(905212)Chemical Engineering Principles (2)

CHAPTER 9:
Balances on Reactive Processes

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9.5 Process with Unknown Outlet Conditions: Adiabatic Reactors

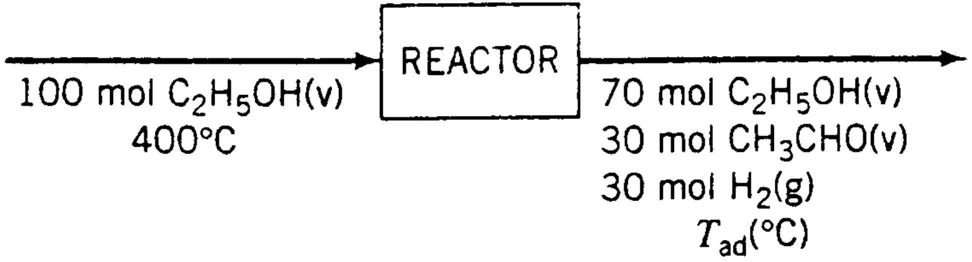
Example 9.5.3 : Energy Balance On an Adiabatic Reactor

The dehydrogenation of ethanol to form acetaldehyde

$$C_2H_5OH(v) \rightarrow CH_3CHO(v) + H_2(g)$$

is carried out in a continuous adiabatic reactor. Ethanol vapor is fed to the reactor at 400°C, and a conversion of 30% is obtained. Calculate the product temperature.

Basis: 100 mol Feed



REACTOR

100 mol $C_2H_5OH(v)$
400°C

70 mol $C_2H_5OH(v)$
30 mol $CH_3CHO(v)$
30 mol $H_2(g)$
T_{ad}(°C)

9.5 Process with Unknown Outlet Conditions: Adiabatic Reactors

The open system energy balance neglecting kinetic and potential energy changes and shaft work and setting $Q = 0$ for this adiabatic reactor is

$$\Delta H = \xi \, \Delta \hat{H}_r^\circ + \sum n_{\text{out}} \hat{H}_{\text{out}} - \sum n_{\text{in}} \hat{H}_{\text{in}} = 0$$

References: $C_2H_5OH(v)$, $CH_3CHO(v)$, $H_2(g)$ at 25°C and 1 atm

Substance	n_{in} (mol)	$\hat{H}_{\text{in}}$ (kJ/mol)	n_{out} (mol)	$\hat{H}_{\text{out}}$ (kJ/mol)
C_2H_5OH	100.0	$\hat{H}_1$	70.0	$\hat{H}_2$
CH_3CHO	—	—	30.0	$\hat{H}_3$
H_2	—	—	30.0	$\hat{H}_4$

9.5 Process with Unknown Outlet Conditions: Adiabatic Reactors

The open system energy balance neglecting kinetic and potential energy changes and shaft work and setting $Q = 0$ for this adiabatic reactor is

$$\Delta H = \xi \Delta \hat{H}_r^\circ + \sum n_{\text{out}} \hat{H}_{\text{out}} - \sum n_{\text{in}} \hat{H}_{\text{in}} = 0$$

$$\xi = \frac{|(n_{CH_3CHO})_{\text{out}} - (n_{CH_3CHO})_{\text{in}}|}{|\nu_{CH_3CHO}|} = \frac{|30.0 \text{ mol} - 0 \text{ mol}|}{1} = 30.0 \text{ mol}$$

$$\Delta \hat{H}_r^\circ = \sum \nu_i \Delta \hat{H}_f^\circ = (-1)(\Delta \hat{H}_f^\circ)_{C_2H_5OH(v)} + (1)(\Delta \hat{H}_f^\circ)_{CH_3CHO(v)} + (1)(\Delta \hat{H}_f^\circ)_{H_2(g)}$$

$$= [(-1)(-235.31) + (1)(-166.2) + (1)(0)] \text{ kJ/mol} = 69.11 \text{ kJ/mol}$$

Calculate Inlet Enthalpy

$$\hat{H}_1 = \int_{25^\circ C}^{400^\circ C} (C_p)_{C_2H_5OH} \xrightarrow{C_p \text{ from Table B.2}} \hat{H}_1 = 33.79 \text{ kJ/mol}$$

9.5 Process with Unknown Outlet Conditions: Adiabatic Reactors

Outlet Enthalpies

$$\hat{H}_i = \int_{25°\text{C}}^{T_{\text{ad}}} C_{pi}(T)\,dT, \quad i = 1, 2, 3$$

Solve the Energy Balance for T_{ad}

$$\Delta H = \xi\,\Delta\hat{H}_r^\circ + (70.0\text{ mol})\hat{H}_2 + (30.0\text{ mol})\hat{H}_3 + (30.0\text{ mol})\hat{H}_4 - (100.0\text{ mol})\hat{H}_1 = 0$$

$$\Big\Downarrow \text{Substitute for } \xi\ (= 30.0\text{ mol}),\ \Delta\hat{H}_r^\circ\ (= 69.11\text{ kJ/mol}),\ \hat{H}_1\ (= 33.79\text{ kJ/mol}),\text{ and } \hat{H}_2 \text{ through } \hat{H}_4$$

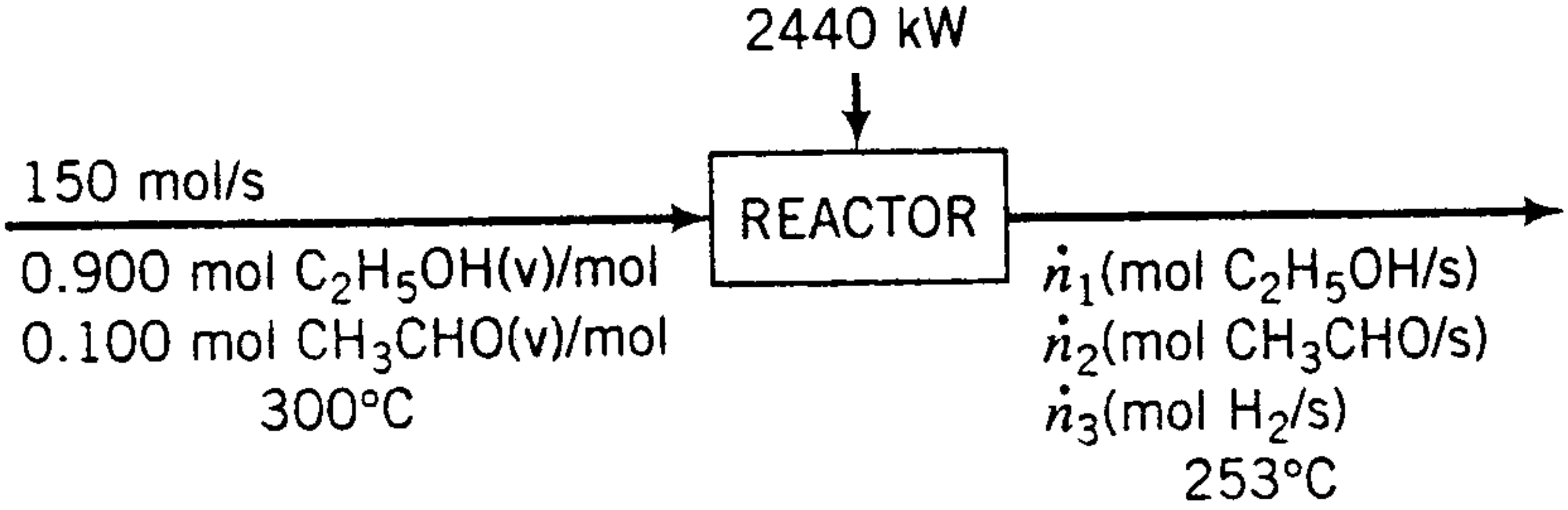
$$\Delta H = 5.190 \times 10^{-10}T_{\text{ad}}^4 + 2.813 \times 10^{-6}T_{\text{ad}}^3 + 7.492 \times 10^{-3}T_{\text{ad}}^2 + 6.673T_{\text{ad}} - 1477 = 0$$

This equation can be solved using an equation-solving program or a spreadsheet.[6] The solution is

$$\boxed{T_{\text{ad}} = 185°\text{C}}$$

Example 9.5.4: Simultaneous Mass & Energy

The ethanol dehydrogenation reaction of Example 9.5-3 is carried out with the feed entering at 300°C. The feed contains 90.0 mole% ethanol and the balance acetaldehyde and enters the reactor at a rate of 150 mol/s. To keep the temperature from dropping too much and thereby decreasing the reaction rate to an unacceptably low level, heat is transferred to the reactor. When the heat addition rate is 2440 kW, the outlet temperature is 253°C. Calculate the fractional conversion of ethanol achieved in the reactor.



