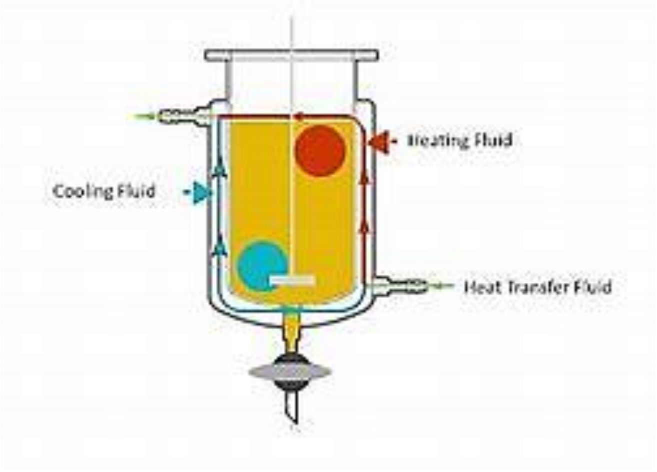
Reactor Design II



Week 7
Energy Balance in Reactors with Exchange

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Introduction

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- Chemical Reaction Engineering (CRE) examines the principles of energy transfer in reactors.

- This lecture focuses on reactors with heat exchange and user-friendly energy balance equations to optimize reactor design and operation.

Topics to be Addressed

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- - Fundamentals of Reactors with Heat Exchange
- - Energy Balance Derivations and Assumptions
- - Adiabatic Operation and Heat Exchange Systems
- - Reversible Reactions and Temperature Effects
- - Practical Examples and User-Friendly Equations

Objectives

- By the end of this lecture, students will be able to:

- - Understand energy balance principles for reactors with heat exchange.
- - Apply energy balance equations to adiabatic and heat exchange systems.
- - Analyze reversible reactions and their temperature dependencies.
- - Use user-friendly equations to simplify reactor design and operation.

Introduction

- Heat exchange in reactors is crucial for controlling reaction rates and ensuring efficiency.

- This session includes discussions on adiabatic and heat exchange systems, constant and variable temperature profiles, and reversible reaction analysis.

Last Lecture

Energy Balance Fundamentals

$$\sum F_{i0}E_{i0} - \sum F_iE_i + \dot{Q} - \dot{W} = \frac{dE_{sys}}{dt}$$

Substituting for $\dot{W}$

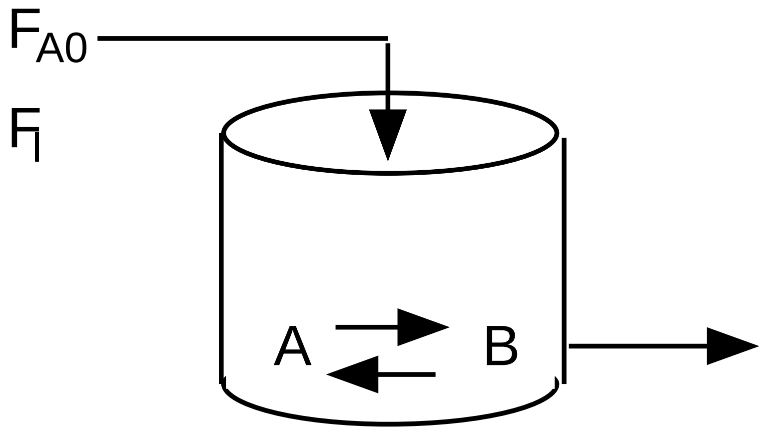
$$\sum F_{i0}\overbrace{\left[U_{i0} + P_0\tilde{V}_{i0}\right]}^{H_{i0}} - \sum F_i\overbrace{\left[U_i + P\tilde{V}_i\right]}^{H_i} + \dot{Q} - \dot{W}_S = \frac{dE_{sys}}{dt}$$

$$\boxed{\sum F_{i0}H_{i0} - \sum F_iH_i + \dot{Q} - \dot{W}_S = \frac{dE_{sys}}{dt}}$$

$$\dot{Q} - \dot{W}_S + \sum F_{i0}H_{i0} - \sum F_iH_i = 0$$

- Reactors with Heat Exchange
- User friendly Energy Balance Derivations
  - Adiabatic
  - Heat Exchange Constant T_a
  - Heat Exchange Variable T_a Co-current
  - Heat Exchange Variable T_a Counter Current

Adiabatic Operation CSTR



Elementary liquid phase reaction carried out in a CSTR

The feed consists of both - Inerts I and Species A with the ratio of inerts I to the species A being 2 to 1.

Adiabatic Operation CSTR

- Assuming the reaction is irreversible for CSTR, $A \rightarrow B$, ($K_C = 0$) what reactor volume is necessary to achieve 80% conversion?
- If the exiting temperature to the reactor is 360K, what is the corresponding reactor volume?
- Make a Levenspiel Plot and then determine the PFR reactor volume for 60% conversion and 95% conversion. Compare with the CSTR volumes at these conversions.
- Now assume the reaction is reversible, make a plot of the equilibrium conversion as a function of temperature between 290K and 400K.

