

# Lecture # 21 CHE331A

**Energy Balance  
for reactors:  
Batch, CSTR,  
PFR/PBR**

**Adiabatic  
Reactors**

**Non-adiabatic  
Reactors**

**Multiple reactors  
and  
inter-stage  
cooling**

**Multiple steady  
states**

**Energy balance  
and its application  
to Reactors**

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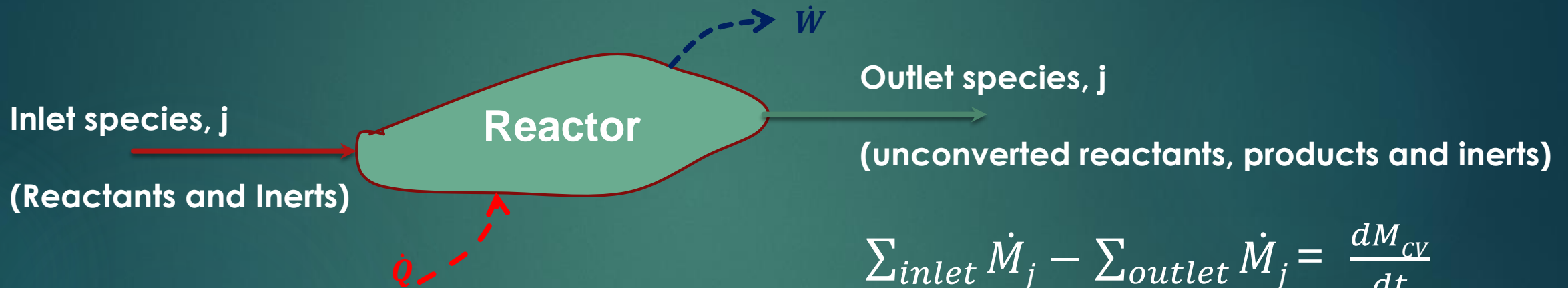
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# Back to the Past and the way forward

- For a control volume (Reactor) the three balances can be applied



**In – Out + Generation = Accumulation**

$$\sum_{inlet} \dot{M}_j - \sum_{outlet} \dot{M}_j = \frac{dM_{cv}}{dt}$$

$\dot{M}_j \rightarrow \frac{\text{mass of species } j}{\text{time}}$

$$(F_j)_{inlet} - (F_j)_{outlet} + G_j = \frac{d(N_j)_{cv}}{dt}$$

$F_j \rightarrow \frac{\text{moles of species 'j'}}{\text{time}}$        $G_j \rightarrow \frac{\text{moles of 'j' generated}}{\text{time}}$

$(N_j)_{cv} \rightarrow \text{moles of 'j' in CV}$

$$\sum_{inlet} \dot{E} - \sum_{outlet} \dot{E} + \dot{Q} - \dot{W} = \frac{dE_{cv}}{dt}$$

$\dot{E} \rightarrow \frac{\text{Energy (Enthalpy)}}{\text{time}}$



# For non-isothermal reactors Energy Balance is required for Design/Analysis

- ▶ For Batch Reactor:  $\dot{Q} - \dot{W} = \frac{dE_{cv}}{dt}$        $\sum_{inlet} \dot{E} = 0 = \sum_{outlet} \dot{E}$
- ▶ For flow reactor at steady state:  $\sum_i F_{i0} h_{i0,T_0} - \sum_i F_i h_{i,T} + \dot{Q} - \dot{W} = 0$   
(Assuming ideal solutions)
- ▶  $F_{i0} h_{i0}$  and  $F_i h_i$  are the enthalpy/time of the inlet/outlet stream
- ▶ Reaction:  $A + \frac{b}{a} B \rightarrow \frac{c}{a} C + \frac{d}{a} D$

$$\sum_{i,inlet} F_{i0} h_{i0,T_0} = F_{A0} h_{A0,T_0} + F_{B0} h_{B0,T_0} + F_{C0} h_{C0,T_0} + F_{D0} h_{D0,T_0} + F_{I0} h_{I0,T_0}$$

- ▶ and

$$\sum_{i,outlet} F_i h_{i,T} = F_A h_{A,T} + F_B h_{B,T} + F_C h_{C,T} + F_D h_{D,T} + F_I h_{I,T}$$



# Energy balance for reacting flow systems in more detail

- Recall from stoichiometric table:  $F_{i0} = F_{A0}(\theta_i)$  and  $F_i = F_{A0} \left( \theta_i + \frac{\mu_i}{a} X \right)$

$$\sum_i F_{i0} h_{i0} - \sum_i F_i h_i = F_{A0} \sum_i \theta_i h_{i0} - F_{A0} \sum_i \left[ \left( \theta_i + \frac{\mu_i}{a} X \right) h_i \right]$$

