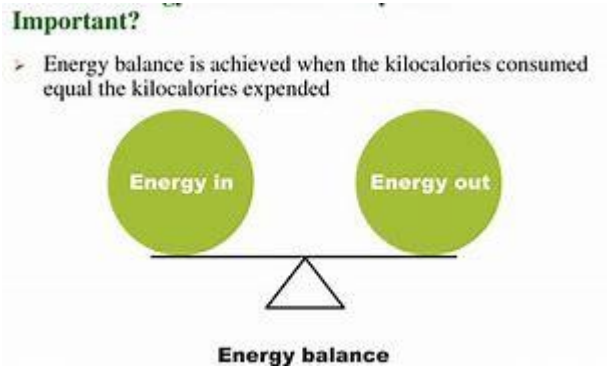
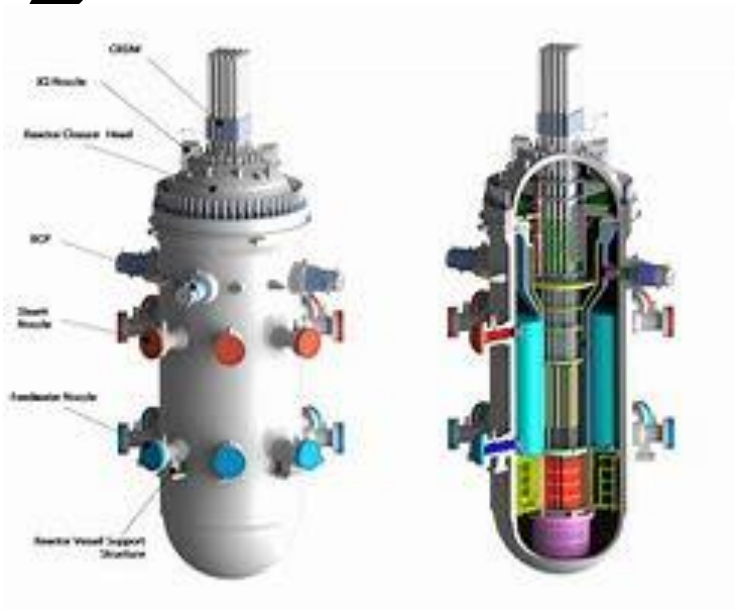
Reactor Design II





Week 6

Energy Balance in Reactors

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Introduction

- Chemical Reaction Engineering (CRE) involves understanding the energy balance in reactor systems.

- This lecture focuses on energy balance fundamentals, adiabatic reactors, and the equations necessary to analyze energy transfer in chemical processes.

Topics to be Addressed

- - Fundamentals of Energy Balance
- - Energy Balance Equations and Assumptions
- - Adiabatic Reactor Design and Analysis
- - Introduction to Heat Effects in Reactors
- - Case Studies and Practical Applications

Objectives

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

- - Understand the principles of energy balance in chemical reactors.
- - Apply energy balance equations to different reactor configurations.
- - Analyze adiabatic reactor performance.
- - Relate heat effects to reactor design and operation.

Introduction

- Energy balance analysis is critical for designing efficient reactors and optimizing their performance.

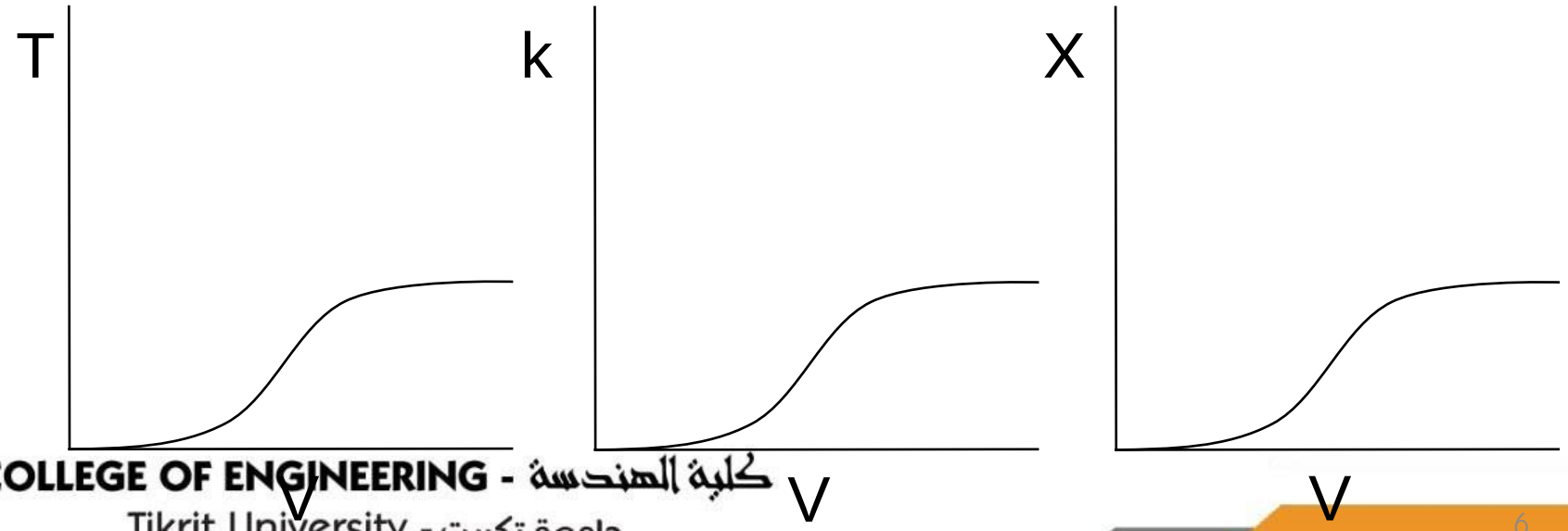
- This session covers theoretical frameworks and practical applications, including the design of adiabatic reactors and the use of user-friendly equations.