2440 kW

150 mol/s

0.900 mol $C_2H_5OH(v)$/mol

0.100 mol $CH_3CHO(v)$/mol

300°C

REACTOR

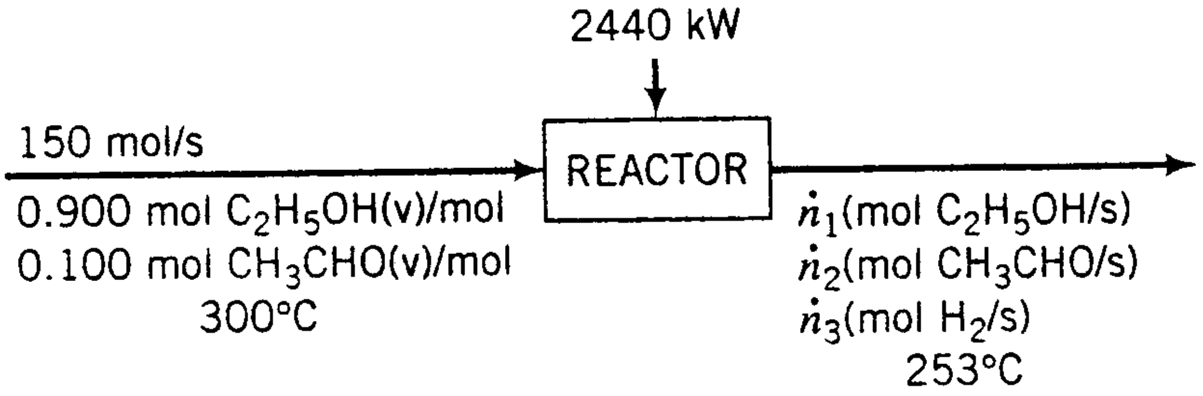
$\dot{n}_1$(mol C_2H_5OH/s)

$\dot{n}_2$(mol CH_3CHO/s)

$\dot{n}_3$(mol H_2/s)

253°C

$$C_2H_5OH \longrightarrow CH_3CHO + H_2$$



2440 kW

150 mol/s

0.900 mol $C_2H_5OH(v)$/mol

0.100 mol $CH_3CHO(v)$/mol

300°C

REACTOR

$\dot{n}_1$(mol C_2H_5OH/s)

$\dot{n}_2$(mol CH_3CHO/s)

$\dot{n}_3$(mol H_2/s)

253°C

$$C_2H_5OH \longrightarrow CH_3CHO + H_2$$

$$\begin{array}{l} \quad 3 \text{ unknown labeled variables } (\dot{n}_1, \dot{n}_2, \dot{n}_3) \\ -\ 2 \text{ independent atomic species balances (C and H)} \\ \underline{-\ 1 \text{ energy balance}} \\ =\ 0 \text{ degrees of freedom} \end{array}$$

Balance on C

$$\frac{150\text{ mol}}{\text{s}}\left|\frac{0.900\text{ mol }C_2H_5OH}{\text{mol}}\right|\frac{2\text{ mol C}}{1\text{ mol }C_2H_5OH}+\frac{150\text{ mol}}{\text{s}}\left|\frac{0.100\text{ mol }CH_3CHO}{\text{mol}}\right|\frac{2\text{ mol C}}{1\text{ mol }CH_3CHO}$$

$$=\frac{\dot{n}_1(\text{mol }C_2H_5OH)}{\text{s}}\left|\frac{2\text{ mol C}}{1\text{ mol }C_2H_5OH}\right.+\frac{\dot{n}_2(\text{mol }CH_3CHO)}{\text{s}}\left|\frac{2\text{ mol C}}{1\text{ mol }CH_3CHO}\right.$$

$$\Downarrow$$

$$\dot{n}_1+\dot{n}_2 = 150\text{ mol/s} \qquad (1)$$

Balance on H

$$[(150)(0.900)(6)+(150)(0.100)(4)]\text{ mol H/s} = 6\dot{n}_1+4\dot{n}_2+2\dot{n}_3 \quad \text{(Convince yourself)}$$

$$\Downarrow$$

$$3\dot{n}_1+2\dot{n}_2+\dot{n}_3 = 435\text{ mol H/s} \qquad (2)$$

Energy Balance

$$\dot{Q} = \Delta\dot{H} = \sum \dot{n}_{\text{out}}\hat{H}_{\text{out}} - \sum \dot{n}_{\text{in}}\hat{H}_{\text{in}}$$

$$\hat{H}_i = \Delta\hat{H}^\circ_{fi} + \int_{25^\circ C}^{T} C_{pi}(T)\,dT$$

References: C(s), H_2(g), O_2(g) at 25°C and 1 atm

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)
C_2H_5OH	135	−212.19	$\dot{n}_1$	−216.81
CH_3CHO	15	−147.07	$\dot{n}_2$	−150.90
H_2	—	—	$\dot{n}_3$	6.595

$$2440 \text{ kJ/s} = [-216.81\dot{n}_1 - 150.90\dot{n}_2 + 6.595\dot{n}_3 - (135)(-212.19) - (15)(-147.07)] \text{ kJ/s}$$

$$\Downarrow$$

$$216.81\dot{n}_1 + 150.90\dot{n}_2 - 6.595\dot{n}_3 = 28{,}412 \text{ kJ/s} \tag{3}$$

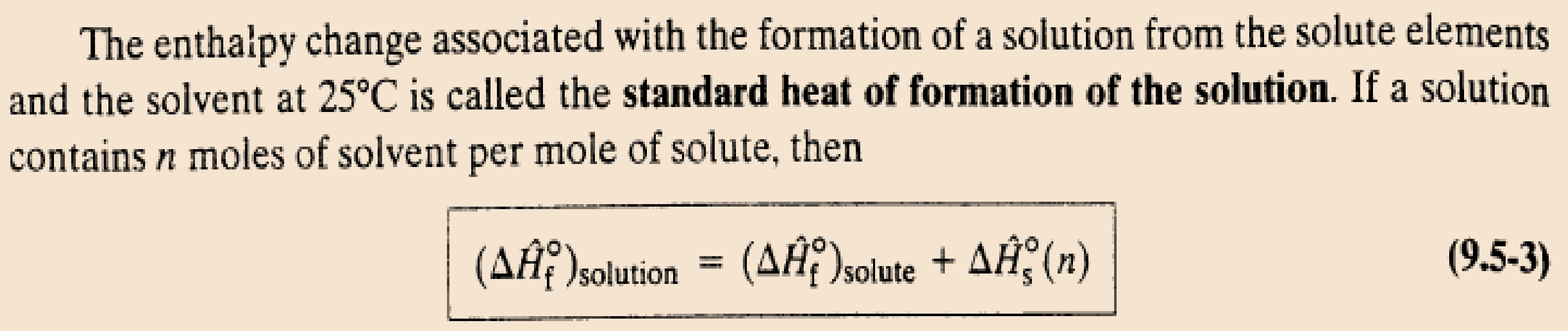
Solving Equations 1 through 3 simultaneously yields

$$\dot{n}_1 = 92.0 \text{ mol } C_2H_5OH\text{/s}$$

$$\dot{n}_2 = 58.0 \text{ mol } CH_3CHO\text{/s}$$

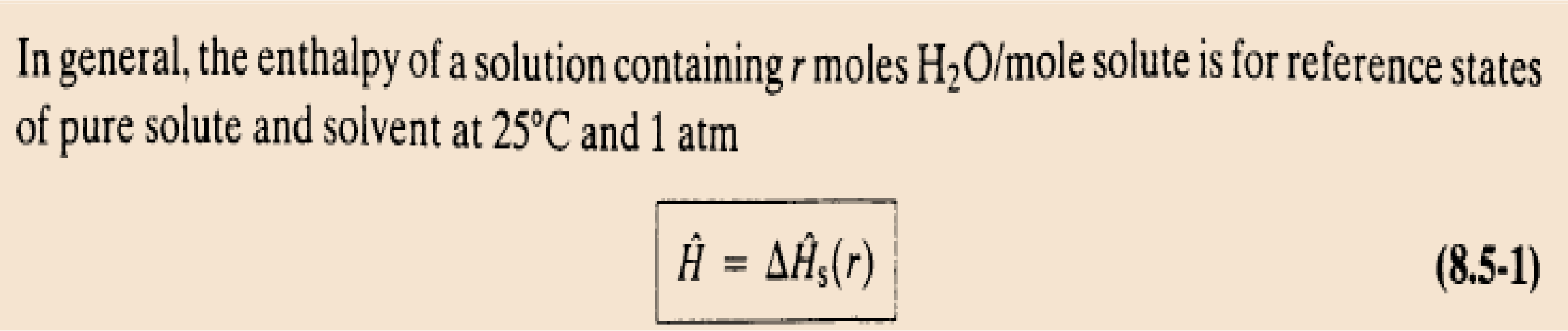
$$\dot{n}_3 = 43.0 \text{ mol } H_2\text{/s}$$

