

## ASSIGNMENT - 7



$$\Delta H_r^\circ = 69.36 \text{ kJ/mol}$$

q) The reaction is endothermic. To keep the temperature constant, the reactor will have to be heated. Under the adiabatic conditions, the temperature will decrease. The energy required to break the reactant bonds is more than the energy released when the product bonds are formed.

b)  $\Delta U_r^\circ = \Delta H_r^\circ - RT \left[ \sum_{\text{gaseous products}} v_i - \sum_{\text{gaseous reactants}} v_i \right]$

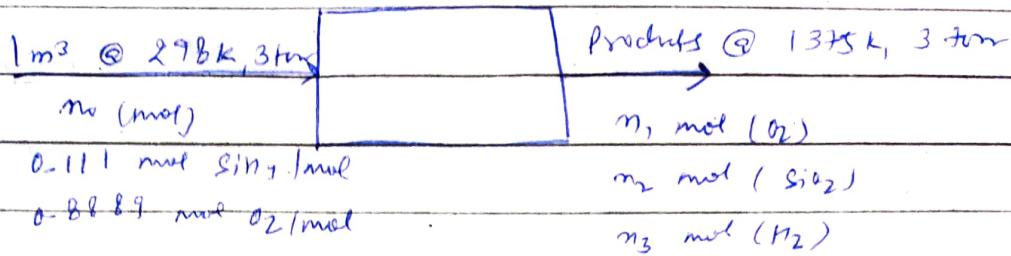
$$= 69.36 - 8.314 \times 10^{-3} \times 298 \times (7-0)$$

$$\Rightarrow 52 \text{ kJ/mol}$$

$\Delta U_r^\circ$  is the change in internal energy when 1-g mole of  $\text{Ca}(\text{l})$  and 5 g-moles of  $\text{H}_2\text{o}(\text{l})$  @  $25^\circ\text{C}$  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  $\text{H}_2(\text{g})$  @  $25^\circ\text{C}$  and 1 atm.

Q =  $\Delta U = \frac{n_{\text{CaO}} \Delta U_r^\circ}{V_{\text{CaO}}} = \frac{150 \times 52}{64.10} = 121.7 \text{ kJ}$

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## Ideal Gas Law

$$n = \frac{1 \text{ m}^3}{298 \text{ K}} \times \frac{273 \text{ K}}{760 \text{ torr}} \times \frac{1 \text{ mol}}{22.4 \times 10^{-3} \text{ m}^3} = 0.1614 \text{ mol}$$

$$m = n_i + v_i \epsilon$$

$$SiH_4 \Rightarrow O = 0.111 (0.1617) - 8$$

$$\varrho = 0.0179 \text{ mol}$$

$$O_2 \Rightarrow n_1 = 0.8889 (0.1619) - 8$$

$$n_1 = 0.1257 \text{ mol } (\text{O}_2)$$

$$S_1 O_2 \Rightarrow n_2 = \frac{g}{M} = 0.0129 \text{ mol } (S_1 O_2)$$

$$H_2 \Rightarrow m_3 = 2.8 - 0.0358 \text{ mol}(H_2)$$

b7

$$\Delta \hat{H}_f^\circ = (\Delta \hat{H}_f^\circ)_{S, O_2(s)} - (\Delta \hat{H}_f^\circ)_{S, H_2(g)}$$

$$= [-851 - (-619)] \text{ kJ/mol} = -789.1 \text{ kJ/mol}$$

References :- SiH<sub>4</sub>(g), O<sub>2</sub>(g), SiO<sub>2</sub>(s), H<sub>2</sub>(g) @ 298 K

Substance	$n_{in}$ (mol/h)	$\dot{H}_{in}$ (kJ/mol)	$n_{out}$ (mol/h)	$\dot{H}_{out}$ (kJ/mol)
$SiH_4$	0.0179	0	-	-
$O_2$	0.1935	0	0.1256	$\dot{H}_1$
$SiO_2$	-	-	0.0179	$\dot{H}_2$
$H_2$	-	-	0.0358	$\dot{H}_3$

$$O_2 (g, 1375 \text{ K}) \Rightarrow \hat{H}_1 = \hat{H}_{O_2} (1102^\circ\text{C}) = 36.14 \text{ kJ/mol}$$