Today's Lecture

Energy Balance, Rationale and Overview

Let's calculate the volume necessary to achieve a conversion, X, in a PFR for a first-order, exothermic and adiabatic reaction.

The temperature profile might look something like this:



Energy Balance, Rationale and Overview

Mole Balance:

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

Rate Law:

$$r_A = -k_i \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right] C_A$$

Stoichiometry:

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

Combine:

$$\frac{dX}{dV} = \frac{k_i \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]}{F_{A0}} C_{A0}(1 - X)$$

Energy Balance, Rationale and Overview

$$\frac{dX}{dV} = \frac{k_i \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]}{F_{A0}} C_{A0}(1 - X)$$

We cannot solve this equation because we don't have X either as a function of V or T.

We need another equation. That equation is:

The Energy Balance

User Friendly Equations Relate T and X or F_i

1. Adiabatic CSTR, PFR, Batch or PBR

$$\dot{W}_S = 0 \qquad \Delta\hat{C}_P = 0$$

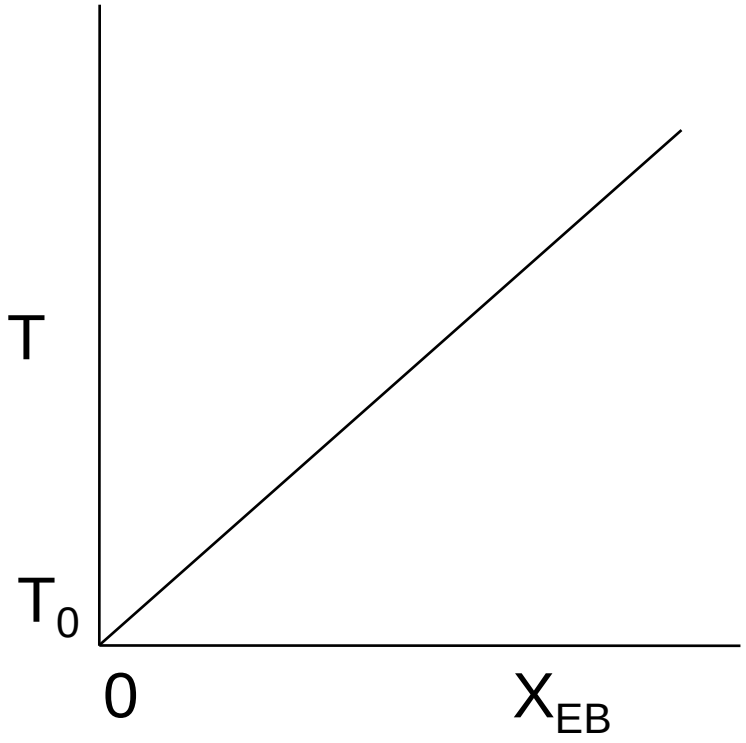
$$X_{EB} = \frac{\sum \Theta_i C_{P_i} \left(T - T_0\right)}{-\Delta H^o_{Rx}}$$

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

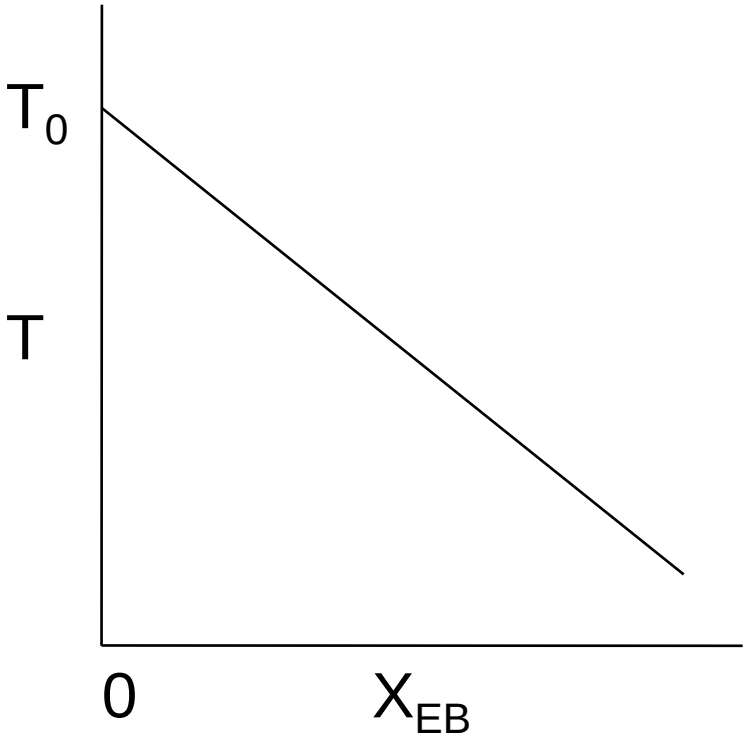
$$T = T_0 + \frac{\left(-\Delta H^o_{Rx}\right) X_{EB}}{\sum \Theta_i C_{P_i}}$$