9.5c Thermochemistry of Solutions



The enthalpy change associated with the formation of a solution from the solute elements and the solvent at 25°C is called the **standard heat of formation of the solution**. If a solution contains n moles of solvent per mole of solute, then

$$\boxed{(\Delta\hat{H}_f^\circ)_{\text{solution}} = (\Delta\hat{H}_f^\circ)_{\text{solute}} + \Delta\hat{H}_s^\circ(n)} \qquad \textbf{(9.5-3)}$$

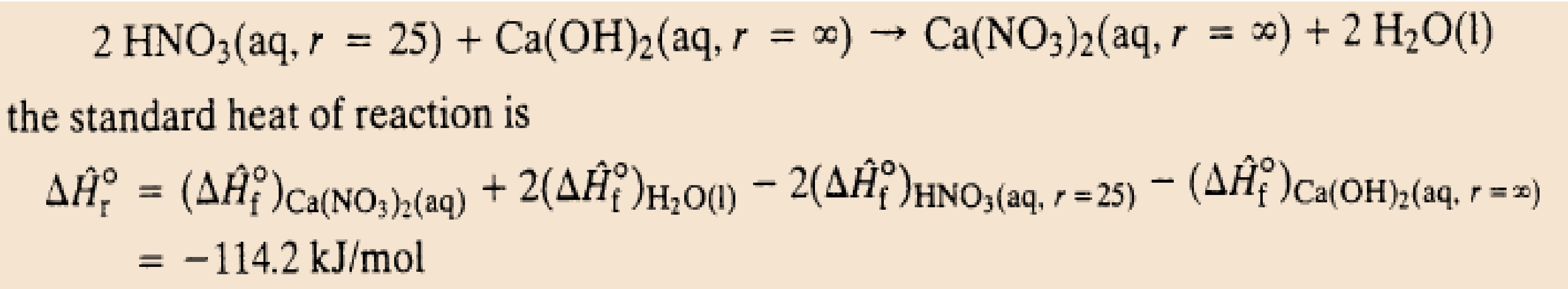


In general, the enthalpy of a solution containing r moles H_2O/mole solute is for reference states of pure solute and solvent at 25°C and 1 atm

$$\boxed{\hat{H} = \Delta\hat{H}_s(r)} \qquad \textbf{(8.5-1)}$$

9.5c Thermochemistry of Solutions

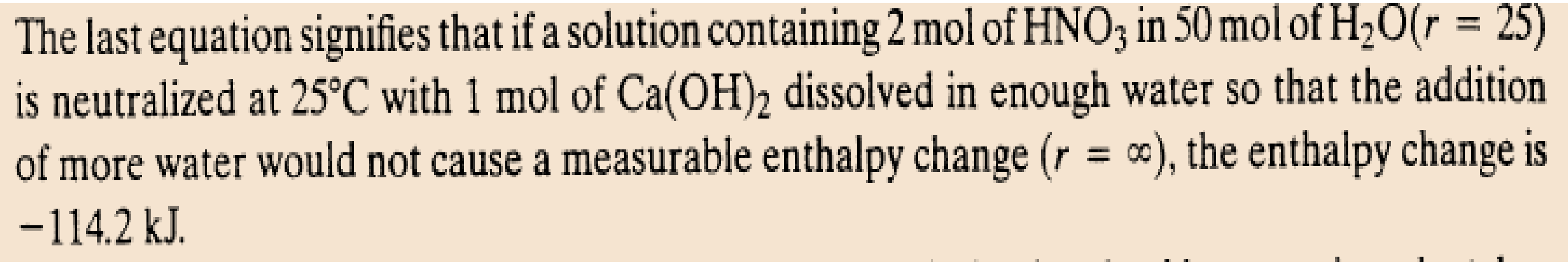
Standard Hear of Reaction ($\Delta\hat{H}_r^o$) Involving solutions



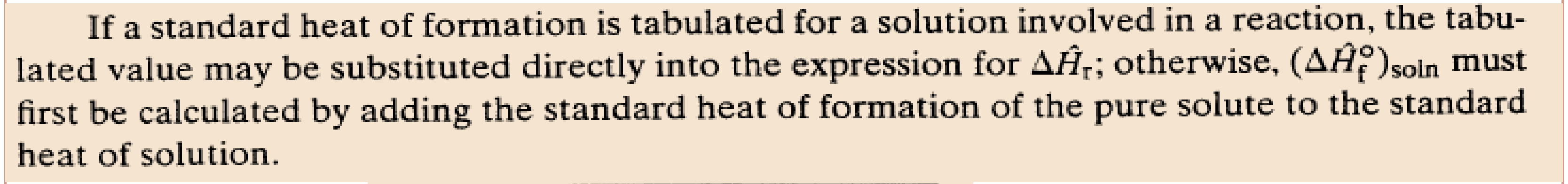
$$2\,HNO_3(aq, r = 25) + Ca(OH)_2(aq, r = \infty) \rightarrow Ca(NO_3)_2(aq, r = \infty) + 2\,H_2O(l)$$

the standard heat of reaction is

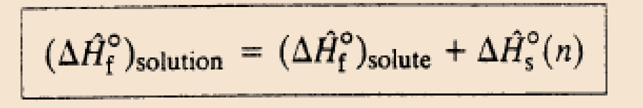
$$\Delta\hat{H}_r^\circ = (\Delta\hat{H}_f^\circ)_{Ca(NO_3)_2(aq)} + 2(\Delta\hat{H}_f^\circ)_{H_2O(l)} - 2(\Delta\hat{H}_f^\circ)_{HNO_3(aq,\, r=25)} - (\Delta\hat{H}_f^\circ)_{Ca(OH)_2(aq,\, r=\infty)}$$
$$= -114.2 \text{ kJ/mol}$$



The last equation signifies that if a solution containing 2 mol of HNO_3 in 50 mol of $H_2O(r = 25)$ is neutralized at 25°C with 1 mol of $Ca(OH)_2$ dissolved in enough water so that the addition of more water would not cause a measurable enthalpy change ($r = \infty$), the enthalpy change is −114.2 kJ.



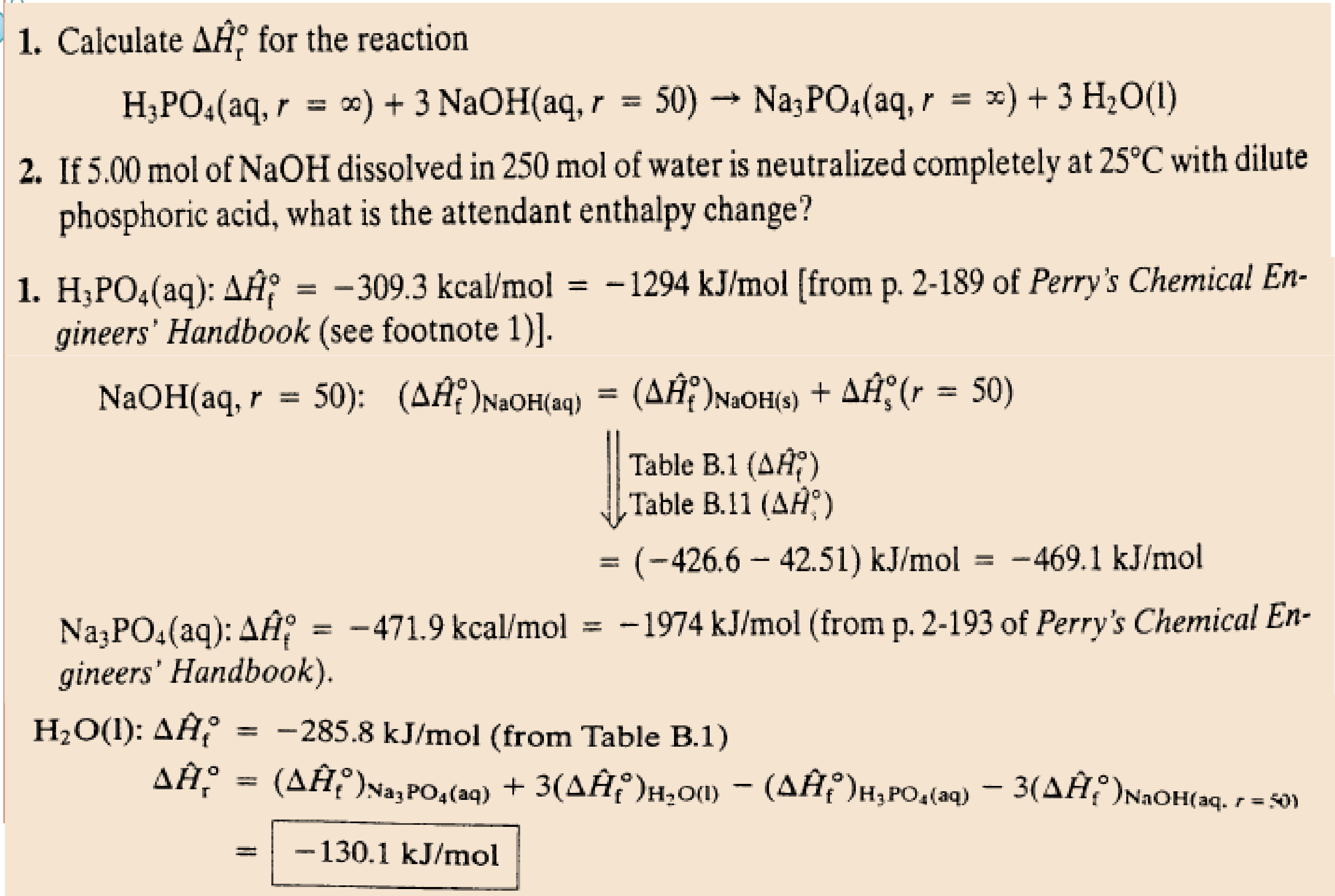
If a standard heat of formation is tabulated for a solution involved in a reaction, the tabulated value may be substituted directly into the expression for $\Delta\hat{H}_r$; otherwise, $(\Delta\hat{H}_f^\circ)_{soln}$ must first be calculated by adding the standard heat of formation of the pure solute to the standard heat of solution.



