$

$$x = a R^b \qquad a = \exp(-6.00) = 2.49 \times 10^{-3}$$

$$R = 38.3 \Rightarrow x = 0.288 \frac{\text{moles CO}}{\text{mol}}$$

$$\underline{\text{Theoretical } O_2}: \quad \frac{175 \text{ kmol}}{\text{h}} \left| \frac{0.288 \text{ kmol CO}}{\text{kmol}} \right| \frac{0.5 \text{ kmol } O_2}{\text{kmol CO}}$$

$$+ \frac{175 \text{ kmol}}{\text{h}} \left| \frac{0.212 \text{ kmol } H_2}{\text{kmol}} \right| \frac{0.5 \text{ kmol } O_2}{\text{kmol } H_2} = 43.75 \frac{\text{kmol } O_2}{\text{h}}$$

$$\underline{\text{Air fed:}} \quad \frac{43.75 \text{ kmol } O_2 \text{ required}}{\text{h}} \left| \frac{1 \text{ kmol air}}{0.21 \text{ kmol } O_2} \right| \frac{1.2 \text{ kmol air fed}}{1 \text{ kmol air required}} = \underline{\underline{250 \frac{\text{kmol air}}{\text{h}}}}$$

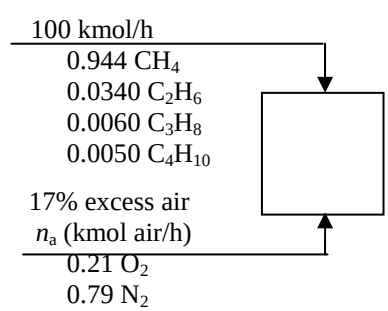
4.67 **a.**

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

$$C_4H_{10} + \frac{13}{2}O_2 \rightarrow 4CO_2 + 5H_2O$$



$$\underline{\text{Theoretical } O_2}: \frac{0.944(100)\text{kmol } CH_4}{\text{h}} \left| \frac{2 \text{ kmol } O_2}{1 \text{ kmol } CH_4} \right. + \frac{0.0340(100)\text{kmol } C_2H_6}{\text{h}} \left| \frac{3.5 \text{ kmol } O_2}{1 \text{ kmol } C_2H_6} \right.$$

$$+ \frac{0.0060(100)\text{kmol } C_3H_8}{\text{h}} \left| \frac{5 \text{ kmol } O_2}{1 \text{ kmol } C_3H_3} \right. + \frac{0.0050(100)\text{kmol } C_4H_{10}}{\text{h}} \left| \frac{6.5 \text{ kmol } O_2}{1 \text{ kmol } C_4H_{10}} \right.$$

$$= 207.0 \text{ kmol } O_2/\text{h}$$

4.67 (cont'd)

Air feed rate: $n_f = \dfrac{207.0 \text{ kmol } O_2}{\text{h}} \left| \dfrac{1 \text{ kmol air}}{0.21 \text{ kmol } O_2} \right| \dfrac{1.17 \text{ kmol air fed}}{\text{kmol air req.}} = \underline{\underline{1153 \text{ kmol air/h}}}$

b. $\underline{\underline{n_a = n_f\left(2x_1 + 3.5x_2 + 5x_3 + 6.5x_4\right)\left(1 + P_{xs}/100\right)\left(1/0.21\right)}}$

c. $\dot{n}_f = aR_f$, $(\dot{n}_f = 75.0 \text{ kmol / h},\ R_f = 60) \Rightarrow \dot{n}_f = 1.25R_f$

$\dot{n}_a = bR_a$, $(\dot{n}_a = 550 \text{ kmol / h},\ R_a = 25) \Rightarrow \dot{n}_a = 22.0R_a$

$$x_i = kA_i \ \Rightarrow\ \sum_i x_i = k\sum_i A_i = 1 \ \Rightarrow\ k = \frac{1}{\sum_i A_i}$$

$$\Rightarrow\ x_i = \frac{A_i}{\sum_i A_i}\ ,\ i = \text{CH}_4,\ \text{C}_2\text{H}_4,\ \text{C}_3\text{H}_8,\ \text{C}_4\text{H}_{10}$$

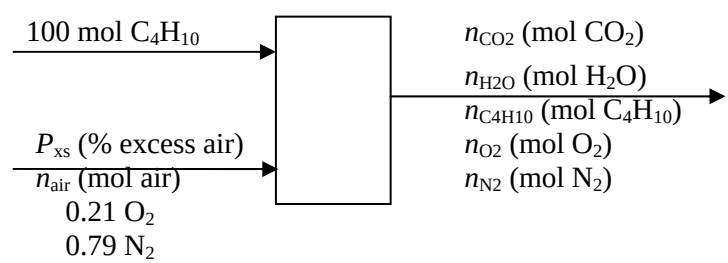
Run	P_{xs}	R_f	A_1	A_2	A_3	A_4
1	15%	62	248.7	19.74	6.35	1.48
2	15%	83	305.3	14.57	2.56	0.70
3	15%	108	294.2	16.61	4.78	2.11

Run	n_f	x_1	x_2	x_3	x_4	n_a	R_a
1	77.5	0.900	0.0715	0.0230	0.0054	934	42.4
2	103.8	0.945	0.0451	0.0079	0.0022	1194	54.3
3	135.0	0.926	0.0523	0.0150	0.0066	1592	72.4

d. Either of the flowmeters could be in error, the fuel gas analyzer could be in error, the flowmeter calibration formulas might not be linear, or the stack gas analysis could be incorrect.

4.68 **a.** $C_4H_{10} + 13/2\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$

Basis: 100 mol C_4H_{10}



D.F. analysis

6 unknowns (n, n_1, n_2, n_3, n_4, n_5)

-3 atomic balances (C, H, O)

-1 N_2 balance

-1 % excess air

-1 % conversion

0 D.F.

4.68 (cont'd)

b. i) Theoretical oxygen = (100 mol C_4H_{10})(6.5 mol O_2/mol C_4H_{10}) = 650 mol O_2

$$n_{air} = (650 \text{ mol } O_2)(1 \text{ mol air} / 0.21 \text{ mol } O_2) = 3095 \text{ mol air}$$