Adiabatic

Exothermic



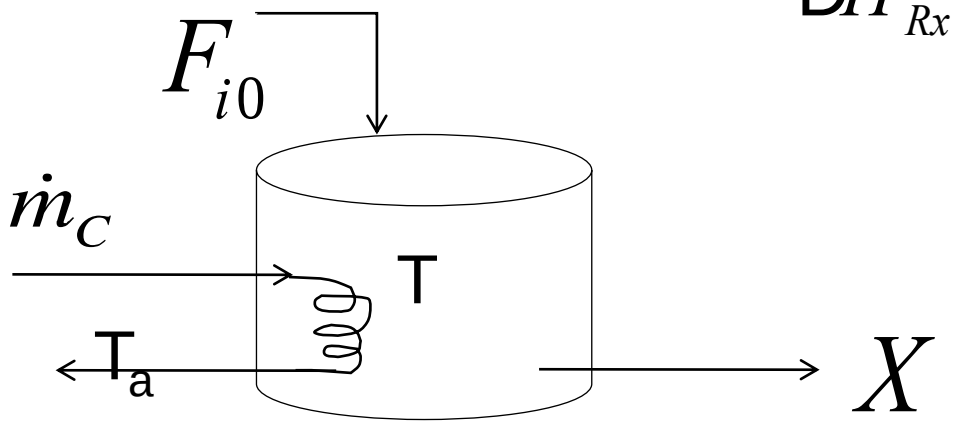
Endothermic



and X or F_i

2. CSTR with heat exchange: $UA(T_a-T)$ and a large coolant flow rate

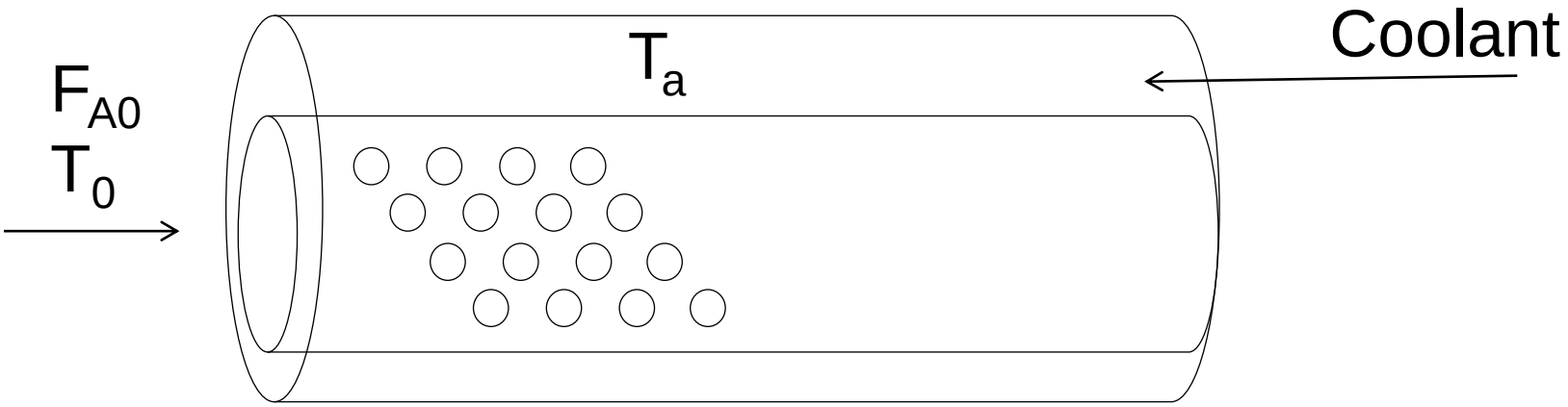
$$X_{EB} = \frac{\left(\frac{UA}{F_{A0}}(T - T_a)\right) + \sum Q_i C_{P_i}(T - T_0)}{-\Delta H^o_{Rx}}$$



User Friendly Equations Relate T

and X or F_i

3. PFR/PBR with heat exchange



3A. PFR in terms of conversion

$$\frac{dT}{dV} = \frac{\overbrace{r_A \Delta H_{Rx}(T)}^{Q_g} - \overbrace{Ua(T - T_a)}^{Q_r}}{F_{A0}\left(\sum \Theta_i C_{Pi} + \Delta C_p X\right)} = \frac{Q_g - Q_r}{F_{A0}\left(\sum \Theta_i C_{Pi} + \Delta C_p X\right)}$$

and X or F_i

3B. PBR in terms of conversion

$$\frac{dT}{dW} = \frac{r_A' \Delta H_{Rx}(T) - \frac{Ua}{\rho_b}(T - T_a)}{F_{A0}\left(\sum \Theta_i C_{Pi} + \Delta C_p X\right)}$$

3C. PBR in terms of molar flow rates

$$\frac{dT}{dW} = \frac{r_A' \Delta H_{Rx}(T) - \frac{Ua}{\rho_b}(T - T_a)}{\sum F_i C_{Pi}}$$

and X or F_i

3D. PFR in terms of molar flow rates

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

4. Batch

$$\frac{dT}{dt} = \frac{(r_A V)(\Delta H_{Rx}) - UA(T - T_a)}{\sum N_i C_{P_i}}$$

User Friendly Equations Relate T

and X or F_i

5. For Semibatch or unsteady CSTR

$$\frac{dT}{dt} = \frac{\dot{Q} - \dot{W}_S - \sum_{i=1}^{n} F_{i0}\left(C_{P_i}\left(T - T_{i0}\right) + \left[-\Delta H_{Rx}\left(T\right)\right]\left(-r_A V\right)\right)}{\sum_{i=1}^{n} N_i C_{P_i}}$$

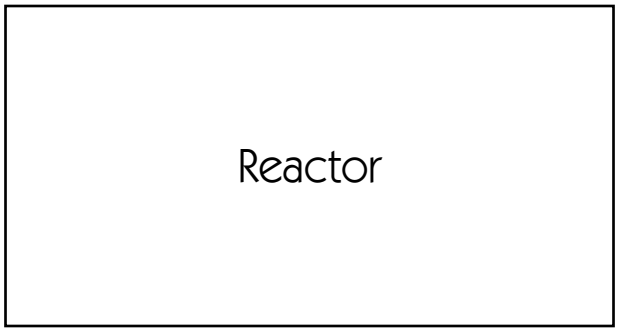
6. For multiple reactions in a PFR (q reactions and m species)

$$\frac{dT}{dV} = \frac{\sum_{i=1}^{q} r_{ij}\Delta H_{Rx_{ij}} - Ua\left(T - T_a\right)}{\sum_{j=1}^{m} F_i C_{Pj}}$$

Let's look where these User Friendly Equations came from.

