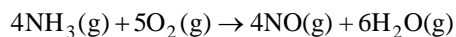


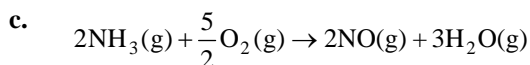
## CHAPTER NINE

### 9.1



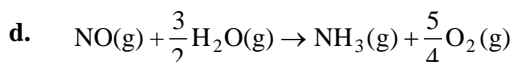
$$\Delta \hat{H}_r^\circ = -904.7 \text{ kJ/mol}$$

- a. When 4 g-moles of  $\text{NH}_3(\text{g})$  and 5 g-moles of  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$  and 1 atm react to form 4 g-moles of  $\text{NO}(\text{g})$  and 6 g-moles of water vapor at  $25^\circ\text{C}$  and 1 atm, the change in enthalpy is -904.7 kJ.
- b. Exothermic at  $25^\circ\text{C}$ . The reactor must be cooled to keep the temperature constant. The temperature would increase under adiabatic conditions. The energy required to break the molecular bonds of the reactants is less than the energy released when the product bonds are formed.



Reducing the stoichiometric coefficients of a reaction by half reduces the heat of reaction by half.

$$\Delta \hat{H}_r^\circ = -\frac{904.7}{2} = \underline{\underline{-452.4 \text{ kJ/mol}}}$$



Reversing the reaction reverses the sign of the heat of reaction. Also reducing the stoichiometric coefficients to one-fourth reduces the heat of reaction to one-fourth.

$$\Delta \hat{H}_r^\circ = -\frac{(-904.7)}{4} = \underline{\underline{+226.2 \text{ kJ/mol}}}$$

e.  $\dot{m}_{\text{NH}_3} = 340 \text{ g/s}$

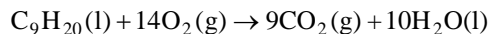
$$\dot{n}_{\text{NH}_3} = \frac{340 \text{ g}}{\text{s}} \left| \frac{1 \text{ mol}}{17.03 \text{ g}} \right| = 20.0 \text{ mol/s}$$

$$\dot{Q} = \Delta \dot{H} = \frac{\dot{n}_{\text{NH}_3} \Delta \hat{H}_r^\circ}{\nu_{\text{NH}_3}} = \frac{20.0 \text{ mol NH}_3}{\text{s}} \left| \frac{-904.7 \text{ kJ}}{4 \text{ mol NH}_3} \right| = \underline{\underline{-4.52 \times 10^3 \text{ kJ/s}}}$$

The reactor pressure is low enough to have a negligible effect on enthalpy.

- f. Yes. Pure water can only exist as vapor at 1 atm above  $100^\circ\text{C}$ , but in a mixture of gases, it can exist as vapor at lower temperatures.

### 9.2



$$\Delta \hat{H}_r^\circ = -6124 \text{ kJ/mol}$$

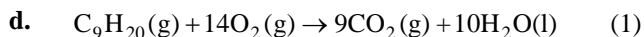
- a. When 1 g-mole of  $\text{C}_9\text{H}_{20}(\text{l})$  and 14 g-moles of  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$  and 1 atm react to form 9 g-moles of  $\text{CO}_2(\text{g})$  and 10 g-moles of water vapor at  $25^\circ\text{C}$  and 1 atm, the change in enthalpy is -6124 kJ.
- b. Exothermic at  $25^\circ\text{C}$ . The reactor must be cooled to keep the temperature constant. The temperature would increase under adiabatic conditions. The energy required to break the molecular bonds of the reactants is less than the energy released when the product bonds are formed.

c. 
$$\dot{Q} = \Delta \dot{H} = \frac{\dot{n}_{\text{C}_9\text{H}_{20}} \Delta \hat{H}_r^\circ}{\nu_{\text{C}_9\text{H}_{20}}} = \frac{25.0 \text{ mol C}_9\text{H}_{20}}{\text{s}} \left| \frac{-6124 \text{ kJ}}{1 \text{ mol C}_9\text{H}_{20}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-1.53 \times 10^5 \text{ kW}}}$$

## 9.2 (cont'd)

Heat Output =  $1.53 \times 10^5$  kW.

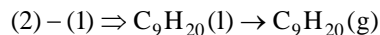
The reactor pressure is low enough to have a negligible effect on enthalpy.



$$\Delta \hat{H}_r^\circ = -6171 \text{ kJ/mol}$$



$$\Delta \hat{H}_r^\circ = -6124 \text{ kJ/mol}$$

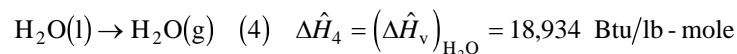
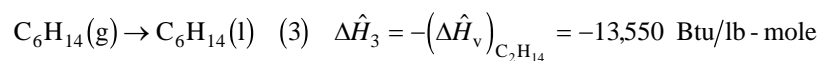
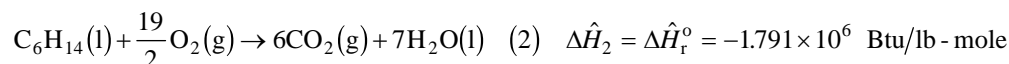
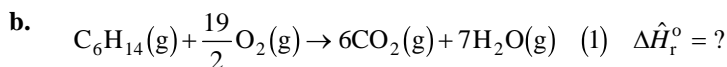


$$\Delta \hat{H}_v^\circ(\text{C}_9\text{H}_{20}, 25^\circ\text{C}) = -6124 \text{ kJ/mol} - (-6171 \text{ kJ/mol}) = \underline{\underline{47 \text{ kJ/mol}}}$$

- e. Yes. Pure n-nonane can only exist as vapor at 1 atm above  $150.6^\circ\text{C}$ , but in a mixture of gases, it can exist as a vapor at lower temperatures.

## 9.3

- a. Exothermic. The reactor will have to be cooled to keep the temperature constant. The temperature would increase under adiabatic conditions. The energy required to break the reactant bonds is less than the energy released when the product bonds are formed.

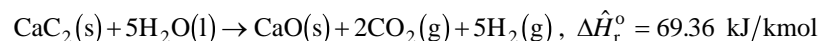


$(1) = (2) + (3) + 7 \times (4) \xRightarrow{\text{Hess's law}} \Delta \hat{H}_1 = \Delta \hat{H}_2 + \Delta \hat{H}_3 + 7\Delta \hat{H}_4 = \underline{\underline{-1.672 \times 10^6 \text{ Btu/lb-mole}}}$

c.  $\dot{m} = 120 \text{ lb}_m/\text{s} \quad \xRightarrow{M_{\text{O}_2}=32.0} \quad \dot{n} = 3.75 \text{ lb-mole/s}$

$$\dot{Q} = \Delta \dot{H} = \frac{\dot{n}_{\text{O}_2} \Delta \hat{H}_r^\circ}{v_{\text{O}_2}} = \frac{3.75 \text{ lb-mole/s}}{9.5} \left| \frac{-1.672 \times 10^6 \text{ Btu}}{1 \text{ lb-mole O}_2} \right| = \underline{\underline{-6.60 \times 10^5 \text{ Btu/s (from reactor)}}}$$

## 9.4



- a. Endothermic. The reactor will have to be heated to keep the temperature constant. The temperature would decrease under adiabatic conditions. The energy required to break the reactant bonds is more than the energy released when the product bonds are formed.

b.

$$\Delta \hat{U}_r^\circ = \Delta \hat{H}_r^\circ - RT \left[ \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right] = 69.36 \frac{\text{kJ}}{\text{mol}} - \frac{8.314 \text{ J}}{\text{mol} \cdot \text{K}} \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| \left| \frac{298 \text{ K}}{10^3 \text{ J}} \right| (7-0)$$

$$= \underline{\underline{52.0 \text{ kJ/mol}}}$$

## 9.4 (cont'd)

$\Delta \hat{U}_r^\circ$  is the change in internal energy when 1 g-mole of  $\text{CaC}_2(\text{s})$  and 5 g-moles of  $\text{H}_2\text{O}(\text{l})$  at  $25^\circ\text{C}$  and 1 atm react to form 1 g-mole of  $\text{CaO}(\text{s})$ , 2 g-moles of  $\text{CO}_2(\text{g})$  and 5 g-moles of  $\text{H}_2(\text{g})$  at  $25^\circ\text{C}$  and 1 atm.

$$\text{c. } Q = \Delta U = \frac{n_{\text{CaC}_2} \Delta \hat{U}_r^\circ}{v_{\text{CaC}_2}} = \frac{150 \text{ g CaC}_2}{64.10 \text{ g}} \left| \frac{1 \text{ mol}}{1 \text{ mol CaC}_2} \right| \frac{52.0 \text{ kJ}}{1 \text{ mol CaC}_2} = \underline{\underline{121.7 \text{ kJ}}}$$

Heat must be transferred to the reactor.

## 9.5

$$\text{a. } \underline{\text{Given reaction} = (1) - (2)} \xRightarrow{\text{Hess's law}} \Delta \hat{H}_r^\circ = \Delta \hat{H}_{r1}^\circ - \Delta \hat{H}_{r2}^\circ = (1226 - 18,935) \text{ Btu/lb-mole} \\ = \underline{\underline{-17,709 \text{ Btu/lb-mole}}}$$

$$\text{b. } \underline{\text{Given reaction} = (1) - (2)} \xRightarrow{\text{Hess's law}} \Delta \hat{H}_r^\circ = \Delta \hat{H}_{r1}^\circ - \Delta \hat{H}_{r2}^\circ = (-121,740 + 104,040) \text{ Btu/lb-mole} \\ = \underline{\underline{-17,700 \text{ Btu/lb-mole}}}$$

$$\text{9.6 a. } \text{Reaction (3)} = 0.5 \times (1) - (2) \xRightarrow{\text{Hess's law}} \Delta \hat{H}_r^\circ = 0.5 \left( -326.2 \frac{\text{kJ}}{\text{mol}} \right) - \left( -285.8 \frac{\text{kJ}}{\text{mol}} \right) = \underline{\underline{122.7 \frac{\text{kJ}}{\text{mol}}}}$$

b. Reactions (1) and (2) are easy to carry out experimentally, but it would be very hard to decompose methanol with only reaction (3) occurring.

$$\text{9.7 a. } \text{N}_2(\text{g}) + \text{O}_2(\text{g}) \rightarrow 2\text{NO}(\text{g}), \Delta \hat{H}_r^\circ = 2(\Delta \hat{H}_f^\circ)_{\text{NO}(\text{g})} = 2 \left( \overset{\text{Table B.1}}{\downarrow} 90.37 \frac{\text{kJ}}{\text{mol}} \right) = \underline{\underline{180.74 \text{ kJ/mol}}}$$

$$\text{b. } n - \text{C}_5\text{H}_{12}(\text{g}) + \frac{11}{2} \text{O}_2(\text{g}) \rightarrow 5\text{CO}(\text{g}) + 6\text{H}_2\text{O}(\text{l}) \\ \Delta \hat{H}_r^\circ = 5(\Delta \hat{H}_f^\circ)_{\text{CO}(\text{g})} + 6(\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} - (\Delta \hat{H}_f^\circ)_{n - \text{C}_5\text{H}_{12}(\text{g})} \\ = [(5)(-110.52) + (6)(-285.84) - (-146.4)] \text{ kJ/mol} = \underline{\underline{-2121.2 \text{ kJ/mol}}}$$

$$\text{c. } \text{C}_6\text{H}_{14}(\text{l}) + \frac{19}{2} \text{O}_2(\text{g}) \rightarrow 6\text{CO}_2(\text{g}) + 7\text{H}_2\text{O}(\text{g}) \\ \Delta \hat{H}_r^\circ = 6(\Delta \hat{H}_f^\circ)_{\text{CO}_2} + 7(\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{g})} - (\Delta \hat{H}_f^\circ)_{\text{C}_6\text{H}_{14}(\text{l})} \\ = [(6)(-393.5) + 7(-241.83) - (-198.8)] \text{ kJ/mol} = \underline{\underline{-3855 \text{ kJ/mol}}}$$

$$\text{d. } \text{Na}_2\text{SO}_4(\text{l}) + 4\text{CO}(\text{g}) \rightarrow \text{Na}_2\text{S}(\text{l}) + 4\text{CO}_2(\text{g}) \\ \Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{S}(\text{l})} + 4(\Delta \hat{H}_f^\circ)_{\text{CO}_2(\text{g})} - (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{l})} - 4(\Delta \hat{H}_f^\circ)_{\text{CO}(\text{g})} \\ = [(-373.2 + 6.7) + (4)(-393.5) - (-1384.5 + 24.3) - 4(-110.52)] \text{ kJ/mol} = \underline{\underline{-138.2 \text{ kJ/mol}}}$$

9.8

a. 
$$\Delta \hat{H}_{r1}^{\circ} = (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_2\text{Cl}_4(\text{l})} - (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_4(\text{g})} \Rightarrow (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_2\text{Cl}_4(\text{l})} = -385.76 + 52.28 = \underline{\underline{-333.48 \text{ kJ/mol}}}$$

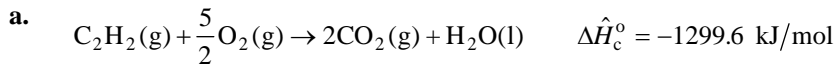
$$\Delta \hat{H}_{r2}^{\circ} = (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{HCl}_3(\text{l})} + (\Delta \hat{H}_f^{\circ})_{\text{HCl}(\text{g})} - (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_2\text{Cl}_4(\text{l})} = -276.2 - 92.31 + 333.48 = \underline{\underline{-35.03 \text{ kJ/mol}}}$$

b. Given reaction = (1) + (2)  $\Rightarrow -385.76 - 35.03 = \underline{\underline{-420.79 \text{ kJ/mol}}}$

c. 
$$\dot{Q} = \Delta \dot{H} = \frac{300 \text{ mol C}_2\text{HCl}_3}{\text{h}} \left| \frac{-420.79 \text{ kJ}}{\text{mol}} \right| = \underline{\underline{-1.26 \times 10^5 \text{ kJ/h}}} (= -35 \text{ kW})$$

Heat is evolved.

9.9



The enthalpy change when 1 g-mole of  $\text{C}_2\text{H}_2(\text{g})$  and 2.5 g-moles of  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$  and 1 atm react to form 2 g-moles of  $\text{CO}_2(\text{g})$  and 1 g-mole of  $\text{H}_2\text{O}(\text{l})$  at  $25^\circ\text{C}$  and 1 atm is -1299.6 kJ.

b. 
$$\Delta \hat{H}_c^{\circ} = 2(\Delta \hat{H}_f^{\circ})_{\text{CO}_2(\text{g})} + (\Delta \hat{H}_f^{\circ})_{\text{H}_2\text{O}(\text{l})} - (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_2(\text{g})}$$

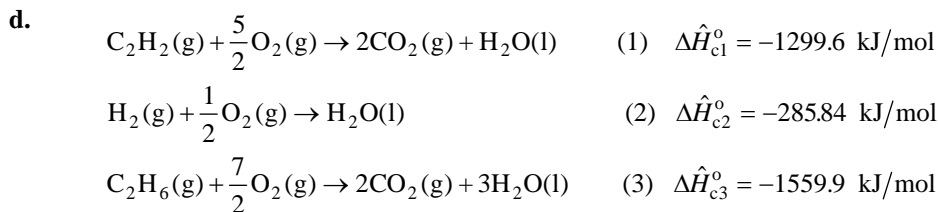
$$\begin{array}{c} \text{Table B.1} \\ \downarrow \\ = [2(-393.5) + (-285.84) - (226.75)] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-1299.6 \frac{\text{kJ}}{\text{mol}}}} \end{array}$$

c. (i) 
$$\Delta \hat{H}_r^{\circ} = (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_6(\text{g})} - (\Delta \hat{H}_f^{\circ})_{\text{C}_2\text{H}_2(\text{g})}$$

$$\begin{array}{c} \text{Table B.1} \\ \downarrow \\ = [(-84.67) - (226.75)] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-311.4 \frac{\text{kJ}}{\text{mol}}}} \end{array}$$

(ii) 
$$\Delta \hat{H}_r^{\circ} = (\Delta \hat{H}_c^{\circ})_{\text{C}_2\text{H}_2(\text{g})} + 2(\Delta \hat{H}_c^{\circ})_{\text{H}_2(\text{g})} - (\Delta \hat{H}_c^{\circ})_{\text{C}_2\text{H}_6(\text{g})}$$

$$\begin{array}{c} \text{Table B.1} \\ \downarrow \\ = [(-1299.6) + 2(-285.84) - (-1559.9)] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-311.4 \frac{\text{kJ}}{\text{mol}}}} \end{array}$$



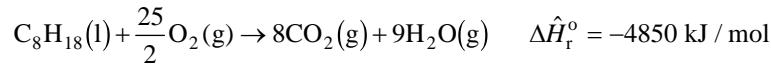
The acetylene dehydrogenation reaction is (1) + 2 × (2) – (3)

Hess's law 
$$\Rightarrow \Delta \hat{H}_r^{\circ} = \Delta \hat{H}_{c1}^{\circ} + 2 \times \Delta \hat{H}_{c2}^{\circ} - \Delta \hat{H}_{c3}^{\circ}$$

$$= (-1299.6 + 2(-285.84) - (-1559.9)) \text{ kJ/mol} = \underline{\underline{-311.4 \text{ kJ/mol}}}$$

9.10

a.



When 1 g-mole of  $\text{C}_8\text{H}_{18}(\text{l})$  and 12.5 g-moles of  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$  and 1 atm react to form 8 g-moles of  $\text{CO}_2(\text{g})$  and 9 g-moles of  $\text{H}_2\text{O}(\text{g})$ , the change in enthalpy equals -4850 kJ.

b. Energy balance on reaction system (not including heated water):

$$\Delta E_k, \Delta E_p, W = 0 \Rightarrow Q = \Delta U = n(\text{mol C}_8\text{H}_{18} \text{ consumed}) \Delta\hat{U}_\text{c}^\circ (\text{kJ/mol})$$

$$(C_p)_{\text{H}_2\text{O}(\text{l})} \text{ from Table B.2} = 75.4 \times 10^{-3} \text{ kJ/mol} \cdot ^\circ\text{C}$$

$$-Q = m_{\text{H}_2\text{O}} (C_p)_{\text{H}_2\text{O}(\text{l})} \Delta T = \frac{1.00 \text{ kg}}{18.0 \times 10^{-3} \text{ kg}} \left| \frac{1 \text{ mol}}{18.0 \times 10^{-3} \text{ kg}} \right| \left| \frac{75.4 \times 10^{-3} \text{ kJ}}{\text{mol} \cdot ^\circ\text{C}} \right| \left| \frac{21.34^\circ\text{C}}{1} \right| = 89.4 \text{ kJ}$$

$$Q = \Delta U \Rightarrow -89.4 \text{ kJ} = \frac{2.01 \text{ g C}_8\text{H}_{18} \text{ consumed}}{114.2 \text{ g}} \left| \frac{1 \text{ mol C}_8\text{H}_{18}}{114.2 \text{ g}} \right| \left| \frac{\Delta\hat{U}_\text{c}^\circ (\text{kJ})}{1 \text{ mol C}_8\text{H}_{18}} \right|$$

$$\Rightarrow \Delta\hat{U}_\text{c}^\circ = -5079 \text{ kJ/mol}$$

$$\Delta\hat{H}_\text{c}^\circ = \Delta\hat{U}_\text{c}^\circ + RT \left[ \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right]$$

$$= -5079 \text{ kJ/mol} + \frac{8.314 \text{ J}}{\text{mol} \cdot \text{K}} \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| \left| \frac{298 \text{ K}}{1} \right| \left| \frac{(8 + 9 - 12.5)}{1} \right|$$

$$\Rightarrow \Delta\hat{H}_\text{c}^\circ = -5068 \text{ kJ/mol}$$

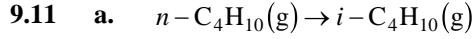
$$\% \text{ difference} = \frac{(-5068) - (-4850)}{|-5068|} \times 100 = -4.3 \%$$

c.

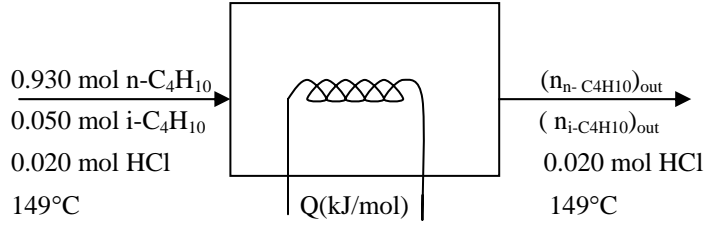
$$\Delta\hat{H}_\text{c}^\circ = 8(\Delta\hat{H}_\text{f}^\circ)_{\text{CO}_2(\text{g})} + 9(\Delta\hat{H}_\text{f}^\circ)_{\text{H}_2\text{O}(\text{g})} - (\Delta\hat{H}_\text{f}^\circ)_{\text{C}_8\text{H}_{18}(\text{l})}$$

$$\Rightarrow (\Delta\hat{H}_\text{f}^\circ)_{\text{C}_8\text{H}_{18}(\text{l})} = [8(-393.5) + 9(-241.83) + 5068] \text{ kJ/mol} = -256.5 \text{ kJ/mol}$$

There is no practical way to react carbon and hydrogen such that 2,3,3-trimethylpentane is the only product.



Basis: 1 mol feed gas



$$(n_{\text{n-C}_4\text{H}_{10}})_{\text{out}} = 0.930(1 - 0.400) = \underline{\underline{0.560 \text{ mol}}}$$

$$(n_{\text{i-C}_4\text{H}_{10}})_{\text{out}} = 0.050 + 0.930 \times 0.400 = \underline{\underline{0.420 \text{ mol}}}$$

$$\xi = \frac{|(n_{\text{n-C}_4\text{H}_{10}})_{\text{out}} - (n_{\text{n-C}_4\text{H}_{10}})_{\text{in}}|}{|v_{\text{n-C}_4\text{H}_{10}}|} = \frac{|0.560 - 0.930|}{|1|} = \underline{\underline{0.370 \text{ mol}}}$$

b.  $\Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{i\text{-C}_4\text{H}_{10}} - (\Delta \hat{H}_f^\circ)_{n\text{-C}_4\text{H}_{10}} \xRightarrow{\text{Table B.1}} \Delta \hat{H}_r^\circ = [-134.5 - (-124.7)] \text{ kJ/mol} = \underline{\underline{-9.8 \text{ kJ/mol}}}$

c. References:  $n\text{-C}_4\text{H}_{10}(\text{g})$ ,  $i\text{-C}_4\text{H}_{10}(\text{g})$  at  $25^\circ\text{C}$

substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$n\text{-C}_4\text{H}_{10}$	1	$\hat{H}_1$	0.600	$\hat{H}_1$
$i\text{-C}_4\text{H}_{10}$	—	—	0.400	$\hat{H}_2$

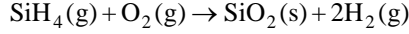
$$\hat{H}_1 = \left[ \int_{25}^{149} \overset{\text{Table B.2}}{\downarrow} C_p dT \right] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{14.29 \text{ kJ/mol}}} \quad \hat{H}_2 = \left[ \int_{25}^{149} \overset{\text{Table B.2}}{\downarrow} C_p dT \right] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{14.14 \text{ kJ/mol}}}$$

$$Q = \Delta H = \xi [\Delta \hat{H}_r^\circ + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i] = 0.370 [-9.8 + (1)(14.142) - (1)(14.287)] \text{ kJ} \\ = \underline{\underline{-3.68 \text{ kJ}}}$$

$$\text{For } 325 \text{ mol/h fed, } \dot{Q} = \frac{-9.8 \text{ kJ}}{1 \text{ mol feed}} \left| \frac{325 \text{ mol feed}}{\text{h}} \right| \left| \frac{1 \text{ h}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-0.90 \text{ kW}}}$$

d.  $\Delta \hat{H}_r(149^\circ\text{C}) = \frac{-3.68 \text{ kJ}}{0.370 \text{ mol}} = \underline{\underline{-9.95 \text{ kJ/mol}}}$

9.12 a.



Ideal Gas Equation of state :  $n_o = \frac{1 \text{ m}^3}{298 \text{ K}} \left| \frac{273 \text{ K}}{760 \text{ torr}} \right| \left| \frac{3.00 \text{ torr}}{22.4 \times 10^{-3} \text{ m}^3} \right| = 0.1614 \text{ mol}$

$$n_i = n_{io} + \nu_i \xi$$

$$\text{SiH}_4 : 0 = 0.1111(0.1614 \text{ mol}) - \xi \Rightarrow \xi = 0.0179 \text{ mol}$$

$$\text{O}_2 : n_1 = 0.8889(0.1614 \text{ mol}) - \xi = 0.1256 \text{ mol O}_2$$

$$\text{SiO}_2 : n_2 = \xi = 0.0179 \text{ mol SiO}_2$$

$$\text{H}_2 : n_3 = 2\xi = 0.0358 \text{ mol H}_2$$

b.  $\Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{\text{SiO}_2(\text{s})} - (\Delta \hat{H}_f^\circ)_{\text{SiH}_4(\text{g})}$   
 $= [-851 - (-61.9)] \text{ kJ/mol} = -789.1 \text{ kJ/mol}$

References :  $\text{SiH}_4(\text{g}), \text{O}_2(\text{g}), \text{SiO}_2(\text{g}), \text{H}_2(\text{g})$  at 298 K

Substance	$n_{\text{in}}$ (mol/h)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol/h)	$\hat{H}_{\text{out}}$ (kJ/mol)
SiH <sub>4</sub>	0.0179	0	—	—
O <sub>2</sub>	0.1435	0	0.1256	$\hat{H}_1$
SiO <sub>2</sub>	—	—	0.0179	$\hat{H}_2$
H <sub>2</sub>	—	—	0.0358	$\hat{H}_3$

Table B.8  
↓

$$\text{O}_2(\text{g}, 1375\text{K}): \hat{H}_1 = \hat{H}_{\text{O}_2}(1102^\circ\text{C}) = 36.14 \text{ kJ/mol}$$

$$\text{SiO}_2(\text{s}, 1375\text{K}): \hat{H}_2 = \int_{298}^{1375} (C_p)_{\text{SiO}_2(\text{s})} dT = 79.18 \text{ kJ/mol}$$

Table B.8  
↓

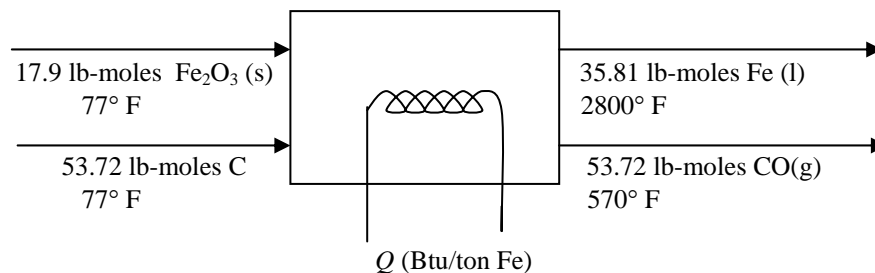
$$\text{H}_2(\text{g}, 1375\text{K}): \hat{H}_3 = \hat{H}_{\text{H}_2}(1102^\circ\text{C}) = 32.35 \text{ kJ/mol}$$

c.  $Q = \Delta H = \xi \Delta \hat{H}_r^\circ + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = -7.01 \text{ kJ/m}^3 \text{ feed}$

$$\dot{Q} = \frac{-7.01 \text{ kJ}}{\text{m}^3} \left| \frac{27.5 \text{ m}^3}{\text{h}} \right| \left| \frac{1 \text{ h}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = -0.0536 \text{ kW} \text{ (transferred from reactor)}$$

9.13 a.  $\text{Fe}_2\text{O}_3(\text{s}) + 3\text{C}(\text{s}) \rightarrow 2\text{Fe}(\text{s}) + 3\text{CO}(\text{g})$ ,  $\Delta\hat{H}_r(77^\circ\text{F}) = 2.111 \times 10^5$  Btu/lb - mole

Basis:  $\frac{2000 \text{ lb}_m \text{ Fe}}{55.85 \text{ lb}_m} = 35.81 \text{ lb - moles Fe produced}$   
 53.72 lb - moles CO produced  
 17.9 lb - moles  $\text{Fe}_2\text{O}_3$  fed  
 53.72 lb - moles C fed



b. References:  $\text{Fe}_2\text{O}_3(\text{s})$ ,  $\text{C}(\text{s})$ ,  $\text{Fe}(\text{s})$ ,  $\text{CO}(\text{g})$  at  $77^\circ\text{F}$

Substance	$n_{\text{in}}$ (lb - moles)	$\hat{H}_{\text{in}}$ (Btu/lb - mole)	$n_{\text{out}}$ (lb - moles)	$\hat{H}_{\text{out}}$ (Btu/lb - mole)
$\text{Fe}_2\text{O}_3(\text{s}, 77^\circ\text{F})$	17.91	0	—	—
$\text{C}(\text{s}, 77^\circ\text{F})$	53.72	0	—	—
$\text{Fe}(\text{l}, 2800^\circ\text{F})$	—	—	35.81	$\hat{H}_1$
$\text{CO}(\text{g}, 570^\circ\text{F})$	—	—	53.72	$\hat{H}_2$

$$\text{Fe}(\text{l}, 2800^\circ\text{F}): \hat{H}_1 = \int_{77}^{2794} (C_p)_{\text{Fe}(\text{s})} dT + \Delta\hat{H}_m(2794^\circ\text{F}) + \int_{2794}^{2800} (C_p)_{\text{Fe}(\text{l})} dT = \underline{\underline{28400 \text{ Btu/lb - mole}}}$$

$$\text{CO}(\text{g}, 570^\circ\text{F}): \hat{H}_2 = \hat{H}_{\text{CO}}(570^\circ\text{F}) \overset{\substack{\uparrow \\ \text{(interpolating} \\ \text{from Table B.9)}}}{=} \underline{\underline{3486 \text{ Btu/lb - mole}}}$$

c.  $Q = \Delta H = \frac{n_{\text{Fe}} \Delta\hat{H}_r^0}{\nu_{\text{Fe}}} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i$

$$= \frac{(35.81)(2.111 \times 10^5)}{2} + (35.81)(28400) + (53.72)(3486) - 0 = \underline{\underline{4.98 \times 10^6 \text{ Btu / ton Fe produced}}}$$

d. Effect of any pressure changes on enthalpy are neglected.

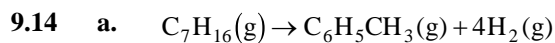
Specific heat of  $\text{Fe}(\text{s})$  is assumed to vary linearly with temperature from  $77^\circ\text{F}$  to  $570^\circ\text{F}$ .

Specific heat of  $\text{Fe}(\text{l})$  is assumed to remain constant with temperature.

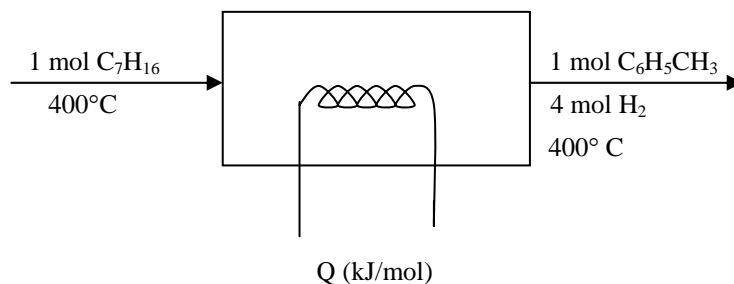
Reaction is complete.

No vaporization occurs.





Basis: 1 mol  $\text{C}_7\text{H}_{16}$



b.

References:  $\text{C}(\text{s}), \text{H}_2(\text{g})$  at  $25^\circ\text{C}$

substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$\text{C}_7\text{H}_{16}$	1	$\hat{H}_1$	—	—
$\text{C}_6\text{H}_5\text{CH}_3$	—	—	1	$\hat{H}_2$
$\text{H}_2$	—	—	4	$\hat{H}_3$

$$\text{C}_7\text{H}_{16}(\text{g}, 400^\circ\text{C}): \hat{H}_1 = (\Delta\hat{H}_f^\circ)_{\text{C}_7\text{H}_{16}(\text{g})} + \left[ \int_{25}^{400} \overset{0.2427}{C_p} dT \right]$$

$$= (-187.8 + 91.0) \text{ kJ/mol} = \underline{\underline{-96.8 \text{ kJ/mol}}}$$

$$\text{C}_6\text{H}_5\text{CH}_3(\text{g}, 400^\circ\text{C}): \hat{H}_2 = (\Delta\hat{H}_f^\circ)_{\text{C}_6\text{H}_5\text{CH}_3(\text{g})} + \left[ \int_{25}^{400} \overset{\text{Table B.2}}{C_p} dT \right]$$

$$= (+50 + 60.2) \text{ kJ/mol} = \underline{\underline{110.2 \text{ kJ/mol}}}$$

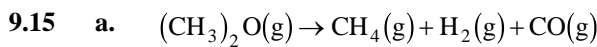
$$\text{H}_2(\text{g}, 400^\circ\text{C}): \hat{H}_3 = \overset{\text{Table B.8}}{\hat{H}_{\text{H}_2}(400^\circ\text{C})} = \underline{\underline{10.89 \text{ kJ/mol}}}$$

c.

$$Q = \Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i$$

$$= [(1)(110.2) + (4)(10.89) - (1)(-96.8)] \text{ kJ} = 251 \text{ kJ (transferred to reactor)}$$

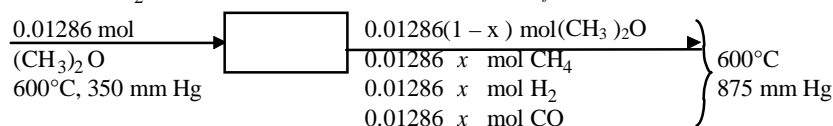
d.  $\Delta\hat{H}_r(400^\circ\text{C}) = \frac{251 \text{ kJ}}{1 \text{ mol C}_7\text{H}_{16} \text{ react}} = \underline{\underline{251 \text{ kJ/mol}}}$



Moles charged: (Assume ideal gas)

$$\frac{2.00 \text{ liters} \mid 273 \text{ K} \mid 350 \text{ mm Hg} \mid 1 \text{ mol}}{873 \text{ K} \mid 760 \text{ mm Hg} \mid 22.4 \text{ liters(STP)}} = 0.01286 \text{ mol } (\text{CH}_3)_2\text{O}$$

Let  $x$  = fraction  $(\text{CH}_3)_2\text{O}$  decomposed (Clearly  $x < 1$  since  $P_f < 3P_0$ )



$$\text{Total moles in tank at } t = 2h = 0.01286[(1-x) + 3x] = 0.01286(1+2x) \text{ mol}$$

$$\frac{P_f V}{P_0 V} = \frac{n_f RT}{n_0 RT} \Rightarrow \frac{n_f}{n_0} = \frac{P_f}{P_0} \Rightarrow \frac{0.01286(1+2x)}{0.01286} = \frac{875}{350} \Rightarrow x = 0.75 \Rightarrow \underline{\underline{75\% \text{ decomposed}}}$$

b. References:  $\text{C}(\text{s})$ ,  $\text{H}_2(\text{g})$ ,  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$

substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$(\text{CH}_3)_2\text{O}(\text{g})$	0.01286	$\hat{H}_1$	$0.25 \times 0.01286$	$\hat{H}_1$
$\text{CH}_4(\text{g})$	—	—	$0.75 \times 0.01286$	$\hat{H}_2$
$\text{H}_2(\text{g})$	—	—	$0.75 \times 0.01286$	$\hat{H}_3$
$\text{CO}(\text{g})$	—	—	$0.75 \times 0.01286$	$\hat{H}_4$

$$\begin{aligned} (\text{CH}_3)_2\text{O}(\text{g}, 600^\circ\text{C}): \hat{H}_1 &= (\Delta\hat{H}_f^\circ)_{(\text{CH}_3)_2\text{O}} + \left[ \int_{298}^{873} \overset{\text{given}}{C_p} dT \right] \frac{\text{J}}{\text{mol}} \times \frac{1 \text{ kJ}}{10^3 \text{ J}} = (-180.16 + 62.40) \text{ kJ/mol} \\ &= \underline{\underline{-118 \text{ kJ/mol}}} \end{aligned}$$

$$\text{CH}_4(\text{g}, 600^\circ\text{C}): \hat{H}_2 = (\Delta\hat{H}_f^\circ)_{\text{CH}_4} + \left[ \int_{25}^{600} \overset{\text{Table B.2}}{C_p} dT \right] = -74.85 + 29.46 = \underline{\underline{-45.39 \text{ kJ/mol}}}$$

$$\text{H}_2(\text{g}, 600^\circ\text{C}): \hat{H}_3 = \overset{\text{Table B.8}}{\hat{H}_{\text{H}_2}(600^\circ\text{C})} = \underline{\underline{16.81 \text{ kJ/mol}}}$$

$$\text{CO}(\text{g}, 600^\circ\text{C}): \hat{H}_4 = (\Delta\hat{H}_f^\circ)_{\text{CO}} + \overset{\text{Table B.8}}{\hat{H}_{\text{CO}}(600^\circ\text{C})} = -110.52 + 17.57 \text{ kJ/mol} = \underline{\underline{-92.95 \text{ kJ/mol}}}$$

c. For the reaction of parts (a) and (b), the enthalpy change and extent of reaction are :

$$\Delta H = \sum n_{\text{out}} \hat{H}_{\text{out}} - \sum n_{\text{in}} \hat{H}_{\text{in}} = [-1.5515 - (-1.5175)] \text{ kJ} = -0.0340 \text{ kJ}$$

9.15 (cont'd)

$$\xi = \frac{(n_{\text{CH}_4})_{\text{out}} - (n_{\text{CH}_4})_{\text{in}}}{\nu_{\text{CH}_4}} = \frac{0.75 \times 0.01286}{1} \text{ mol} = 0.009645 \text{ mol}$$

$$\Delta H = \xi \Delta \hat{H}_r(600^\circ\text{C}) \Rightarrow \Delta \hat{H}_r(600^\circ\text{C}) = \frac{-0.0340 \text{ kJ}}{0.009645} = \underline{\underline{-3.53 \text{ kJ/mol}}}$$

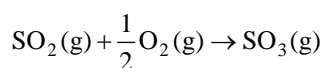
$$\Delta \hat{U}_r(600^\circ\text{C}) = \Delta \hat{H}_r(600^\circ\text{C}) - RT \left[ \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right]$$

d.

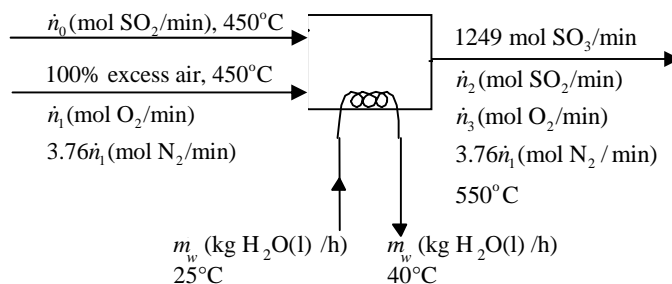
$$= -3.53 \text{ kJ/mol} - \frac{8.314 \text{ J}}{\text{mol} \cdot \text{K}} \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| \left| \frac{873 \text{ K}}{1} \right| \left| \frac{(1+1+1-1)}{1} \right| = \underline{\underline{-18.0 \text{ kJ/mol}}}$$

$$Q = \xi \Delta \hat{U}_r(600^\circ\text{C}) = (0.009645 \text{ mol})(-18.0 \text{ kJ/mol}) = \underline{\underline{-0.174 \text{ kJ}}} \text{ (transferred from reactor)}$$

9.16 a.



$$\text{Basis: } \frac{100 \text{ kg SO}_3}{\text{min}} \left| \frac{10^3 \text{ mol SO}_3}{80.07 \text{ kg SO}_3} \right| = 1249 \text{ mol SO}_3/\text{min}$$



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

$$\text{SO}_3 \text{ balance: } \frac{\dot{n}_0 \text{ (mol SO}_2 \text{ fed)}}{\text{min}} \left| \frac{0.65 \text{ mol SO}_2 \text{ react}}{1 \text{ mol SO}_2 \text{ fed}} \right| \left| \frac{1 \text{ mol SO}_3 \text{ produced}}{1 \text{ mol SO}_2 \text{ react}} \right| = 1249 \frac{\text{mol SO}_3}{\text{min}}$$

$$\Rightarrow \dot{n}_0 = \underline{\underline{1922 \text{ mol SO}_2 / \text{min fed}}}$$

$$\text{100\% excess air: } \dot{n}_1 = \frac{1922 \text{ mol SO}_2}{\text{min}} \left| \frac{0.5 \text{ mol O}_2 \text{ reqd}}{1 \text{ mol SO}_2} \right| \left| \frac{(1+1) \text{ mol O}_2 \text{ fed}}{1 \text{ mol O}_2 \text{ reqd}} \right| = \underline{\underline{1922 \text{ mol O}_2 / \text{min fed}}}$$

$$\text{N}_2 \text{ balance: } 3.76(1922) = \underline{\underline{7227 \text{ mol / min (in \& out)}}}$$

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

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

**9.16 (cont'd)**

**b.**

$$\text{Extent of reaction : } \xi = \frac{(\dot{n}_{\text{SO}_2})_{\text{out}} - (\dot{n}_{\text{SO}_2})_{\text{in}}}{|\nu_{\text{SO}_2}|} = \frac{|673 - 1922|}{|1|} = \underline{\underline{1249 \text{ mol / min}}}$$

$$\Delta \hat{H}_r^o = (\Delta \hat{H}_f^o)_{\text{SO}_3(\text{g})} - (\Delta \hat{H}_f^o)_{\text{SO}_2(\text{g})} \xrightarrow{\text{Table B.1}} = -395.18 - (-296.9) = \underline{\underline{-99.28 \text{ kJ / mol}}}$$

References :  $\text{SO}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$ ,  $\text{SO}_3(\text{g})$  at  $25^\circ \text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol / min)	$\hat{H}_{\text{in}}$ (kJ / mol)	$\dot{n}_{\text{out}}$ (mol / min)	$\hat{H}_{\text{out}}$ (kJ / mol)
$\text{SO}_2$	1922	$\hat{H}_1$	673	$\hat{H}_4$
$\text{O}_2$	1922	$\hat{H}_2$	1298	$\hat{H}_5$
$\text{N}_2$	7227	$\hat{H}_3$	7227	$\hat{H}_6$
$\text{SO}_3$	—	—	1249	$\hat{H}_7$

$$\text{SO}_2(\text{g}, 450^\circ \text{C}) : \hat{H}_1 = \int_{25}^{450} \overset{\text{Table B.2}}{\downarrow} C_p dT = \underline{\underline{19.62 \text{ kJ / mol}}}$$

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

$$\text{N}_2(\text{g}, 450^\circ \text{C}) = \hat{H}_3 = \hat{H}_{\text{N}_2}(450^\circ \text{C}) \xrightarrow{\text{Table B.8}} = \underline{\underline{12.69 \text{ kJ / mol}}}$$

Out :

$$\text{SO}_2(\text{g}, 550^\circ \text{C}) : \hat{H}_4 = \int_{25}^{550} \overset{\text{Table B.2}}{\downarrow} C_p dT = \underline{\underline{24.79 \text{ kJ/mol}}}$$

$$\text{O}_2(\text{g}, 550^\circ \text{C}) = \hat{H}_5 = \hat{H}_{\text{O}_2}(550^\circ \text{C}) \xrightarrow{\text{Table B.8}} = \underline{\underline{16.71 \text{ kJ / mol}}}$$

$$\text{N}_2(\text{g}, 550^\circ \text{C}) = \hat{H}_6 = \hat{H}_{\text{N}_2}(550^\circ \text{C}) \xrightarrow{\text{Table B.8}} = \underline{\underline{15.81 \text{ kJ / mol}}}$$

$$\text{SO}_3(\text{g}, 550^\circ \text{C}) : \hat{H}_7 = \int_{25}^{550} \overset{\text{Table B.2}}{\downarrow} C_p dT = \underline{\underline{35.34 \text{ kJ / mol}}}$$

$$\begin{aligned} \dot{Q} &= \Delta \dot{H} = \xi \Delta \hat{H}_r^o + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i \\ &= (1249)(-98.28) + (673)(24.796) + (179.8)(16.711) + (7227)(15.808) + (1249)(35.336) - (1922)(13.362) - (7227)(12.691) \\ &= \frac{-8.111 \times 10^4 \text{ kJ}}{\text{min}} \left| \frac{1 \text{ min}}{60 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-1350 \text{ kW}}} \end{aligned}$$

**c.**

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

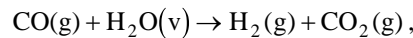
9.16 (cont'd)

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

d.  $\Rightarrow 8.111 \times 10^4 \frac{\text{kJ}}{\text{min}} = \dot{m}_w \left( \frac{\text{kg}}{\text{min}} \right) [167.5 - 104.8] \frac{\text{kJ}}{\text{kg}} \Rightarrow \underline{\underline{\dot{m}_w = 1290 \text{ kg/min cooling water}}}$

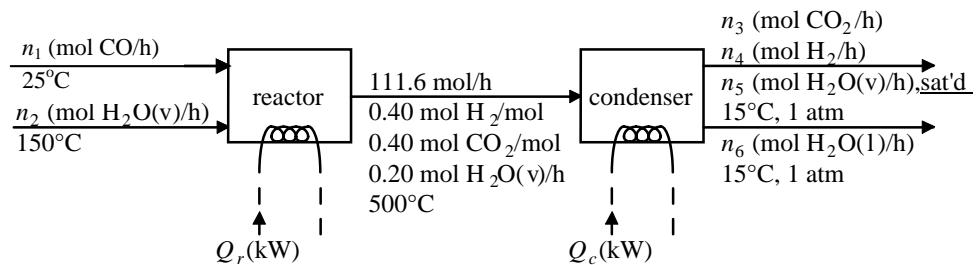
If elemental species were taken as references, the heats of formation of each molecular species would have to be taken into account in the enthalpy calculations and the heat of reaction term would not have been included in the calculation of  $\Delta \dot{H}$ .