100% conversion $\Rightarrow$ $n_{C4H10} = 0$, $n_{O_2} = 0$

$$\left.\begin{array}{l} n_{N2} = (0.79)(3095 \text{ mol}) = 2445 \text{ mol} \\ n_{CO2} = (100 \text{ mol } C_4H_{10} \text{ react})(4 \text{ mol } CO_2/\text{mol } C_4H_{10}) = 400 \text{ mol } CO_2 \\ n_{H2O} = (100 \text{ mol } C_4H_{10} \text{ react})(5 \text{ mol } H_2O/\text{mol } C_4H_{10}) = 500 \text{ mol } H_2O \end{array}\right\} \begin{array}{l} 73.1\% \ N_2 \\ 12.0\% \ CO_2 \\ 14.9\% \ H_2O \end{array}$$

ii) 100% conversion $\Rightarrow$ $n_{C4H10} = 0$

20% excess $\Rightarrow$ n_{air} = 1.2(3095) = 3714 mol (780 mol O_2, 2934 mol N_2)

Exit gas:

400 mol CO_2	10.1% CO_2
500 mol H_2O	12.6% H_2O
130 mol O_2	3.3% O_2
2934 mol N_2	74.0% N_2

iii) 90% conversion $\Rightarrow$ n_{C4H10} = 10 mol C_4H_{10} (90 mol C_4H_{10} react, 585 mol O_2 consumed)

20% excess: n_{air} = 1.2(3095) = 3714 mol (780 mol O_2, 2483 mol N_2)

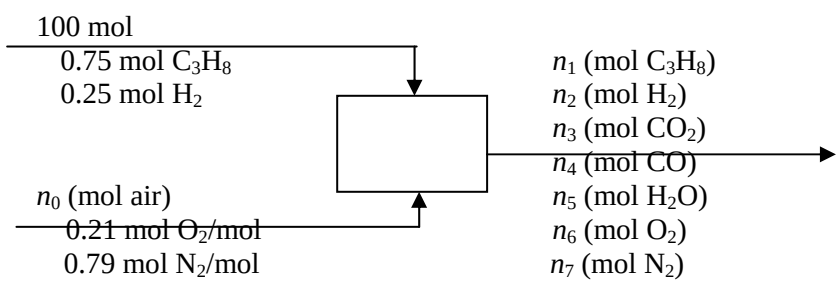
Exit gas:

10 mol C_4H_{10}	0.3% C_4H_{10}
360 mol CO_2	9.1% CO_2
450 mol H_2O (v)	11.4% H_2O
195 mol O_2	4.9% O_2
2934 mol N_2	74.3% N_2

4.69 **a.** $C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$ $\qquad$ $H_2 + 1/2\ O_2 \rightarrow H_2O$

$C_3H_8 + 7/2\ O_2 \rightarrow 3\ CO + 4\ H_2O$

Basis: 100 mol feed gas



Theoretical oxygen: $\dfrac{75 \text{ mol } C_3H_8}{} \left| \dfrac{5 \text{ mol } O_2}{\text{mol } C_3H_8} + \dfrac{25 \text{ mol } H_2}{} \right| \dfrac{0.50 \text{ mol } O_2}{\text{mol } H_2} = 387.5 \text{ mol } O_2$

4.69 (cont'd)

Air feed rate: $n_0 = \dfrac{387.5 \text{ mol } O_2}{\text{h}} \left| \dfrac{1 \text{ kmol air}}{0.21 \text{ kmol } O_2} \right| \dfrac{1.25 \text{ kmol air fed}}{1 \text{ kmol air req'd.}} = 2306.5 \text{ mol air}$

90% propane conversion $\Rightarrow n_1 = 0.100(75 \text{ mol } C_3H_8) = 7.5 \text{ mol } C_3H_8$

(67.5 mol C_3H_8 reacts)

85% hydrogen conversion $\Rightarrow n_2 = 0.150(25 \text{ mol } C_3H_8) = 3.75 \text{ mol } H_2$

95% CO_2 selectivity $\Rightarrow n_3 = \dfrac{0.95(67.5 \text{ mol } C_3H_8 \text{ react})}{} \left| \dfrac{3 \text{ mol } CO_2 \text{ generated}}{\text{mol } C_3H_8 \text{ react}} \right.$

$= 192.4 \text{ mol } CO_2$

5% CO selectivity $\Rightarrow n_3 = \dfrac{0.05(67.5 \text{ mol } C_3H_8 \text{ react})}{} \left| \dfrac{3 \text{ mol CO generated}}{\text{mol } C_3H_8 \text{ react}} \right. = 10.1 \text{ mol CO}$

H balance: $(75 \text{ mol } C_3H_8)\left(8 \dfrac{\text{mol H}}{\text{mol } C_3H_8}\right) + (25 \text{ mol } H_2)(2)$

$= (7.5 \text{ mol } C_3H_8)(8) + (3.75 \text{ mol } H_2)(2) + n_5(\text{mol } H_2O)(2) \Rightarrow n_5 = 291.2 \text{ mol } H_2O$

O balance: $(0.21 \times 2306.5 \text{ mol } O_2)(2 \dfrac{\text{mol O}}{\text{mol } O_2}) = (192.4 \text{ mol } CO_2)(2)$

$+ (10.1 \text{ mol CO})(1) + (291.2 \text{ mol } H_2O)(1) + 2n_6(\text{mol } O_2) \Rightarrow n_6 = 141.3 \text{ mol } O_2$

N_2 balance: $n_7 = 0.79(2306.5) \text{ mol } N_2 = 1822 \text{ mol } N_2$

Total moles of exit gas = (7.5 + 3.75 + 192.4 + 10.1 + 291.2 + 141.3 + 1822) mol

= 2468 mol

CO concentration in exit gas = $\dfrac{10.1 \text{ mol CO}}{2468 \text{ mol}} \times 10^6 = \underline{\underline{4090 \text{ ppm}}}$

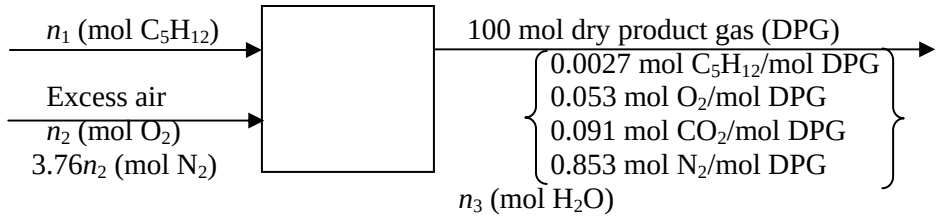
b. If more air is fed to the furnace,

(i) more gas must be compressed (pumped), leading to a higher cost (possibly a larger pump, and greater utility costs)

(ii) The heat released by the combustion is absorbed by a greater quantity of gas, and so the product gas temperature decreases and less steam is produced.