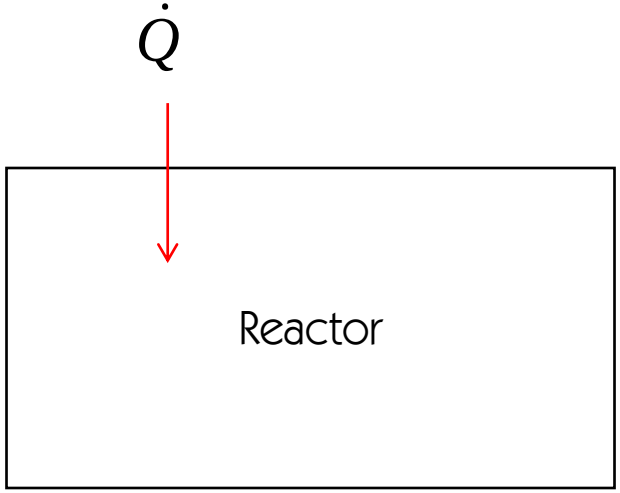
Energy Balance

Reactor with no Spatial Variations



Energy Balance

Reactor with no Spatial Variations



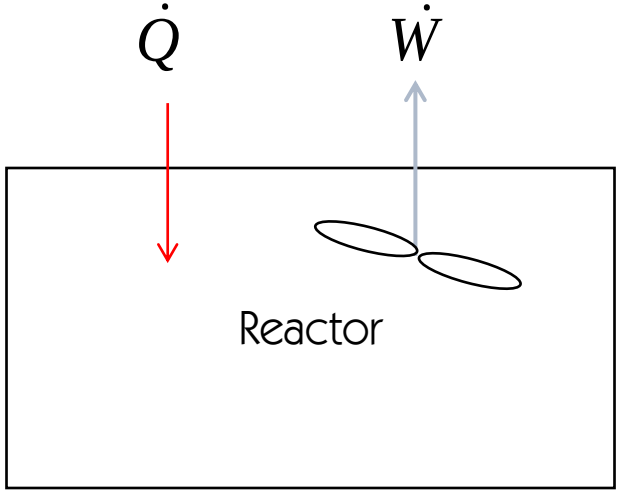
Rate of flow of heat ***to*** the system ***from*** the surroundings

$\dot{Q}$

(J/s)

Energy Balance

Reactor with no Spatial Variations



Rate of flow of heat ***to*** the system ***from*** the surroundings

$\dot{Q}$ (J/s)

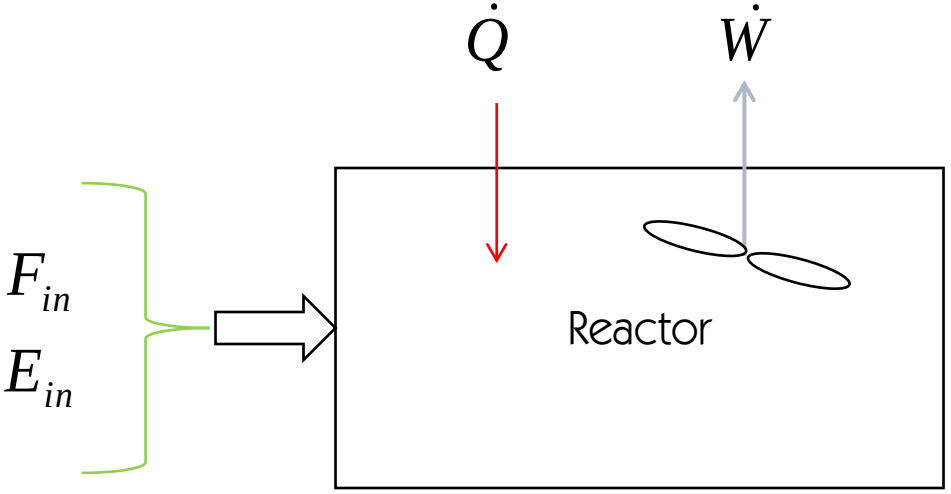
-

Rate of work ***done by*** the system ***on*** the surroundings

$\dot{W}$ (J/s)