9.17



$$\Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{\text{CO}_2(\text{g})} - (\Delta \hat{H}_f^\circ)_{\text{CO(g)}} - (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O(v)}} \overset{\substack{\text{Table B.1} \\ \downarrow}}{=} -41.15 \frac{\text{kJ}}{\text{mol}}$$

a. Basis :  $[2.5 \text{ m}^3(\text{STP}) \text{ product gas/h}] [1000 \text{ mol}/22.4 \text{ m}^3(\text{STP})] = 111.6 \text{ mol/h}$



C balance on reactor :  $\dot{n}_1 = (0.40)(111.6 \text{ mol/h}) = 44.64 \text{ mol CO/h}$

H balance on reactor :  $2\dot{n}_2 = 111.6[(2)(0.40) + (2)(0.20)] \text{ mol/h} \Rightarrow \dot{n}_2 = 66.96 \text{ mol H}_2\text{O(v)/h}$

Steam theoretically required =  $\frac{44.64 \text{ mol CO}}{\text{h}} \left| \frac{1 \text{ mol H}_2\text{O}}{1 \text{ mol CO}} \right. = 44.64 \text{ mol H}_2\text{O}$

% excess steam =  $\frac{(66.96 - 44.64) \text{ mol/h}}{44.64 \text{ mol/h}} \times 100\% = \underline{\underline{50\% \text{ excess steam}}}$

CO<sub>2</sub> balance on condenser :  $\dot{n}_3 = (0.40)(111.6 \text{ mol/h}) = 44.64 \text{ mol CO}_2/\text{h}$

H<sub>2</sub> balance on condenser:  $\dot{n}_4 = (0.40)(111.6 \text{ mol/h}) = 44.64 \text{ mol H}_2/\text{h}$

Saturation of condenser outlet gas:

$$y_{\text{H}_2\text{O}} = \frac{p_w^*(15^\circ\text{C})}{p} \Rightarrow \frac{\dot{n}_5 (\text{mol H}_2\text{O/h})}{(44.64 + 44.64 + \dot{n}_5) (\text{mol/h})} = \frac{12.788 \text{ mm Hg}}{760 \text{ mm Hg}} \Rightarrow \dot{n}_5 = 1.53 \text{ mol H}_2\text{O(v)/h}$$

H<sub>2</sub>O balance on condenser:  $(111.6)(0.20) \text{ mol H}_2\text{O/h} = 1.53 + \dot{n}_6$   
 $\Rightarrow \dot{n}_6 = 20.8 \text{ mol H}_2\text{O/h condensed} = \underline{\underline{0.374 \text{ kg/h}}}$

**9.17 (cont'd)**

**b. Energy balance on condenser**

References :  $\text{H}_2(\text{g})$ ,  $\text{CO}_2(\text{g})$  at  $25^\circ\text{C}$ ,  $\text{H}_2\text{O}$  at reference point of steam tables

Substance	$\dot{n}_{\text{in}}$ mol / h	$\hat{H}_{\text{in}}$ kJ / mol	$\dot{n}_{\text{out}}$ mol / h	$\hat{H}_{\text{out}}$ kJ / mol
$\text{CO}_2(\text{g})$	44.64	$\hat{H}_1$	44.64	$\hat{H}_4$
$\text{H}_2(\text{g})$	44.64	$\hat{H}_2$	44.64	$\hat{H}_5$
$\text{H}_2\text{O}(\text{v})$	22.32	$\hat{H}_3$	1.53	$\hat{H}_6$
$\text{H}_2\text{O}(\text{l})$	—	—	20.80	$\hat{H}_7$

Enthalpies for  $\text{CO}_2$  and  $\text{H}_2$  from Table B.8

$$\text{CO}_2(\text{g}, 500^\circ\text{C}) : \hat{H}_1 = \hat{H}_{\text{CO}_2}(500^\circ\text{C}) = 21.34 \text{ kJ / mol}$$

$$\text{H}_2(\text{g}, 500^\circ\text{C}) : \hat{H}_2 = \hat{H}_{\text{H}_2}(500^\circ\text{C}) = 13.83 \text{ kJ / mol}$$

$$\text{H}_2\text{O}(\text{v}, 500^\circ\text{C}) : \hat{H}_3 = 3488 \frac{\text{kJ}}{\text{kg}} \times \left( \frac{18 \text{ kg}}{10^3 \text{ mol}} \right) = 62.86 \text{ kJ/mol}$$

$$\text{CO}_2(\text{g}, 15^\circ\text{C}) : \hat{H}_4 = \hat{H}_{\text{CO}_2}(15^\circ\text{C}) = -0.552 \text{ kJ/mol}$$

$$\text{H}_2(\text{g}, 15^\circ\text{C}) : \hat{H}_5 = \hat{H}_{\text{H}_2}(15^\circ\text{C}) = -0.432 \text{ kJ / mol}$$

$$\text{H}_2\text{O}(\text{v}, 15^\circ\text{C}) : \hat{H}_6 = 2529 \frac{\text{kJ}}{\text{kg}} \times \left( \frac{18.0 \text{ kg}}{10^3 \text{ mol}} \right) = 45.52 \text{ kJ/mol}$$

$$\text{H}_2\text{O}(\text{l}, 15^\circ\text{C}) : \hat{H}_7 = 62.9 \frac{\text{kJ}}{\text{kg}} \times \left( \frac{18.0 \text{ kg}}{10^3 \text{ mol}} \right) = 1.13 \text{ kJ/mol}$$

$$\dot{Q} = \Delta \dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = \frac{(49.22 - 2971.8) \text{ kJ}}{\text{h}} \left| \frac{1 \text{ h}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-0.812 \text{ kW}}}$$

(heat transferred from condenser)

**c. Energy balance on reactor :**

References :  $\text{H}_2(\text{g})$ ,  $\text{C}(\text{s})$ ,  $\text{O}_2(\text{g})$  at  $25^\circ\text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol / h)	$\hat{H}_{\text{in}}$ (kJ / mol)	$\dot{n}_{\text{out}}$ (mol / h)	$\hat{H}_{\text{out}}$ (kJ / mol)
$\text{CO}(\text{g})$	44.64	$\hat{H}_1$	—	—
$\text{H}_2\text{O}(\text{v})$	66.96	$\hat{H}_2$	22.32	$\hat{H}_3$
$\text{H}_2(\text{g})$	—	—	44.64	$\hat{H}_4$
$\text{CO}_2(\text{g})$	—	—	44.64	$\hat{H}_5$

$$\text{CO}(\text{g}, 25^\circ\text{C}) : \hat{H}_1 = (\Delta \hat{H}_f^\circ)_{\text{CO}} \stackrel{\text{Table B.1}}{=} \underline{\underline{-110.52 \text{ kJ / mol}}}$$

$$\text{H}_2\text{O}(\text{v}, 150^\circ\text{C}) : \hat{H}_2 = (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{v})} + \hat{H}_{\text{H}_2\text{O}}(150^\circ\text{C}) \stackrel{\text{Tables B.1, B.8}}{=} \underline{\underline{-237.56 \text{ kJ/mol}}}$$

**9.17 (cont'd)**

$$\text{H}_2\text{O}(\text{v}, 500^\circ\text{C}) : \hat{H}_3 = (\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{v})} + \hat{H}_{\text{H}_2\text{O}}(500^\circ\text{C}) \stackrel{\text{Tables B.1, B.8}}{=} \underline{\underline{-224.82 \text{ kJ/mol}}}$$

$$\text{H}_2(\text{g}, 500^\circ\text{C}) : \hat{H}_4 = \hat{H}_{\text{H}_2}(500^\circ\text{C}) \stackrel{\text{Table B.8}}{=} \underline{\underline{13.83 \text{ kJ/mol}}}$$

$$\text{CO}_2(\text{g}, 500^\circ\text{C}) : \hat{H}_5 = (\Delta\hat{H}_f^\circ)_{\text{CO}_2} + \hat{H}_{\text{CO}_2}(500^\circ\text{C}) \stackrel{\text{Tables B.1, B.8}}{=} \underline{\underline{-372.16 \text{ kJ/mol}}}$$

$$Q = \Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = \frac{[-21013.83 - (-20839.96)] \text{ kJ}}{\text{h}} \left| \frac{1 \text{ h}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-0.0483 \text{ kW}}}$$

(heat transferred from reactor)

**d.**

Benefits

Preheating CO  $\Rightarrow$  more heat transferred from reactor (possibly generate additional steam for plant)

Cooling CO  $\Rightarrow$  lower cooling cost in condenser.

9.18 b.

References : FeO(s), CO(g), Fe(s), CO<sub>2</sub>(g) at 25°C

Substance	$n_{in}$ (mol)	$\hat{H}_{in}$ (kJ / mol)	$n_{out}$ (mol)	$\hat{H}_{out}$ (kJ / mol)
FeO	1.00	0	$n_1$	$\hat{H}_1$
CO	$n_0$	$\hat{H}_0$	$n_2$	$\hat{H}_2$
Fe	—	—	$n_3$	$\hat{H}_3$
CO <sub>2</sub>	—	—	$n_4$	$\hat{H}_4$

$$Q = \xi \Delta \hat{H}_r^o + \sum n_{out} \hat{H}_{out} - \sum n_{in} \hat{H}_{in}$$

$$\Rightarrow Q = \xi \Delta \hat{H}_r^o + n_1 \hat{H}_1 + n_2 \hat{H}_2 + n_3 \hat{H}_3 + n_4 \hat{H}_4 - n_0 \hat{H}_0$$

Fractional Conversion :  $X = \frac{(1.00 - n_1)}{1.00} \Rightarrow \underline{\underline{n_1 = 1 - X}}$

CO consumed :  $\frac{1 \text{ mol CO}}{1 \text{ mol FeO consumed}} \mid \frac{(1 - n_1) \text{ mol FeO consumed}}{1 \text{ mol FeO consumed}} = (1 - n_1) \text{ mol CO}$

$$\Rightarrow n_2 = n_0 - (1 - n_1) = \underline{\underline{n_0 - X}}$$

Fe produced :  $n_3 = \frac{1 \text{ mol Fe}}{1 \text{ mol FeO consumed}} \mid \frac{(1 - n_1) \text{ mol FeO consumed}}{1 \text{ mol FeO consumed}} = (1 - n_1) \text{ mol Fe} = \underline{\underline{X}}$

CO<sub>2</sub> produced :  $n_4 = \frac{1 \text{ mol CO}_2}{1 \text{ mol FeO consumed}} \mid \frac{(1 - n_1) \text{ mol FeO consumed}}{1 \text{ mol FeO consumed}} = (1 - n_1) \text{ mol CO}_2 = \underline{\underline{X}}$

Extent of reaction :  $\xi = \frac{|(n_{CO})_{out} - (n_{CO})_{in}|}{|\nu_{CO}|} = \frac{|n_2 - n_0|}{1} = \underline{\underline{X}}$

$$\hat{H}_i = \int_{25}^T C_{pi} dT \quad \text{for } i = 0, 1, 2, 3, 4$$

$$\hat{H}_0 = 0.02761 (T_0 - 298) + 2.51 \times 10^{-6} (T_0^2 - 298^2)$$

$$\Rightarrow \underline{\underline{\hat{H}_0 = (-8.451 + 0.02761 T_0 + 2.51 \times 10^{-6} T_0^2) \text{ kJ / mol}}}$$

$$\hat{H}_1 = 0.0528 (T - 298) + 3.1215 \times 10^{-6} (T^2 - 298^2) + 3.188 \times 10^2 (1/T - 1/298)$$

$$\Rightarrow \underline{\underline{\hat{H}_1 = (-17.0814 + 0.0528 T + 3.1215 \times 10^{-6} T^2 + 3.188 \times 10^2 / T) \text{ kJ / mol}}}$$

$$\hat{H}_2 = (0.02761 (T - 298) + 2.51 \times 10^{-6} (T^2 - 298^2))$$

$$\Rightarrow \underline{\underline{\hat{H}_2 = (-8.451 + 0.02761 T + 2.51 \times 10^{-6} T^2) \text{ kJ / mol}}}$$

$$\hat{H}_3 = 0.01728 (T - 298) + 1.335 \times 10^{-5} (T^2 - 298^2)$$

$$\Rightarrow \underline{\underline{\hat{H}_3 = (-6.335 + 0.01728 T + 1.335 \times 10^{-5} T^2) \text{ kJ / mol}}}$$

$$\hat{H}_4 = 0.04326 (T - 298) + 0.573 \times 10^{-5} (T^2 - 298^2) + 8.18 \times 10^2 (1/T - 1/298)$$

$$\Rightarrow \underline{\underline{\hat{H}_4 = (-16.145 + 0.04326 T + 0.573 \times 10^{-5} T^2 + 8.18 \times 10^2 / T) \text{ kJ / mol}}}$$



**9.18 (cont'd)**

**c.**  $n_0 = 2.0$  mol CO,  $T_0 = 350$  K,  $T = 550$  K, and  $X = 0.700$  mol FeO reacted/mol FeO fed  
 $\Rightarrow n_1 = 1 - 0.7 = 0.3$ ,  $n_2 = 2 - 0.7 = 1.3$ ,  $n_3 = 0.7$ ,  $n_4 = 0.7$ ,  $\xi = 0.7$

Summary :  $\hat{H}_0 = 1.520$  kJ/mol,  $\hat{H}_1 = 13.48$  kJ/mol,  $\hat{H}_2 = 7.494$  kJ/mol,

$\hat{H}_3 = 7.207$  kJ/mol,  $\hat{H}_4 = 10.87$  kJ/mol

$\Delta\hat{H}_r^\circ = -16.48$  kJ/mol

$Q = (0.7)(-16.48) + (0.3)(13.48) + (1.3)(7.494) + (0.7)(7.207) + (0.7)(10.87) - (2)(1.520)$

$\Rightarrow \underline{\underline{Q = 11.86 \text{ kJ}}}$

**d.**

no	To	X	T	Xi	n1	n2	n3	n4	H0	H1	H2	H3	H4	Q
1	400	1	298	1	0	0	1	1	2.995	0	0	0	0	-19.48
1	400	1	400	1	0	0	1	1	2.995	5.335	2.995	2.713	4.121	-12.64
1	400	1	500	1	0	0	1	1	2.995	10.737	5.982	5.643	8.553	-5.279
1	400	1	600	1	0	0	1	1	2.995	16.254	9.019	8.839	13.237	2.601
1	400	1	700	1	0	0	1	1	2.995	21.864	12.11	12.303	18.113	10.941
1	400	1	800	1	0	0	1	1	2.995	27.555	15.24	16.033	23.152	19.71
1	400	1	900	1	0	0	1	1	2.995	33.321	18.43	20.031	28.339	28.895
1	400	1	1000	1	0	0	1	1	2.995	39.159	21.67	24.295	33.663	38.483

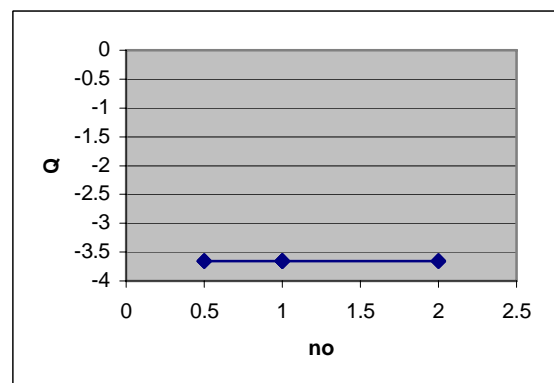
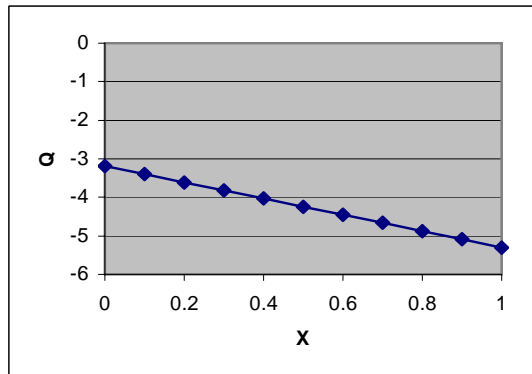
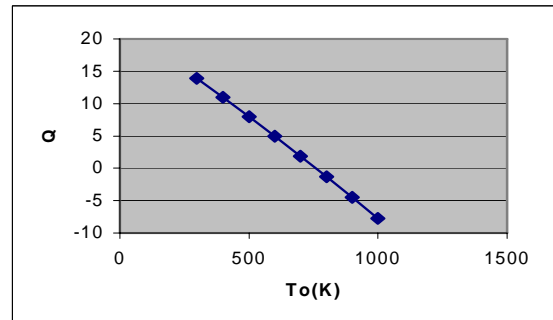
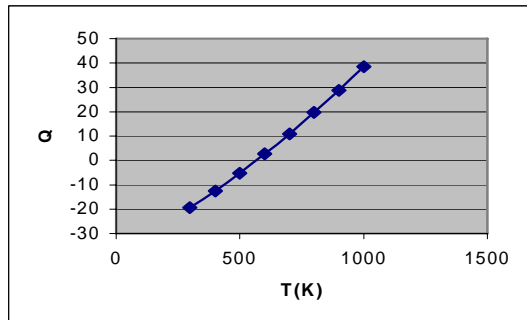
no	To	X	T	Xi	n1	n2	n3	n4	H0	H1	H2	H3	H4	Q
1	298	1	700	1	0	0	1	1	0	21.864	12.11	12.303	18.113	13.936
1	400	1	700	1	0	0	1	1	2.995	21.864	12.11	12.303	18.113	10.941
1	500	1	700	1	0	0	1	1	5.982	21.864	12.11	12.303	18.113	7.954
1	600	1	700	1	0	0	1	1	9.019	21.864	12.11	12.303	18.113	4.917
1	700	1	700	1	0	0	1	1	12.11	21.864	12.11	12.303	18.113	1.83
1	800	1	700	1	0	0	1	1	15.24	21.864	12.11	12.303	18.113	-1.308
1	900	1	700	1	0	0	1	1	18.43	21.864	12.11	12.303	18.113	-4.495
1	1000	1	700	1	0	0	1	1	21.67	21.864	12.11	12.303	18.113	-7.733

no	To	X	T	Xi	n1	n2	n3	n4	H0	H1	H2	H3	H4	Q
1	400	0	500	0	1	1	0	0	2.995	10.737	5.55	5.643	8.533	13.72
1	400	0.1	500	0.1	0.9	0.9	0.1	0.1	2.995	10.737	5.55	5.643	8.533	11.82
1	400	0.2	500	0.2	0.8	0.8	0.2	0.2	2.995	10.737	5.55	5.643	8.533	9.92
1	400	0.3	500	0.3	0.7	0.7	0.3	0.3	2.995	10.737	5.55	5.643	8.533	8.02
1	400	0.4	500	0.4	0.6	0.6	0.4	0.4	2.995	10.737	5.55	5.643	8.533	6.12
1	400	0.5	500	0.5	0.5	0.5	0.5	0.5	2.995	10.737	5.55	5.643	8.533	4.22
1	400	0.6	500	0.6	0.4	0.4	0.6	0.6	2.995	10.737	5.55	5.643	8.533	2.32
1	400	0.7	500	0.7	0.3	0.3	0.7	0.7	2.995	10.737	5.55	5.643	8.533	0.42
1	400	0.8	500	0.8	0.2	0.2	0.8	0.8	2.995	10.737	5.55	5.643	8.533	-1.48
1	400	0.9	500	0.9	0.1	0.1	0.9	0.9	2.995	10.737	5.55	5.643	8.533	-3.38
1	400	1	500	1	0	0	1	1	2.995	10.737	5.55	5.643	8.533	-5.28

no	To	X	T	Xi	n1	n2	n3	n4	H0	H1	H2	H3	H4	Q
0.5	400	0.5	400	0.5	0.5	0.0	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
0.6	400	0.5	400	0.5	0.5	0.1	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
0.8	400	0.5	400	0.5	0.5	0.3	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
1.0	400	0.5	400	0.5	0.5	0.5	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653

**9.18 (cont'd)**

1.2	400	0.5	400	0.5	0.5	0.7	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
1.4	400	0.5	400	0.5	0.5	0.9	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
1.6	400	0.5	400	0.5	0.5	1.1	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
1.8	400	0.5	400	0.5	0.5	1.3	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653
2.0	400	0.5	400	0.5	0.5	1.5	0.5	0.5	2.995	5.335	2.995	2.713	4.121	-3.653



**9.19 a.** Fermentor capacity : 550,000 gal

Solution volume :  $(0.9 \times 550,000) = 495,000$  gal

Final reaction mixture :

$$\begin{cases} 0.071 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH} / \text{lb}_m \text{ solution} \\ 0.069 \text{ lb}_m (\text{yeast, other species}) / \text{lb}_m \text{ solution} \\ 0.86 \text{ lb H}_2\text{O} / \text{lb}_m \text{ solution} \end{cases}$$

Mass of tank contents :  $\frac{495,000 \text{ gal}}{7.4805 \text{ gal}} \times \frac{1 \text{ ft}^3}{1 \text{ ft}^3} \times \frac{65.52 \text{ lb}_m}{1 \text{ ft}^3} = 4335593 \text{ lb}_m$

Mass of ethanol produced :  $\frac{4.336 \times 10^6 \text{ lb}_m \text{ solution}}{1 \text{ lb}_m \text{ solution}} \times \frac{0.071 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}}{1 \text{ lb}_m \text{ solution}} = \underline{\underline{3.078 \times 10^5 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}}}$

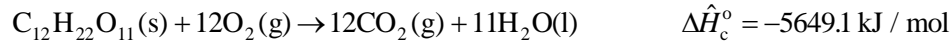
$\Rightarrow \frac{3.078 \times 10^5 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}}{46.1 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}} \times \frac{1 \text{ lb - mole C}_2\text{H}_5\text{OH}}{46.1 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}} = 6677 \text{ lb - mole C}_2\text{H}_5\text{OH}$

$\Rightarrow \frac{307827 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}}{49.67 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}} \times \frac{1 \text{ ft}^3 \text{ C}_2\text{H}_5\text{OH}}{49.67 \text{ lb}_m \text{ C}_2\text{H}_5\text{OH}} \times \frac{7.4805 \text{ gal}}{1 \text{ ft}^3} = 46,360 \text{ gal C}_2\text{H}_5\text{OH}$

9.19 (cont'd)

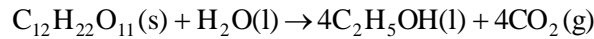
$$\text{Makeup water required : } 495,000 \text{ gal} - \frac{46,360 \text{ gal C}_2\text{H}_5\text{OH}}{2.6 \text{ gal C}_2\text{H}_5\text{OH}} \left| \frac{25 \text{ gal mash}}{2.6 \text{ gal C}_2\text{H}_5\text{OH}} \right| = 4.9 \times 10^4 \text{ gal}$$

b. 
$$\text{Acres reqd. : } \frac{46,360 \text{ gal C}_2\text{H}_5\text{OH}}{1 \text{ batch}} \left| \frac{1 \text{ bu}}{2.6 \text{ gal C}_2\text{H}_5\text{OH}} \right| \left| \frac{1 \text{ acre}}{101 \text{ bu}} \right| \left| \frac{1 \text{ batch}}{8 \text{ h}} \right| \left| \frac{24 \text{ h}}{1 \text{ day}} \right| \left| \frac{330 \text{ days}}{1 \text{ year}} \right| = 1.75 \times 10^5 \frac{\text{acres}}{\text{year}}$$



$$\Delta \hat{H}_c^\circ = 12 \Delta \hat{H}_f^\circ(\text{CO}_2) + 11 \Delta \hat{H}_f^\circ(\text{H}_2\text{O}) - \Delta \hat{H}_f^\circ(\text{C}_{12}\text{H}_{22}\text{O}_{11})$$

$$\Rightarrow \Delta \hat{H}_f^\circ(\text{C}_{12}\text{H}_{22}\text{O}_{11}) = -2217.14 \text{ kJ/mol}$$



$$\Delta \hat{H}_r^\circ = 4 \Delta \hat{H}_f^\circ(\text{C}_2\text{H}_5\text{OH}) + 4 \Delta \hat{H}_f^\circ(\text{CO}_2) - \Delta \hat{H}_f^\circ(\text{C}_{12}\text{H}_{22}\text{O}_{11}) - \Delta \hat{H}_f^\circ(\text{H}_2\text{O}) = -184.5 \text{ kJ/mol}$$

c. 
$$\Rightarrow \Delta \hat{H}_r^\circ = \frac{-181.5 \text{ kJ}}{1 \text{ mol}} \left| \frac{453.6 \text{ mol}}{1 \text{ lb-mole}} \right| \left| \frac{0.9486 \text{ Btu}}{1 \text{ kJ}} \right| = -7.811 \times 10^4 \text{ Btu/lb-mole}$$

Moles of maltose :

$$\frac{4.336 \times 10^6 \text{ lb}_m \text{ solution}}{1 \text{ lb}_m \text{ solution}} \left| \frac{0.071 \text{ lb C}_2\text{H}_5\text{OH}}{1 \text{ lb}_m \text{ solution}} \right| \left| \frac{1 \text{ lb-mole C}_2\text{H}_5\text{OH}}{46.1 \text{ lb C}_2\text{H}_5\text{OH}} \right| \left| \frac{1 \text{ lb-mole C}_{12}\text{H}_{22}\text{O}_{11}}{4 \text{ lb-mole C}_2\text{H}_5\text{OH}} \right|$$

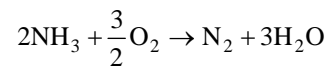
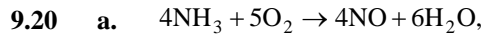
$$= 1669 \text{ lb-moles C}_{12}\text{H}_{22}\text{O}_{11} \Rightarrow \xi = n_{\text{C}_{10}\text{H}_{22}\text{O}_{11}} = 1669 \text{ lb-moles}$$

$$Q = \xi \Delta \hat{H}_r + m C_p (95^\circ \text{F} - 85^\circ \text{F})$$

$$= (1669 \text{ lb-moles}) \left( -7.811 \times 10^4 \frac{\text{Btu}}{\text{lb-mole}} \right) + (4.336 \times 10^6 \text{ lb}_m) \left( 0.95 \frac{\text{Btu}}{\text{lb}^\circ \text{F}} \right) (10^\circ \text{F})$$

d. 
$$= -8.9 \times 10^7 \text{ Btu} \quad (\text{heat transferred from reactor})$$

Brazil has a shortage of natural reserves of petroleum, unlike Venezuela.



References:  $\text{N}_2(\text{g}), \text{H}_2(\text{g}), \text{O}_2(\text{g}),$  at  $25^\circ \text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol/min)	$\hat{H}_{\text{in}}$ (kJ/mol)	$\dot{n}_{\text{out}}$ (mol/min)	$\hat{H}_{\text{out}}$ (kJ/mol)
NH <sub>3</sub>	100	$\hat{H}_1$	—	—
Air	900	$\hat{H}_2$	—	—
NO	—	—	90	$\hat{H}_3$
H <sub>2</sub> O	—	—	150	$\hat{H}_4$
N <sub>2</sub>	—	—	716	$\hat{H}_5$
O <sub>2</sub>	—	—	69	$\hat{H}_6$

$$\hat{H}_i = \Delta \hat{H}_{fi}^\circ + \int_{25}^T C_{pi} dT$$

Table B.1  
↓

$$\text{NH}_3(\text{g}, 25^\circ \text{C}): \hat{H}_1 = (\Delta \hat{H}_f^\circ)_{\text{NH}_3} = \underline{\underline{-46.19 \text{ kJ/mol}}}$$

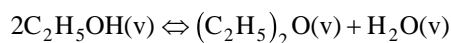
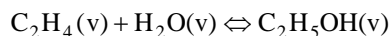
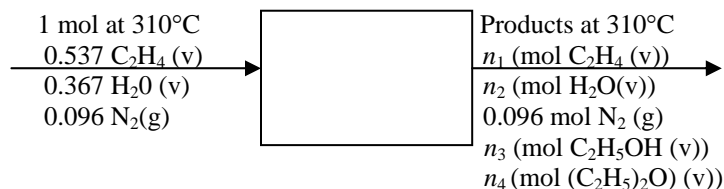
## 9.20 (cont'd)

$$\begin{aligned}
 \text{Air(g, } 150^\circ\text{C): } \hat{H}_2 &= \overset{\text{Table B.8}}{\downarrow} \underline{\underline{3.67 \text{ kJ/mol}}} \\
 \text{NO(g, } 700^\circ\text{C): } \hat{H}_3 &= 90.37 + \overset{\text{Table B.1, Table B.2}}{\downarrow} \int_{25}^{700} C_p dT = \underline{\underline{111.97 \text{ kJ/mol}}} \\
 \text{H}_2\text{O(g, } 700^\circ\text{C): } \hat{H}_4 &= \overset{\text{Table B.1, Table B.8}}{\downarrow} \underline{\underline{-216.91 \text{ kJ/mol}}} \\
 \text{N}_2\text{(g, } 700^\circ\text{C): } \hat{H}_5 &= \overset{\text{Table B.8}}{\downarrow} \underline{\underline{20.59 \text{ kJ/mol}}} \\
 \text{O}_2\text{(g, } 700^\circ\text{C): } \hat{H}_6 &= \overset{\text{Table B.8}}{\downarrow} \underline{\underline{21.86 \text{ kJ/mol}}}
 \end{aligned}$$

b.  $\dot{Q} = \Delta \dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = -4890 \text{ kJ/min} \times (1 \text{ min} / 60\text{s}) = \underline{\underline{-81.5 \text{ kW}}}$   
 (heat transferred from the reactor)

- c. If molecular species had been chosen as references for enthalpy calculations, the extents of each reaction would have to be calculated and Equation 9.5-1b used to determine  $\Delta \dot{H}$ . The value of  $\dot{Q}$  would remain unchanged.

9.21 a. Basis: 1 mol feed



5% ethylene conversion:  $(0.537)(0.05) = 0.02685 \text{ mol C}_2\text{H}_4 \text{ consumed}$   
 $\Rightarrow n_1 = (0.95)(0.537) = 0.510 \text{ mol C}_2\text{H}_4$

90% ethanol yield:

$$n_3 = \frac{0.02685 \text{ mol C}_2\text{H}_4 \text{ consumed}}{1 \text{ mol C}_2\text{H}_4} \times \frac{0.9 \text{ mol C}_2\text{H}_5\text{OH}}{1 \text{ mol C}_2\text{H}_4} = 0.02417 \text{ mol C}_2\text{H}_5\text{OH}$$

C balance:  $(2)(0.537) = (2)(0.510) + (2)(0.02417) + 4n_4 \Rightarrow n_4 = 1.415 \times 10^{-3} \text{ mol } (\text{C}_2\text{H}_5)_2\text{O}$

O balance:  $0.367 = n_2 + 0.02417 + 1.415 \times 10^{-3} \Rightarrow n_2 = 0.3414 \text{ mol H}_2\text{O}$

## 9.21 (cont'd)

References: C(s), H<sub>2</sub>(g), O<sub>2</sub>(g) at 25°C, N<sub>2</sub>(g) at 310°C

substance	$n_{in}$ (mol)	$\hat{H}_{in}$ (kJ/mol)	$n_{out}$ (mol)	$\hat{H}_{out}$ (kJ/mol)
C <sub>2</sub> H <sub>4</sub>	0.537	$\hat{H}_1$	0.510	$\hat{H}_1$
H <sub>2</sub> O	0.367	$\hat{H}_2$	0.3414	$\hat{H}_2$
N <sub>2</sub>	0.096	0	0.096	0
C <sub>2</sub> H <sub>5</sub> OH	—	—	0.02417	$\hat{H}_3$
(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	—	—	$1.415 \times 10^{-3}$	$\hat{H}_4$

$$\underline{\text{C}_2\text{H}_4(\text{g}, 310^\circ\text{C})} : \hat{H}_1 = (\Delta\hat{H}_f^\circ)_{\text{C}_2\text{H}_4} + \int_{25}^{310} C_p dT \Rightarrow (52.28 + 16.41) = 68.69 \text{ kJ/mol}$$

Table B.1 for  $\Delta\hat{H}_f^\circ$   
Table B.2 for  $C_p$

$$\underline{\text{H}_2\text{O}(\text{g}, 310^\circ\text{C})} : \hat{H}_2 = (\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{v})} + \hat{H}_{\text{H}_2\text{O}(\text{v})}(310^\circ\text{C}) \Rightarrow (-241.83 + 9.93) = -231.90 \text{ kJ/mol}$$

Table B.1  
Table B.8

**b.**  $\underline{\text{C}_2\text{H}_5\text{OH}(\text{g}, 310^\circ\text{C})} : \hat{H}_3 = (\Delta\hat{H}_f^\circ)_{\text{C}_2\text{H}_5\text{OH}(\text{g})} + \int_{25}^{310} C_p dT \Rightarrow (-235.31 + 24.16) = -211.15 \text{ kJ/mol}$

Table B.1  
Table B.2

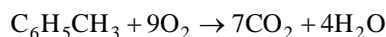
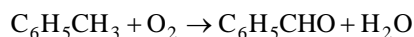
$$\underline{(\text{C}_2\text{H}_5)_2\text{O}(\text{g}, 310^\circ\text{C})} : \hat{H}_4 = (\Delta\hat{H}_f^\circ)_{(\text{C}_2\text{H}_5)_2\text{O}(\text{l})} + \Delta\hat{H}_v(25^\circ\text{C}) + \int_{25}^{310} C_p dT = (-272.8 + 26.05 + 42.52)$$

$$= -204.2 \text{ kJ/mol}$$

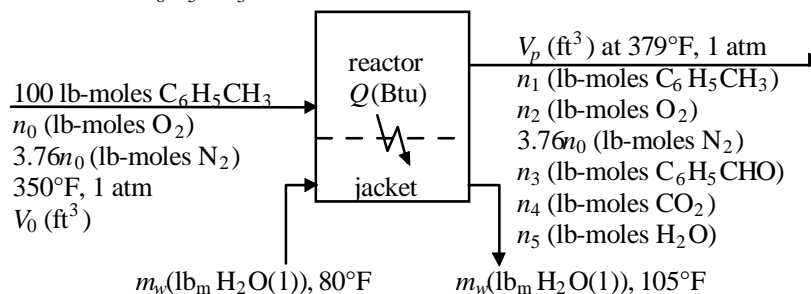
Energy balance:  $Q = \Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = -1.3 \text{ kJ} \Rightarrow \underline{\underline{1.3 \text{ kJ transferred from reactor/mol feed}}}$

To suppress the undesired side reaction. Separation of unconsumed reactants from products and recycle of ethylene.

## 9.22



Basis: 100 lb-mole of C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> fed to reactor.



Strategy:

All material and energy balances will be performed for the assumed basis of 100 lb-mole C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub>. The calculated quantities will then be scaled to the known flow rate of water in the product gas (29.3 lb<sub>m</sub>/4 h).

## 9.22 (cont'd)

<u>Plan of attack:</u>	% excess air $\Rightarrow n_0$	Ideal gas equation of state $\Rightarrow V_0$
	13% $C_6H_5CHO$ formation $\Rightarrow n_3$	Ideal gas equation of state $\Rightarrow V_p$
	0.5% $CO_2$ formation $\Rightarrow n_4$	E. B. on reactor $\Rightarrow Q$
	C balance $\Rightarrow n_1$	E. B. on jacket $\Rightarrow m_w$
	H balance $\Rightarrow n_5$	Scale $V_0, V_p, Q, m_w$ by $(\dot{n}_5)_{\text{actual}} / (n_5)_{\text{basis}}$
	O balance $\Rightarrow n_2$	

100% excess air:

$$n_0 = \frac{100 \text{ lb - moles } C_6H_5CH_3}{1 \text{ mole } C_6H_5CH_3} \left| \frac{1 \text{ mol } O_2 \text{ reqd}}{1 \text{ mole } C_6H_5CH_3} \right| \frac{(1+1) \text{ mole } O_2 \text{ fed}}{1 \text{ mol } O_2 \text{ reqd}} = 200 \text{ lb - moles } O_2$$

$$N_2 \text{ feed (\& output)} = 3.76(200) \text{ lb - moles } N_2 = 752 \text{ lb - moles } N_2$$

$$\begin{aligned} \underline{13\% \rightarrow C_6H_5CHO} \Rightarrow n_3 &= \frac{100 \text{ lb-moles } C_6H_5CH_3}{1 \text{ mole } C_6H_5CH_3 \text{ fed}} \left| \frac{0.13 \text{ mole } C_6H_5CH_3 \text{ react}}{1 \text{ mole } C_6H_5CH_3 \text{ fed}} \right| \frac{1 \text{ mole } C_6H_5CHO \text{ formed}}{1 \text{ mole } C_6H_5CH_3 \text{ react}} \\ &= 13 \text{ lb-moles } C_6H_5CHO \end{aligned}$$

$$\underline{0.5\% \rightarrow CO_2} \Rightarrow n_4 = \frac{(100)(0.005) \text{ lb - moles } C_6H_5CH_3 \text{ react}}{1 \text{ mole } C_6H_5CH_3} \left| \frac{7 \text{ moles } CO_2}{1 \text{ mole } C_6H_5CH_3} \right| = 3.5 \text{ lb - moles } CO_2$$

$$\begin{aligned} \text{C balance: } & \downarrow \text{mol C/mole } C_7H_8 \\ (100)(7) \text{ lb - moles C} &= 7n_1 + (13)(7) + (3.5)(1) \Rightarrow n_1 = 86.5 \text{ lb - moles } C_6H_5CH_3 \end{aligned}$$

$$\underline{\text{H balance:}} \quad (100)(8) \text{ lb - moles H} = (86.5)(8) + (13)(6) + 2n_5 \Rightarrow n_5 = 15.0 \text{ lb - moles } H_2O(v)$$

$$\underline{\text{O balance:}} \quad (200)(2) \text{ lb - moles O} = 2n_2 + (13)(1) + (3.5)(2) + (15)(1) \Rightarrow n_2 = 182.5 \text{ lb - moles } O_2$$

Ideal gas law – inlet:

$$V_0 = \frac{(100 + 200 + 752) \text{ lb - moles}}{1 \text{ lb - moles}} \left| \frac{359 \text{ ft}^3 (\text{STP})}{492^\circ \text{ R}} \right| \frac{(350 + 460)^\circ \text{ R}}{492^\circ \text{ R}} = 6.218 \times 10^5 \text{ ft}^3$$

Ideal gas law – outlet:

$$V_p = \frac{\left( \begin{matrix} C_7H_8 & O_2 & C_7H_8O & CO_2 & H_2O & N_2 \\ 86.5 & 182.5 & 13 & 3.5 & 15 & 752 \end{matrix} \right) \text{ lb - moles}}{1 \text{ lb - mole}} \left| \frac{359 \text{ ft}^3}{492^\circ \text{ R}} \right| \frac{(379 + 460)^\circ \text{ R}}{492^\circ \text{ R}} = 6.443 \times 10^5 \text{ ft}^3$$

## 9.22 (cont'd)

Energy balance on reactor (excluding cooling jacket)

References: C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C (77°F)

substance	$n_{in}$ (lb - moles)	$\hat{H}_{in}$ (Btu/lb - mole)	$n_{out}$ (lb - moles)	$\hat{H}_{out}$ (Btu/lb - mole)
C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	100	$\hat{H}_1$	86.5	$\hat{H}_4$
O <sub>2</sub>	200	$\hat{H}_2$	182.5	$\hat{H}_5$
N <sub>2</sub>	752	$\hat{H}_3$	752	$\hat{H}_6$
C <sub>6</sub> H <sub>5</sub> CHO	—	—	13	$\hat{H}_7$
CO <sub>2</sub>	—	—	3.5	$\hat{H}_8$
H <sub>2</sub> O	—	—	15	$\hat{H}_9$

Enthalpies:

$$C_6H_5CH_3(g, T): \hat{H}(T) = \left[ \overset{\text{Table B.1}}{\downarrow} \Delta \hat{H}_f^\circ (\text{kJ/mol}) \times \frac{430.28 \text{ Btu/lb - mole}}{1 \text{ kJ/mol}} + 31 \frac{\text{Btu}}{\text{lb - mole} \cdot ^\circ \text{F}} (T - 77)^\circ \text{F} \right]$$

$$C_6H_5CH_3(g, 350^\circ \text{F}): \hat{H}_1 = 2.998 \times 10^4 \text{ Btu/lb - mole}$$

$$C_6H_5CH_3(g, 379^\circ \text{F}): \hat{H}_4 = 3.088 \times 10^4 \text{ Btu/lb - mole}$$

$$C_6H_5CHO(g, T): \hat{H}(T) = [-17200 + 31(T - 77)^\circ \text{F}] \text{ Btu/lb - mole}$$

$$\Rightarrow \hat{H}_7 = -7.83 \times 10^3 \text{ Btu/lb - mole}$$

$$O_2(g, 350^\circ \text{F}): \hat{H}_2 = \hat{H}_{O_2}(350^\circ \text{F}) \overset{\text{Table B.9}}{\downarrow} = 1.972 \times 10^3 \text{ Btu/lb - mole}$$

$$N_2(g, 350^\circ \text{F}): \hat{H}_3 = \hat{H}_{N_2}(350^\circ \text{F}) \overset{\text{Table B.9}}{\downarrow} = 1.911 \times 10^3 \text{ Btu/lb - mole}$$

$$O_2(g, 379^\circ \text{F}): \hat{H}_5 = \hat{H}_{O_2}(379^\circ \text{F}) \overset{\text{Table B.9}}{\downarrow} = 2.186 \times 10^3 \text{ Btu/lb - mole}$$

$$N_2(g, 379^\circ \text{F}): \hat{H}_6 = \hat{H}_{N_2}(379^\circ \text{F}) \overset{\text{Table B.9}}{\downarrow} = 2.116 \times 10^3 \text{ Btu/lb - mole}$$

$$CO_2(g, 379^\circ \text{F}): \hat{H}_8 = (\Delta \hat{H}_f^\circ)_{CO_2(g)} + \hat{H}_{CO_2}(379^\circ \text{F}) \overset{\text{Table B.1 and B.9}}{\downarrow} = -1.664 \times 10^5 \text{ Btu/lb - mole}$$

$$H_2O(g, 379^\circ \text{F}): \hat{H}_9 = (\Delta \hat{H}_f^\circ)_{H_2O(g)} + \hat{H}_{H_2O}(379^\circ \text{F}) \overset{\text{Table B.1 and B.9}}{\downarrow} = -1.016 \times 10^5 \text{ Btu/lb - mole}$$

Energy Balance :

$$Q = \Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = -2.376 \times 10^6 \text{ Btu}$$

Energy balance on cooling jacket:

$$Q = \Delta H = m_w \int_{80}^{105} (C_p)_{H_2O(l)} dT$$

$$\Downarrow \quad Q = +2.376 \times 10^4 \text{ Btu}, \quad C_p = 1.0 \text{ Btu/(lb}_m \cdot ^\circ \text{F)}$$

$$2.376 \times 10^6 \text{ Btu} = m_w (\text{lb}_m) \times 1.0 \frac{\text{Btu}}{\text{lb}_m \cdot ^\circ \text{F}} \times (105 - 80)^\circ \text{F} \Rightarrow m_w = 9.504 \times 10^4 \text{ lb}_m \text{ H}_2\text{O(l)}$$

9.22(cont'd)

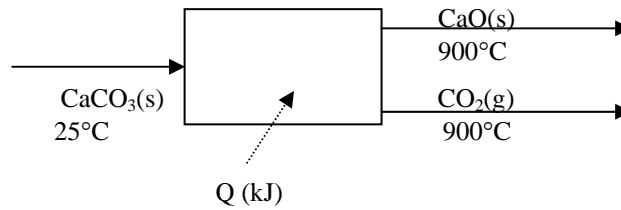
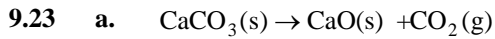
$$\text{Scale factor: } \frac{(\dot{n}_5)_{\text{actual}}}{(n_5)_{\text{basis}}} = \frac{29.3 \text{ lb}_m \text{ H}_2\text{O}}{4 \text{ h}} \left| \frac{1 \text{ b-mole H}_2\text{O}}{18.016 \text{ lb}_m \text{ H}_2\text{O}} \right| \frac{1}{15.0 \text{ lb-moles H}_2\text{O}} = 0.02711 \text{ h}^{-1}$$

a.  $V_0 = (6.218 \times 10^5 \text{ ft}^3)(0.02711 \text{ h}^{-1}) = \underline{1.69 \times 10^4 \text{ ft}^3/\text{h}} \text{ (feed)}$

$$V_p = (6.443 \times 10^5 \text{ ft}^3)(0.02711 \text{ h}^{-1}) = \underline{1.75 \times 10^4 \text{ ft}^3/\text{h}} \text{ (product)}$$

b.  $Q = (-2.376 \times 10^6 \text{ Btu})(0.02711 \text{ h}^{-1}) = \underline{-6.44 \times 10^4 \text{ Btu/h}}$

$$\dot{m}_w = (9.504 \times 10^4 \text{ Btu})(0.02711 \text{ h}^{-1}) = \frac{2577 \text{ lb}_m}{\text{h}} \left| \frac{1 \text{ ft}^3}{62.4 \text{ lb}_m} \right| \frac{7.4805 \text{ gal}}{1 \text{ ft}^3} \left| \frac{1 \text{ h}}{60 \text{ min}} \right| = \underline{5.15 \text{ gal H}_2\text{O}/\text{min}}$$



$$\text{Basis: } 1000 \text{ kg CaCO}_3 = \frac{1000 \text{ kg}}{0.100 \text{ kg}} \left| \frac{1 \text{ mol}}{0.100 \text{ kg}} \right| = 10.0 \text{ kmol CaCO}_3 \Rightarrow \begin{matrix} 10.0 \text{ kmol CaO(s) produced} \\ 10.0 \text{ kmol CO}_2(\text{g}) \text{ produced} \\ 10.0 \text{ kmol CaCO}_3(\text{s}) \text{ fed} \end{matrix}$$

References: Ca(s), C(s), O<sub>2</sub>(g) at 25°C

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
CaCO <sub>3</sub>	10 <sup>4</sup>	$\hat{H}_1$	—	—
CaO	—	—	10 <sup>4</sup>	$\hat{H}_2$
CO <sub>2</sub>	—	—	10 <sup>4</sup>	$\hat{H}_3$

$$\text{CaCO}_3(\text{s}, 25^\circ\text{C}) : \hat{H}_1 = (\Delta\hat{H}_f^\circ)_{\text{CaCO}_3(\text{s})} \xrightarrow{\text{Table B.1}} = -1206.9 \text{ kJ/mol}$$

$$\text{CaO}(\text{s}, 900^\circ\text{C}) : \hat{H}_2 = (\Delta\hat{H}_f^\circ)_{\text{CaO}(\text{s})} + \int_{298}^{1173} C_p dT \xrightarrow{\text{Table B.1, Table B.2}} = (-635.6 + 48.54) \text{ kJ/mol} = -587.06 \text{ kJ/mol}$$

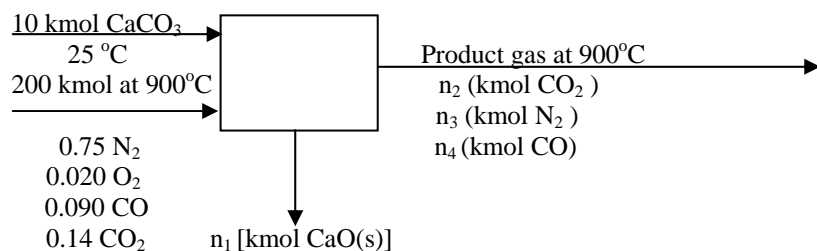
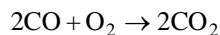
$$\text{CO}_2(\text{g}, 900^\circ\text{C}) : \hat{H}_3 = (\Delta\hat{H}_f^\circ)_{\text{CO}_2(\text{g})} + \hat{H}_{\text{CO}_2}(900^\circ\text{C}) \xrightarrow{\text{Table B.1, Table B.8}} = (-393.5 + 42.94) \text{ kJ/mol} = -350.56 \text{ kJ/mol}$$

$$\text{Energy balance: } Q = \Delta H = \left( \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i \right) = \underline{2.7 \times 10^6 \text{ kJ}}$$



### 9.23 (cont'd)

b. Basis : 1000 kg  $\text{CaCO}_3$  fed  $\Rightarrow$  10.0 kmol  $\text{CaCO}_3$



10 kmol  $\text{CaCO}_3$  react  $\Rightarrow n_1 = 10.0$  kmol  $\text{CaO}$

$$n_2 = (0.14)(200) + \frac{10.0 \text{ kmol } \text{CaCO}_3 \text{ react}}{1 \text{ kmol } \text{CO}_2} \left| \frac{1 \text{ kmol } \text{CO}_2}{1 \text{ kmol } \text{O}_2} + \frac{4 \text{ kmol } \text{O}_2 \text{ react}}{1 \text{ kmol } \text{O}_2} \right| \frac{2 \text{ kmol } \text{CO}_2}{1 \text{ kmol } \text{O}_2} = 46 \text{ kmol } \text{CO}_2$$

$$n_3 = (0.75)(200) = 150 \text{ kmol } \text{N}_2$$

C balance:  $(10.0)(1) + (200)(0.09)(1) + (200)(0.14)(1) = 46(1) + n_4(1) \Rightarrow n_4 = 10.0$  kmol  $\text{CO}$

References :  $\text{Ca}(\text{s})$ ,  $\text{C}(\text{s})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$  at  $25^\circ\text{C}$

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$\text{CaCO}_3$	10.0	$\hat{H}_1$	—	—
$\text{CaO}$	—	—	10	-587.06
$\text{CO}_2$	28	-350.56	46	-350.56
$\text{CO}$	18	$\hat{H}_2$	10	$\hat{H}_2$
$\text{O}_2$	4.0	$\hat{H}_3$	—	—
$\text{N}_2$	150	$\hat{H}_4$	150	$\hat{H}_4$

Table B.1

$$\text{CaCO}_3(\text{s}, 25^\circ\text{C}) : \hat{H}_1 = (\Delta \hat{H}_f^\circ)_{\text{CaCO}_3(\text{s})} = -1206.9 \text{ kJ/mol}$$

Table B.1,  
Table B.8

$$\text{CO}(\text{g}, 900^\circ\text{C}) : \hat{H}_1 = (\Delta \hat{H}_f^\circ)_{\text{CO}(\text{g})} + \hat{H}_{\text{CO}}(900^\circ\text{C}) = (-110.52 + 27.49) \text{ kJ/mol} = -83.03 \text{ kJ/mol}$$

Table B.8

$$\text{O}_2(\text{g}, 900^\circ\text{C}) : \hat{H}_2 = \hat{H}_{\text{O}_2}(900^\circ\text{C}) = 28.89 \text{ kJ/mol}$$

Table B.8

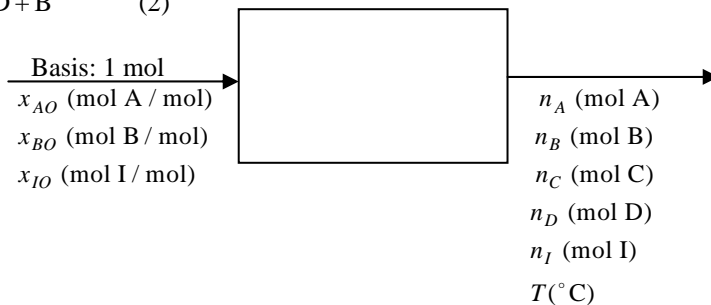
$$\text{N}_2(\text{g}, 900^\circ\text{C}) : \hat{H}_3 = \hat{H}_{\text{N}_2}(900^\circ\text{C}) = 27.19 \text{ kJ/mol}$$

$$Q = \Delta H = \left( \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i \right) = 0.44 \times 10^6 \text{ kJ}$$

$$\% \text{ reduction in heat requirement} = \left| \frac{2.7 \times 10^6 - 0.44 \times 10^6}{2.7 \times 10^6} \right| \times 100 = 83.8\%$$

c. The hot combustion gases raise the temperature of the limestone, so that less heat from the outside is needed to do so. Additional thermal energy is provided by the combustion of  $\text{CO}$ .

