Lecture # 23 CHE331A

Energy Balance for reactors:

Batch, CSTR, PFR/PBR

Adiabatic and non-adiabatic Reactors

Multiple reactors and inter-stage cooling

Analysis of CSTRs and the presence of Multiple States

Tubular reactors (PFR/PBR) with Heat exchange

(non-adiabatic)

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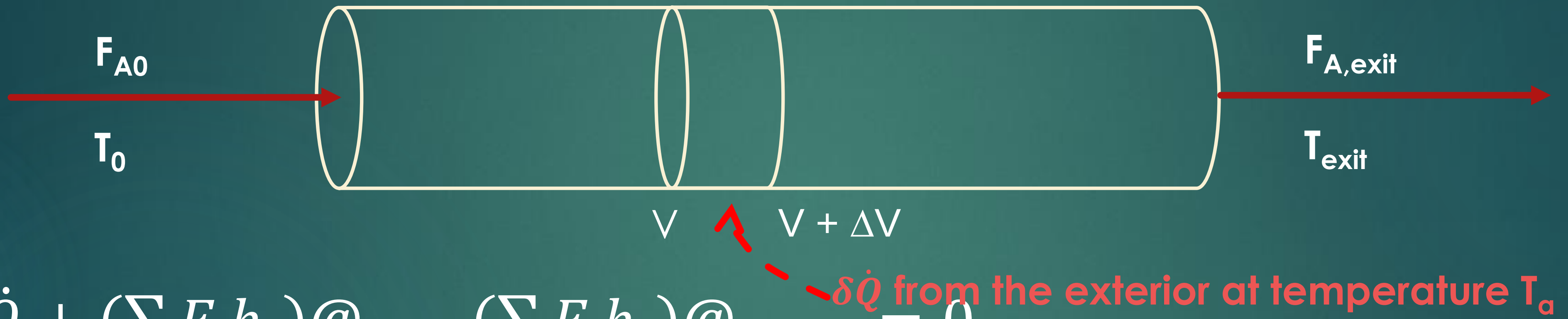
Tubular reactors (PFR) with Heat Exchange

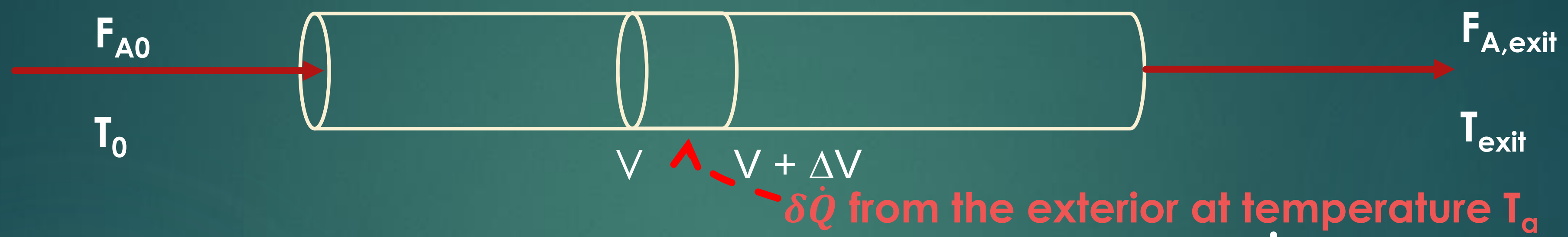
- Energy balance equation with no shaft work (assuming ideal solutions):
  for a **differential** volume element:



- $\delta\dot{Q} + (\sum F_i h_i)@_V - (\sum F_i h_i)@_{V+\Delta V} = 0$
- $\delta\dot{Q} = U.\Delta A.(T_a - T) = U.a.\Delta V(T_a - T)$
- Where: $U \; - \; overall\ heat\ transfer\ coefficient$ and

  $a \; - heat\ exchange\ area\ per\ unit\ volume = \frac{\pi D L}{\pi \frac{D^2}{4} L}\ or\ a = \frac{4}{D}$

Differential analysis of a PFR exchanging heat with the environment at constant temperature



- $\delta\dot{Q} + (\sum F_i h_i)@_V - (\sum F_i h_i)@_{V+\Delta V} = 0$ with $\delta\dot{Q} = U.a.\Delta V.(T_a - T)$
- Diving by ΔV and taking limits of ΔV → 0
- $U.a(T_a - T) - \frac{d(\sum F_i h_i)}{dV} = 0$ F_i and h_i are varying with V
- $U.a.(T_a - T) - \sum h_i \frac{d(F_i)}{dV} - \sum F_i \frac{d(h_i)}{dV} = 0$
- We need to analyze the two derivatives: $\frac{d(F_i)}{dV}$ and $\frac{d(h_i)}{dV}$

