



open

Heat orxn method

$$\Delta \dot{H} = \sum_j \dot{H}_{f,j} + \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i$$

convenient for single rxns when you know  $\Delta H_{rxn}$

Ref state has to be the conditions  $\Delta H_{rxn}$

Heat of Formation

$$Q = \Delta \dot{H} = \sum_{out} n_i \hat{H}_i - \sum_{in} n_i \hat{H}_i$$

$$= [ \dot{n}_{2CO_2} \hat{H}_{2CO_2} + \dot{n}_{2CO} \hat{H}_{2CO} + \dot{n}_{2H_2O} \hat{H}_{2H_2O} + \dot{n}_{2CH_4} \hat{H}_{2CH_4} + \dot{n}_{2O_2} \hat{H}_{2O_2} ]$$

$$- [ \dot{n}_{1CH_4} \hat{H}_{1CH_4} + \dot{n}_{1O_2} \hat{H}_{1O_2} ] \quad \text{material balances} \quad \dot{n}_{out} = \dot{n}_{in} + \sum_j \dot{v}_j \dot{v}_j$$

Ref state:  $C(25^\circ C, 1 \text{ atm}, s)$   
 $H_2(25^\circ C, 1 \text{ atm}, g)$   
 $O_2(25^\circ C, 1 \text{ atm}, g)$

For non-reactive systems we can choose the ref. state to be anything (inlet condition)

Outlet

$$\hat{H}_{2\text{CO}_2} = \Delta H_{f, \text{CO}_2}^\circ + \int_{25^\circ\text{C}}^{T_2} C_{P, \text{CO}_2, g} dT + 0$$

↑  
for ideal gas  
 $\Delta H = 0$  for  $\Delta P$

$$\Delta H_{f, \text{CO}_2}^\circ = -393 \text{ kJ/mol}$$

$$C_{P, \text{CO}_2, g} = 36.11 \times 10^{-3} + 4.233 \times 10^{-5} T + 2.887 \times 10^{-8} T^2 + 7.464 \times 10^{-12} T^3$$

$$\hat{H}_{2\text{CO}} = \Delta H_{f, \text{CO}}^\circ + \int_{25^\circ\text{C}}^{T_2} C_{P, \text{CO}, g} dT + 0$$

$\text{C}(25^\circ\text{C}, 1\text{atm}, \text{s})$   
 $\text{O}_2(25^\circ\text{C}, 1\text{atm}, \text{g})$  } Ref. states

ⓐ ↓  
 $\text{CO}_2(25^\circ\text{C}, 1\text{atm}, \text{g})$

ⓑ ↓  
 $\text{CO}_2(T_2, 1\text{atm}, \text{g})$

ⓒ ↓  
 $\text{CO}_2(T_2, P_2, \text{g})$  } process condition stream 2

$\text{C}(25^\circ\text{C}, 1\text{atm}, \text{s})$   
 $\text{O}_2(25^\circ\text{C}, 1\text{atm}, \text{g})$  } Ref. state

↓  
 $\text{CO}(25^\circ\text{C}, 1\text{atm}, \text{g})$

↓  
 $\text{CO}(T_2, 1\text{atm}, \text{g})$

↓  
 $\text{CO}(T_2, P_2, \text{g})$

Side note: For non-reactive systems, make your life easy + set inlet conditions as ref.  $\hat{H}_{ii} = 0$

$$\hat{H}_{2i} = \underbrace{\quad}_{\Delta P} \underbrace{\quad}_{\Delta T} \underbrace{\quad}_{\Delta \text{phase}}$$