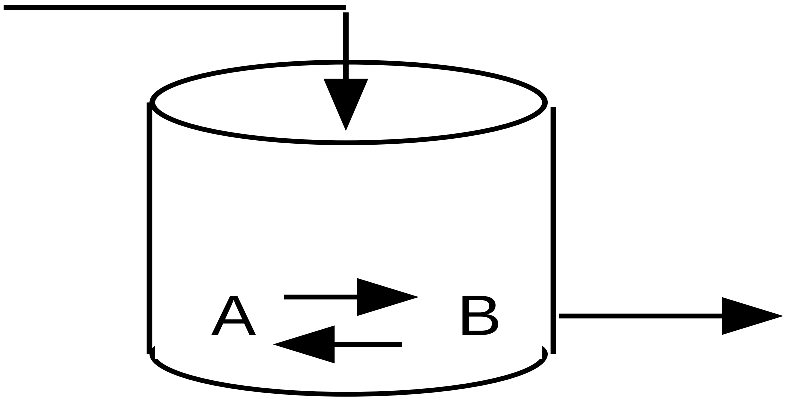
CSTR: Adiabatic Example

$$F_{A0} = 5\frac{mol}{min}$$

$$\Delta H_{Rxn} = -20000\frac{cal}{mol\ A}$$ (exothermic)

$$T_0 = 300\ K$$

$$F_I = 10\frac{mol}{min}$$



$$T = ?$$
$$X = ?$$

1) Mole Balances:

$$V = \frac{F_{A0}X}{-r_A\big|_{exit}}$$

CSTR: Adiabatic Example

2) Rate Laws:

$$-r_A = k\left[C_A - \frac{C_B}{K_C}\right]$$

$$k = k_1 e^{\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)}$$

$$K_C = K_{C1}\exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$$

3) Stoichiometry:

$$C_A = C_{A0}(1 - X)$$

$$C_B = C_{A0}X$$

CSTR: Adiabatic Example

4) Energy Balance

Adiabatic, $\Delta C_p=0$

$$T = T_0 + \frac{(-\Delta H_{Rx})X}{\sum \Theta_i C_{P_i}} = T_0 + \frac{(-\Delta H_{Rx})X}{C_{P_A} + \Theta_I C_{P_I}}$$

$$T = 300 + \left[\frac{-(-20{,}000)}{164+(2)(18)}\right]X = 300 + \frac{20{,}000}{164+36}X$$

$$\boxed{T = 300 + 100X}$$

CSTR: Adiabatic Example

Irreversible for Parts (a) through (c)

$$-r_A = kC_{A0}(1-X)\,(\text{i.e.,}\ K_C = \infty)$$

(a) Given X = 0.8, find T and V

$$\text{Given } X \xrightarrow{Calc} T \xrightarrow{Calc} k \xrightarrow{Calc} -r_A \xrightarrow{Calc} V$$

$$T \rightarrow Calc\ \ K_C \rightarrow -r_A$$

(if reversible)

CSTR: Adiabatic Example

Given X, Calculate T and V

$$V = \frac{F_{A0}X}{-r_A|_{exit}} = \frac{F_{A0}X}{kC_{A0}(1-X)}$$

$$T = 300 + 100(0.8) = 380\text{K}$$

$$k = 0.1\exp\frac{10{,}000}{1.989}\left[\frac{1}{298} - \frac{1}{380}\right] = 3.81$$

$$V = \frac{F_{A0}X}{-r_A} = \frac{(5)(0.8)}{(3.81)(2)(1-0.8)} = 2.82\,\text{dm}^3$$

CSTR: Adiabatic Example

Given T, Calculate X and V

(b) $\text{Given X} \xrightarrow{\text{Calc}} \text{T} \xrightarrow{\text{Calc}} \text{k} \xrightarrow{\text{Calc}} -\text{r}_\text{A} \xrightarrow{\text{Calc}} \text{V}$

$\text{T} \rightarrow \text{Calc K}_\text{C} \rightarrow -\text{r}_\text{A}$

(if reversible)