4.70 **a.** $C_5H_{12} + 8\ O_2 \rightarrow 5\ CO_2 + 6\ H_2O$

Basis: 100 moles dry product gas



3 unknowns (n_1, n_2, n_3)

-3 atomic balances (O, C, H)

-1 N2 balance

-1 D.F. $\Rightarrow$ Problem is overspecified

b. N_2 balance: $3.76\ n_2 = 0.8533\ (100) \Rightarrow n_2 = 22.69$ mol O_2

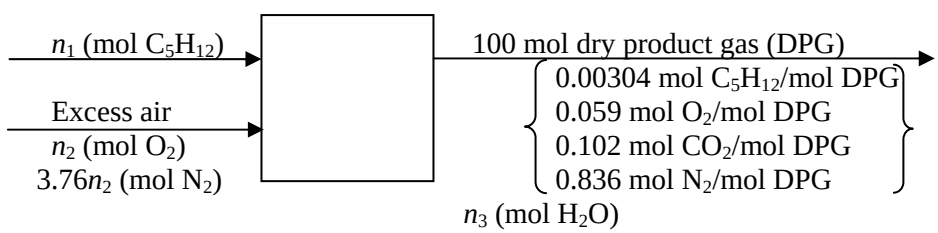
C balance: $5\ n_1 = 5(0.0027)(100) + (0.091)(100) \Rightarrow n_1 = 2.09$ mol C_5H_{12}

H balance: $12\ n_1 = 12(0.0027)(100) + 2n_3 \Rightarrow n_3 = 10.92$ mol H_2O

O balance: $2n_2 = 100[(0.053)(2) + (0.091)(2)] + n_3 \Rightarrow 45.38$ mol O = 39.72 mol O

Since the 4th balance does not close, the given data cannot be correct.

c.



N_2 balance: $3.76\ n_2 = 0.836\ (100) \Rightarrow n_2 = 22.2$ mol O_2

C balance: $5\ n_1 = 100\ (5*0.00304 + 0.102) \Rightarrow n_1 = 2.34$ mol C_5H_{12}

H balance: $12\ n_1 = 12(0.00304)(100) + 2n_3 \Rightarrow n_3 = 12.2$ mol H_2O

O balance: $2n_2 = 100[(0.0590)(2) + (0.102)(2)] + n_3 \Rightarrow 44.4$ mol O = 44.4 mol O √

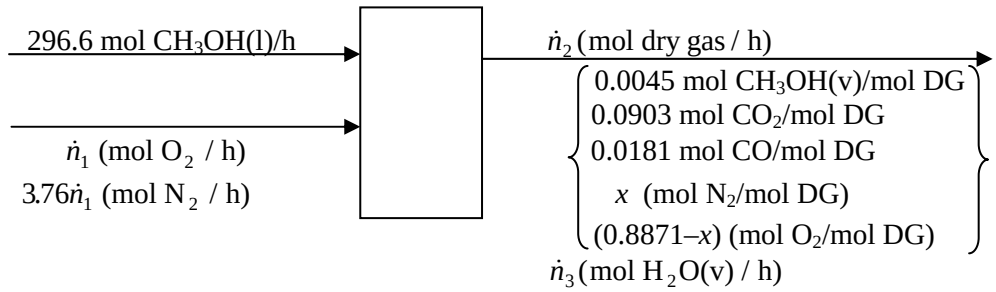
Fractional conversion of C_5H_{12}: $\dfrac{2.344 - 100 \times 0.00304}{2.344} = \underline{\underline{0.870 \text{ mol react/mol fed}}}$

Theoretical O_2 required: 2.344 mol C_5H_{12} (8 mol O_2/mol C_5H_{12}) = 18.75 mol O_2

% excess air: $\dfrac{22.23 \text{ mol } O_2 \text{ fed} - 18.75 \text{ mol } O_2 \text{ required}}{18.75 \text{ mol } O_2 \text{ required}} \times 100\% = \underline{\underline{18.6\% \text{ excess air}}}$

4.71 **a.** $\frac{12\text{ L CH}_3\text{OH}}{\text{h}}\left|\frac{1000\text{ ml}}{\text{L}}\right|\frac{0.792\text{ g}}{\text{ml}}\left|\frac{\text{mol}}{32.04\text{ g}}\right. = 296.6\text{ mol CH}_3\text{OH / h}$

$CH_3OH + 3/2\ O_2 \rightarrow CO_2 + 2\ H_2O$, $CH_3OH + O_2 \rightarrow CO + 2\ H_2O$



4 unknowns $(\dot{n}_1, \dot{n}_2, \dot{n}_3, x)$ – 4 balances (C, H, O, N_2) = 0 D.F.

b. Theoretical O_2: 296.6 (1.5) = 444.9 mol O_2 / h

C balance: 296.6 = $\dot{n}_2$ (0.0045 + 0.0903 + 0.0181) $\Rightarrow$ $\dot{n}_2$ = 2627 mol/h

H balance: 4 (296.6) = $\dot{n}_2$ (4*0.0045) + 2 $\dot{n}_3$ $\Rightarrow$ $\dot{n}_3$ = 569.6 mol H_2O / h

O balance: $296.6 + 2n_1 = 2627[0.0045 + 2(0.0903) + 0.0181 + 2(0.8871 - x)] + 569.6$

N_2 balance: 3.76 $\dot{n}_1$ = x (2627)

Solving simultaneously $\Rightarrow$ $\dot{n}_1 = 574.3$ mol O_2 / h, x = 0.822 mol N_2 / mol DG

Fractional conversion: $\frac{296.6 - 2627(0.0045)}{296.6} = \underline{\underline{0.960\text{ mol CH}_3\text{OH react/mol fed}}}$

% excess air: $\frac{574.3 - 444.9}{444.9} \times 100\% = \underline{\underline{29.1\%}}$

Mole fraction of water: $\frac{569.6\text{ mol H}_2\text{O}}{(2627 + 569.6)\text{ mol}} = \underline{\underline{0.178\text{ mol H}_2\text{O/mol}}}$

c. Fire, CO toxicity. Vent gas to outside, install CO or hydrocarbon detector in room, trigger alarm if concentrations are too high

4.72 **a.** G.C. Say n_s mols fuel gas constitute the sample injected into the G.C. If x_{CH_4} and $x_{C_2H_6}$ are the mole fractions of methane and ethane in the fuel, then

$$\frac{n_s(\text{mol})x_{C_2H_6}(\text{mol C}_2\text{H}_2/\text{mol})(2\text{ mol C}/1\text{ mol C}_2\text{H}_6)}{n_s(\text{mol})x_{CH_4}(\text{mol CH}_4/\text{mol})(1\text{ mol C}/1\text{ mol CH}_4)} = \frac{20}{85}$$