Energy Balance

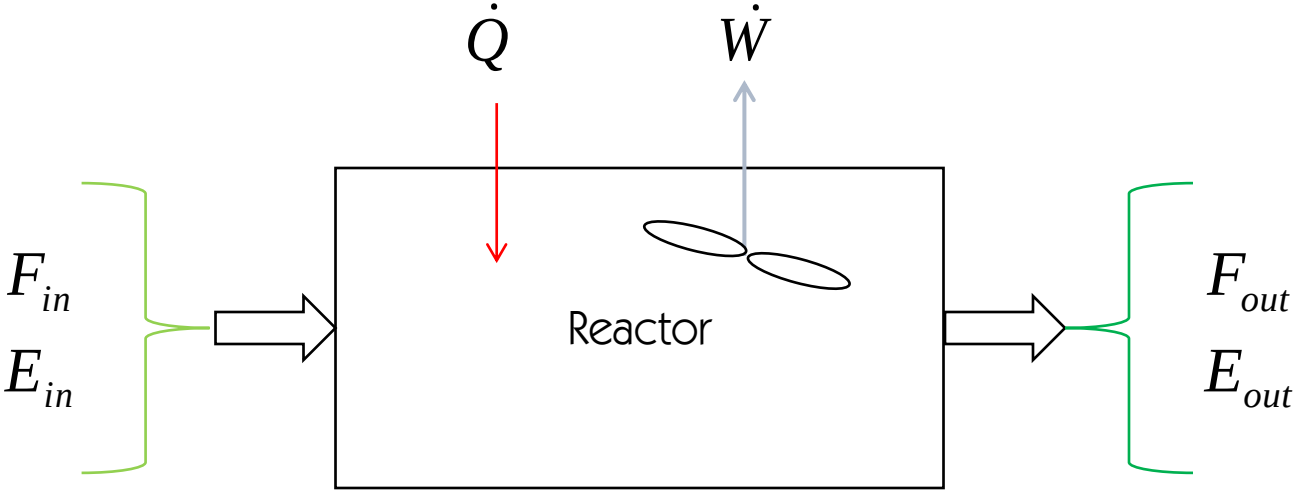
Reactor with no Spatial Variations



Rate of flow of heat ***to*** the system ***from*** the surroundings	-	Rate of work ***done by*** the system ***on*** the surroundings	+	Rate of energy added to the system by mass flow ***into*** the system
$\dot{Q}$	-	$\dot{W}$	+	$F_{in}E_{in}$
(J/s)		(J/s)		(J/s)

Energy Balance

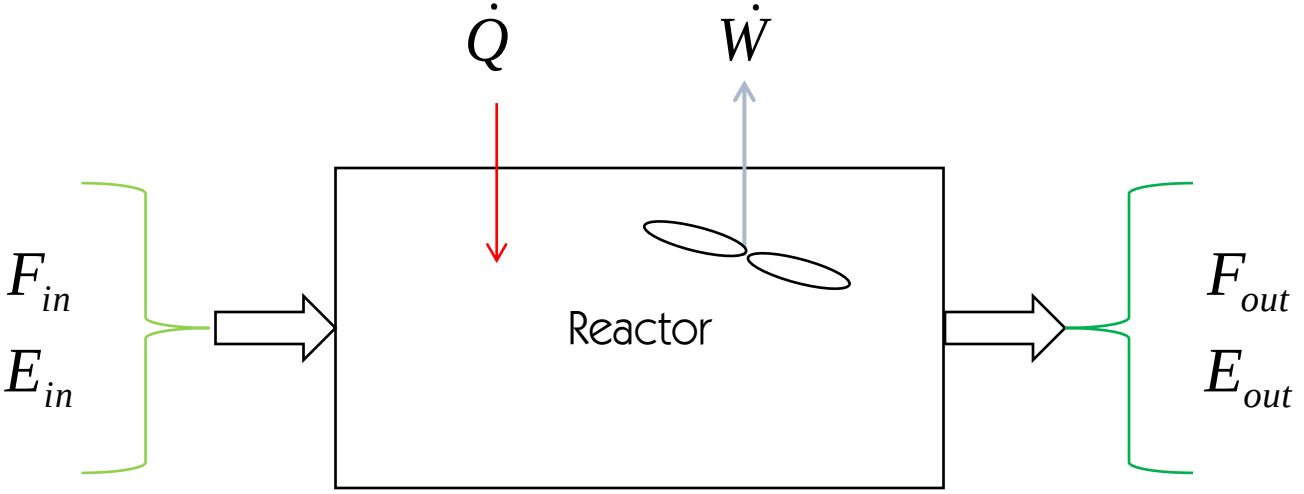
Reactor with no Spatial Variations



Rate of flow of heat ***to*** the system ***from*** the surroundings	-	Rate of work ***done by*** the system ***on*** the surroundings	+	Rate of energy added to the system by mass flow ***into*** the system	-	Rate of energy leaving system by mass flow ***out*** of the system
$\dot{Q}$	-	$\dot{W}$	+	$F_{in}E_{in}$	-	$F_{out}E_{out}$
(J/s)		(J/s)		(J/s)		(J/s)