$$\boxed{(\Delta\hat{H}_f^\circ)_{solution} = (\Delta\hat{H}_f^\circ)_{solute} + \Delta\hat{H}_s^\circ(n)}$$

9.5c Thermochemistry of Solutions

Standard Hear of Neutralization Reaction ($\Delta\hat{H}_r^o$)



1. Calculate $\Delta\hat{H}_r^\circ$ for the reaction

$$H_3PO_4(aq, r = \infty) + 3\,NaOH(aq, r = 50) \rightarrow Na_3PO_4(aq, r = \infty) + 3\,H_2O(l)$$

2. If 5.00 mol of NaOH dissolved in 250 mol of water is neutralized completely at 25°C with dilute phosphoric acid, what is the attendant enthalpy change?

1. $H_3PO_4(aq)$: $\Delta\hat{H}_f^\circ = -309.3$ kcal/mol $= -1294$ kJ/mol [from p. 2-189 of *Perry's Chemical Engineers' Handbook* (see footnote 1)].

$$NaOH(aq, r = 50):\quad (\Delta\hat{H}_f^\circ)_{NaOH(aq)} = (\Delta\hat{H}_f^\circ)_{NaOH(s)} + \Delta\hat{H}_s^\circ(r = 50)$$

$$\Big\Downarrow \begin{array}{l}\text{Table B.1 } (\Delta\hat{H}_f^\circ) \\ \text{Table B.11 } (\Delta\hat{H}_s^\circ)\end{array}$$

$$= (-426.6 - 42.51)\text{ kJ/mol} = -469.1\text{ kJ/mol}$$

$Na_3PO_4(aq)$: $\Delta\hat{H}_f^\circ = -471.9$ kcal/mol $= -1974$ kJ/mol (from p. 2-193 of *Perry's Chemical Engineers' Handbook*).

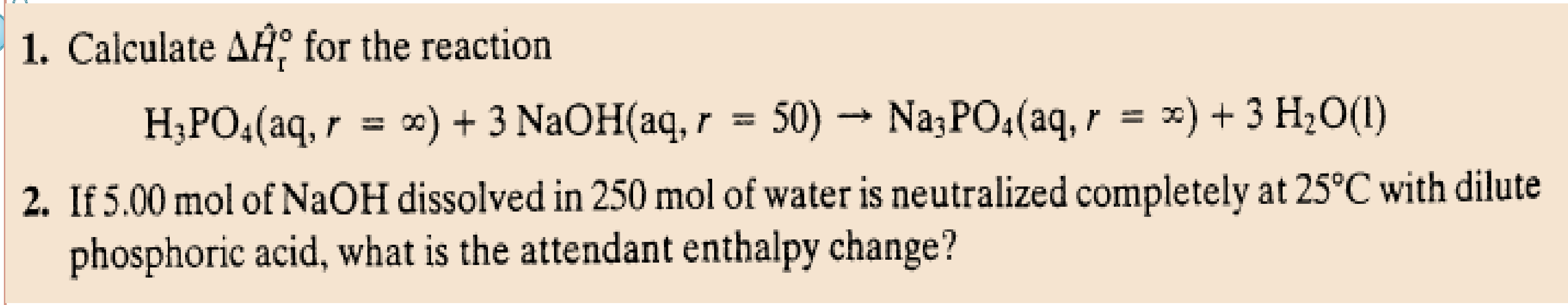
$H_2O(l)$: $\Delta\hat{H}_f^\circ = -285.8$ kJ/mol (from Table B.1)

$$\Delta\hat{H}_r^\circ = (\Delta\hat{H}_f^\circ)_{Na_3PO_4(aq)} + 3(\Delta\hat{H}_f^\circ)_{H_2O(l)} - (\Delta\hat{H}_f^\circ)_{H_3PO_4(aq)} - 3(\Delta\hat{H}_f^\circ)_{NaOH(aq,\, r=50)}$$

$$= \boxed{-130.1\text{ kJ/mol}}$$

9.5c Thermochemistry of Solutions

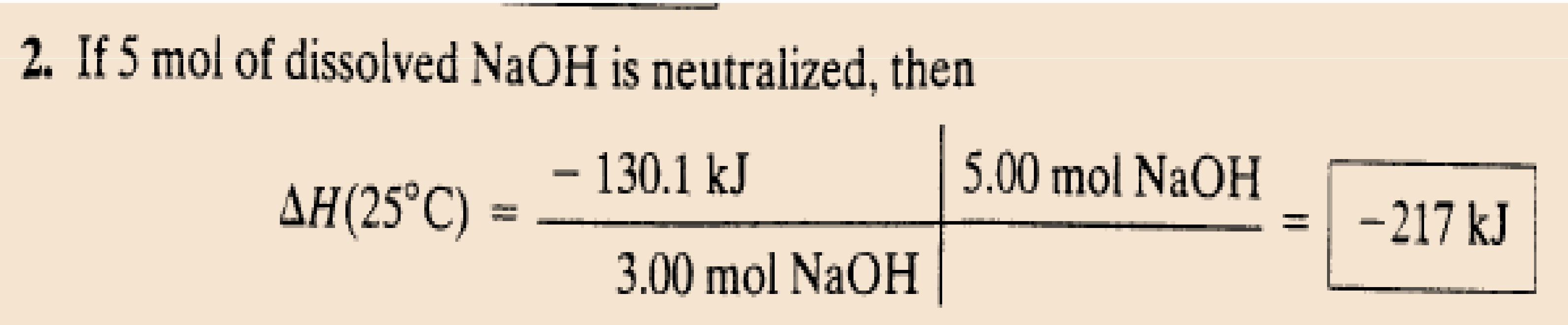
Standard Hear of Neutralization Reaction ($\Delta\hat{H}_r^o$)



1. Calculate $\Delta\hat{H}_r^\circ$ for the reaction

$$H_3PO_4(aq, r = \infty) + 3\,NaOH(aq, r = 50) \rightarrow Na_3PO_4(aq, r = \infty) + 3\,H_2O(l)$$

2. If 5.00 mol of NaOH dissolved in 250 mol of water is neutralized completely at 25°C with dilute phosphoric acid, what is the attendant enthalpy change?



2. If 5 mol of dissolved NaOH is neutralized, then

$$\Delta H(25^\circ C) = \frac{-130.1\ \text{kJ}}{3.00\ \text{mol NaOH}}\left|\frac{5.00\ \text{mol NaOH}}{}\right. = \boxed{-217\ \text{kJ}}$$

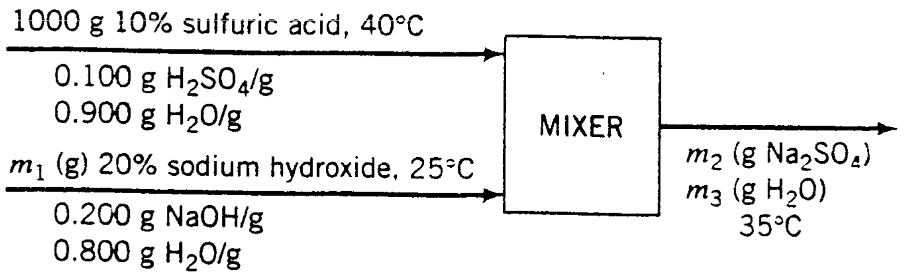
Take home Example 9.5.6

Energy Balance on a Neutralization Process

A 10.0 wt% aqueous solution of H_2SO_4 at 40°C is to be neutralized with a 20.0 wt% aqueous solution of NaOH at 25°C in a continuous reactor. At what rate in kJ/kg H_2SO_4 solution must heat be removed from the reactor if the product solution emerges at 35°C?