$\Downarrow$

$$\frac{x_{C_2H_6}(\text{mol C}_2\text{H}_6/\text{mol fuel})}{x_{CH_4}(\text{mol CH}_4/\text{mol fuel})} = 0.1176\text{ mole C}_2\text{H}_6/\text{mole CH}_4 \text{ in fuel gas}$$

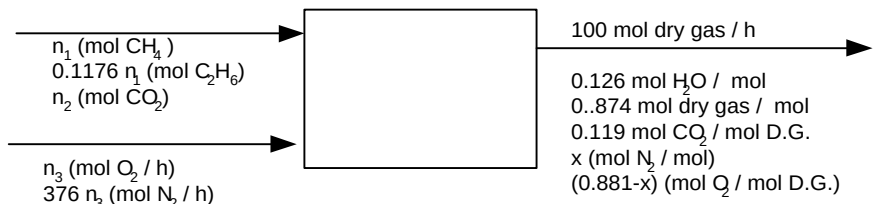
4.72 (cont'd)

Condensation measurement: $\dfrac{(1.134\text{ g } H_2O)(1\text{ mol}/18.02\text{ g})}{0.50\text{ mol product gas}} = 0.126\dfrac{\text{mole } H_2O}{\text{mole product gas}}$

Basis: 100 mol product gas. Since we have the most information about the product stream composition, we choose this basis now, and would subsequently scale to the given fuel and air flow rates if it were necessary (which it is not).

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

$$C_2H_6 + \frac{7}{2}O_2 \rightarrow 2CO_2 + 3H_2O$$



Strategy: H balance $\Rightarrow n_1$; C balance $\Rightarrow n_2$; $\left.\begin{matrix} N_2 \text{ balance} \\ O \text{ balance} \end{matrix}\right\} \Rightarrow n_3, x$

H balance: $4n_1 + (6)(0.1176n_1) = (100)(0.126)(2) \Rightarrow n_1 = 5.356 \text{ mol } CH_4$ in fuel

$\Rightarrow 0.1176(5.356) = 0.630$ mol C_2H_6 in fuel

C balance: $5.356 + (2)(0.630) + n_2 = (100)(0.874)(0.119) \Rightarrow n_2 = 3.784 \text{ mol } CO_2$ in fuel

Composition of fuel: $5.356 \text{ mol } CH_4$, $0.630 \text{ mol } C_2H_6$, $3.784 \text{ mols } CO_2$

$\Rightarrow \underline{\underline{0.548\ CH_4,\ 0.064\ C_2H_6,\ 0.388\ CO_2}}$

N_2 balance: $3.76n_3 = (100)(0.874)x$

O balance: $(2)(3.784) + 2n_3 = (100)(0.126) + (100)(0.874)(2)[0.119 + (0.881 - x)]$

Solve simultaneously: $n_3 = 18.86 \text{ mols } O_2 \text{ fed}$, $x = 0.813$

Theoretical O_2: $\dfrac{5.356 \text{ mol } CH_4}{} \left| \dfrac{2 \text{ mol } O_2}{1 \text{ mol } CH_4} \right. + \dfrac{0.630 \text{ mol } C_2H_6}{} \left| \dfrac{3.5 \text{ mol } O_2}{1 \text{ mol } CH_4} \right.$

$= 12.92 \text{ mol } O_2$ required

Desired O_2 fed: $\dfrac{(5.356 + 0.630 + 3.784) \text{ mol fuel}}{} \left| \dfrac{7 \text{ mol air}}{1 \text{ mol fuel}} \right| \dfrac{0.21 \text{ mol } O_2}{\text{mol air}} = \underline{14.36 \text{ mol } O_2}$

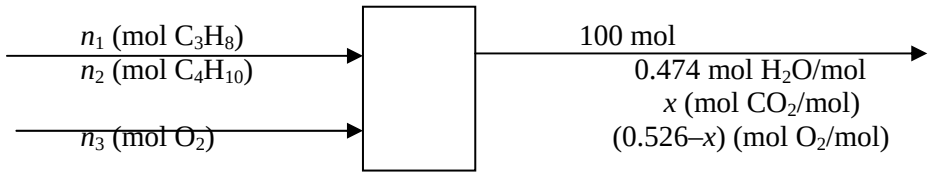
Desired % excess air: $\dfrac{14.36 - 12.92}{12.92} \times 100\% = \underline{\underline{11\%}}$

b. Actual % excess air: $\dfrac{18.86 - 12.92}{12.92} \times 100\% = \underline{\underline{46\%}}$

Actual molar feed ratio of air to fuel: $\dfrac{(18.86/0.21) \text{ mol air}}{9.77 \text{ mol feed}} = \underline{\underline{9:1}}$

4.73 **a.** $C_3H_8 + 5\ O_2 \rightarrow 3\ CO_2 + 4\ H_2O$, $C_4H_{10} + 13/2\ O_2 \rightarrow 4\ CO_2 + 5\ H_2O$

Basis 100: mol product gas



Dry product gas contains 69.4% CO_2 $\Rightarrow \dfrac{x}{0.526 - x} = \dfrac{69.4}{30.6} \Rightarrow x = 0.365\ \text{mol}\ CO_2/\text{mol}$

3 unknowns (n_1, n_2, n_3) – 3 balances (C, H, O) = 0 D.F.