- 9.24 a.  $A + B \rightarrow C$  (1)  
 $2C \rightarrow D + B$  (2)



Fractional conversion:  $f_A = \frac{\text{mol A consumed}}{\text{mol A feed}} = \frac{x_{AO} - n_A}{x_{AO}} \Rightarrow n_A = x_{AO}(1 - f_A)$

C generated:  $n_0 = \frac{x_{AO}(\text{mol A fed})}{\text{mol A fed}} \left| \frac{f_A(\text{mol A consumed})}{\text{mol A fed}} \right| \left| \frac{Y_C(\text{mol C generated})}{\text{mol A consumed}} \right|$   
 $\Rightarrow n_C = x_{AO} f_A Y_C$

D generated:  $n_D = 0.5 \times \text{mol C consumed} = (1/2) \times (\text{mol A consumed} - \text{mol C out})$   
 $\Rightarrow n_D = (1/2)(x_{AO} f_A - n_C)$

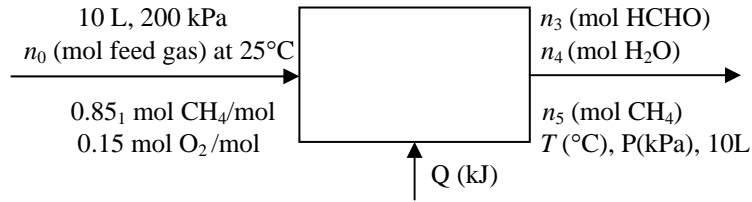
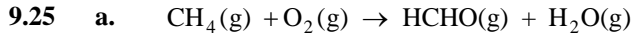
Balance on B: mol B out = mol B in – mol B consumed in (1) + mol B generated in (2)  
 $= \text{mol B in} - \text{mol A consumed in (1)} + \text{mol D generated in (2)}$   
 $\Rightarrow n_B = x_{BO} - x_{AO} f_A + n_D$

Balance on I: mol I out = mol I in  $\Rightarrow n_I = x_{IO}$

b.

Species	Formula	DHf	a	b	c	d
A	C2H4(v)	52.28	0.04075	1.15E-04	-6.89E-08	1.77E-11
B	H2O(v)	-241.83	0.03346	6.88E-06	7.60E-09	-3.59E-12
C	C2H5OH(v)	-235.31	0.06134	1.57E-04	-8.75E-08	1.98E-11
D	C4H10O(v)	-246.75	0.08945	4.03E-04	-2.24E-07	0
I	N2(g)	0	0.02900	2.20E-05	5.72E-09	-2.87E-12
Tf	Tp	xA0	xB0	xI0	fA	YC
310	310	0.537	0.367	0.096	0.05	0.90
Species	n(in) (mol)	H(in) (kJ/mol)	n(out) (mol)	H(out) (kJ/mol)		
A	0.537	68.7	0.510	68.7		
B	0.367	-231.9	0.341	-231.9		
C	0	-211.2	0.024	-211.2		
D	0	-204.2	0.001	-204.2		
I	0.096	9.4	0.096	9.4		
Q(kJ) =	-1.31					

- c. For  $T_f = 125^\circ\text{C}$ ,  $Q = \underline{7.90 \text{ kJ}}$ . Raising  $T_p$ , lowering  $f_A$ , and raising  $Y_C$  all increase  $Q$ .



$$\text{Basis: } n_0 = \frac{200 \text{ kPa}}{1 \text{ kPa}} \left| \frac{1000 \text{ Pa}}{1 \text{ kPa}} \right| \left| \frac{10 \text{ L}}{1 \text{ L}} \right| \left| \frac{10^{-3} \text{ m}^3}{1 \text{ L}} \right| \left| \frac{1 \text{ mol K}}{8.314 \text{ m}^3 \text{ Pa}} \right| \left| \frac{1}{298 \text{ K}} \right|$$

$$= 0.8072 \text{ mol feed gas mixture}$$

$$0.8072 \text{ mol feed gas mixture} \Rightarrow (0.85)(0.8072) = 0.6861 \text{ mol CH}_4,$$

$$\Rightarrow (0.15)(0.8072) = 0.1211 \text{ mol O}_2$$

$$\text{CH}_4 \text{ consumed: } \frac{1 \text{ mol CH}_4}{1 \text{ mol O}_2 \text{ fed}} \left| \frac{0.1211 \text{ mol O}_2 \text{ fed}}{1 \text{ mol O}_2 \text{ fed}} \right| = 0.1211 \text{ mol CH}_4$$

$$\Rightarrow n_5 = (0.6861 - 0.1211) \text{ mol CH}_4 = 0.5650 \text{ mol CH}_4$$

$$\text{HCHO produced: } n_3 = \frac{1 \text{ mol HCHO}}{1 \text{ mol CH}_4 \text{ consumed}} \left| \frac{0.1211 \text{ mol CH}_4 \text{ consumed}}{1 \text{ mol CH}_4 \text{ consumed}} \right| = 0.1211 \text{ mol HCHO}$$

$$\text{H}_2\text{O produced: } n_4 = \frac{1 \text{ mol H}_2\text{O}}{1 \text{ mol CH}_4 \text{ consumed}} \left| \frac{0.1211 \text{ mol CH}_4 \text{ consumed}}{1 \text{ mol CH}_4 \text{ consumed}} \right| = 0.1211 \text{ mol H}_2\text{O}$$

$$\text{Extent of reaction: } \xi = \frac{|(n_{\text{O}_2})_{\text{out}} - (n_{\text{O}_2})_{\text{in}}|}{|\nu_{\text{O}_2}|} = \frac{|0 - 0.1211|}{|1|} = 0.1211 \text{ mol}$$

References:  $\text{CH}_4(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{HCHO}(\text{g})$ ,  $\text{H}_2\text{O}(\text{g})$ , at  $25^\circ\text{C}$

Substance	$n_{\text{in}}$ mol	$\hat{U}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{U}_{\text{out}}$ kJ/mol
CH <sub>4</sub>	0.6861	0	0.5650	$\hat{U}_1$
O <sub>2</sub>	0.1211	0	—	—
HCHO	—	—	0.1211	$\hat{U}_2$
H <sub>2</sub> O	—	—	0.1211	$\hat{U}_3$

$$\hat{U}_i = \int_{25}^T (C_v)_i dT = \int_{25}^T (C_p - R)_i dT \quad i = 1, 2, 3$$

Using  $(C_p)_i$  from Table B.2 and  $R = 8.314 \times 10^{-3} \text{ kJ/mol} \cdot \text{K}$ :

$$\hat{U}_1 = (0.02599 T + 2.7345 \times 10^{-5} T^2 + 0.1220 \times 10^{-8} T^3 - 2.75 \times 10^{-12} T^4 - 0.6670) \text{ kJ/mol}$$

$$\hat{U}_2 = (0.02597 T + 2.1340 \times 10^{-5} T^2 - 2.1735 \times 10^{-12} T^4 - 0.6623) \text{ kJ/mol}$$

$$\hat{U}_3 = (0.02515 T + 0.3440 \times 10^{-5} T^2 + 0.2535 \times 10^{-8} T^3 - 0.8983 \times 10^{-12} T^4 - 0.6309) \text{ kJ/mol}$$

9.25 (cont'd)

$$Q = \frac{100 \text{ J}}{\text{s}} \left| \frac{85 \text{ s}}{1} \right| \left| \frac{1 \text{ kJ}}{1000 \text{ J}} \right| = 8.5 \text{ kJ}$$

$$\Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{\text{HCHO}} + (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}} - (\Delta \hat{H}_f^\circ)_{\text{CH}_4} \overset{\text{Table B.1}}{=} ((-115.90) + (-241.83) - (-74.85)) \text{ kJ / mol}$$

$$= -282.88 \text{ kJ / mol}$$

$$\Delta \hat{U}_r^\circ = \Delta \hat{H}_r^\circ - RT \left( \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right)$$

$$= -282.88 \text{ kJ / mol} - \frac{8.314 \text{ J}}{\text{mol K}} \left| \frac{298 \text{ K}}{1} \right| \left| \frac{(1 + 1 - 1 - 1)}{1} \right| \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| = -282.88 \text{ kJ / mol}$$

Energy Balance :

$$Q = \xi \Delta \hat{U}_r^\circ + \sum (n_i)_{\text{out}} (\hat{U}_i)_{\text{out}} - \sum (n_i)_{\text{in}} (\hat{U}_i)_{\text{in}}$$

$$= (0.1211)(-282.88 \text{ kJ / mol}) + 0.5650 \hat{U}_1 + 0.1211 \hat{U}_2 + 0.1211 \hat{U}_3$$

Substitute for  $\hat{U}_1$  through  $\hat{U}_3$  and  $Q$

$$0 = 0.02088 T + 1.845 \times 10^{-5} T^2 + 0.09963 \times 10^{-8} T^3 - 1.926 \times 10^{-12} T^4 - 43.29 \text{ kJ / mol}$$

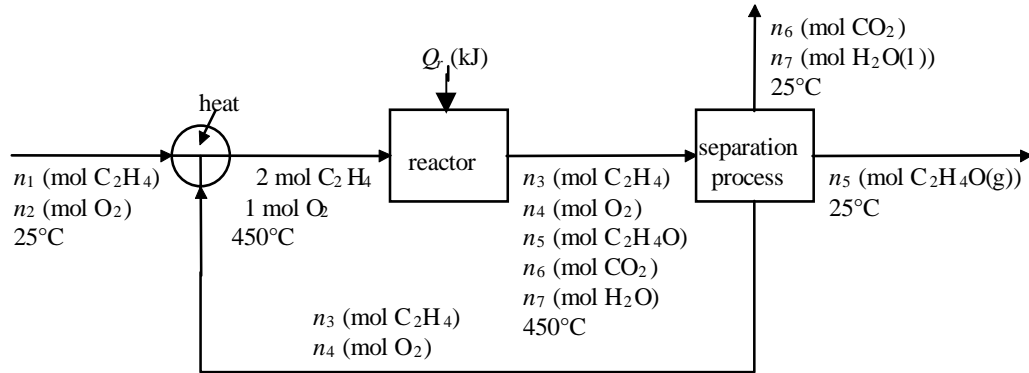
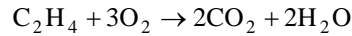
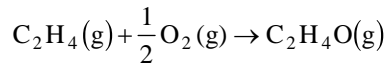
Solve for  $T$  using E - Z Solve  $\Rightarrow T = 1091^\circ \text{C} = 1364 \text{ K}$

$$\Rightarrow P = nRT / V = \frac{0.8072 \text{ mol}}{1} \left| \frac{8.314 \text{ m}^3 \cdot \text{Pa}}{\text{mol} \cdot \text{K}} \right| \left| \frac{1364 \text{ K}}{10 \text{ L}} \right| \left| \frac{1 \text{ L}}{10^{-3} \text{ m}^3} \right| = 915 \times 10^3 \text{ Pa} = \underline{\underline{915 \text{ kPa}}}$$

- b. Add heat to raise the reactants to a temperature at which the reaction rate is significant.
- c. Side reaction :  $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ .  $T$  would have been higher (more negative heat of reaction for combustion of methane), volume and total moles would be the same, therefore  $P = nRT / V$  would be greater.

9.26 a.

Basis: 2 mol C<sub>2</sub>H<sub>4</sub> fed to reactor



25% conversion  $\Rightarrow 0.500 \text{ mol C}_2\text{H}_4 \text{ consumed} \Rightarrow n_3 = \underline{\underline{1.50 \text{ mol C}_2\text{H}_4}}$

70% yield  $\Rightarrow n_5 = \frac{0.500 \text{ mol C}_2\text{H}_4 \text{ consumed}}{1 \text{ mol C}_2\text{H}_4} \times \frac{0.700 \text{ mol C}_2\text{H}_4\text{O}}{1 \text{ mol C}_2\text{H}_4} = \underline{\underline{0.350 \text{ mol C}_2\text{H}_4\text{O}}}$

C balance on reactor:  $(2)(2) = (2)(1.50) + (2)(0.350) + n_6 \Rightarrow n_6 = \underline{\underline{0.300 \text{ mol CO}_2}}$

Water formed:  $n_7 = \frac{0.300 \text{ mol CO}_2}{1 \text{ mol CO}_2} \times \frac{1 \text{ mol H}_2\text{O}}{1 \text{ mol CO}_2} = \underline{\underline{0.300 \text{ mol H}_2\text{O}}}$

O balance on reactor:  $(2)(1) = 2n_4 + 0.350 + (2)(0.300) + 0.300 \Rightarrow n_4 = \underline{\underline{0.375 \text{ mol O}_2}}$

Overall C balance:  $2n_1 = n_6 + 2n_5 = 0.300 + (2)(0.350) \Rightarrow n_1 = \underline{\underline{0.500 \text{ mol C}_2\text{H}_4}}$

Overall O balance:  $2n_2 = 2n_6 + n_7 + n_5 = (2)(0.300) + (0.300) + (0.350) \Rightarrow n_2 = \underline{\underline{0.625 \text{ mol O}_2}}$

Feed stream: 44.4% C<sub>2</sub>H<sub>4</sub>, 55.6% O<sub>2</sub>      Reactor inlet: 66.7% C<sub>2</sub>H<sub>4</sub>, 33.3% O<sub>2</sub>

Recycle stream: 80.0% C<sub>2</sub>H<sub>4</sub>, 20.0% O<sub>2</sub>

Reactor outlet: 53.1% C<sub>2</sub>H<sub>4</sub>, 13.3% O<sub>2</sub>, 12.4% C<sub>2</sub>H<sub>4</sub>O, 10.6% CO<sub>2</sub>, 10.6% H<sub>2</sub>O

Mass of ethylene oxide  $= \frac{0.350 \text{ mol C}_2\text{H}_4\text{O}}{1 \text{ mol}} \times \frac{44.05 \text{ g}}{1 \text{ mol}} \times \frac{1 \text{ kg}}{10^3 \text{ g}} = 0.0154 \text{ kg}$

b. References for enthalpy calculations: C(s), H<sub>2</sub>(g), O<sub>2</sub>(g) at 25°C

$$\hat{H}_i(T) = \Delta \hat{H}_{fi}^0 + \int_{25}^T C_p dT \text{ for C}_2\text{H}_4$$

$$= \Delta \hat{H}_f^0 + \int_{298}^{T+273} C_p dT \text{ for C}_2\text{H}_4\text{O}$$

$$= \Delta \hat{H}_{fi}^0 + \hat{H}_i(\text{table B.8}) \text{ for O}_2, \text{CO}_2, \text{H}_2\text{O}(\text{g})$$

$$= \Delta \hat{H}_f^0 \text{ for H}_2\text{O}(\text{l})$$

9.26 (cont'd)

Overall Process					Reactor				
Substance	$n_{in}$ (mol)	$\hat{H}_{in}$ (kJ/mol)	$n_{out}$ (mol)	$\hat{H}_{out}$ (kJ/mol)	substance	$n_{in}$ (mol)	$\hat{H}_{in}$ (kJ/mol)	$n_{out}$ (mol)	$\hat{H}_{out}$ (kJ/mol)
C <sub>2</sub> H <sub>4</sub>	0.500	52.28	—	—	C <sub>2</sub> H <sub>4</sub>	2	79.26	150	79.26
O <sub>2</sub>	0.625	0	—	—	O <sub>2</sub>	1	13.37	0.375	13.37
C <sub>2</sub> H <sub>4</sub> O	—	—	0.350	-51.00	C <sub>2</sub> H <sub>4</sub> O	—	—	0.350	-19.99
CO <sub>2</sub>	—	—	0.300	-393.5	CO <sub>2</sub>	—	—	0.300	-374.66
H <sub>2</sub> O(l)	—	—	0.300	-285.84	H <sub>2</sub> O(g)	—	—	0.300	-226.72

Energy balance on process:  $Q = \Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = \underline{\underline{-248 \text{ kJ}}}$

Energy balance on reactor:  $Q = \Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = \underline{\underline{-236 \text{ kJ}}}$

c. Scale to 1500 kg C<sub>2</sub>H<sub>4</sub>O/day :

C<sub>2</sub>H<sub>4</sub>O production for initial basis =  $(0.350 \text{ mol}) \left( \frac{44.05 \text{ kg}}{10^3 \text{ mol}} \right) = 0.01542 \text{ kg C}_2\text{H}_4\text{O}$

$\Rightarrow \text{Scale factor} = \frac{1500 \text{ kg/day}}{0.01542 \text{ kg}} = 9.73 \times 10^4 \text{ day}^{-1}$

In initial basis, fresh feed contains  $\left\{ \begin{array}{l} 0.500 \text{ mol C}_2\text{H}_4 \\ 0.625 \text{ mol O}_2 \end{array} \right\} \begin{array}{l} \overline{M} = (0.500)(28.05 \text{ g C}_2\text{H}_4/\text{mol}) + (0.625)(32.0 \text{ g O}_2/\text{mol}) \\ = 34.025 \times 10^{-3} \text{ kg} \end{array}$

Fresh feed rate =  $(34.025 \times 10^{-3} \text{ kg})(9.73 \times 10^4 \text{ day}^{-1}) = \underline{\underline{3310 \text{ kg/day (44.4\% C}_2\text{H}_4, 55.6\% \text{ O}_2)}}$

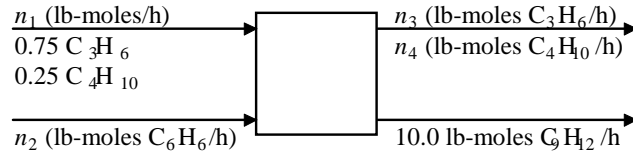
$Q_{\text{process}} = \frac{(-248 \text{ kJ})(9.73 \times 10^4 \text{ day}^{-1})}{24 \text{ hr}} \left| \frac{1 \text{ day}}{24 \text{ hr}} \right| \left| \frac{1 \text{ hr}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-279 \text{ kW}}}$

$Q_{\text{reactor}} = \frac{(-236 \text{ kJ})(9.73 \times 10^4 \text{ day}^{-1})}{24 \text{ hr}} \left| \frac{1 \text{ day}}{24 \text{ hr}} \right| \left| \frac{1 \text{ hr}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-265 \text{ kW}}}$

9.27 a.

Basis:  $\frac{1200 \text{ lb}_m \text{ C}_9\text{H}_{12}}{\text{h}} \left| \frac{1 \text{ lb - mole}}{120 \text{ lb}_m} \right. = 10.0 \text{ lb - moles cumene produced/h}$

Overall process :



Benzene balance:  $\dot{n}_2 = \frac{10.0 \text{ lb - moles C}_9\text{H}_{12} \text{ produced}}{\text{h}} \left| \frac{1 \text{ mole C}_6\text{H}_6 \text{ consumed}}{1 \text{ mole C}_9\text{H}_{12} \text{ produced}} \right.$

$$= \frac{10.0 \text{ lb - moles C}_6\text{H}_6}{\text{h}} \left| \frac{78.1 \text{ lb}_m \text{ C}_6\text{H}_6}{1 \text{ lb - mole}} \right. = \underline{\underline{781 \text{ lb}_m \text{ C}_6\text{H}_6/\text{h}}}$$

Propylene balance:  $0.75\dot{n}_1 = \dot{n}_3 + \frac{10.0 \text{ lb - moles C}_9\text{H}_{12}}{\text{h}} \left| \frac{1 \text{ mole C}_3\text{H}_6}{1 \text{ mole C}_9\text{H}_{12}} \right.$

(input=output+consumption)

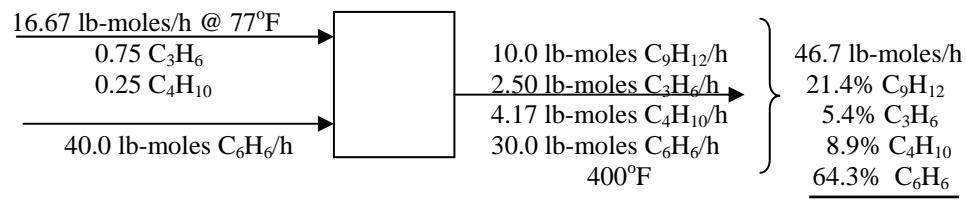
$$\Rightarrow 0.75\dot{n}_1 = \dot{n}_3 + 10 \quad \left. \begin{array}{l} \Rightarrow \dot{n}_1 = 16.67 \text{ lb - moles/h} \\ 20\% \text{ C}_3\text{H}_6 \text{ unreacted} \Rightarrow \dot{n}_3 = 0.20(0.75\dot{n}_1) \end{array} \right\} \Rightarrow \dot{n}_3 = 2.50 \text{ lb - moles C}_3\text{H}_6/\text{h}$$

Mass flow rate of C<sub>3</sub>H<sub>6</sub> / C<sub>4</sub>H<sub>10</sub> feed =  $\frac{(0.75)(16.67) \text{ lb - moles C}_3\text{H}_6}{\text{h}} \left| \frac{42.08 \text{ lb}_m \text{ C}_3\text{H}_6}{1 \text{ lb - mole}} \right.$

$$+ \frac{(0.25)(16.67) \text{ lb - moles C}_4\text{H}_{10}}{\text{h}} \left| \frac{58.12 \text{ lb}_m \text{ C}_4\text{H}_{10}}{1 \text{ lb - mole}} \right. = \underline{\underline{768 \text{ lb}_m/\text{h}}}$$

Reactor :

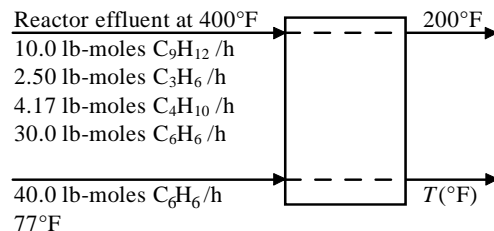
Benzene feed rate =  $\frac{10.0 \text{ lb - moles fresh feed}}{\text{h}} \left| \frac{(3+1) \text{ moles fed to reactor}}{1 \text{ mole fresh feed}} \right. = 40 \text{ lb - moles C}_6\text{H}_6/\text{h}$



Overhead from T1  $\Rightarrow \left. \begin{array}{l} 2.50 \text{ lb - moles C}_3\text{H}_6/\text{h} \\ 4.17 \text{ lb - moles C}_4\text{H}_{10}/\text{h} \end{array} \right\} \Rightarrow \frac{6.67 \text{ lb - moles/h}}{37.5\% \text{ C}_3\text{H}_6}$

$$\underline{\underline{62.5\% \text{ C}_4\text{H}_{10}}}$$

b. Heat exchanger :



**9.27 (cont'd)**

Energy balance:  $\Delta H = 0 \Rightarrow \sum n_i (\hat{H}_{i, \text{out}} - \hat{H}_{i, \text{in}}) = \sum n_i C_{pi} (T_{\text{out}} - T_{\text{in}})_i = 0$

(Assume adiabatic)

$$\left[ \frac{10 \text{ lb - moles } \text{C}_9\text{H}_{12}}{\text{h}} \mid \frac{120 \text{ lb}_m}{1 \text{ lb - mole}} \mid \frac{0.40 \text{ Btu}}{1 \text{ lb}_m \cdot ^\circ \text{F}} \right] (200^\circ \text{F} - 400^\circ \text{F}) + \overset{\text{C}_3\text{H}_6}{\downarrow} (2.50)(42.08)(0.57)(200^\circ \text{F} - 400^\circ \text{F})$$

$$+ \overset{\text{C}_4\text{H}_{10}}{\downarrow} (4.17)(58.12)(0.55)(200^\circ \text{F} - 400^\circ \text{F}) + \overset{\text{C}_6\text{H}_6 \text{ in}}{\uparrow} (30.0)(78.11)(0.45)(200^\circ \text{F} - 400^\circ \text{F})$$

$$+ \overset{\text{C}_6\text{H}_6 \text{ fed}}{\uparrow} (40.0)(78.11)(0.45)(T - 77^\circ \text{F}) = 0 \Rightarrow \underline{\underline{T = 323^\circ \text{F}}}$$

(Refer to flow chart of Part b:  $T = 323^\circ \text{F}$ )

References :  $\text{C}_3\text{H}_6(\text{l})$ ,  $\text{C}_4\text{H}_{10}(\text{l})$ ,  $\text{C}_6\text{H}_6(\text{l})$ ,  $\text{C}_9\text{H}_{12}(\text{l})$  at  $77^\circ \text{F}$

$$\hat{H}_i (\text{Btu/lb - mole}) = C_{pi} (\text{Btu/lb}_m \cdot ^\circ \text{F}) M_i (\text{lb}_m / \text{lb - mole}) (T - 77) (^\circ \text{F})$$

Substance	$\dot{n}_{\text{in}}$ (lb - mole / h)	$\hat{H}_{\text{in}}$ (Btu / lb - mole)	$\dot{n}_{\text{out}}$ (lb - mole / h)	$\hat{H}_{\text{out}}$ (Btu / lb - mole)
$\text{C}_3\text{H}_6$	12.0	0	2.50	7750
$\text{C}_4\text{H}_{10}$	4.17	0	4.17	10330
$\text{C}_6\text{H}_6$	40.0	8650	30.0	11350
$\text{C}_9\text{H}_{12}$	—	—	10.0	15530

Energy balance on reactor :

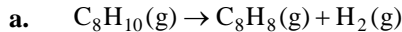
$$Q = \Delta H = \frac{\dot{n}_{\text{C}_9\text{H}_{12}} \Delta \hat{H}_r^\circ}{v_{\text{C}_9\text{H}_{12}}} + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

$$= \frac{(10.0)(-39520)}{(1)} + (2.50)(7750) + (4.17)(10330) + (30.0)(11350) + (10.0)(15530)$$

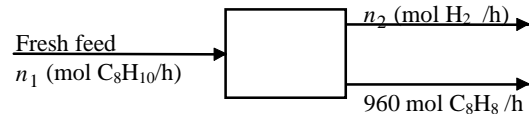
$$- (40.0)(8650) = \underline{\underline{-183000 \text{ Btu/h (heat removal)}}}$$

**9.28**

Basis :  $\frac{100 \text{ kg } \text{C}_8\text{H}_8}{\text{h}} \mid \frac{10^3 \text{ g}}{1 \text{ kg}} \mid \frac{1 \text{ mol}}{104.15 \text{ g}} = 960 \text{ mol/h styrene produced}$



Overall system



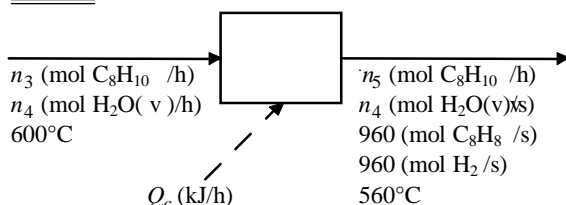
Fresh feed rate:  $\dot{n}_1 = \frac{960 \text{ mol } \text{C}_8\text{H}_8}{\text{h}} \mid \frac{1 \text{ mol } \text{C}_8\text{H}_{10}}{1 \text{ mol } \text{C}_8\text{H}_8} = \underline{\underline{960 \text{ mol } \text{C}_8\text{H}_{10}/\text{h} \text{ fresh feed}}}$

H<sub>2</sub> balance :  $\dot{n}_2 = \frac{960 \text{ mol } \text{C}_8\text{H}_{10}}{\text{h}} \mid \frac{1 \text{ mol } \text{H}_2}{1 \text{ mol } \text{C}_8\text{H}_{10}} = 960 \text{ mol } \text{H}_2/\text{h}$



## 9.28 (cont'd)

Reactor :

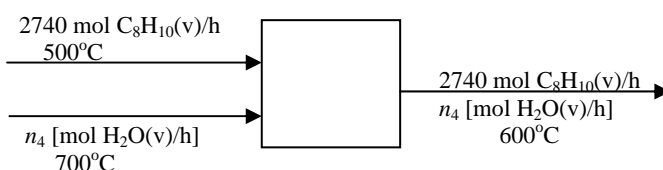


$$\underline{\text{35\% 1-pass conversion}} \Rightarrow \frac{0.35n_3(\text{mol C}_8\text{H}_{10} \text{ react})}{\text{h}} \left| \frac{1 \text{ mol C}_8\text{H}_8}{1 \text{ mol C}_8\text{H}_{10}} \right| = 960 \text{ mol C}_8\text{H}_8/\text{h}$$

$$\Rightarrow \dot{n}_3 = 2740 \text{ mol C}_8\text{H}_{10}/\text{h} \text{ fed to reactor}$$

$$\Rightarrow \underline{\underline{\text{Recycle rate} = (2740 - 960) = 1780 \text{ mol C}_8\text{H}_{10}/\text{h} \text{ recycled}}}$$

Reactor feed mixing point



Energy balance:  $\Delta H = 2740\Delta\hat{H}_{\text{C}_8\text{H}_{10}} + \dot{n}_4\Delta\hat{H}_{\text{H}_2\text{O}} = 0(\text{kJ/h})$   
(Neglect  $Q$ ,  $\Delta E_k$ )

$$\Delta\hat{H}_{\text{C}_8\text{H}_{10}} = \left[ \int_{500}^{600} \underbrace{(118 + 0.30T)}_{\hat{C}_p} dT \right] \frac{\text{J}}{\text{mol} \cdot ^\circ\text{C}} \times \frac{1 \text{ kJ}}{10^3 \text{ J}} = 28.3 \text{ kJ/mol}$$

$$\Delta\hat{H}_{\text{H}_2\text{O}} \xRightarrow[\text{P}=1 \text{ bar}]{\text{Table B.8}} = -3.9 \text{ kJ/mol}$$

$$(2740)(28.3) + \dot{n}_4(-3.9) = 0 \Rightarrow \underline{\underline{\dot{n}_4 = 1.99 \times 10^4 \text{ mol H}_2\text{O} / \text{h}}}$$

Ethylbenzene preheater (A) :

b.

$$\frac{960 \text{ mol fresh feed}}{\text{h}} + \frac{1780 \text{ mol recycled}}{\text{h}} = \frac{2740 \text{ mol EB(l)}}{\text{h}} \text{ at } 25^\circ\text{C}$$

$$\Rightarrow \frac{2740 \text{ mol EB(v)}}{\text{h}} \text{ at } 500^\circ\text{C}$$

$$\Delta\hat{H} = \int_{25}^{136} C_{pt} dT + \Delta\hat{H}_v(136^\circ\text{C}) + \int_{136}^{500} C_{pv} dT = (20.2 + 36.0 + 77.7) \text{ kJ/mol} = 133.9 \text{ kJ/mol}$$

$$\dot{Q}_A = \Delta\dot{H} = \frac{2740 \text{ mol C}_8\text{H}_{10}}{\text{h}} \left| \frac{133.9 \text{ kJ}}{\text{mol C}_8\text{H}_{10}} \right| = \underline{\underline{3.67 \times 10^5 \text{ kJ/h (preheater)}}}$$

Steam generator (F) :

$$19400 \text{ mol/h H}_2\text{O(l, } 25^\circ\text{C)} \rightarrow 19400 \text{ mol/h H}_2\text{O(v, } 700^\circ\text{C, } 1 \text{ atm)}$$

$$\text{Table B.5} \Rightarrow \hat{H}(\text{l, } 25^\circ\text{C}) = 104.8 \text{ kJ/kg ;}$$

$$\text{Table B.7} \Rightarrow \hat{H}(\text{v, } 700^\circ\text{C, } 1 \text{ atm} \approx 1 \text{ bar}) = 3928 \text{ kJ/kg}$$

9.28 (cont'd)

$$\dot{Q}_F = \Delta \dot{H} = \frac{19400 \text{ mol H}_2\text{O}}{\text{h}} \left| \frac{18.0 \text{ g}}{1 \text{ mol}} \right| \left| \frac{1 \text{ kg}}{10^3 \text{ g}} \right| \left| \frac{(3928 - 104.8) \text{ kJ}}{\text{kg}} \right|$$

$$= 1.34 \times 10^6 \text{ kJ/h (steam generator)}$$

Reactor (C) :

References:  $\text{C}_8\text{H}_8(\text{v})$ ,  $\text{C}_8\text{H}_{10}(\text{v})$ ,  $\text{H}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{v})$  at  $600^\circ\text{C}$

$$\hat{H}_i(560^\circ\text{C}) = \int_{600}^{560} (C_{pv})_i dT \text{ for } \text{C}_8\text{H}_{10}, \text{C}_8\text{H}_8$$

$\approx \hat{H}(T)$  for  $\text{H}_2, \text{H}_2\text{O}$  (interpolating from Table B.8)

Substance	$\dot{n}_{\text{in}}$ (mol/h)	$\hat{H}_{\text{in}}$ (kJ/mol)	$\dot{n}_{\text{out}}$ (mol/h)	$\hat{H}_{\text{out}}$ (kJ/mol)
$\text{C}_8\text{H}_{10}$	2740	0	1780	-11.68
$\text{H}_2\text{O}$	19900	0	19900	-1.56
$\text{C}_8\text{H}_8$	—	—	960	-10.86
$\text{H}_2$	—	—	960	-1.19

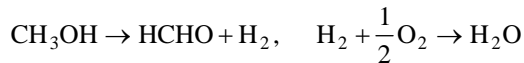
Energy balance :

$$\dot{Q}_c = \Delta \dot{H} = \frac{960 \text{ mol C}_8\text{H}_8 \text{ produced}}{\text{h}} \left| \frac{124.5 \text{ kJ}}{1 \text{ mol C}_8\text{H}_8} \right| + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

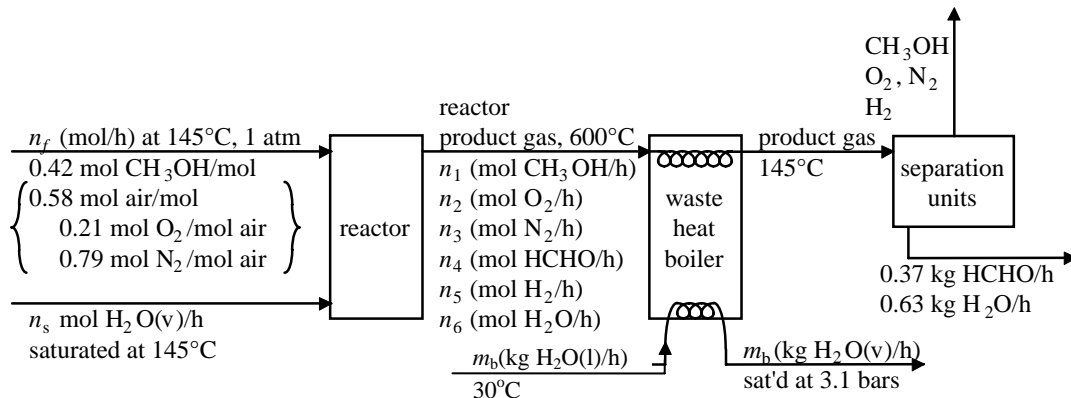
$$= 5.61 \times 10^4 \text{ kJ/h (reactor)}$$

- c. This is a poorly designed process as shown. The reactor effluents are cooled to  $25^\circ\text{C}$ , and then all but the hydrogen are reheated after separation. Probably less cooling is needed, and in any case provisions for heat exchange should be included in the design.

9.29



a.



b.

In the absence of data to the contrary, we assume that the separation of methanol from formaldehyde is complete.

Methanol vaporizer:

The product stream, which contains 42 mole %  $\text{CH}_3\text{OH}(\text{v})$ , is saturated at  $T_m(^{\circ}\text{C})$  and 1 atm.

**9.29 (cont'd)**

$$y_m P = p_m^*(T_m) \Rightarrow (0.42)(760 \text{ mmHg}) = 319.2 \text{ mmHg} = p_m^*(T_m)$$

$$\xrightarrow{\text{Antoine equation}} p_m^* = 319.2 \text{ mmHg} \Rightarrow T_m = \underline{\underline{44.1^\circ \text{C}}}$$

**c. Moles HCHO formed :**

$$= \frac{36 \times 10^6 \text{ kg solution}}{350 \text{ days}} \left| \frac{0.37 \text{ kg HCHO}}{1 \text{ kg solution}} \right| \left| \frac{1 \text{ kmol}}{30.03 \text{ kg HCHO}} \right| \left| \frac{1 \text{ day}}{24 \text{ h}} \right| = 52.80 \frac{\text{kmol HCHO}}{\text{h}}$$

but if all the HCHO is recovered, then this equals  $\dot{n}_4$ , or  $\dot{n}_4 = 52.80 \text{ kmol HCHO/h}$

70% conversion :

$$\frac{52.80 \text{ kmol HCHO}}{\text{h}} \left| \frac{1 \text{ kmol CH}_3\text{OH react}}{1 \text{ kmol HCHO formed}} \right| \left| \frac{1 \text{ kmol CH}_3\text{OH fed}}{0.70 \text{ kmol CH}_3\text{OH react}} \right| \left| \frac{1 \text{ kmol feed gas}}{0.42 \text{ kmol CH}_3\text{OH}} \right| = \dot{n}_f$$

$$\Rightarrow \dot{n}_f = 179.59 \text{ kmol/h}$$

Methanol unreacted:

$$\dot{n}_1 = \frac{(0.42)(179.59) \text{ kmol CH}_3\text{OH fed}}{\text{h}} \left| \frac{(1-0.70) \text{ kmol CH}_3\text{OH fed}}{1 \text{ kmol CH}_3\text{OH fed}} \right| = 22.63 \frac{\text{kmol CH}_3\text{OH}}{\text{h}}$$

$$\underline{\text{N}_2 \text{ balance:}} \quad \dot{n}_3 = (179.6 \text{ kmol/h})(0.58)(0.79) = 82.29 \text{ kmol N}_2/\text{h}$$

Four reactor stream variables remain unknown —  $\dot{n}_s$ ,  $\dot{n}_2$ ,  $\dot{n}_5$ , and  $\dot{n}_6$  — and four relations are available — H and O balances, the given  $\text{H}_2$  content of the product gas (5%), and the energy balance. The solution is tedious but straightforward.

$$\underline{\text{H balance:}} \quad (179.6)(0.42)(4) + 2\dot{n}_s = (22.63)(4) + (52.8)(2) + 2\dot{n}_5 + 2\dot{n}_6$$

$$\Rightarrow \dot{n}_s = \dot{n}_5 + \dot{n}_6 - 52.80 \quad (1)$$

$$\underline{\text{O balance:}} \quad (179.6)(0.42)(1) + (179.6)(0.58)(0.21)(2) + \dot{n}_s = (22.63)(1) + 2\dot{n}_2 + (52.80)(1) + \dot{n}_6$$

$$\Rightarrow \dot{n}_s = 2\dot{n}_2 + \dot{n}_6 - 43.75 \quad (2)$$

$$\underline{\text{H}_2 \text{ content:}} \quad \frac{\dot{n}_5}{22.63 + \dot{n}_2 + 82.29 + 52.89 + \dot{n}_5 + \dot{n}_6} = 0.05 \Rightarrow 19\dot{n}_5 - \dot{n}_2 - \dot{n}_6 = 157.72 \quad (3)$$

References : C(s),  $\text{H}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$  at  $25^\circ \text{C}$

$$H = \Delta \hat{H}_f^\circ + \int_{25}^T \overset{\text{Table B.2}}{\downarrow} C_p dT$$

or Table B.8 for  $\text{O}_2$ ,  $\text{N}_2$  and  $\text{H}_2$

9.29 (cont'd)

substance	$\dot{n}_{in}$ kmol / h	$\hat{H}_{in}$ kJ / kmol	$\dot{n}_{out}$ kmol / h	$\hat{H}_{out}$ kJ / kmol
CH <sub>3</sub> OH	75.43	-195220	22.63	-163200
O <sub>2</sub>	21.88	3620	$n_2$	18410
N <sub>2</sub>	82.29	3510	82.29	17390
H <sub>2</sub> O	$n_s$	-237740	$n_6$	-220920
HCHO	—	—	52.80	-88800
H <sub>2</sub>	—	—	$n_5$	16810

Energy Balance :

$$\Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = 0 \Rightarrow 18410n_2 + 16810n_5 - 220920n_6 + 237704n_s = -7.406 \times 10^6 \quad (4)$$

We now have four equations in four unknowns. Solve using E-Z Solve.

$$\dot{n}_s = \frac{58.8 \text{ kmol H}_2\text{O(v)}}{\text{h}} \left| \frac{18.02 \text{ kg}}{1 \text{ kmol}} \right| = \underline{\underline{1060 \text{ kg steam fed/h}}}$$

$$\dot{n}_2 = 2.26 \text{ kmol O}_2/\text{h}, \dot{n}_5 = 13.58 \text{ kmol H}_2/\text{h}, \dot{n}_6 = 98.00 \text{ kmol H}_2\text{O/h}$$

Summarizing, the product gas component flow rates are 22.63 kmol CH<sub>3</sub>OH/h, 2.26 kmol O<sub>2</sub>/h, 82.29 kmol N<sub>2</sub>/h, 52.80 kmol HCHO/h, 13.58 kmol H<sub>2</sub>/h, and 98.02 kmol H<sub>2</sub>O/h

$$\Rightarrow \underline{\underline{\frac{272 \text{ kmol/h product gas}}{8\% \text{ CH}_3\text{OH}, 0.8\% \text{ O}_2, 30\% \text{ N}_2, 19\% \text{ HCHO}, 5\% \text{ H}_2, 37\% \text{ H}_2\text{O}}}}$$

d.

Energy balance on waste heat boiler. Since we have already calculated specific enthalpies of all components of the product gas at the boiler inlet (at 600°C), and for all but two of them at the boiler outlet (at 145°C), we will use the same reference states for the boiler calculation

Reference States: C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C for reactor gas

H<sub>2</sub>O(l) at triple point for boiler water

Substance	$\dot{n}_{in}$ kmol/h	$\hat{H}_{in}$ kJ/kmol	$\dot{n}_{out}$ mol	$\hat{H}_{out}$ kJ/mol
CH <sub>3</sub> OH	22.63	-163200	22.63	-195220
O <sub>2</sub>	2.26	18410	2.26	3620
N <sub>2</sub>	82.29	17390	82.29	3510
H <sub>2</sub> O	98.02	-220920	98.02	-237730
HCHO	52.80	-88800	52.80	-111350
H <sub>2</sub>	13.58	16810	13.58	3550
H <sub>2</sub> O	$m_b$ (kg/h)	125.7 (kJ/kg)	$m_b$ (kg/h)	2726.1 (kJ/kg)

**9.29 (cont'd)**

Energy Balance :

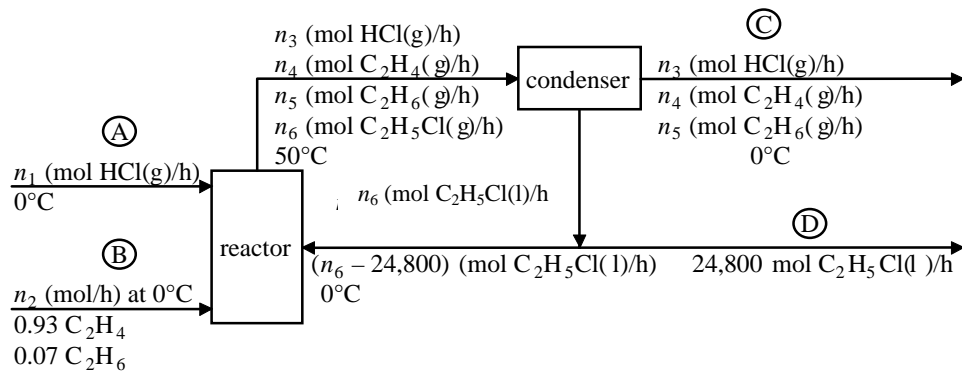
$$\Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = 0$$

$$\Rightarrow m_b (2726.1 - 125.7) - 4.92 \times 10^6 = 0$$

$$\Rightarrow m_b = 1892 \text{ kg steam/h}$$

**9.30 a.  $\text{C}_2\text{H}_4 + \text{HCl} \rightarrow \text{C}_2\text{H}_5\text{Cl}$**

Basis:  $\frac{1600 \text{ kg C}_2\text{H}_5\text{Cl(l)}}{\text{h}} \left| \frac{10^3 \text{ g}}{1 \text{ kg}} \right| \frac{1 \text{ mol}}{64.52 \text{ g}} = 24800 \text{ mol/h C}_2\text{H}_5\text{Cl}$



Product composition data:

$$n_3 = 0.015n_1 \quad (1)$$

$$n_4 = 0.015(0.93n_2) = 0.01395n_2 \quad (2)$$

$$n_5 = 0.07n_2 \quad (3)$$

Overall Cl balance :

$$\frac{n_1 (\text{mol HCl/h})}{1 \text{ mol HCl}} \left| \frac{1 \text{ mol Cl}}{1 \text{ mol HCl}} \right| = (n_3)(1) + (24800)(1) \quad (4)$$

Solve (4) simultaneously with (1)  $\Rightarrow n_1 = 25180 \text{ mol/h} = \underline{\underline{25.18 \text{ kmol HCl fed / h}}}$

$$n_3 = 378 \text{ mol HCl(g)/h}$$

Overall C balance :

$$n_2 (0.93)(2) + n_2 (0.07)(2) = 2n_4 + 2n_5 + (2)(24800)$$

From Eqs. (2) and (3)  $\Rightarrow 2n_2 [0.93 + 0.07 - 0.0139 - 0.07] = (2)(24800)$

$$n_2 = 27070 \text{ mol fed/h} = \underline{\underline{27.07 \text{ kmol/h of Feed B}}}$$

**b.**  $\left. \begin{array}{l} n_3 = 378 \text{ mol HCl/h} \\ n_4 = 0.01395(27070) = 378 \text{ mol C}_2\text{H}_4/\text{h} \\ n_5 = 0.07(27070) = 1895 \text{ mol C}_2\text{H}_6/\text{h} \end{array} \right\} \underline{\underline{\begin{array}{l} 2.65 \text{ kmol / h of Product C} \\ 14.3\% \text{ HCl, } 14.3\% \text{ C}_2\text{H}_4, 71.4\% \text{ C}_2\text{H}_6 \end{array}}}$

**9.30 (cont'd)**

c.

