

SOLUTION TO ASSIGNMENT 4

(Equations refer to chapter #4 of Principles of Combustion by K K Kuo)

4.4 Solution: Neglecting dissociation, the following chemical reaction occurs:



A) Prior to solving, we want to simplify eqn (4-104) to solve for T_2 . The approximate Rankine-Hugoniot equation is given by eqn (4-104):

$$e_2 - e_1 = \frac{R_2 T_2}{2 \gamma_2} \quad (\text{assuming } P_2 \gg P_1)$$

Knowing:

$$e_2 - e_1 = (h_2 - h_1) - \left(\frac{P_2}{\rho_2} - \frac{P_1}{\rho_1} \right) \quad (\text{eqn (4-41)})$$

and:

$$h = C_p T + h^\circ \quad \text{where } h^\circ = \sum_{i=1}^N Y_i \Delta h_{f,i}^\circ \quad \text{eqn (4-17)}$$

substituting:

$$C_{p_2} T_2 + h_2^\circ - C_{p_1} T_1 - h_1^\circ - \left(\frac{P_2}{\rho_2} - \frac{P_1}{\rho_1} \right) = \frac{R_2 T_2}{2 \gamma_2}$$

put T_2 terms on LHS:

$$T_2 \left(C_{p_2} - \frac{R_2}{2 \gamma_2} \right) = (h_1^\circ - h_2^\circ) + C_{p_1} T_1 + \left(\frac{P_2}{\rho_2} - \frac{P_1}{\rho_1} \right)$$

$P = \rho R T$ (ideal gas assumption); and again putting T_2 terms on LHS:

$$T_2 \left(C_{p_2} - \frac{R_2}{2 \gamma_2} - R_2 \right) = (h_1^\circ - h_2^\circ) + C_{p_1} T_1 - R_1 T_1$$

$$T_2 \left[C_{p_2} - R_2 \left(1 + \frac{1}{2 \gamma_2} \right) \right] = (h_1^\circ - h_2^\circ) + T_1 (C_{p_1} - R_1)$$

for ideal gases:

$$C_p - C_v = R \quad \text{and} \quad \gamma = \frac{C_p}{C_v}$$

simplifying :

$$T_2 \left(\gamma_2 C_{V_2} - R_2 \left(1 + \frac{1}{2\gamma_2} \right) \right) = (h_1^\circ - h_2^\circ) + T_1 C_{V_1}$$

divide by C_{V_2} :

$$T_2 \left[\gamma_2 - \frac{R_2}{C_{V_2}} \left(1 + \frac{1}{2\gamma_2} \right) \right] = \frac{h_1^\circ - h_2^\circ}{C_{V_2}} + \frac{C_{V_1}}{C_{V_2}} T_1$$

$$T_2 = \left[\frac{h_1^\circ - h_2^\circ}{C_{V_2}} + \frac{C_{V_1}}{C_{V_2}} T_1 \right] \frac{1}{\gamma_2 - (\gamma_2 - 1) \left(1 + \frac{1}{2\gamma_2} \right)}$$

or simplifying:

$$T_2 = \frac{2\gamma_2}{\gamma_2 + 1} \left[\frac{h_1^\circ - h_2^\circ}{C_{V_2}} + \frac{C_{V_1}}{C_{V_2}} T_1 \right] \quad \textcircled{A}$$

B) Solving for $h_1^\circ - h_2^\circ$

$$h_1^\circ - h_2^\circ = -\Delta H_{R, T_0} \quad (\text{at standard state } T = 298.15 \text{ K}) \quad [\text{eqn (1-140)}]$$

$$-\Delta H_{R, T_0} = -\sum_{i=1}^N \gamma_i'' \Delta H_{f, M_i}^\circ + \sum_{i=1}^N \gamma_i' \Delta H_{f, M_i}^\circ \quad (\Delta H_{f, M_i}^\circ \text{ in Table 1.2})$$

$$-\Delta H_{R, T_0} = -\left[2(-57.798) + 3(0) \right] + \left[2(0) + 0 + 3(0) \right]$$

$$= 115.596 \text{ Kcal}$$

$$= 483.654 \text{ KJ}$$

$$\text{on a molar basis } \Delta \bar{h}^\circ = \frac{\Delta H^\circ}{N_p} = \frac{483.654}{5} = 96.731 \text{ KJ/mol}$$

C) For the reactants:

- specific heat on a molar basis:

$$\bar{C}_{p,} = \sum_{i=1}^N X_i \bar{C}_{p_i}$$

reactants total moles = 2 + 1 + 3 = 6

$$\therefore X_{H_2} = 2/6 = .33333, X_{O_2} = 1/6 = .16667, X_{N_2} = 3/6 = .5$$

at 298.15° (From Table 1.4):

for O_2 : $C_p = 7.017 \text{ cal/mol-K} = 29.359 \text{ J/mol-K}$

for H_2 : $C_p = 6.892 \text{ cal/mol-K} = 28.836 \text{ J/mol-K}$

for N_2 : $C_p = 6.960 \text{ cal/mol-K} = 29.121 \text{ J/mol-K}$

$$\therefore \bar{C}_{p1} = (.33333)(28.836) + (.16667)(29.359) + (.5)(29.121)$$
$$= 29.066 \text{ J/mol-K}$$

$$\bar{C}_{v1} = \bar{C}_{p1} - R_1 = 29.066 - 8.314 = 20.752 \text{ J/mol-K}$$

D) For the products: Since T_2 is not known, we will have to iterate. Assume $T_2 = 3000 \text{ K}$ for the first iteration.

