WEEK 11

Balances on Reactive Systems

Heat of Reaction (Chap 9)

- Heat of reaction: endothermic, exothermic

  The heat of reaction (or enthalpy) of reaction $\Delta\hat{H}_r(T,P)$ is the enthalpy change for a process in which stoichiometric quantities of reactants at temperature T and pressure P react completely in a single reaction to form products at the same temperature and pressure.

  Ex: CaC_2 (s) + $2H_2O$(l) -> $Ca(OH)_2$(s) + C_2H_2(g)

  Calcium carbide　　Calcium hydroxide　　Acetylene

$$\Delta\hat{H}_r\left(25^o C, 1atm\right) = -125.4 \quad KJ/mol$$

  Ex: 2A + B → 3C

$$\Delta\hat{H}_r\left(100^o C, 1atm\right) = -50 \quad KJ/mol$$

  -50KJ/(2 mole of A consumed) = -50 KJ/(1 mole of B consumed)
  = -50kJ/(3 moles of A produced)

Heat of Reaction

If for example, you know that 150 moles of C were generated per second:

$\Delta\dot{H} =$ [-50 kJ/(3 moles of C generated)]*150 mole C/s

$\Delta\dot{H} = -2500 kJ/s$ enthalpy change

In general

$$\Delta H = \frac{\Delta\hat{H}_r\left(T_0, P_0\right)}{\left|\nu_A\right|} n_{A,r}$$

Stoichiometric coefficient (negative: reactant; positive: product)

Heat of Reaction

- Remember: extent of reaction ξ
- As a result $\xi = \frac{|n_{Aout} - n_{Ain}|}{|\nu_A|} = \frac{n_{A,r}}{|\nu_A|}$

$$\Delta H = \xi \Delta \hat{H}_r \left(T_0, P_0\right)$$

$\Delta \hat{H}_r (-)$: exothermic

$\Delta \hat{H}_r (+)$: endothermic

- At low P we have $\Delta \hat{H}_r (T)$

<u>Standard heat of reaction</u>: $\hat{H}_r^0$ heat of reaction when both reactants and products are at specified reference temperature and pressure, usually 25^{o}C and 1 atm.

Examples: Heat of Reaction

- To do in class: Page 443, Ex. 9.1-1

$$\dot{\xi} = \frac{|\dot{n}_{Aout} - \dot{n}_{Ain}|}{|\nu_A|} = \frac{\dot{n}_{A,r}}{|\nu_A|} \qquad \Delta\dot{H} = \xi\Delta\hat{H}_r^0$$

- To do in class: Page 443, Ex. 9.1-2

$$\Delta\hat{H}_{r2}^0 = 2\Delta\hat{H}_{r1}^0$$ Heat of reaction also doubles

- To do in class: Page 443, Ex. 9.1-3

$$\Delta\hat{H}_r = H_{products} - H_{reactants}$$ $H_2O(l)$ -> $H_2O(v)$

$\Delta\hat{H}_v(+)$: Heat of vaporization

9.3 Formation reactions and heat of formation

- Heat of formation: page 628, B1

- Heat of reaction: $\Delta\hat{H}_r^0 = \sum_i \nu_i \Delta\hat{H}_{fi}^0 = \sum_{products} |\nu_i| \Delta\hat{H}_{fi}^0 - \sum_{reactants} |\nu_i| \Delta\hat{H}_{fi}^0$

- To do in class: Page 447, Ex. 9.3-1

- To do in class: Page 449, Ex. 9.4-1

9.5 Energy balances on reactive processes

1. Draw and label flowchart
2. Use material balances including equilibrium relationships
3. Choose reference states and calculate enthalpies
4. Generate an enthalpy table
5. Calculate $\Delta \dot{H}$
6. Use energy balance with the calculated enthalpy.
7. To do in class: furnace example