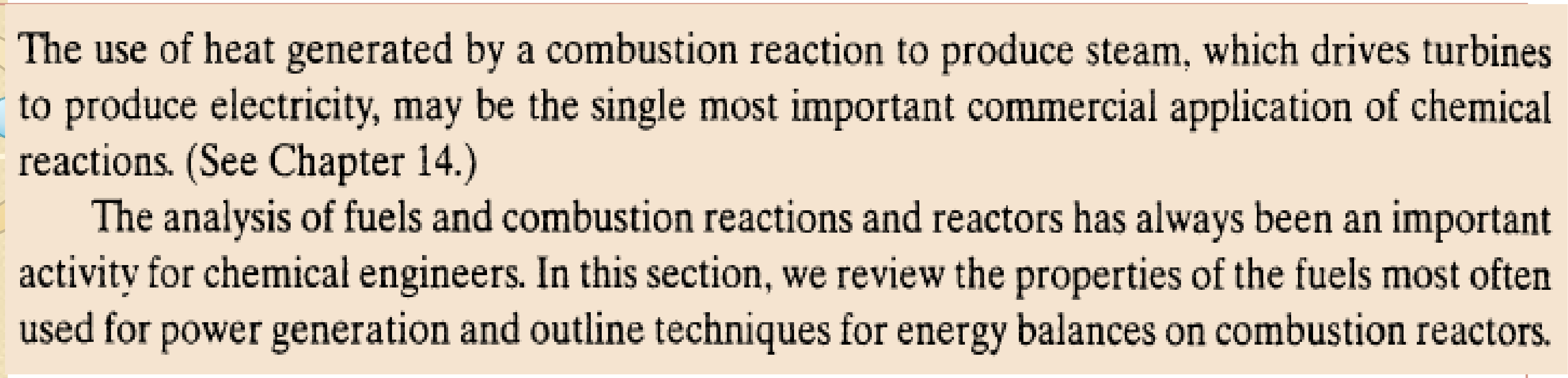
Basis: 1 kg H_2SO_4 Solution

$$H_2SO_4(aq, 10\%) + 2\,NaOH(aq, 20\%) \rightarrow Na_2SO_4(aq) + 2\,H_2O(l)$$



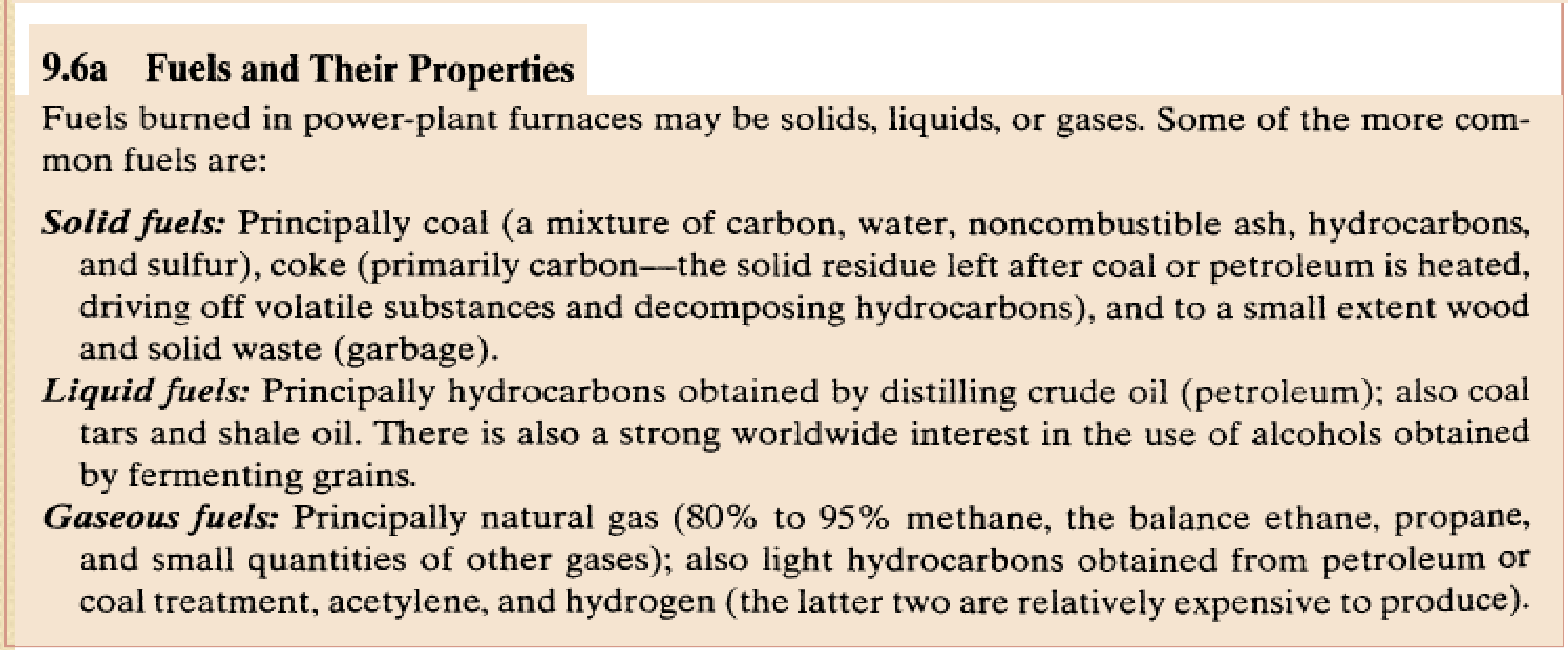
Make sure that you understand all the steps

9.6 Fuels and Combustion



The use of heat generated by a combustion reaction to produce steam, which drives turbines to produce electricity, may be the single most important commercial application of chemical reactions. (See Chapter 14.)

The analysis of fuels and combustion reactions and reactors has always been an important activity for chemical engineers. In this section, we review the properties of the fuels most often used for power generation and outline techniques for energy balances on combustion reactors.



9.6a Fuels and Their Properties

Fuels burned in power-plant furnaces may be solids, liquids, or gases. Some of the more common fuels are:

Solid fuels: Principally coal (a mixture of carbon, water, noncombustible ash, hydrocarbons, and sulfur), coke (primarily carbon—the solid residue left after coal or petroleum is heated, driving off volatile substances and decomposing hydrocarbons), and to a small extent wood and solid waste (garbage).

Liquid fuels: Principally hydrocarbons obtained by distilling crude oil (petroleum); also coal tars and shale oil. There is also a strong worldwide interest in the use of alcohols obtained by fermenting grains.

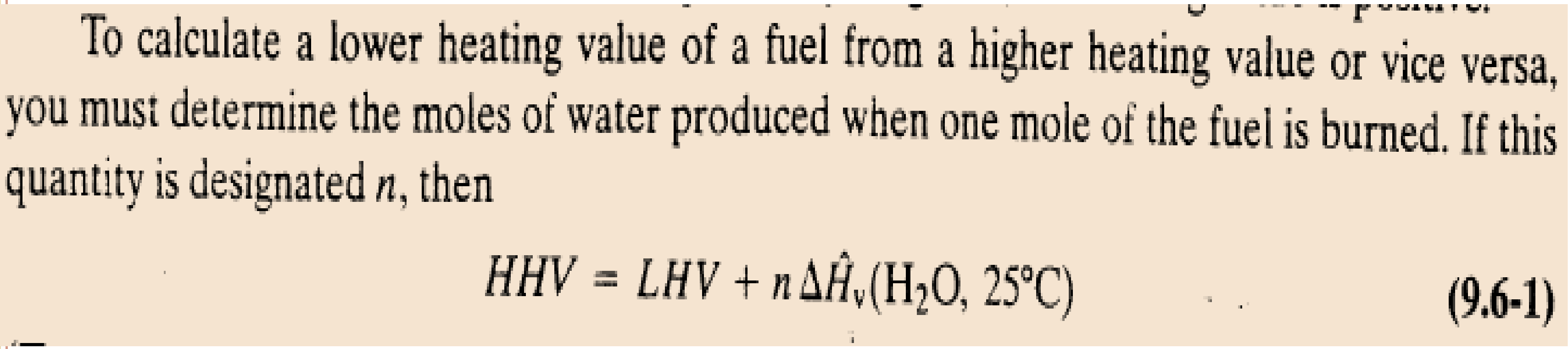
Gaseous fuels: Principally natural gas (80% to 95% methane, the balance ethane, propane, and small quantities of other gases); also light hydrocarbons obtained from petroleum or coal treatment, acetylene, and hydrogen (the latter two are relatively expensive to produce).