O balance: $2\ n_3 = 152.6 \Rightarrow n_3 = 76.3$ mol O_2

$$\left.\begin{array}{l}\text{C balance}: 3\,n_1 + 4\,n_2 = 36.5 \\ \text{H balance}: 8\,n_1 + 10\,n_2 = 94.8\end{array}\right\} \Rightarrow \begin{array}{l} n_1 = 7.1\ \text{mol}\ C_3H_8 \\ n_2 = 3.8\ \text{mol}\ C_4H_{10}\end{array} \Rightarrow \underline{\underline{65.1\%\ C_3H_8,\ 34.9\%\ C_4H_{10}}}$$

b. n_c=100 mol (0.365 mol CO_2/mol)(1mol C/mol CO_2) = 365 mol C

n_h = 100 mol (0.474 mol H_2O/mol)(2mol H/mol H_2O)=94.8 mol H

$\Rightarrow$ 27.8%C, 72.2% H

From a:

$$\frac{7.10\ \text{mol}\ C_3H_8 \left| \dfrac{3\ \text{mol C}}{\text{mol}\ C_3H_8} \right. + 3.80\ \text{mol}\ C_4H_{10} \left| \dfrac{4\ \text{mol C}}{\text{mol}\ C_4H_{10}} \right.}{7.10\ \text{mol}\ C_3H_8 \left| \dfrac{11\ \text{mol (C + H)}}{\text{mol}\ C_3H_8} \right. + 3.80\ \text{mol}\ C_4H_{10} \left| \dfrac{14\ \text{mol (C + H)}}{\text{mol}\ C_4H_{10}} \right.} \times 100\% = \underline{\underline{27.8\%\ C}}$$

4.74 Basis: 100 kg fuel oil

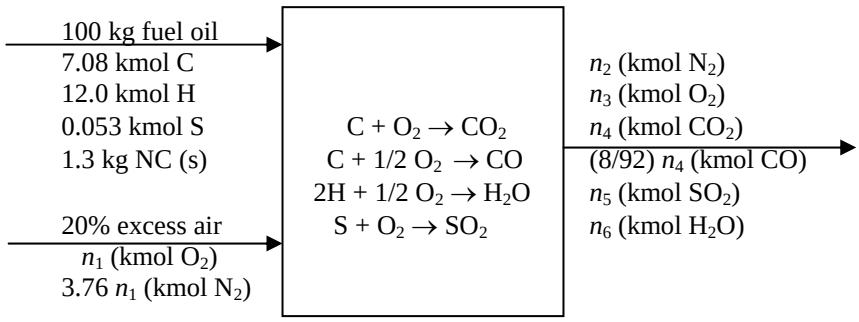
Moles of C in fuel: $\dfrac{100\ \text{kg}}{} \left| \dfrac{0.85\ \text{kg C}}{\text{kg}} \right| \dfrac{1\ \text{kmol C}}{12.01\ \text{kg C}} = 7.08\ \text{kmol C}$

Moles of H in fuel: $\dfrac{100\ \text{kg}}{} \left| \dfrac{0.12\ \text{kg H}}{\text{kg}} \right| \dfrac{1\ \text{kmol H}}{1\ \text{kg H}} = 12.0\ \text{kmol H}$

Moles of S in fuel: $\dfrac{100\ \text{kg}}{} \left| \dfrac{0.017\ \text{kg S}}{\text{kg}} \right| \dfrac{1\ \text{kmol S}}{32.064\ \text{kg S}} = 0.053\ \text{kmol S}$

1.3 kg non-combustible materials (NC)

4.74 (cont'd)



Theoretical O_2:

$$\frac{7.08\text{ kmol C}}{}\left|\frac{1\text{ kmol O}_2}{1\text{ kmol C}}\right. + \frac{12\text{ kmol H}}{}\left|\frac{.5\text{ kmol O}_2}{2\text{ kmol H}}\right. + \frac{0.053\text{ kmol S}}{}\left|\frac{1\text{ kmol O}_2}{1\text{ kmol S}}\right. = 10.133\text{ kmol O}_2$$

20 % excess air: $n_1 = 1.2(10.133) = 12.16$ kmol O_2 fed

O balance: $2\,(12.16) = 2\,(6.5136) + 0.5664 + 2\,(0.053) + 6 + 2\,n_3 \Rightarrow n_3 = 2.3102$ kmol O_2

C balance: $7.08 = n_4 + 8n_4/92 \Rightarrow n_4 = 6.514$ mol CO_2

$\Rightarrow 8\,(6.514)/92 = 0.566$ mol CO

S balance: $n_5 = 0.53$ kmol SO_2

H balance: $12 = 2n_6 \Rightarrow n_6 = 6.00$ kmol H_2O

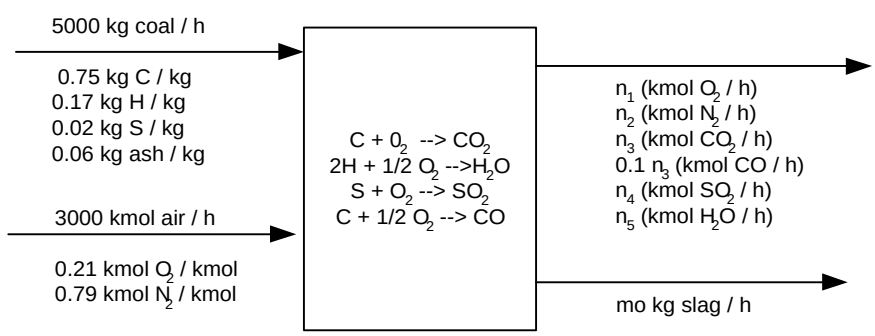
N_2 balance: $n2 = 3.76(12.16) = 45.72$ kmol N_2

Total moles of stack gas = (6.514 + 0.566 + 0.053 + 6.00 + 2.310 + 45.72) kmol

= 61.16 kmol

$\Rightarrow$ 10.7% CO, 0.92% CO, 0.087% SO_2, 9.8% H_2O, 3.8% O_2, 74.8% N_2

4.75 a. Basis: 5000 kg coal/h; 50 kmol air/min = 3000 kmol air/h



Theoretical O_2:

C: $$\frac{0.75(5000)\text{ kg C}}{\text{h}}\left|\frac{1\text{ kmol C}}{12.01\text{ kg C}}\right|\frac{1\text{ kmol O}_2}{1\text{ kmol C}} = 312.2\text{ kmol O}_2/\text{h}$$

4.75 (cont'd)

H: $\dfrac{0.17(5000)\text{ kg H}}{\text{h}}\left|\dfrac{1\text{ kmol H}}{1.01\text{ kg H}}\right|\dfrac{1\text{ kmol H}_2\text{O}}{2\text{ kmol H}}\left|\dfrac{1\text{ kmol O}_2}{2\text{ kmol H}_2\text{O}}\right. = 210.4\text{ kmol O}_2/\text{h}$

S: $\dfrac{0.02(5000)\text{ kg S}}{\text{h}}\left|\dfrac{1\text{ kmol S}}{32.06\text{ kg S}}\right|\dfrac{1\text{ kmol O}_2}{1\text{ kmol S}} = 3.1\text{ kmol O}_2/\text{h}$

Total = (312.2+210.4 + 3.1) kmol O_2/h = 525.7 kmol O_2/h

$\underline{\text{O}_2\text{ fed}}$ = $0.21(3000) = 630\text{ kmol O}_2/\text{h}$

