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

Course: Material and Energy Balances UCH301

Course Instructor:

Dr. R. K. Gupta, Professor, Chemical Engineering

Adiabatic flame temperature

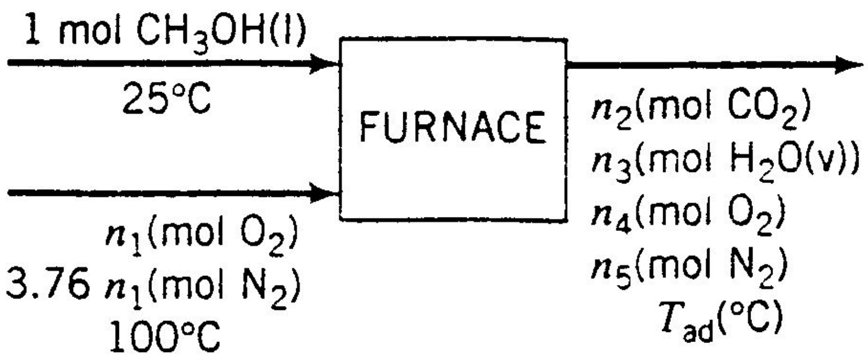
- The highest achievable temperature reached if the reactor is adiabatic and all of the energy released by the combustion goes to raise the temperature of the combustion products. This temperature is called the **adiabatic flame temperature,** T_{ad}.

Problem

- Liquid methanol is to be burned with 100% excess air. The engineer designing the furnace must calculate the highest temperature that the furnace walls will have to withstand so that an appropriate material of construction can be chosen. Perform this calculation, assuming that the methanol is fed at 25°C and the air enters at 100°C.

Solution

$$CH_3OH(l) + \frac{3}{2} O_2 \rightarrow CO_2 + 2 H_2O(l): \quad \Delta \hat{H}_c^\circ = -726.6 \text{ kJ/mol}$$



- Heat of combustion in case of H_2O vapor product = -726.6+44(2) = -636.6 kJ/mol

Energy balance

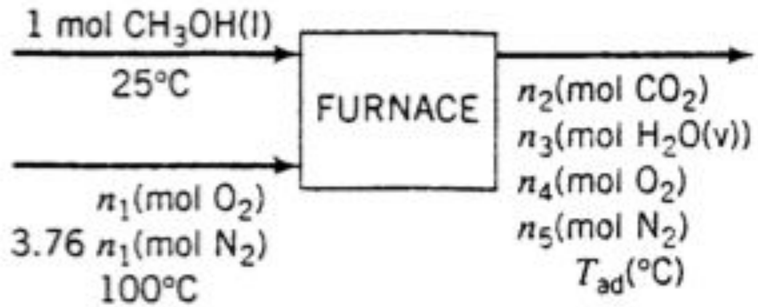
BASIS: 1 Mol of Methanol burned

$$\Delta\dot{H} = \dot{n}_f \Delta\hat{H}_c^\circ + \sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{ad}) - \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{feed})$$

- Also ΔH = 0, since Q =0; therefore

$$\sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{ad}) = -\dot{n}_f \Delta\hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{feed})$$

$$CH_3OH(l) + \tfrac{3}{2}\, O_2 \rightarrow CO_2 + 2\, H_2O(l): \quad \Delta \hat{H}_c^\circ = -726.6 \text{ kJ/mol}$$



Material balance (for complete combustion):

1.5 mol O_2 required for 1 mol of methanol.

O_2 supplied 100% excess: $n_1 = 1.5*2 = 3$ mol

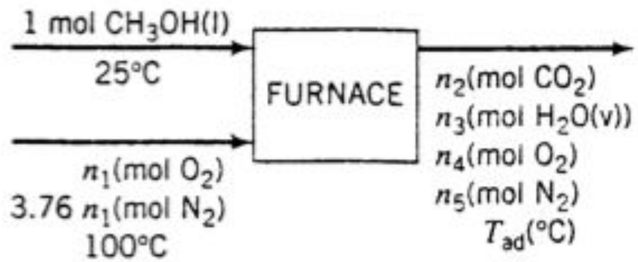
CO_2 produced: $n_2 = 1$ mol

H_2O produced: $n_3 = 2$ mol

O_2 unreacted: $n_4 = 1.\ 5$ mol

N_2 out: $n_5 = 11.28$ mol of N_2

$$CH_3OH(l) + \frac{3}{2} O_2 \rightarrow CO_2 + 2 H_2O(l): \quad \Delta \hat{H}_c^\circ = -726.6 \text{ kJ/mol}$$



References: $CH_3OH(l)$, O_2, N_2 at 25°C

$CH_3OH(l, 25°C)$: $\hat{H} = 0$

Air (100°C): $\hat{H} = 2.191$ kJ/mol (from Table

$$\sum_{\text{out}} \dot{n}_i \hat{H}_i(T_{\text{ad}}) = -\dot{n}_f \Delta \hat{H}_c^\circ + \sum_{\text{in}} \dot{n}_i \hat{H}_i(T_{\text{feed}})$$

Evaluating R.H.S. of the equation:

$$-n_{ethanol} \Delta H_C^0 + \sum_{in} n_i H_i = -(1 \times -638.6) + \{1 \times 0 + 14.28 * 2.191\} = 669.74\, kJ$$

- The heat capacities of product gas components can be estimated by using the following equations for C_ps:
- $$(C_p)_{CO_2} = 0.03611 + 4.233 \times 10^{-5}T - 2.887 \times 10^{-8}T^2 + 7.464 \times 10^{-12}T^3$$

$$(C_p)_{H_2O(g)} = 0.03346 + 0.688 \times 10^{-5}T + 0.7604 \times 10^{-8}T^2 - 3.593 \times 10^{-12}T^3$$

$$(C_p)_{O_2} = 0.02910 + 1.158 \times 10^{-5}T - 0.6076 \times 10^{-8}T^2 + 1.311 \times 10^{-12}T^3$$

$$(C_p)_{N_2} = 0.02900 + 0.2199 \times 10^{-5}T + 0.5723 \times 10^{-8}T^2 - 2.871 \times 10^{-12}T^3$$

$$\sum niCpi = 0.4378 + 9.826\times10^{-5}T + 4.178\times10^{-8}T^2 - 30.14\times10^{-12}T^3$$

$$\sum_{out} n_i C_{pi} = \int_{25}^{T_{ad}} 0.4378 + 9.826\times10^{-5}T + 4.178\times10^{-8}T^2 - 30.14\times10^{-12}T^3$$

$$= 0.4378T_{ad} + 4.913\times10^{-5}T_{ad}^2 + 1.393\times10^{-8}T_{ad}^3 - 7.535\times10^{-12}T_{ad}^4 - 11.845$$

$$\sum_{out} n_i C_{pi} = 0.4378T_{ad} + 4.913\times10^{-5}T_{ad}^2 + 1.393\times10^{-8}T_{ad}^3 - 7.535\times10^{-12}T_{ad}^4 - 11.845$$

$$\sum_{out} n_i C_{pi} = 669.74\,kJ$$

$$0.4378T_{ad} + 4.913\times10^{-5}T_{ad}^2 + 1.393\times10^{-8}T_{ad}^3 - 7.535\times10^{-12}T_{ad}^4 - 11.845 = 669.74\,kJ$$

Solving this equation gives:

$T_{ad} = 1256\ ^0C$