9.6 Fuels and Combustion

✓Heating value of a combustible material is the negative of the standard heat of combustion. Since $-\Delta\hat{H}_c^o$ is always negative, heating value is positive

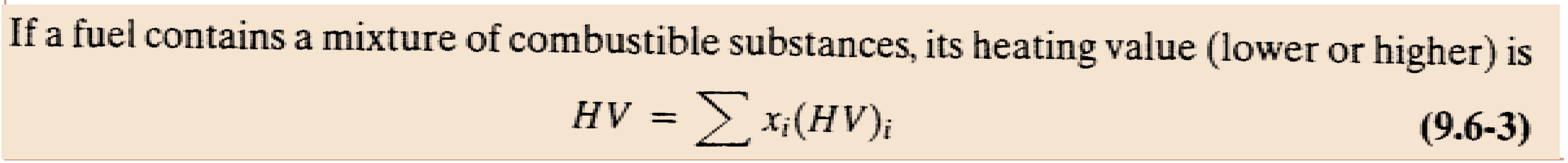
✓The Higher Heating Value (HHV) or total heating value or gross heating value is $-\Delta\hat{H}_c^o$ with H_2O (l) as combustion product

✓The Lower Heating Value (LHV) or net heating value is the value based on with H_2O (v) as a product



To calculate a lower heating value of a fuel from a higher heating value or vice versa, you must determine the moles of water produced when one mole of the fuel is burned. If this quantity is designated n, then

$$HHV = LHV + n\,\Delta\hat{H}_v(\mathrm{H_2O},\ 25^\circ\mathrm{C}) \qquad \textbf{(9.6-1)}$$



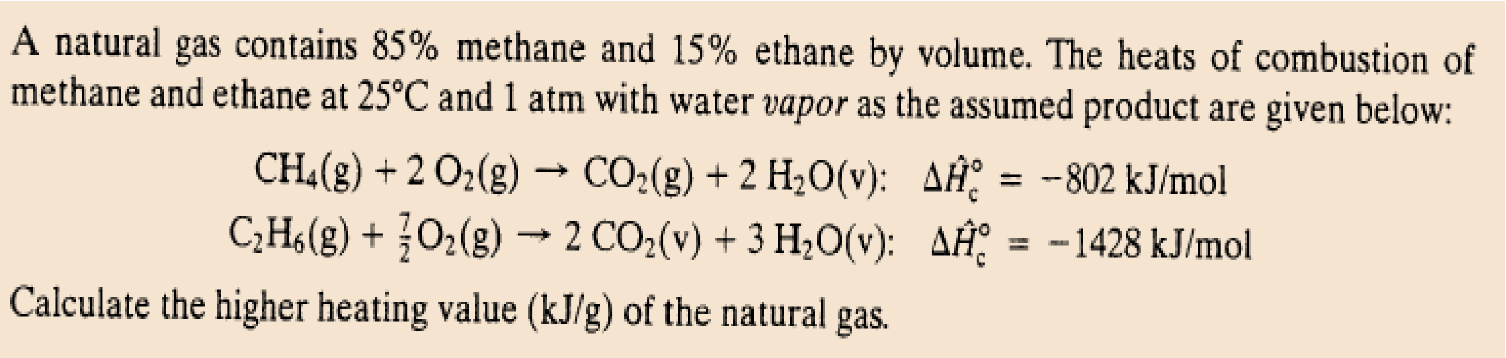
If a fuel contains a mixture of combustible substances, its heating value (lower or higher) is

$$HV = \sum x_i (HV)_i \qquad \textbf{(9.6-3)}$$

x_i is the mass fraction

9.6 Fuels and Combustion

Example 9.6-1: Calculation of Heating Value



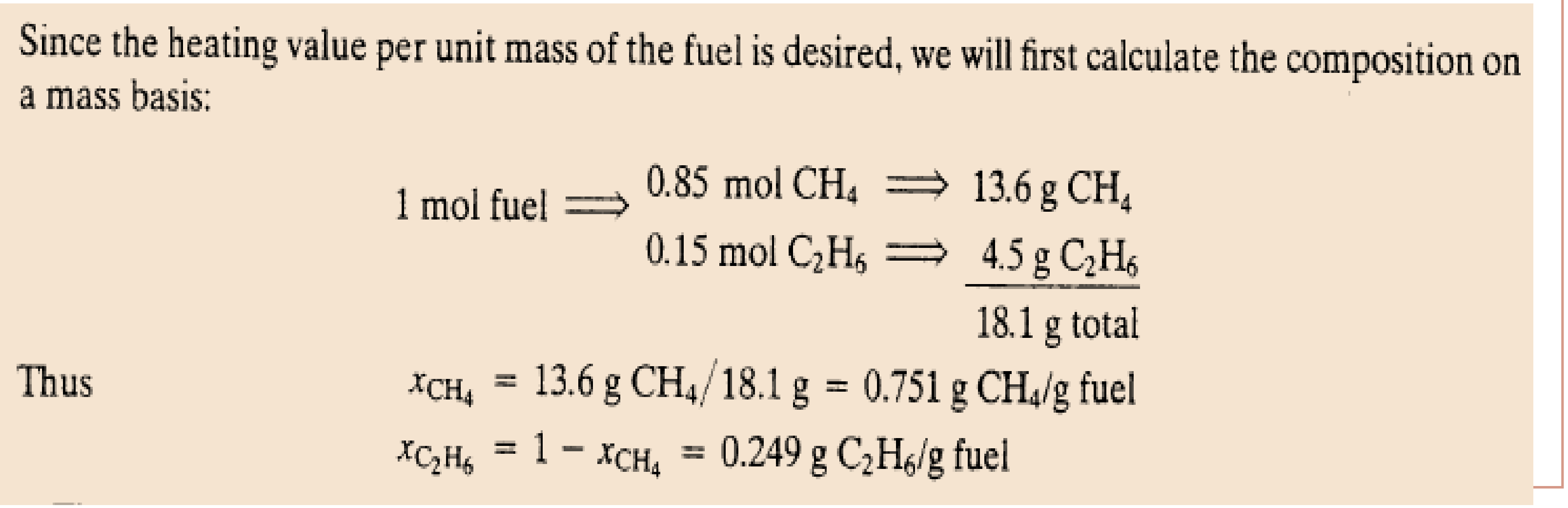
A natural gas contains 85% methane and 15% ethane by volume. The heats of combustion of methane and ethane at 25°C and 1 atm with water *vapor* as the assumed product are given below:

$$CH_4(g) + 2\,O_2(g) \rightarrow CO_2(g) + 2\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -802 \text{ kJ/mol}$$

$$C_2H_6(g) + \tfrac{7}{2}O_2(g) \rightarrow 2\,CO_2(v) + 3\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -1428 \text{ kJ/mol}$$

Calculate the higher heating value (kJ/g) of the natural gas.

$$HHV = x_{CH_4}(HHV)_{CH_4} + x_{C_2H_6}(HHV)_{C_2H_6}$$



Since the heating value per unit mass of the fuel is desired, we will first calculate the composition on a mass basis:

$$1 \text{ mol fuel} \Longrightarrow \begin{array}{l} 0.85 \text{ mol } CH_4 \Longrightarrow 13.6 \text{ g } CH_4 \\ 0.15 \text{ mol } C_2H_6 \Longrightarrow \underline{4.5 \text{ g } C_2H_6} \\ \qquad\qquad\qquad\qquad\quad 18.1 \text{ g total} \end{array}$$

Thus

$$x_{CH_4} = 13.6 \text{ g } CH_4/18.1 \text{ g} = 0.751 \text{ g } CH_4/\text{g fuel}$$

$$x_{C_2H_6} = 1 - x_{CH_4} = 0.249 \text{ g } C_2H_6/\text{g fuel}$$

9.6 Fuels and Combustion

Example 9.6-1: Calculation of Heating Value

A natural gas contains 85% methane and 15% ethane by volume. The heats of combustion of methane and ethane at 25°C and 1 atm with water *vapor* as the assumed product are given below:

$$CH_4(g) + 2\,O_2(g) \rightarrow CO_2(g) + 2\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -802 \text{ kJ/mol}$$

$$C_2H_6(g) + \tfrac{7}{2}O_2(g) \rightarrow 2\,CO_2(v) + 3\,H_2O(v): \quad \Delta\hat{H}_c^\circ = -1428 \text{ kJ/mol}$$

Calculate the higher heating value (kJ/g) of the natural gas.

