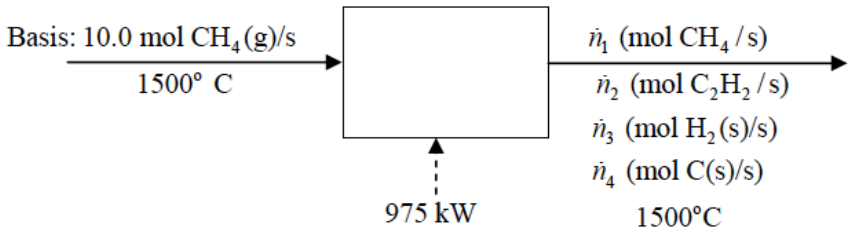
Introduction to Chemical Engineering I

Problem Sheet - Week 10

Problem 1

9.36

$$2CH_4 \rightarrow C_2H_2 + 3H_2$$
$$C_2H_2 \rightarrow 2C(s) + H_2$$



a.

60% conversion $\Rightarrow \dot{n}_1 = 10(1-0.600) = \underline{\underline{4.00 \text{ mol } CH_4/s}}$

C balance: $10(1) = 4(1) + 2\dot{n}_2 + \dot{n}_4 \Rightarrow 2\dot{n}_2 + \dot{n}_4 = 6$ (1)

H balance: $10(4) = 4(4) + 2\dot{n}_2 + 2\dot{n}_3 \Rightarrow 2\dot{n}_2 + 2\dot{n}_3 = 24$ (2)

References for enthalpy calculations : C(s), $H_2(g)$ at 25°C

$$H_i = \left(\Delta\hat{H}_f^\circ\right)_i + C_{pi}(1500-25),\ i = CH_4, C_2H_2, C, H_2$$

Substance	$\dot{n}_{in}$ (mol/s)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/s)	$\hat{H}_{out}$ (kJ/mol)
$CH_4(g)$	10	41.68	4	41.68
$C_2H_2(g)$	–	–	$\dot{n}_2$	303.45
$H_2(g)$	–	–	$\dot{n}_3$	45.72
C(s)	–	–	$\dot{n}_4$	32.45

Energy Balance: $Q = \Delta H \Rightarrow 975 \text{ kJ/s} = \sum_{out} \dot{n}_i\hat{H}_i - \sum_{in} \dot{n}_i\hat{H}_i$ (3)

Solve (1) - (3) simultaneously $\Rightarrow$
$\dot{n}_2 = \underline{\underline{2.50 \text{ mol } C_2H_2/s}}$
$\dot{n}_3 = \underline{\underline{9.50 \text{ mol } H_2/s}}$
$\dot{n}_4 = \underline{\underline{1.00 \text{ mol C/s}}}$

$$\text{Yield of acetylene} = \frac{2.50 \text{ mol } C_2H_2/s}{6.00 \text{ mol } CH_4 \text{ consumed/s}} = \underline{\underline{0.417 \text{ mol } C_2H_2/\text{mol } CH_4 \text{ consumed}}}$$

b.

If no side reaction,

$\dot{n}_1 = 10.0(1-0.600) = \underline{\underline{4.00 \text{ mol } CH_4/s}}$

$\dot{n}_3 = 0 \Rightarrow \dot{n}_2 = \underline{\underline{3.00 \text{ mol } C_2H_2/s}}$, $\dot{n}_4 = \underline{\underline{9.00 \text{ mol } H_2/s}}$

$$\text{Yield of acetylene} = \frac{3.00 \text{ mol } C_2H_2/s}{6.00 \text{ mol } CH_4 \text{ consumed/s}} = \underline{\underline{0.500 \text{ mol } C_2H_2/\text{mol } CH_4 \text{ consumed}}}$$

$$\text{Reactor Efficiency} = \frac{0.417}{0.500} = \underline{\underline{0.834}}$$

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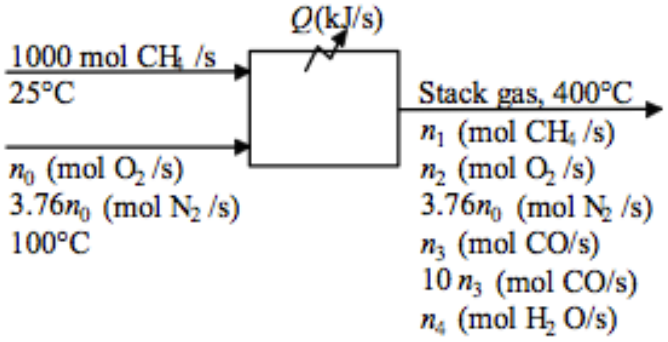
Problem 2

9.55 **a.**

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O \qquad CH_4 + \frac{3}{2}O_2 \rightarrow CO + 2H_2O$$