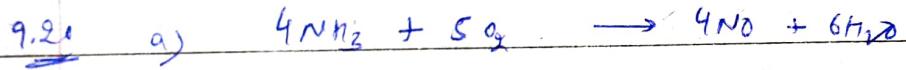
$$SiO_2 (s, 1375 \text{ K}) \Rightarrow \hat{H}_2 = \int_{298}^{1375} (C_p)_{SiO_2(s)} dT = 79.18 \text{ kJ/mol}$$

$$H_2 (g, 1375 \text{ K}) \Rightarrow \hat{H}_3 = \hat{H}_{H_2} (1102^\circ\text{C}) = 32.35 \text{ kJ/mol}$$

$$\textcircled{c} \quad Q = \Delta H = \sum_{\text{out}} \Delta H_i^{\circ} + \sum_{\text{out}} n_i \hat{H}_i - \sum_{\text{in}} n_i \hat{H}_i^{\circ} = -7.01 \text{ kJ/m}^3$$

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

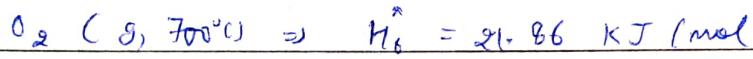
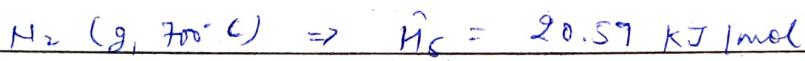
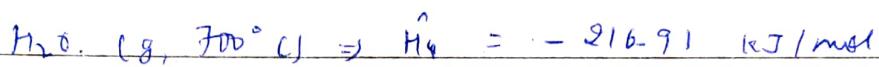
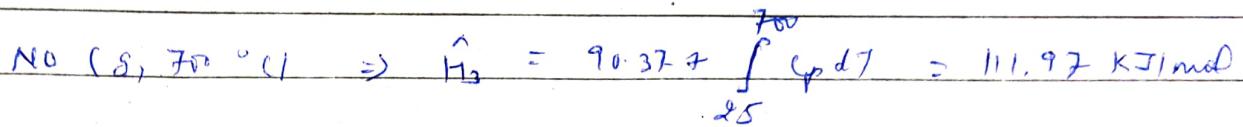
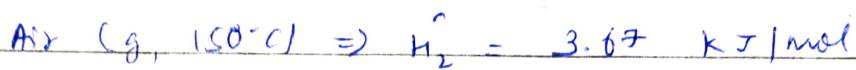
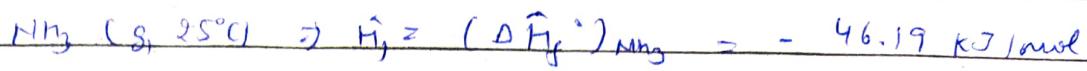
(transferred from reactor)



References :  $N_2(g)$ ,  $N_2(s)$ ,  $O_2(s)$  @  $25^\circ\text{C}$

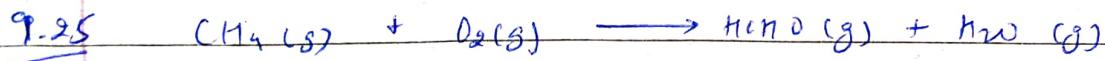
Substance	$n_{\text{in}}$ (mol/m <sup>3</sup> )	$\hat{H}_{\text{in}}$ (kJ/mol)	$n_{\text{out}}$ (mol/m <sup>3</sup> )	$\hat{H}_{\text{out}}$ (kJ/mol)
$NH_3$	100	$\hat{H}_1$	-	-
Air	900	$\hat{H}_2$	-	-
$NO$	-	-	90	$\hat{H}_3$
$H_2O$	-	-	150	$\hat{H}_4$
$H_2$	-	-	716	$\hat{H}_5$
$O_2$	-	-	69	$\hat{H}_6$

$$\hat{H}_f = \Delta \hat{H}_{f,i} + \int_{25}^T q_p dT$$



b)  $\dot{Q} = \Delta H = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i$   
 $= -4890 \times \left(\frac{1}{60}\right) = -81.5 \text{ kJ}$

c) for enthalpy calculations, if molecular species had been chosen as references, the extents of each reaction would have to be calculated to determine  $\Delta H$ . The value of  $\dot{Q}$  would've remain unchanged.