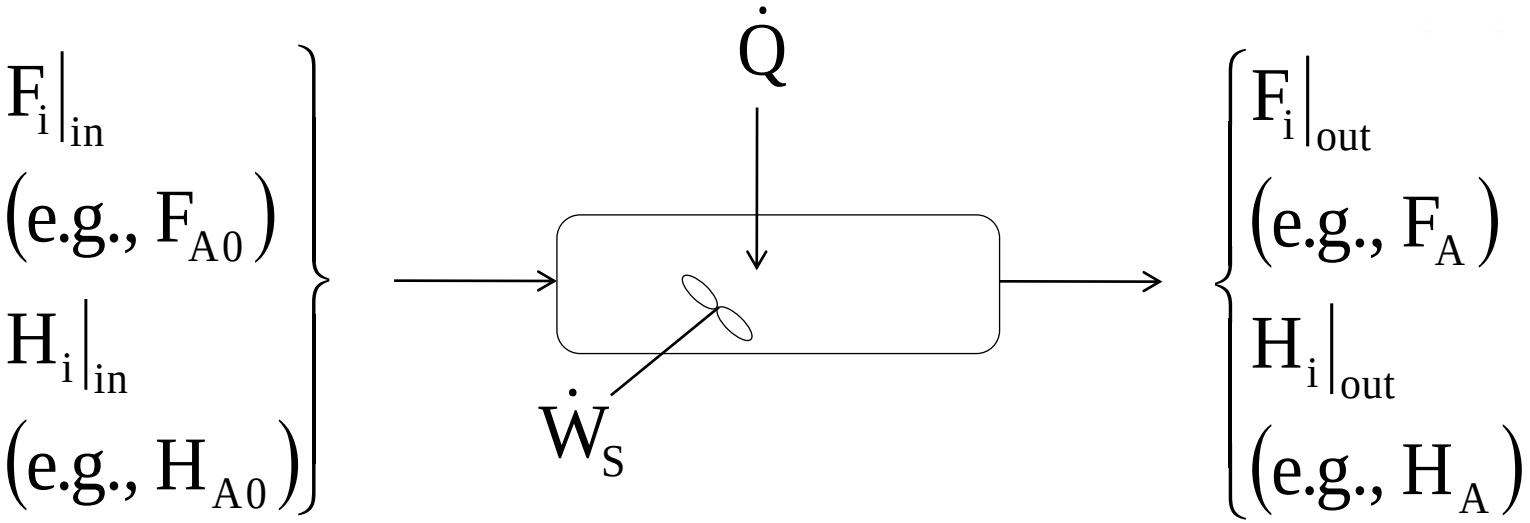
Energy Balance

Reactor with no Spatial Variations



Rate of accumulation of energy ***within*** the system	=	Rate of flow of heat ***to*** the system ***from*** the surroundings	-	Rate of work ***done by*** the system ***on*** the surroundings	+	Rate of energy added to the system by mass flow ***into*** the system	-	Rate of energy leaving system by mass flow ***out*** of the system
$\frac{d\hat{E}_{sys}}{dt}$ (J/s)	=	$\dot{Q}$ (J/s)	-	$\dot{W}$ (J/s)	+	$F_{in}E_{in}$ (J/s)	-	$F_{out}E_{out}$ (J/s)

Energy Balance



Energy Balance on an open system: schematic.

$$\dot{Q} - \dot{W}_S + \sum F_{i0} E_{i0}\Big|_{in} - \sum F_i E_i\Big|_{out} = \frac{dE_{system}}{dt} \quad (1)$$

OK folks, here is what we are going to do to put the above equation into a usable form.

1. *Replace Ui by Ui=Hi-PVi*
2. Express H_i in terms of heat capacities
3. Express Fi in terms of either conversion or rates of reaction
4. Define ΔH_{Rx}
5. Define ΔC_P
6. Manipulate so that the overall energy balance is in terms of the User Friendly Equations.

Intro to Heat Effects

Assumptions:

$$E_i = U_i + \cancel{PE_i}^{=0} + \cancel{KE_i}^{=0}$$ Other energies small compared to internal

$$\dot{W} = \text{flow work} + \text{shaft work}$$

$$\text{flow work} = -\sum F_{i0} P_0 \tilde{V}_{i0} + \sum F_i P \tilde{V}_i \qquad \left(\tilde{V} = \frac{m^3}{mol} \right)$$

Recall:

$$H_i = U_i + P\tilde{V}_i$$

Intro to Heat Effects

Substituting for $\dot{W}$

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

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

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

Steady State: $\dot{Q} - \dot{W}_S + \sum F_{i0}H_{i0} - \sum F_i H_i = 0$

Intro to Heat Effects

General Energy Balance :

$$\dot{Q} - \dot{W}_S + \sum F_{i0} H_{i0} - \sum F_i H_i = \frac{dE_{system}}{dt}$$

For Steady State Operation:

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

Intro to Heat Effects

$$\sum F_{i0} H_{i0} = F_{A0} \sum \Theta_i H_{i0}$$

$$\sum F_i H_i = F_{A0} \sum \left(\Theta_i + \upsilon_i X \right) H_i = F_{A0} \sum \Theta_i H_i + F_{A0} X \overbrace{\sum \upsilon_i H_i}^{\Delta H_{Rx}}$$

$$\dot{Q} - \dot{W}_S + F_{A0} \left(\sum \Theta_i \left(H_{i0} - H_i \right) + F_{A0} X \Delta H_{Rx} \right) = 0$$

Intro to Heat Effects

For No Phase Changes

$$H_i(T) = H_i^0(T_R) + \int_{T_R}^{T} C_{Pi}\,dT$$

→ Enthalpy of formation at temperature T_R

Constant Heat Capacities

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

$$H_{i0} - H_i = C_{Pi}(T - T_0)$$

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

Heat of reaction at temperature T

Intro to Heat Effects

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

$$\mathrm{D}H_R\left(T\right) = \mathrm{D}H_R^o\left(T_R\right) + \mathrm{D}\hat{C}_P\left(T - T_R\right)$$

$$\sum \upsilon_i \hat{C}_{Pi} = \Delta\hat{C}_P = \frac{d}{a}\hat{C}_{PD} + \frac{c}{a}\hat{C}_{PC} - \frac{b}{a}\hat{C}_{PB} - \hat{C}_{PA}$$

Substituting back into the Energy Balance

$$\dot{Q} - \dot{W}_S - F_{A0}X\left[\Delta H_R^o\left(T_R\right) + \Delta\hat{C}_P\left(T - T_R\right)\right] - F_{A0}\sum \Theta_i \tilde{C}_{Pi}\left(T - T_{i0}\right) = 0$$

Adiabatic (Q=0) and no Work $(\dot{W}_S = 0)$

Intro to Heat Effects

$$\Delta H_{Rx} = \frac{d}{a} H_D + \frac{c}{a} H_C - \frac{b}{a} H_B - H_A$$

$$\Delta C_P = \frac{d}{a} C_{PD} + \frac{c}{a} C_{PC} - \frac{b}{a} C_{PB} - C_{PA}$$

Intro to Heat Effects

$$\dot{Q} - \dot{W}_S + F_{A0}\left(\sum \Theta_i \left(H_{i0} - H_i\right) + F_{A0} X \Delta H_{Rx}\right) = 0$$