Basis: 1000 mol CH_4/h fed



90% combustion $\Rightarrow \dot{n}_1 = 0.10(1000) = 100$ mol CH_4/s

Theoretical O_2 required = 2000 mol/s

10% excess O_2 $\Rightarrow$ O_2 fed=1.1(2000 mol/s)=2200 mol/s

C balance:

$$(1000 \text{ mol } CH_4/\text{s})(1 \text{ mol C/mol } CH_4) = (100)(1) + \dot{n}_3(1) + 10\dot{n}_3(1) \Rightarrow \dot{n}_3 = 81.8 \text{ mol CO/s}$$

$$\Rightarrow 10\dot{n}_3 = 818 \text{ mol } CO_2/\text{s}$$

H balance: $(1000)(4) = (100)(4) + 2\dot{n}_4 \Rightarrow \dot{n}_4 = 1800$ mol H_2O/s

O balance: $(2200)(2) = 2\dot{n}_2 + (81.8)(1) + (818)(2) + (1800)(1) \Rightarrow \dot{n}_2 = 441$ mol O_2/s

References: C(s), H_2(g), O_2(g), N_2(g) at 25°C

Substance	$\dot{n}_{in}$ (mol/s)	$\hat{H}_{in}$ (kJ/mol)	$\dot{n}_{out}$ (mol/s)	$\hat{H}_{out}$ (kJ/mol)
CH_4	1000	–74.85	100	–57.62
O_2	2200	2.24	441	11.72
N_2	8272	2.19	8272	11.15
CO	–	–	81.8	–99.27
CO_2	–	–	818	–377.2
H_2O	–	–	1800	–228.63

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$$\hat{H} = \overset{\text{Table B.1}}{\Delta\hat{H}_f^o} + \int_{25}^{T} \overset{\text{Table B.2}}{C_p}\, dT \text{ for } CH_4$$

$$= \Delta\hat{H}_f^o + \overset{\text{Table B.8}}{\hat{H}_i(T)} \text{ for others}$$

Energy balance: $\dot{Q} = \Delta\dot{H} = \sum_{out} \dot{n}_i \hat{H}_i - \sum_{in} \dot{n}_i \hat{H}_i = \underline{\underline{-5.85\times10^5 \text{ kJ/s (kW)}}}$

b.

(i) T_{air} ↑ (increases) $\Rightarrow -\dot{Q}\uparrow$

(ii) %XS ↑ $\Rightarrow -\dot{Q}\downarrow$ (more energy required to heat additional O_2 and N_2 to 400°C, therefore less energy transferred.)

(iii) $S_{CO_2/CO}\uparrow \Rightarrow -\dot{Q}\uparrow$ (reaction to form CO2 has a greater heat of combustion and so releases more thermal energy)

(iv) $T_{stack}\uparrow \Rightarrow -\dot{Q}\downarrow$ (more energy required to heat combustion products)

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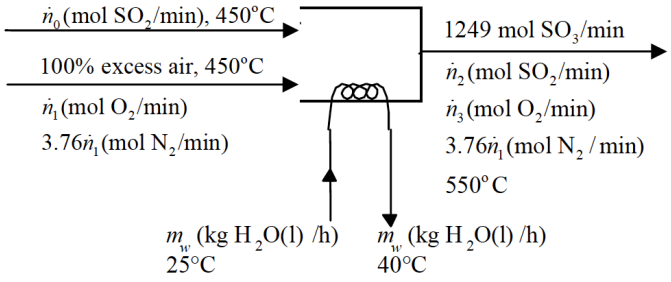
Additional problem

9.16 **a.**

$$SO_2(g) + \frac{1}{2}O_2(g) \rightarrow SO_3(g)$$

$$\underline{\text{Basis}}: \quad \frac{100 \text{ kg } SO_3}{\text{min}} \left| \frac{10^3 \text{ mol } SO_3}{80.07 \text{ kg } SO_3} \right| = 1249 \text{ mol } SO_3/\text{min}$$



Assume low enough pressure for $\hat{H}$ to be independent of P.

$$\underset{(\text{Generation=output})}{SO_3 \text{ balance}}: \quad \frac{\dot{n}_0 \text{ (mol } SO_2 \text{ fed)}}{\text{min}} \left| \frac{0.65 \text{ mol } SO_2 \text{ react}}{1 \text{ mol } SO_2 \text{ fed}} \right| \frac{1 \text{ mol } SO_3 \text{ produced}}{1 \text{ mol } SO_2 \text{ react}} = 1249 \frac{\text{mol } SO_3}{\text{min}}$$

$$\Rightarrow \dot{n}_0 = \underline{\underline{1922 \text{ mol } SO_2 / \text{ min fed}}}$$

$$\underline{100\% \text{ excess air}}: \quad \dot{n}_1 = \frac{1922 \text{ mol } SO_2}{\text{min}} \left| \frac{0.5 \text{ mol } O_2 \text{ reqd}}{1 \text{ mol } SO_2} \right| \frac{(1+1) \text{ mol } O_2 \text{ fed}}{1 \text{ mol } O_2 \text{ reqd}} = \underline{\underline{1922 \text{ mol } O_2/\text{min fed}}}$$

$$\underline{N_2 \text{ balance}}: \quad 3.76(1922) = \underline{\underline{7227 \text{ mol/min (in \& out)}}}$$

$$\underline{65\% \text{ conversion}}: \quad \dot{n}_2 = 1922(1-0.65) \text{ mol/s} = \underline{\underline{673 \text{ mol } SO_2/\text{min out}}}$$

$$\underline{\text{O balance:}} \quad (2)(1922) + (2)(1922) = (3)(1249) + (2)(673) + 2\dot{n}_3 \Rightarrow \dot{n}_3 = 1298 \text{ mol/min out}$$

