Lecture # 25 CHE331A

Energy Balance for reactors:

Batch, CSTR, PFR/PBR

Adiabatic Reactors

(CSTR, PFR, PBR)

Non-adiabatic Reactors

PFR

(including an example)

Reversible reactions, Multiple reactors & inter-stage cooling

CSTR and Heat Effects

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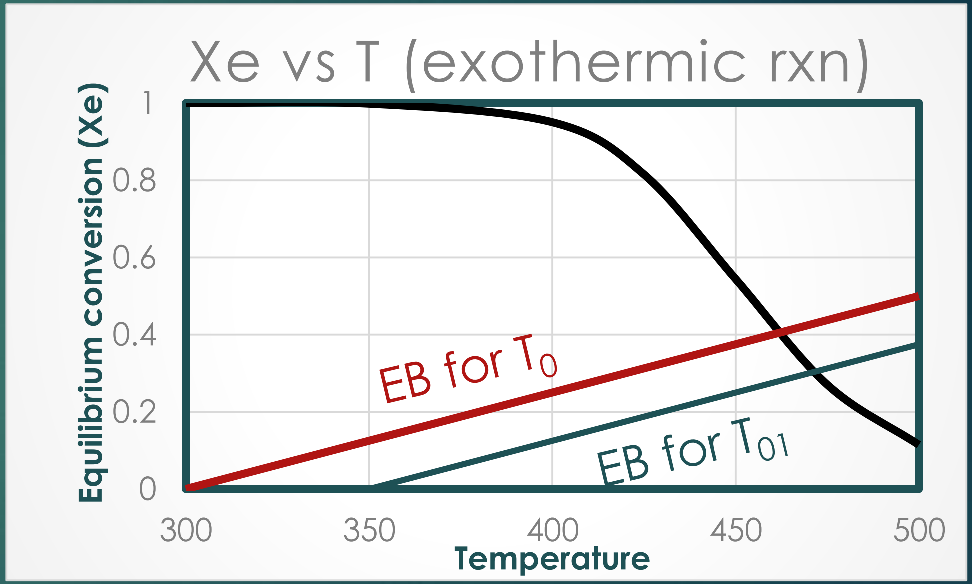
Equilibrium considerations (reversible reations)

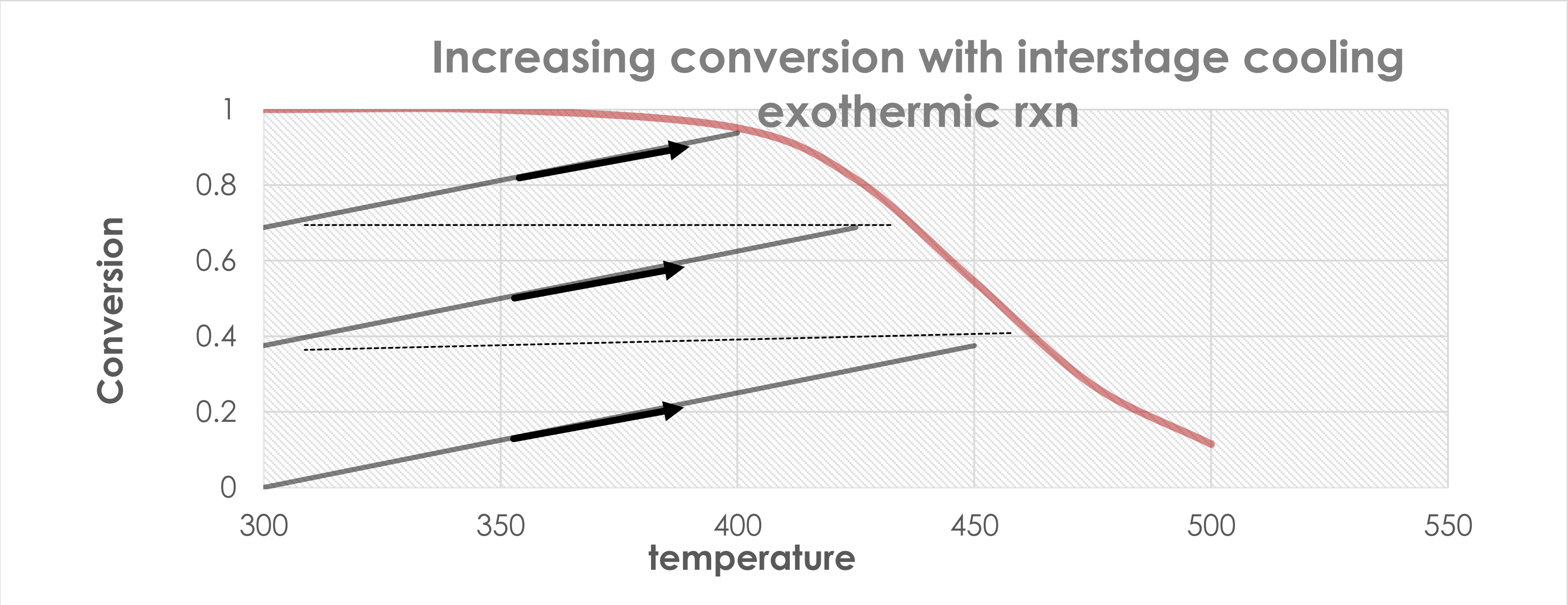
- For reversible reactions knowing equilibrium conversion is important
- For a reversible reaction $A \rightleftharpoons B$; $X_e = \frac{K_C(T)}{1+K_C(T)}$
- Maximum conversion that can be achieved adiabatically is given by the intersection of the X_e vs T curve and the Energy Balance equation, X_{EB} vs T