$$-r_A = kC_{A0}(1-X)\ \text{(Irreversible)}$$

$$T = 360K$$

$$X = \frac{T-300}{100} = 0.6$$

$$k = 1.83\,\text{min}^{-1}$$

$$V = \frac{(5)(0.6)}{(1.83)(2)(0.4)} = 2.05\,dm^3$$

CSTR: Adiabatic Example

(c) Levenspiel Plot

$$\frac{F_{A0}}{-r_A} = \frac{F_{A0}}{kC_{A0}(1-X)}$$

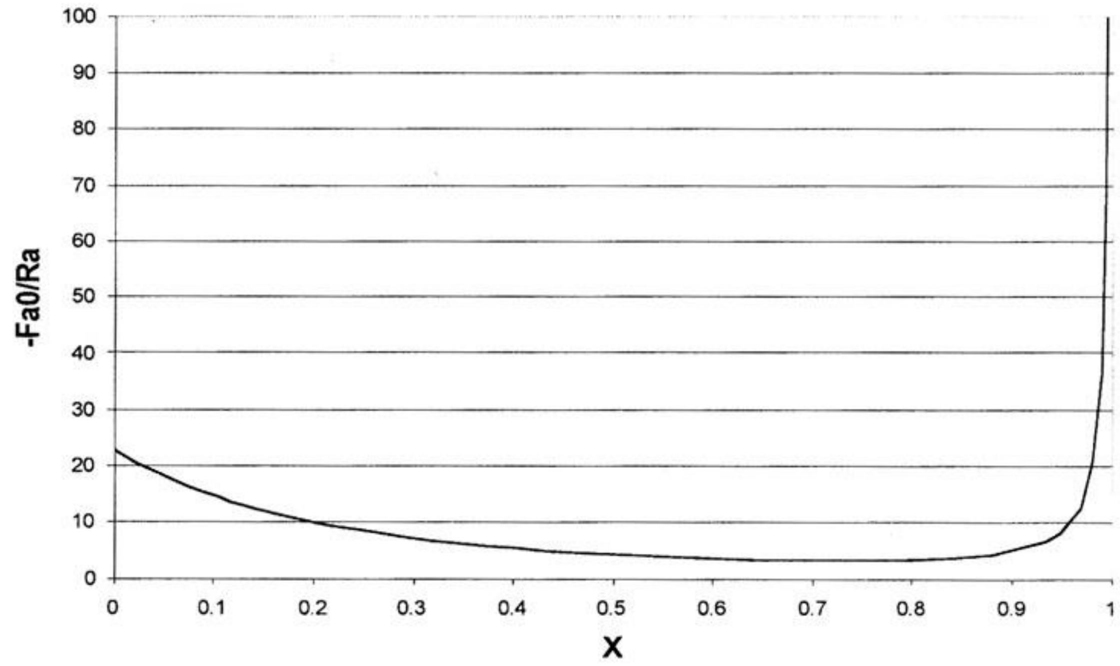
$$T = 300 + 100X$$

$$\text{Choose } X \xrightarrow{Calc} T \xrightarrow{Calc} k \xrightarrow{Calc} -r_A \xrightarrow{Calc} \frac{F_{A0}}{-r_A}$$

CSTR: Adiabatic Example

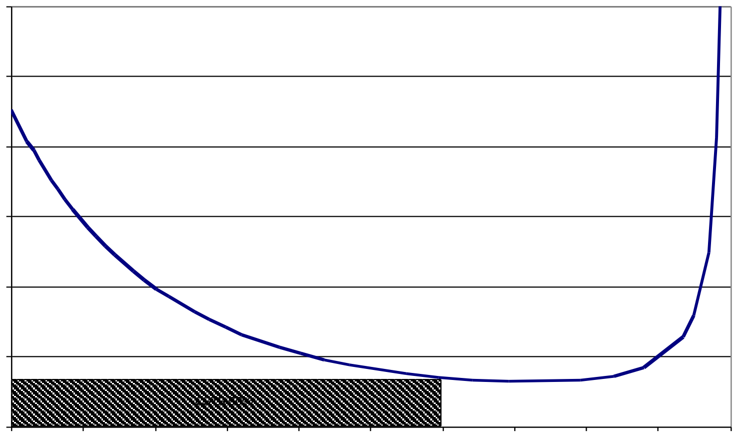
(c) Levenspiel Plot

X	T(K)	$\frac{F_{A0}}{-r_A}\left(dm^3\right)$
0	300	25
0.1	310	14.4
0.2	320	9.95
0.4	340	5.15
0.6	360	3.42
0.8	380	3.87
0.9	390	4.16
0.95	395	8.0