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9.16 (cont'd)

b.

$$\text{Extent of reaction}: \quad \dot{\xi} = \frac{\left|(\dot{n}_{SO_2})_{out} - (\dot{n}_{SO_2})_{in}\right|}{\left|\nu_{SO_2}\right|} = \frac{|673 - 1922|}{|1|} = \underline{\underline{1249 \text{ mol / min}}}$$

$$\Delta\hat{H}_r^\circ = (\Delta\hat{H}_f^\circ)_{SO_3(g)} - (\Delta\hat{H}_f^\circ)_{SO_2(g)} \overset{\text{Table B.1}}{=} -395.18 - (-296.9) = \underline{\underline{-99.28 \text{ kJ / mol}}}$$

References: $SO_2(g)$, $O_2(g)$, $N_2(g)$, $SO_3(g)$ at 25°C

Substance	$\dot{n}_{in}$ (mol / min)	$\hat{H}_{in}$ (kJ / mol)	$\dot{n}_{out}$ (mol / min)	$\hat{H}_{out}$ (kJ / mol)
SO_2	1922	$\hat{H}_1$	673	$\hat{H}_4$
O_2	1922	$\hat{H}_2$	1298	$\hat{H}_5$
N_2	7227	$\hat{H}_3$	7227	$\hat{H}_6$
SO_3	–	–	1249	$\hat{H}_7$

$$SO_2(g,450^\circ C): \quad \hat{H}_1 = \int_{25}^{450} \overset{\text{Table B.2}}{C_p}\, dT = \underline{19.62 \text{ kJ / mol}}$$

$$O_2(g,450^\circ C) = \hat{H}_2 = \hat{H}_{O_2}(450^\circ C) \overset{\text{Table B.8}}{=} \underline{13.36 \text{ kJ / mol}}$$

$$N_2(g,450^\circ C) = \hat{H}_3 = \hat{H}_{N_2}(450^\circ C) \overset{\text{Table B.8}}{=} \underline{12.69 \text{ kJ / mol}}$$

Out:

$$SO_2(g,550^\circ C): \quad \hat{H}_4 = \int_{25}^{550} \overset{\text{Table B.2}}{C_p}\, dT = \underline{\underline{24.79 \text{ kJ/mol}}}$$

$$O_2(g,550^\circ C) = \hat{H}_5 = \hat{H}_{O_2}(550^\circ C) \overset{\text{Table B.8}}{=} \underline{16.71 \text{ kJ / mol}}$$

$$N_2(g,550^\circ C) = \hat{H}_6 = \hat{H}_{N_2}(550^\circ C) \overset{\text{Table B.8}}{=} \underline{\underline{15.81 \text{ kJ / mol}}}$$

$$SO_3(g,550^\circ C): \quad \hat{H}_7 = \int_{25}^{550} \overset{\text{Table B.2}}{C_p}\, dT = \underline{\underline{35.34 \text{ kJ / mol}}}$$

$$\dot{Q} = \Delta\dot{H} = \dot{\xi}\Delta\hat{H}_r^\circ + \sum_{out} \dot{n}_i\hat{H}_i - \sum_{in} \dot{n}_i\hat{H}_i$$

$$= (1249)(-98.28) + (673)(24.796) + (179.8)(16.711) + (7227)(15.808) + (1249)(35.336) - (19$$

$$-1922(13.362) - (7227)(12.691)$$

$$= \frac{-8.111\times10^4 \text{ kJ}}{\text{min}} \left| \frac{1 \text{ min}}{60 \text{ s}} \right| \frac{1 \text{ kW}}{1 \text{ kJ/s}} = \underline{\underline{-1350 \text{ kW}}}$$

c.

Assume system is adiabatic, so that $\dot{Q}_{\text{lost from reactor}} = \dot{Q}_{\text{gained by cooling water}}$

$$\dot{Q} = \Delta\dot{H} = \dot{m}_w \left[\underset{\text{Table B.5}}{\hat{H}_w}(1,\ 40^\circ C) - \underset{\text{Table B.5}}{\hat{H}_w}(1,\ 25^\circ C) \right]$$

d.

$$\Rightarrow 8.111\times10^4 \frac{\text{kJ}}{\text{min}} = \dot{m}_w \left(\frac{\text{kg}}{\text{min}}\right)[167.5 - 104.8]\frac{\text{kJ}}{\text{kg}} \Rightarrow \underline{\underline{\dot{m}_w = 1290 \text{ kg/min cooling water}}}$$

If elemental species were taken as references, the heats of formation of each molecular species would have to be taken into account in the enthalpy calculations and the heat of reaction term would not have been included in the calculation of $\Delta\dot{H}$.