$T(^\circ C), P(kPa), 10L$	$n_3 (\text{mol } H_2O)$
$n_1 (\text{mol fuel gas})$	$n_2 (\text{mol } H_2O)$
$@ 25^\circ C$	$\rightarrow$
0.85 mol	$n_5 (\text{mol } CH_4)$
( $n_4 (\text{mol})$ )	$T(^\circ C), P(kPa), 10L$
0.15 mol ( $O_2 (\text{mol})$ )	$Q (\text{kJ})$

$$\text{Basis: } n_0 = 200 \text{ kDa} \quad | \begin{matrix} 10^3 \text{ Pa} & 10^2 & 10^{-3} \text{ m}^3 & 1 \text{ mol k} \\ 1 \text{ kDa} & 12 & 8.314 \text{ m}^3 \text{ Pa} & 298 \text{ K} \end{matrix} |$$

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

$$\text{CH}_4 \Rightarrow 0.65 (0.8072) = 0.6861 \text{ mol CH}_4$$

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

$$\text{CH}_4 \text{ consumed: } | \begin{matrix} 1 \text{ mol CH}_4 & 0.1211 \text{ mol O}_2 \text{ fed} \\ 1 \text{ mol O}_2 \text{ fed} \end{matrix} | = 0.1211 \text{ mol CH}_4$$

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

$$\text{HCHO produced: } | \begin{matrix} 1 \text{ mol HCHO} & 0.1211 \text{ mol CH}_4 \text{ consumed} \\ 1 \text{ mol CH}_4 & \text{consumed} \end{matrix} | = 0.1211 \text{ mol HCHO}$$

$$\text{H}_2\text{O produced: } n_T = | \begin{matrix} 1 \text{ mol H}_2\text{O} & 0.1211 \text{ mol CH}_4 \text{ consumed} \\ 1 \text{ mol CH}_4 & \text{consumed} \end{matrix} | = 0.1211 \text{ mol H}_2\text{O}$$

$$\text{Extent of reaction: } \xi = \left| \frac{(n_{O_2})_{\text{out}} - (n_{O_2})_{\text{in}}}{n_{O_2}} \right| = \left| \frac{0 - 0.1211}{0.1211} \right| = 1$$

References:  $\text{CH}_4(g)$ ,  $\text{O}_2(g)$ ,  $\text{HCHO}(g)$ ,  $\text{H}_2\text{O}(g)$ , @ 25°C

Substance	$n_{\text{in}}$	$\hat{U}_{\text{in}}$	$n_{\text{out}}$	$\hat{U}_{\text{out}}$
	mol	KJ/mol	mol	KJ/mol
$\text{CH}_4$	0.6861	0	0.5650	$\hat{U}_1$
$\text{O}_2$	0.1211	0	-	-
$\text{HCHO}$	-	-	0.1211	$\hat{U}_2$
$\text{H}_2\text{O}$	-	-	0.1211	$\hat{U}_3$

$$\hat{U}_i = \int_{25}^T (C_V)_i dT = \int_{25}^T (4-R)_i dT \quad i = 1, 2, 3$$

from table B.2 use  $(C_P)_i$

$$\hat{U}_1 = (0.025997 + 2.7345 \times 10^{-5} T^2 + 0.1220 \times 10^{-8} T^3 - 2.75 \times 10^{-12} T^4 - 0.6670) \text{ kJ/mol}$$

$$\hat{U}_2 = (0.025977 + 2.1340 \times 10^{-5} T^2 - 2.1735 \times 10^{-12} T^4 - 0.6623) \text{ kJ/mol}$$

$$\hat{U}_3 = (0.025757 + 0.3470 \times 10^{-5} T^2 + 0.2535 \times 10^{-8} T^3 - 0.8983 \times 10^{-12} T^4 - 0.6309) \text{ kJ/mol}$$

$$Q = \frac{100 \text{ J}}{\text{s}} \left| \frac{8.5 \text{ s}}{10^3 \text{ J}} \right| = 8.5 \text{ kJ}$$

$$\begin{aligned} \Delta \hat{H}_r^\circ &= (\Delta \hat{H}_f^\circ)_{\text{CH}_3O} + (\Delta \hat{H}_f^\circ)_{\text{H}_2O} - (\Delta \hat{H}_f^\circ)_{\text{CH}_3} \\ &= [(-115.90) + (-241.83) - (-74.85)] \text{ kJ/mol} \\ &= -262.88 \text{ kJ/mol} \end{aligned}$$

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

$$\begin{aligned} &= -262.88 \text{ kJ/mol} - \frac{8.314}{\text{mol K}} \left| \frac{298 \text{ K}}{(1+1)-1-1} \right| \frac{1 \text{ kJ}}{10^3 \text{ J}} \\ &= -262.88 \text{ kJ/mol} \end{aligned}$$