- $\sum_i F_{i0} h_{i0} - \sum_i F_i h_i = F_{A0} \sum [\theta_i (h_{i0} - h_i)] - (F_{A0} X) \sum \left[ \left( \frac{\mu_i}{a} \right) h_i \right] = F1 - F2$
- $F1 = F_{A0} \left[ (h_{A0,T0} - h_{A,T}) + \theta_B (h_{B0,T0} - h_{B,T}) + \theta_C (h_{C0,T0} - h_{C,T}) + \theta_D (h_{D0,T0} - h_{D,T}) + \theta_I (h_{I0,T0} - h_{I,T}) \right]$
- $F2 = (F_{A0} X) \left[ \frac{d}{a} h_{D,T} + \frac{c}{a} h_{C,T} - \frac{b}{a} h_{B,T} - h_{A,T} \right] = (F_{A0} X) \Delta h_{Rxn,T}$
- Where,  $\Delta h_{Rxn,T}$  is the  $\frac{\text{heat of reaction}}{\text{mol A}}$  at T (joules/mol A)



# Energy balance flow systems ... some more

- ▶  $\sum_i F_{i0} h_{i0} - \sum_i F_i h_i + \dot{Q} - \dot{W} = 0$
- ▶  $F_{A0} \sum [\theta_i (h_{i0} - h_i)] - F_{A0} X \Delta h_{Rxn,T} + \dot{Q} - \dot{W} = 0 \quad (1)$
- ▶ Usually, enthalpy of a species ' $i$ ' is given with reference to enthalpy of formation at 298 K, i.e.,  $h_{i,T} = h_{i,T_R}^0 + \int_{T_R}^T C_{p,i} dT$ ; (no phase change)
- ▶  $C_{p,i}$  is a function of temperature and is given by:  $C_{p,i} = \alpha_i + \beta_i T + \gamma_i T^2$
- ▶ For constant heat capacity:  
$$h_{i,T} = h_{i,T_R}^0 + C_{p,i} (T - T_R)$$
$$h_{i,T_0} = h_{i,T_R}^0 + C_{p,i} (T_0 - T_R)$$
- ▶ After substitution Equation (1) above becomes:

$$-F_{A0} \sum [\theta_i C_{p,i} (T - T_0)] - F_{A0} X \Delta h_{Rxn}(T) + \dot{Q} - \dot{W} = 0$$



# Energy balance ... continued

- ▶ The heat of reaction,  $\Delta h_{Rxn}(T)$ , is given by
- ▶  $\Delta h_{Rxn}(T) = \frac{d}{a} h_D(T) + \frac{c}{a} h_C(T) - \frac{b}{a} h_B(T) - h_A(T)$
- ▶ Usually,  $\Delta h_{Rxn}(T)$ , is given at  $T_R$ ,  $\Delta h_{Rxn}^0(T_R)$
- ▶ Defining  $\Delta C_p = \frac{d}{a} C_{P,D} + \frac{c}{a} C_{P,C} - \frac{b}{a} C_{P,B} - C_{P,A}$ 
  - $C_{P,i}$  is the constant heat capacity of species  $i$
- ▶  $\Delta h_{Rxn}(T) = \Delta h_{Rxn}^0(T_R) + \Delta C_p(T - T_R)$

$$\dot{Q} - \dot{W} - F_{A0} \sum [\theta_i C_{P,i}(T - T_o)] - F_{A0} X [\Delta h_{Rxn}^0(T_R) + \Delta C_p(T - T_R)] = 0$$





# Finally we get the relationship between temperature and conversion

►  $\dot{Q} - \dot{W} - F_{A0} \sum [\theta_i C_{P,i} (T - T_o)] - F_{A0} X [\Delta h_{Rxn}^0 (T_R) + \Delta C_p (T - T_R)] = 0$

► *For no shaft work and adiabatic operations:  $\dot{Q} = 0 = \dot{W}$*

►  $X = \frac{\sum [\theta_i C_{P,i} (T - T_o)]}{[-\Delta h_{Rxn}^0 (T_R) + \Delta C_p (T - T_R)]} \rightarrow X = X(T) \quad \text{need } T = T(X)$

$$T = \frac{X [-\Delta h_{Rxn}^0 (T_R)] + \sum [\theta_i C_{P,i} T_o] + X \Delta C_p T_R}{\sum \theta_i C_{P,i} + X \Delta C_p}$$

► For  $A \rightarrow P$   $\Delta C_p = 0$  and pure A as the inlet

$$T = T_o + \frac{X [-\Delta h_{Rxn}^0 (T_R)]}{C_{P,A}}$$

► The same expression referred to before