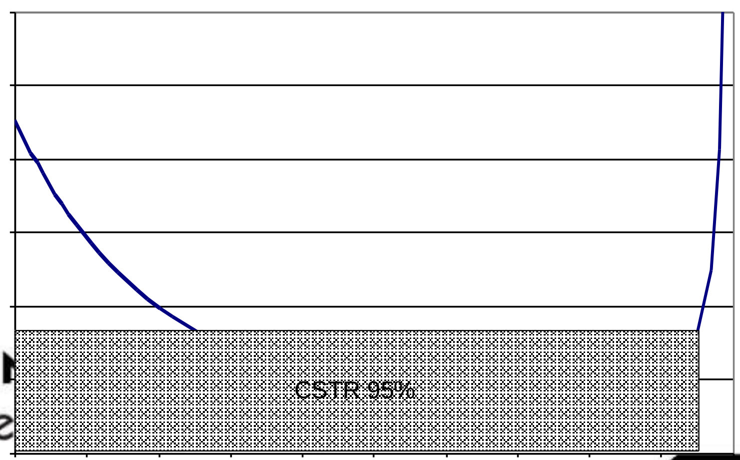


CSTR: Adiabatic Example

CSTR X = 0.6 T = 360 K

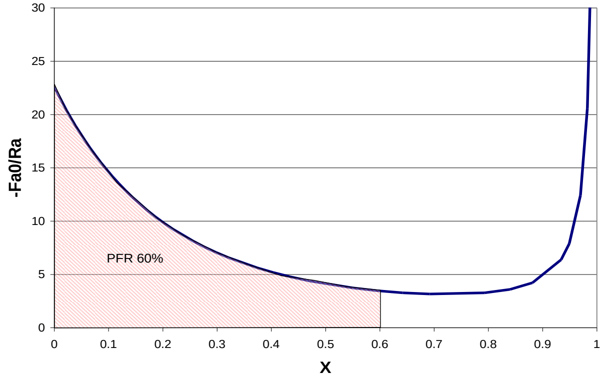


CSTR X = 0.95 T = 395 K

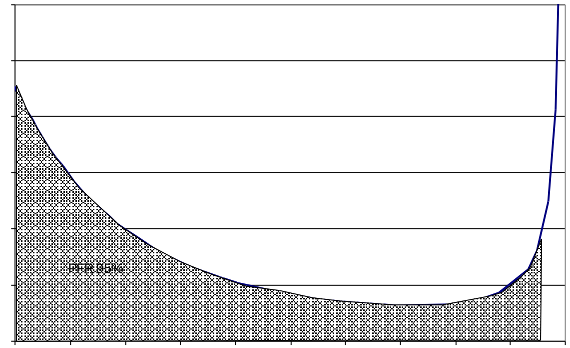


CSTR: Adiabatic Example

PFR X = 0.6



PFR X = 0.95



CSTR: Adiabatic Example - Summary

CSTR	X = 0.6	T = 360	V = 2.05 dm^3
PFR	X = 0.6	T_{exit} = 360	V = 5.28 dm^3
CSTR	X = 0.95	T = 395	V = 7.59 dm^3
PFR	X = 0.95	T_{exit} = 395	V = 6.62 dm^3

Energy Balance in terms of Enthalpy

$$\sum F_i H_i \Big|_V - \sum F_i H_i \Big|_{V+\Delta V} + Ua(T_a - T)\Delta V = 0$$

$$\frac{-d\sum F_i H_i}{dV} + Ua(T_a - T) = 0$$

$$\frac{-d\sum F_i H_i}{dV} = -\left[\sum F_i \frac{dH_i}{dV} + \sum H_i \frac{dF_i}{dV}\right]$$

PFR Heat Effects

$$\frac{dF_i}{dV} = r_i = \upsilon_i\left(-r_A\right)$$

$$H_i = H_i^0 + C_{Pi}\left(T - T_R\right)$$

$$\frac{dH_i}{dV} = C_{Pi}\frac{dT}{dV}$$

$$\frac{-d\sum F_i H_i}{dV} = -\left[\sum F_i C_{Pi}\frac{dT}{dV} + \sum H_i \upsilon_i\left(-r_A\right)\right]$$

$$\sum \upsilon_i H_i = \Delta H_{Rx}$$

PFR Heat Effects

$$-\left[\sum C_{Pi}F_i\frac{dT}{dV}+\Delta H_{Rx}(-r_A)\right]+Ua\left(T_a-T\right)=0$$

$$\sum F_iC_{Pi}\frac{dT}{dV}=\Delta H_{Rx}r_A-Ua\left(T-T_a\right)$$

$$\boxed{\frac{dT}{dV}=\frac{\left(\Delta H_{Rx}\right)\left(-r_A\right)-Ua\left(T-T_a\right)}{\sum F_iC_{Pi}}}$$

Need to determine T_a

Heat Exchange:

$$\frac{dT}{dV}=\frac{(-r_A)(-\Delta H_{Rx})-Ua(T-T_a)}{\sum F_i C_{P_i}}$$

$$\sum F_i C_{P_i}=F_{A0}\left[\sum \Theta_i C_{P_i}+\Delta C_P X\right], \text{ if } \Delta C_P=0 \text{ then}$$

$$\frac{dT}{dV}=\frac{(-r_A)(-\Delta H_{Rx})-Ua(T-T_a)}{F_{A0}\sum \Theta_i C_{P_i}}$$

Need to determine T_a

Heat Exchange Example: Case 1 - Adiabatic

Energy Balance:

Adiabatic (Ua=0) and ΔC_P=0

$$T = T_0 + \frac{\left(-\Delta H_{Rx}\right)X}{\sum \Theta_i C_{P_i}} \qquad (16A)$$

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A. Constant Ta e.g., Ta = 300K

B. Variable T_a Co-Current

$$\frac{dT_a}{dV}=\frac{Ua\left(T-T_a\right)}{\dot{m}C_{P_{cool}}},V=0 \quad T_a=T_{ao} \qquad (17C)$$

C. Variable T_a Counter Current

$$\frac{dT_a}{dV}=\frac{Ua\left(T_a-T\right)}{\dot{m}C_{P_{cool}}} \quad V=0 \quad T_a=?\ \text{Guess}$$

Guess T_a at V = 0 to match T_{a0} = T_{a0} at exit, i.e., V = V_f

Heat Exchanger Energy Balance

Variable T_a Co-current

Coolant Balance:

In - Out + Heat Added = 0

$$\dot{m}_C H_C\big|_V - \dot{m}_C H_C\big|_{V+\Delta V} + Ua\Delta V\left(T - T_a\right) = 0$$

$$-\dot{m}_C \frac{dH_C}{dV} + Ua\left(T - T_a\right) = 0$$

$$\mathrm{H_C = H_C^0 + C_{PC}\left(T_a - T_r\right)}$$

$$\frac{\mathrm{dH_C}}{\mathrm{dV}} = \mathrm{C_{PC}} \frac{\mathrm{dT_a}}{\mathrm{dV}}$$

$$\boxed{\frac{dT_a}{dV} = \frac{Ua\left(T - T_a\right)}{\dot{m}_C C_{PC}}, \; V = 0 \quad T_a = T_{a0}}$$