A PFR with heat exchange … some more

- The two derivatives: $\frac{d(F_i)}{dV}$ and $\frac{d(h_i)}{dV}$
- The mol balance equation gives: $\frac{d(F_i)}{dV} = r_i = v_i(-r_A)$
- And, $\frac{d(h_i)}{dV} = C_{p,i}\frac{dT}{dV}$ (assuming constant specific heat)
- Substituting in: $U.a.(T_a - T) - \sum h_i \frac{d(F_i)}{dV} - \sum F_i \frac{d(h_i)}{dV} = 0$ we have
- $U.a.(T_a - T) - \sum h_i v_i(-r_A) - \sum F_i C_{p,i}\frac{dT}{dV} = 0$ with $\sum h_i v_i = \Delta h_{Rxn,T}$
- Thus,

$$\boxed{\frac{dT}{dV} = \frac{\Delta h_{Rxn,T}(r_A) + U.a.(T_a - T)}{\sum F_i C_{p,i}}}$$

PFR with heat exchange … continued

- The change in temp with V is given by: $\frac{dT}{dV} = \frac{r_A \Delta h_{Rxn,T} + U.a(T_a - T)}{\sum F_i C_{p,i}}$
- $r_A \Delta h_{Rxn,T}$ is the heat generated during reaction and
- $U.a.(T - T_a)$ is the heat removed from the reactor
- To design/analyze the PFR with heat exchange the two coupled ODEs need to be solved simultaneously
  - One is the mol balance (MB) ODE and the other is the energy balance (EB) ODE

$$\frac{d(F_i)}{dV} = r_i$$

$$\frac{dT}{dV} = \frac{r_A \Delta h_{Rxn,T} + U.a.(T_a - T)}{\sum F_i C_{p,i}}$$

The energy balance equation in terms of conversion and for a PFR

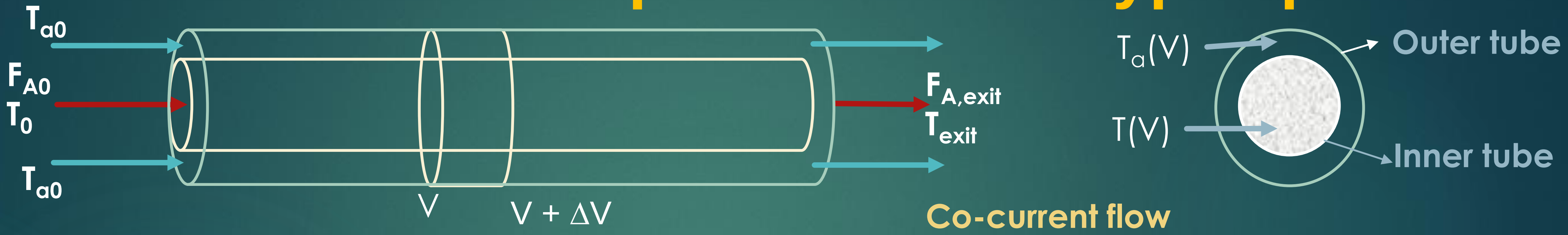
$$\frac{dT}{dV} = \frac{r_A \Delta h_{Rxn,T} + U.a.(T_a - T)}{\sum F_i C_{p,i}}$$

- Substituting: $F_i = F_{A0}(\theta_i + v_i X)$, and $\Delta h_{Rxn,T} = \Delta h^0_{Rxn,T_R} + \Delta C_p (T - T_R)$

$$\boxed{\frac{dT}{dV} = \frac{r_A\left[\Delta h^0_{Rxn,T_R} + \Delta C_p (T - T_R)\right] + U.a.(T_a - T)}{F_{A0} \sum \left(\theta_i C_{P,i} + \Delta C_P X\right)} = g(X,T)}$$

- Thus, $\frac{dT}{dV} = g(X,T)$ and $\frac{dX}{dV} = \frac{-r_A}{F_{A0}} = f(X,T)$ needs to be solved
  - Boundary conditions of $T = T_0\ and\ X = 0\ at\ V = 0$
- Check if you get the same expression for adiabatic PFR where $U = 0$