Excess air: $\dfrac{630-525.7}{525.7}\times 100\% = \underline{\underline{19.8\%\text{ excess air}}}$

b. Balances:

C: $\dfrac{(0.94)(0.75)(5000)\text{ kg C react}}{\text{h}}\left|\dfrac{1\text{ kmol C}}{12.01\text{ kg C}}\right. = \dot{n}_3 + 0.1\dot{n}_3$

$\Rightarrow \dot{n}_3 = 266.8\text{ kmol CO}_2/\text{h},\ 0.1\dot{n}_3 = 26.7\text{ kmol CO/h}$

H: $\dfrac{(0.17)(5000)\text{ kg H}}{\text{h}}\left|\dfrac{1\text{ kmol H}}{1.01\text{ kg H}}\right|\dfrac{1\text{ kmol H}_2\text{O}}{2\text{ kmol H}}\right. = n_5 \Rightarrow n_5 = 420.8\text{ kmol H}_2\text{O/h}$

S: (from part a) $\dfrac{3.1\text{ kmol O}_2\ (\text{for SO}_2)}{\text{h}}\left|\dfrac{1\text{ kmol SO}_2}{1\text{ kmol O}_2}\right. = \dot{n}_4 \Rightarrow \dot{n}_4 = 3.1\text{ kmol SO}_2/\text{h}$

$\underline{\text{N}_2}$: $(0.79)(3000)\text{ kmol N}_2/\text{h} = \dot{n}_2 \Rightarrow \dot{n}_2 = 2370\text{ kmol N}_2/\text{h}$

O: $(0.21)(3000)(2) = 2\dot{n}_1 + 2(266.8) + 1(26.68) + 2(3.1) + (1)(420.8)$

$\Rightarrow \dot{n}_1 = 136.4\text{ kmol O}_2/\text{h}$

Stack gas total $= 3223$ kmol/h

Mole fractions:

$x_{CO} = 26.7/3224 = \underline{\underline{8.3\times 10^{-3}\text{ mol CO/mol}}}$

$x_{SO_2} = 3.1/3224 = \underline{\underline{9.6\times 10^{-4}\text{ mol SO}_2/\text{mol}}}$

c. $\text{SO}_2 + \frac{1}{2}\text{O}_2 \rightarrow \text{SO}_3$

$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$

$\dfrac{3.1\text{ kmol SO}_2}{\text{h}}\left|\dfrac{1\text{ kmol SO}_3}{1\text{ kmol SO}_2}\right|\dfrac{1\text{ kmol H}_2\text{SO}_4}{1\text{ kmol SO}_3}\right|\dfrac{98.08\text{ kg H}_2\text{SO}_4}{\text{kmol H}_2\text{SO}_4}\right. = \underline{\underline{304\text{ kg H}_2\text{SO}_4/\text{h}}}$

4.76 a. Basis: 100 g coal as received (c.a.r.). Let a.d.c. denote air-dried coal; v.m. denote volatile matter

$$\frac{100\text{ g c.a.r.}}{}\left|\frac{1.147\text{ g a.d.c.}}{1.207\text{ g c.a.r.}}\right. = 95.03\text{ g air - dried coal; } 4.97\text{ g } H_2O \text{ lost by air drying}$$

$$\frac{95.03\text{ g a.d.c}}{}\left|\frac{(1.234-1.204)\text{ g } H_2O}{1.234\text{ g a.d.c.}}\right. = 2.31\text{ g } H_2O \text{ lost in second drying step}$$

Total $H_2O = 4.97\text{ g} + 2.31\text{ g} = \underline{7.28\text{ g moisture}}$

$$\frac{95.03\text{ g a.d.c}}{}\left|\frac{(1.347-0.811)\text{ g (v.m.}+H_2O)}{1.347\text{ g a.d.c.}}\right. - 2.31\text{ g } H_2O = \underline{35.50\text{ g volatile matter}}$$

$$\frac{95.03\text{ g a.d.c}}{}\left|\frac{0.111\text{ g ash}}{1.175\text{ g a.d.c.}}\right. = \underline{8.98\text{ g ash}}$$

Fixed carbon $= (100 - 7.28 - 35.50 - 8.98)\text{g} = \underline{48.24\text{ g fixed carbon}}$

$$\begin{array}{l} 7.28\text{ g moisture} \\ 48.24\text{ g fixed carbon} \\ 35.50\text{ g volatile matter} \\ 8.98\text{ g ash} \\ \hline 100\text{ g coal as received} \end{array} \Rightarrow \begin{array}{l} \underline{\underline{7.3\%\text{ moisture}}} \\ \underline{\underline{48.2\%\text{ fixed carbon}}} \\ \underline{\underline{35.5\%\text{ volatile matter}}} \\ \underline{\underline{9.0\%\text{ ash}}} \end{array}$$

b. Assume volatile matter is all carbon and hydrogen.

$$C + CO_2 \rightarrow CO_2: \quad \frac{1\text{ mol } O_2}{1\text{ mol C}}\left|\frac{1\text{ mol C}}{12.01\text{ g C}}\right|\frac{10^3\text{ g}}{1\text{ kg}}\left|\frac{1\text{ mol air}}{0.21\text{ mol } O_2}\right. = 396.5\text{ mol air/kg C}$$

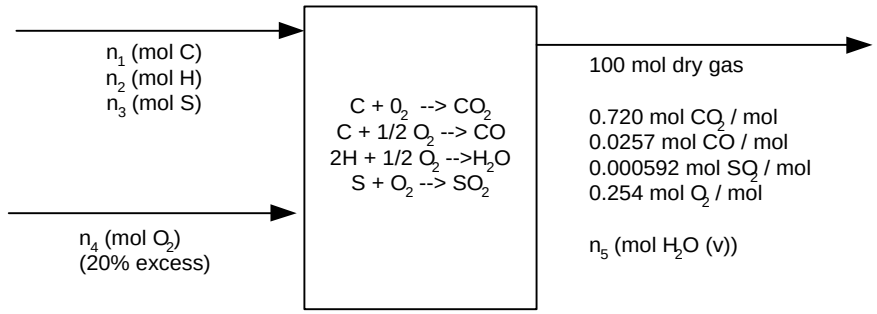
$$2H + \frac{1}{2}O_2 \rightarrow H_2O: \quad \frac{0.5\text{ mol } O_2}{2\text{ mol H}}\left|\frac{1\text{ mol H}}{1.01\text{ g H}}\right|\frac{10^3\text{ g}}{1\text{ kg}}\left|\frac{1\text{ mol air}}{0.21\text{ mol } O_2}\right. = 1179\text{ mol air/kg H}$$