References:  $C_2H_4(g)$ ,  $C_2H_6(g)$ ,  $C_2H_5Cl(g)$ ,  $HCl(g)$  at  $0^\circ C$

$$C_2H_4(g, 50^\circ C): \hat{H} = \int_0^{50} C_p dT \xRightarrow{\text{Table B.2}} 2.181 \text{ kJ/mol}$$

$$C_2H_6(g, 50^\circ C): \hat{H} = \int_0^{50} C_p dT \xRightarrow{\text{Table B.2}} 2.512 \text{ kJ/mol}$$

$$HCl(g, 50^\circ C): \hat{H} = \int_0^{50} C_p dT \xRightarrow{\text{Table B.2}} 1.456 \text{ kJ/mol}$$

$$C_2H_5Cl(l, 0^\circ C): \hat{H} = -\Delta \hat{H}_v(0^\circ C) = -24.7 \text{ kJ/mol}$$

$$C_2H_5Cl(g, 50^\circ C): \hat{H} = \int_0^{50} C_{pv} dT = 2.709 \text{ kJ/mol}$$

substance	$n_{in}$ mol	$\hat{H}_{in}$ kJ / mol	$n_{out}$ mol	$\hat{H}_{out}$ kJ / mol
HCl	25180	0	378	1.456
$C_2H_4$	25175	0	378	2.181
$C_2H_6$	1895	0	1895	2.512
$C_2H_5Cl$	$n_6 - 24800$	-24.7	$n_6$	2.709

Energy balance:

$$\Delta H = 0 \Rightarrow \frac{n_A \Delta \hat{H}_r(0^\circ C)}{\nu_A} + \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = 0$$

$$\Rightarrow \frac{(25180 - 378) \text{ mol HCl react}}{h} \left| \frac{-64.5 \text{ kJ}}{1 \text{ mol HCl}} \right| + (378)(1.456) + (378)(2.181) + (1895)(2.512)$$

$$+ 2.709n_6 - (n_6 - 24800)(-24.7) = 0 \Rightarrow n_6 = 80490 \text{ mol } C_2H_5Cl/h \text{ in reactor effluent}$$

$$\begin{aligned} \underline{C_2H_5Cl \text{ recycled}} &= \frac{80490 \text{ mol condensed}}{h} - \frac{24800 \text{ mol product}}{h} = 55690 \frac{\text{mol}}{h} \\ &= 55.7 \frac{\text{kmol recycled}}{h} \end{aligned}$$

d.

$C_p$  is a linear function of temperature.

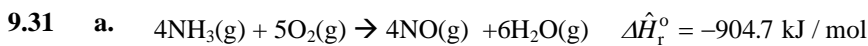
$\Delta \hat{H}_v$  is independent of temperature.

100% condensation of ethylbenzene in the heat exchanger is assumed.

Heat of mixing and influence of pressure on enthalpy is neglected.

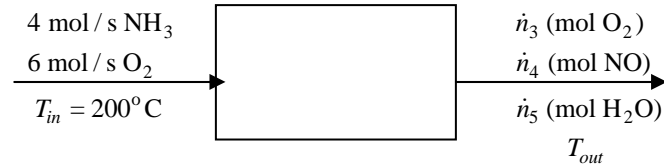
Reactor is adiabatic.

No  $C_2H_4$  or  $C_2H_6$  is absorbed in the ethyl chloride product.



Basis: 10 mol/s Feed gas

9.31 (cont'd)



$$\text{O}_2 \text{ consumed} : \frac{5 \text{ mol O}_2}{4 \text{ mol NH}_3} \left| \frac{4 \text{ mol NH}_3 \text{ fed}}{\text{s}} \right. = 5 \text{ mol/s} \Rightarrow \dot{n}_3 = (6 - 1) \text{ mol O}_2 / \text{s} = \underline{\underline{1 \text{ mol O}_2 / \text{s}}}$$

$$\text{NO produced} : \dot{n}_4 = \frac{4 \text{ mol NO produced}}{4 \text{ mol NH}_3} \left| \frac{4 \text{ mol NH}_3 \text{ fed}}{\text{s}} \right. = \underline{\underline{4 \text{ mol NO/s}}}$$

$$\text{H}_2\text{O produced} : \dot{n}_5 = \frac{6 \text{ mol H}_2\text{O produced}}{4 \text{ mol NH}_3} \left| \frac{4 \text{ mol NH}_3 \text{ fed}}{\text{s}} \right. = \underline{\underline{6 \text{ mol H}_2\text{O/s}}}$$

$$\text{Extent of reaction} : \dot{\xi} = \frac{(\dot{n}_{\text{NH}_3})_{\text{out}} - (\dot{n}_{\text{NH}_3})_{\text{in}}}{|\nu_{\text{NH}_3}|} = \frac{|0 - 4|}{|4|} = \underline{\underline{1 \text{ mol/s}}}$$

- b. Well-insulated reactor, so no heat loss  
 No absorption of heat by container wall  
 Neglect kinetic and potential energy changes;  
 No shaft work  
 No side reactions.

- c. References : NH<sub>3</sub>(g), O<sub>2</sub>(g), NO(g), H<sub>2</sub>O(g) at 25°C, 1atm

Substance	$\dot{n}_{\text{in}}$ (mol / s)	$\hat{H}_{\text{in}}$ (kJ / mol)	$\dot{n}_{\text{out}}$ (mol / s)	$\hat{H}_{\text{out}}$ (kJ / mol)
NH <sub>3</sub> (g)	4.00	$\hat{H}_1$	—	—
O <sub>2</sub> (g)	6.00	$\hat{H}_2$	1.00	$\hat{H}_3$
NO(g)	—	—	4.00	$\hat{H}_4$
H <sub>2</sub> O(g)	—	—	6.00	$\hat{H}_5$

$$\hat{H}_1 = \int_{25}^{200} (C_p)_{\text{NH}_3} dT \stackrel{\text{Table B.2}}{=} 6.74 \text{ kJ / mol}, \quad \hat{H}_2 = \hat{H}_{\text{O}_2}(200^\circ\text{C}) \stackrel{\text{Table B.8}}{=} 5.31 \text{ kJ / mol}$$

Using  $(C_p)_i$  from Table B.2 :

$$\hat{H}_3 = (0.0291 T_{\text{out}} + 0.5790 \times 10^{-5} T_{\text{out}}^2 - 0.2025 \times 10^{-8} T_{\text{out}}^3 + 0.3278 \times 10^{-12} T_{\text{out}}^4 - 0.7311) \text{ kJ/mol}$$

$$\hat{H}_4 = (0.0295 T_{\text{out}} + 0.4094 \times 10^{-5} T_{\text{out}}^2 - 0.0975 \times 10^{-8} T_{\text{out}}^3 + 0.0913 \times 10^{-12} T_{\text{out}}^4 - 0.7400) \text{ kJ/mol}$$

$$\hat{H}_5 = (0.03346 T_{\text{out}} + 0.3440 \times 10^{-5} T_{\text{out}}^2 + 0.2535 \times 10^{-8} T_{\text{out}}^3 - 0.8983 \times 10^{-12} T_{\text{out}}^4 - 0.8387) \text{ kJ/mol}$$

Energy Balance:  $\Delta \dot{H} = 0$

$$\Delta \dot{H} = \dot{\xi} \Delta \hat{H}_r^\circ + \sum_{i=3}^5 (n_i)_{\text{out}} (\hat{H}_i)_{\text{out}} - \sum_{i=1}^2 (n_i)_{\text{in}} (\hat{H}_i)_{\text{in}}$$

9-31 (cont'd)

$$\Rightarrow \Delta \dot{H} = \dot{\xi} \Delta \hat{H}_r^\circ + (1.00) \hat{H}_3 + (4.00) \hat{H}_4 + (6.00) \hat{H}_5 - (4.00) \hat{H}_1 - (6.00) \hat{H}_2$$

↓ Substitute for  $\dot{\xi}$ ,  $\Delta \hat{H}_r^\circ$ , and  $\hat{H}_1$  through  $\hat{H}_6$

$$\Delta \dot{H} = (0.3479 T_{\text{out}} + 4.28 \times 10^{-5} T_{\text{out}}^2 + 0.9285 \times 10^{-8} T_{\text{out}}^3 - 4.697 \times 10^{-12} T_{\text{out}}^4) - 972.24 \text{ kJ/mol} = 0$$

$$\text{E-Z Solve} \Rightarrow \underline{\underline{T_{\text{out}} = 2223^\circ\text{C}}}$$

- d. If only the first term from Table B.2 is used,  $\hat{H}_i = \int_{25}^T (C_{pi}) dT = C_{pi} (T - 25)$

$$\hat{H}_1 = 0.03515(200 - 25) = 6.15 \text{ kJ/mol}, \hat{H}_2 = 5.31 \text{ kJ/mol}, \hat{H}_3 = 0.0291(T_{\text{out}} - 25),$$

$$\hat{H}_4 = 0.0295(T_{\text{out}} - 25), \hat{H}_5 = 0.03346(T_{\text{out}} - 25)$$

$$\text{E.B. } \Delta \dot{H} = \dot{\xi} \Delta \hat{H}_r^\circ + (1.00) \hat{H}_3 + (4.00) \hat{H}_4 + (6.00) \hat{H}_5 - (4.00) \hat{H}_1 - (6.00) \hat{H}_2 = 0$$

↓ Substitute for  $\dot{\xi}$  ( $= 1 \text{ mol/s}$ ),  $\Delta \hat{H}_r^\circ$  ( $= -904.7 \text{ kJ/mol}$ ) and  $\hat{H}_1$  through  $\hat{H}_6$

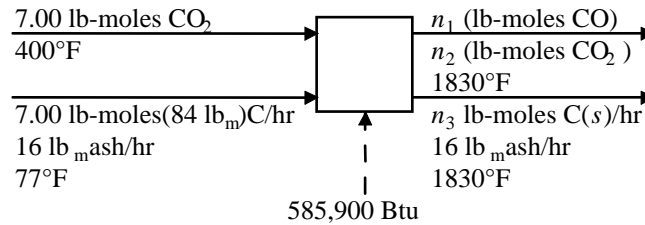
$$0 = 0.3479 T_{\text{out}} - 969.86 \Rightarrow \underline{\underline{T_{\text{out}} = 2788^\circ\text{C}}} \Rightarrow \% \text{ error} = \frac{2788^\circ\text{C} - 2223^\circ\text{C}}{2223^\circ\text{C}} \times 100 = \underline{\underline{25\%}}$$

- e. If the higher temperature were used as the basis, the reactor design would be safer (but more expensive).

9.32

Basis : 100 lb<sub>m</sub> coke fed

$$\Rightarrow 84 \text{ lb}_m \text{ C} \Rightarrow 7.00 \text{ lb-moles C fed} \Rightarrow 7.00 \text{ lb-moles CO}_2 \text{ fed}$$



- a.  $\text{C(s)} + \text{CO}_2(\text{g}) \rightarrow 2\text{CO(g)}$ ,

$$\Delta \hat{H}_r^\circ \left( 77^\circ\text{F} \right) = \left( \Delta \hat{H}_c^\circ \right)_{\text{CO}_2(\text{g})} - 2 \left( \Delta \hat{H}_c^\circ \right)_{\text{CO(g)}}$$

$$= \frac{[-393.50 - (2)(-282.99)] \text{ kJ}}{\text{mol}} \left| \frac{0.9486 \text{ Btu}}{1 \text{ kJ}} \right| \frac{453.6 \text{ mols}}{1 \text{ lb-mole}} = 74,210 \text{ Btu/lb-mole}$$

Let  $x$  = fractional conversion of C and CO<sub>2</sub> :

↓

$$n_1 = \frac{7.00x(\text{lb-moles C reacted})}{1 \text{ lb-mole C reacted}} \left| \frac{2 \text{ lb-moles CO formed}}{1 \text{ lb-mole C reacted}} \right| = 14.0x \text{ lb-moles CO}$$

$$n_2 = 7.00(1 - x) \text{ lb-moles CO}_2$$

$$n_3 = 7.00(1 - x) \text{ lb-moles C(s)}$$

References for enthalpy calculations: C(s), CO<sub>2</sub>(g), CO(g), ash at 77°F



**9.32 (cont'd)**

$$\text{CO}_2(\text{g}, 400^\circ\text{F}): \hat{H} = \hat{H}_{\text{CO}_2}(400^\circ\text{F}) \xRightarrow{\text{Table B.9}} 3130 \text{ Btu/lb - mole}$$

$$\text{CO}_2(\text{g}, 1830^\circ\text{F}): \hat{H} = \hat{H}_{\text{CO}_2}(1830^\circ\text{F}) \xRightarrow{\text{Table B.9}} 20,880 \text{ Btu/lb - mole}$$

$$\text{CO}(\text{g}, 1830^\circ\text{F}): \hat{H} = \hat{H}_{\text{CO}}(1830^\circ\text{F}) \xRightarrow{\text{Table B.9}} 13,280 \text{ Btu/lb - mole}$$

$$\text{Solid (1830}^\circ\text{F): } \hat{H} = \frac{0.24 \text{ Btu}}{\text{lb}_m \cdot ^\circ\text{F}} \bigg| \frac{(1830 - 77)^\circ\text{F}}{1} = 420 \text{ Btu/lb}_m$$

Mass of solids (emerging)

$$= \frac{7.00(1-x) \text{ lb - moles C}}{1 \text{ lb - mole}} \bigg| \frac{12.0 \text{ lb}_m}{1 \text{ lb - mole}} + 16 \text{ lb}_m = (100 - 84x) \text{ lb}_m$$

substance	$n_{\text{in}}$ (lb - moles)	$\hat{H}_{\text{in}}$ (Btu/lb - mole)	$n_{\text{out}}$ (lb - moles)	$\hat{H}_{\text{out}}$ (Btu/lb - mole)
CO <sub>2</sub>	7.00	3130	$7.00(1-x)$	20,890
CO	—	—	$14.0x$	13,280
	(lb <sub>m</sub> )	(Btu/lb <sub>m</sub> )	(lb <sub>m</sub> )	(Btu/lb <sub>m</sub> )
solid	100	0	$100 - 84x$	420

Extent of reaction:  $n_{\text{CO}} = (n_{\text{CO}})_o + \nu_{\text{CO}}\xi \Rightarrow 14.0x = 2\xi \Rightarrow \xi(\text{lb - moles}) = 7.0x$

Energy balance:

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

$$585,900 \text{ Btu} = \frac{7.0x \text{ (lb - moles)}}{1 \text{ lb - mole}} \bigg| \frac{74,210 \text{ Btu}}{1 \text{ lb - mole}} + 7.00(1-x)(20,880)$$

$$+ (14.0x)(13,280) + (100 - 84x)(420) - (7.00)(3130)$$

$$\Downarrow$$

$$x = 0.801 \Rightarrow \underline{\underline{80.1\% \text{ conversion}}}$$

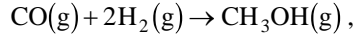
**b.**

Advantages of CO. Gases are easier to store and transport than solids, and the product of the combustion is CO<sub>2</sub>, which is a much lower environmental hazard than are the products of coke combustion.

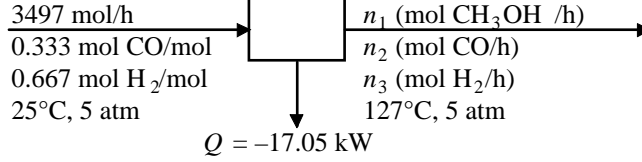
Disadvantages of CO. It is highly toxic and dangerous if it leaks or is not completely burned, and it has a lower heating value than coke. Also, it costs something to produce it from coke.

9.33

$$\text{Basis : } \frac{17.1 \text{ m}^3}{\text{h}} \left| \frac{10^3 \text{ L}}{1 \text{ m}^3} \right| \frac{273 \text{ K}}{298 \text{ K}} \left| \frac{5.00 \text{ atm}}{1.00 \text{ atm}} \right| \frac{1 \text{ mol}}{22.4 \text{ L(STP)}} = 3497 \text{ mol/h feed}$$



$$\Delta \hat{H}_r^o = (\Delta \hat{H}_f^o)_{\text{CH}_3\text{OH(g)}} - (\Delta \hat{H}_f^o)_{\text{CO(g)}} = -90.68 \text{ kJ/mol}$$



Let  $f$  = fractional conversion of CO (which also equals the fractional conversion of  $\text{H}_2$ , since CO and  $\text{H}_2$  are fed in stoichiometric proportion).

$$\text{CO reacted : } = \frac{(3497)(0.333) \text{ mol CO feed}}{\text{mol feed}} \left| \frac{f (\text{mol react})}{1} \right| = 1166f (\text{mol CO react})$$

$$\text{CH}_3\text{OH produced : } \dot{n}_1 = \frac{1166f \text{ mol CO react}}{\text{mol CO}} \left| \frac{1 \text{ mol CH}_3\text{OH}}{1 \text{ mol CO}} \right| = 1166f \text{ mol CH}_3\text{OH/h}$$

$$\text{CO remaining : } \dot{n}_2 = 1166(1-f) \text{ mol CO/h}$$

$$\begin{aligned} \text{H}_2 \text{ remaining : } \dot{n}_3 &= (3497)(0.667) \text{ mol H}_2 \text{ fed} - \frac{1166f \text{ mol CO react}}{\text{mol CO}} \left| \frac{2 \text{ mol H}_2 \text{ react}}{1 \text{ mol CO react}} \right| \\ &= 2332(1-f) \text{ mol H}_2/\text{h} \end{aligned}$$

Reference states :  $\text{CO(g)}$ ,  $\text{H}_2\text{(g)}$ ,  $\text{CH}_3\text{OH(g)}$  at  $25^\circ\text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol/h)	$\hat{H}_{\text{in}}$ (kJ/mol)	$\dot{n}_{\text{out}}$ (mol/h)	$\hat{H}_{\text{out}}$ (kJ/mol)
CO	1166	0	$1166(1-f)$	$\hat{H}_1$
H <sub>2</sub>	2332	0	$2332(1-f)$	$\hat{H}_2$
CH <sub>3</sub> OH	—	—	$1166f$	$\hat{H}_3$

$$\text{CO(g, } 127^\circ\text{C)}: \hat{H}_1 = \hat{H}_{\text{CO}}(127^\circ\text{C}) \xrightarrow{\text{Table B.8}} 2.99 \text{ kJ/mol}$$

$$\text{H}_2\text{(g, } 127^\circ\text{C)}: \hat{H}_2 = \hat{H}_{\text{H}_2}(127^\circ\text{C}) \xrightarrow{\text{Table B.8}} 2.943 \text{ kJ/mol}$$

$$\text{CH}_3\text{OH(g, } 127^\circ\text{C)}: \hat{H}_3 = \int_{25}^{122} C_p dT \xrightarrow{\text{Table B.2}} 5.009 \text{ kJ/mol}$$

$$\text{Energy balance : } \dot{Q} = \Delta \dot{H} = \xi \Delta \hat{H}_r^o + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i$$

$$\begin{aligned} \Rightarrow \frac{-17.05 \text{ kJ}}{\text{s}} \left| \frac{3600 \text{ s}}{1 \text{ h}} \right| &= (1166f)(-90.68) \frac{\text{kJ}}{\text{h}} + [1166(1-f)](2.99) \\ &\quad + [2332(1-f)](2.993) + [1166f(5.009)](\text{kJ/h}) \end{aligned}$$

$$\Rightarrow 1.102 \times 10^5 f = 7.173 \times 10^4 \Rightarrow f = 0.651 \text{ mol CO(or H}_2\text{) converted/mol fed}$$

### 9.33 (cont'd)

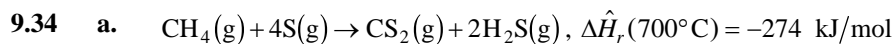
$$\dot{n}_1 = 1166(0.651) = 759.1 \text{ mol/h}$$

$$\dot{n}_2 = 1166(1 - 0.651) = 406.9 \text{ mol/h}$$

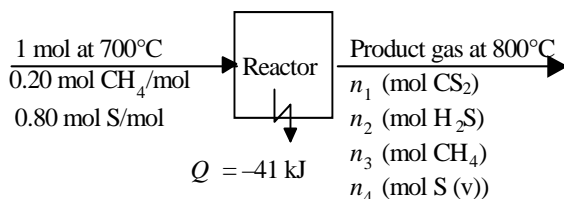
$$\dot{n}_3 = 2332(1 - 0.651) = 813.9 \text{ mol/h}$$

↓

$$\dot{n}_{\text{tot}} = 1980 \frac{\text{mol}}{\text{h}} \Rightarrow V_{\text{out}} = \frac{1980 \text{ mol}}{\text{h}} \left| \frac{22.4 \text{ L(STP)}}{1 \text{ mol}} \right| \left| \frac{400 \text{ K}}{273 \text{ K}} \right| \left| \frac{1.00 \text{ atm}}{5.00 \text{ atm}} \right| \left| \frac{1 \text{ m}^3}{10^3 \text{ L}} \right| = \underline{\underline{13.0 \text{ m}^3/\text{h}}}$$



Basis : 1 mol of feed



Let  $f$  = fractional conversion of  $\text{CH}_4$  (which also equals fractional conversion of  $\text{S}$ , since the species are fed in stoichiometric proportion)

$$\text{Moles } \text{CH}_4 \text{ reacted} = 0.20f, \text{ Extent of reaction} = \xi(\text{mol}) = 0.20f$$

$$n_3 = 0.20(1 - f) \text{ mol } \text{CH}_4$$

$$n_4 = 0.80 \text{ mol S fed} - \frac{0.20f(\text{mol } \text{CH}_4 \text{ react})}{1 \text{ mol } \text{CH}_4 \text{ react}} \left| \frac{4 \text{ mol S react}}{1 \text{ mol } \text{CH}_4 \text{ react}} \right| = 0.80(1 - f) \text{ mol S}$$

$$n_1 = \frac{0.20f \text{ mol } \text{CH}_4 \text{ react}}{1 \text{ mol } \text{CH}_4} \left| \frac{1 \text{ mol } \text{CS}_2}{1 \text{ mol } \text{CH}_4} \right| = 0.20f \text{ mol } \text{CS}_2$$

$$n_2 = \frac{0.20f \text{ mol } \text{CH}_4 \text{ react}}{1 \text{ mol } \text{CH}_4} \left| \frac{2 \text{ mol } \text{H}_2\text{S}}{1 \text{ mol } \text{CH}_4} \right| = 0.40f \text{ mol } \text{H}_2\text{S}$$

References:  $\text{CH}_4(\text{g}), \text{S}(\text{g}), \text{CS}_2(\text{g}), \text{H}_2\text{S}(\text{g})$  at  $700^\circ\text{C}$  (temperature at which  $\Delta \hat{H}_r$  is known)

substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$\text{CH}_4$	0.20	0	$0.20(1 - f)$	$\hat{H}_1$
$\text{S}$	0.80	0	$0.80(1 - f)$	$\hat{H}_2$
$\text{CS}_2$	—	—	$0.20f$	$\hat{H}_3$
$\text{H}_2\text{S}$	—	—	$0.40f$	$\hat{H}_4$

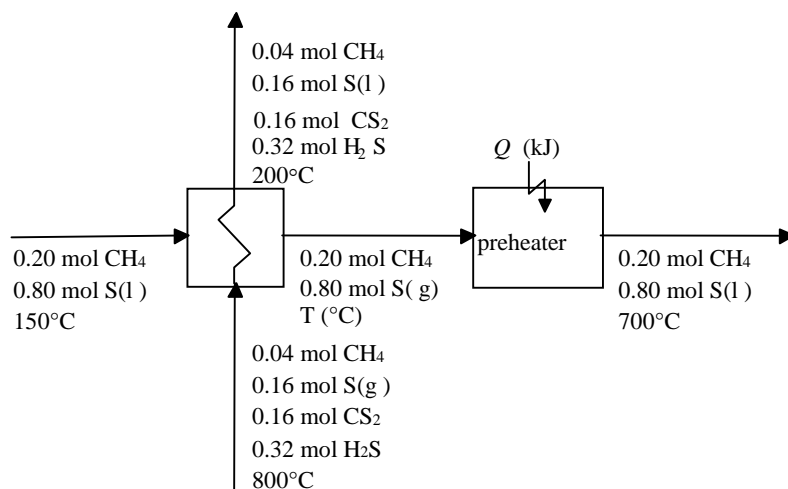
$$\hat{H}_{\text{out}} = C_{pi}(800 - 700) \Rightarrow \begin{cases} \text{CH}_4(\text{g}, 800^\circ\text{C}): \hat{H}_1 = 7.14 \text{ kJ/mol} \\ \text{S}(\text{g}, 800^\circ\text{C}): \hat{H}_2 = 3.64 \text{ kJ/mol} \\ \text{CS}_2(\text{g}, 800^\circ\text{C}): \hat{H}_3 = 3.18 \text{ kJ/mol} \\ \text{H}_2\text{S}(\text{g}, 800^\circ\text{C}): \hat{H}_4 = 4.48 \text{ kJ/mol} \end{cases}$$

### 9.34 (cont'd)

Energy balance on reactor:

$$\begin{aligned}\dot{Q} = \Delta \dot{H} &= \xi \Delta \hat{H}_r + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = 41 \frac{\text{kJ}}{\text{s}} \\ &= \frac{(0.20f)(-274.0)}{(1)} + [0.20(1-f)(7.140) + 0.80(1-f)(3.640) + 0.20f(3.180) + 0.40f(4.480)] \\ \Rightarrow f &= 0.800\end{aligned}$$

b.



System: Heat exchanger-preheater combination. Assume the heat exchanger is adiabatic, so that the only heat transferred to the system from its surroundings is  $Q$  for the preheater.

References :  $\text{CH}_4(\text{g}), \text{S}(\text{l}), \text{CS}_2(\text{g}), \text{H}_2\text{S}(\text{g})$  at  $200^\circ\text{C}$

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
$(\text{CH}_4)_{150^\circ, 700^\circ}$	0.20	$\hat{H}_1$	0.20	$\hat{H}_7$
$(\text{CH}_4)_{800^\circ, 200^\circ}$	0.04	$\hat{H}_2$	0.04	0
S(l)	0.80	$\hat{H}_3$	0.16	0
S(g)	0.16	$\hat{H}_4$	0.80	$\hat{H}_8$
$\text{CS}_2$	0.16	$\hat{H}_5$	0.16	0
$\text{H}_2\text{S}$	0.32	$\hat{H}_6$	0.32	0

$$\hat{H}_i = C_{pi}(T - 200) \text{ for all substances but S}$$

$$= (C_p)_{\text{S(l)}}(T - 200) \text{ for S(l)}$$

$$= (C_p)_{\text{S(l)}} \left( \frac{444.6 - 200}{T_b} \right) + \frac{\Delta \hat{H}_v}{= 83.7 \text{ kJ/mol}} (T_b) + (C_p)_{\text{S(g)}}(T - 444.6) \text{ for S(g)}$$

**9.34 (cont'd)**

$$\text{CH}_4(\text{g}, 150^\circ\text{C}): \hat{H}_1 = -3.57 \text{ kJ/mol}$$

$$\text{CH}_4(\text{g}, 800^\circ\text{C}): \hat{H}_2 = 42.84 \text{ kJ/mol}$$

$$\text{S}(\text{l}, 150^\circ\text{C}): \hat{H}_3 = -1.47 \text{ kJ/mol}$$

$$\text{S}(\text{g}, 800^\circ\text{C}): \hat{H}_4 = 103.83 \text{ kJ/mol}$$

$$\text{CS}_2(\text{g}, 800^\circ\text{C}): \hat{H}_5 = 19.08 \text{ kJ/mol}$$

$$\text{H}_2\text{S}(\text{g}, 800^\circ\text{C}): \hat{H}_6 = 26.88 \text{ kJ/mol}$$

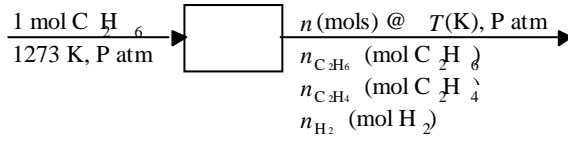
$$\text{CH}_4(\text{g}, 700^\circ\text{C}): \hat{H}_7 = 35.7 \text{ kJ/mol}$$

$$\text{S}(\text{g}, 700^\circ\text{C}): \hat{H}_8 = 100.19 \text{ kJ/mol}$$

$$\text{Energy balance: } Q(\text{kJ}) = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i \Rightarrow Q = 59.2 \text{ kJ} \Rightarrow \underline{\underline{59.2 \text{ kJ/mol feed}}}$$

- c. The energy economy might be improved by insulating the reactor better. The reactor effluent will emerge at a higher temperature and transfer more heat to the fresh feed in the first preheater, lowering (and possibly eliminating) the heat requirement in the second preheater.

## 9.35

Basis: 1 mol C<sub>2</sub>H<sub>6</sub> fed to reactor

a.  $\text{C}_2\text{H}_6 \rightleftharpoons \text{C}_2\text{H}_4 + \text{H}_2$ ,  $K_p = \frac{x_{\text{C}_2\text{H}_4} x_{\text{H}_2}}{x_{\text{C}_2\text{H}_6}} P = 7.28 \times 10^6 \exp[-17,000 / T(K)]$  (1)

Fractional conversion =  $f$  (mols C<sub>2</sub>H<sub>6</sub> react/mol fed)

$$\left. \begin{aligned} \xi(\text{mol}) &= f \\ n_{\text{C}_2\text{H}_6} &= (1-f)(\text{mol C}_2\text{H}_6) \\ n_{\text{C}_2\text{H}_4} &= f(\text{mol C}_2\text{H}_4) \\ n_{\text{H}_2} &= f(\text{mol H}_2) \\ n &= 1+f(\text{mols}) \end{aligned} \right\} \Rightarrow \begin{aligned} x_{\text{C}_2\text{H}_6} &= \frac{1-f}{1+f} \frac{\text{mol C}_2\text{H}_6}{\text{mol}} \\ x_{\text{C}_2\text{H}_4} &= \frac{f}{1+f} \frac{\text{mol C}_2\text{H}_4}{\text{mol}} \\ x_{\text{H}_2} &= \frac{f}{1+f} \frac{\text{mol H}_2}{\text{mol}} \end{aligned}$$

$$K_p = \frac{x_{\text{C}_2\text{H}_4} x_{\text{H}_2}}{x_{\text{C}_2\text{H}_6}} P \Rightarrow K_p = \frac{\frac{f^2}{(1+f)^2} P}{\frac{(1-f)}{(1+f)}} = \frac{f^2 P}{(1-f)(1+f)} = \frac{f^2}{1-f^2} P$$

$$(1-f^2)K_p = f^2 P \Rightarrow f = \left( \frac{K_p}{P + K_p} \right)^{1/2} \quad (2)$$

b. References: C<sub>2</sub>H<sub>6</sub>(g), C<sub>2</sub>H<sub>4</sub>(g), H<sub>2</sub>(g) at 1273 K

Energy balance:

$$\Delta H = 0 \Rightarrow \xi \Delta \hat{H}_r(1273 \text{ K}) + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i$$

$$(\hat{H}_i)_{\text{in}} = 0 \text{ (inlet temperature = reference temperature)}$$

$$(\hat{H}_i)_{\text{out}} = \int_{1273}^T C_{pi} dT$$

 $\Downarrow$  energy balance

$$f \Delta \hat{H}_r(1273 \text{ K}) + (1-f) \int_{1273}^T (C_p)_{\text{C}_2\text{H}_6} dT + f \int_{1273}^T (C_p)_{\text{C}_2\text{H}_4} dT + f \int_{1273}^T (C_p)_{\text{H}_2} dT = 0$$

 $\Downarrow$  rearrange, reverse limits and change signs of integrals

$$\frac{1-f}{f} = \frac{\Delta \hat{H}_r(1273 \text{ K}) - \int_T^{1273} (C_p)_{\text{C}_2\text{H}_4} dT - \int_T^{1273} (C_p)_{\text{H}_2} dT}{\underbrace{\int_T^{1273} (C_p)_{\text{C}_2\text{H}_6} dT}_{\phi(T)}} \quad (3)$$

$$\frac{1-f}{f} = \phi(T) \Rightarrow 1-f = f\phi(T) \Rightarrow f = \frac{1}{1+\phi(T)} \quad (4)$$

9.35 (cont'd)

$$\phi(T) = \frac{145600 - \int_T^{1273} (9.419 + 0.1147T) dT - \int_T^{1273} (26.90 + 4.167 \times 10^{-3} T) dT}{\int_T^{1273} (11.35 + 0.1392T) dT}$$

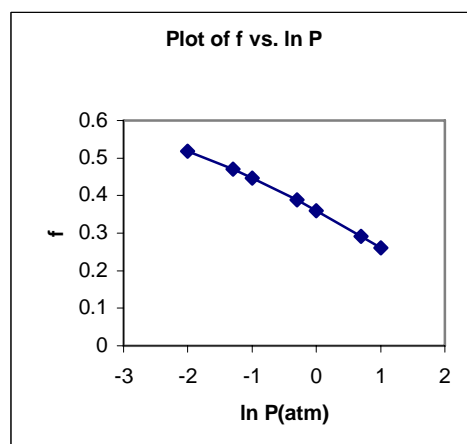
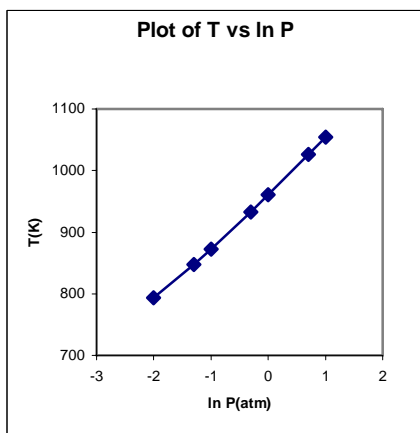
$$\Rightarrow \phi(T) = \frac{3052 + 36.2T + 0.05943T^2}{127240 - 11.3T - 0.0696T^2}$$

c.  $\left( \frac{K_p}{1 + K_p} \right)^{1/2} = \frac{1}{1 + \phi(T)} \Rightarrow \left( \frac{K_p}{1 + K_p} \right)^{1/2} - \frac{1}{1 + \phi(T)} = \psi(T) = 0$

$\phi(T)$  given by expression of Part b.  $K_p(T)$  given by Eq. (1)

d.

P (atm)	T (K)	f	K <sub>p</sub> (atm)	Phi	Psi
0.01	794	0.518	0.0037	0.93152	-0.0001115
0.05	847.4	0.47	0.0141	1.12964	-0.0002618
0.1	872.3	0.446	0.025	1.24028	0.00097743
0.5	932.8	0.388	0.0886	1.57826	3.41E-05
1	960.3	0.36	0.1492	1.77566	4.69E-05
5	1026	0.292	0.4646	2.42913	-2.57E-05
10	1055	0.261	0.7283	2.83692	-7.54E-05



e. C \*\*PROGRAM FOR PROBLEM 9-35

```

WRITE (5, 1)
1  FORMAT ('1', 20X, 'SOLUTION TO PROBLEM 9-35//')
T = 1200.0
TLAST = 0.0
PSIL = 0.0

```

### 9.35 (cont'd)

```

C  **DECREMENT BY 50 DEG. AND LOOK FOR A SIGN IN PSI
    DO 10I =1, 20
    CALL PSICAL (T, PHI, PSI)
    IF ((PSIL*PSI).LT.0.0) GO TO 40
    TLAST = T
    PSIL = PSI
    T = T - 50.
10  CONTINUE
40  IF (T.GE.0.0) GO TO 45
    WRITE (3, 2)
    2  FORMAT (1X, 'T LESS THAN ZERO -- ERROR')
    STOP
C  **APPLY REGULA-FALSI
45  DO 50 I = 1, 20
    IF (I.NE.1) T2L = T2
    T2 = (T*PSIL-TLAST*PSI)/(PSIL-PSI)
    IF (ABS(T2-T2L).LT.0.01) GO TO 99
    CALL PSICAL (T2, PHIT, PSIT)
    IF (PSIT.EQ.0) GO TO 99
    IF ((PBIT*PBIL).GT.0.0) PSIL = PSIT
    IF ((PSIT*PSIL).GT.0.0) TLAST = T2
    IF ((PSIT*PSI).GT.0.0) PSI = PSIT
    IF ((PSIT*PSI).GT.0.0) T = T2
50  CONTINUE
    IF (I.EQ.20) WRITE (3, 3)
    3  FORMAT ('0', 'REGULA-FALSI DID NOT CONVERGE IN 20 ITERATIONS')
93  STOP
    END
    SUBROUTINE PSICAL (T, PHI, PSI)
    REAL KF
    PHI = (3052 + 36.2*T + 36.2*T + 0.05943*T**2)/(127240. - 11.35*T
    * - 0.0636*T**2)
    KP = 7.28E6*EXP(-17000./T)
    FBI = SQRT((KP/(1. + KP)) - 1./12. + PHI)
    WRITE (3, 1) T, PSI
    1  FORMAT (6X, 'T =', F6.2, 4X, 'PSI =', E11.4)
    RETURN
    END

```

OUTPUT: SOLUTION TO PROBLEM 9-35

```

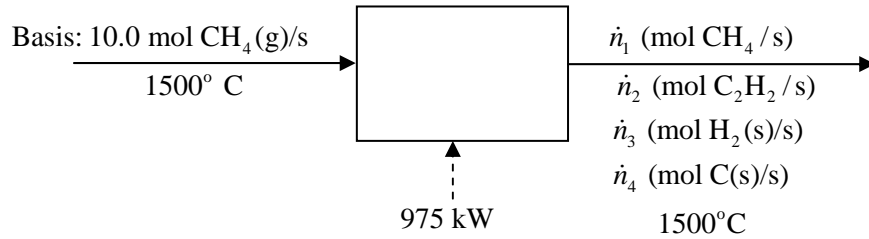
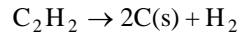
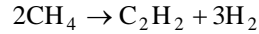
T = 1200.00  PSI = 0.8226E + 00
T = 1150.00  PSI = 0.7048E + 00
T = 1100.00  PSI = 0.5551E + 00
T = 1050.00  PSI = 0.3696E + 00
T = 1000.00  PSI = 0.1619E + 00
T = 950.00   PSI = -0.3950E - 01
T = 959.80   PSI = -0.1824E - 02
T = 960.25   PSI = -0.7671E - 04
T = 960.27   PSI = -0.3278E - 05

```

Solution:  $T = 960.3 \text{ K}$ ,  $f = 0.360 \text{ mol C}_2\text{H}_6 \text{ reacted/mol fed}$



9.36



a.

$$\text{60\% conversion} \Rightarrow \dot{n}_1 = 10(1 - 0.600) = \underline{\underline{4.00 \text{ mol CH}_4/\text{s}}}$$

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

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

References for enthalpy calculations : C(s), H<sub>2</sub>(g) at 25°C

$$H_i = \left( \Delta \hat{H}_f^\circ \right)_i + C_{pi}(1500 - 25), \quad i = \text{CH}_4, \text{C}_2\text{H}_2, \text{C}, \text{H}_2$$

Substance	$\dot{n}_{\text{in}}$ (mol/s)	$\hat{H}_{\text{in}}$ (kJ/mol)	$\dot{n}_{\text{out}}$ (mol/s)	$\hat{H}_{\text{out}}$ (kJ/mol)
CH <sub>4</sub> (g)	10	41.68	4	41.68
C <sub>2</sub> H <sub>2</sub> (g)	—	—	$\dot{n}_2$	303.45
H <sub>2</sub> (g)	—	—	$\dot{n}_3$	45.72
C(s)	—	—	$\dot{n}_4$	32.45

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

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

$$\text{Yield of acetylene} = \frac{2.50 \text{ mol C}_2\text{H}_2/\text{s}}{6.00 \text{ mol CH}_4 \text{ consumed/s}} = \underline{\underline{0.417 \text{ mol C}_2\text{H}_2/\text{mol CH}_4 \text{ consumed}}}$$

b.

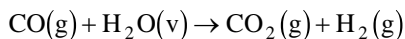
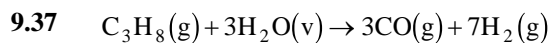
If no side reaction,

$$\dot{n}_1 = 10.0(1 - 0.600) = \underline{\underline{4.00 \text{ mol CH}_4/\text{s}}}$$

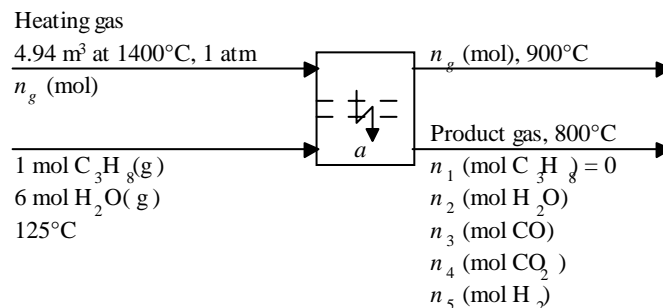
$$\dot{n}_3 = 0 \Rightarrow \dot{n}_2 = \underline{\underline{3.00 \text{ mol C}_2\text{H}_2/\text{s}}}, \quad \dot{n}_4 = \underline{\underline{9.00 \text{ mol H}_2/\text{s}}}$$

$$\text{Yield of acetylene} = \frac{3.00 \text{ mol C}_2\text{H}_2/\text{s}}{6.00 \text{ mol CH}_4 \text{ consumed/s}} = \underline{\underline{0.500 \text{ mol C}_2\text{H}_2/\text{mol CH}_4 \text{ consumed}}}$$

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



Basis: 1 mol  $\text{C}_3\text{H}_8$  fed



$$n_g = \frac{4.94 \text{ m}^3}{1 \text{ m}^3} \left| \frac{10^3 \text{ L}}{1 \text{ m}^3} \right| \left| \frac{273 \text{ K}}{1673 \text{ K}} \right| \left| \frac{1 \text{ mol}}{22.4 \text{ L}} \right| = 35.99 \text{ mol heating gas}$$

Let  $\xi_1$  and  $\xi_2$  be the extents of the two reactions.

$$\begin{aligned} n_1 &= 1 - \xi_1 \xRightarrow{n_1=0} \xi_1 = 1 \text{ mol} & n_4 &= \xi_2 \\ n_2 &= 6 - 3\xi_1 - \xi_2 \xRightarrow{\xi_1=1} n_2 = 3 - \xi_2 & n_5 &= 7\xi_1 + \xi_2 \xRightarrow{\xi_1=1} n_5 = 7 + \xi_2 \\ n_3 &= 3\xi_1 - \xi_2 \xRightarrow{\xi_1=1} n_3 = 3 - \xi_2 \end{aligned}$$

References:  $\text{C}(\text{s})$ ,  $\text{H}_2(\text{g})$ ,  $\text{O}_2(\text{g})$  at 25°C, heating gas at 900°C

$$\hat{H}_i = \Delta \hat{H}_{\text{fi}}^0 + \int_{25}^T C_{p,i} dT \quad \text{for } \text{C}_3\text{H}_8$$

= Table B.8 for  $\text{CO}_2$ ,  $\text{H}_2$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}$

$$= \int_{900}^T C_p dT = C_p (T - 900) \quad \text{for heating gas}$$

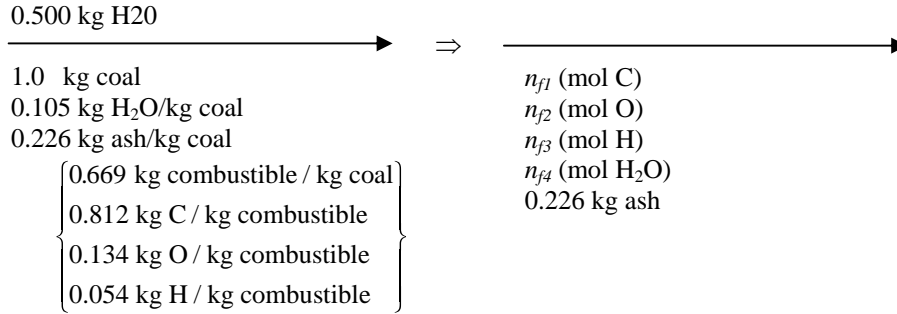
Substance	$n_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
$\text{C}_3\text{H}_8$	1	-95.39	0	—
$\text{H}_2\text{O}$	6	-238.43	$3 - \xi_2$	-212.78
$\text{CO}$	—	—	$3 - \xi_2$	-86.39
$\text{CO}_2$	—	—	$\xi_2$	-356.15
$\text{H}_2$	—	—	$7 + \xi_2$	22.85
heating gas	35.99	200.00	35.99	0

Energy Balance :

$$\begin{aligned} \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i &= 0 \Rightarrow \xi_2 = 2.00 \text{ mol} \Rightarrow n_2 = 1 \text{ mol } \text{H}_2\text{O}, n_3 = 1 \text{ mol } \text{CO}, \\ n_4 &= 1 \text{ mol } \text{CO}_2, n_5 = 9 \text{ mol } \text{H}_2 \Rightarrow \underline{\underline{7.7 \text{ mol } \% \text{H}_2\text{O}, 7.7\% \text{CO}, 15.4\% \text{CO}_2, 69.2\% \text{H}_2}} \end{aligned}$$

- 9.38 a. Any C consumed in reaction (2) is lost to reaction (1). Without the energy released by reaction (2) to compensate for the energy consumed by reaction (1), the temperature in the adiabatic reactor and hence the reaction rate would drop.

