Lecture # 24 CHE331A

Energy Balance for reactors:

Batch, CSTR, PFR/PBR

Adiabatic Reactors

(CSTR, PFR, PBR)

Non-adiabatic Reactors

PFR

An example of PFR, Multiple reactors & inter-stage cooling

GOUTAM DEO
CHEMICAL ENGINEERING DEPARTMENT
IIT KANPUR

The cracking of acetone to ketene and methane

- The cracking reaction is a key step in the production of Acetic Anhydride (example 8-5, 4th Edition)
- $CH_3COCH_3(A) \rightarrow CH_2CO(B) + CH_4(C)$ 1st order, irreversible

$$k = 3.58 exp\left[34{,}222\left(\frac{1}{1035} - \frac{1}{T}\right)\right] \; s^{-1}$$

  - Reactor: PFR, 1000 numbers of 1” schedule 40 tubes, total volume = 5 m^3
  - Inlet: 7850 kg acetone per hour T_0 = 1035 K P = 162 kPa (isobaric)
  - Case I: Adiabatic PFR
  - Case II: Constant T heating media; U = 110 J/m^2.s.K T_a = 1150 K
  - Case III: Variable temp heating medium
- Plot Conversion and temperature along the length of the reactor

Design/Analysis of the PFR used for vapor phase cracking of acetone

- Mol Balance for PFR: $\frac{dX}{dV} = -\frac{r_A}{F_{A0}}$ Rate law: $-r_A = k.C_A$
- Stoichiometry: $C_A = C_{A0}\frac{(1-X)}{(1+\varepsilon X)}\frac{T_0}{T}$ $\varepsilon = y_{A0}\delta = 1 * (1 + 1 - 1) = 1$
- Thus, $-r_A = k.C_A = k.C_{A0}\frac{(1-X)}{(1+X)}\frac{T_0}{T}$ and $\boxed{\frac{dX}{dV} = -\frac{k}{\dot{v}_0}\frac{(1-X)}{(1+X)}\frac{T_0}{T}}$ (A)
- Calculation of the inlet conditions:
  - $F_{A0} = \frac{7850\ kg/h}{58\ kg/kmol} * \frac{1}{1000\ Tubes} * \frac{1\ hr}{3600\ s} * \frac{1000\ mol}{1\ kmol} = 0.0376\ mol/s$
  - $C_{A0} = \frac{P_{A0}}{RT} = \frac{162\ kPa}{8.31 * 1035\ (kPa.m^3)/(kmol.K)} = 0.0188\frac{kmol}{m^3} = 18.8\ mol/m^3$
  - $\dot{v}_0 = \frac{F_{A0}}{C_{A0}} = 2.037\frac{dm^3}{s}$ $V = \frac{5\ m^3}{1000\ tubes} = 5\ dm^3$

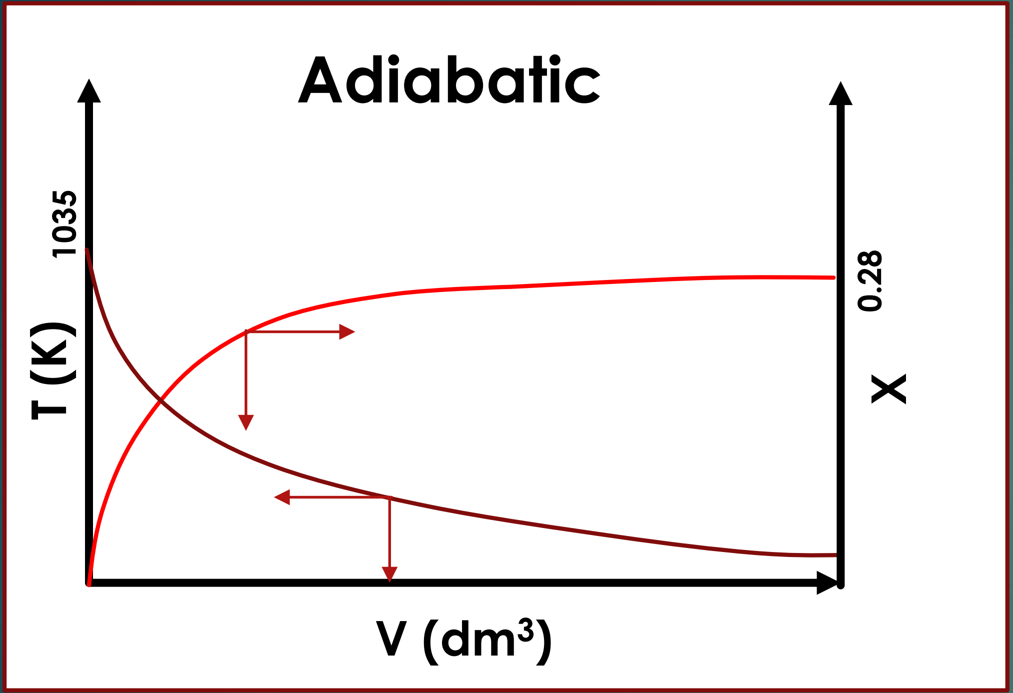
The vapor phase cracking of acetone … continued