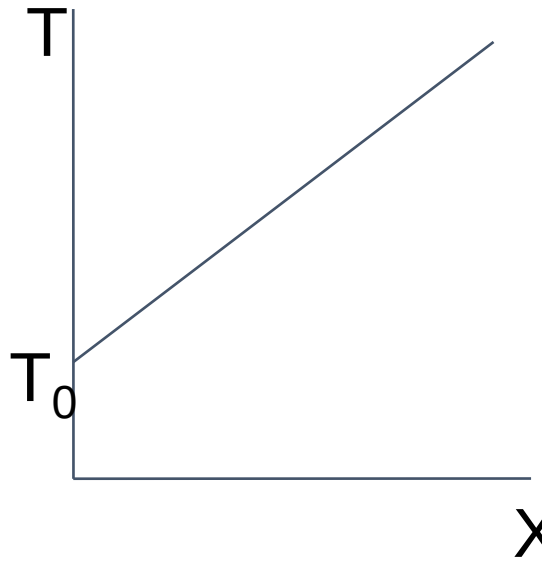
Substituting back into the Energy Balance

$$\dot{Q} - \dot{W}_S - F_{A0} X \left[\Delta H_R^o \left(T_R\right) + \Delta \hat{C}_P \left(T - T_R\right)\right] - F_{A0} \sum \Theta_i \tilde{C}_{Pi} \left(T - T_{i0}\right) = 0$$

Adiabatic Energy Balance

Adiabatic (Q=0) and no Work $(\dot{W}_S = 0)$

$$T = T_0 - \frac{X\left[\Delta H_R^o(T_R) + \Delta \hat{C}_P(T - T_R)\right]}{\sum \Theta_i \tilde{C}_{Pi} + X\Delta \hat{C}_P} = T_0 - \frac{X\left[\Delta H_R(T)\right]}{\sum \Theta_i \tilde{C}_{Pi} + X\Delta \hat{C}_P}$$



Exothermic

Example: Adiabatic PFR

$A \leftrightarrow B$

1) Mole Balance: $$\frac{dX}{dV} = -\frac{r_A}{F_{A0}}$$

2) Rate Laws: $$r_A = -k\left[C_A - \frac{C_B}{k_C}\right] \qquad k = k_1 \exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T}\right)\right]$$

$$\Delta C_P = 0 \qquad k_C = k_{C2} \exp\left[\frac{\Delta H_X^0}{k}\left(\frac{1}{T_2} - \frac{1}{T}\right)\right]$$

Example: Adiabatic PFR

$A \leftrightarrow B$

3) Stoichiometry:

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

$$C_B = C_{A0}X$$

4) Energy Balance

$$T = T_0 + \frac{-\Delta H_X^0 X}{\sum \theta_i C_{Pi}}$$

First need to calculate the maximum conversion which is at the *adiabatic equilibrium conversion*.