- b. Basis : 1.00 kg coal fed (+0.500 kg H<sub>2</sub>O)

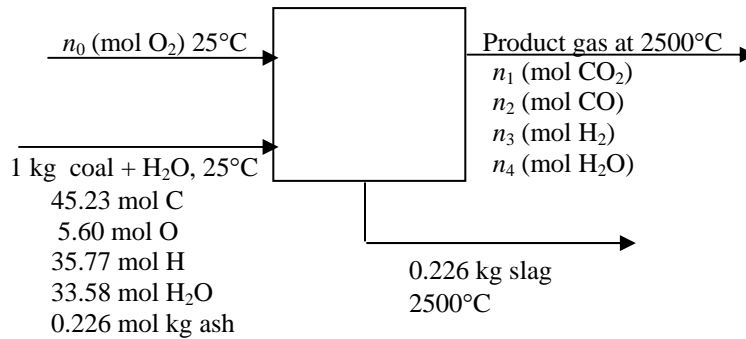


$$n_{f1} = [(1.00)(0.669)(0.812) \text{ kg C}] [1 \text{ mol C} / 12.01 \times 10^{-3} \text{ kg}] = 45.23 \text{ mol C}$$

$$n_{f2} = (1.00)(0.669)(0.134) / 16.0 \times 10^{-3} = 5.6 \text{ mol O}$$

$$n_{f3} = (1.00)(0.669)(0.054) / 1.01 \times 10^{-3} = 35.77 \text{ mol H}$$

$$n_{f4} = [(0.500 + 0.105) \text{ kg}] [1 \text{ mol H}_2\text{O} / 18.016 \times 10^{-3} \text{ kg}] = 33.58 \text{ mol H}_2\text{O}$$



$$\text{Reactive oxygen (O) available} = (2n_0 + 5.60) \text{ mol O}$$

$$\text{Oxygen consumed by H (2H+O} \rightarrow \text{H}_2\text{O)} : \frac{35.77 \text{ mol H}}{2 \text{ mol H}} \left| \frac{1 \text{ mol O}}{2 \text{ mol H}} \right| = 17.88 \text{ mol O}$$

$$\Rightarrow \text{Reactive O remaining} = (2n_0 + 5.60) - 17.88 = (2n_0 - 12.28) \text{ mol O}$$

$$\text{CO}_2 \text{ formed (C+2O} \rightarrow \text{CO}_2) : n_1 = \frac{(2n_0 - 12.28) \text{ mol O}}{2 \text{ mol O}} \left| \frac{1 \text{ mol CO}_2}{2 \text{ mol O}} \right| = \underline{\underline{(n_0 - 6.14) \text{ mol CO}_2}}$$

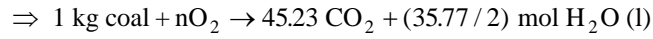
$$\text{C balance : } 45.23 = n_1 + n_2 \xRightarrow{n_1 = n_0 - 6.14} n_2 = \underline{\underline{(51.37 - n_0) \text{ mol CO}}}$$

$$\text{O balance : } 2n_0 + 5.60 + 33.58 = 2n_1 + n_2 + n_4 \xRightarrow{n_1 = n_0 - 6.14, n_2 = 51.37 - n_0} n_4 = \underline{\underline{(n_0 + 0.06) \text{ mol H}_2\text{O}}}$$

$$\text{H balance : } 35.77 + 2(33.58) = 2n_3 + 2n_4 \xRightarrow{n_4 = n_0 + 0.06} n_3 = \underline{\underline{(51.37 - n_0) \text{ mol H}_2}}$$

### 9.38 (cont'd)

c. 1 kg coal contains 45.23 mol C and 35.77 mol H



$$\Delta \hat{H}_r = -21,400 \text{ kJ} = 45.23(\Delta \hat{H}_f^\circ)_{\text{CO}_2} + (35.77 / 2)(\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O(l)}} - (\Delta \hat{H}_f^\circ)_{\text{coal}}$$

$$\Rightarrow \underline{\underline{(\Delta \hat{H}_f^\circ)_{\text{coal}} = -1510 \text{ kJ / kg}}}$$

References : C(s), O<sub>2</sub>(g), H<sub>2</sub>(g), ash(s) at 25°C

Substance	$n_{in}$ (mol)	$\hat{H}_{in}$ (kJ/mol)	$n_{out}$ (mol)	$\hat{H}_{out}$ (kJ/mol)
CO <sub>2</sub>	—	—	$n_0 - 6.14$	$\hat{H}_1$
CO	—	—	$51.37 - n_0$	$\hat{H}_2$
H <sub>2</sub>	—	—	$51.37 - n_0$	$\hat{H}_3$
H <sub>2</sub> O	33.58	$\hat{H}_0$	$n_0 + 0.06$	$\hat{H}_4$
Coal	1 kg	-1510 kJ/kg	—	—
Ash(slag)	(in coal)	0	0.266 kg	$\hat{H}_5$ (kJ/kg)

$$\hat{H}_i = \Delta \hat{H}_{fi}^\circ + C_{pi}(2500 - 25), \quad i = 1, 3$$

$$\hat{H}_1 = -393.5 + 0.0508(2475) = -267.8 \text{ kJ/mol CO}_2$$

$$\hat{H}_2 = -110.52 + 0.0332(2475) = -28.35 \text{ kJ/mol CO}$$

$$\hat{H}_3 = 0.0300(2475) = 74.25 \text{ kJ/mol H}_2$$

$$\hat{H}_4 = -241.83 + 0.0395(2475) = -144.07 \text{ kJ/mol H}_2\text{O}$$

$$\hat{H}_5 = (\Delta \hat{H}_m)_{\text{ash}} + 1.4(2475) = 710 + 1.4(2475) = 4175 \text{ kJ/kg ash}$$

Energy Balance

$$\Delta H = \sum n_{out} \hat{H}_{out} - \sum n_{in} \hat{H}_{in} = 0 \Rightarrow n_0 = \underline{\underline{35.4 \text{ mol O}_2}}$$

9.39

$$\text{Mass of H}_2\text{SO}_4 = \frac{3 \text{ m}^3}{1 \text{ m}^3} \left| \frac{10^3 \text{ L}}{1 \text{ m}^3} \right| \left| \frac{1 \text{ mol H}_2\text{SO}_4}{\text{L}} \right| = 3000 \text{ mol H}_2\text{SO}_4 \left( \frac{98.02 \text{ g}}{1 \text{ mol}} \right) = 2.941 \times 10^5 \text{ g H}_2\text{SO}_4$$

$$\text{Mass of solution} = \frac{3 \text{ m}^3}{1 \text{ m}^3} \left| \frac{10^3 \text{ L}}{1 \text{ m}^3} \right| \left| \frac{10^3 \text{ mL}}{\text{L}} \right| \left| \frac{1.064 \text{ g}}{1 \text{ mL}} \right| = 3.192 \times 10^6 \text{ g solution}$$

$$\Rightarrow \text{Moles of H}_2\text{O} = (3.192 \times 10^6 - 2.941 \times 10^5) \text{ g H}_2\text{O} \left( \frac{1 \text{ mol}}{18.02 \text{ g}} \right) = 1.61 \times 10^5 \text{ mol H}_2\text{O}$$

$$n \left( \frac{\text{mol H}_2\text{O}}{\text{mol H}_2\text{SO}_4} \right) = \frac{1.61 \times 10^5 \text{ mol H}_2\text{O}}{3000 \text{ mol H}_2\text{SO}_4} = 53.6 \text{ mol H}_2\text{O/mol H}_2\text{SO}_4$$

$$(\Delta \hat{H}_f)_{\text{H}_2\text{SO}_4(\text{aq}, r=53.6)} = (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{l})} + (\Delta \hat{H}_s)_{\text{H}_2\text{SO}_4(\text{aq}, r=53.6)} = (-811.32 - 73.39) \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-884.7 \text{ kJ/mol}}}$$

↑  
Table B.1
↑  
Table B.11

$$H = (3000 \text{ mol H}_2\text{SO}_4)(-884.7 \text{ kJ/mol H}_2\text{SO}_4) = \underline{\underline{-2.65 \times 10^6 \text{ kJ}}}$$

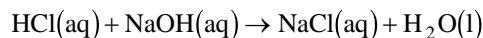
9.40

$$\text{HCl(aq): } \Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{\text{HCl(g)}} + (\Delta \hat{H}_s^\circ)_\infty \xrightarrow{\text{Tables B.1, B.11}} = -92.31 - 75.14 = -167.45 \text{ kJ/mol}$$

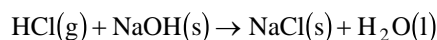
$$\text{NaOH(aq): } \Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{\text{NaOH(s)}} + (\Delta \hat{H}_s^\circ)_\infty \xrightarrow{\text{Tables B.1, B.11}} = -426.6 - 42.89 = -469.49 \text{ kJ/mol}$$

$$\text{NaCl(aq): } \Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{\text{NaCl(s)}} + (\Delta \hat{H}_s^\circ)_\infty \xrightarrow{\text{Table B.1}} = -411.0 + 4.87 = -406.1 \text{ kJ/mol}$$

↓  
Table B.1
↓  
Given



$$\Delta \hat{H}_r^\circ = [-406.1 - 285.84 - (-167.45) - (-469.49)] = \underline{\underline{-55.0 \text{ kJ/mol}}}$$



$$\begin{aligned} \Delta \hat{H}_r^\circ &= \sum_{\text{products}} \nu_i \Delta \hat{H}_f^\circ - \sum_{\text{reactants}} \nu_i \Delta \hat{H}_f^\circ \\ &= [-411.0 - 285.84 - (-92.31) - (-426.6)] \text{ kJ/mol} = \underline{\underline{-177.9 \text{ kJ/mol}}} \end{aligned}$$

The difference between the two calculated values equals

$$\left\{ (\Delta \hat{H}_s)_{\text{NaCl}} - (\Delta \hat{H}_s)_{\text{HCl}} - (\Delta \hat{H}_s)_{\text{NaOH}} \right\}.$$



$$\text{Basis: } 1 \text{ mol H}_2\text{SO}_4 \text{ soln} \Rightarrow \left. \begin{aligned} 0.10 \text{ mol H}_2\text{SO}_4 \times (98.08 \text{ g/mol}) &= 9.808 \text{ g H}_2\text{SO}_4 \\ 0.90 \text{ mol H}_2\text{O} \times (18.02 \text{ g/mol}) &= 16.22 \text{ g H}_2\text{O} \end{aligned} \right\}$$

$$\Rightarrow \frac{26.03 \text{ g soln}}{1.27 \text{ g}} \left| \frac{1 \text{ cm}^3}{\text{g}} \right| = 20.49 \text{ cm}^3$$

$$\Rightarrow \frac{0.10 \text{ mol H}_2\text{SO}_4}{1 \text{ mol H}_2\text{SO}_4} \left| \frac{2 \text{ mol NaOH}}{1 \text{ mol H}_2\text{SO}_4} \right| \left| \frac{1 \text{ liter caustic soln}}{3 \text{ mol NaOH}} \right| \left| \frac{10^3 \text{ cm}^3}{1 \text{ L}} \right| = 66.67 \text{ cm}^3 \text{ NaOH(aq)}$$

9.41 (cont'd)

$$\text{Volume ratio} = \frac{66.67 \text{ cm}^3 \text{ NaOH(aq)}}{20.49 \text{ cm}^3 \text{ H}_2\text{SO}_4 \text{ (aq)}} = \underline{\underline{3.25 \text{ cm}^3 \text{ caustic solution} / \text{cm}^3 \text{ acid solution}}}$$

b.  $\text{H}_2\text{SO}_4 \text{ (aq): } r = 9 \text{ mol H}_2\text{O} / 1 \text{ mol H}_2\text{SO}_4$

$$(\Delta \hat{H}_f^\circ)_{\text{soln}} = (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(l)} + (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{aq}, r=9)} = (-811.32 - 65.23) \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-877 \text{ kJ/mol H}_2\text{SO}_4}}$$

NaOH(aq): The solution fed contains  $(66.67 \text{ cm}^3)(1.13 \text{ g/cm}^3) = 75.34 \text{ g}$ , and

$$(0.2 \text{ mol NaOH})(40.00 \text{ g/mol}) = 8.00 \text{ g NaOH}$$

$$\Rightarrow (75.34 - 8.00) \text{ g H}_2\text{O} \Rightarrow (67.39 \text{ g H}_2\text{O})(1 \text{ mol}/18.02 \text{ g}) = 3.74 \text{ mol H}_2\text{O}$$

$$\Rightarrow r = 3.74 \text{ mol H}_2\text{O} / 0.20 \text{ mol NaOH} = 18.7 \text{ mol H}_2\text{O} / \text{mol NaOH}$$

$$(\Delta \hat{H}_f^\circ)_{\text{soln}} = (\Delta \hat{H}_f^\circ)_{\text{NaOH(s)}} + (\Delta \hat{H}_s^\circ)_{\text{NaOH(s)(aq}, r=18.7)} = (-426.6 - 42.8) \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-469.4 \text{ kJ/mol NaOH}}}$$

Na<sub>2</sub>SO<sub>4</sub> (aq):

$$(\Delta \hat{H}_f^\circ)_{\text{soln}} = (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(s)} + (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{aq})} = (-1384.5 - 1.17) \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-1385.7 \text{ kJ/mol Na}_2\text{SO}_4}}$$

Extent of reaction:  $(n_{\text{H}_2\text{SO}_4})_{\text{final}} = (n_{\text{H}_2\text{SO}_4})_{\text{fed}} + \nu_{\text{H}_2\text{SO}_4} \xi \Rightarrow 0 = 0.10 \text{ mol} - (1)\xi \Rightarrow \xi = 0.10 \text{ mol}$

Energy Balance:

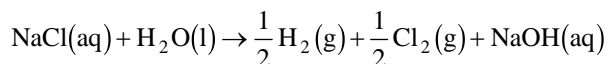
$$\begin{aligned} Q = \Delta H &= \xi \left[ (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{aq})} + 2(\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}(l)} - (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{aq})} - 2(\Delta \hat{H}_f^\circ)_{\text{NaOH(aq)}} \right] \\ &= (0.10 \text{ mol}) \left[ -1385.7 + 2(-285.84) - (-876.55) - (2)(-469.4) \right] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{-14.2 \text{ kJ}}} \end{aligned}$$

9.42 a.

NaCl(aq):  $\Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{\text{NaCl(s)}} + (\Delta \hat{H}_s^\circ)_\infty \overset{\substack{\text{Table B.1,} \\ \text{given}}}{=} (-411.0 + 4.87) \text{ kJ/mol} = \underline{\underline{-406.1 \text{ kJ/mol}}}$

NaOH(aq):

$$\Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{\text{NaOH(s)}} + (\Delta \hat{H}_s^\circ)_\infty \overset{\substack{\text{Table B.1} \\ \downarrow}}{=} (-426.6 - 42.89) \text{ kJ/mol} = \underline{\underline{-469.5 \text{ kJ/mol}}}$$

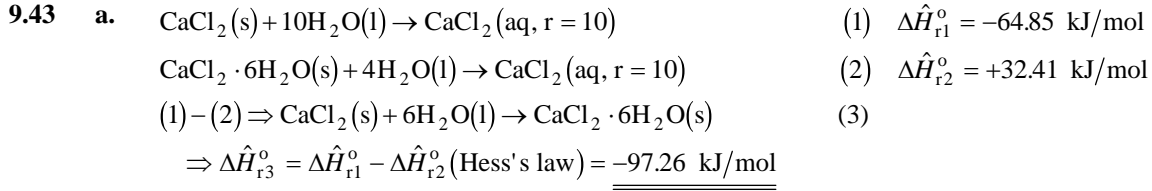


$$\Delta \hat{H}_r^\circ = [-469.5 - (-406.1) - (-285.84)] \text{ kJ/mol} = \underline{\underline{222.44 \text{ kJ/mol}}}$$

b. 

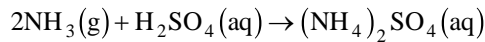
8500 ktonne Cl <sub>2</sub>	10 <sup>3</sup> tonne	10 <sup>3</sup> kg	10 <sup>3</sup> g	1 mol Cl <sub>2</sub>	222.44 kJ
yr	1 ktonne	1 tonne	1 kg	70.91 g Cl <sub>2</sub>	0.5 mol Cl <sub>2</sub>

$$\frac{10^3 \text{ J}}{1 \text{ kJ}} \left| \frac{2.778 \times 10^{-7} \text{ kW} \cdot \text{h}}{1 \text{ J}} \right| \left| \frac{1 \text{ MW} \cdot \text{h}}{10^3 \text{ kW} \cdot \text{h}} \right| = \underline{\underline{1.48 \times 10^7 \text{ MW} \cdot \text{h} / \text{yr}}}$$



b. From (1),  $\Delta\hat{H}_{r1}^\circ = (\Delta\hat{H}_f^\circ)_{\text{CaCl}_2(\text{aq}, r=10)} - (\Delta\hat{H}_f^\circ)_{\text{CaCl}_2(\text{s})}$   
 $\Rightarrow (\Delta\hat{H}_f^\circ)_{\text{CaCl}_2(\text{aq}, r=10)} = (-64.85 - 794.96) \text{ kJ/mol} = \underline{\underline{-859.81 \text{ kJ/mol}}}$

9.44 Basis: 1 mol  $(\text{NH}_4)_2\text{SO}_4$  produced



a.

References : Elements at 25°C

$$\text{NH}_3(\text{g}, 75^\circ\text{C}): \hat{H} = \Delta\hat{H}_f^\circ + \int_{25}^{75} C_p dT = (-46.19 + 1.83) \text{ kJ/mol} = -44.36 \text{ kJ/mol} \text{ (Table B.1, B.2)}$$

$$\text{H}_2\text{SO}_4(\text{aq}, 25^\circ\text{C}): \hat{H} = (\Delta\hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{aq})} = -907.51 \text{ kJ/mol H}_2\text{SO}_4 \text{ (Table B.1)}$$

$$(\text{NH}_4)_2\text{SO}_4(\text{aq}, 25^\circ\text{C}): \hat{H} = (\Delta\hat{H}_f^\circ)_{(\text{NH}_4)_2\text{SO}_4(\text{aq})} = -1173.1 \text{ kJ/mol } (\text{NH}_4)_2\text{SO}_4 \text{ (Table B.1)}$$

Energy balance:

$$Q = \Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = (1)(-1173.1) - (2)(-44.36) - (1)(-907.51) \text{ kJ}$$

$$= -177 \text{ kJ} \Rightarrow 177 \frac{\text{kJ withdrawn}}{\text{mol } (\text{NH}_4)_2\text{SO}_4 \text{ produced}}$$

b. 1 mole %  $(\text{NH}_4)_2\text{SO}_4$  solution  $\Rightarrow \frac{1 \text{ mol } (\text{NH}_4)_2\text{SO}_4}{100 \text{ mol solution}} \times \frac{132 \text{ g}}{\text{mol}} = 132 \text{ g } (\text{NH}_4)_2\text{SO}_4$

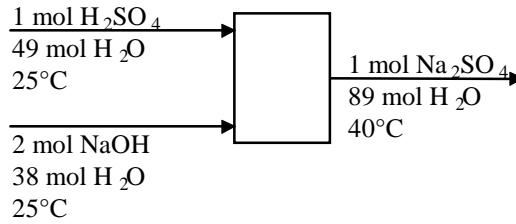
$$\frac{99 \text{ mol H}_2\text{O}}{100 \text{ mol solution}} \times \frac{18 \text{ g}}{\text{mol}} = \frac{1782 \text{ g H}_2\text{O}}{1914 \text{ g solution}}$$

The heat transferred from the reactor in part (a) now goes to heat the product solution from

$$25^\circ\text{C to } T_{\text{final}} \Rightarrow 177 \text{ kJ} = \frac{1.914 \text{ g}}{10^3 \text{ g}} \times \frac{1 \text{ kg}}{\text{kg}} \times \frac{4.184 \text{ kJ}}{\text{kg}^\circ\text{C}} \times (T - 25)^\circ\text{C} \Rightarrow T_{\text{final}} = \underline{\underline{47.1^\circ\text{C}}}$$

c. In a real reactor, the final solution temperature will be less than the value calculated in part b, due to heat loss to the surroundings. The final temperature will therefore be less than 47.1°C.

9.45 a.  $\text{H}_2\text{SO}_4(\text{aq}) + 2\text{NaOH}(\text{aq}) \rightarrow \text{Na}_2\text{SO}_4(\text{aq}) + 2\text{H}_2\text{O}(\text{aq})$  Basis: 1 mol  $\text{H}_2\text{SO}_4$  fed



Reference states:  $\text{Na}(\text{s}), \text{H}_2(\text{g}), \text{S}(\text{s}), \text{O}_2(\text{g})$  at  $25^\circ\text{C}$

$\text{H}_2\text{SO}_4(\text{aq}, r = 49, 25^\circ\text{C})$ :

$$\begin{aligned} n\hat{H} &= (1 \text{ mol } \text{H}_2\text{SO}_4) \left[ (\Delta\hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{l})} + \Delta\hat{H}_s^\circ(r = 49) \right] (\text{kJ/mol}) + 49(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} \\ &= (1)[-811.3 - 73.3] = -884.6 \text{ kJ} + 49(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} \end{aligned}$$

$\text{NaOH}(\text{aq}, r = 19, 25^\circ\text{C})$ :

$$\begin{aligned} n\hat{H} &= (2 \text{ mol } \text{NaOH}) \left[ (\Delta\hat{H}_f^\circ)_{\text{NaOH}(\text{s})} + \Delta\hat{H}_s^\circ(r = 19) \right] (\text{kJ/mol}) + 38(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} \\ &= (2)[-426.6 - 42.8] = -938.8 \text{ kJ} + 38(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} \end{aligned}$$

$\text{Na}_2\text{SO}_4(\text{aq}, r = 89, 40^\circ\text{C})$ :

$$\frac{1 \text{ kmol } \text{Na}_2\text{SO}_4}{1 \text{ kmol}} \left| \frac{142.0 \text{ kg}}{1 \text{ kmol}} \right| = 0.142 \text{ kg}, \quad \frac{89 \text{ kmol } \text{H}_2\text{O}}{1 \text{ kmol}} \left| \frac{18.02 \text{ kg}}{1 \text{ kmol}} \right| = 1.604 \text{ kg} \Rightarrow 1.746 \text{ kg}$$

$$n\hat{H} = (1 \text{ mol } \text{Na}_2\text{SO}_4) \left[ (\Delta\hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4} + (\Delta\hat{H}_s^\circ)_{\text{Na}_2\text{SO}_4} \right] + 89(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} + mC_p(40 - 25)$$

$$\begin{aligned} &\Downarrow \\ &\Delta\hat{H}_f^\circ = -1384.5 \text{ kJ/mol (Table B.1)} \\ &\Delta\hat{H}_s^\circ = -1.2 \text{ kJ/mol} \\ &m = 1.746 \text{ kg}, C_p \approx (C_p)_{\text{H}_2\text{O}(\text{l})} = 4.814 \text{ kJ/(kg}\cdot^\circ\text{C)} \\ &\Downarrow \\ n\hat{H} &= -1276 \text{ kJ} + 89(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} \end{aligned}$$

$$\text{Energy balance: } Q = \Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = 547.4 + 2(\Delta\hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})}^{+285.84 \text{ kJ/mol}} = -24.3 \text{ kJ}$$

Mass of acid fed

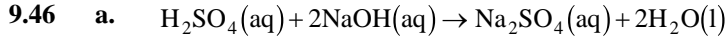
$$\frac{1 \text{ mol } \text{H}_2\text{SO}_4}{1 \text{ mol}} \left| \frac{98.08 \text{ g } \text{H}_2\text{SO}_4}{1 \text{ mol}} \right| + \frac{49 \text{ mol } \text{H}_2\text{O}}{1 \text{ mol}} \left| \frac{18.02 \text{ g } \text{H}_2\text{O}}{1 \text{ mol}} \right| = 981 \text{ g} = 0.981 \text{ kg}$$

$$\Rightarrow \frac{Q}{M_{\text{acid}}} = \frac{-24.3 \text{ kJ}}{0.981 \text{ kg acid}} \Rightarrow 24.8 \text{ kJ / kg acid transferred from reactor contents}$$

b. If the reactor is adiabatic, the heat transferred from the reactor of Part(a) instead goes to heat the product solution from  $40^\circ\text{C}$  to  $T_f$

$$\Rightarrow 24.3 \times 10^3 \text{ J} = \frac{1.746 \text{ kg}}{\text{kg}\cdot^\circ\text{C}} \left| \frac{4.184 \text{ kJ}}{\text{kg}\cdot^\circ\text{C}} \right| (T_f - 40)^\circ\text{C} \Rightarrow T_f = \underline{\underline{43^\circ\text{C}}}$$





$\text{H}_2\text{SO}_4$  solution:

$$75 \text{ ml of } 4\text{M } \text{H}_2\text{SO}_4 \text{ solution} \Rightarrow \frac{4 \text{ mol } \text{H}_2\text{SO}_4}{1 \text{ L acid soln}} \left| \frac{1 \text{ L}}{10^3 \text{ mL}} \right| \frac{75 \text{ mL}}{1} = 0.30 \text{ mol } \text{H}_2\text{SO}_4$$

$$(75 \text{ mL})(1.23 \text{ g/mL}) = 92.25 \text{ g}, \quad (0.3 \text{ mol } \text{H}_2\text{SO}_4)(98.08 \text{ g/mol}) = 29.42 \text{ g } \text{H}_2\text{SO}_4$$

$$\Rightarrow (92.25 - 29.42) \text{ g } \text{H}_2\text{O} \Rightarrow (62.83 \text{ g } \text{H}_2\text{O})(1 \text{ mol}/18.02 \text{ g}) = 3.49 \text{ mol } \text{H}_2\text{O}$$

$$\Rightarrow r = 3.49 \text{ mol } \text{H}_2\text{O} / 0.30 \text{ mol } \text{H}_2\text{SO}_4 = 11.63 \text{ mol } \text{H}_2\text{O} / \text{mol } \text{H}_2\text{SO}_4$$

$$\begin{aligned} (\Delta \hat{H}_f^\circ)_{\text{soln}} &= (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{l})} + (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{aq}, r=11.63)} \quad \begin{array}{c} \text{Table B.1,} \\ \text{Table B.11} \\ \downarrow \end{array} \quad (-811.32 - 67.42) \frac{\text{kJ}}{\text{mol}} \\ &= -878.74 \text{ kJ/mol } \text{H}_2\text{SO}_4 \end{aligned}$$

NaOH solution required:

$$\frac{0.30 \text{ mol } \text{H}_2\text{SO}_4}{1 \text{ mol } \text{H}_2\text{SO}_4} \left| \frac{2 \text{ mol NaOH}}{1 \text{ mol } \text{H}_2\text{SO}_4} \right| \left| \frac{1 \text{ L NaOH(aq)}}{12 \text{ mol NaOH}} \right| \left| \frac{10^3 \text{ mL}}{1 \text{ L}} \right| = \underline{\underline{50.00 \text{ mL NaOH(aq)}}}$$

$$(50.00 \text{ mL})(1.37 \text{ g/mL}) = 68.5 \text{ g}$$

$$\frac{12 \text{ mol NaOH}}{1 \text{ L NaOH(aq)}} \left| \frac{1 \text{ L}}{10^3 \text{ mL}} \right| \left| \frac{50 \text{ mL}}{1} \right| = 0.60 \text{ mol NaOH} \quad \begin{array}{c} 40 \text{ g/mol NaOH} \\ \Rightarrow \end{array} 24.00 \text{ g NaOH}$$

$$\Rightarrow (68.5 - 24.00) \text{ g } \text{H}_2\text{O} \Rightarrow (44.5 \text{ g } \text{H}_2\text{O})(1 \text{ mol}/18.02 \text{ g}) = 2.47 \text{ mol } \text{H}_2\text{O}$$

$$\Rightarrow r = 2.47 \text{ mol } \text{H}_2\text{O} / 0.6 \text{ mol NaOH} = \frac{4.12 \text{ mol } \text{H}_2\text{O}}{\text{mol NaOH}}$$

$$\begin{aligned} (\Delta \hat{H}_f^\circ)_{\text{soln}} &= (\Delta \hat{H}_f^\circ)_{\text{NaOH(s)}} + (\Delta \hat{H}_s^\circ)_{\text{NaOH(s)(aq}, r=4.12)} = (-426.6 - 35.10) \frac{\text{kJ}}{\text{mol}} \\ &= -461.70 \text{ kJ/mol NaOH} \end{aligned}$$

$\text{Na}_2\text{SO}_4(\text{aq})$ :

$$(\Delta \hat{H}_f^\circ)_{\text{soln}} = (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{s})} + (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{aq})} = (-1384.5 - 1.17) \frac{\text{kJ}}{\text{mol}} = -1385.7 \text{ kJ/mol } \text{Na}_2\text{SO}_4$$

$$m_{\text{total}} = \text{total mass of reactants or products} = (92.25 \text{ g } \text{H}_2\text{SO}_4 \text{ soln} + 68.5 \text{ g NaOH}) = 160.75 \text{ g} = 0.161 \text{ kg}$$

$$\text{Extent of reaction: } (n_{\text{H}_2\text{SO}_4})_{\text{final}} = (n_{\text{H}_2\text{SO}_4})_{\text{fed}} + \nu_{\text{H}_2\text{SO}_4} \xi \Rightarrow 0 = 0.30 \text{ mol} - (1) \xi \Rightarrow \xi = 0.30 \text{ mol}$$

Standard heat of reaction

$$\Delta \hat{H}_r^\circ = (\Delta \hat{H}_f^\circ)_{\text{Na}_2\text{SO}_4(\text{aq})} + 2(\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O}(\text{l})} - (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{SO}_4(\text{aq})} - 2(\Delta \hat{H}_f^\circ)_{\text{NaOH(aq)}}$$

$$\text{Energy Balance: } Q = \Delta H = \xi \Delta \hat{H}_r^\circ + m_{\text{total}} C_p (T - 25)^\circ \text{C}$$

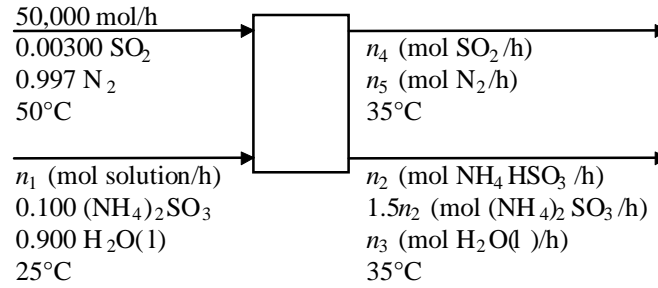
$$= (0.30 \text{ mol})(155.2 \text{ kJ/mol}) + (0.161 \text{ kg}) \left( 4.184 \frac{\text{kJ}}{\text{kg } ^\circ \text{C}} \right) (T - 25)^\circ \text{C} = 0 \Rightarrow T = \underline{\underline{94^\circ \text{C}}}$$

**b.** Volumes are additive.

Heat transferred to and through the container wall is negligible.

9.47

Basis : 50,000 mol flue gas/h



90% SO<sub>2</sub> removal:  $\dot{n}_4 = 0.100(0.00300)(50,000 \text{ mol/h}) = 15.0 \text{ mol SO}_2/\text{h}$

N<sub>2</sub> balance:  $\dot{n}_5 = (0.997)(50,000 \text{ mol/h}) = 49,850 \text{ mol N}_2/\text{h}$

NH<sub>4</sub><sup>+</sup> balance:  $(2)(0.100)(\dot{n}_1) = \dot{n}_2 + (1.5)(2)\dot{n}_2 \Rightarrow \dot{n}_1 = 20\dot{n}_2$

S balance:  $0.100\dot{n}_1 + (0.00300)(50,000) = 15.0 + \dot{n}_2 + 1.5\dot{n}_2 \Rightarrow \dot{n}_2 = 270 \text{ mol NH}_4\text{HSO}_3/\text{h}$

H<sub>2</sub>O balance:  $\dot{n}_3 = (0.900)(5400) - \frac{270 \text{ mol NH}_4\text{HSO}_3 \text{ produced}}{\text{h}} \left| \frac{1 \text{ mol H}_2\text{O consumed}}{2 \text{ mol NH}_4\text{HSO}_3 \text{ produced}} \right|$   
 $= 4725 \text{ mol H}_2\text{O(l)/h}$

Heat of reaction:

$$\Delta \hat{H}_r^\circ = 2(\Delta \hat{H}_f^\circ)_{\text{NH}_4\text{HSO}_4(\text{aq})} - (\Delta \hat{H}_f^\circ)_{(\text{NH}_4)_2\text{SO}_3(\text{aq})} - (\Delta \hat{H}_f^\circ)_{\text{SO}_2(\text{g})} - (\Delta \hat{H}_f^\circ)_{\text{H}_2\text{O(l)}}$$

$$= 2(-760) - (-890) - (-296.90) - (-285.84) \text{ kJ/mol} = -47.3 \text{ kJ/mol}$$

References : N<sub>2</sub>(g), SO<sub>2</sub>(g), (NH<sub>4</sub>)<sub>2</sub>SO<sub>3</sub>(aq), NH<sub>4</sub>HSO<sub>3</sub>(aq), H<sub>2</sub>O(l) at 25°C

SO<sub>2</sub>(g, 50°C):  $\hat{H} = \int_{25}^{50} (C_p)_{\text{SO}_2} dT = 1.01 \text{ kJ/mol}$  ( $C_p$  from Table B.2)

SO<sub>2</sub>(g, 35°C):  $\hat{H} = \int_{25}^{35} (C_p)_{\text{SO}_2} dT = 0.40 \text{ kJ/mol}$

N<sub>2</sub>(g, 50°C):  $\hat{H} = 0.73 \text{ kJ/mol}$  (Table B.8)

N<sub>2</sub>(g, 35°C):  $\hat{H} = 0.292 \text{ kJ/mol}$

Entering solution:  $\hat{H} = 0$ 

Effluent solution at 35°C

$$\dot{m}(\text{g/h}) = \frac{270 \text{ mol NH}_4\text{HSO}_3}{\text{h}} \left| \frac{99 \text{ g}}{\text{mol}} \right|$$

$$+ \frac{1.5 \times 270 \text{ mol (NH}_4)_2\text{SO}_3}{\text{h}} \left| \frac{116 \text{ g}}{\text{mol}} \right| + \frac{4725 \text{ mol H}_2\text{O}}{\text{h}} \left| \frac{18 \text{ g}}{1 \text{ mol}} \right| = 159,000 \frac{\text{g}}{\text{h}}$$

$$\dot{n}\hat{H} = mC_p\Delta T = \frac{159,000 \text{ g}}{\text{h}} \left| \frac{4 \text{ J}}{\text{g}^\circ\text{C}} \right| \left| \frac{(35 - 25)^\circ\text{C}}{10^3 \text{ J}} \right| = 6360 \text{ kJ/h}$$

Extent of reaction:

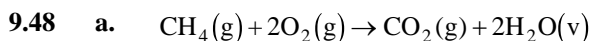
$$(\dot{n}_{\text{NH}_4\text{HSO}_3})_{\text{out}} = (\dot{n}_{\text{NH}_4\text{HSO}_3})_{\text{in}} + \nu_{\text{NH}_4\text{HSO}_3} \dot{\xi} \Rightarrow 270 \text{ mol/h} = 0 + 2\dot{\xi} \Rightarrow \dot{\xi} = 135 \text{ mol/h}$$

9.47 (cont'd)

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

$$Q = \frac{135 \text{ mol}}{\text{h}} \left| \frac{-47.3 \text{ kJ}}{\text{mol}} \right| + (15) \overset{\text{SO}_2 \text{ out}}{(0.40)} + (49,850) \overset{\text{N}_2 \text{ out}}{(0.292)}$$

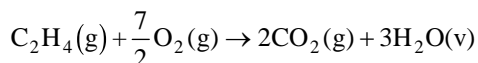
$$+ \overset{\text{effluent solution}}{6360} - (50,000)(0.003)(1.01) - (49,850)(0.73) = \frac{-22,000 \text{ kJ}}{\text{h}} \left| \frac{1 \text{ h}}{3600 \text{ s}} \right| \left| \frac{1 \text{ kW}}{1 \text{ kJ/s}} \right| = \underline{\underline{-6.11 \text{ kW}}}$$



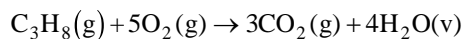
$$\overset{\text{Table B.1 HHV}}{\downarrow} \quad \overset{\text{at } 25^\circ\text{C}}{\downarrow}$$

$$\text{HHV} = 890.36 \text{ kJ/mol}, \text{ LHV} = -\Delta\hat{H}_c^\circ - 2(\Delta\hat{H}_v)_{\text{H}_2\text{O}} = [890.36 - 2(44.01)] \text{ kJ/mol}$$

$$= 802.34 \text{ kJ/mol CH}_4$$



$$\text{HHV} = 1559.9 \text{ kJ/mol}, \text{ LHV} = [1559.9 - 3(44.01)] \text{ kJ/mol} = 1427.87 \text{ kJ/mol C}_2\text{H}_6$$



$$\text{HHV} = 2220.0 \text{ kJ/mol}, \text{ LHV} = [2220.0 - 4(44.01)] \text{ kJ/mol} = 2043.96 \text{ kJ/mol C}_3\text{H}_8$$

$$(\text{HHV})_{\text{natural gas}} = (0.875)(890.36 \text{ kJ/mol}) + (0.070)(1559.9 \text{ kJ/mol}) + (0.020)(2200.00 \text{ kJ/mol})$$

$$= \underline{\underline{933 \text{ kJ/mol}}}$$

$$(\text{LHV})_{\text{natural gas}} = (0.875)(802.34 \text{ kJ/mol}) + (0.070)(1427.87 \text{ kJ/mol}) + (0.020)(2043.96 \text{ kJ/mol})$$

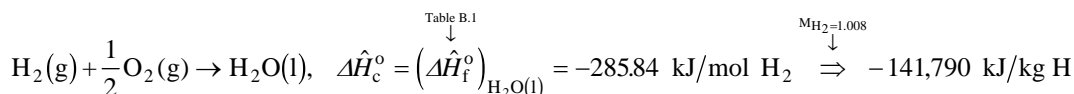
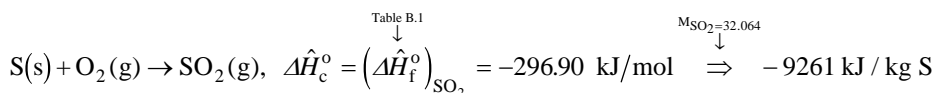
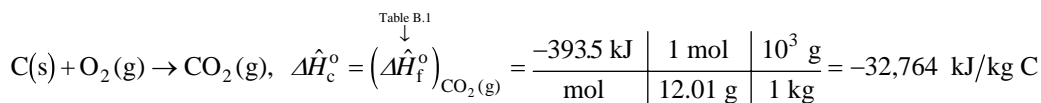
$$= \underline{\underline{843 \text{ kJ/mol}}}$$

b. 1 mol natural gas  $\Rightarrow [(0.875 \text{ mol CH}_4) \left( 16.04 \frac{\text{g}}{\text{mol}} \right) + (0.070 \text{ mol C}_2\text{H}_6) \left( 30.07 \frac{\text{g}}{\text{mol}} \right) + (0.020 \text{ mol C}_3\text{H}_8) \left( 44.09 \frac{\text{g}}{\text{mol}} \right) + (0.035 \text{ mol N}_2) \left( 28.02 \frac{\text{g}}{\text{mol}} \right)] \times \frac{1 \text{ kg}}{10^3 \text{ g}} = 0.01800 \text{ kg}$

$$\Rightarrow \frac{843 \text{ kJ}}{\text{mol}} \left| \frac{1 \text{ mol}}{0.01800 \text{ kg}} \right| = \underline{\underline{46800 \text{ kJ/kg}}}$$

- c. The enthalpy change when 1 kg of the natural gas at 25°C is burned completely with oxygen at 25°C and the products CO<sub>2</sub>(g) and H<sub>2</sub>O(v) are brought back to 25°C.

9.49



**9.49 (cont'd)**
**a.**

$$\text{H available for combustion} = \text{total H} - \text{H in H}_2\text{O}; \text{ latter is } \frac{x_0 \text{ (kg O)}}{\text{kg coal}} \left| \frac{2 \text{ kg H}}{16 \text{ kg O}} \right|$$

↑  
in water

$$\text{Eq. (9.6-3)} \Rightarrow \underline{\underline{HHV = 32,764C + 141,790 \left( H - \frac{O}{8} \right) + 9261S}}$$

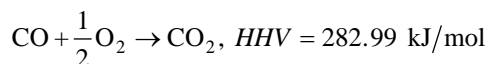
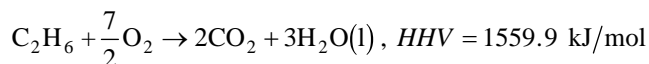
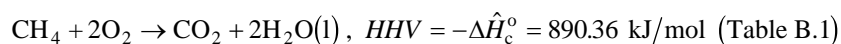
This formula does not take into account the heats of formation of the chemical constituents of coal.

**b.**  $C = 0.758, H = 0.051, O = 0.082, S = 0.016 \Rightarrow (HHV)_{\text{Dulong}} = 31,646 \text{ kJ/kg coal}$

$$1 \text{ kg coal} \Rightarrow \frac{0.016 \text{ kg S}}{32.06 \text{ kg S burned}} \left| \frac{64.07 \text{ kg SO}_2 \text{ formed}}{32.06 \text{ kg S burned}} \right| = 0.0320 \text{ kg SO}_2/\text{kg coal}$$

$$\phi = \frac{0.0320 \text{ kg SO}_2/\text{kg coal}}{31,646 \text{ kJ/kg coal}} = \underline{\underline{1.01 \times 10^{-6} \text{ kg SO}_2/\text{kJ}}}$$

**c.** Diluting the stack gas lowers the mole fraction of SO<sub>2</sub>, but does not reduce SO<sub>2</sub> emission rates. The dilution does not affect the kg SO<sub>2</sub>/kJ ratio, so there is nothing to be gained by it.

**9.50**


$$\text{Initial moles charged: } \frac{2.000 \text{ L}}{\text{(Assume ideal gas)}} \left| \frac{273.2 \text{ K}}{(25 + 273.2) \text{ K}} \right| \left| \frac{2323 \text{ mm Hg}}{760 \text{ mm Hg}} \right| \left| \frac{1 \text{ mol}}{22.4 \text{ L(STP)}} \right| = 0.25 \text{ mol}$$

$$\text{Average mol. wt.: } (4.929 \text{ g})/(0.25 \text{ mol}) = 19.72 \text{ g/mol}$$

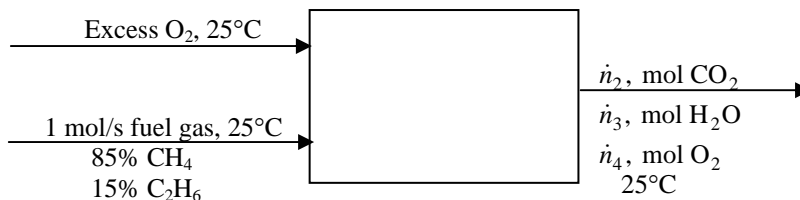
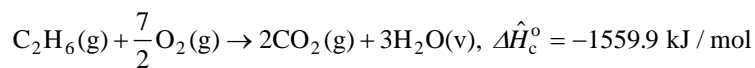
$$\text{Let } x_1 = \text{mol CH}_4/\text{mol gas}, x_2 = \text{mol C}_2\text{H}_6/\text{mol gas} \Rightarrow (1 - x_1 - x_2) \text{ mol CO (mol gas)}$$

$$\overline{MW} = 19.72 \Rightarrow x_1(16.04 \text{ g/mol CH}_4) + x_2(30.07) + (1 - x_1 - x_2)(28.01) = 19.72 \quad (1)$$

$$\overline{HHV} = 963.7 \text{ kJ/mol} \Rightarrow x_1(890.36) + x_2(1559.9) + (1 - x_1 - x_2)(282.99) = 963.7 \quad (2)$$

Solving (1) & (2) simultaneously yields

$$x_1 = \underline{\underline{0.725 \text{ mol CH}_4/\text{mol}}}, x_2 = \underline{\underline{0.188 \text{ mol C}_2\text{H}_6/\text{mol}}}, 1 - x_1 - x_2 = \underline{\underline{0.087 \text{ mol CO/mol}}}$$

**9.51 a.** Basis : 1 mol/s fuel gas


### 9.51 (cont'd)

$$1 \text{ mol/s fuel gas} \Rightarrow 0.85 \text{ mol CH}_4 / \text{s} , 0.15 \text{ mol C}_2\text{H}_6 / \text{s}$$

$$\text{Theoretical oxygen} = \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \left| \frac{0.85 \text{ mol CH}_4}{\text{s}} \right| + \frac{3.5 \text{ mol O}_2}{1 \text{ mol C}_2\text{H}_6} \left| \frac{0.15 \text{ mol C}_2\text{H}_6}{\text{s}} \right| = 2.225 \text{ mol O}_2 / \text{s}$$

$$\text{Assume 10\% excess O}_2 \Rightarrow \text{O}_2 \text{ fed} = 1.1 \times 2.225 = 2.448 \text{ mol O}_2 / \text{s}$$

$$\text{C balance : } \dot{n}_2 = (0.85)(1) + (0.15)(2) \Rightarrow \dot{n}_2 = 1.15 \text{ mol CO}_2 / \text{s}$$

$$\text{H balance : } 2\dot{n}_3 = (0.85)(4) + (0.15)(6) \Rightarrow \dot{n}_3 = 2.15 \text{ mol H}_2\text{O} / \text{s}$$

$$10\% \text{ excess O}_2 \Rightarrow \dot{n}_4 = (0.1)(2.225) \text{ mol O}_2 / \text{s} = 0.223 \text{ mol O}_2 / \text{s}$$

$$\text{Extents of reaction: } \dot{\xi}_1 = \dot{n}_{\text{CH}_4} = 0.85 \text{ mol/s}, \quad \dot{\xi}_2 = \dot{n}_{\text{C}_2\text{H}_6} = 0.15 \text{ mol/s}$$

$$\text{Reference states: CH}_4(\text{g}), \text{C}_2\text{H}_6(\text{g}), \text{N}_2(\text{g}), \text{O}_2(\text{g}), \text{H}_2\text{O}(\text{l}), \text{CO}_2(\text{g}) \text{ at } 25^\circ\text{C}$$

(We will use the values of  $\Delta\hat{H}_c^\circ$  given in Table B.1, which are based on  $\text{H}_2\text{O}(\text{l})$  as a combustion product, and so must choose the liquid as a reference state for water)

Substance	$\dot{n}_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$\dot{n}_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
CH <sub>4</sub>	0.85	0	—	—
C <sub>2</sub> H <sub>6</sub>	0.15	0	—	—
O <sub>2</sub>	2.225	0	0.223	0
CO <sub>2</sub>	—	—	1.15	0
H <sub>2</sub> O(v)	—	—	2.15	$H_1$

$$\hat{H}_1 = \Delta\hat{H}_v(25^\circ\text{C}) = 44.01 \text{ kJ/mol}$$

Energy Balance :

$$\begin{aligned} \dot{Q} &= \dot{n}_{\text{CH}_4} (\Delta\hat{H}_c^\circ)_{\text{CH}_4} + \dot{n}_{\text{C}_2\text{H}_6} (\Delta\hat{H}_c^\circ)_{\text{C}_2\text{H}_6} + \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i \\ &= (0.85 \text{ mol/s CH}_4)(-890.36 \text{ kJ/mol}) + (0.15 \text{ mol/s C}_2\text{H}_6)(-1559.9 \text{ kJ/mol}) \\ &\quad + (2.15 \text{ mol/s H}_2\text{O})(44.01 \text{ kJ/mol}) = -896 \text{ kW} \\ &\Rightarrow \underline{\underline{-\dot{Q} = 896 \text{ kW}}} \text{ (transferred from reactor)} \end{aligned}$$

- b. Constant Volume Process.** The flowchart and stoichiometry and material balance calculations are the same as in part (a), except that amounts replace flow rates (mol instead of mol/s, etc.)

$$1 \text{ mol fuel gas} \Rightarrow 0.85 \text{ mol CH}_4, 0.15 \text{ mol C}_2\text{H}_6$$

$$\text{Theoretical oxygen} = 2.225 \text{ mol O}_2$$

$$\text{Assume 10\% excess O}_2 \Rightarrow \text{O}_2 \text{ fed} = 1.1 \times 2.225 = 2.448 \text{ mol O}_2$$

$$\text{C balance : } n_2 = (0.85)(1) + (0.15)(2) \Rightarrow n_2 = 1.15 \text{ mol CO}_2$$

$$\text{H balance : } 2n_3 = (0.85)(4) + (0.15)(6) \Rightarrow n_3 = 2.15 \text{ mol H}_2\text{O}$$

$$10\% \text{ excess O}_2 \Rightarrow n_4 = (0.1)(2.225) \text{ mol O}_2 = 0.223 \text{ mol O}_2$$

### 9.51 (cont'd)

Reference states:  $\text{CH}_4(\text{g})$ ,  $\text{C}_2\text{H}_6(\text{g})$ ,  $\text{N}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{l})$ ,  $\text{CO}_2(\text{g})$  at  $25^\circ\text{C}$

For a constant volume process the heat released or absorbed is determined by the internal energy of reaction.