Instead of a heat exchange with an exterior source other at constant temperature other types possible



- Energy balance for the coolant (heat transferred from reactor to T_a):

$$\dot{m}_c h_{c,V} - \dot{m}_c h_{c,V+\Delta V} + U.a.\Delta V(T - T_a) = 0$$

- Dividing by ΔV and taking limits: $-\dot{m}_c \dfrac{dh_c}{dV} + U.a.(T - T_a) = 0$

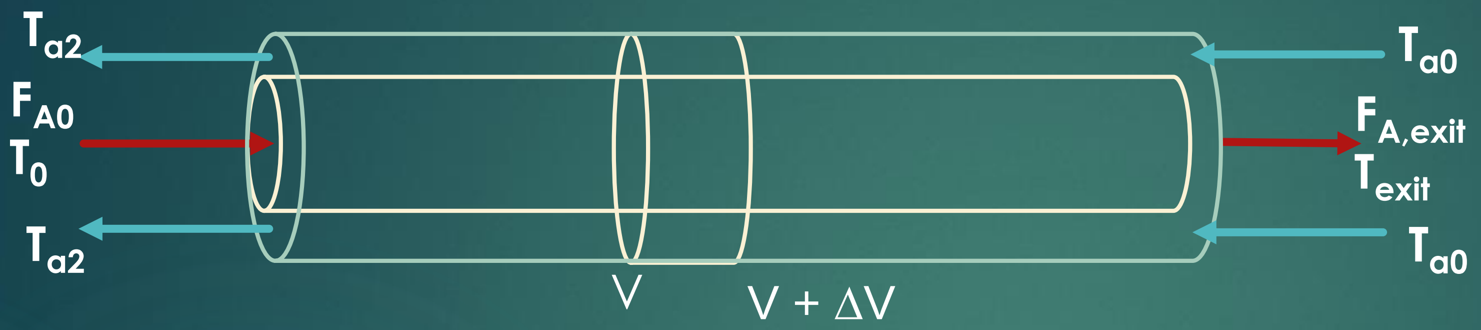
- For constant $C_{P,c}$ of the coolant: $\dfrac{dh_c}{dV} = C_{P,c}\dfrac{dT_a}{dV}$ substituting above,

$$\frac{dT_a}{dV} = \frac{U.a.(T - T_a)}{\dot{m}_c.C_{P,c}}$$

With: $T_a = T_{a0}$ & $T = T_0$ at $V = 0$

This is another ODE that needs to Solved simultaneously

The case of counter-current heat exchange with a coolant



Counter-current flow

- Energy balance for the coolant (heat transferred from reactor to T_a):

$$\dot{m}_c h_{c,V+\Delta V} - \dot{m}_c h_{c,V} + U.a.\Delta V(T - T_a) = 0$$

- And, $\dot{m}_c \frac{dh_c}{dV} + U.a.(T - T_a) = 0$, Further $\frac{dh_c}{dV} = C_{P,c}\frac{dT_a}{dV}$

$$\frac{dT_a}{dV} = \frac{U.a.(T_a - T)}{\dot{m}_c.C_{P,c}}$$

With: $T_a = T_{a2}$ & $T = T_0$ at $V = 0$

With: $T_a = T_{a0}$ & $T = T$ at $V = V$

- Usually, the inlet conditions are know, i.e., T_{a0}
- Thus, to find the exit conversion we need to do trial-and-error

The ODEs that need to be solved for different cases: A Summary

- Mol Balance ODE: $$F_{A0}\frac{dX}{dV} = -r_A$$ **With:** X = 0 at V = 0
- Energy Balance with exterior at constant temperature:

$$\frac{dT}{dV} = \frac{r_A \Delta h_{Rxn,T} + U.a.(T_a - T)}{\sum F_i C_{p,i}}$$

With: T = T at V = 0

- Energy Balance with exterior with variable temp (co-current):

$$\frac{dT_a}{dV} = \frac{U.a.(T - T_a)}{\dot{m}_c.C_{P,c}}$$

With: $T_a = T_{a0}$ at V = 0

- Energy Balance with exterior with variable temp (counter-current)

$$\frac{dT_a}{dV} = \frac{U.a.(T_a - T)}{\dot{m}_c.C_{P,c}}$$

With: $T_a = T_{a2}$ at V = 0

Such that: $T_a = T_{a0}$ at V = V