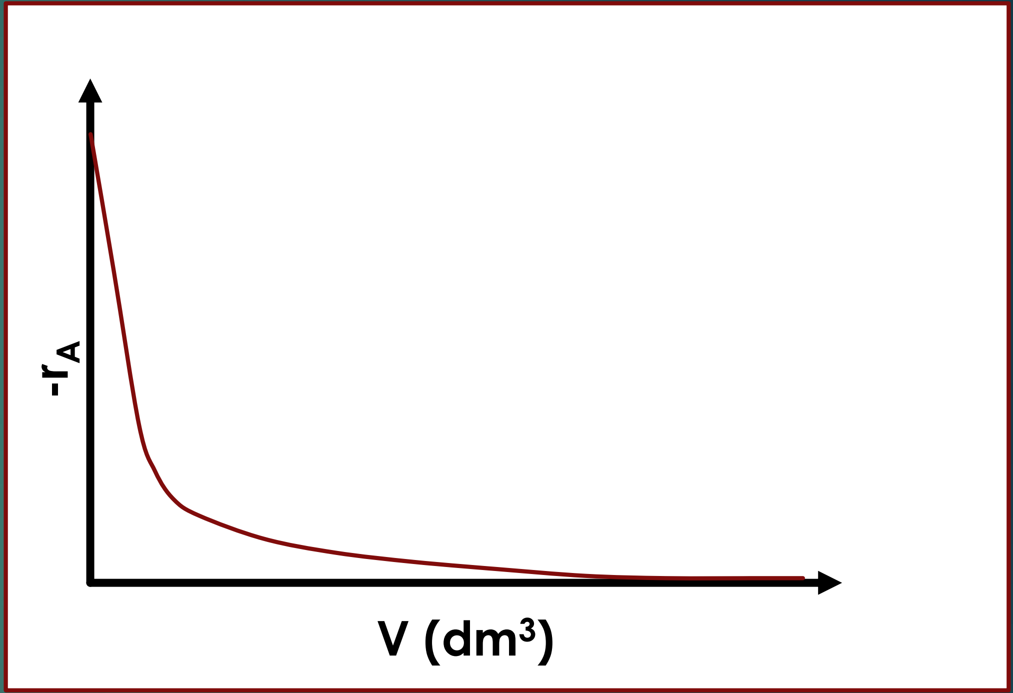
- Calculation of Energy Balance Parameters:
- Based on the standard heats of formation of species A, B and C
  - $\Delta h^0_{Rxn,T_R=298\,K} = -61.09 - 74.81 - (-216.67)\,\frac{\text{kJ}}{\text{mol}} = 80770\,\frac{\text{J}}{\text{mol}}$ (endothermic)
  - $\Delta C_p = C_{p,C} + C_{p,B} - C_{p,A} = 83 + 71 - 163 = -9\,\frac{J}{mol.K}$
  - $\sum(\theta_i C_{P,i}) = C_{p,A} = 163\,\frac{J}{mol.K}$ since pure A enters
- Case I (Adiabatic reactor):

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

- We have: $$\boxed{\frac{dT}{dV} = \frac{r_A\left[\Delta h^0_{Rxn,T_R} + \Delta C_p(T-T_R)\right]}{F_{A0}(C_{P,A} + X\Delta C_P)}}$$ (B) Solve (A) and (B)

Variation of conversion and temperature with volume determined by solving the 2 ODEs