Example: Adiabatic PFR

Differential equations

1 d(T)/d(t) = 1

Explicit equations

1 Kc1 = 1000

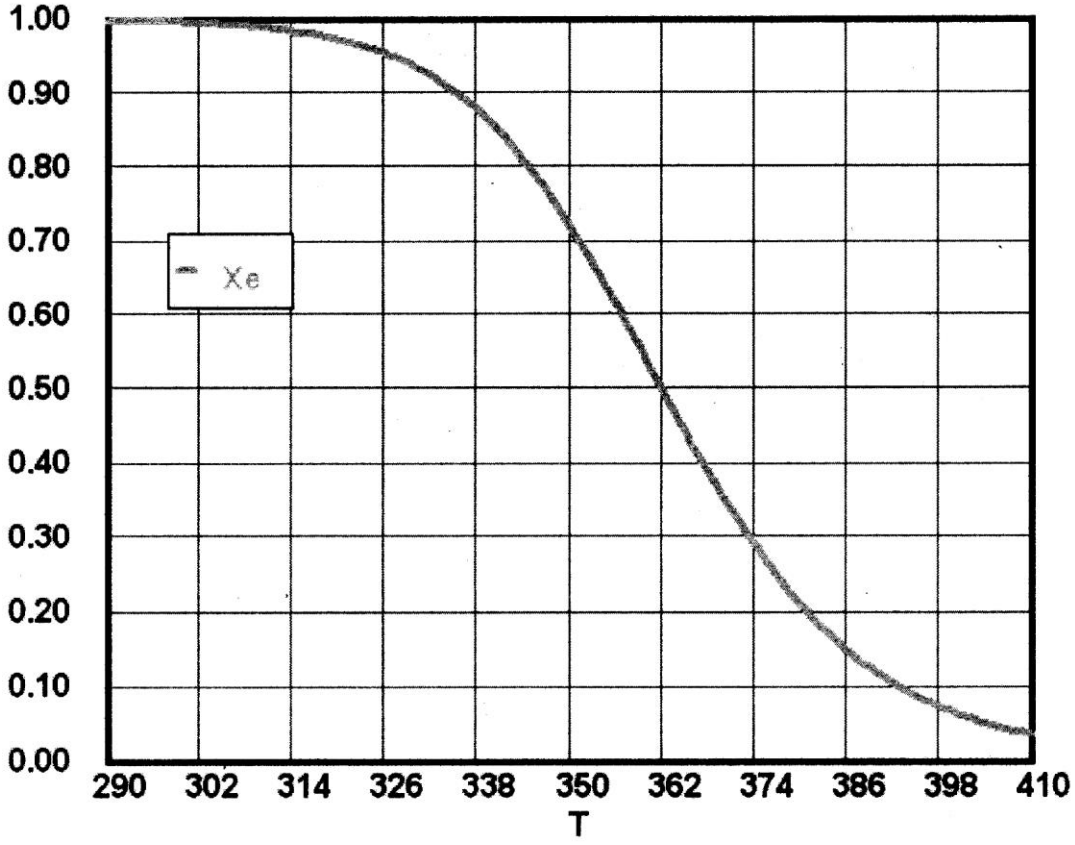
2 T1 = 290

3 R = 1.987

4 DeltaH = -20000

5 Kc = Kc1*exp((DeltaH/R)*(1/T1-1/T))

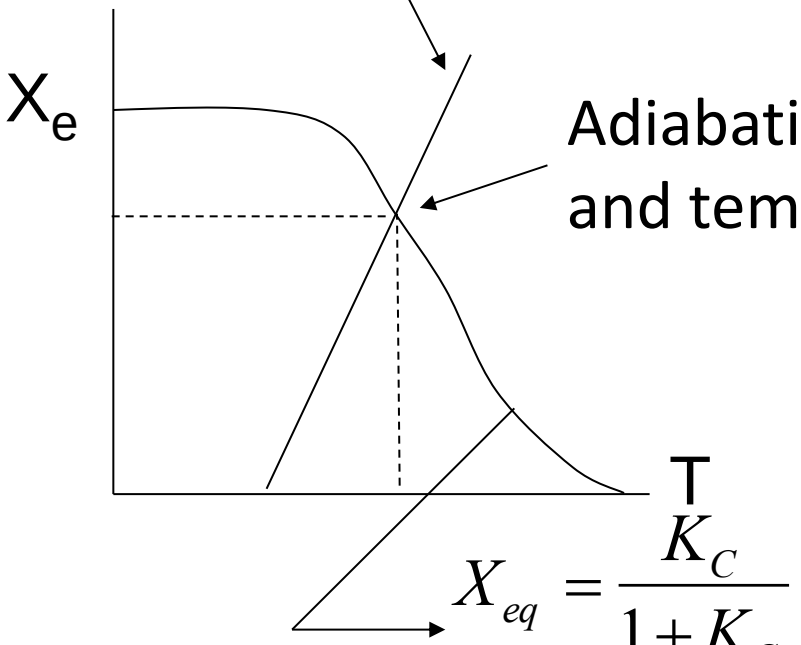
6 Xe = Kc/(1+Kc)



Example: Adiabatic PFR

$A \leftrightarrow B$

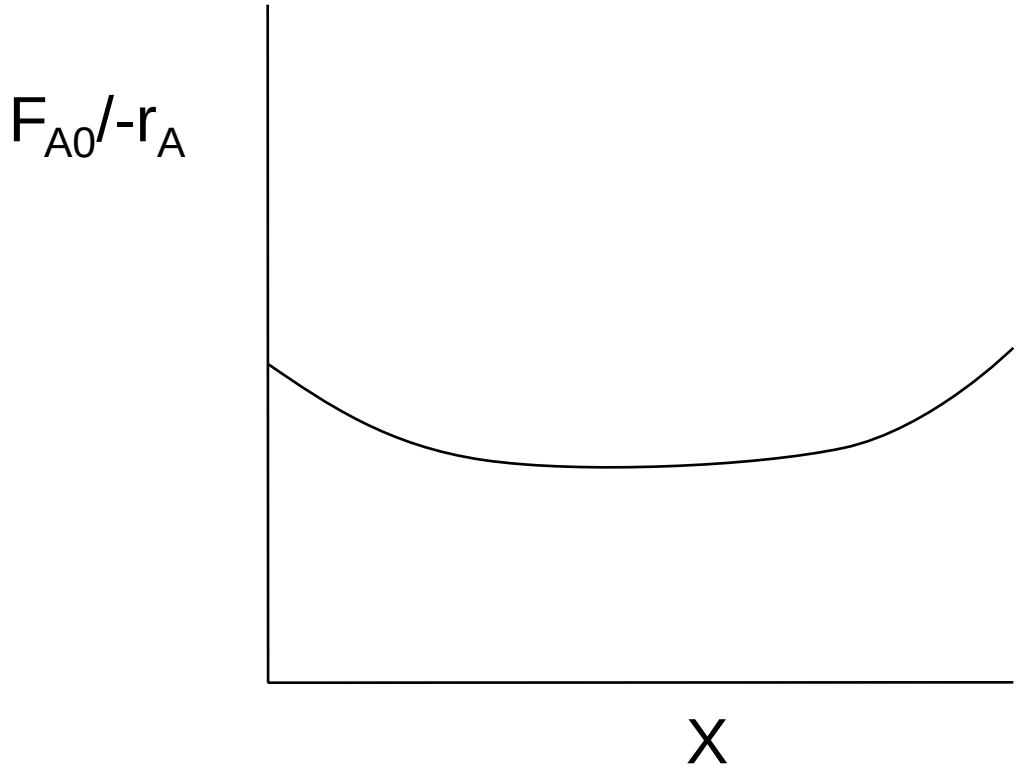
$$T = T_0 + \frac{-\Delta H_X^0 X}{\sum \theta_i C_{Pi}}$$



Adiabatic equilibrium conversion and temperature

Example: Adiabatic PFR

We can now form a table. Set X, then calculate T, $-V_A$, and $F_{A0}/-r_A$, increment X, then plot $F_{A0}/-r_A$ vs. X:



Are you ready?

Summary

- In this lecture, we covered:

- - Fundamentals of energy balance and its importance in reactor design.
- - Key equations and assumptions for analyzing energy transfer.
- - Design principles of adiabatic reactors.
- - Introduction to heat effects in chemical reactions.

- Energy balance is essential for optimizing reactor performance and ensuring safe and efficient processes.