The higher heating values of the components are calculated from the given heats of combustion (which are the negatives of the lower heating values) as follows:

$$\begin{aligned}(HHV)_{CH_4} &= (LHV)_{CH_4} + n_{H_2O}(\Delta\hat{H}_v)_{H_2O} \\ &= \left[802\,\frac{\text{kJ}}{\text{mol } CH_4} + \frac{2\text{ mol } H_2O}{\text{mol } CH_4}\left(44.013\,\frac{\text{kJ}}{\text{mol } H_2O}\right)\right]\frac{1\text{ mol}}{16.0\text{ g } CH_4} \\ &= 55.6\text{ kJ/g}\end{aligned}$$

$$\begin{aligned}(HHV)_{C_2H_6} &= \left[1428\,\frac{\text{kJ}}{\text{mol } C_2H_6} + \frac{3\text{ mol } H_2O}{\text{mol } C_2H_6}\left(44.013\,\frac{\text{kJ}}{\text{mol } H_2O}\right)\right]\frac{1\text{ mol}}{30.0\text{ g } C_2H_6} \\ &= 52.0\text{ kJ/g}\end{aligned}$$

The higher heating value of the mixture is from Equation 9.6-3:

$$\begin{aligned}HHV &= x_{CH_4}(HHV)_{CH_4} + x_{C_2H_6}(HHV)_{C_2H_6} \\ &= [(0.751)(55.6) + (0.249)(52.0)]\text{ kJ/g} = \boxed{54.7\text{ kJ/g}}\end{aligned}$$

9.6 Fuels and Combustion

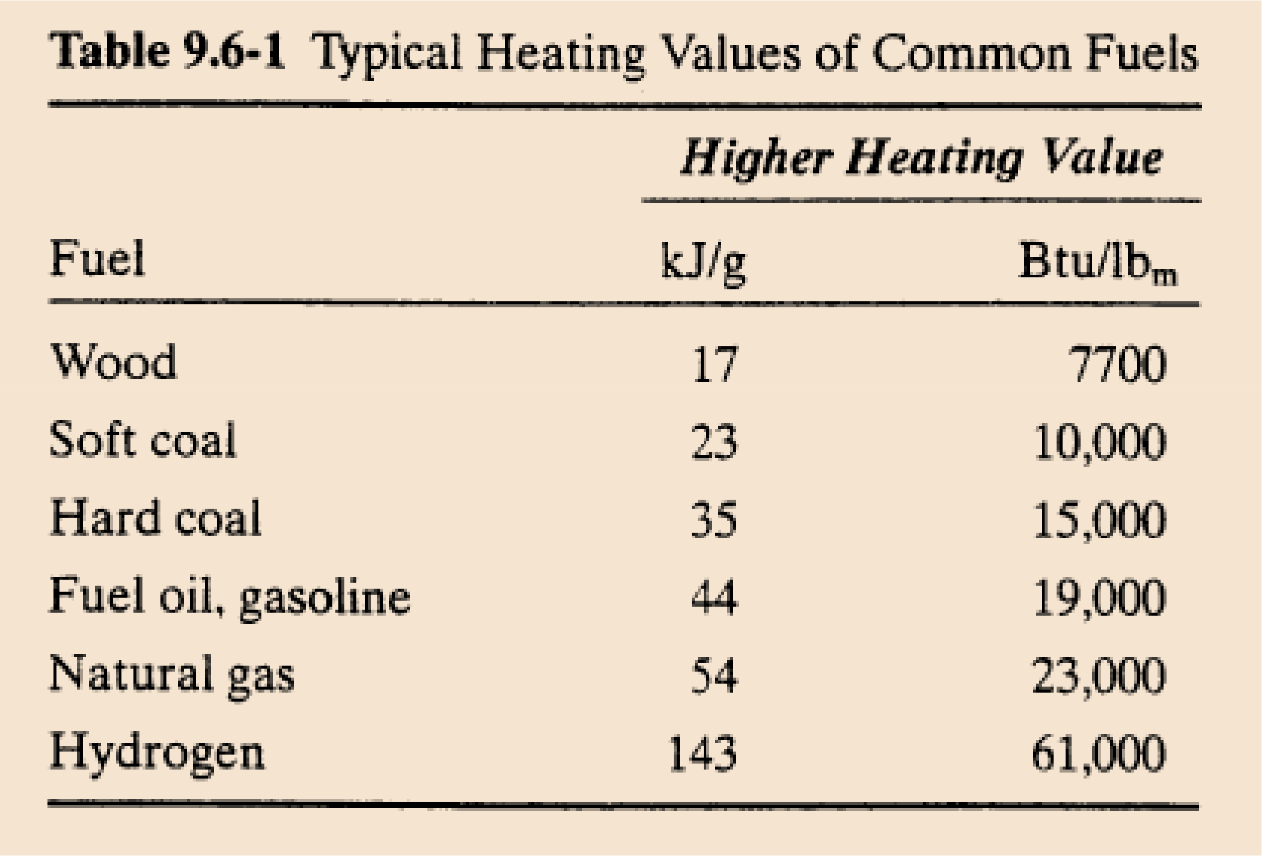
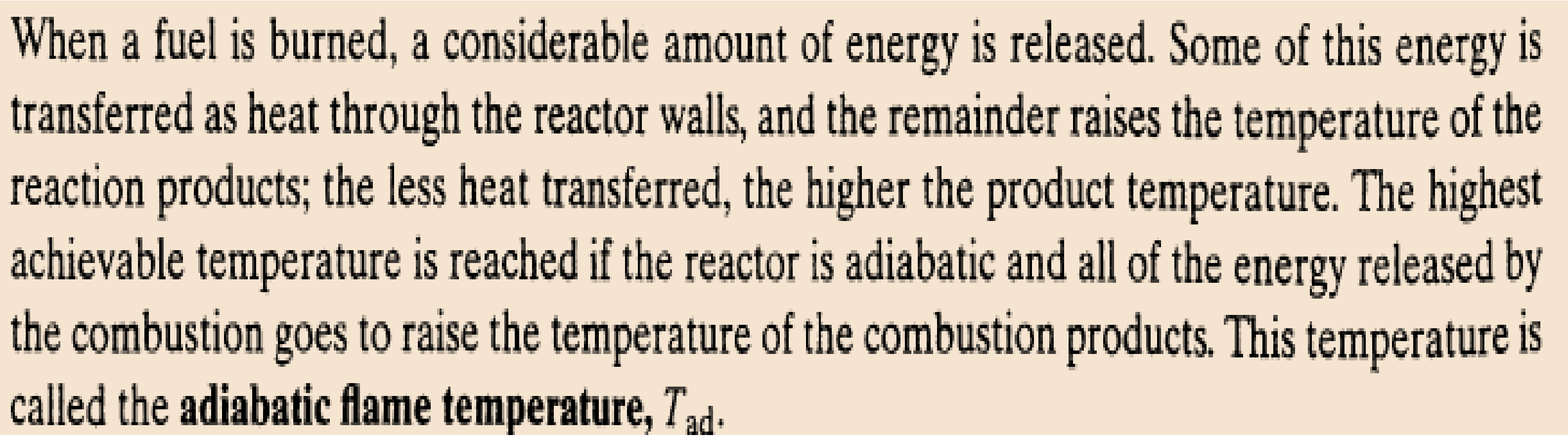


Table 9.6-1 Typical Heating Values of Common Fuels

	Higher Heating Value	
Fuel	kJ/g	Btu/lb$_m$
Wood	17	7700
Soft coal	23	10,000
Hard coal	35	15,000
Fuel oil, gasoline	44	19,000
Natural gas	54	23,000
Hydrogen	143	61,000

9.6b Adiabatic Flame Temperature



When a fuel is burned, a considerable amount of energy is released. Some of this energy is transferred as heat through the reactor walls, and the remainder raises the temperature of the reaction products; the less heat transferred, the higher the product temperature. The highest achievable temperature is reached if the reactor is adiabatic and all of the energy released by the combustion goes to raise the temperature of the combustion products. This temperature is called the **adiabatic flame temperature,** T_{ad}.

$$\Delta\dot{H} = \dot{n}_f \Delta\hat{H}_c^\circ + \sum_{out} \dot{n}_i \hat{H}_i(T_{ad}) - \sum_{in} \dot{n}_i \hat{H}_i(T_{feed})$$

$\dot{Q} = \Delta\dot{H}$, or $\Delta\dot{H} = 0$ for an adiabatic reactor)

$$\sum_{out} \dot{n}_i \hat{H}_i(T_{ad}) = -\dot{n}_f \Delta\hat{H}_c^\circ + \sum_{in} \dot{n}_i \hat{H}_i(T_{feed})$$

9.6b Adiabatic Flame Temperature

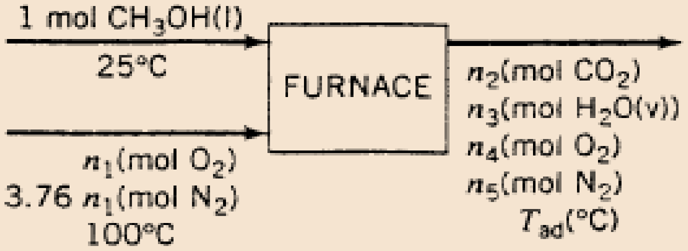
Calculation of an Adiabatic Flame Temperature

Liquid methanol is to be burned with 100% excess air. The engineer designing the furnace must calculate the highest temperature that the furnace walls will have to withstand so that an appropriate material of construction can be chosen. Perform this calculation, assuming that the methanol is fed at 25°C and the air enters at 100°C.