Heat Exchanger Energy Balance

Variable T_a Counter-current

In - Out + Heat Added = 0

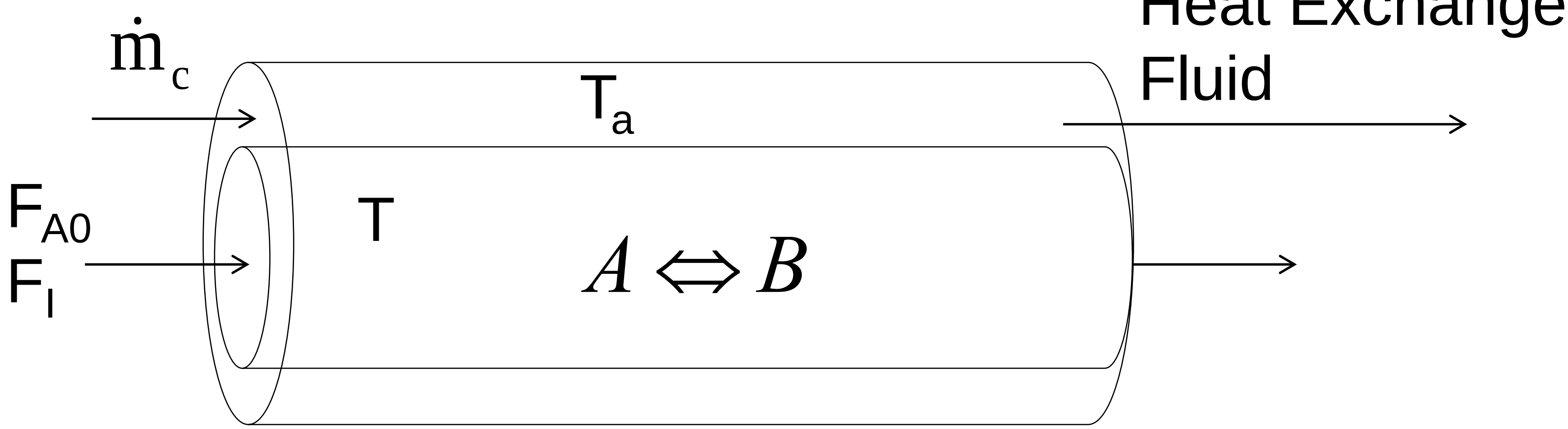
$$\dot{m}_C H_C\big|_{V+\Delta V} - \dot{m}_C H_C\big|_V + Ua\Delta V\left(T - T_a\right) = 0$$

$$\dot{m}_C \frac{dH_C}{dV} + Ua\left(T - T_a\right) = 0$$

$$\frac{dT_a}{dV} = \frac{Ua\left(T_a - T\right)}{\dot{m}_C C_{PC}}$$

Heat Exchanger – Example
Case 1 – Constant T_a

Elementary liquid phase reaction carried out in a PFR



The feed consists of both inerts I and species A with the ratio of inerts to the species A being 2 to 1.

Heat Exchanger – Example

Case 1 – Constant T_a

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1) Mole Balance:

$$(1)\quad \frac{dX}{dV} = -r_A / F_{A0}$$

2) Rate Laws:

$$(2)\quad r_A = -k\left[C_A - \frac{C_B}{K_C}\right]$$

$$(3)\quad k = k_1 \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

$$(4)\quad K_C = K_{C2} \exp\left[\frac{\Delta H_{Rx}}{R}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$$

Heat Exchanger – Example

Case 1 – Constant T_a

3) Stoichiometry: $C_A = C_{A0}(1-X) \quad (5)$

$$C_B = C_{A0}X \qquad (6)$$

4) Heat Effects:

$$\frac{dT}{dV} = \frac{(\Delta H_R)(-r_A) - Ua(T - T_a)}{F_{A0}\sum \theta_i C_{Pi}} \qquad (7)$$

$$(\Delta C_P = 0)$$

$$X_{eq} = \frac{k_C}{1+k_C} \qquad (8)$$

$$\sum \theta_i C_{Pi} = C_{PA} + \theta_I C_{PI} \qquad (9)$$

Heat Exchanger – Example
Case 1 – Constant T_a

Parameters:

$$\Delta H_R, \quad E, \quad R, \quad T_1, \quad T_2,$$

$$k_1, \quad k_{C2}, \quad Ua, \quad T_a, \quad F_{A0},$$

$$C_{A0}, \quad C_{PA}, \quad C_{PI}, \quad \theta_I,$$

$$rate = -r_A$$

PFR Heat Effects

Heat generated   Heat removed

$$\frac{dT}{dV} = \frac{Q_g - Q_r}{\sum F_i C_{Pi}}$$

$$\sum F_i C_{Pi} = \sum F_{A0}\left(q_i + u_i X\right) C_{Pi} = F_{A0}\left[\sum q_i C_{Pi} + DC_P X\right]$$

$$\boxed{\frac{dT}{dV} = \frac{(DH_R)(r_A) - Ua(T - T_a)}{F_{A0}\left[\sum q_i C_{Pi} + DC_P X\right]}}$$

Heat Exchanger – Example

Case 2 – Adiabatic

Mole Balance:

$$\frac{dX}{dV} = \frac{-r_A}{F_{A0}}$$

Energy Balance:

Adiabatic and $\Delta C_P = 0$

$Ua = 0$

$$T = T_0 + \frac{\left(-\Delta H_{Rx}\right)X}{\sum \Theta_i C_{P_i}} \qquad (16A)$$

