CHE 205 MASS AND ENERGY BALANCES

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BALANCES ON REACTIVE PROCESSES:

GENERAL PROCEDURE

HEAT OF REACTION METHOD

Single reaction and standard heat of reaction is known

HEAT OF FORMATION METHOD

multiple reactions and when standard heat of reaction is not known
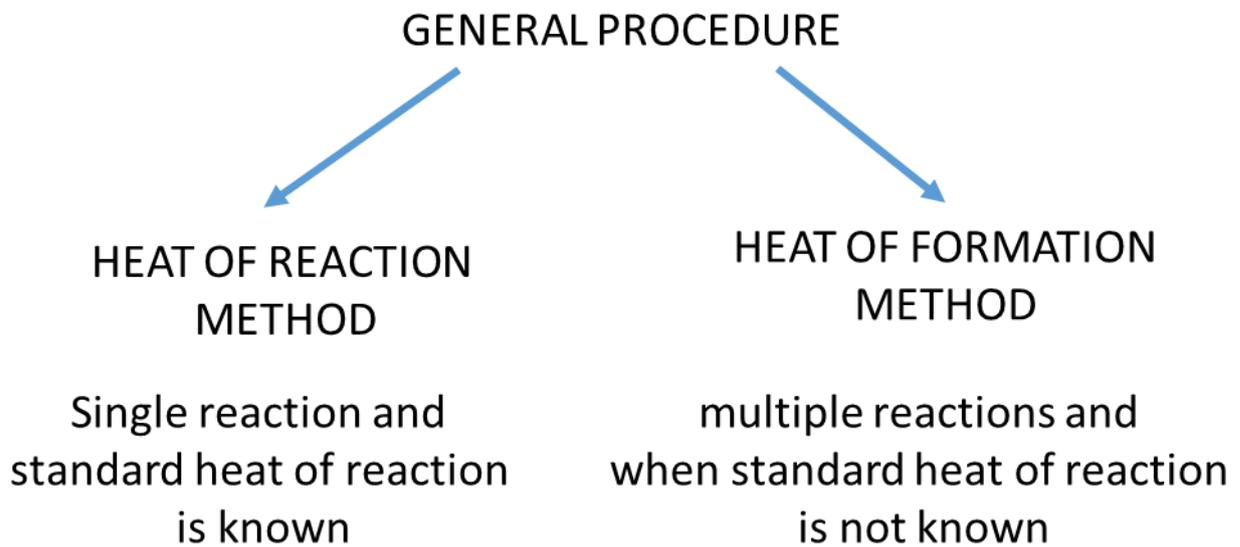
HEAT OF REACTION METHOD:

1. Complete all the material balance calculations.

2. Choose the reference states for specific enthalpy calculations. The references are the reactants and products at 25°C and 1 atm in the phases.

3. For a single reaction calculate the extent of reaction

4. Prepare the inlet and outlet enthalpy table.

5. Calculate each unknown enthalpy according to the reference state.

6. Calculate ΔH for the reactor.

$$\Delta H = \xi \Delta H_r^o + \sum n_{out} H_{out} - \sum n_{in} H_{in}$$

7. Substitute the calculated value of ΔH in the energy balance equation.

$$\Delta H = \sum n_{out} H_{out} - \sum n_{in} H_{in}$$

HEAT OF FORMATION METHOD

1. Complete all the material balance calculations.

2. Choose the reference states for specific enthalpy calculations. The references are the elemental species that constitute the reactant and product species (C_s, $O_{2(g)}$, $H_{2(g)}$) at 25°C and 1 atm.

3. Prepare the inlet and outlet enthalpy table.

4. Calculate each unknown enthalpy according to the reference state.

5. Calculate ΔH for the reactor.

$$\Delta H = \sum n_{out} H_{out} - \sum n_{in} H_{in}$$

6. Substitute the calculated value of ΔH in the energy balance equation.

YOUR TURN

I.

n-Butane (n-C_4H_{10}) at 25 °C is burned with excess air (at 100 °C) in a continuous combustion chamber

$$C_4H_{10} \, (g) + 13/2 \, O_2 \, (g) \rightarrow 4CO_2 \, (g) + 5H_2O \, (g)$$
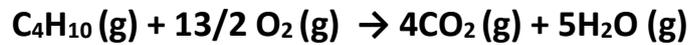
The product gas (at 250°C) contains 0.25 mol% butane, 5.9 mol% oxygen (O_2), 11.4 mol% carbon dioxide (CO_2) and the balance nitrogen on dry basis.

a) Assume 100 mol of dry product as basis. Draw and label the flow chart.
b) Calculate the fractional conversion of n-butane (mol reacted/ mol fed), amount of water (mol H_2O (g)) leaving the combustion chamber and the amount of excess air.
c) Calculate the amount of heat that is transferred to or from the combustion chamber if n-butane enters at 25°C, air enters at 100°C and all the products leave at 250°C.

II.

Ammonia is oxidized in a continuous reactor;

$$4 \, NH_{3 \, (g)} + 5 \, O_{2 \, (g)} \rightarrow 4 \, NO_{(g)} + 6 \, H_2O_{(v)}$$
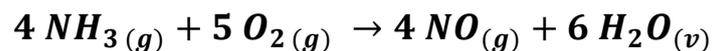
$$\Delta Hr^0 = -904.7 \text{ kJ/mol}$$

The feed stream (containing NH_3 and O_2) enters at 200°C and the products (O_2, NO and H_2O) leave at 1200°C. The mole ratio of NH_3 to O_2 in the feed is 2:3 (NH_3 / O_2 = 2:3). Draw and label the flow chart. Calculate the required heat transfer to or from the reactor.

III.

A superheated gas mixture at 600°C and 1 atm flowing at a rate of 28.5 m^3 (STP)/h is to be cooled to 450°C in an adiabatic spray cooler. The gas mixture contains 17.1 mole % water vapor , H_2O (v) and has a dry-basis composition of 7.5 mole% CO, 11.5% CO_2, 1% O_2 and 80 % N_2. A liquid water at 20°C is sprayed into the hot gas at a rate of m (kg H_2O (l)/ h). Calculate the liquid water feed rate (m) in kg/h.

28.5 m^3/h   gas mixture
(superheated) at 600°C

m (kg $H_2O_{(l)}$ / h),   20°C

Spray Cooler

450°C (superheated)

CO
CO_2
O_2
N_2
$H_2O_{(v)}$