- $X_{EB} = \frac{\sum[\theta_i C_{P,i}(T-T_o)]}{[-\Delta h^0_{Rxn}(T_R)+\Delta C_p(T-T_R)]} = \frac{C_{P,A}(T-T_0)}{-\Delta h_{Rxn,T}}$
- Increasing inlet temperature T_0 to T_{01} decreases maximum conversion that can be achieved

Multiple reactors with inter-stage cooling or heating

- Higher conversions can be achieved by adiabatic operations by connecting reactors in series with inter-stage cooling/heating

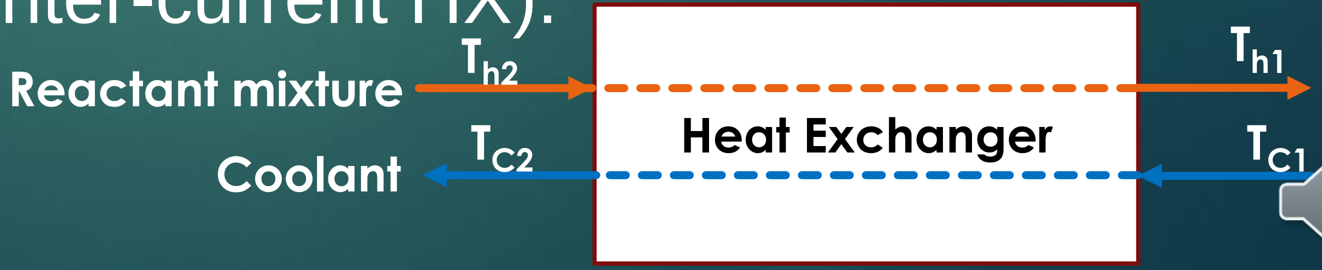


Think about endothermic reactions!

Calculation of heat transfer area of heat exchanger

- Calculate exit temperature of reactor (exothermic reaction):
  - For inlet temperature T_0, X_e is calculated, e.g., $X_e = 0.42$ for $T_0 = 300$ K
  - Design adiabatic reactor for $0.95*X_e$, e.g., $X = 0.40$
  - Energy balance equation: $T_{oulet} = 300 + 400X$, $T_{oulet} = 460$ K
- Cool down temperature to T_{inlet} (to 2nd reactor) = 350 K (for example)
- Heat load for cooling reaction outlet: $\dot{Q} + \sum F_{i0} h_{i0} - \sum F_i h_i = 0$
- For example, $\dot{Q} = -220 \frac{kcal}{s}$ mass flow rate of coolant is calculated
- Heat transfer area from (counter-current HX):

$$\dot{Q} = UA \frac{[(T_{h2} - T_{C2}) - (T_{h1} - T_{C1})]}{ln\left(\frac{T_{h2} - T_{C2}}{T_{h1} - T_{C1}}\right)}$$