Substance	$n_{\text{in}}$ mol	$\hat{U}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{U}_{\text{out}}$ kJ/mol
$\text{CH}_4$	0.85	0	—	—
$\text{C}_2\text{H}_6$	0.15	0	—	—
$\text{O}_2$	2.225	0	0.223	0
$\text{CO}_2$	—	—	1.15	0
$\text{H}_2\text{O}(\text{v})$	—	—	2.15	$\hat{U}_1$

$$\hat{U}_1 = \Delta \hat{U}_{\text{v}}(25^\circ\text{C}) = \Delta \hat{H}_{\text{v}}(25^\circ\text{C}) - RT = 44.01 \text{ kJ/mol} - \frac{8.314 \text{ J}}{\text{mol K}} \left| \frac{1 \text{ kJ}}{1000 \text{ J}} \right| \frac{298 \text{ K}}{1} = 41.53 \frac{\text{kJ}}{\text{mol}}$$

$$\text{Eq. (9.1-5)} \Rightarrow \Delta \hat{U}_{\text{c}}^{\circ} = \Delta \hat{H}_{\text{c}}^{\circ} - RT \left( \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right)$$

$$\Rightarrow (\Delta \hat{U}_{\text{c}}^{\circ})_{\text{CH}_4} = (-890.36 \text{ kJ/mol}) - \frac{8.314 \text{ J}}{\text{mol K}} \left| \frac{298 \text{ K}}{1} \right| \frac{(1+2-1-2)}{10^3 \text{ J}} \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| = -890.36 \frac{\text{kJ}}{\text{mol}}$$

$$(\Delta \hat{U}_{\text{c}}^{\circ})_{\text{C}_2\text{H}_6} = (-1559.9 \text{ kJ/mol}) - \frac{8.314 \text{ J}}{\text{mol K}} \left| \frac{298 \text{ K}}{1} \right| \frac{(3+2-3.5-1)}{10^3 \text{ J}} \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| = -1561.14 \frac{\text{kJ}}{\text{mol}}$$

Energy balance:

$$\begin{aligned} Q = \Delta U &= n_{\text{CH}_4} (\Delta \hat{U}_{\text{c}}^{\circ})_{\text{CH}_4} + n_{\text{C}_2\text{H}_6} (\Delta \hat{U}_{\text{c}}^{\circ})_{\text{C}_2\text{H}_6} + \sum_{\text{out}} n_i \hat{U}_i - \sum_{\text{in}} n_i \hat{U}_i \\ &= (0.85 \text{ mol/s CH}_4)(-890.36 \text{ kJ/mol}) + (0.15 \text{ mol/s C}_2\text{H}_6)(-1561.14 \text{ kJ/mol}) \\ &\quad + (2.15 \text{ mol/s H}_2\text{O})(41.53 \text{ kJ/mol}) = -902 \text{ kJ} \\ &\Rightarrow \underline{\underline{-Q = 902 \text{ kJ}}} \text{ (transferred from reactor)} \end{aligned}$$

- c. Since the  $\text{O}_2$  (and  $\text{N}_2$  if air were used) are at  $25^\circ\text{C}$  at both the inlet and outlet of this process, their specific enthalpies or internal energies are zero and their amounts therefore have no effect on the calculated values of  $\Delta \hat{H}$  and  $\Delta U$ .

- 9.52 a.  $\dot{n}_{\text{fuel}}(-\Delta \hat{H}_{\text{c}}^{\circ}) = \dot{W}_s - \dot{Q}_l$  (Rate of heat release due to combustion = shaft work + rate of heat loss)

$$\begin{aligned} \dot{V}(\text{gal}) &\left| \frac{28.317 \text{ L}}{1 \text{ gal}} \right| \left| \frac{0.700 \text{ kg}}{1 \text{ L}} \right| \left| \frac{10^3 \text{ g}}{1 \text{ kg}} \right| \left| \frac{49 \text{ kJ}}{1 \text{ g}} \right| \\ &= \frac{100 \text{ hp}}{1.341 \times 10^{-3} \text{ hp}} \left| \frac{1 \text{ J/s}}{1 \text{ hp}} \right| \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| \left| \frac{3600 \text{ s}}{1 \text{ h}} \right| + \frac{15 \times 10^6 \text{ kJ}}{298 \text{ h}} \Rightarrow \underline{\underline{\dot{V} = 2.5 \text{ gal/h}}} \end{aligned}$$

- b. The work delivered would be less since more of the energy released by combustion would go into heating the exhaust gas.
- c. Heat loss increases as  $T_a$  decreases.  
Lubricating oil becomes thicker, so more energy goes to overcoming friction.

9.53

a.

Energy balance:  $\Delta U = 0 \Rightarrow \frac{n(\text{lb}_m \text{ fuel burned})}{\text{lb}_m} \left| \frac{\Delta \hat{U}_c^\circ (\text{Btu})}{\text{lb}_m} + mC_v(T_{\text{out}} - 77^\circ \text{F}) = 0 \right.$

$$\Rightarrow (0.00215)\Delta \hat{U}_c^\circ + (4.62 \text{ lb}_m)(0.900 \text{ Btu/lb}_m \cdot ^\circ \text{F})(87.06^\circ \text{F} - 77.00^\circ \text{F}) = 0$$

$$\Rightarrow \Delta \hat{U}_c^\circ = \underline{\underline{-19500 \text{ Btu/lb}_m}}$$

b. The reaction for which we determined  $\Delta \hat{U}_c^\circ$  isThe higher heating value is  $\Delta \hat{H}_r$  for the reaction

Eq. (9.1-5) on p. 441  $\Rightarrow \Delta \hat{H}_{c1}^\circ = \Delta \hat{U}_{c1}^\circ + RT(b + c - a)$

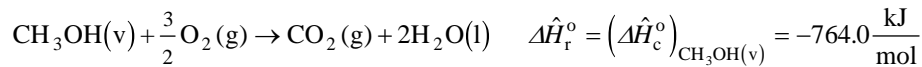
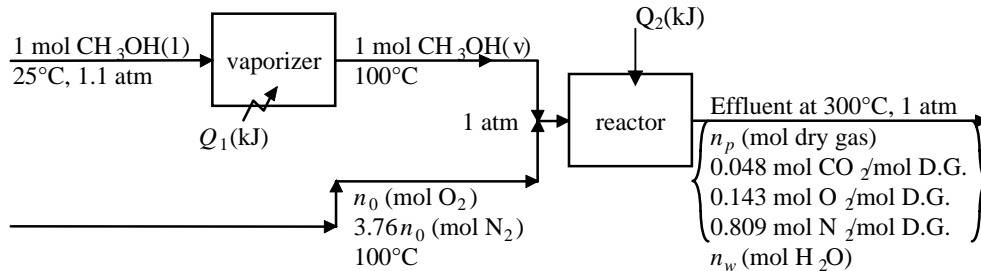
Eq. (9.6-1) on p. 462  $\Rightarrow \underset{(HHV)}{-\Delta \hat{H}_{c2}^\circ} = \underset{(LHV)}{-\Delta \hat{H}_{c1}^\circ} + c\Delta \hat{H}_v(\text{H}_2\text{O}, 77^\circ \text{F})$

To calculate the higher heating value, we therefore need

 $a = \text{lb-moles of O}_2 \text{ that react with 1 lb}_m \text{ fuel oil}$  $b = \text{lb-moles of CO}_2 \text{ formed when 1 lb}_m \text{ fuel oil is burned}$  $c = \text{lb-moles of H}_2\text{O formed when 1 lb}_m \text{ fuel oil is burned}$ 

9.54

a.

Basis: 1 mol CH<sub>3</sub>OH fed and burned

Overall C balance:  $\frac{1 \text{ mol CH}_3\text{OH}}{1 \text{ mol CH}_3\text{OH}} \left| \frac{1 \text{ mol C}}{1 \text{ mol CH}_3\text{OH}} = n_p(0.048)(1) \Rightarrow n_p = 20.83 \text{ mol dry gas} \right.$

N<sub>2</sub> balance:  $3.76n_0 = (20.83)(0.809) \Rightarrow n_0 = 4.482 \text{ mol O}_2$

Theoretical O<sub>2</sub>:  $(1 \text{ mol CH}_3\text{OH})(1.5 \text{ mol O}_2/\text{mol CH}_3\text{OH}) = 1.5 \text{ mol O}_2$

% excess air  $= \frac{(4.482 - 1.5) \text{ mol O}_2}{1.5 \text{ mol O}_2} \times 100\% = \underline{\underline{200\% \text{ excess air}}}$

H balance:  $(1 \text{ mol CH}_3\text{OH})(4 \text{ mol H}/1 \text{ mol CH}_3\text{OH}) = n_w(2) \Rightarrow n_w = 2 \text{ mol H}_2\text{O}$

(An atomic O balance  $\Rightarrow 9.96 \text{ mol O} = 9.96 \text{ mol O}$ , so that the results are consistent.)

$p_w^* = \frac{n_w}{n_w + n_p} \times P = \frac{2 \text{ mol H}_2\text{O}}{(2 + 20.83) \text{ mol}} \times 760 \text{ mm Hg} = 66.58 \text{ mm Hg} = p_w^*(T_{dp}) \xrightarrow{\text{Table B.3}} \underline{\underline{T_{dp} = 44.1^\circ \text{C}}}$

9.54 (cont'd)

b. Energy balance on vaporizer:

$$Q_1 = \Delta H = n\Delta\hat{H} = 1 \text{ mol} \left[ \int_{25}^{64.7} \underset{\substack{\uparrow \\ \text{Table B.2}}}{C_{pl}} dT + \underset{\substack{\uparrow \\ \text{Table B.1}}}{\Delta\hat{H}_v} + \int_{64.7}^{100} \underset{\substack{\uparrow \\ \text{Table B.2}}}{C_{pv}} dT \right] \frac{\text{kJ}}{\text{mol}} = \underline{\underline{40.33 \text{ kJ}}}$$

References : CH<sub>3</sub>OH(v), N<sub>2</sub>(g), O<sub>2</sub>(g), CO<sub>2</sub>(g), H<sub>2</sub>O(l) at 25°C

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ / mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ / mol)
CH <sub>3</sub> OH	1.00	3.603	—	—
N <sub>2</sub>	16.85	2.187	16.85	8.118
O <sub>2</sub>	4.482	2.235	2.98	8.470
CO <sub>2</sub>	—	—	1.00	11.578
H <sub>2</sub> O	—	—	2.00	53.58

$$\begin{aligned} \hat{H}(T) &= \hat{H}_i \text{ for N}_2, \text{ O}_2, \text{ CO}_2 \text{ (Table B.8)} \\ &= \Delta\hat{H}_v(25^\circ\text{C}) + \hat{H}_i \text{ for H}_2\text{O(v)} \text{ (Eq. 9.6-2a on p. 462, Table B.8)} \\ &= \int_{25}^T C_p dT \text{ for CH}_3\text{OH(v)} \text{ (Table B.2)} \end{aligned}$$

(Note: H<sub>2</sub>O(l) was chosen as the reference state since the given value of  $\Delta\hat{H}_c^\circ$  presumes liquid water as the product.)

Extent of reaction:  $(n_{\text{CH}_3\text{OH}})_{\text{out}} = (n_{\text{CH}_3\text{OH}})_{\text{in}} + \nu_{\text{CH}_3\text{OH}}\xi \Rightarrow 0 = 1 \text{ mol} - \xi \Rightarrow \xi = 1 \text{ mol}$

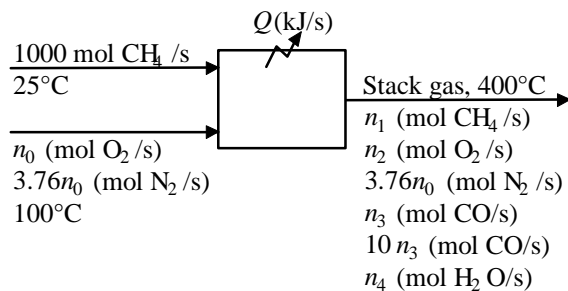
Energy balance on reactor:  $Q_2 = \xi\Delta\hat{H}_c^\circ + \sum_{\text{out}} n_i\hat{H}_i - \sum_{\text{in}} n_i\hat{H}_i$

$$\begin{aligned} &= (1)(-764.0) + [(16.85)(8.118) + \dots - (4.482)(2.235)] \text{ kJ} \\ &\quad \text{(Table B.1)} \\ &= -534 \text{ kJ} \Rightarrow \underline{\underline{534 \text{ kJ}}} \text{ transferred from reactor} \end{aligned}$$

9.55 a.



Basis: 1000 mol CH<sub>4</sub>/h fed



90% combustion  $\Rightarrow \dot{n}_1 = 0.10(1000) = 100 \text{ mol CH}_4/\text{s}$

Theoretical O<sub>2</sub> required = 2000 mol/s



### 9.55 (cont'd)

$$10\% \text{ excess } \underline{\text{O}_2} \Rightarrow \text{O}_2 \text{ fed} = 1.1(2000 \text{ mol/s}) = 2200 \text{ mol/s}$$

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:  $(1000)(4) = (100)(4) + 2\dot{n}_4 \Rightarrow \dot{n}_4 = 1800 \text{ mol H}_2\text{O/s}$

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

References: C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C

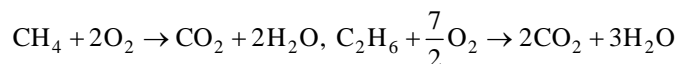
Substance	$\dot{n}_{\text{in}}$ (mol/s)	$\hat{H}_{\text{in}}$ (kJ/mol)	$\dot{n}_{\text{out}}$ (mol/s)	$\hat{H}_{\text{out}}$ (kJ/mol)
CH <sub>4</sub>	1000	-74.85	100	-57.62
O <sub>2</sub>	2200	2.24	441	11.72
N <sub>2</sub>	8272	2.19	8272	11.15
CO	—	—	81.8	-99.27
CO <sub>2</sub>	—	—	818	-377.2
H <sub>2</sub> O	—	—	1800	-228.63

$$\begin{aligned} \hat{H} &= \Delta \hat{H}_f^0 + \int_{25}^T \underset{\substack{\text{Table B.1} \\ \downarrow}}{C_p} dT \text{ for CH}_4 \\ &\quad \downarrow \substack{\text{Table B.2} \\ \text{Table B.8}} \\ &= \Delta \hat{H}_f^0 + \hat{H}_1(T) \text{ for others} \end{aligned}$$

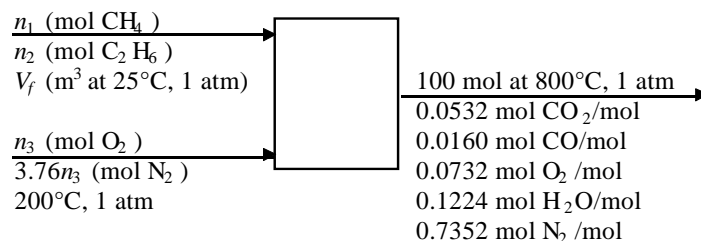
Energy balance:  $\dot{Q} = \Delta \dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = \underline{\underline{-5.85 \times 10^5 \text{ kJ/s (kW)}}}$

- b.**
- (i)  $T_{\text{air}} \uparrow$  (increases)  $\Rightarrow -\dot{Q} \uparrow$
  - (ii) %XS  $\uparrow \Rightarrow -\dot{Q} \downarrow$  (more energy required to heat additional O<sub>2</sub> and N<sub>2</sub> to 400°C, therefore less energy transferred.)
  - (iii)  $S_{\text{CO}_2/\text{CO}} \uparrow \Rightarrow -\dot{Q} \uparrow$  (reaction to form CO<sub>2</sub> has a greater heat of combustion and so releases more thermal energy)
  - (iv)  $T_{\text{stack}} \uparrow \Rightarrow -\dot{Q} \downarrow$  (more energy required to heat combustion products)

9.56



Basis : 100 mol stack gas. Assume ideal gas behavior.



a.

N<sub>2</sub> balance:  $3.76n_3 = (100)(0.7352) \text{ mol N}_2 \Rightarrow n_3 = 19.55 \text{ mol O}_2 \text{ fed}$

C balance:  $n_1(1) + n_2(2) = (100)(0.0532)(1) + (100)(0.0160)(1)$   
H balance:  $n_1(4) + n_2(6) = (100)(0.1224)(2)$

$$\left. \begin{array}{l} n_1(1) + n_2(2) = 1.164 \\ n_1(4) + n_2(6) = 2.448 \end{array} \right\} \Rightarrow \begin{array}{l} n_1 = 3.72 \text{ mol CH}_4 \\ n_2 = 1.60 \text{ mol C}_2\text{H}_6 \end{array}$$

$$V_f = \frac{(3.72 + 1.60) \text{ mol fuel gas}}{1 \text{ mol}} \left| \frac{22.4 \text{ L(STP)}}{1 \text{ mol}} \right| \left| \frac{298.2 \text{ K}}{273.2 \text{ K}} \right| \left| \frac{1 \text{ m}^3}{10^3 \text{ L}} \right| = 0.130 \text{ m}^3$$

$$\text{Theoretical O}_2 = \frac{3.72 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \right| + \frac{1.60 \text{ mol C}_2\text{H}_6}{1 \text{ mol C}_2\text{H}_6} \left| \frac{3.5 \text{ mol O}_2}{1 \text{ mol C}_2\text{H}_6} \right| = 13.04 \text{ mol O}_2$$

Fuel composition:  $\left. \begin{array}{l} 3.72 \text{ mol CH}_4 \\ 1.60 \text{ mol C}_2\text{H}_6 \end{array} \right\} \Rightarrow \begin{array}{l} 69.9 \text{ mole\% CH}_4 \\ 30.1 \text{ mole\% C}_2\text{H}_6 \end{array}$

% Excess air:  $\frac{(19.55 - 13.04) \text{ mol O}_2 \text{ in excess}}{13.04 \text{ mol O}_2 \text{ required}} \times 100\% = \underline{\underline{50\% \text{ excess air}}}$

b.

References : C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C

Substance	$n_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
CH <sub>4</sub>	3.72	-74.85	—	—
C <sub>2</sub> H <sub>6</sub>	1.60	-84.67	—	—
O <sub>2</sub>	19.55	5.31	7.32	25.35
N <sub>2</sub>	73.52	5.13	73.52	23.86
CO	—	—	1.60	-86.39
CO <sub>2</sub>	—	—	5.32	-356.1
H <sub>2</sub> O	—	—	12.24	-212.78

### 9.56 (cont'd)

$$\begin{aligned}
 \hat{H} &= \overset{\text{Table B.1}}{\downarrow} \Delta \hat{H}_f^o + \overset{\text{Table B.2, for CH}_4, \text{C}_2\text{H}_6}{\downarrow} \int_{25}^T C_p \, dT \\
 &= \Delta \hat{H}_f^o + \overset{\text{Table B.8}}{\downarrow} \hat{H}_i(T) \text{ for O}_2, \text{N}_2, \text{CO}, \text{CO}_2, \text{H}_2\text{O}(\text{v})
 \end{aligned}$$

Energy balance:

$$Q = \Delta H = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = \frac{-2764 \text{ kJ}}{0.130 \text{ m}^3 \text{ fuel}} = \underline{\underline{-2.13 \times 10^4 \text{ kJ/m}^3 \text{ fuel}}}$$

9.57

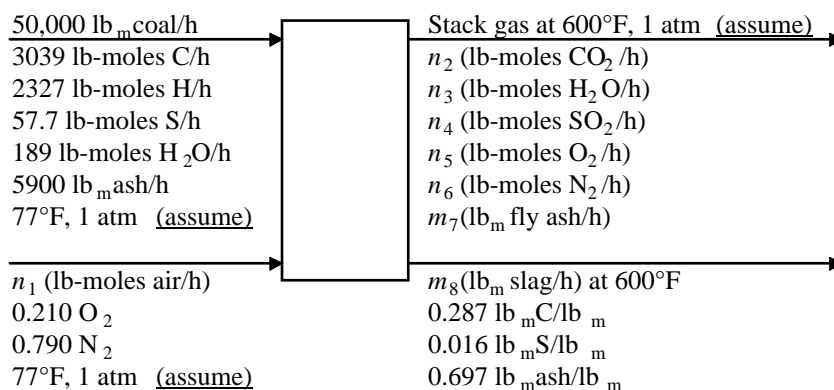
$$\text{Basis: } 50000 \text{ lb}_m \text{ coal fed/h} \Rightarrow \frac{(0.730)(50000) \text{ lb}_m \text{ C}}{\text{h}} \left| \frac{1 \text{ lb-mole C}}{12.01 \text{ lb}_m} \right. = 3039 \text{ lb-mole C/h}$$

$$(0.047)(50000)/1.01 = 2327 \text{ lb-moles H/h (does not include H in water)}$$

$$(0.037)(50000)/32.07 = 57.7 \text{ lb-moles S/h}$$

$$(0.068)(50000)/18.02 = 189 \text{ lb-moles H}_2\text{O/h}$$

$$(0.118)(50000) = 5900 \text{ lb}_m \text{ ash/h}$$



a. Feed rate of air:

$$\text{O}_2 \text{ required to oxidize carbon } (\text{C} + \text{O}_2 \rightarrow \text{CO}_2) = \frac{3039 \text{ lb-moles C}}{\text{h}} \left| \frac{1 \text{ lb-mole O}_2}{1 \text{ lb-mole C}} \right. = 3039 \text{ lb-moles O}_2/\text{h}$$

$$\text{Air fed: } \dot{n}_1 = \frac{1.5 \times 3039 \text{ lb-moles O}_2 \text{ fed}}{\text{h}} \left| \frac{1 \text{ mole air}}{0.210 \text{ mole O}_2} \right. = 21710 \text{ lb-moles air/h}$$

$$30\% \text{ ash in coal emerges in slag} \Rightarrow 0.697 \dot{m}_8 = 0.30(5900 \text{ lb}_m/\text{h}) \Rightarrow \dot{m}_8 = 2540 \text{ lb}_m \text{ slag/h}$$

$$\Rightarrow \dot{m}_7 = 0.700(5900) = 4130 \text{ lb}_m \text{ fly ash/h}$$

$$\text{C balance: } 3039(\text{lb-moles C/h}) = \dot{n}_2 + (0.287)(2540)/12.01$$

$$\Rightarrow \dot{n}_2 = 2978 \text{ lb-moles CO}_2/\text{h} \xrightarrow{M_{\text{CO}_2}=44.01} 1.31 \times 10^5 \text{ lb}_m \text{ CO}_2/\text{h}$$

$$\text{H balance: } 2327(\text{lb-moles H/h}) + (189)(2) = 2\dot{n}_3$$

$$\Rightarrow \dot{n}_3 = 1352.5 \text{ lb-moles H}_2\text{O/h} \xrightarrow{M_{\text{H}_2\text{O}}=18.02} 2.44 \times 10^4 \text{ lb}_m \text{ H}_2\text{O/h}$$

$$\text{N}_2 \text{ balance: } \dot{n}_6 = (0.790)21710 \text{ lb-moles/h} = 17150 \text{ lb-moles N}_2/\text{h} \xrightarrow{M_{\text{N}_2}=28.02} 4.81 \times 10^5 \text{ lb}_m \text{ N}_2/\text{h}$$

$$\text{S balance: } 57.7(\text{lb-moles S/h}) = (1)\dot{n}_4 + 0.016(2540)/32.06$$

$$\Rightarrow \dot{n}_4 = 56.4 \text{ lb-moles SO}_2/\text{h} \xrightarrow{M_{\text{SO}_2}=64.2} 3620 \text{ lb}_m \text{ SO}_2/\text{h}$$

$$\text{O balance: } \underbrace{(189)(1)}_{(\text{coal})} + \underbrace{(0.21)(21710)(2)}_{(\text{air})} = \underbrace{(2978)(2)}_{(\text{CO}_2)} + \underbrace{(1352.5)(1)}_{(\text{H}_2\text{O})} + \underbrace{(56.4)(2)}_{(\text{SO}_2)} + \underbrace{2\dot{n}_5}_{(\text{O}_2)}$$

$$\Rightarrow \dot{n}_5 = 943 \text{ lb-moles O}_2/\text{h} \Rightarrow 30200 \text{ lb}_m \text{ O}_2/\text{h}$$

9.57 (cont'd)

Summary of component mass flow rates

Stack gas at 600° F, 1 atm

$$\left. \begin{array}{l} 2978 \text{ lb-moles CO}_2/\text{h} \Rightarrow \underline{\underline{131000 \text{ lb}_m \text{ CO}_2/\text{h}}} \\ 1352.5 \text{ lb-moles H}_2\text{O}/\text{h} \Rightarrow \underline{\underline{24400 \text{ lb}_m \text{ H}_2\text{O}/\text{h}}} \\ 56.4 \text{ lb-moles SO}_2/\text{h} \Rightarrow \underline{\underline{3620 \text{ lb}_m \text{ SO}_2/\text{h}}} \\ 943 \text{ lb-moles O}_2/\text{h} \Rightarrow \underline{\underline{30200 \text{ lb}_m \text{ O}_2/\text{h}}} \\ 17150 \text{ lb-moles N}_2/\text{h} \Rightarrow \underline{\underline{48100 \text{ lb}_m \text{ N}_2/\text{h}}} \\ \underline{\underline{4130 \text{ lb}_m \text{ fly ash/h}}} \end{array} \right\} 674,350 \text{ lb}_m \text{ stack gas/h}$$

Check:  $[50000 + (21710)(29)]_{\text{in}} \Leftrightarrow [674350 + 2540]_{\text{out}}$   
 $\Rightarrow (679600)_{\text{in}} \Leftrightarrow (676900)_{\text{out}} \text{ (0.4\% roundoff error)}$

Total molar flow rate = 22480 lb-moles/h at 600° F, 1 atm (excluding fly ash)

$$\Rightarrow V = \frac{22480 \text{ lb-moles}}{\text{h}} \left| \frac{359 \text{ ft}^3 (\text{STP})}{1 \text{ lb-mole}} \right| \frac{1060^\circ \text{R}}{492^\circ \text{R}} = \underline{\underline{1.74 \times 10^7 \text{ ft}^3/\text{h}}}$$

b. References: Coal components, air at 77° F  $\Rightarrow \sum_{\text{in}} n_i \hat{H}_i = 0$

Stack gas:  $n\hat{H} = \frac{674350 \text{ lb}_m}{\text{h}} \left| \frac{7.063 \text{ Btu}}{\text{lb-mole} \cdot ^\circ \text{F}} \right| \frac{1 \text{ lb-mole}}{28.02 \text{ lb}_m} \frac{(600 - 77)^\circ \text{F}}{1} = 8.90 \times 10^7 \text{ Btu/h}$

Slag:  $n\hat{H} = \frac{2540 \text{ lb}_m}{\text{h}} \left| \frac{0.22 \text{ Btu}}{\text{lb}_m \cdot ^\circ \text{F}} \right| \frac{(600 - 77)^\circ \text{F}}{1} = 2.92 \times 10^5 \text{ Btu/h}$

Energy balance:  $Q = \Delta H = n_{\text{coal burned}} \Delta \hat{H}_c^\circ (77^\circ \text{F}) + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i$   
 $= \frac{5 \times 10^4 \text{ lb}_m}{\text{h}} \left| \frac{-1.8 \times 10^4 \text{ Btu}}{\text{lb}_m} \right| + (8.90 \times 10^7 + 2.92 \times 10^5) \text{ Btu/h}$   
 $= -8.11 \times 10^8 \text{ Btu/h}$

Power generated =  $\frac{(0.35)(8.11 \times 10^8) \text{ Btu}}{\text{h}} \left| \frac{1 \text{ hr}}{3600 \text{ s}} \right| \frac{1 \text{ W}}{9.486 \times 10^{-4} \text{ Btu/s}} \left| \frac{1 \text{ MW}}{10^6 \text{ W}} \right| = \underline{\underline{83.1 \text{ MW}}}$

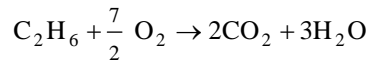
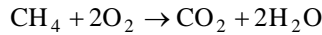
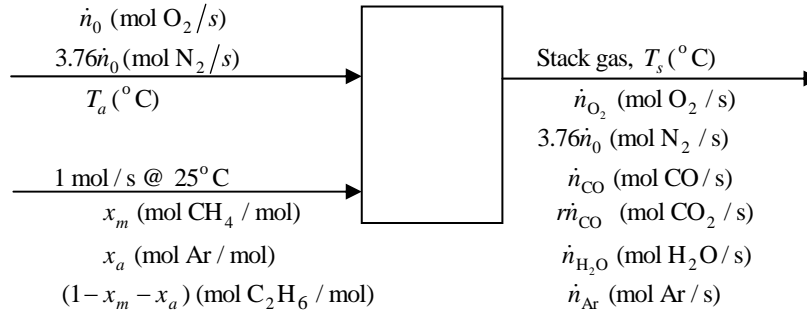
c.  $\hat{Q} = (-8.11 \times 10^8 \text{ Btu/h}) / (5000 \text{ lb}_m \text{ coal/h}) = -1.62 \times 10^4 \text{ Btu/lb}_m \text{ coal}$

$$\Rightarrow \frac{-\hat{Q}}{HHV} = \frac{1.62 \times 10^4 \text{ Btu/lb}_m}{1.80 \times 10^4 \text{ Btu/lb}_m} = \underline{\underline{0.901}}$$

Some of the heat of combustion goes to vaporize water and heat the stack gas.

d.  $-\hat{Q}/HHV$  would be closer to 1. Use heat exchange between the entering air and the stack gas.

9.58 b. Basis : 1 mol fuel gas/s



Percent excess air:  $\dot{n}_0 = (1 + \frac{P_{xs}}{100})[2x_m + 3.5(1 - x_m - x_a)]$

C balance:  $x_m + 2(1 - x_m - x_a) = (1 + r)\dot{n}_{\text{CO}} \Rightarrow \dot{n}_{\text{CO}} = \frac{x_m + 2(1 - x_m - x_a)}{(1 + r)}$

H balance:  $4x_m + 6(1 - x_m - x_a) = 2\dot{n}_{\text{H}_2\text{O}} \Rightarrow \dot{n}_{\text{H}_2\text{O}} = 2x_m + 3(1 - x_m - x_a)$

O balance:  $2\dot{n}_0 = 2\dot{n}_{\text{O}_2} + \dot{n}_{\text{CO}} + 2r\dot{n}_{\text{CO}} + \dot{n}_{\text{H}_2\text{O}} \Rightarrow \dot{n}_{\text{O}_2} = \dot{n}_0 - \dot{n}_{\text{CO}}(1 + 2r) / 2 - \dot{n}_{\text{H}_2\text{O}} / 2$

References : C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C

Substance	$n_{in}$	$\hat{H}_{in}$	$n_{out}$	$\hat{H}_{out}$
CH <sub>4</sub>	$x_m$	0	—	—
C <sub>2</sub> H <sub>6</sub>	$(1 - x_m - x_A)$	0	—	—
A	$x_A$	0	$x_A$	$\hat{H}_3$
O <sub>2</sub>	$n_o$	$\hat{H}_1$	$n_{\text{O}_2}$	$\hat{H}_4$
N <sub>2</sub>	$3.76n_o$	$\hat{H}_2$	$3.76n_o$	$\hat{H}_5$
CO	—	—	$n_{\text{CO}}$	$\hat{H}_6$
CO <sub>2</sub>	—	—	$r n_{\text{CO}}$	$\hat{H}_7$
H <sub>2</sub> O	—	—	$n_{\text{H}_2\text{O}}$	$\hat{H}_8$

c. 
$$\hat{H}_i = (\Delta\hat{H}_f)_i + \int_{25}^{T_a \text{ or } T_s} C_{p,i} dT$$

Given :  $x_m = 0.85$ ,  $x_a = 0.05$ ,  $P_{xs} = 5\%$ ,  $r = 10.0$ ,  $T_a = 150^\circ\text{C}$ ,  $T_s = 700^\circ\text{C}$

$\Rightarrow n_o = 2.153$ ,  $n_{\text{CO}} = 0.0955$ ,  $n_{\text{H}_2\text{O}} = 2.00$ ,  $n_{\text{O}_2} = 0.1500$

$\hat{H}_1 (\text{kJ/mol}) = 8.091$ ,  $\hat{H}_2 = 29.588$ ,  $\hat{H}_3 = 0.702$ ,  $\hat{H}_4 = 3.279$ ,

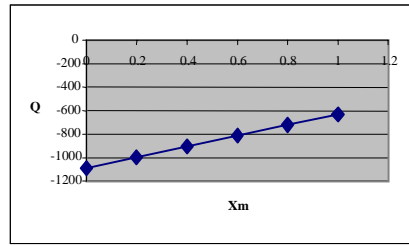
$\hat{H}_5 = 166.72$ ,  $\hat{H}_6 = -8567$ ,  $\hat{H}_7 = -345.35$ ,  $\hat{H}_8 = -433.82$

Energy balance:  $\dot{Q} = \sum \dot{n}_{out} \hat{H}_{out} - \sum \dot{n}_{in} \hat{H}_{in} = \underline{\underline{-655 \text{ kW}}}$

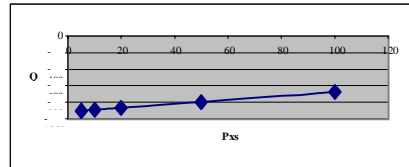
9.58 (cont'd)

d. Xa Pxs r Ta Ts Q

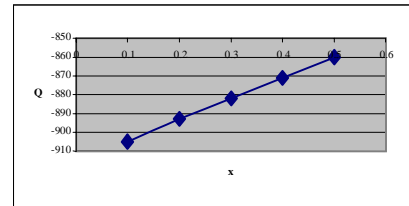
0.0	5	10	150	700	-
0.0	5	10	150	700	-
0.0	5	10	150	700	-
0.0	5	10	150	700	-
0.0	5	10	150	700	-
0.0	5	10	150	700	-



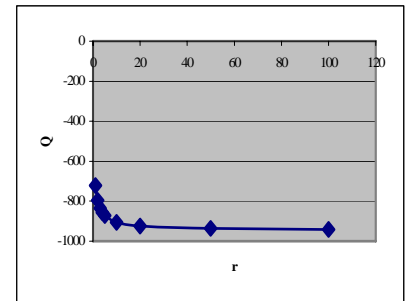
0.1	5	10	150	700	-
0.1	10	10	150	700	-
0.1	20	10	150	700	-
0.1	50	10	150	700	-
0.1	100	10	150	700	-



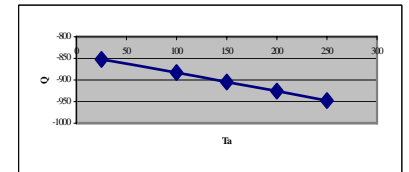
0.1	5	10	150	700	-
0.2	5	10	150	700	-
0.3	5	10	150	700	-
0.4	5	10	150	700	-
0.5	5	10	150	700	-



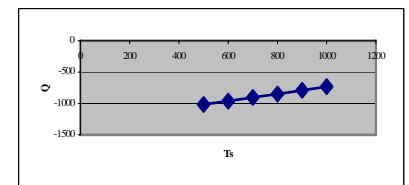
0.1	5	1	150	700	-722
0.1	5	2	150	700	-796
0.1	5	3	150	700	-834
0.1	5	4	150	700	-856
0.1	5	5	150	700	-871
0.1	5	10	150	700	-905
0.1	5	20	150	700	-924
0.1	5	50	150	700	-936
0.1	5	100	150	700	-941



0.1	5	10	25	700	-852
0.1	5	10	100	700	-883
0.1	5	10	150	700	-905
0.1	5	10	200	700	-926
0.1	5	10	250	700	-948



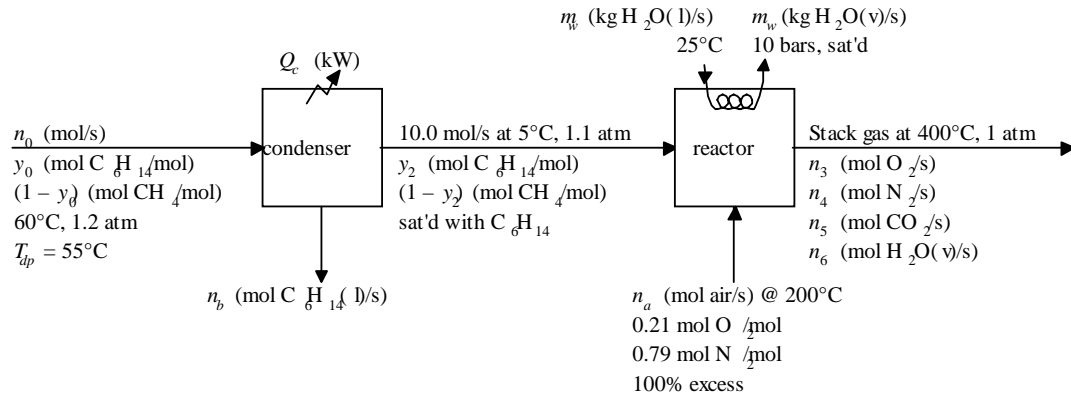
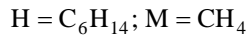
0.1	5	10	150	500	-1014
0.1	5	10	150	600	-960
0.1	5	10	150	700	-905
0.1	5	10	150	800	-848
0.1	5	10	150	900	-790
0.1	5	10	150	1000	-731



9.59

a.

Basis:  $\frac{207.4 \text{ liters}}{\text{s}} \mid \frac{273.2 \text{ K}}{278.2 \text{ K}} \mid \frac{1.1 \text{ atm}}{1.0 \text{ atm}} \mid \frac{1 \text{ mol}}{22.4 \text{ liters(STP)}} = 10.0 \text{ mols/s fuel gas to furnace}$



Antoine Eq.  
↓

$$T_{dp} = 55^\circ\text{C} \Rightarrow y_0 P = p_H^*(55^\circ\text{C}) = 483.3 \text{ mm Hg}$$

$$\Rightarrow y_0 = \frac{483.3 \text{ mm Hg}}{1.2 \times 760 \text{ mm Hg}} = 0.530 \text{ mol C}_6\text{H}_{14}/\text{mol} \Rightarrow 0.470 \text{ mol CH}_4/\text{mol}$$

Saturation at condenser outlet:

$$y_2 = \frac{p_H^*(5^\circ\text{C})}{P} = \frac{58.89 \text{ mm Hg}}{1.1 \times 760 \text{ mm Hg}} = 0.070 \text{ mol C}_6\text{H}_{14}/\text{mol} = 0.93\% \text{ mol CH}_4/\text{mol}$$

Methane balance on condenser:  $\dot{n}_0(1 - y_0) = 10.0(1 - y_2) \xRightarrow[y_2=0.070]{y_0=0.530} \dot{n}_0 = 19.78 \text{ mol/s}$

Hexane balance on condenser:  $\dot{n}_0 y_0 = \dot{n}_b + 10.0 y_2 \xRightarrow[\dot{n}_0=19.78, y_0=0.530, y_2=0.070]{\dot{n}_b=9.78 \text{ mol C}_6\text{H}_{14}/\text{s condensed}}$

$$\text{Volume of condensate} = \frac{9.78 \text{ mol C}_6\text{H}_{14}(\text{l})}{\text{s}} \mid \frac{86.17 \text{ g}}{\text{mol}} \mid \frac{\text{cm}^3}{0.659 \text{ g}} \mid \frac{1 \text{ L}}{10^3 \text{ cm}^3} \mid \frac{3600 \text{ s}}{1 \text{ h}}$$

$$= 4600 \text{ L C}_6\text{H}_{14}(\text{l})/\text{h}$$

b.

References :  $\text{CH}_4(\text{g}, 5^\circ\text{C}), \text{C}_6\text{H}_{14}(\text{l}, 5^\circ\text{C})$

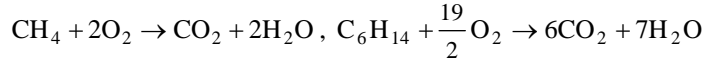
Substance	$\dot{n}_{\text{in}}$ (mol / s)	$\hat{H}_{\text{in}}$ (kJ / mol)	$\dot{n}_{\text{out}}$ (mol / s)	$\hat{H}_{\text{out}}$ (kJ / mol)
CH <sub>4</sub>	9.30	1.985	9.30	0
C <sub>6</sub> H <sub>14</sub> (v)	10.48	41.212	0.70	32.940
C <sub>6</sub> H <sub>14</sub> (l)	—	—	9.78	0

$$\text{CH}_4(\text{g}): \hat{H} = \int_5^T \downarrow_{\text{Table B.2}} C_p dT \quad \text{C}_6\text{H}_{14}(\text{v}): \hat{H} = \int_5^{T_b} \downarrow_{\text{Table B.1}} C_{pR} dT + \Delta \hat{H}_v + \int_{T_b}^T \downarrow_{\text{Table B.1}} C_{pV} dT$$

Condenser energy balance:  $\dot{Q}_c = \Delta \dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = -427 \text{ kW}$



9.59 (cont'd)



$$\text{Theoretical O}_2: \frac{9.30 \text{ mol CH}_4}{\text{s}} \left| \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \right| + \frac{0.70 \text{ mol C}_6\text{H}_{14}}{\text{s}} \left| \frac{9.5 \text{ mol O}_2}{1 \text{ mol C}_6\text{H}_{14}} \right| = 25.3 \text{ mol O}_2/\text{s}$$

$$100\% \text{ excess} \Rightarrow (\text{O}_2)_{\text{fed}} = 2 \times (\text{O}_2)_{\text{theor.}} \Rightarrow 0.21\dot{n}_a = 2 \times 25.3 \Rightarrow \dot{n}_a = 240.95 \text{ mol air/s}$$

$$\text{N}_2 \text{ balance: } 0.79(240.95) = \dot{n}_4 \Rightarrow \dot{n}_4 = 190.35 \text{ mol N}_2/\text{s}$$

C balance:

$$\frac{9.30 \text{ mol CH}_4}{\text{s}} \left| \frac{1 \text{ mol C}}{1 \text{ mol CH}_4} \right| + \frac{0.70 \text{ mol C}_6\text{H}_{14}}{\text{s}} \left| \frac{6 \text{ mol C}}{1 \text{ mol C}_6\text{H}_{14}} \right| = \frac{\dot{n}_5 (\text{mol CO}_2)}{\text{s}} \left| \frac{1 \text{ mol C}}{1 \text{ mol CO}_2} \right|$$

$$\Rightarrow \dot{n}_5 = 13.5 \text{ mol CO}_2/\text{s}$$

H balance:

$$(9.30 \text{ mol CH}_4/\text{s})(4 \text{ mol H/mol CH}_4) + (0.70)(14) = \dot{n}_6(2) \Rightarrow \dot{n}_6 = 23.5 \text{ mol H}_2\text{O}$$

$$\text{Since combustion is complete, } (\text{O}_2)_{\text{remaining}} = (\text{O}_2)_{\text{excess}} = \frac{1}{2}(\text{O}_2)_{\text{fed}} \Rightarrow \dot{n}_3 = 25.3 \text{ mol O}_2/\text{s}$$

References : C(s), H<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g) at 25°C for reactor side, H<sub>2</sub>O(l) at triple point for steam side (reference state for steam tables)

Substance	$\dot{n}_{\text{in}}$ mol / s	$\hat{H}_{\text{in}}$ kJ / mol	$\dot{n}_{\text{out}}$ mol / s	$\hat{H}_{\text{out}}$ kJ / mol
CH <sub>4</sub>	9.30	-75.553	—	—
C <sub>6</sub> H <sub>14</sub> (v)	0.70	-170.07	—	—
O <sub>2</sub>	50.6	5.31	25.3	11.72
N <sub>2</sub>	190.35	5.13	190.35	11.15
CO <sub>2</sub>	—	—	13.5	-377.15
H <sub>2</sub> O(v)	—	—	23.5	-228.60
H <sub>2</sub> O(boiler water)	$\dot{m}_w$ (kg / s)	104.8	$\dot{m}_w$ (kg / s)	2776.2

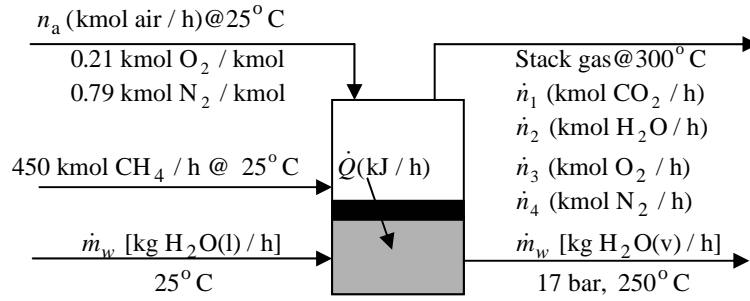
$$\begin{array}{c} \text{Table B.1 and B.2} \\ \downarrow \\ \hat{H}(T) = \Delta\hat{H}_f^\circ + \int_{25}^T C_p dT \quad \text{for CH}_4, \text{C}_6\text{H}_{14} \end{array}$$

$$\begin{array}{c} \text{Table B.1 and B.8} \\ \downarrow \\ = \Delta\hat{H}_f^\circ + \hat{H}_i(T) \quad \text{for O}_2, \text{N}_2, \text{CO}_2, \text{H}_2\text{O}(v) \end{array}$$

Energy balance on reactor (assume adiabatic):

$$\Delta\dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = 0 \Rightarrow -8468 + \dot{m}_w (2776.2 - 104.8) = 0 \Rightarrow \dot{m}_w = \underline{\underline{3.2 \text{ kg steam/s}}}$$

9.60 a. Basis: 450 kmol CH<sub>4</sub> fed/h CH<sub>4</sub> + 2O<sub>2</sub> → CO<sub>2</sub> + 2H<sub>2</sub>O



$$\text{Air fed: } \dot{n}_a = \frac{450 \text{ kmol CH}_4}{\text{h}} \left| \frac{2 \text{ kmol O}_2 \text{ req'd}}{1 \text{ kmol CH}_4} \right| \frac{1.2 \text{ kmol O}_2 \text{ fed}}{1 \text{ kmol O}_2 \text{ req'd}} \left| \frac{1 \text{ kmol air}}{0.21 \text{ kmol O}_2} \right|$$

$$= 5143 \text{ kmol air/h}$$

$$450 \text{ kmol/h CH}_4 \text{ react} \Rightarrow \dot{n}_1 = 450 \text{ kmol CO}_2/\text{h}, \dot{n}_2 = 900 \text{ kmol H}_2\text{O/h}$$

$$\text{N}_2 \text{ balance: } \dot{n}_4 = (0.79)(5143 \times 10^6 \text{ mol/h}) = 4060 \text{ kmol N}_2/\text{h}$$

Molecular O<sub>2</sub> balance:

$$\dot{n}_3 = (0.21)(5143) \frac{\text{mol O}_2 \text{ fed}}{\text{h}} - \frac{450 \text{ kmol CH}_4 \text{ react}}{\text{h}} \left| \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \right| = 180 \text{ kmol O}_2/\text{h}$$

$$\left. \begin{array}{l} 450 \text{ kmol CO}_2/\text{h} \\ 900 \text{ kmol H}_2\text{O/h} \\ 4060 \text{ kmol N}_2/\text{h} \\ 180 \text{ kmol O}_2/\text{h} \end{array} \right\} \Rightarrow \begin{array}{l} y_{\text{CO}_2} = 0.0805 \\ y_{\text{H}_2\text{O}} = 0.161 \\ y_{\text{N}_2} = 0.726 \\ y_{\text{O}_2} = 0.0322 \end{array}$$

$$5590 \text{ kmol/h}$$

Mean heat capacity of stack gas

$$\bar{C}_p = \sum y_i C_{pi} = (0.0805)(0.0423) + (0.161)(0.0343) + (0.726)(0.0297) + (0.0322)(0.0312)$$

$$= 0.0315 \text{ kJ/mol} \cdot ^\circ\text{C}$$

Energy balance on furnace (combustion side only)

References: CH<sub>4</sub>(g), CO<sub>2</sub>(g), O<sub>2</sub>(g), N<sub>2</sub>(g), H<sub>2</sub>O(l) at 25°C

Substance	$\dot{n}_{\text{in}}$ (kmol/h)	$\hat{H}_{\text{in}}$ (kJ/kmol)	$\dot{n}_{\text{out}} \hat{H}_{\text{out}}$ (kJ/h)
CH <sub>4</sub>	450	0	—
Air	5143	0	—
Stack gas	—	—	$\dot{H}_p$

Extent of reaction:

$$\xi = \dot{n}_{\text{CH}_4} = 450 \text{ kmol/h}$$

9.60 (cont'd)

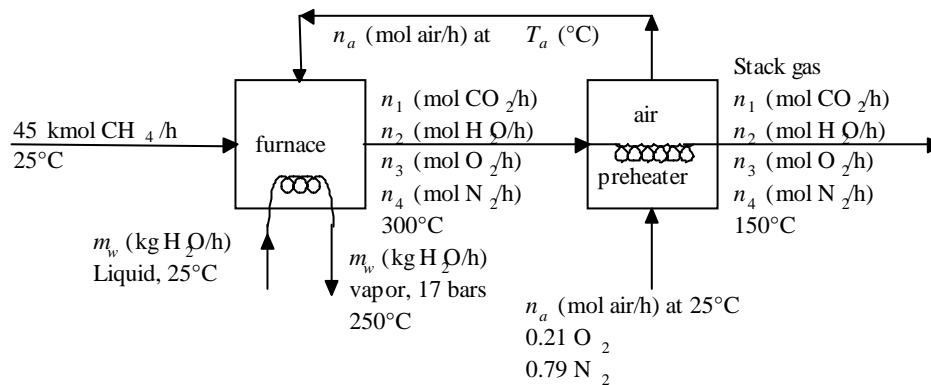
$$\begin{aligned}\dot{H}_p &= \dot{n}_2 (\Delta \hat{H}_v)_{\text{H}_2\text{O}(25^\circ\text{C})} + \dot{n}_{\text{stack gas}} (\bar{C}_p)_{\text{stack gas}} (T_{\text{stack gas}} - 25^\circ\text{C}) \\ &= \frac{180 \text{ kmol H}_2\text{O}}{\text{h}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{44.01 \text{ kJ}}{\text{mol}} + \frac{5590 \text{ kmol}}{\text{h}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{0.0315 \text{ kJ}}{\text{mol} \cdot ^\circ\text{C}} (300 - 25)^\circ\text{C} \\ &= \underline{\underline{5.63 \times 10^7 \text{ kJ/h}}}\end{aligned}$$

$$\begin{aligned}\dot{Q} = \Delta \dot{H} &= \xi (\Delta \hat{H}_c^\circ)_{\text{CH}_4} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i \\ &= \left( 450 \frac{\text{kmol}}{\text{h}} \right) \left( 1000 \frac{\text{mol}}{\text{kmol}} \right) \left( -890.36 \frac{\text{kJ}}{\text{mol}} \right) + 5.63 \times 10^7 \frac{\text{kJ}}{\text{h}} = \underline{\underline{-3.44 \times 10^8 \frac{\text{kJ}}{\text{h}}}}\end{aligned}$$

Energy balance on steam boiler

$$\begin{aligned}\dot{Q} = \dot{m}_w \Delta \hat{H}_w &\Rightarrow +3.44 \times 10^8 \frac{\text{kJ}}{\text{h}} = \left[ \dot{m}_w \left( \frac{\text{kg}}{\text{h}} \right) \right] \left[ (2914 - 105) \frac{\text{kJ}}{\text{kg}} \right] \\ &\Rightarrow \underline{\underline{\dot{m}_w = 1.23 \times 10^5 \text{ kg steam/h}}}\end{aligned}$$

b.