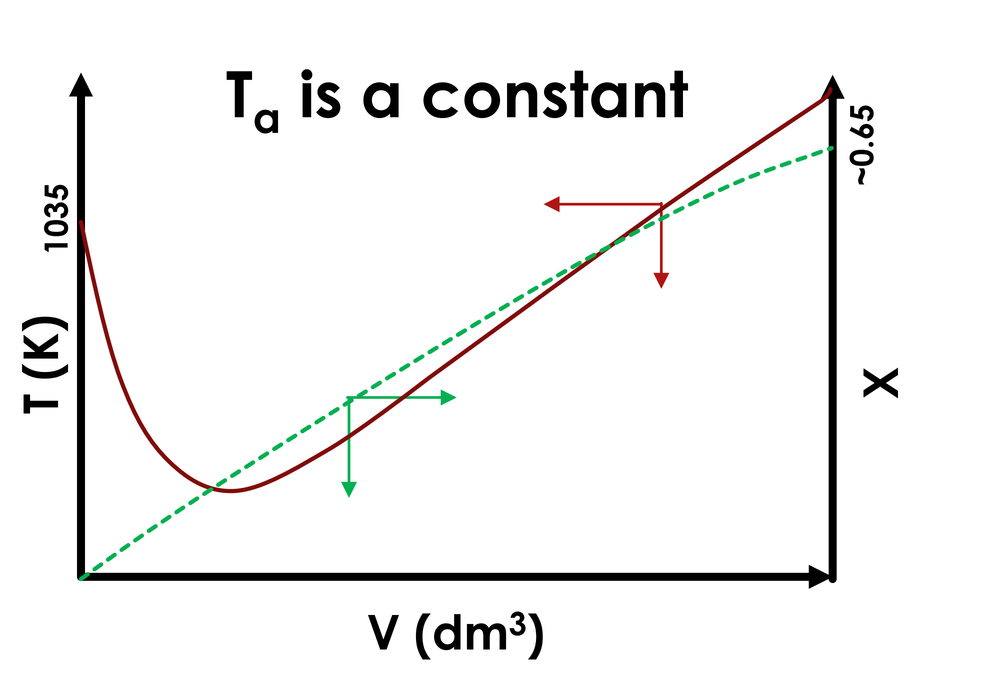


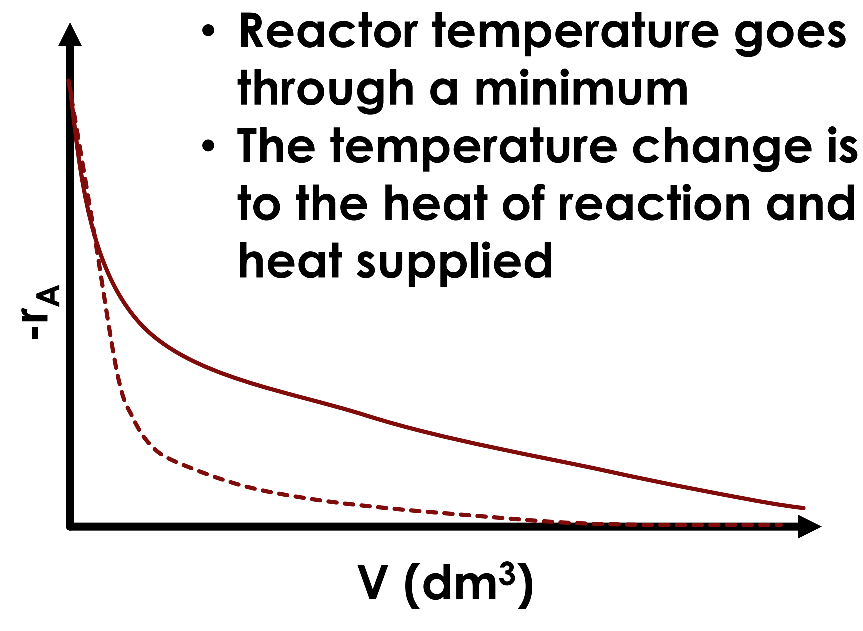


- As temperature drops due to endothermic reaction, the rate also drops rapidly
- Conversion may be increased if a hot diluent is added to provide the sensible heat
  - Not too much diluent since the concentration will also drop

Cracking of acetone in a PFR with a constant heating medium (Case II)

- Heat transfer parameters: $a = \frac{4}{D} = 150\ m^{-1}$; $U.a = 16500\ \frac{J}{m^3.s.K}$
- Energy balance equation: $\frac{dT}{dV} = \frac{r_A\left[\Delta h^0_{Rxn,T_R} + \Delta C_p(T - T_R)\right] + U.a.(T_a - T)}{F_{A0}(C_{P,A} + X\Delta C_P)}$ (C)
- For final volume = 1 dm^3 (compared to 5 dm^3) Solve ODEs (A) and (C)





- Reactor temperature goes through a minimum
- The temperature change is due to the heat of reaction and heat supplied

Cracking of acetone in a PFR with a variable heating medium (Case III)

- $$\frac{dX}{dV} = -\frac{k}{\dot{v}_0}\frac{(1-X)}{(1+X)}\frac{T_0}{T} \qquad \text{(A)}$$ $$\frac{dT}{dV} = \frac{r_A\left[\Delta h^0_{Rxn,T_R} + \Delta C_p(T-T_R)\right] + U.a.(T_a - T)}{F_{A0}(C_{P,A} + X\Delta C_P)} \qquad \text{(C)}$$
- $$\frac{dT_a}{dV} = \frac{U.a.(T-T_a)}{\dot{m}_c.C_{P,c}}$$ (co-current, air at 1250 K as heating medium) (D)