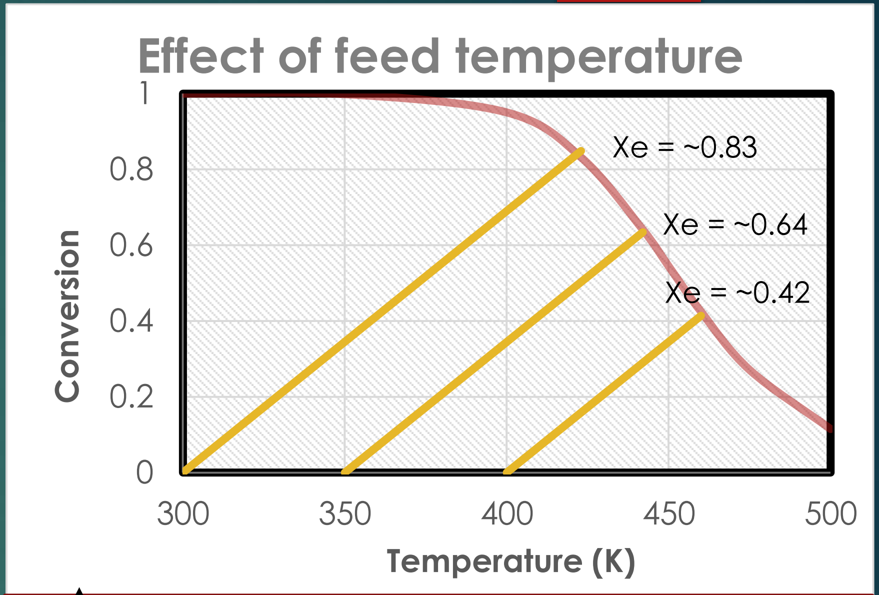
Optimum feed temperature for an adiabatic reactor with fixed size or catalyst weight

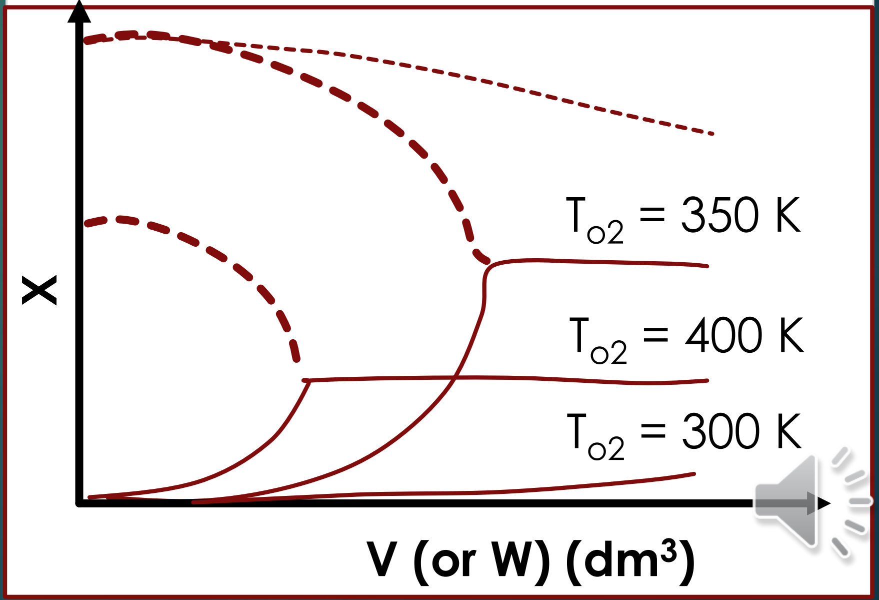
- Low feed temperature: X_e is high, rate is low
- High feed temperature: low X_e and high rate
- For a fixed size or catalyst weight, X_e is

achieved at the beginning of the reactor for high feed temperature and the rest of the reactor is at equilibrium

  - For low feed temperatures equilibrium conversion may not be reached

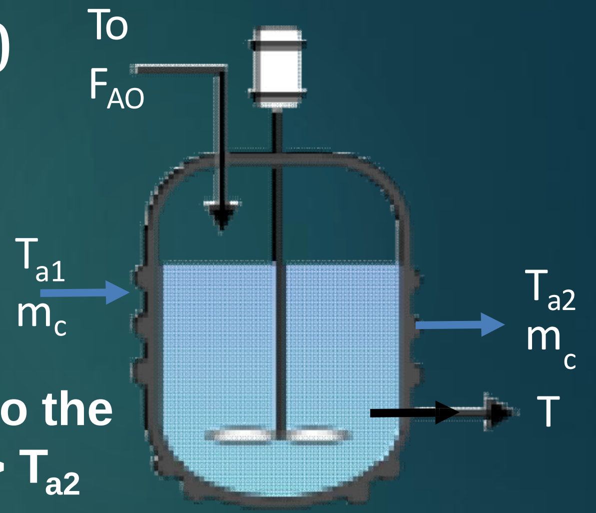
- Optimum feed temperature exists for a given size or catalyst weight (Section 8-5, Fogler)





CSTR with Heat Effects

- The temperature is the same inside the CSTR, but not equal to T_0
- EB: $\dot{Q} - \dot{W} - F_{A0}\sum[\theta_i C_{P,i}(T - T_o)] - F_{A0}X\Delta h_{Rxn}(T) = 0$
- Substituting MB: $F_{A0}X = -r_A V$ in EB
- $\dot{Q} - \dot{W} - F_{A0}\sum[\theta_i C_{P,i}(T - T_o)] + r_A V\Delta h_{Rxn}(T) = 0$