Additional Parameters

(17A) & (17B)

$$T_0, \sum \Theta_i C_{P_i} = C_{P_A} + \Theta_I C_{P_I}$$

Adiabatic PFR

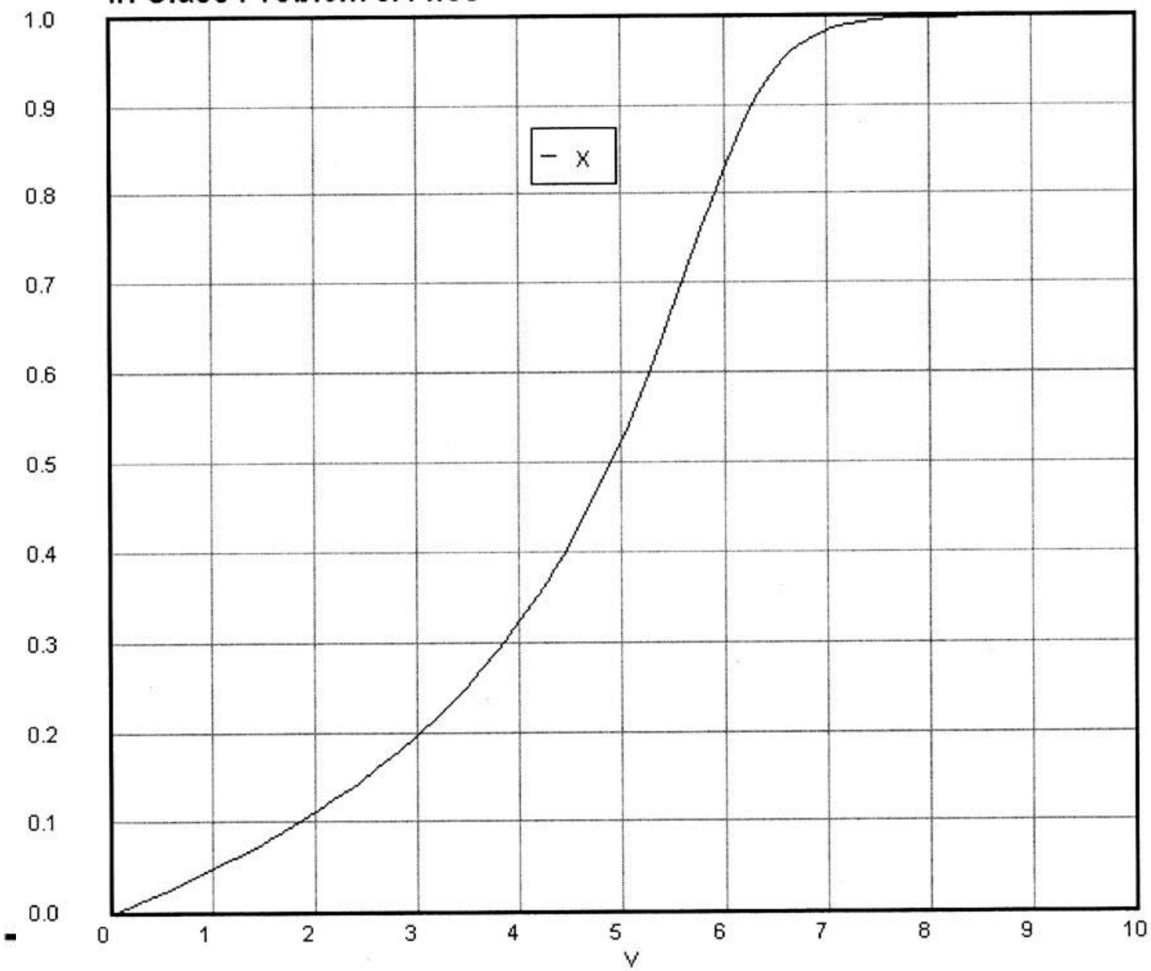
Differential equations

1 d(X)/d(V) = -ra/Fao

Explicit equations

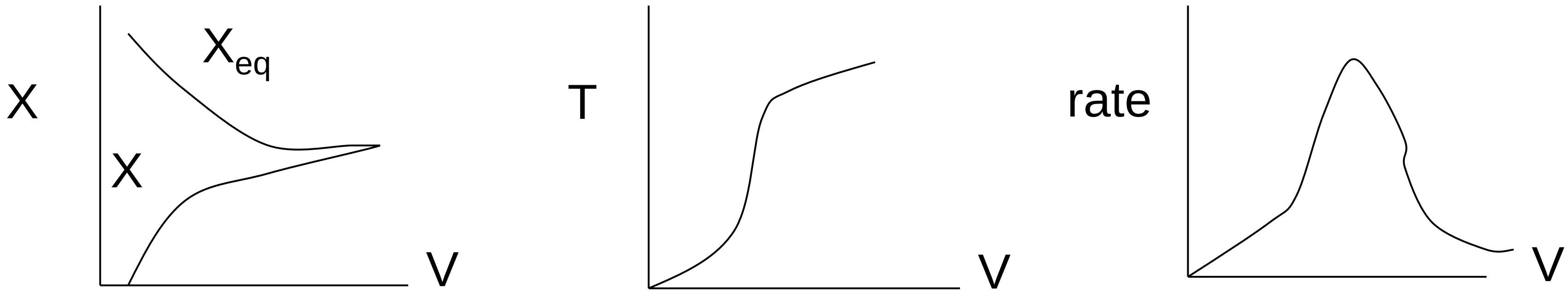
1 k1 = 0.1
2 Cao = 2
3 DH = -20000
4 To = 300
5 CpI = 18
6 Cpa = 164
7 ThetaI = 2
8 sumCp = Cpa+ThetaI*CpI
9 T = To+(-DH)*X/sumCp
10 Fao = 5
11 E = 10000
12 R = 1.987
13 T1 = 298
14 Ca = Cao*(1-X)
15 k = k1*exp(E/R*(1/T1-1/T))