$$\underline{\text{Air required:}} \quad \frac{1000\text{ kg coal}}{}\left|\frac{0.482\text{ kg C}}{\text{kg coal}}\right|\frac{396.5\text{ mol air}}{\text{kg C}}$$

$$+\frac{1000\text{ kg}}{}\left|\frac{0.355\text{ kg v.m.}}{\text{kg}}\right|\frac{6\text{ kg C}}{7\text{ kg v.m.}}\left|\frac{396.5\text{ mol air}}{\text{kg C}}\right.$$

$$+\frac{1000\text{ kg}}{}\left|\frac{0.355\text{ kg v.m.}}{\text{kg}}\right|\frac{1\text{ kg H}}{7\text{ kg v.m.}}\left|\frac{1179\text{ mol air}}{\text{kg H}}\right. = \underline{\underline{3.72\times10^5\text{ mol air}}}$$

4.77 **a.** Basis 100 mol dry fuel gas. <u>Assume no solid or liquid products!</u>

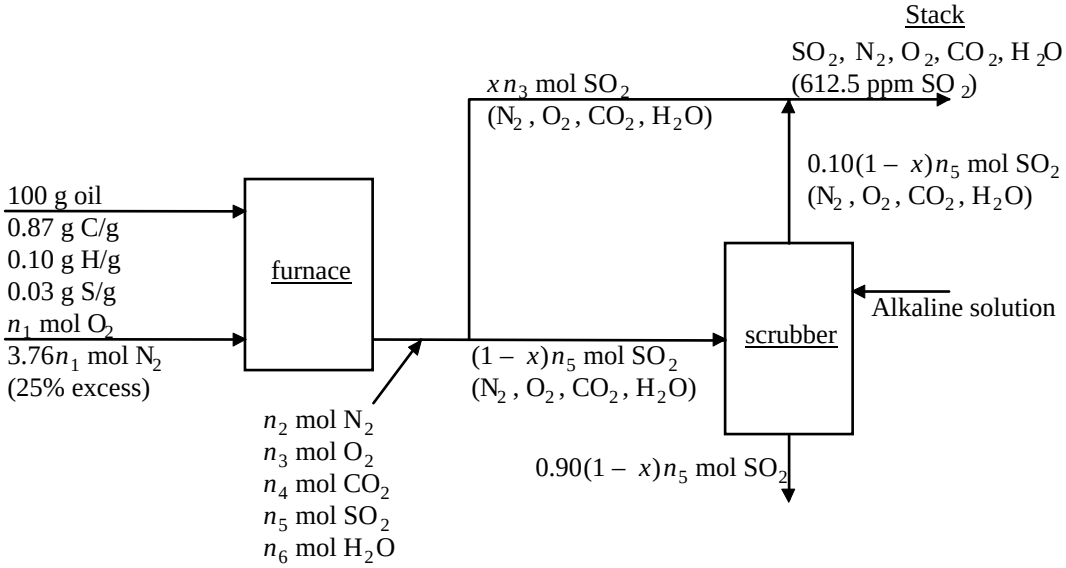


$$\left.\begin{array}{l}\underline{\text{H balance:}}\ \ n_2 = 2\,n_5 \\ \underline{\text{O balance:}}\ \ 2\,n_4 = 100\,[\,2(0.720) + 0.0257 + 2\,(0.000592) + 2\,(0.254)] + n_5 \\ \underline{20\,\%\ \text{excess}\ O_2:}\ \ (1.20)\,(74.57 + 0.0592 + 0.25\,n_2\,] = n_4\end{array}\right\}$$

$\Rightarrow$ n_2 = 183.6 mol H, n_4 = 144.6 mol O_2, n_5 = 91.8 mol H_2O

Total moles in feed: 258.4 mol (C+H+S) $\Rightarrow$ <u>28.9% C, 71.1% H, 0.023% S</u>

4.78 <u>Basis: 100 g oil</u>



$$\underline{CO_2}:\ \frac{0.87(100)\text{g C}}{}\left|\ \frac{1\text{ mol C}}{12.01\text{ g C}}\ \right|\ \frac{1\text{ mol }CO_2}{1\text{ mol C}} \Rightarrow n_4 = 7.244\text{ mol }CO_2\begin{pmatrix}7.244\text{ mol }O_2\\ \text{consumed}\end{pmatrix}$$

$$\underline{H_2O}:\ \frac{0.10(100)\text{g H}}{}\left|\ \frac{1\text{ mol H}}{1.01\text{ g H}}\ \right|\ \frac{1\text{ mol }H_2O}{2\text{ mol H}} \Rightarrow n_6 = 4.95\text{ mol }H_2O\begin{pmatrix}2.475\text{ mol }O_2\\ \text{consumed}\end{pmatrix}$$

4.78 (cont'd)

$\underline{SO_2}$: $\dfrac{0.03(100)\text{g S}}{} \left| \dfrac{1 \text{ mol S}}{32.06 \text{ g S}} \right| \dfrac{1 \text{ mol } SO_2}{1 \text{ mol S}} \Rightarrow n_5 = 0.0936 \text{ mol } SO_2 \left(\begin{matrix} 0.0956 \text{ mol } O_2 \\ \text{consumed} \end{matrix} \right)$

$\underline{25\% \text{ excess } O_2}$: $n_1 = 1.25(7.244 + 2.475 + 0.0936) \Rightarrow 12.27 \text{ mol } O_2$

$\underline{O_2 \text{ balance}}$: $n_3 = 12.27 \text{ mol } O_2 \text{ fed} - (7.244 + 2.475 + 0.0936) \text{ mol } O_2 \text{ consumed}$

$= 2.46 \text{ mol } O_2$

$\underline{N_2 \text{ balance}}$: $n_2 = 3.76(12.27 \text{ mol}) = 46.14 \text{ mol } N_2$

$\underline{SO_2 \text{ in stack } (SO_2 \text{ balance around mixing point})}$:

$$x\underbrace{(0.0936)}_{n_5} + 0.10(1-x)(0.0936) = 0.00936 + 0.0842x(\text{mol } SO_2)$$