Heat added to the reactor: $T_{a1} > T_{a2}$

- Rate of heat transfer from HX to the reactor: $\dot{Q} = UA\frac{(T_{a1}-T_{a2})}{ln\left(\frac{T-T_{a1}}{T-T_{a2}}\right)}$
- Energy balance (heating media): $\dot{Q} = \dot{m}_C C_{P,C}(T_{a1} - T_{a2}) = UA\frac{(T_{a1}-T_{a2})}{ln\left(\frac{T-T_{a1}}{T-T_{a2}}\right)}$

Further analysis of the heating media

- $\dot{m}_C C_{P,C}(T_{a1} - T_{a2}) = UA \frac{(T_{a1}-T_{a2})}{ln\left(\frac{T-T_{a1}}{T-T_{a2}}\right)}$ which is solved for T_{a2}
- $T_{a2} = T - (T - T_{a1})exp\left(\frac{-UA}{\dot{m}_C C_{P,C}}\right)$; exponent is small and expanded as
- $e^{-x} = 1 - x + \frac{x^2}{2!}$ ... neglecting 2nd and higher order terms, then

$$(T_{a1} - T_{a2}) = (T_{a1} - T)\left[1 - \left(1 - \frac{UA}{\dot{m}_C C_{P,C}}\right)\right] = (T_{a1} - T)\left(\frac{UA}{\dot{m}_C C_{P,C}}\right)$$

- Further: $\dot{Q} = \dot{m}_C C_{P,C}(T_{a1} - T_{a2}) = \dot{m}_C C_{P,C}(T_{a1} - T)\left(\frac{UA}{\dot{m}_C C_{P,C}}\right)$
- And, for large flow rates of heating/cooling media, $T_{a1} \cong T_{a2} = T_a$

$$\dot{Q} = UA(T_a - T)$$

Further analysis of the CSTR with heat effects

- $\dot{Q} - \dot{W} - F_{A0} \sum\left[\theta_i C_{P,i}(T - T_o)\right] - F_{A0} X \Delta h_{Rxn}(T) = 0,$
- Substituting for $\dot{Q}$ and neglecting $\dot{W}$ in the above equation
- $UA(T_a - T) - F_{A0} \sum\left[\theta_i C_{P,i}(T - T_o)\right] - F_{A0} X \Delta h_{Rxn}(T) = 0$
  - Dividing by F_{A0} and in terms of conversion: $X = \dfrac{\frac{UA(T-T_a)}{F_{A0}} + \sum\left[\theta_i C_{P,i}(T-T_o)\right]}{-\Delta h_{Rxn}(T)}$
  - To size CSTR the MB, $V = \dfrac{F_{A0} X}{-r_A(X,T)}$, is also used
- For $\sum \theta_i C_{P,i} = C_{P,0}$, then
- $UA(T_a - T) - F_{A0} C_{P,0}(T - T_o) - F_{A0} X \Delta h_{Rxn}(T) = 0$

$$C_{P,0}\left(\frac{UA}{F_{A0} C_{P,0}}\right) T_a + C_{P,0} T_0 - C_{P,0}\left(\frac{UA}{F_{A0} C_{P,0}} + 1\right) T - X \Delta h_{Rxn}(T)$$

Analysis of CSTR with heat effects … continued

- $C_{P,0}\left(\frac{UA}{F_{A0}C_{P,0}}\right)T_a + C_{P,0}T_0 - C_{P,0}\left(\frac{UA}{F_{A0}C_{P,0}} + 1\right)T - X\Delta h_{Rxn}(T) = 0$
- Define two parameters: $\kappa = \left(\frac{UA}{F_{A0}C_{P,0}}\right)$ and $T_c = \frac{\kappa T_a + T_0}{1+\kappa}$
- Then, $-X\Delta h_{Rxn}(T) = C_{P,0}(1+\kappa)(T - T_c)$
- Thus, we can find $X\ or\ T$ from the above

$$X = \frac{C_{P,0}(1+\kappa)(T-T_c)}{-\Delta h_{Rxn}(T)}$$

OR

$$T = T_c + \frac{-X\Delta h_{Rxn}(T)}{C_{P,0}(1+\kappa)}$$

- Three methods for design/analysis of a CSTR with heat effects
  - Given X, find V and T
  - Given T, find X and V
  - Given V, find X and T

See example 8-8 For production of propylene glycol