Department of Chemical Engineering Thapar Institute of Engineering & Technology, Patiala

Course: Material and Energy Balances UCH301

Course Instructor:

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Heat of Reaction from ΔH^0_f

- Determine the standard heat of reaction for the combustion of liquid *n*-pentane, assuming $H_2O(l)$ is a combustion product.

$$C_5H_{12}(l) + 8\,O_2(g) \rightarrow 5\,CO_2(g) + 6\,H_2O(l)$$

Solution

The heat of reaction from the ΔH^0_f data:

Data for ΔH^0_f from Table:

- $\Delta H^0_{f,\ CO2(g)}$ = -393.5 kJ/mol; $\Delta H^0_{f,H2O(l)}$ = -285.84 kJ/mol
- $\Delta H^0_{f,C5H12(l)}$ = -173 k J/mol

$$\Delta H^0_r = \sum(\Delta H^0_f)\text{products} - \sum(\Delta H^0_f)\text{reactants}$$

$$\Delta \hat{H}_r^\circ = [5(-393.5) + 6(-285.84) - (-173.0)]\ \text{kJ/mol}$$

$$= \boxed{-3509\ \text{kJ/mol}}$$

Heat of Reaction from ΔH_c

- Calculate the standard heat of reaction for the dehydrogenation of ethane:

$$C_2H_6(g) \rightarrow C_2H_4(g) + H_2(g)$$

Data:

$$(\Delta \hat{H}_c^\circ)_{C_2H_6} = -1559.9 \text{ kJ/mol}$$

$$(\Delta \hat{H}_c^\circ)_{C_2H_4} = -1411.0 \text{ kJ/mol}$$

$$(\Delta \hat{H}_c^\circ)_{H_2} = -285.84 \text{ kJ/mol}$$

- The heat of reaction is:

$\Delta H^0_r = \sum(\Delta H^0_c)\text{reactants} - \sum(\Delta H^0_c)\text{products}$

$$H_r^0 = (-1559.9) - (-1411.0 - 285.84) = 136.9 \frac{kJ}{mol}$$

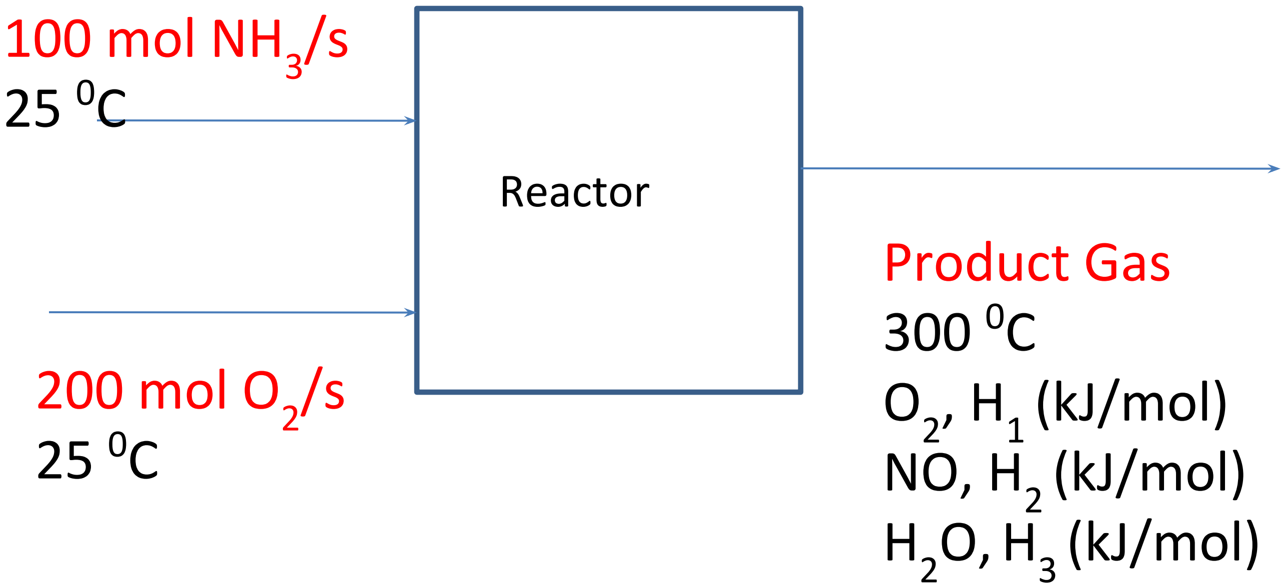
Problem

The standard heat of reaction for the oxidation of ammonia is given below:

$4NH_3(g) + 5O_2(g) \longrightarrow 4NO(g) + 6\ H_2O(v) \qquad \Delta H^0_r = -904.7\ kJ/mol$

One hundred mol of NH_3 per second and 200 mol O_2 per second at 25 ^0C are fed to a reactor in which NH_3 is completely consumed. The product gas emerges from the reactor at 300 ^0C. Calculate the rate at which heat must be transferred to or from the reactor.

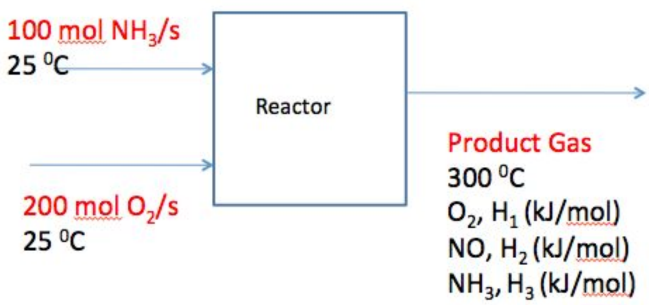
Solution


100 mol NH_3/s
25 ^{0}C
200 mol O_2/s
25 ^{0}C
Reactor
Product Gas
300 ^{0}C
O_2, H_1 (kJ/mol)
NO, H_2 (kJ/mol)
H_2O, H_3 (kJ/mol)

- Basis:100 mol/s NH_3 feed
- Data

Reference (g, 25^{0}C), for all species

Component	Mol/s (inlet)	Hin kJ/mol	Mol/s outlet	Hout kJ/mol
NH_3	100	0		
O_2	200	0	?	H_1=?
NO	-	-	?	H_2=?
H_2O	-	-	?	H_3=?



$4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6\,H_2O(v) \quad \Delta H^0_r = -904.7$ kJ/mol

- Energy balance for the process:

$$Q = \Delta H = \Delta H^0_r + \sum n_i H_{i\,(out)} - \sum n_i H_{i\,(In)}$$

Material balance (for n_i, at outlet):

- Mloes of NH_3 consumed = 100 mol/s
- Therefore O_2 Consumed = 100*(5/4)= 125 mol/s
- O_2 out = 200 -125 = 75 mol/s
- NO out = NH_3 Consumed = 100 mol/s
- H_2O out = (6/4)*100 =150 mol/s

H_1 = 8.470 kJ/mol (from table)

$H_2 = H_2 = \int C_{p,NO}\, dT$

C_p[kJ/(mol·°C)] or [kJ/(mol·K)] $= a + bT + cT^2 + dT^3$

$C_{p,NO}(T) = a + bT + CT^2 + dT^3$ kJ/(mol.°C)

$$H_2 = \int_{T=25^0 C}^{T=300^0 C} (\mathrm{a} + \mathrm{bT} + \mathrm{CT}^2 + \mathrm{dT}^3)\, dT$$

Where, $a \times 10^3 = 29.5$; $b \times 10^5 = 0.8188$; $C \times 10^8 = -0.2925$; $d \times 10^{12} = 0.3652$

Evaluating the integral $\rightarrow$ H_2 = 8.453 kJ/mol

H_3 = 9.57 kJ/mol (from table)

Reference (g, 25^0C), for all species

Component	Mol/s (inlet)	Hin kJ/mol	Mol/s outlet	Hout kJ/mol
NH_3	100	0		
O_2	200	0	?	H_1=?
NO	-	-	?	H_2=?
H_2O	-	-	?	H_3=?

$$Q = \Delta H = \Delta H^0_r + \sum n_{out} H_{out} - \sum n_{in} H_{in}$$

$$= (100/4)*(-904.7)+ [75*8.47+100*8.453+ 150*9.57 -100*0-200*0] = -19700 \text{ kJ/s}$$

$$Q = \Delta H = -19700 \text{ kJ/s}$$

Therefore, 19700 kJ/s heat must be removed from the reactor to keep temperature at 300 ^{0}C