E.B. on overall process: The material balances and the energy balance are identical to those of part (a), except that the stack gas exits at 150°C instead of 300°C.

References:  $\text{CH}_4(\text{g})$ ,  $\text{CO}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{l})$  at 25°C (furnace side)

$\text{H}_2\text{O}(\text{l})$  at triple point (steam table reference) (steam tube side)

Substance	$\dot{n}_{\text{in}}$ (kmol/h)	$\hat{H}_{\text{in}}$ (kJ/kmol)	$\dot{n}_{\text{out}} \hat{H}_{\text{out}}$ (kJ/h)
$\text{CH}_4$	450	0	—
Air	5143	0	—
Stack gas	—	—	$\dot{H}_p$
$\text{H}_2\text{O}$	$\dot{m}_w$ (kg/h)	105 kJ/kg	$\dot{m}_w$ (kg/h) 2914 kJ/kg

$$\begin{aligned}\dot{H}_p &= \dot{n}_2 (\Delta \hat{H}_v)_{\text{H}_2\text{O}(25^\circ\text{C})} + \dot{n}_{\text{stack gas}} (\bar{C}_p)_{\text{stack gas}} (T_{\text{stack gas}} - 25^\circ\text{C}) \\ &= \frac{180 \text{ kmol H}_2\text{O}}{\text{h}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{44.01 \text{ kJ}}{\text{mol}} + \frac{5590 \text{ kmol}}{\text{h}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{0.0315 \text{ kJ}}{\text{mol} \cdot ^\circ\text{C}} (150 - 25)^\circ\text{C} \\ &= \underline{\underline{2.99 \times 10^7 \text{ kJ/h}}}\end{aligned}$$

### 9.60 (cont'd)

$$\Delta \dot{H} = \dot{\xi}(\Delta \hat{H}_c^\circ)_{\text{CH}_4} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = 0$$

$$\Rightarrow \left( 450 \frac{\text{kmol}}{\text{h}} \right) \left( 1000 \frac{\text{mol}}{\text{kmol}} \right) \left( -890.36 \frac{\text{kJ}}{\text{mol}} \right) + 2.99 \times 10^7 \frac{\text{kJ}}{\text{h}}$$

$$+ \left[ \dot{m}_w \left( \frac{\text{kg}}{\text{h}} \right) \right] \left[ (2914 - 105) \frac{\text{kJ}}{\text{kg}} \right] = 0 \Rightarrow m_w = \underline{\underline{1.32 \times 10^5 \text{ kg steam/h}}}$$

Energy balance on preheater:  $\Delta \dot{H} = (\Delta \dot{H})_{\text{stack gas}} + (\Delta \dot{H})_{\text{air}} = 0$

$$(\Delta H)_{\text{stack gas}} = n \bar{C}_p \Delta T = \frac{5590 \text{ kmol}}{\text{h}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{0.0315 \text{ kJ}}{\text{mol} \cdot ^\circ\text{C}} \frac{(150 - 300)^\circ\text{C}}{1} = -2.64 \times 10^7 \frac{\text{kJ}}{\text{h}}$$

$$(-\Delta H)_{\text{stack gas}} = (\Delta H)_{\text{air}} = n_a \hat{H}_{\text{air}}(T_a) \Rightarrow \hat{H}_{\text{air}}(T_a) = \frac{2.64 \times 10^7 \text{ kJ/h}}{5143 \text{ kmol/h}} \left| \frac{1 \text{ kmol}}{10^3 \text{ mol}} \right| = 5.133 \frac{\text{kJ}}{\text{mol}}$$

$$\hat{H}_{\text{air}} = 5.133 \text{ kJ/mol} \quad \text{Table B.8} \quad \underline{\underline{T_a = 199^\circ\text{C}}}$$

- c. The energy balance on the furnace includes the term  $-\sum n_{\text{in}} \hat{H}_{\text{in}}$ . If the air is preheated and the stack gas temperature remains the same, this term and hence  $\dot{Q}$  become more negative, meaning that more heat is transferred to the boiler water and more steam is produced. The stack gas is a logical heating medium since it is available at a high temperature and costs nothing.

### 9.61

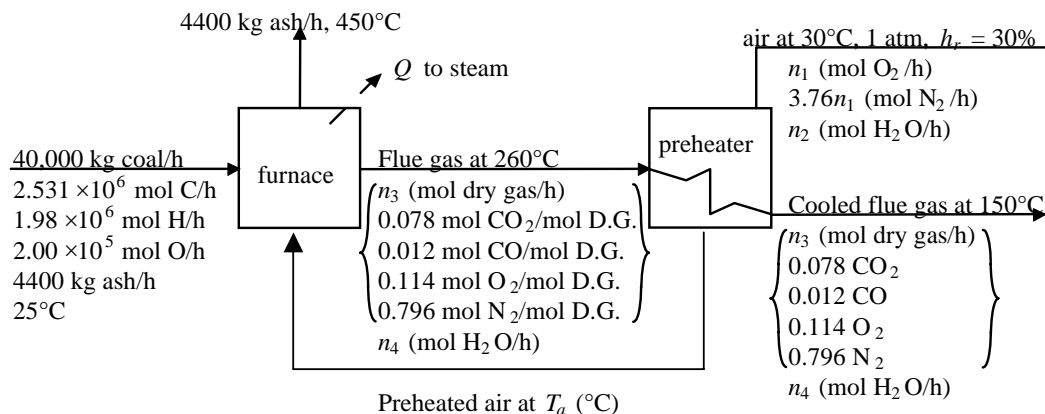
Basis: 40000 kg coal/h  $\Rightarrow \frac{(0.76 \times 40000) \text{ kg C}}{\text{h}} \left| \frac{10^3 \text{ g}}{1 \text{ kg}} \right| \frac{1 \text{ mol C}}{12.01 \text{ g}} = 2.531 \times 10^6 \text{ mol C/h}$

Assume coal enters at 25°C

$$[(0.05 \times 4000) \text{ kg H/h}] \left( \frac{10^3}{1.01} \right) = 1.98 \times 10^6 \text{ mol H/h}$$

$$[(0.08 \times 4000) \text{ kg O/h}] \left( \frac{10^3}{16.0} \right) = 2.00 \times 10^5 \text{ mol O/h}$$

$$(0.11 \times 40000) = 4400 \text{ kg ash/h}$$



#### a. Overall system balances

C balance:  $2.531 \times 10^6 = 0.078n_3 + 0.012n_3 \Rightarrow n_3 = 2.812 \times 10^7 \text{ mol/h dry flue gas}$

N<sub>2</sub> balance:  $3.76n_1 = (0.796)(2.812 \times 10^7) \Rightarrow n_1 = 5.95 \times 10^6 \text{ mol O}_2/\text{h}$   $(3.76)(5.95 \times 10^6)$   
 $= 224 \times 10^7 \text{ mol N}_2/\text{h}$

### 9.61 (cont'd)

30% relative humidity (inlet air):

$$y_{\text{H}_2\text{O}} P = 0.30 p_{\text{H}_2\text{O}}^*(30^\circ\text{C}) \Rightarrow \frac{\dot{n}_2}{5.95 \times 10^6 + 2.24 \times 10^7 + n_2} (760 \text{ mm Hg}) = 0.300 (31.824 \text{ mm Hg})$$

Table B.3  
↓

$$\Rightarrow \dot{n}_2 = 3.61 \times 10^5 \text{ mol H}_2\text{O/h}$$

Volumetric flow rate of inlet air:

$$\dot{V} = \frac{(5.95 \times 10^6 + 2.24 \times 10^7 + 3.61 \times 10^5) \text{ mol}}{\text{h}} \left| \frac{22.4 \text{ liters(STP)}}{1 \text{ mol}} \right| \left| \frac{1 \text{ m}^3}{10^3 \text{ liters}} \right| = 6.43 \times 10^5 \text{ SCM/h}$$

Air/fuel ratio:  $\frac{6.43 \times 10^5 \text{ m}^3 \text{ air/h}}{40000 \text{ kg coal/h}} = \underline{\underline{16.1 \text{ SCM air/kg coal}}}$

H balance:  $\underbrace{1.98 \times 10^6 \text{ mol H/h}}_{\text{H in coal}} + 2 \underbrace{(3.61 \times 10^5) \text{ mol H/h}}_{\text{H in water vapor}} = 2\dot{n}_4 \Rightarrow \dot{n}_4 = 1.351 \times 10^6 \text{ mol H}_2\text{O/h}$

H<sub>2</sub>O content of stack gas =  $\frac{1.357 \times 10^6 \text{ mol H}_2\text{O/h}}{(1.357 \times 10^6 + 2.812 \times 10^7) \text{ mol/h}} \times 100\% = \underline{\underline{4.6\% \text{ H}_2\text{O}}}$

#### b. Energy balance on stack gas in preheater

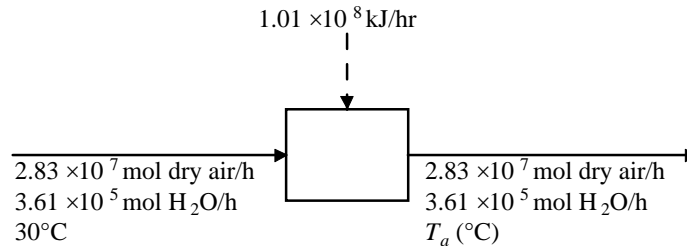
References: CO<sub>2</sub>, CO, O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O(v) at 25°C

Substance	$n_{\text{in}}$ mol/h	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol/h	$\hat{H}_{\text{out}}$ kJ/mol
CO <sub>2</sub>	$2.193 \times 10^6$	4.942	$2.193 \times 10^6$	9.738
CO	$0.337 \times 10^6$	3669	$0.337 \times 10^6$	6.961
O <sub>2</sub>	$3.706 \times 10^6$	3758	$3.206 \times 10^6$	7.193
N <sub>2</sub>	$22.38 \times 10^6$	3655	$72.38 \times 10^6$	6.918
H <sub>2</sub> O	$1.357 \times 10^6$	4266	$1.351 \times 10^6$	8135

$\hat{H}_i(T)$  from Table B.8 for inlet       $\hat{H}_i(T) = \int_{T_a}^{T} \overset{\text{Table B.2}}{\underset{\downarrow}{C_p}} dT$  for outlet

$$Q = \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = \underline{\underline{-1.01 \times 10^8 \text{ kJ/h}}} \text{ (Heat transferred from stack gas)}$$

Air preheating



(We assume preheater is adiabatic, so that  $Q_{\text{stack gas}} = -Q_{\text{air}}$ )

Energy balance on air:

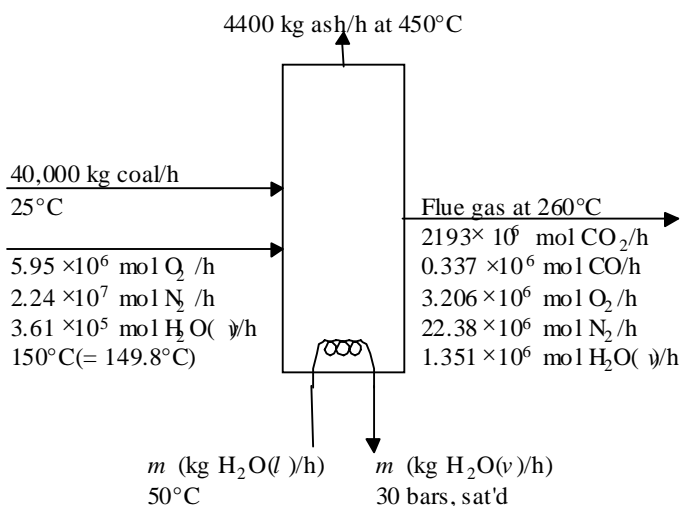
$$Q = \Delta H \Rightarrow 1.01 \times 10^8 \text{ kJ/hr} = \sum_{30}^{T_a} \int n_i (C_p)_i dT = \int_{30}^{T_a} n_{\text{dry air}} \overset{\text{Table B.2}}{\underset{\downarrow}{(C_p)_{\text{dry air}}}} dT + \int_{30}^{T_a} n_{\text{H}_2\text{O}} \overset{\text{Table B.2}}{\underset{\downarrow}{(C_p)_{\text{H}_2\text{O}}}} dT$$

9.61 (cont'd)

$$\Rightarrow 1.01 \times 10^8 = 8.31 \times 10^5 (T_a - 30) + 59.92(T_a^2 - 30^2) + 0.031(T_a^3 - 30^3) - 1.42 \times 10^{-5}(T_a^4 - 30^4)$$

$$\Rightarrow T_a = 150^\circ \text{C}$$

c.



References for energy balance on furnace:  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{O}_2$ ,  $\text{N}_2$ ,  $\text{H}_2\text{O(l)}$ , coal at  $25^\circ \text{C}$

(Must choose  $\text{H}_2\text{O(l)}$  since we are given the higher heating value of the coal.)

substance	$n_{\text{in}}$	$\hat{H}_{\text{in}}$	$n_{\text{out}}$	$\hat{H}_{\text{out}}$	
Coal	40000	0	—	—	$n(\text{kg/h})$
Ash	—	—	4400	412.25	$\hat{H}(\text{kJ/kg})$
$\text{O}_2$	$5.95 \times 10^6$	3.758	$3.206 \times 10^6$	7.193	$n(\text{mol/h})$ $\hat{H}(\text{kJ/mol})$
$\text{N}_2$	$2.24 \times 10^7$	3.655	$2.24 \times 10^7$	6.918	
$\text{CO}_2$	—	—	$2.193 \times 10^6$	9.738	
$\text{CO}$	—	—	$0.337 \times 10^6$	6.961	
$\text{H}_2\text{O}$	$3.61 \times 10^5$	48.28	$1.351 \times 10^6$	52.14	

(Furnace only — exclude boiler water)

Heat transferred from furnace

$$Q = n_{\text{coal}} \Delta \hat{H}_i^o + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i$$

$$= \left( 4 \times 10^4 \frac{\text{kg}}{\text{h}} \right) \left( -2.5 \times 10^4 \frac{\text{kJ}}{\text{kg}} \right) + \left( 2.74 \times 10^3 - \underset{\substack{\uparrow \\ \hat{H} \text{ of preheated air}}}{1.22 \times 10^8}} \frac{\text{kJ}}{\text{kg}} \right)$$

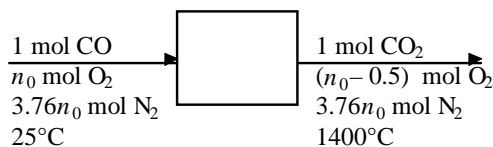
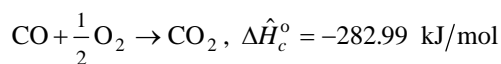
$$= -8.76 \times 10^8 \text{ kJ/h}$$

Heat transferred to boiler water:  $0.60(8.76 \times 10^8 \text{ kJ/h}) = 5.25 \times 10^8 \text{ kJ/h}$

Energy balance on boiler:  $\dot{Q}(\text{kJ/h}) = \dot{m} \left( \frac{\text{kg}}{\text{h}} \right) \left[ \hat{H}(\text{H}_2\text{O(l)}, 30b, \text{sat'd}) - \hat{H}(\text{H}_2\text{O(l)}, 50^\circ \text{C}) \right]$

$$\Rightarrow 5.25 \times 10^8 \text{ kJ/h} = \dot{m} \left[ \underset{\substack{\uparrow \\ \text{Table B.6}}}{2802.3} - \underset{\substack{\uparrow \\ \text{Table B.5}}}{209.3} \right] \frac{\text{kJ}}{\text{kg}} \Rightarrow \underline{\underline{\dot{m} = 2.02 \times 10^5 \text{ kg steam/h}}}$$

9.62

Basis : 1 mol CO burned.

a. Oxygen in product gas:  $n_1 = n_0 (\text{mol O}_2 \text{ fed}) - \frac{1 \text{ mol CO react}}{1 \text{ mol CO}} \left| \frac{0.5 \text{ mol O}_2}{1 \text{ mol CO}} \right| = n_0 - 0.5$

References: CO, CO<sub>2</sub>, O<sub>2</sub>, N<sub>2</sub> at 25°C

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
CO	1	0	—	—
O <sub>2</sub>	$n_0$	0	$n_0 - 0.5$	$\hat{H}_1$
N <sub>2</sub>	$3.76n_0$	0	$3.76n_0$	$\hat{H}_2$
CO <sub>2</sub>	—	—	1	$\hat{H}_3$

Table B.8  
↓

$$\text{O}_2(\text{g}, 1400^\circ\text{C}): \hat{H}_1 = \hat{H}_{\text{O}_2}(1400^\circ\text{C}) = 47.07 \text{ kJ/mol}$$

Table B.8  
↓

$$\text{N}_2(\text{g}, 1400^\circ\text{C}): \hat{H}_2 = \hat{H}_{\text{N}_2}(1400^\circ\text{C}) = 44.51 \text{ kJ/mol}$$

Table B.8  
↓

$$\text{CO}_2(\text{g}, 1400^\circ\text{C}): \hat{H}_3 = \hat{H}_{\text{CO}_2}(1400^\circ\text{C}) = 71.89 \text{ kJ/mol}$$

E.B.:

$$\Delta H = n_{\text{CO}} \Delta \hat{H}_c^\circ + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = -282.99 + 47.07(n_0 - 0.5) + 44.51(3.76n_0) + 71.89 = 0$$

$$\Rightarrow n_0 = 1.094 \text{ mol O}_2$$

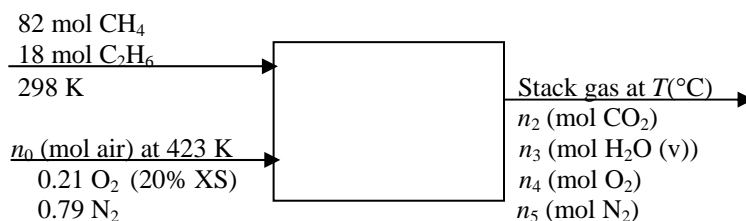
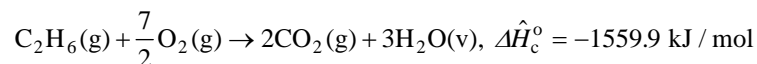
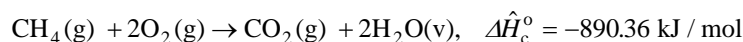
$$\text{Theoretical O}_2 = (1 \text{ mol CO})(0.5 \text{ mol O}_2 / \text{mol CO}) = 0.500 \text{ mol O}_2$$

$$\text{Excess oxygen: } \frac{1.094 \text{ mol fed} - 0.500 \text{ mol reqd.}}{0.500 \text{ mol}} \times 100\% = 119\% \text{ excess oxygen}$$

- b. Increase %XS air  $\Rightarrow T_{\text{ad}}$  would decrease, since the heat liberated by combustion would go into heating a larger quantity of gas (i.e., the additional N<sub>2</sub> and unconsumed O<sub>2</sub>).

9.63

- a. Basis : 100 mol natural gas  $\Rightarrow$  82 mol CH<sub>4</sub>, 18 mol C<sub>2</sub>H<sub>6</sub>



### 9.63 (cont'd)

$$\text{Theoretical oxygen} = \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \left| \frac{82 \text{ mol CH}_4}{1 \text{ mol CH}_4} \right| + \frac{3.5 \text{ mol O}_2}{1 \text{ mol C}_2\text{H}_6} \left| \frac{18 \text{ mol C}_2\text{H}_6}{1 \text{ mol C}_2\text{H}_6} \right| = 227 \text{ mol O}_2$$

$$\text{Air fed : } n_1 = \frac{1.2 \times 227 \text{ mol O}_2}{0.21 \text{ mol O}_2} \left| \frac{1 \text{ mol air}}{0.21 \text{ mol O}_2} \right| = 1297.14 \text{ mol air}$$

$$\text{C balance : } n_2 = (82.00)(1) + (18.00)(2) \Rightarrow n_2 = 118.00 \text{ mol CO}_2$$

$$\text{H balance : } 2n_3 = (82.00)(4) + (18.00)(6) \Rightarrow n_3 = 218.00 \text{ mol H}_2\text{O}$$

$$\text{20\% excess air, complete combustion} \Rightarrow n_4 = (0.2)(227) \text{ mol O}_2 = 45.40 \text{ mol O}_2$$

$$\text{N}_2 \text{ balance : } n_5 = (0.79)(1297.14) = 1024.63 \text{ mol N}_2$$

$$\text{Extents of reaction: } \xi_1 = n_{\text{CH}_4} = 82 \text{ mol}, \quad \xi_2 = n_{\text{C}_2\text{H}_6} = 18 \text{ mol}$$

$$\text{Reference states: CH}_4(\text{g}), \text{C}_2\text{H}_6(\text{g}), \text{N}_2(\text{g}), \text{O}_2(\text{g}), \text{H}_2\text{O}(\text{l}) \text{ at } 298 \text{ K}$$

(We will use the values of  $\Delta \hat{H}_c^\circ$  given in Table B.1, which are based on  $\text{H}_2\text{O}(\text{l})$  as a combustion product, and so must choose the liquid as a reference state for water.)

$$\begin{aligned} \hat{H}_i(T) &= C_{p,i}(T - 298 \text{ K}) \text{ for all species but water} \\ &= \Delta \hat{H}_{\text{v,H}_2\text{O}}(298 \text{ K}) + C_{p,\text{H}_2\text{O}}(T - 298 \text{ K}) \text{ for water} \end{aligned}$$

Substance	$n_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
CH <sub>4</sub>	82.00		—	—
C <sub>2</sub> H <sub>6</sub>	18.00	0	—	—
O <sub>2</sub>	272.40	4.14	45.40	$0.0331(T - 298)$
N <sub>2</sub>	1024.63	3.91	1024.63	$0.0313(T - 298)$
CO <sub>2</sub>	—	—	118.00	$0.0500(T - 298)$
H <sub>2</sub> O(v)	—	—	218.00	$44.013 + 0.0385(T - 298)$

$$\text{Energy balance : } \Delta H = 0$$

$$\begin{aligned} \xi_1 (\Delta \hat{H}_c^\circ)_{\text{CH}_4} + \xi_2 (\Delta \hat{H}_c^\circ)_{\text{C}_2\text{H}_6} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i &= 0 \\ \Rightarrow (82.00 \text{ mol CH}_4)(-890.36 \text{ kJ/mol}) + (18.00 \text{ mol C}_2\text{H}_6)(-1559.90 \text{ kJ/mol}) \\ &+ [(45.40)(0.0331) + (1024.63)(0.0313) + (118.00)(0.0500) + (218.00)(0.0385)](T - 298) \\ &+ (218.00)(44.01) - (272.40)(4.14) - (1024.63)(3.91) = 0 \end{aligned}$$

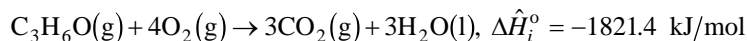
**b.** Solving for  $T$  using E-Z Solve  $\Rightarrow T = 2317 \text{ K}$

Increase % excess air  $\Rightarrow T_{\text{out}}$  decreases. (Heat of combustion has more gas to heat)

% methane increases  $\Rightarrow T_{\text{out}}$  might decrease. (lower heat of combustion, but heat released goes into heating fewer moles of gas.)



9.64

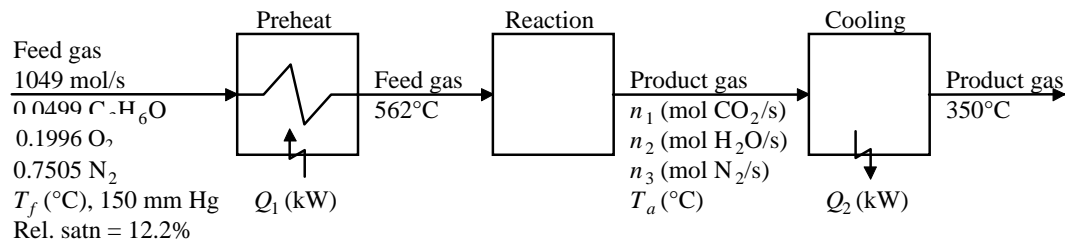


$$\text{Basis: } \frac{1410 \text{ m}^3(\text{STP}) \text{ feed gas}}{\text{min}} \left| \frac{10^3 \text{ mol}}{22.4 \text{ m}^3(\text{STP})} \right| \frac{1 \text{ min}}{60 \text{ s}} = 1049 \text{ mol/s feed gas}$$

Stoichiometric proportion:

$$1 \text{ mol C}_3\text{H}_6\text{O} \Rightarrow 4 \text{ mol O}_2 \Rightarrow 4 \times 3.76 = 15.04 \text{ mol N}_2 \Rightarrow (1 + 4 + 15.04) = 20.04 \text{ mol}$$

$$y_{\text{C}_3\text{H}_6\text{O}} = \frac{1 \text{ mol C}_3\text{H}_6\text{O}}{20.04 \text{ mol}} = 0.0499 \frac{\text{mol C}_3\text{H}_6\text{O}}{\text{mol}}, y_{\text{O}_2} = \frac{4}{20.04} = 0.1996 \text{ mol O}_2/\text{mol}$$



a. Relative saturation = 12.2%  $\Rightarrow y_{\text{C}_3\text{H}_6\text{O}} P = 0.122 p_{\text{C}_3\text{H}_6\text{O}}^*(T_f)$

$$\Rightarrow p^* = \frac{(0.0499)(1500 \text{ mm Hg})}{0.122} = 613.52 \text{ mm Hg} \xrightarrow{\text{Table B.4}} T_f = 50.0^\circ \text{C}$$

b. Feed contains (1049 mol/s)(0.0499 C<sub>3</sub>H<sub>6</sub>O/mol) = 52.34 mol C<sub>3</sub>H<sub>6</sub>O/s

$$(1049)(0.1996) = 209.4 \text{ mol O}_2/\text{s}$$

$$(1049)(0.7505) = 787.3 \text{ mol N}_2/\text{s}$$

$$\Rightarrow \text{Product contains } \left. \begin{array}{l} n_1 = (52.34)(3) = 157.0 \text{ mol CO}_2/\text{s} \\ n_2 = (52.34)(3) = 157.0 \text{ mol H}_2\text{O}/\text{s} \\ n_3 = 787.3 \text{ mol N}_2/\text{s} \end{array} \right\} \Rightarrow \begin{array}{l} 14.25 \text{ mole\% CO}_2 \\ 14.25\% \text{ H}_2\text{O} \\ 71.5\% \text{ N}_2 \end{array}$$

References: C<sub>3</sub>H<sub>6</sub>O(g), O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>O(l), CO<sub>2</sub> at 25°C

Substance	$\dot{n}_{\text{in}}$ (mols)	$\hat{H}_{\text{in}}$ (kJ/mol) (562°C)	$\dot{n}_{\text{out}}$ (mols)	$\hat{H}_{\text{out}}$ (kJ/mol) T <sub>a</sub>
C <sub>3</sub> H <sub>6</sub> O	52.34	67.66	—	—
O <sub>2</sub>	209.4	17.72	—	—
N <sub>2</sub>	787.3	17.18	787.3	0.032(T <sub>a</sub> - 25)
CO <sub>2</sub>	—	—	157.0	0.052(T <sub>a</sub> - 25)
H <sub>2</sub> O	—	—	157.0	44.013 + 0.040(T <sub>a</sub> - 25)

Energy balance on reactor:

$$\Delta H = n_{\text{C}_3\text{H}_6\text{O}} \Delta \hat{H}_c^\circ + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = 0 \text{ (kJ/s)}$$

$$\Rightarrow (5234 \text{ mol/s}) \left( -1821.1 \frac{\text{kJ}}{\text{mol}} \right) + 39.638(T_a - 25) + 157.0(44.013) - 2.078 \times 10^4 = 0 \Rightarrow T_a = 2780^\circ \text{C}$$

9.64 (cont'd)

c.

Preheating step: References:  $\text{C}_3\text{H}_6(\text{g})$ ,  $\text{O}_2$ ,  $\text{N}_2$  at  $25^\circ\text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol/s)	$\hat{H}_{\text{in}}$ (kJ/mol) ( $50^\circ\text{C}$ )	$\dot{n}_{\text{out}}$ (mol/s)	$\hat{H}_{\text{out}}$ (kJ/mol) ( $562^\circ\text{C}$ )
$\text{C}_3\text{H}_6\text{O}$	52.34	3.15	52.34	67.66
$\text{O}_2$	209.4	0.826	209.4	17.72
$\text{N}_2$	787.3	0.775	787.3	16.65

$$\text{E.B.} \Rightarrow \dot{Q}_1 = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = \underline{\underline{1.94 \times 10^4 \text{ kW}}}$$

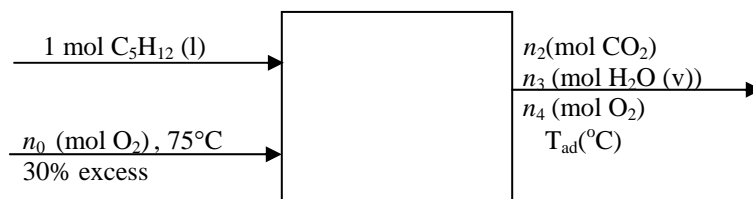
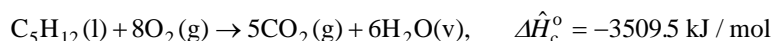
Cooling step: References:  $\text{CO}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{v})$ ,  $\text{N}_2(\text{g})$  at  $25^\circ\text{C}$

Substance	$n_{\text{in}}$ (mol)	$\hat{H}_{\text{in}}$ (kJ/mol) ( $2871^\circ\text{C}$ )	$n_{\text{out}}$ (mol)	$\hat{H}_{\text{out}}$ (kJ/mol) ( $350^\circ\text{C}$ )
$\text{CO}_2$	157.0	142.3	157.0	16.25
$\text{H}_2\text{O}$	157.0	108.15	157.0	12.35
$\text{N}_2$	787.3	88.23	787.3	10.08

$$\text{E.B.} \Rightarrow Q_2 = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = \underline{\underline{-9.64 \times 10^4 \text{ kW}}}$$

Exchange heat between the reactor feed and product gases.

9.65 a. Basis : 1 mol  $\text{C}_5\text{H}_{12}(\text{l})$



$$\underline{\underline{\text{Theoretical oxygen}}} = \frac{1 \text{ mol C}_5\text{H}_{12}}{1 \text{ mol C}_5\text{H}_{12}} \left| \frac{8 \text{ mol O}_2}{1 \text{ mol C}_5\text{H}_{12}} \right. = 8 \text{ mol O}_2$$

$$\underline{\underline{30\% \text{ excess}}} \Rightarrow n_0 = 1.3 \times 8 = 10.4 \text{ mol O}_2$$

$$\underline{\underline{\text{C balance:}}} \quad n_2 = (1)(5) \Rightarrow n_2 = 5 \text{ mol CO}_2$$

$$\underline{\underline{\text{H balance:}}} \quad 2n_3 = (1)(12) \Rightarrow n_3 = 6 \text{ mol H}_2\text{O}$$

$$\underline{\underline{30\% \text{ excess O}_2, \text{ complete combustion}}} \Rightarrow n_4 = (0.3)(8) \text{ mol O}_2 = 2.4 \text{ mol O}_2$$

Reference states:  $\text{C}_5\text{H}_{12}(\text{l})$ ,  $\text{O}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{l})$ ,  $\text{CO}_2(\text{g})$  at  $25^\circ\text{C}$

(We will use the values of  $\Delta \hat{H}_c^0$  given in Table B.1, which are based on  $\text{H}_2\text{O}(\text{l})$  as a combustion product, and so must choose the liquid as a reference state for water)

9.65 (cont'd)

substance	$n_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
C <sub>5</sub> H <sub>12</sub>	1.00	0	—	—
O <sub>2</sub>	10.40	$\hat{H}_1$	2.40	$\hat{H}_2$
CO <sub>2</sub>	—	—	5.00	$\hat{H}_3$
H <sub>2</sub> O	—	—	6.00	$\hat{H}_4$

$$\hat{H}_i = \int_{25}^T (C_p)_i dT \quad i = 2, 3$$

$$= \Delta \hat{H}_v(25^\circ \text{C}) + \int_{25}^T (C_p)_{\text{H}_2\text{O}(\text{v})} dT \quad \text{for H}_2\text{O}(\text{v})$$

Table B.8  
↓

$$\hat{H}_1 = \hat{H}_{\text{O}_2}(75^\circ \text{C}) = 1.48 \text{ kJ/mol}$$

Substituting  $(C_p)_i$  from Table B.2 :

$$\hat{H}_2 = (0.0291 T_{\text{ad}} + 0.579 \times 10^{-5} T_{\text{ad}}^2 - 0.2025 \times 10^{-8} T_{\text{ad}}^3 + 0.3278 \times 10^{-12} T_{\text{ad}}^4 - 0.7311) \frac{\text{kJ}}{\text{mol}}$$

$$\hat{H}_3 = (0.03611 T_{\text{ad}} + 2.1165 \times 10^{-5} T_{\text{ad}}^2 - 0.9623 \times 10^{-8} T_{\text{ad}}^3 + 1.866 \times 10^{-12} T_{\text{ad}}^4 - 0.9158) \frac{\text{kJ}}{\text{mol}}$$

$$\hat{H}_4 = 44.01 + (0.03346 T_{\text{ad}} + 0.3440 \times 10^{-5} T_{\text{ad}}^2 + 0.2535 \times 10^{-8} T_{\text{ad}}^3 - 0.8983 \times 10^{-12} T_{\text{ad}}^4 - 0.838) \frac{\text{kJ}}{\text{mol}}$$

$$\Rightarrow \hat{H}_4 = 43.17 + (0.03346 T_{\text{ad}} + 0.3440 \times 10^{-5} T_{\text{ad}}^2 + 0.2535 \times 10^{-8} T_{\text{ad}}^3 - 0.8983 \times 10^{-12} T_{\text{ad}}^4) \frac{\text{kJ}}{\text{mol}}$$

Energy balance :  $\Delta H = 0$

$$n_{\text{C}_5\text{H}_{12}} (\Delta \hat{H}_c^\circ)_{\text{C}_5\text{H}_{12}(\text{l})} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i = 0$$

$$(1 \text{ mol C}_5\text{H}_{12})(-3509.5 \text{ kJ/mol}) + (2.40) \hat{H}_2 + (5.00) \hat{H}_3 + (6.00) \hat{H}_4 - (10.40)(\hat{H}_1) = 0$$

↓ Substitute for  $\hat{H}_1$  through  $\hat{H}_4$

$$\Delta \hat{H} = (0.4512 T_{\text{ad}} + 14.036 \times 10^{-5} T_{\text{ad}}^2 - 3.777 \times 10^{-8} T_{\text{ad}}^3 + 4.727 \times 10^{-12} T_{\text{ad}}^4) - 3272.20 \text{ kJ/mol} = 0$$

$$\Rightarrow f(T_{\text{ad}}) = -3272.20 + 0.4512 T_{\text{ad}} + 14.036 \times 10^{-5} T_{\text{ad}}^2 - 3.777 \times 10^{-8} T_{\text{ad}}^3 + 4.727 \times 10^{-12} T_{\text{ad}}^4 = 0$$

$$\text{Check : } \frac{-3272.20}{4.727 \times 10^{-12}} = -6.922 \times 10^{14}$$

$$\text{Solving for } T_{\text{ad}} \text{ using E-Z Solve} \Rightarrow \underline{\underline{T_{\text{ad}} = 4414^\circ \text{C}}}$$

**b.**

Terms	$T_{\text{ad}}$	% Error
1	7252	64.3%
2	3481	-21.1%
3	3938	-10.8%

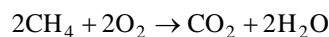
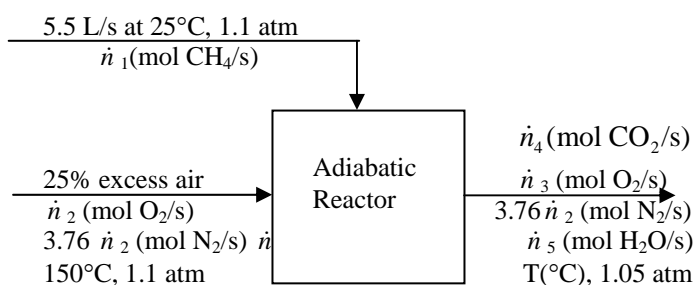
9.65 (cont'd)

c.

T	f(T)	f'(T)	Tnew
7252	6.05E+03	3.74	5634
5634	1.73E+03	1.82	4680
4680	3.10E+02	1.22	4426
4426	1.41E+01	1.11	4414
4414	3.11E-02	1.11	4414

d. The polynomial formulas are only applicable for  $T \leq 1500^\circ\text{C}$

9.66



$$\text{Fuel feed rate} := \frac{5.50 \text{ L}}{\text{s}} \left| \frac{273 \text{ K}}{298 \text{ K}} \right| \left| \frac{1.1 \text{ atm}}{1.0 \text{ atm}} \right| \left| \frac{\text{mol}}{22.4 \text{ L(STP)}} \right| = 0.247 \text{ mol CH}_4 / \text{s}$$

$$\text{Theoretical O}_2 = 2 \times 0.247 = 0.494 \text{ mol O}_2 / \text{s}$$

$$\begin{aligned} 25\% \text{ excess air} &\Rightarrow \dot{n}_2 = 1.25(0.494) = 0.6175 \text{ mol O}_2 / \text{s} \\ &\Rightarrow 3.76 \times 0.6175 = 2.32 \text{ mol N}_2 / \text{s} \end{aligned}$$

$$\begin{aligned} \text{Complete combustion} &\Rightarrow \dot{\xi} = n_1 = 0.247 \text{ mol} / \text{s}, \dot{n}_4 = 0.247 \text{ mol CO}_2 / \text{s}, \dot{n}_5 = 0.494 \text{ mol H}_2\text{O} / \text{s} \\ \dot{n}_3 &= 0.6175 \text{ mol O}_2 \text{ fed} / \text{s} - 0.494 \text{ mol consumed} / \text{s} \\ &= 0.124 \text{ mol O}_2 / \text{s} \end{aligned}$$

References:  $\text{CH}_4, \text{O}_2, \text{N}_2, \text{CO}_2, \text{H}_2\text{O}$  at  $25^\circ\text{C}$

Substance	$\dot{n}_{\text{in}}$ (mol / s)	$\hat{H}_{\text{in}}$ (kJ / mol)	$\dot{n}_{\text{out}}$ (mol / s)	$\hat{H}_{\text{out}}$ (kJ / mol)
CH <sub>4</sub>	0.247	0	—	—
O <sub>2</sub>	0.6175	$\hat{H}_1$	0.124	$\hat{H}_3$
N <sub>2</sub>	2.32	$\hat{H}_2$	2.32	$\hat{H}_4$
CO <sub>2</sub>	—	—	0.247	$\hat{H}_5$
H <sub>2</sub> O	—	—	0.497	$\hat{H}_6$

$$\hat{H}_1 = \hat{H}(\text{O}_2, 150^\circ\text{C}) \xrightarrow{\text{Table B.8}} 3.78 \text{ kJ/mol}$$

$$\hat{H}_2 = \hat{H}(\text{N}_2, 150^\circ\text{C}) \xrightarrow{\text{Table B.8}} 3.66 \text{ kJ/mol}$$

$$(\Delta \hat{H}_c^\circ)_{\text{CH}_4} = -890.36 \text{ kJ/mol}$$

$$\hat{H}_i = \int_{25}^T C_{p,i} dT, \quad i = 3 - 5$$

9.66 (cont'd)

$$\hat{H}_b = (\Delta \hat{H}_v)_{\text{H}_2\text{O}(25^\circ\text{C})} + \int_{25}^T (C_p)_{\text{H}_2\text{O}(v)} dT$$

a. Energy Balance

$$\Delta \dot{H} = \dot{\xi}(\Delta \hat{H}_c^\circ)_{\text{CH}_4} + \sum \dot{n}_{\text{out}} \hat{H}_{\text{out}} - \sum \dot{n}_{\text{in}} \hat{H}_{\text{in}} = 0$$

Table B.2 for  $C_{pi}(T)$ ,  $(\Delta \hat{H}_v)_{\text{H}_2\text{O}} = 44.01 \text{ kJ/mol}$

$$0.247(-890.36) + 0.494(44.01) + 0.0963(T - 25) + 1.02 \times 10^{-5}(T^2 - 25^2) + 0.305 \times 10^{-8}(T^3 - 25^3) - 1.61 \times 10^{-12}(T^4 - 25^4) - 0.6175(3.78) - 2.32(3.66) = 0$$

$$\Rightarrow -211.4 + 0.0963T_{ad} + 1.02 \times 10^{-5}T_{ad}^2 + 0.305 \times 10^{-8}T_{ad}^3 - 1.61 \times 10^{-12}T_{ad}^4 = 0 \Rightarrow \underline{\underline{T = 1832^\circ\text{C}}}$$

b. In product gas,

$$T = 1832^\circ\text{C}, P = 1.05 \times 760 = 798 \text{ mmHg}$$

$$y_{\text{H}_2\text{O}} = \frac{0.494 \text{ mol/s}}{(0.124 + 2.32 + 0.247 + 0.494) \text{ mol/s}} = 0.155 \text{ mol H}_2\text{O/mol}$$

Raoult's law:  $y_{\text{H}_2\text{O}}P = p_{\text{H}_2\text{O}}^*(T_{dp}) \Rightarrow p_{\text{H}_2\text{O}}^* = (0.155)(798) = 124 \text{ mmHg} \xRightarrow{\text{Table B.3}} \underline{\underline{T_{dp} = 56^\circ\text{C}}}$

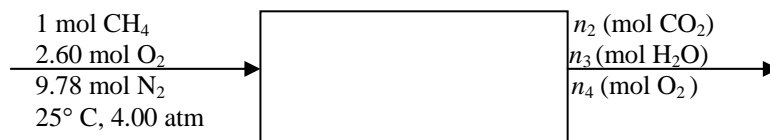
$$\text{Degr. superheat} = 1832^\circ\text{C} - 56^\circ\text{C} = \underline{\underline{1776^\circ\text{C}}}$$

9.67 a.  $\text{CH}_4(\text{l}) + 2\text{O}_2(\text{g}) \rightarrow \text{CO}_2(\text{g}) + 2\text{H}_2\text{O}(\text{v})$

Basis: 1 mol  $\text{CH}_4$

$$\text{Theoretical oxygen} = \frac{1 \text{ mol CH}_4}{1 \text{ mol CH}_4} \left| \frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \right| = 2.00 \text{ mol O}_2$$

$$\underline{30\% \text{ excess air}} \Rightarrow 1.30(2.00) = 2.60 \text{ mol O}_2, \Rightarrow 3.76 \times 2.60 = 9.78 \text{ mol N}_2$$



$$\underline{\text{Complete combustion}} \Rightarrow n_2 = 1.00 \text{ mol CO}_2, n_3 = 2.00 \text{ mol H}_2\text{O}$$

$$\underline{2.00 \text{ mol O}_2 \text{ consumed}} \Rightarrow n_4 = (2.60 - 2.00) \text{ mol O}_2 = 0.60 \text{ mol O}_2$$

$$\underline{\text{Internal energy of reaction:}} \text{ Eq. (9.1-5)} \Rightarrow \Delta \hat{U}_c^\circ = \Delta \hat{H}_c^\circ - RT \left( \sum_{\text{gaseous products}} \nu_i - \sum_{\text{gaseous reactants}} \nu_i \right)$$

$$\Rightarrow (\Delta \hat{U}_c^\circ)_{\text{CH}_4} = \left( -890.36 \frac{\text{kJ}}{\text{mol}} \right) - \frac{8.314 \text{ J}}{\text{mol K}} \left| \frac{298 \text{ K}}{10^3 \text{ J}} \right| (1 + 2 - 1 - 2) = -890.36 \frac{\text{kJ}}{\text{mol}}$$

$$\hat{U} = \int_{25}^T (C_v) dT \xRightarrow{\text{Ideal Gas}} \int_{25}^T (C_p - R_g) dT$$

$$\text{If } C_p \text{ is independent of } T \Rightarrow \hat{U} = (C_p - R_g)(T - 25^\circ\text{C})$$

9.67 (cont'd)

b. Reference states:  $\text{CH}_4(\text{g})$ ,  $\text{N}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{H}_2\text{O}(\text{l})$ ,  $\text{CO}_2(\text{g})$  at  $25^\circ\text{C}$

(We will use the values of  $\Delta\hat{H}_c^0$  given in Table B.1, which are based on  $\text{H}_2\text{O}(\text{l})$  as a combustion product, and so must choose the liquid as a reference state for water.)