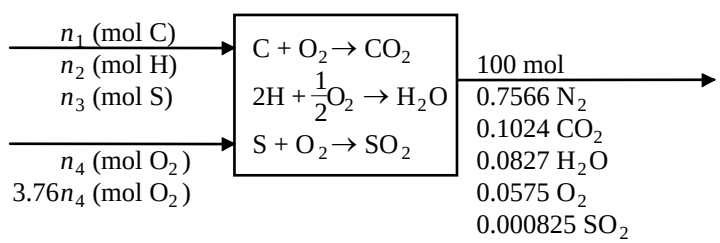
$\underline{\text{Total dry gas in stack}}$ (Assume no CO_2, O_2, or N_2 is absorbed in the scrubber)

$$\underset{(CO_2)}{7.244} + \underset{(O_2)}{2.46} + \underset{(N_2)}{46.14} + \underset{(SO_2)}{(0.00936 + 0.0842x)} = 55.85 + 0.0842x(\text{mol dry gas})$$

$\underline{612.5 \text{ ppm } SO_2 (\text{dry basis}) \text{ in stack gas}}$

$$\frac{0.00936 + 0.0842x}{55.85 + 0.0842x} = \frac{612.5}{1.0 \times 10^6} \Rightarrow x = 0.295 \Rightarrow \underline{\underline{30\% \text{ bypassed}}}$$

4.79 $\underline{\text{Basis: 100 mol stack gas}}$



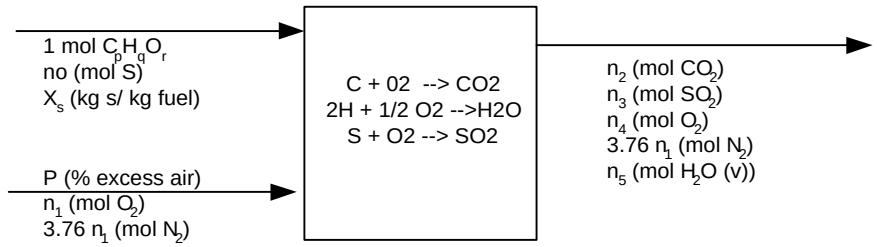
a. $\left.\begin{matrix} \underline{\text{C balance}}: & n_1 = (100)(0.1024) = 10.24 \text{ mol C} \\ \underline{\text{H balance}}: & n_2 = (100)(0.0827)(2) = 16.54 \text{ mol H} \end{matrix}\right\} \Rightarrow \dfrac{10.24 \text{ mol C}}{16.54 \text{ mol H}} = \underline{\underline{0.62 \ \dfrac{\text{mol C}}{\text{mol H}}}}$

The C/H mole ratio of CH_4 is 0.25, and that of C_2H_6 is 0.333; no mixture of the two could have a C/H ratio of 0.62, so the fuel could not be the natural gas.

b. $\underline{\text{S balance}}$: $n_3 = (100)(0.000825) = 0.0825 \text{ mol S}$

$$\left.\begin{matrix} (10.24 \text{ mol C})(12.0 \text{ g/1 mol}) = 122.88 \text{ g C} \\ (16.54 \text{ mol H})(1.01 \text{ g/1 mol}) = 16.71 \text{ g H} \\ (0.0825 \text{ mol S})(32.07 \text{ g/1 mol}) = 2.65 \text{ g S} \end{matrix}\right\} \Rightarrow \begin{matrix} \dfrac{122.88}{16.71} = \underline{\underline{7.35 \text{ g C/g H}}} \\ \dfrac{2.65}{142.24} \times 100\% = \underline{\underline{1.9\% \text{ S}}} \end{matrix} \Rightarrow \underline{\underline{\text{No. 4 fuel oil}}}$$

4.80 a. Basis: 1 mol $C_pH_qO_r$



Hydrocarbon mass:

$$\left.\begin{aligned} &p\text{ (mol C) (12 g / mol) = 12 p (g C)} \\ &q\text{ (mol H) (1 g / mol) = q (g H)} \\ &r\text{ (mol O) (16 g / mol) = 16 r (g O)} \end{aligned}\right\} \Rightarrow \text{(12 p + q + 16 r) g fuel}$$

S in feed:

$$n_o = \frac{(12\,p + q + 16r)\text{ g fuel}}{} \left| \frac{X_s\text{ (g S)}}{(1 - X_s)\text{ (g fuel)}} \right| \frac{1\text{ mol S}}{32.07\text{ g S}} = \frac{X_s(12\,p + q + 16\,r)}{32.07(1 - X_s)}\text{ (mol S)} \quad (1)$$

Theoretical O_2:

$$\frac{p\text{ (mol C)}}{} \left| \frac{1\text{ mol O}_2}{1\text{ mol C}} + \frac{q\text{ (mol H)}}{} \right| \frac{0.5\text{ mol O}_2}{2\text{ mol H}} - \frac{(r\text{ mol O})}{} \left| \frac{1\text{ mol O}_2}{2\text{ mol O}} \right.$$

$$= (p + 1/4\,q - 1/2\,r)\text{ mol O}_2$$

% excess $\Rightarrow n_1 = (1 + P/100)\,(p + 1/4\,q - ½\,r)$ mol O_2 fed (2)

C balance: $n_2 = p$ (3)

H balance: $n_5 = q/2$ (4)

S balance: $n_3 = n_0$ (5)

O balance: $r + 2n_1 = 2n_2 + 2n_3 + 2n_4 + n_5 \Rightarrow n_4 = ½\,(r + 2n_1 - 2n_2 - 2n_3 - n_5)$ (6)

Given: $p = 0.71$, $q = 1.1$, $r = 0.003$, $X_s = 0.02$ $P = 18\%$ excess air

(1) $\Rightarrow n_0 = 0.00616$ mol S (5) $\Rightarrow n_3 = 0.00616$ mol SO_2

(2) $\Rightarrow n_1 = 1.16$ mol O_2 fed (6) $\Rightarrow n_4 = 0.170$ mol O_2

(3) $\Rightarrow n_2 = 0.71$ mol CO_2 (4) $\Rightarrow n_5 = 0.55$ mol H_2O

(3.76*1.16) mol N_2 = 4.36 mol N_2

Total moles of dry product gas = $n_2 + n_3 + n_4 + 3.76\,n_1$=5.246 mol dry product gas

Dry basis composition

y_{CO2} = (0.710 mol CO_2/ 5.246 mol dry gas) * 100% = 13.5% CO_2

y_{O2} = (0.170 / 5.246) * 100% = 3.2% O_2

y_{N2} = (4.36 / 5.246) * 100% = 83.1% N_2

y_{SO2} = (0.00616 / 5.246) * 10^6 = 1174 ppm SO_2