Doing energy balance

$$\begin{aligned} \dot{Q} &= \dot{q}_0 \hat{v}_0 + \sum (m_i)_{out} (\hat{v}_i)_{out} - \sum (m_i)_{in} (\hat{v}_i)_{in} \\ &= (0.12\text{mol}) (-262.88 \text{ kJ/mol}) + 0.5750 \hat{v}_7 + 0.12\text{mol} \hat{v}_2 \\ &\quad + 0.12\text{mol} \hat{v}_3 \end{aligned}$$

$$\begin{aligned} 0 &= 0.02088T + 1.845 \times 10^{-5}T^2 + 0.099032 \times 10^{-8}T^3 \\ &\quad - 1.726 \times 10^{-12}T^4 - 43.29 \text{ kJ/mol} \end{aligned}$$

$$\Rightarrow T = 1091^\circ\text{C} = 1364 \text{ K}$$

$$P = \frac{nRT}{V} = \frac{0.8072 \text{ mol}}{\text{mol}} \left| \frac{8.314 \text{ J mol}^{-1} \text{ K}^{-1}}{\text{mol} \cdot \text{K}} \right| \left| \frac{1364 \text{ K}}{10 \text{ L}} \right| \left| \frac{1 \text{ L}}{10^{-3} \text{ m}^3} \right|$$

$$\underline{P = 915 \text{ kPa}}$$

b) Rather than running the reactor adiabatically, heat should be added to the feed mixture to raise the temperature of reactants to an extent at which the reaction rate is significant.

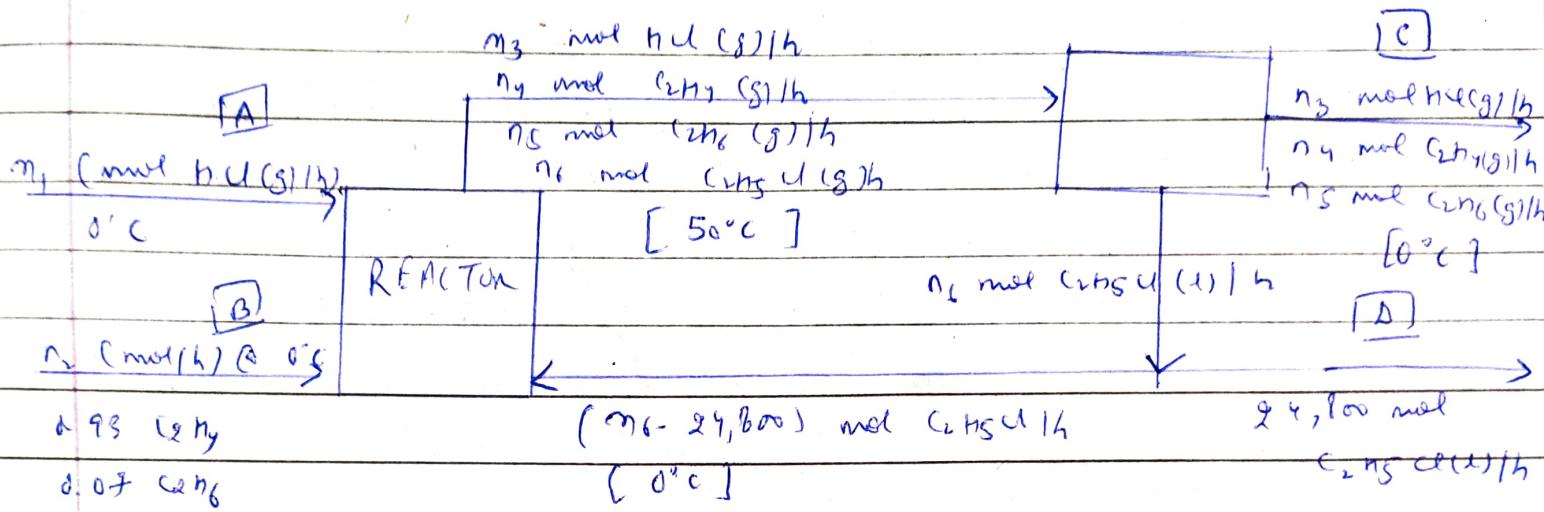
c) The side reaction is:  $\text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}$ . T would have been higher (more negative heat of reaction for combustion of methane). Volume & total moles would be the same so  $P = \frac{nRT}{V}$  would be greater.