Substance	$n_{\text{in}}$ mol	$\hat{U}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{U}_{\text{out}}$ kJ/mol
$\text{CH}_4$	1.00	0	—	—
$\text{O}_2$	2.60	0	0.60	$\hat{U}_1$
$\text{N}_2$	9.78	0	9.78	$\hat{U}_2$
$\text{CO}_2$	—	—	1.00	$\hat{U}_3$
$\text{H}_2\text{O}(\text{v})$	—	—	2.00	$\hat{U}_4$

Part a

$$\begin{aligned}\hat{U}_i &= (C_p - R_g)(T - 25) \quad \text{for all species except } \text{H}_2\text{O}(\text{v}) \\ &= \Delta\hat{U}_v(25^\circ\text{C}) + (C_p - R_g)(T - 25) = \left[ \Delta\hat{H}_v(25^\circ\text{C}) - R_g T_{\text{ref}} \right] + (C_p - R_g)(T - 25) \quad \text{for } \text{H}_2\text{O}(\text{v})\end{aligned}$$

Substituting given values of  $(C_p)_i$  and  $R_g = 8.314 \times 10^{-3} \text{ kJ/mol}$  yields

$$\hat{U}_1 = (0.033 - 8.314 \times 10^{-3})(T - 25) \text{ kJ/mol} = (0.02469T - 0.6172) \text{ kJ/mol}$$

$$\hat{U}_2 = (0.032 - 8.314 \times 10^{-3})(T - 25) \text{ kJ/mol} = (0.02369T - 0.5922) \text{ kJ/mol}$$

$$\hat{U}_3 = (0.052 - 8.314 \times 10^{-3})(T - 25) \text{ kJ/mol} = (0.04369T - 1.0922) \text{ kJ/mol}$$

$$\hat{U}_4 = \left[ 44.01 \frac{\text{kJ}}{\text{mol}} - \left( 8.314 \times 10^{-3} \frac{\text{kJ}}{\text{mol} \cdot \text{K}} \right) (298 \text{ K}) \right] + (0.040 - 8.314 \times 10^{-3})(T - 25) \frac{\text{kJ}}{\text{mol}}$$

$$\Rightarrow \hat{U}_4 = 41.53 \frac{\text{kJ}}{\text{mol}} + (0.052 - 8.314 \times 10^{-3})(T - 25) \frac{\text{kJ}}{\text{mol}} = (0.03167T - 40.74) \frac{\text{kJ}}{\text{mol}}$$

Energy Balance

$$Q = n_{\text{CH}_4} (\Delta\hat{U}_c^0)_{\text{CH}_4} + \sum_{\text{out}} n_i \hat{U}_i - \sum_{\text{in}} n_i \hat{U}_i = 0$$

$$\Rightarrow Q = (1.00)(-890.36 \text{ kJ/mol}) + (0.60)\hat{U}_1 + (9.78)\hat{U}_2 + (1.00)\hat{U}_3 + (2.00)\hat{U}_4 = 0$$

Substituting  $\hat{U}_1$  through  $\hat{U}_4$

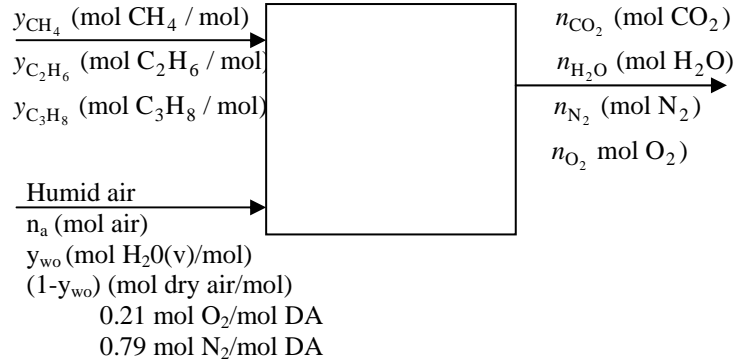
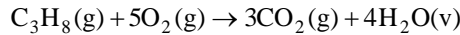
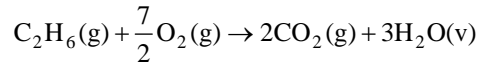
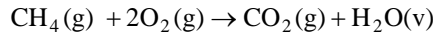
$$0.3557 T - 816.19 = 0 \Rightarrow \underline{\underline{T = 2295^\circ\text{C}}}$$

Ideal Gas Equation of State  $\Rightarrow \frac{P_f}{P_i} = \frac{T_f}{T_i} \Rightarrow P_f = \left( \frac{(2295 + 273) \text{ K}}{(25 + 273) \text{ K}} \right) \times 4.00 \text{ atm} = \underline{\underline{34.5 \text{ atm}}}$

- c.
- Heat loss to and through reactor wall
  - Tank would expand at high temperatures and pressures

9.68

b. 1 mol natural gas

Basis : 1 g-mole natural gasTheoretical oxygen :

$$\frac{2 \text{ mol O}_2}{1 \text{ mol CH}_4} \left| \frac{y_{\text{CH}_4} (\text{mol CH}_4)}{1 \text{ mol C}_2\text{H}_6} \right| + \frac{3.5 \text{ mol O}_2}{1 \text{ mol C}_2\text{H}_6} \left| \frac{y_{\text{C}_2\text{H}_6} (\text{mol C}_2\text{H}_6)}{1 \text{ mol C}_3\text{H}_8} \right| + \frac{5 \text{ mol O}_2}{1 \text{ mol C}_3\text{H}_8} \left| \frac{y_{\text{C}_3\text{H}_8} (\text{mol C}_3\text{H}_8)}{1 \text{ mol C}_3\text{H}_8} \right|$$

$$= (2y_{\text{CH}_4} + 3.5y_{\text{C}_2\text{H}_6} + 5y_{\text{C}_3\text{H}_8})$$

$$\text{Excess oxygen: } 0.21n_a(1 - y_{w0}) = \left(1 + \frac{P_{xs}}{100}\right) (2y_{\text{CH}_4} + 3.5y_{\text{C}_2\text{H}_6} + 5y_{\text{C}_3\text{H}_8}) \text{ mol O}_2$$

$$\Rightarrow n_a = \left(1 + \frac{P_{xs}}{100}\right) (2y_{\text{CH}_4} + 3.5y_{\text{C}_2\text{H}_6} + 5y_{\text{C}_3\text{H}_8}) \frac{1}{0.21(1 - y_{w0})} \text{ mol air}$$

Feed components

$$(n_{\text{O}_2})_{\text{in}} = 0.21n_a(1 - y_{w0}), (n_{\text{N}_2})_{\text{in}} = 0.79n_a(1 - y_{w0}), (n_{\text{H}_2\text{O}})_{\text{in}} = n_a y_{w0}$$

$$\text{N}_2 \text{ in product gas: } n_{\text{N}_2} = (n_{\text{N}_2})_{\text{in}} \text{ mol N}_2$$

CO<sub>2</sub> in product gas :

$$n_{\text{CO}_2} = \frac{1 \text{ mol CO}_2}{1 \text{ mol CH}_4} \left| \frac{n_{\text{CH}_4} (\text{mol CH}_4)}{1 \text{ mol C}_2\text{H}_6} \right| + \frac{2 \text{ mol CO}_2}{1 \text{ mol C}_2\text{H}_6} \left| \frac{n_{\text{C}_2\text{H}_6} (\text{mol C}_2\text{H}_6)}{1 \text{ mol C}_3\text{H}_8} \right| + \frac{3 \text{ mol CO}_2}{1 \text{ mol C}_3\text{H}_8} \left| \frac{n_{\text{C}_3\text{H}_8} (\text{mol C}_3\text{H}_8)}{1 \text{ mol C}_3\text{H}_8} \right|$$

$$= (n_{\text{CH}_4} + 2n_{\text{C}_2\text{H}_6} + 3n_{\text{C}_3\text{H}_8}) \text{ mol CO}_2$$

H<sub>2</sub>O in product gas :

$$n_{\text{H}_2\text{O}} = \frac{1 \text{ mol H}_2\text{O}}{1 \text{ mol CH}_4} \left| \frac{n_{\text{CH}_4} (\text{mol CH}_4)}{1 \text{ mol C}_2\text{H}_6} \right| + \frac{3 \text{ mol H}_2\text{O}}{1 \text{ mol C}_2\text{H}_6} \left| \frac{n_{\text{C}_2\text{H}_6} (\text{mol C}_2\text{H}_6)}{1 \text{ mol C}_3\text{H}_8} \right| + \frac{4 \text{ mol H}_2\text{O}}{1 \text{ mol C}_3\text{H}_8} \left| \frac{n_{\text{C}_3\text{H}_8} (\text{mol C}_3\text{H}_8)}{1 \text{ mol C}_3\text{H}_8} \right|$$

$$= [2n_{\text{CH}_4} + 3n_{\text{C}_2\text{H}_6} + 4n_{\text{C}_3\text{H}_8} + n_a(1 - y_{w0})] \text{ mol H}_2\text{O}$$

$$\text{O}_2 \text{ in product gas: } n_{\text{O}_2} = \frac{P_{xs}}{100} (2n_{\text{CH}_4} + 3.5n_{\text{C}_2\text{H}_6} + 5n_{\text{C}_3\text{H}_8}) \text{ mol O}_2$$

**9.68 (cont'd)**

c. References : C(s), H<sub>2</sub>(g) at 25°C

$$\hat{H}_{\text{CH}_4}(T) = (\Delta H_f^\circ)_{\text{CH}_4} + \int_{25}^T (C_p)_{\text{CH}_4} dT$$

Using  $(\Delta H_f^\circ)_{\text{CH}_4}$  from Table B.1 and  $(C_p)_{\text{CH}_4}$  from Table B.2

$$\hat{H}_{\text{CH}_4}(T) = -74.85 \text{ kJ/mol} + \left( \int_{25}^T (0.03431 + 5.469 \times 10^{-5} T + 0.3661 \times 10^{-8} T^2 - 11.00 \times 10^{-12} T^3) dT \right) \text{ kJ/mol}$$

$$\Rightarrow \hat{H}_{\text{CH}_4}(T) = [-75.72 + 3.431 \times 10^{-2} T + 2.734 \times 10^{-5} T^2 + 0.122 \times 10^{-8} T^3 - 2.75 \times 10^{-12} T^4] \text{ kJ/mol}$$

Substance	$n_{\text{in}}$ mol	$\hat{H}_{\text{in}}$ kJ/mol	$n_{\text{out}}$ mol	$\hat{H}_{\text{out}}$ kJ/mol
CH <sub>4</sub>	$n_1$	$\hat{H}_1$	—	—
C <sub>2</sub> H <sub>6</sub>	$n_2$	$\hat{H}_2$	—	—
C <sub>3</sub> H <sub>8</sub>	$n_3$	$\hat{H}_3$	—	—
O <sub>2</sub>	$n_4$	$\hat{H}_4$	$n_7$	$\hat{H}_7$
N <sub>2</sub>	$n_5$	$\hat{H}_5$	$n_8$	$\hat{H}_8$
CO <sub>2</sub>	$n_6$	—	$n_9$	$\hat{H}_9$
H <sub>2</sub> O	—	—	$n_{10}$	$\hat{H}_{10}$

$$\Delta H = \sum_{i=4}^7 (n_i)_{\text{out}} (H_i)_{\text{out}} - \sum_{i=1}^6 (n_i)_{\text{in}} (H_i)_{\text{in}}$$

$$\hat{H}_i = a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4$$

$$\sum_{i=1}^6 (n_i)_{\text{in}} (H_i)_{\text{in}} = \sum_{i=1}^3 (n_i)_{\text{in}} \hat{H}_i(T_f) + \sum_{i=4}^6 (n_i)_{\text{in}} \hat{H}_i(T_a)$$

$$\Rightarrow \Delta H = \sum_{i=4}^7 (n_i)_{\text{out}} (a_i + b_i T + c_i T^2 + d_i T^3 + e_i T^4)_{\text{out}} - \sum_{i=1}^3 (n_i)_{\text{in}} \hat{H}_i(T_f) - \sum_{i=4}^6 (n_i)_{\text{in}} \hat{H}_i(T_a)$$

$$\Rightarrow \Delta H = \sum_{i=1}^7 (n_i)_{\text{out}} a_i + \sum_{i=4}^7 (n_i)_{\text{out}} b_i T + \sum_{i=1}^7 (n_i)_{\text{out}} c_i T^2 + \sum_{i=1}^7 (n_i)_{\text{out}} d_i T^3 + \sum_{i=1}^7 (n_i)_{\text{out}} e_i T^4$$

$$- \sum_{i=1}^3 (n_i)_{\text{in}} \hat{H}_i(T_f) - \sum_{i=4}^6 (n_i)_{\text{in}} \hat{H}_i(T_a)$$

$$= \alpha_0 + \alpha_1 T + \alpha_2 T^2 + \alpha_3 T^3 + \alpha_4 T^4$$

$$\text{where } \alpha_0 = \sum_{i=1}^7 (n_i)_{\text{out}} a_i - \sum_{i=1}^3 (n_i)_{\text{in}} \hat{H}_i(T_f) - \sum_{i=4}^6 (n_i)_{\text{in}} \hat{H}_i(T_a)$$

$$\alpha_1 = \sum_{i=1}^7 (n_i)_{\text{out}} b_i \quad \alpha_2 = \sum_{i=1}^7 (n_i)_{\text{out}} c_i$$

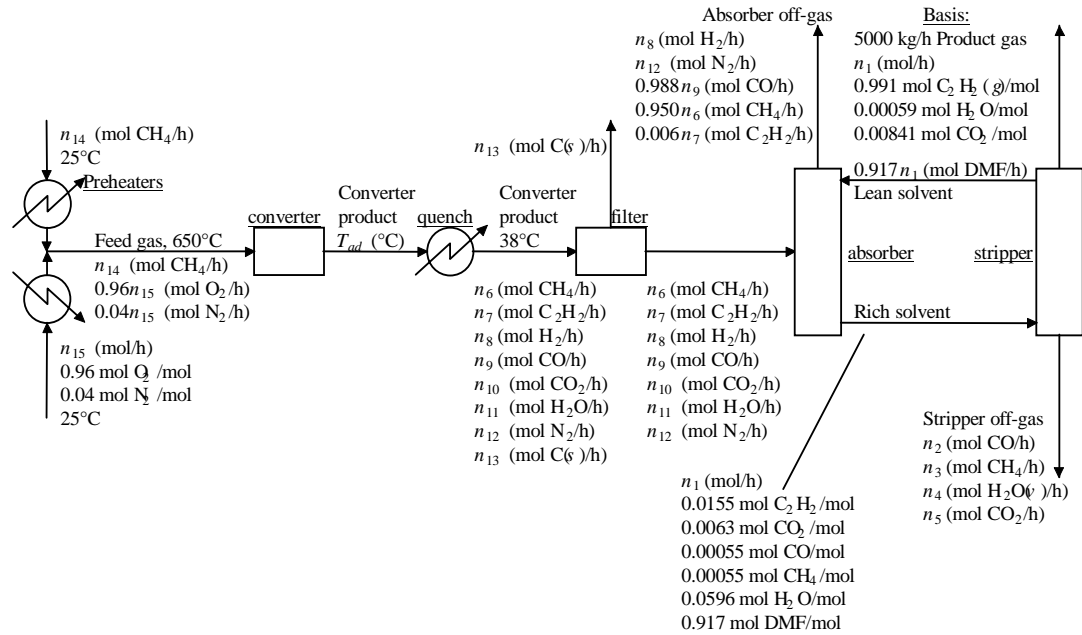
$$\alpha_3 = \sum_{i=1}^7 (n_i)_{\text{out}} d_i \quad \alpha_4 = \sum_{i=1}^7 (n_i)_{\text{out}} e_i$$



## 9.68 (cont'd)

d.	Run 1	Run 2	Run 3	Run 4	Run 5	Run 6
yCH4	0.75	0.86	0.75	0.75	0.75	0.75
yC2H6	0.21	0.1	0.21	0.21	0.21	0.21
yC3H8	0.04	0.04	0.04	0.04	0.04	0.04
Tf	40	40	150	40	40	40
Ta	150	150	150	250	150	150
Pxs	25	25	25	25	100	25
ywo	0.0306	0.0306	0.0306	0.0306	0.0306	0.1
nO2i	3.04	2.84	3.04	3.04	4.87	3.04
nN2	11.44	10.67	11.44	11.44	18.31	11.44
nH2Oi	0.46	0.43	0.46	0.46	0.73	1.61
HCH4	-74.3	-74.3	-70	-74.3	-74.3	-74.3
HC2H6	-83.9	-83.9	-77	-83.9	-83.9	-83.9
HC3H8	-102.7	-102.7	-93	-102.7	-102.7	-102.7
HO2i	3.6	3.6	3.6	6.6	3.6	3.6
HN2i	3.8	3.8	3.8	6.9	3.8	3.8
HH2Oi	-237.6	-237.6	-237.6	-234.1	-237.6	-237.6
nCO2	1.29	1.18	1.29	1.29	1.29	1.29
nH2O	2.75	2.61	2.75	2.75	3.02	3.9
nO2	0.61	0.57	0.61	0.61	2.44	0.61
nN2	11.44	10.67	11.44	11.44	18.31	11.44
<b>Tad</b>	<b>1743.1</b>	<b>1737.7</b>	<b>1750.7</b>	<b>1812.1</b>	<b>1237.5</b>	<b>1633.6</b>
alph0	-1052	-978.9	-1057	-1099	-1093	-1058
alph1	0.4892	0.4567	0.4892	0.4892	0.7512	0.5278
alph2	0.0001	1.00E-04	0.0001	0.0001	0.0001	0.0001
alph3	-3.00E-08	-3.00E-08	-3.00E-08	-3.00E-08	-4.00E-08	-2.00E-08
alph4	3.00E-12	3.00E-12	3.00E-12	3.00E-12	4.00E-12	2.00E-12
Delta H	3.00E-07	9.00E-06	-4.00E-07	-1.00E-04	-1.00E-05	6.00E-04

Species	a	b	c	d	e
		x 10 <sup>2</sup>	x 10 <sup>5</sup>	x 10 <sup>8</sup>	x 10 <sup>12</sup>
CH4	-75.72	3.431	2.734	0.122	-2.75
C2H6	-85.95	4.937	6.96	-1.939	1.82
C3H8	-105.6	6.803	11.3	-4.37	7.928
O2	-0.731	2.9	0.11	0.191	-0.718
N2	-0.728	2.91	0.579	-0.203	0.328
H2O	-242.7	3.346	0.344	0.254	-0.898
CO2	-394.4	3.611	2.117	-0.962	1.866



Average M.W. of product gas:

$$\bar{M} = 0.991(26.04) + 0.00059(18.016) + 0.00841(44.01) = 26.19 \text{ g/mol}$$

Molar flow rate of product gas:  $n_0 = \frac{5000 \text{ kg}}{\text{day}} \left| \frac{10^3 \text{ g}}{1 \text{ kg}} \right| \left| \frac{1 \text{ mol}}{26.19 \text{ g}} \right| \left| \frac{1 \text{ day}}{24 \text{ h}} \right| = 7955 \text{ mol/h}$

Material balances -- plan of attack (refer to flow chart):

Stripper balances: C<sub>2</sub>H<sub>2</sub>  $\Rightarrow n_1$ , CO  $\Rightarrow n_2$ , CH<sub>4</sub>  $\Rightarrow n_3$ , H<sub>2</sub>O  $\Rightarrow n_4$ , CO<sub>2</sub>  $\Rightarrow n_5$

Absorber balances: CH<sub>4</sub>  $\Rightarrow n_6$ , C<sub>2</sub>H<sub>2</sub>  $\Rightarrow n_7$ , CO  $\Rightarrow n_9$ , CO<sub>2</sub>  $\Rightarrow n_{10}$ , H<sub>2</sub>O  $\Rightarrow n_{11}$

$$\left\{ \begin{array}{l} 5.67\% \text{ soot formation} \\ \text{converter C balance} \end{array} \right\} \Rightarrow n_{13}, n_{14}, \text{ converter H balance} \Rightarrow n_8$$

$$\text{Converter O balance} \Rightarrow n_{15}, \text{ converter N}_2 \text{ balance} \Rightarrow n_{12}$$

Stripper balances:

$$\text{C}_2\text{H}_2: 0.0155n_1 = 0.991(7955 \text{ mol/h}) \Rightarrow n_1 = 5.086 \times 10^5 \text{ mol/h}$$

$$\text{CO: } (0.00055)(5.086 \times 10^5) = n_2 \Rightarrow n_2 = 79.7 \text{ mol CO/h}$$

$$\text{CH}_4: (0.00055)(5.086 \times 10^5) = n_3 \Rightarrow n_3 = 79.7 \text{ mol CH}_4/\text{h}$$

$$\text{H}_2\text{O: } (0.0596)(5.086 \times 10^5) = n_4 + (0.00059)(7955) \Rightarrow n_4 = 30308 \text{ mol H}_2\text{O/h}$$

$$\text{CO}_2: (0.0068)(5.086 \times 10^5) = n_5 + (0.00841)(7955) \Rightarrow n_5 = 3392 \text{ mol CO}_2/\text{h}$$

Absorber balances

$$\text{CH}_4: n_6 = 0.950n_6 + (0.00055)(5.086 \times 10^5) = n_6 \Rightarrow 5595 \text{ mol CH}_4/\text{h}$$

**9.69 (cont'd)**

$$\text{C}_2\text{H}_2: n_7 = (0.0155)(5.086 \times 10^5) + 0.006n_7 \Rightarrow n_7 = 7931 \text{ mol C}_2\text{H}_2/\text{h}$$

$$\text{CO}: n_9 = 0.988n_9 + (0.00055)(5.086 \times 10^5) \Rightarrow n_9 = 23311 \text{ mol CO/h}$$

$$\text{CO}_2: n_{10} = (0.0068)(5.086 \times 10^5) = 3458 \text{ mol CO}_2/\text{h}$$

$$\text{H}_2\text{O}: n_{11} = (0.0596)(5.086 \times 10^5) = 30313 \text{ mol H}_2\text{O/h}$$

$$\text{Soot formation: } \frac{n_{13} = (0.0567)n_{14}(\text{mol CH}_4)}{\text{h}} \left| \frac{1 \text{ mol C}}{1 \text{ mol CH}_4} \right. \Rightarrow n_{13} = 0.0567n_{14} \quad (1)$$

Converter C balance:

$$n_{14} = (5595 \text{ mol CH}_4/\text{h})(1 \text{ mol C/mol CH}_4) + (7931)(2) + (23311)(1) + (3458)(1) + n_{13}$$

$$\Rightarrow n_{14} = n_{13} + 48226 \quad (2)$$

$$\text{Solve (1) \& (2) simultaneously } \Rightarrow n_{13} = 2899 \text{ mol C(s)/h}, n_{14} = 51120 \text{ mol CH}_4/\text{h}$$

$$\text{Converter H balance: } \frac{51120 \text{ mol CH}_4}{\text{h}} \left| \frac{4 \text{ mol H}}{1 \text{ mol CH}_4} \right. = \overset{\text{CH}_4}{(5595)(4)} + \overset{\text{C}_2\text{H}_2}{(7931)(2)} + \overset{\text{H}_2}{2n_8} + \overset{\text{H}_2\text{O}}{(30313)(2)}$$

$$\Rightarrow n_8 = 52816 \text{ mol H}_2/\text{h}$$

$$\text{Converter O balance: } (0.96n_{15})(2) = \frac{23311 \text{ mol CO}}{\text{h}} \left| \frac{1 \text{ mol O}}{1 \text{ mol CO}} \right. + \overset{\text{CO}_2}{(3458)(2)} + \overset{\text{H}_2\text{O}}{(30313)(1)}$$

$$\Rightarrow n_{15} = 31531 \text{ mol/h}$$

$$\text{Converter N}_2 \text{ balance: } (0.04)(31531)n_{12} \Rightarrow n_{12} = 1261 \text{ mol N}_2/\text{h}$$

**a. Feed stream flow rates**

$$V_{\text{CH}_4} = \frac{51120 \text{ mol CH}_4}{\text{h}} \left| \frac{0.0244 \text{ m}^3(\text{STP})}{1 \text{ mol}} \right. = \underline{\underline{1145 \text{ SCMH CH}_4}}$$

$$V_{\text{O}_2} = \frac{31531 \text{ mol (O}_2 + \text{N}_2)}{\text{h}} \left| \frac{0.0244 \text{ m}^3(\text{STP})}{1 \text{ mol}} \right. = \underline{\underline{706 \text{ SCMH O}_2(+\text{N}_2)}}$$

**b. Gas feed to absorber**

$$\left. \begin{array}{l} 5595 \text{ mol CH}_4/\text{h} \\ 7931 \text{ mol C}_2\text{H}_2/\text{h} \\ 23311 \text{ mol CO/h} \\ 3458 \text{ mol CO}_2/\text{h} \\ 30313 \text{ mol H}_2\text{O/h} \\ 52816 \text{ mol H}_2/\text{h} \\ 1261 \text{ mol N}_2/\text{h} \\ \hline 1.2469 \times 10^5 \text{ mol/h} \end{array} \right\} \Rightarrow \underline{\underline{125 \text{ kmol/h}}}, \quad \underline{\underline{4.5 \text{ mole\% CH}_4, 6.4 \text{ \% C}_2\text{H}_2, 18.7\% \text{ CO}, 2.8\% \text{ CO}_2, 24.3\% \text{ H}_2\text{O}, 42.4\% \text{ H}_2, 1.0\% \text{ N}_2}}$$

Absorber off-gas

$$\left. \begin{array}{l} 52816 \text{ mol H}_2/\text{h} \\ 1261 \text{ mol N}_2/\text{h} \\ 23031 \text{ mol CO/h} \\ 5315 \text{ mol CH}_4/\text{h} \\ 41.6 \text{ mol C}_2\text{H}_2/\text{h} \\ \hline 8.2471 \times 10^4 \text{ mol/h} \end{array} \right\} \Rightarrow \underline{\underline{82.5 \text{ kmol/h}}}, \quad \underline{\underline{64.1 \text{ mole\% H}_2, 1.5\% \text{ N}_2, 27.9\% \text{ CO}, 6.4\% \text{ CH}_4, 0.06\% \text{ C}_2\text{H}_2}}$$

9.69 (cont'd)

Stripper off-gas

$$\left. \begin{array}{l} 279.7 \text{ mol CO/h} \\ 279.7 \text{ mol CH}_4/\text{h} \\ 30308 \text{ mol H}_2\text{O/h} \\ 3392 \text{ mol CO/h} \\ 3.4259 \times 10^4 \text{ mol/h} \end{array} \right\} \Rightarrow \underline{\underline{34.3 \text{ kmol/h, 0.82\% CO, 0.82\% CH}_4, 88.5\% \text{ H}_2\text{O, 9.9\% CO}_2}}$$

c. DMF recirculation rate =  $0.917 \left( 5.086 \times 10^5 \frac{\text{mol}}{\text{h}} \right) \left( \frac{1 \text{ kmol}}{10^3 \text{ mol}} \right) = \underline{\underline{466 \text{ kmol DMF/h}}}$

d. Overall product yield =  $\frac{(0.991)(7955) \text{ mol C}_2\text{H}_2 \text{ in product gas}}{51120 \text{ mol CH}_4 \text{ in feed/h}} = \underline{\underline{0.154 \frac{\text{mol C}_2\text{H}_2}{\text{mol CH}_4}}}$

The theoretical maximum yield would be obtained if only the reaction  $2\text{CH}_4 \rightarrow \text{C}_2\text{H}_2 + 3\text{H}_2$  occurred, the reaction went to completion, and all the  $\text{C}_2\text{H}_2$  formed were recovered in the product gas. This yield is  $(1 \text{ mol C}_2\text{H}_2/2 \text{ mol CH}_4) = 0.500 \text{ mol C}_2\text{H}_2/2 \text{ mol CH}_4$ .

The ratio of the actual yield to the theoretical yield is  $0.154/0.500 = \underline{\underline{0.308}}$ .

e. Methane preheater

$$\dot{Q}_{\text{CH}_4} = \Delta \dot{H} = \dot{n}_{14} \int_{25}^{650} \underset{\text{CH}_4}{\overset{\text{Table B.2}}{C_p}} dT = \frac{51120 \text{ mol}}{\text{h}} \left| \frac{32824 \text{ J}}{\text{mol}} \right| \left| \frac{1 \text{ h}}{3601 \text{ s}} \right| \left| \frac{1 \text{ kJ}}{10^3 \text{ J}} \right| = \underline{\underline{466 \text{ kW}}}$$

Oxygen preheater

$$\begin{aligned} \dot{Q}_{\text{O}_2} = \Delta \dot{H} &= 0.96 \dot{n}_{15} \overset{\text{Table B.8}}{\hat{H}(\text{O}_2, 650^\circ \text{C})} + 0.04 \dot{n}_{15} \overset{\text{Table B.8}}{\hat{H}(\text{N}_2, 650^\circ \text{C})} \\ &= \left( 31531 \frac{\text{mol}}{\text{h}} \right) \left[ (0.96 \times 20.135 + 0.04 \times 18.99) \frac{\text{kJ}}{\text{mol} \cdot ^\circ \text{C}} \right] \left( \frac{1 \text{ h}}{3600 \text{ s}} \right) = \underline{\underline{176 \text{ kW}}} \end{aligned}$$

f. References :  $\text{C(s)}$ ,  $\text{H}_2(\text{g})$ ,  $\text{O}_2(\text{g})$ ,  $\text{N}_2(\text{g})$  at  $25^\circ \text{C}$

Substance	$\dot{n}_{\text{in}}$	$\hat{H}_{\text{in}}(650^\circ \text{C})$	$\dot{n}_{\text{out}}$	$\hat{H}_{\text{out}}(T_{\text{out}})$	
$\text{CH}_4$	51120	-42.026	5595	$-74.85 + \int_{25}^{T_a} C_p dT$	
$\text{O}_2$	30270	20.125	—	—	
$\text{N}_2$	1261	18.988	1261	$\int_{35}^{T_a} C_p dT$	
$\text{C}_2\text{H}_2$	—	—	7931	$+226.75 \int_{25}^{T_a} C_p dT$	
$\text{H}_2$	—	—	52816	$\int C_p dT$	$n(\text{mol/h})$
$\text{CO}$	—	—	23311	$-110.52 + \int C_p dT$	$\hat{H}(\text{kJ/mol})$
$\text{CO}_2$	—	—	3458	$-393.5 + \int C_p dT$	
$\text{H}_2\text{O}$	—	—	30313	$-241.83 + \int C_p dT$	
$\text{C(s)}$	—	—	2899	$\int C_p dT$	

**9.69 (cont'd)**

$$\hat{H}_i = \underset{\substack{\text{kJ/mol} \\ 25 \\ \text{kJ/mol}\cdot^\circ\text{C}}}{\Delta\hat{H}_i^0} + \int_{25}^T C_{pi} dT$$

$$\sum_{\text{in}} \dot{n}_i \hat{H}_i = -1.575 \times 10^6 \text{ kJ/h}$$

$$\sum_{\text{out}} \dot{n}_i \hat{H}_i = -9.888 \times 10^6 \text{ kJ/h} + \int_{25}^{T_{\text{out}}} \left[ 5595(C_p)_{\text{CH}_4} + 1261(C_p)_{\text{N}_2} + 7931(C_p)_{\text{C}_3\text{H}_2} \right. \\ \left. + 52816(C_p)_{\text{H}_2} + 23311(C_p)_{\text{CO}} + 3458(C_p)_{\text{CO}_2} + 3013(C_p)_{\text{H}_2\text{O}(v)} \right] \frac{1 \text{ kJ}}{10^3 \text{ J}} dT \\ + \int_{298}^{T_{ad}+273} (C_p)_{\text{C}(s)} \times \frac{1 \text{ kJ}}{10^3 \text{ J}} dT$$

We will apply the heat capacity formulas of Table B.2, recognizing that we will probably push at least some of them above their upper temperature limits

$$\sum_{\text{out}} \dot{n}_i \hat{H}_i = -9.888 \times 10^6 \text{ kJ/h} + \int_{25}^{T_{ad}} \left( 3902 + 1.2185 - 5.9885 \times 10^{-4} T^2 - 1.0162 \times 10^{-7} T^3 \right) dT \\ + \int_{298}^{T_{ad}+273} \left( 32.411 + 0.031744T - \frac{1.4179 \times 10^6}{T^2} \right) dT$$

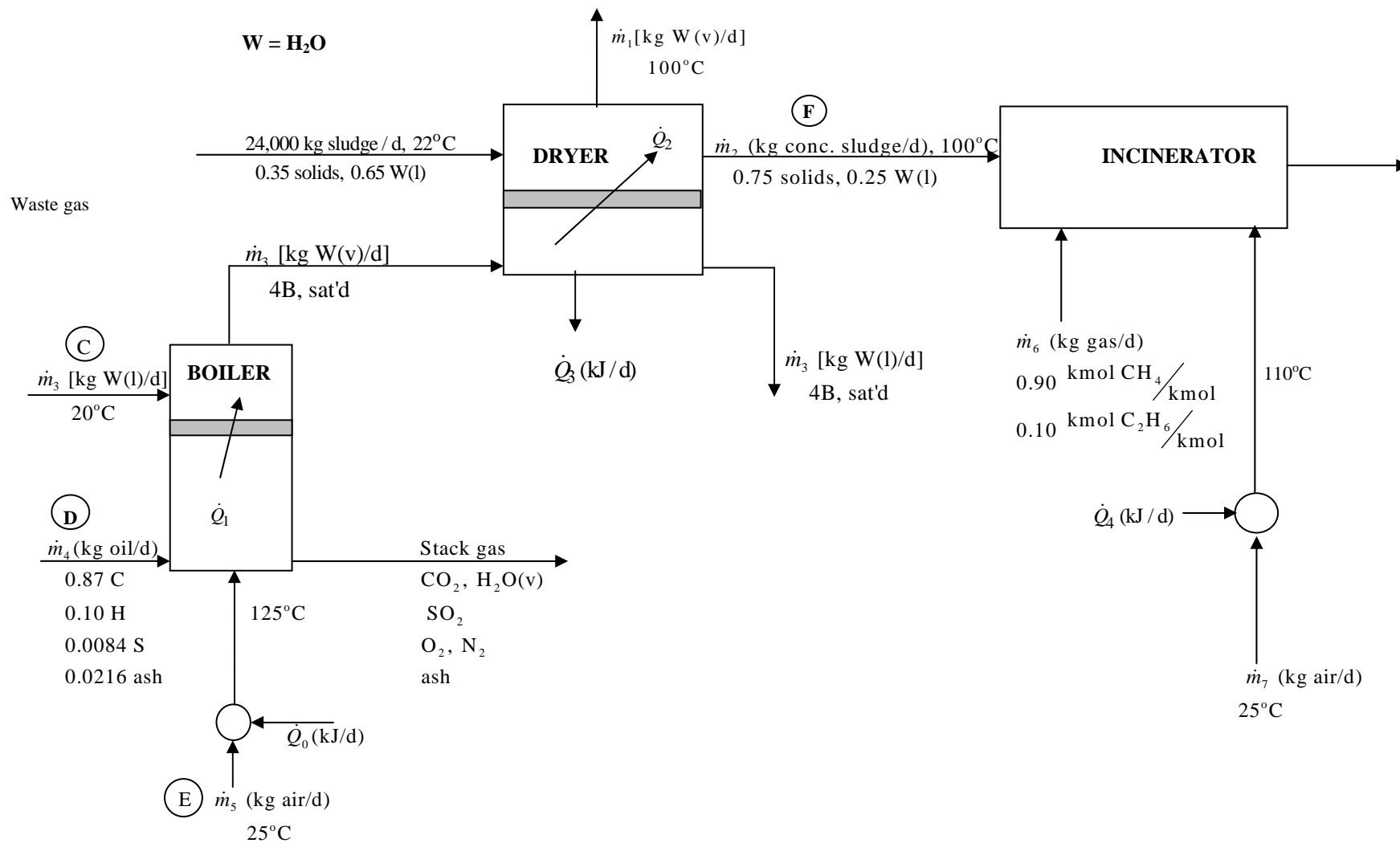
$$\sum_{\text{out}} \dot{n}_i \hat{H}_i = -1.000 \times 10^7 + 3943T_a + 0.6251T_a^2 - 1.996 \times 10^{-4} T_a^3 - 2.5405 \times 10^{-8} T_a^4 + \frac{1.418 \times 10^6}{T_a + 273}$$

Energy balance:  $\Delta\dot{H} = \sum_{\text{out}} \dot{n}_i \hat{H}_i - \sum_{\text{in}} \dot{n}_i \hat{H}_i = 0$

$$\Rightarrow f(T_c) = -8.485 \times 10^6 + 3943T_c + 0.6251T_c^2 - 1.996 \times 10^{-4} T_c^3 - 2.5405 \times 10^{-8} T_c^4 + \frac{1.418 \times 10^6}{T_c + 273} = 0$$

E-Z Solve  
 $\Longrightarrow T_c = \underline{\underline{2032^\circ\text{C}}}$

9.70 a.



## 9.70 (cont'd)

Solids balance on dryer:

$$0.35 \times 24,000 \text{ kg/d} = 0.75\dot{n}_2 \Rightarrow \dot{n}_2 = 11200 \text{ kg/d} \Rightarrow \underline{\underline{F = 11.2 \text{ tonnes/d (conc. sludge)}}}$$

Mass Balance on dryer:  $24,000 = \dot{n}_1 + 11200 \Rightarrow \dot{n}_1 = 12,800 \text{ kg/d}$

Energy balance on sludge side of dryer:

References :  $\text{H}_2\text{O(l, 22}^\circ\text{C)}$ ,  $\text{Solids(22}^\circ\text{C)}$

Substance	$\dot{n}_{\text{in}}$ (kg/d)	$\hat{H}_{\text{in}}$ (kJ/kg)	$\dot{n}_{\text{out}}$ (kg/d)	$\hat{H}_{\text{out}}$ (kJ/kg)
Solids	8400	0	8400	$\hat{H}_1$
$\text{H}_2\text{O(l)}$	15600	0	2800	$\hat{H}_2$
$\text{H}_2\text{O(v)}$	—	—	12800	$\hat{H}_3$

$$\hat{H}_1 = 2.5(100 - 22) = 195.0 \text{ kJ/kg}$$

$$\hat{H}_2 = (419.1 - 92.2) = 326.9 \text{ kJ/kg}$$

$$\hat{H}_3 = (2676 - 92.2) = 2584 \text{ kJ/kg}$$

( $\hat{H}_{\text{water}}$  from Table B.5)

$$\dot{Q}_2 = \sum_{\text{out}} \dot{m}_i \hat{H}_i - \sum_{\text{in}} \dot{m}_i \hat{H}_i \Rightarrow \underline{\underline{\dot{Q}_2 = 3.56 \times 10^7 \text{ kJ/day}}}$$

$$\dot{Q}_{\text{steam}} = \frac{3.56 \times 10^7}{0.55} = 6.47 \times 10^7 \text{ kJ/d} \Rightarrow \underline{\underline{\dot{Q}_3 = 2.91 \times 10^7 \text{ kJ/d}}}$$

Energy balance on steam side of dryer:

$$6.47 \times 10^7 \frac{\text{kJ}}{\text{d}} = \dot{n}_3 \left( \frac{\text{kg}}{\text{d}} \right) \times \overset{\substack{\Delta \hat{H}_v \text{ for} \\ \text{H}_2\text{O(sat'd.)}}}{2133} \left( \frac{\text{kJ}}{\text{kg}} \right) \left( \frac{1 \text{ tonne}}{10^3 \text{ kg}} \right) \Rightarrow \underline{\underline{\dot{n}_3 = 30.3 \text{ tonnes/d (boiler feedwater)}}}$$

Energy balance on steam side of boiler:

$$\dot{Q}_1 = (30300 \frac{\text{kg}}{\text{d}})(2737.6 - 83.9) \frac{\text{kJ}}{\text{kg}} = \underline{\underline{8.04 \times 10^7 \text{ kJ/d}}}$$

$$\underline{\underline{62\% \text{ efficiency}}} \Rightarrow \text{Fuel heating value needed} = \frac{8.04 \times 10^7}{0.62} = 1.3 \times 10^8 \text{ kJ/d}$$

$$\Rightarrow \dot{n}_4 = \frac{1.30 \times 10^8 \text{ kJ/d}}{3.75 \times 10^4 \text{ kJ/kg}} = \underline{\underline{3458 \text{ kg/d}}} \Rightarrow \underline{\underline{D = 3.5 \text{ tonnes/day (fuel oil)}}}$$

Air feed to boiler furnace:  $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$ ,  $4\text{H} + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$ ,  $\text{S} + \text{O}_2 \rightarrow \text{SO}_2$

$$\begin{aligned} (n_{\text{O}_2})_{\text{theo}} &= 3458 \frac{\text{kg}}{\text{d}} \left[ (0.87 \frac{\text{kgC}}{\text{kg}}) \left( \frac{1 \text{ kmol C}}{12 \text{ kg}} \right) \left( \frac{1 \text{ kmol O}_2}{1 \text{ kmol C}} \right) + (0.10) \left( \frac{1}{1} \right) \left( \frac{1}{4} \right) + (0.0084) \left( \frac{1}{32} \right) \left( \frac{1}{1} \right) \right] \\ &= 338 \text{ kmol O}_2/\text{d} \end{aligned}$$

### 9.70 (cont'd)

$$\text{Air fed (25\% excess)} = 1.25(4.76 \frac{\text{kmol air}}{\text{kmol O}_2})(338 \frac{\text{kmol O}_2}{\text{d}}) = 2011 \frac{\text{kmol air}}{\text{d}}$$

$$\Rightarrow \frac{2011 \text{ kmol}}{\text{d}} \left| \frac{29 \text{ kg}}{\text{kmol}} \right| \frac{1 \text{ tonne}}{10^3 \text{ kg}} \Rightarrow \underline{\underline{\dot{E} = 58.3 \text{ tonnes/d (air to boiler)}}}$$

Energy balance on boiler air preheater:

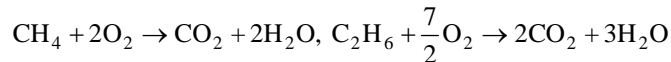
$$\text{Table B.8} \Rightarrow \hat{H}_{\text{air}}(125^\circ \text{C}) = 2.93 \frac{\text{kJ}}{\text{mol}} \Rightarrow \dot{Q}_0 = \frac{2011 \text{ kmol}}{\text{d}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{2.93 \text{ kJ}}{\text{mol}} = \underline{\underline{5.89 \times 10^6 \text{ kJ/d}}}$$

Supplementary fuel for incinerator:

$$\dot{n}_6 = \frac{11.2 \text{ tonne sludge}}{\text{d}} \left| \frac{195 \text{ SCM}}{\text{tonne}} \right| \frac{1 \text{ kmol}}{22.4 \text{ SCM}} = 97.5 \text{ kmol/d}$$

$$\overline{MW}_{\text{gas}} = 0.90 \overline{MW}_{\text{CH}_4} + 0.10 \overline{MW}_{\text{C}_2\text{H}_6} = (0.90)(16) + (0.10)(30) = 17.4 \text{ kg/kmol}$$

$$\dot{M}_{\text{gas}} = (97.5)(17.4) \Rightarrow \underline{\underline{\dot{G} = 1.7 \text{ tonne/d (natural gas)}}}$$



Air feed to incinerator:

$$(\text{air})_{\text{th, sludge}}: \frac{11200 \text{ kg sludge}}{\text{d}} \left| \frac{0.75 \text{ kg sol}}{\text{kg sludge}} \right| \frac{19000 \text{ kJ}}{1 \text{ kg sol}} \left| \frac{2.5 \text{ m}^3(\text{STP}) \text{ air}}{10^4 \text{ kJ}} \right| \frac{1 \text{ kmol}}{22.4 \text{ m}^3(\text{STP})} = 1781 \frac{\text{kmol air}}{\text{d}}$$

$$(\text{air})_{\text{th, gas}}: 97.5 \frac{\text{kmol}}{\text{d}} \left[ 0.90 \frac{\text{kmol CH}_4}{\text{kmol}} \times \frac{2 \text{ kmol O}_2}{\text{kmol CH}_4} + (0.10)(3.5) \right] \left( \frac{4.76 \text{ kmol air}}{1 \text{ kmol O}_2} \right) = 998 \frac{\text{kmol air}}{\text{d}}$$

$$100\% \text{ excess air: } \dot{n}_7 = 2(1781 + 998) \frac{\text{kmol air}}{\text{d}} = 5558 \text{ kmol air/d}$$

$$\Rightarrow \frac{5558 \text{ kmol air}}{\text{d}} \left| \frac{29.0 \text{ kg air}}{1 \text{ kmol air}} \right| \frac{1 \text{ tonne}}{10^3 \text{ kg}} = \underline{\underline{161 \text{ tonne air/d (incinerator air)}}}$$

Energy balance on air preheater :

$$\text{Table B.8} \Rightarrow \hat{H}_{\text{air}}(110^\circ \text{C}) = 2.486 \frac{\text{kJ}}{\text{mol}} \Rightarrow \dot{Q}_4 = \frac{5558 \text{ kmol}}{\text{d}} \left| \frac{10^3 \text{ mol}}{1 \text{ kmol}} \right| \frac{2.486 \text{ kJ}}{\text{mol}} = \underline{\underline{1.38 \times 10^7 \frac{\text{kJ}}{\text{d}}}}$$

- b. Cost of fuel oil, natural gas, fuel oil and air preheating, pumping and compression, piping, utilities, operating personnel, instrumentation and control, environmental monitoring. Lowering environmental hazard might justify lack of profit.
- c. Put hot product gases from boiler and/or incinerator through heat exchangers to preheat both air streams. Make use of steam from dryer.
- d. Sulfur dioxide, possibly NO<sub>2</sub>, fly ash in boiler stack gas, volatile toxic and odorous compounds in gas effluents from dryer and incinerator.