Basis: 1 mol CH_3OH Burned

Assume complete combustion. From Table B.1,

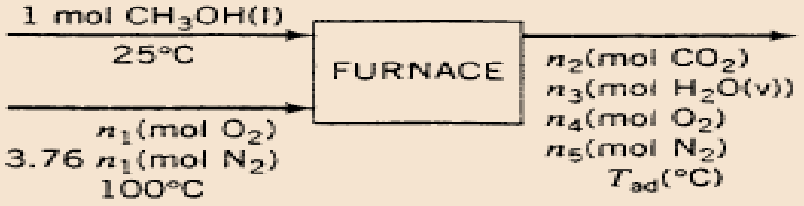
$$CH_3OH(l) + \frac{3}{2}O_2 \rightarrow CO_2 + 2H_2O(l): \quad \Delta\hat{H}_c^\circ = -726.6\ \text{kJ/mol}$$



$$\sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) = -\dot{n}_f\, \Delta\hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}})$$

9.6b Adiabatic Flame Temperature

$$CH_3OH(l) + \tfrac{3}{2}\,O_2 \longrightarrow CO_2 + 2\,H_2O(l): \quad \Delta\hat{H}_c^\circ = -726.6 \text{ kJ/mol}$$



$$\sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) = -\dot{n}_f\,\Delta\hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}})$$

Calculate Component Amounts

$$(n_{O_2})_{\text{theoretical}} = 1.50 \text{ mol}$$

$$n_1 = (2)(1.50 \text{ mol}) = 3.00 \text{ mol } O_2 \text{ fed}$$

$$\Downarrow$$

$$(3.76 \text{ mol } N_2/\text{mol } O_2)(3.00 \text{ mol } O_2) = 11.28 \text{ mol } N_2 \text{ fed}$$

Material balances yield

$$n_2 = 1.00 \text{ mol } CO_2$$

$$n_3 = 2.00 \text{ mol } H_2O$$

$$n_4 = 1.50 \text{ mol } O_2$$

$$n_5 = 11.28 \text{ mol } N_2$$

9.6b Adiabatic Flame Temperature

$$CH_3OH(l) + \tfrac{3}{2}\,O_2 \longrightarrow CO_2 + 2\,H_2O(l): \quad \Delta\hat{H}_c^\circ = -726.6\ \text{kJ/mol}$$

$$\sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) = -\dot{n}_f\,\Delta\hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}})$$

Calculate Feed Component Enthalpies

References: $CH_3OH(l)$, O_2, N_2 at 25°C
CH_3OH(l, 25°C): $\hat{H} = 0$
Air (100°C): $\hat{H} = 2.191$ kJ/mol (from Table B.8)

Evaluate the Right Side of Equation 9.6-4

$$\begin{aligned} -n_f\Delta\hat{H}_c^\circ + \sum_{\text{in}} n_i\hat{H}_i &= -(1.00\ \text{mol}\ CH_3OH)\left(-726.6\ \frac{\text{kJ}}{\text{mol}}\right) \\ &\quad + (1.00\ \text{mol}\ CH_3OH)\left(0\ \frac{\text{kJ}}{\text{mol}}\right) + (14.28\ \text{mol air})\left(2.191\ \frac{\text{kJ}}{\text{mol}}\right) \\ &= 757.9\ \text{kJ} \end{aligned}$$

Calculate Enthalpy of Product Stream

References: $CO_2(g)$, $O_2(g)$, $N_2(g)$, and $H_2O(l)$ at 25°C. (Liquid water is assumed since this is the state for which $\Delta\hat{H}_c$ is known.)

From Table B.2, the heat capacities of the product gases in kJ/(mol·°C) in terms of T(°C) are

$$\begin{aligned}
(C_p)_{CO_2} &= 0.03611 + 4.233 \times 10^{-5}T - 2.887 \times 10^{-8}T^2 + 7.464 \times 10^{-12}T^3 \\
(C_p)_{H_2O(g)} &= 0.03346 + 0.688 \times 10^{-5}T + 0.7604 \times 10^{-8}T^2 - 3.593 \times 10^{-12}T^3 \\
(C_p)_{O_2} &= 0.02910 + 1.158 \times 10^{-5}T - 0.6076 \times 10^{-8}T^2 + 1.311 \times 10^{-12}T^3 \\
(C_p)_{N_2} &= 0.02900 + 0.2199 \times 10^{-5}T + 0.5723 \times 10^{-8}T^2 - 2.871 \times 10^{-12}T^3
\end{aligned}$$

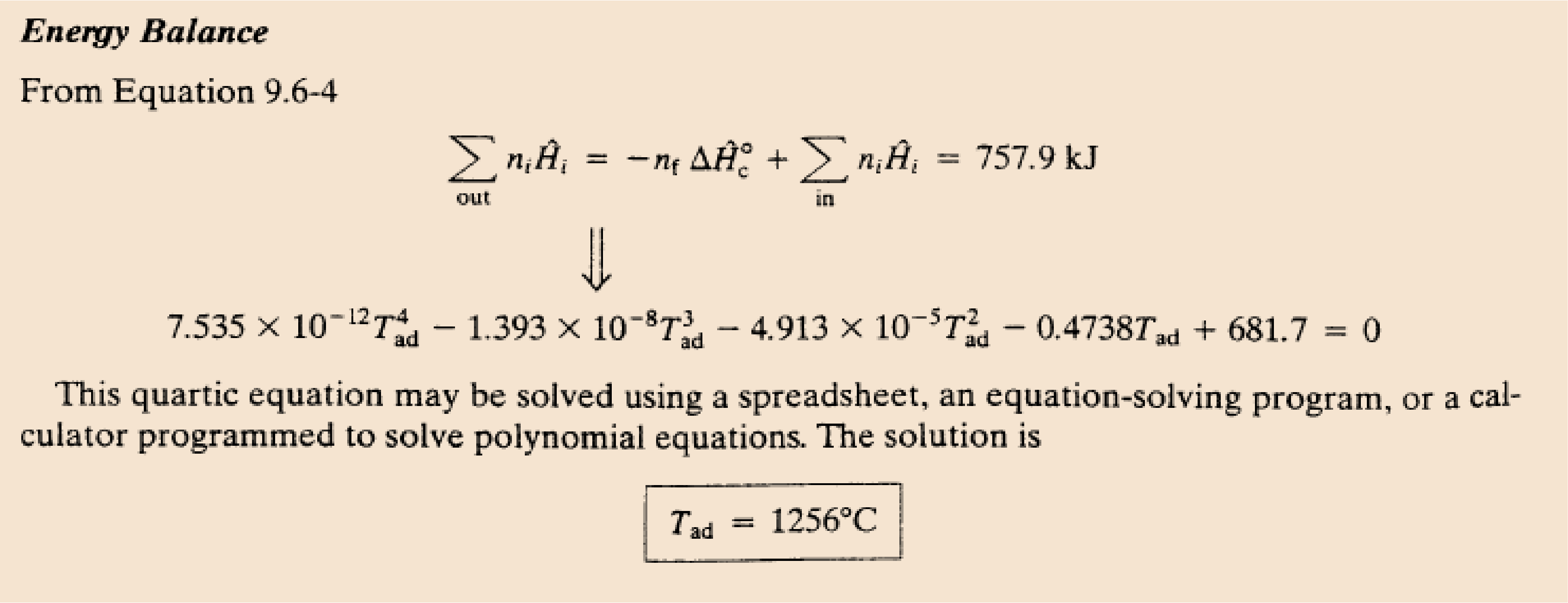
$$\sum n_i C_{pi} = 0.4378 + 9.826 \times 10^{-5}T + 4.178 \times 10^{-8}T^2 - 30.14 \times 10^{-12}T^3$$

$$\Downarrow$$

$$\begin{aligned}
\sum_{\text{out}} n_i \hat{H}_i &= n_3(\Delta\hat{H}_v)_{H_2O} + \int_{25°C}^{T_{ad}} \left(\sum n_i C_{pi}\right) dT \\
&= 88.026 + 0.4378T_{ad} + 4.913 \times 10^{-5}T_{ad}^2 + 1.393 \times 10^{-8}T_{ad}^3 \\
&\quad - 7.535 \times 10^{-12}T_{ad}^4 - 11.845
\end{aligned}$$

$$\Downarrow$$

$$\begin{aligned}
\sum_{\text{out}} n_i \hat{H}_i &= 76.18 + 0.4738T_{ad} + 4.913 \times 10^{-5}T_{ad}^2 + 1.393 \times 10^{-8}T_{ad}^3 \\
&\quad - 7.535 \times 10^{-12}T_{ad}^4
\end{aligned}$$



Energy Balance

From Equation 9.6-4

$$\sum_{\text{out}} n_i\hat{H}_i = -n_{\text{f}}\,\Delta\hat{H}_{\text{c}}^{\circ} + \sum_{\text{in}} n_i\hat{H}_i = 757.9 \text{ kJ}$$

$$\Downarrow$$

$$7.535 \times 10^{-12}T_{\text{ad}}^4 - 1.393 \times 10^{-8}T_{\text{ad}}^3 - 4.913 \times 10^{-5}T_{\text{ad}}^2 - 0.4738T_{\text{ad}} + 681.7 = 0$$

This quartic equation may be solved using a spreadsheet, an equation-solving program, or a calculator programmed to solve polynomial equations. The solution is

$$\boxed{T_{\text{ad}} = 1256^{\circ}\text{C}}$$