Introduction to Chemical Engineering

Problem Sheet 8 – Week 11 – Friday 29 November 2024

Problem 1: Hess's Law (Energy Balance – Reactive)

9.8. Trichloroethylene, a widely used degreasing solvent for machine parts, is produced in a two-step reaction sequence. Ethylene is first chlorinated to yield tetrachloroethane, which is dehydrochlorinated to form trichloroethylene.

$$C_2H_4(g) + 2\,Cl_2(g) \rightarrow C_2H_2Cl_4(l) + H_2(g): \quad \Delta\hat{H}_r^\circ = -385.76 \text{ kJ/mol}$$

$$C_2H_2Cl_4(l) \rightarrow C_2HCl_3(l) + HCl(g)$$

The standard heat of formation of liquid trichloroethylene is -276.2 kJ/mol.

(a) Use the given data and tabulated standard heats of formation of ethylene and hydrogen chloride to calculate the standard heat of formation of tetrachloroethane and the standard heat of the second reaction.

(b) Use Hess's law to calculate the standard heat of the reaction

$$C_2H_4(g) + 2\,Cl_2(g) \rightarrow C_2HCl_3(l) + H_2(g) + HCl(g)$$

(c) If 300 mol/h of $C_2HCl_3(l)$ is produced in the reaction of part (b) and the reactants and products are all at 25°C and 1 atm, how much heat is evolved or absorbed in the process? (Assume $\dot{Q} = \Delta\dot{H}$.)

Solution 1

9.8 **a.**

$$\Delta\hat{H}_{r1}^o = \left(\Delta\hat{H}_f^o\right)_{C_2H_2Cl_4(l)} - \left(\Delta\hat{H}_f^o\right)_{C_2H_4(g)} \Rightarrow \left(\Delta\hat{H}_f^o\right)_{C_2H_2Cl_4(l)} = -385.76 + 52.28 = \underline{\underline{-333.48 \text{ kJ/mol}}}$$

$$\Delta\hat{H}_{r2}^o = \left(\Delta\hat{H}_f^o\right)_{C_2HCl_3(l)} + \left(\Delta\hat{H}_f^o\right)_{HCl(g)} - \left(\Delta\hat{H}_f^o\right)_{C_2H_2Cl_4(l)} = -276.2 - 92.31 + 333.48 = \underline{\underline{-35.03 \text{ kJ/mol}}}$$

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

c.

$$\dot{Q} = \Delta\dot{H} = \frac{300 \text{ mol } C_2HCl_3}{\text{h}}\bigg|\frac{-420.79 \text{ kJ}}{\text{mol}} = \underline{\underline{-1.26\times10^5 \text{ kJ/h}}} \; (= -35 \text{ kW})$$

Heat is evolved.

Problem 2: Heat of Combustion (Energy Balance – Reactive)

9.9. The standard heat of combustion of gaseous acetylene is listed in Table B.1 as -1299.6 kJ/mol.

(a) In your own words, briefly explain what that means. (Your explanation should mention the reference states used to define the tabulated heats of combustion.)

(b) Use tabulated heats of formation to verify the given value of $\Delta\hat{H}_c^\circ$.

(c) Calculate the standard heat of the acetylene hydrogenation reaction

$$C_2H_2(g) + 2H_2(g) \longrightarrow C_2H_6(g)$$

using (i) tabulated heats of formation and (ii) tabulated heats of combustion (Equation 9.4-1).

(d) Write the stoichiometric equations for the combustion reactions of acetylene, hydrogen, and ethane, and use Hess's law to derive the formula you used in part (c-ii).

<u>Note on Equation 9.4-1:</u>

$$\Delta\hat{H}^\circ_r = -\sum_i \nu_i(\Delta\hat{H}^\circ_c)_i = \sum_{reactants} |\nu_i|(\Delta\hat{H}^\circ_c)_i - \sum_{products} |\nu_i|(\Delta\hat{H}^\circ_c)_i$$

Solution 2

9.9

a.

$$C_2H_2(g) + \frac{5}{2}O_2(g) \rightarrow 2CO_2(g) + H_2O(l) \qquad \Delta\hat{H}_c^\circ = -1299.6 \text{ kJ/mol}$$

The enthalpy change when 1 g-mole of $C_2H_2(g)$ and 2.5 g-moles of $O_2(g)$ at 25°C and 1 atm react to form 2 g-moles of $CO_2(g)$ and 1 g-mole of $H_2O(l)$ at 25°C and 1 atm is -1299.6 kJ.

b.

$$\Delta\hat{H}_c^\circ = 2\left(\Delta\hat{H}_f^\circ\right)_{CO_2(g)} + \left(\Delta\hat{H}_f^\circ\right)_{H_2O(l)} - \left(\Delta\hat{H}_f^\circ\right)_{C_2H_2(g)}$$

$$\overset{\text{Table B.1}}{=} \left[2(-393.5) + (-285.84) - (226.75)\right]\frac{\text{kJ}}{\text{mol}} = \underline{\underline{-1299.6 \ \frac{\text{kJ}}{\text{mol}}}}$$

c.

(i) $$\Delta\hat{H}_r^\circ = \left(\Delta\hat{H}_f^\circ\right)_{C_2H_6(g)} - \left(\Delta\hat{H}_f^\circ\right)_{C_2H_2(g)}$$

$$\overset{\text{Table B.1}}{=} \left[(-84.67) - (226.75)\right]\frac{\text{kJ}}{\text{mol}} = \underline{\underline{-311.4 \ \frac{\text{kJ}}{\text{mol}}}}$$

(ii) $$\Delta\hat{H}_r^\circ = \left(\Delta\hat{H}_c^\circ\right)_{C_2H_2(g)} + 2\left(\Delta\hat{H}_c^\circ\right)_{H_2(g)} - \left(\Delta\hat{H}_c^\circ\right)_{C_2H_6(g)}$$

$$\overset{\text{Table B.1}}{=} \left[(-1299.6) + 2(-285.84) - (-1559.9)\right]\frac{\text{kJ}}{\text{mol}} = \underline{\underline{-311.4 \ \frac{\text{kJ}}{\text{mol}}}}$$

d.

$$C_2H_2(g) + \frac{5}{2}O_2(g) \rightarrow 2CO_2(g) + H_2O(l) \qquad (1) \quad \Delta\hat{H}_{c1}^\circ = -1299.6 \text{ kJ/mol}$$

$$H_2(g) + \frac{1}{2}O_2(g) \rightarrow H_2O(l) \qquad (2) \quad \Delta\hat{H}_{c2}^\circ = -285.84 \text{ kJ/mol}$$

$$C_2H_6(g) + \frac{7}{2}O_2(g) \rightarrow 2CO_2(g) + 3H_2O(l) \qquad (3) \quad \Delta\hat{H}_{c3}^\circ = -1559.9 \text{ kJ/mol}$$

The acetylene dehydrogenation reaction is $(1) + 2\times(2) - (3)$

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

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