9.30



Basis:  $\frac{1600 \text{ kg} \text{ Ceng Cl (l)}}{1} \left| \frac{10^3 \text{ g}}{1 \text{ kg}} \right| \left| \frac{1 \text{ mol}}{64.528} \right| = 24800 \text{ mol/h}$

( $\text{H}_2\text{Cl}$ )



### Product composition data

$$m_3 = 0.015m_1 \quad \text{--- (1)}$$

$$m_4 = 0.015(0.93m_2) = 0.01395m_2 \quad \text{--- (2)}$$

$$m_5 = 0.07m_2 \quad \text{--- (3)}$$

### Overall Cl balance

$$\frac{m_1 \text{ (mol HCl/h)}}{1 \text{ mol Cl}} \rightarrow = m_3 \text{ (l)} + 24800 \text{ (l)} - \text{--- (4)}$$

Solving (1) & (4)

$$m_1 = 25780 \text{ mol/h HCl}$$

$$m_3 = 378 \text{ mol HCl(g) / h}$$

Overall C balance

$$m_1 (0.93)(2) + m_2 (0.07)(2) = 2m_3 + 2m_5 + (2)(2460)$$

from ② & ③

$$2m_2 [0.93 + 0.07 - 0.0139 - 0.07] = 2(2460)$$

$m_2 = 270 \text{ mol of feed B/h}$

b)  $n_3 = 378 \text{ mol H}_2/\text{h}$

$$m_4 = 0.01395 (270) = 378 \text{ mol C}_2\text{H}_4/\text{h}$$

$$m_5 = 0.07 (270) = 1895 \text{ mol C}_2\text{H}_6/\text{h}$$

U

2.15 kmol /h of product C

= 14.3% H<sub>2</sub>, 14.3% C<sub>2</sub>H<sub>4</sub>, 71.4% C<sub>2</sub>H<sub>6</sub>

c) References: C<sub>2</sub>H<sub>7</sub>(g), C<sub>2</sub>H<sub>6</sub>(g), C<sub>2</sub>H<sub>5</sub>Cl(g), H<sub>2</sub>(g) @ 0°C

$$(C_2H_7(g), 50^\circ\text{C}) \Rightarrow \hat{H} = \int_0^5 q_p dt = 2.181 \text{ kJ/mol}$$

$$(g H_2(g), 50^\circ\text{C}) \Rightarrow \hat{H} = \int_{50}^0 q_p dt = 2.572 \text{ kJ/mol}$$

$$(g H_5 Cl(g), 50^\circ\text{C}) \Rightarrow \hat{H} = \int_5^{50} q_p dt = 1.756 \text{ kJ/mol}$$

$$(g H_2(g), 1, 0^\circ\text{C}) \Rightarrow \hat{H} = -\Delta H_f(0^\circ\text{C}) = -24.7 \text{ kJ/mol}$$

$$(g H_5 Cl(g), 50^\circ\text{C}) \Rightarrow \hat{H} = \int_0^5 q_p dt = 2.709 \text{ kJ/mol}$$

Substance	min mol	$\hat{H}_{in}$ kJ/mol	max mol	$\hat{H}_{out}$ kJ/mol
H <sub>2</sub>	25780	0	378	1.756
C <sub>2</sub> H <sub>4</sub>	25725	0	372	2.181
C <sub>2</sub> H <sub>6</sub>	1895	0	1895	2.572
C <sub>2</sub> H <sub>5</sub> Cl	$n_6 - 2460$	-24.7	$n_6$	2.709

Energy balance:-  $0 \text{ h}_2\text{o} = n_A \Delta \hat{H}_f(0^\circ\text{C}) + \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i = 0$

$$\Rightarrow (25780 - 378) \text{ mol H}_2 \text{ react} \left| \begin{array}{l} -69.5 \text{ kJ} \\ \text{h} \end{array} \right. + 372 (2.181) + 1895 (2.572)$$

$$+ 378 (1.756) + (n_6 - 2460) (-24.7) = 0$$

$n_6 = 80990 \text{ mol C}_2\text{H}_5\text{Cl}/\text{h}$  in reactor effluent.

$C_2H_5Cl$  recycled = 80490 mol condensed / h - 29800 mol product / h

$$= 55690 \text{ mol/h}$$

$$= 55.7 \text{ kmol recycled / h}$$

- d.
  - $C_p$  is a linear function of temperature
  - $\Delta H_r$  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 ethyl chloride product.