product total moles = 2 + 3 = 5

$$\therefore X_{H_2O} = 2/5 = .4, X_{N_2} = 3/5 = .6$$

at 3000 K: $\bar{C}_{pH_2O} = 12.9 \text{ cal/mol-K} = 53.974 \text{ J/mol-K}$

$$\bar{C}_{pN_2} = 8.861 \text{ cal/mol-K} = 37.074 \text{ J/mol-K}$$

$$\therefore \bar{C}_{p2} = .4(53.974) + .6(37.074) = 43.834 \text{ J/mol-K}$$

$$\bar{C}_{v2} = 43.834 - 8.314 = 35.52 \text{ J/mol-K}$$

$$\gamma_2 = \frac{\bar{C}_{p2}}{\bar{C}_{v2}} = \frac{43.834}{35.52} = 1.234$$

rewriting eqn (A) in terms of molar properties:

$$T_2 = \frac{2\gamma_2}{\gamma_2 + 1} \left[\frac{\Delta H^\circ}{\bar{C}_{v2}} + \frac{(\bar{C}_{v1}/W_1)}{(\bar{C}_{v2}/W_2)} \right]$$

where W_1 is the molecular weight of the unburned mixture and W_2 is the molecular weight of the burned mixture.

$$W_1 = \sum_{i=1}^N X_i W_i$$

$$= (.33333)(2.016) + (.16667)(32.0) + (.5)(28.0)$$

$$= 20.005$$

$$W_2 = (.4)(18.016) + (.6)(28.0)$$

$$= 24.006$$

solving for T_2 :

$$T_2 = \frac{2(1.234)}{2.234} \left[\frac{96,731}{35.52} + \frac{(20.752/20.005)}{(35.52/24.006)} (298.15) \right]$$

$$= 3239.5 \text{ K}$$

E) Second iteration, try $T_2 = 3250$

$$\bar{C}_{P_2} = .4(13.1) + .6(8.900) = 10.58 \text{ cal/mol-K} = 44.267 \text{ J/mol-K}$$

$$\bar{C}_{V_2} = 44.267 - 8.314 = 35.953 \text{ J/mol-K}$$

$$\gamma_2 = \frac{\bar{C}_{P_2}}{\bar{C}_{V_2}} = \frac{44.267}{35.953} = 1.231$$

$$T_2 = \frac{2(1.231)}{2.231} \left[\frac{96,731}{35.953} + \frac{(20.752/20.005)}{(35.953/24.006)} (298.15) \right] = 3197.0$$

interpolating from the secant method:

$$\frac{3239.5 - 3197.0}{3000 - 3250} = -.17 = \frac{T_2 - 3197}{T_2 - 3250}$$

$$T_2 = 3204.7$$

F) For $T_2 = 3204.7$

$$\overline{C_{p_2}} = .4(13.06) + .6(8.893) = 10.56 \text{ cal/mol-K} = 44.182 \text{ J/mol-K}$$

$$\overline{C_{v_2}} = 44.182 - 8.314 = 35.868 \text{ J/mol-K}$$

$$\gamma_2 = \frac{44.182}{35.868} = 1.232$$

$$T_2 = \frac{2(1.232)}{2.232} \left[\frac{96,731}{35.868} + \frac{(20.752/20.005)}{(35.868/24.006)} 298.15 \right] = 3205.7$$

\therefore converged $T_2 = 3205.7$

G) Solving eqn (4-109) for $\frac{p_2}{p_1}$

$$\text{set } X = \frac{p_2}{p_1}, \text{ then } X^2 - \left[\frac{1}{\gamma_2} + 1 - \frac{R_1 T_1}{R_2 T_2} \right] X - \frac{R_1 T_1}{R_2 T_2} = 0$$

$$R_2 = \frac{\overline{R}}{W_2} = \frac{8314.3}{24.006} = 346.34 \text{ J/kg-K}$$

$$R_1 = \frac{8314.3}{20.005} = 415.60 \text{ J/kg-K}$$

$$\frac{R_1 T_1}{R_2 T_2} = \frac{(415.60)(298.15)}{(346.34)(3205.7)} = .1116$$

$$\therefore X^2 - 1.7X - .1116 = 0 \text{ roots } X = 1.763, -0.633 \text{ not possible}$$

$$\therefore \frac{p_2}{p_1} = 1.763$$

speed of sound:

$$C_2 = \sqrt{\gamma_2 R_2 T_2} = \left[1.232(346.34)3205.7 \right]^{1/2} = 1169.5 \text{ m/s}$$

$$U_1 = V_w = \frac{p_2}{p_1} C_2 = 1.763(1169.5) = \underline{2061.9 \text{ m/s}} \text{ ANS (eqn (4-100))}$$

$$\text{also } p_2 = \frac{p_2}{p_1} \left(\frac{R_2 T_2}{R_1 T_1} \right) p_1 = 1.763 \left(\frac{1}{.1116} \right) 1 = 15.797 \text{ atm}$$

Note: The measured U_1 given in Combustion, Flames and Explosions of Gases (Lewis and von Elbe) is 2055 m/s indicating that the assumption of no dissociation is not significant because of the reduced T_f due to the diluent.