In Class Problem 3/11/08



Example: Adiabatic

Find conversion, X_{eq} and T as a function of reactor volume



Heat Exchange

$$\frac{dT}{dV}=\frac{(-r_A)(-\Delta H_{Rx})-Ua(T-T_a)}{\sum F_i C_{P_i}}$$

$$\sum F_i C_{P_i}=F_{A0}\left[\sum \Theta_i C_{P_i}+\Delta C_P X\right], \text{ if } \Delta C_P=0 \text{ then}$$

$$\frac{dT}{dV}=\frac{(-r_A)(-\Delta H_{Rx})-Ua(T-T_a)}{F_{A0}\sum \Theta_i C_{P_i}} \qquad (16B)$$

Need to determine T_a

User Friendly Equations

A. Constant Ta (17B) Ta = 300K

Additional Parameters (18B – (20B):

$$T_a,\ \sum \Theta_i C_{P_i},\ Ua$$

B. Variable T_a Co-Current

$$\frac{dT_a}{dV} = \frac{Ua(T - T_a)}{\dot{m}C_{P_{cool}}} \qquad V = 0 \qquad T_a = T_{ao} \qquad (17C)$$

C. Variable T_a Countercurrent

$$\frac{dT_a}{dV} = \frac{Ua(T_a - T)}{\dot{m}C_{P_{cool}}} \qquad V = 0 \qquad T_a = ?$$

Guess T_a at V = 0 to match T_{a0} = T_{a0} at exit, i.e., V = V_f

Variable T_a Counter-current

Coolant balance:

In - Out + Heat Added = 0

$$\dot{m}_C H_C\big|_V - \dot{m}_C H_C\big|_{V+\Delta V} + Ua\Delta V\left(T - T_a\right) = 0$$

$$-\dot{m}_C \frac{dH_C}{dV} + Ua\left(T - T_a\right) = 0$$

$$\mathrm{H_C = H_C^0 + C_{PC}\left(T_a - T_r\right)}$$

$$\mathrm{\frac{dH_C}{dV} = C_{PC}\frac{dT_a}{dV}}$$

All equations can be used from before except T_a parameter, use differential T_a instead, adding m_C and C_{PC}

$$\frac{dT_a}{dV} = \frac{Ua\left(T - T_a\right)}{\dot{m}_C C_{PC}}, \quad V = 0 \quad T_a = T_{a0}$$

Heat Exchange Energy Balance

Variable T_a Co-current

In - Out + Heat Added = 0

$$\dot{m}_C H_C\big|_{V+\Delta V} - \dot{m}_C H_C\big|_V + Ua\Delta V\left(T - T_a\right) = 0$$

$$\dot{m}_C \frac{dH_C}{dV} + Ua\left(T - T_a\right) = 0$$

$$\boxed{\frac{dT_a}{dV} = \frac{Ua\left(T_a - T\right)}{\dot{m}_C C_{PC}}}$$

All equations can be used from before except dT_a/dV which must be changed to a negative. To arrive at the correct integration we must guess the T_a value at V=0, integrate and see if T_{a0} matches; if not, re-guess the value for T_a at V=0

Derive the user-friendly Energy Balance for a PBR

$$\int_0^W \frac{Ua}{\rho_B}(T_a - T)dW + \sum F_{i0}H_{i0} - \sum F_i H_i = 0$$

Differentiating with respect to W:

$$\frac{Ua}{\rho_B}(T_a - T) + 0 - \sum \frac{dF_i}{dW}H_i - \sum F_i \frac{dH_i}{dW} = 0$$

Derive the user-friendly Energy Balance for a PBR

Mole Balance on species i:

$$\frac{dF_i}{dW} = r_i' = \upsilon_i \left(-r_A' \right)$$

Enthalpy for species i:

$$H_i = H_i^o \left(T_R \right) + \int_{T_R}^{T} C_{Pi} dT$$

Derive the user-friendly Energy Balance for a PBR

Differentiating with respect to W:

$$\frac{dH_i}{dW} = 0 + C_{Pi}\frac{dT}{dW}$$

$$\frac{Ua}{\rho_B}\left(T_a - T\right) + r_A'\sum \upsilon_i H_i - \sum F_i C_{Pi}\frac{dT}{dW} = 0$$

Derive the user-friendly Energy Balance for a PBR

$$\frac{Ua}{\rho_B}(T_a - T) + r_A' \sum \upsilon_i H_i - \sum F_i C_{Pi} \frac{dT}{dW} = 0$$

$$\sum \upsilon_i H_i = \Delta H_R(T)$$

$$F_i = F_{A0}(\Theta_i + \upsilon_i X)$$

Final Form of the Differential Equations in Terms of Conversion:

A:

$$\frac{dT}{dW} = \frac{\frac{Ua}{\rho_B}(T_a - T) + r_A' \Delta H_R(T)}{F_{A0}\left[\sum \Theta_i \tilde{C}_{Pi} + \Delta \hat{C}_P X\right]} = f(X,T)$$

