Example 1.E

The combustion of acetylene fuel with nitrous oxide as oxidant at 25^{o}C *(298 K)* is widely performed in flame emission spectrophotometry. Calculate the maximum temperature attained if the best mixture corresponds to the reaction

$$(C_2H_2) + 3(N_2O) = 2(CO) + (H_2O) + 3(N_2).$$

Assume that water is undissociated.

Given:

$\Delta H^{o}_{298,(C_2H_2)}$ = 54.23 kcal/mole *(226.90 kJ/mol)*.

$\Delta H^{o}_{298,(N_2O)}$ = 19.70 kcal/mole *(82.42 kJ/mol)*.

$\Delta H^{o}_{298,(CO)}$ = -26.42 kcal/mole *(-110.54 kJ/mol)*.

$\Delta H^{o}_{298,(H_2O)}$ = -57.80 kcal/mole *(-241.84 kJ/mol)*.

$$C_{P,(CO)} = 6.8 + 1.0 \times 10^{-3}\, T - 0.11 \times 10^{5}\, T^{-2} \text{ cal/deg/mole}$$
$$\textit{(28.45 + 4.184} \times 10^{-3}\, T - 0.46 \times 10^{5}\, T^{-2} \textit{ J/K/mol).}$$

$$C_{P,(H_2O)} = 7.17 + 2.56 \times 10^{-3}\, T + 0.08 \times 10^{5}\, T^{-2} \text{ cal/deg/mole}$$
$$\textit{(30.0 + 10.71} \times 10^{-3}\, T + 0.33 \times 10^{5}\, T^{-2} \textit{ J/K/mol).}$$

$$C_{P,(N_2)} = 6.5 + 1.0 \times 10^{-3}\, T \text{ cal/deg/mole}$$
$$\textit{(27.20 + 4.184} \times 10^{-3}\, T \textit{ J/K/mol).}$$

Solution: The first step is to calculate the standard enthalpy change of the reaction

$$(C_2H_2) + 3(N_2O) = 2(CO) + (H_2O) + 3(N_2) \qquad (1.E.1)$$

at 25°C. Thus, we have

$$\Delta H^{o}_{298,(1.E.1)} = 2\Delta H^{o}_{298,(CO)} + \Delta H^{o}_{298,(H_2O)} - \Delta H^{o}_{298,(C_2H_2)}$$
$$-3\Delta H^{o}_{298,(N_2O)}$$
$$= (2 \times -26.42) + (-57.80) - (54.23) - (3 \times 19.70)$$
$$= -223.97 \text{ kcal.}$$

In other words, 223.97 kcal of heat is evolved during the reaction (1.E.1), which is used to heat up 2 moles of CO, 1 mole of H_2O and 3 moles of N_2 from 25°C to the final maximum temperature, say T_m. Applying Eq. (1.21), we have

$$\text{Heat evolved} = \int_{298}^{T_m} \Sigma C_{P,\text{product}}\, dT,$$

or

$$223970 = \int_{298}^{T_m} \left[2C_{P,(CO)} + C_{P,(H_2O)} + 3C_{P,(N_2)}\right] dT$$

$$= \int_{298}^{T_m} \Big[(13.6 + 2.0 \times 10^{-3}T - 0.22 \times 10^5 T^{-2}) + (7.17 + 2.56 \times 10^{-3}T + 0.08 \times 10^5 T^{-2}) + (19.5 + 3.0 \times 10^{-3}T)\Big] dT$$

$$= \int_{298}^{T_m} \Big[40.27 + 7.56 \times 10^{-3}T - 0.14 \times 10^5 T^{-2}\Big] dT$$

$$= \Big[40.27\, T + 3.78 \times 10^{-3} T^2 + 0.14 \times 10^5 T^{-1}\Big]_{298}^{T_m}$$

$$= 40.27\,(T_m - 298) + 3.78 \times 10^{-3}\,(T_m^{\,2} - 298^2) + 0.14 \times 10^5 \left(\frac{1}{T_m} - \frac{1}{298}\right)$$

$$= 3.78 \times 10^{-3}\, T_m^{\,2} + 40.27\, T_m + 0.14 \times 10^5\, T_m^{\,-1} - 12383.$$

Neglecting the $T_m^{\,-1}$ term, we have

$$223970 = 3.78 \times 10^{-3}\, T_m^{\,2} + 40.27\, T_m - 12383,$$

or $$3.78 \times 10^{-3}\, T_m^{\,2} + 40.27\, T_m - 236353 = 0.$$

On solving the above equation in T_m and neglecting the negative value, it follows

$$T_m = 4207\ \text{K},$$

or $$T_m = (4207 - 273)^{\circ}\text{C}$$

$$= 3934^{\circ}\text{C}.$$

Thus, the maximum temperature attained is $\underline{3934^{\circ}\text{C}}$.