Derive the user-friendly Energy Balance for a PBR

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Final form of terms of Molar Flow Rate:

$$\frac{dT}{dW} = \frac{\frac{Ua}{\rho_B}\left(T_a - T\right) + r_A{}'\Delta H}{F_i C_{Pi}}$$

B:

$$\boxed{\frac{dX}{dW} = \frac{-r_A{}'}{F_{A0}} = g\left(X, T\right)}$$

Reversible Reactions

$$A + B \Leftrightarrow C + D$$

The rate law for this reaction will follow an elementary **rate law**.

$$-r_A = k\left(C_A C_B - \frac{C_C C_D}{K_C}\right)$$

Where K_e is the concentration equilibrium constant. We know from Le Chaltlier's law that if the reaction is exothermic, K_e will decrease as the temperature is increased and the reaction will be shifted back to the left. If the reaction is endothermic and the temperature is increased, K_e will increase and the reaction will shift to the right.

Reversible Reactions

$$K_C = \frac{K_P}{(RT)^{\delta}}$$

Van’t Hoff Equation:

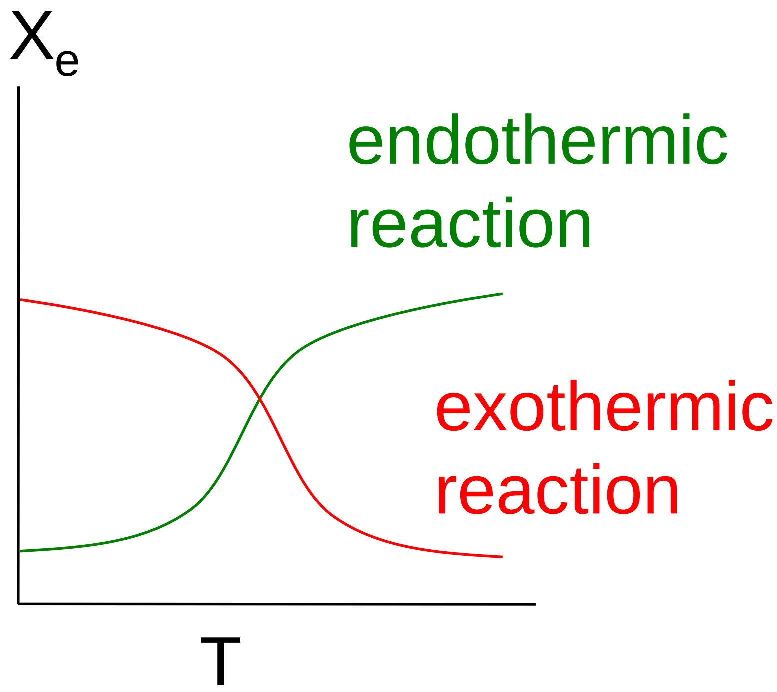
$$\frac{d\ln K_P}{dT} = \frac{\Delta H_R(T)}{RT^2} = \frac{\Delta H_R{}^{o}(T_R) + \Delta\hat{C}_P(T - T_R)}{RT^2}$$

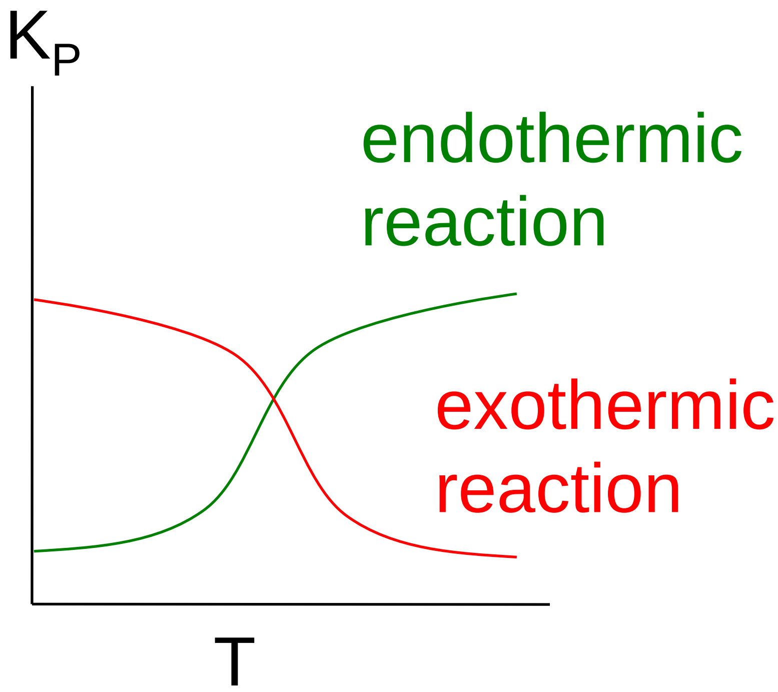
For the special case of $\Delta C_P = 0$

Integrating the Van’t Hoff Equation gives:

$$K_P(T_2) = K_P(T_1)\exp\left[\frac{\Delta H^{o}{}_R(T_R)}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

Reversible Reactions





Are you ready?

Summary

- In this lecture, we covered:

- - Energy balance fundamentals for reactors with heat exchange.
- - Adiabatic and heat exchange reactor design principles.
- - Analysis of reversible reactions and temperature effects.
- - Practical application of user-friendly equations.

- Heat exchange considerations are vital for optimizing reactor performance and efficiency.