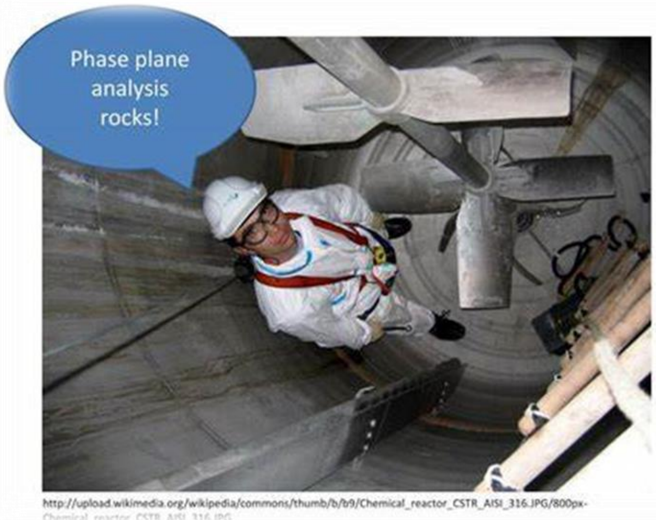
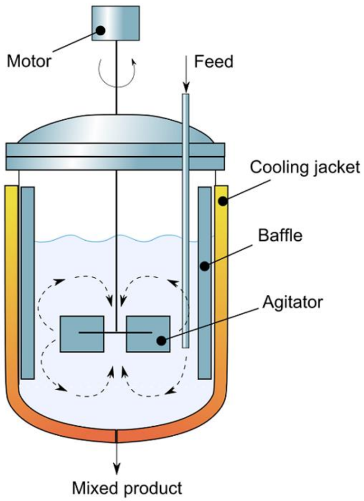
Reactor Design II





Week 9
CSTR With Heat Effects

Saba A. Gheni, Ph.D.
Chemical Engineering Department
ghenis@tu.edu.iq

Introduction

- Chemical Reaction Engineering (CRE) explores reactor design, including heat effects and stability.

- This lecture focuses on Continuous Stirred Tank Reactors (CSTRs) with heat effects, multiple steady states, and the concepts of ignition and extinction temperatures.

Topics to be Addressed

- - Fundamentals of CSTR with Heat Effects
- - Unsteady-State and Steady-State Energy Balances
- - Multiple Steady States (MSS): Analysis and Stability
- - Ignition and Extinction Temperatures
- - Practical Examples and Case Studies

Objectives

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

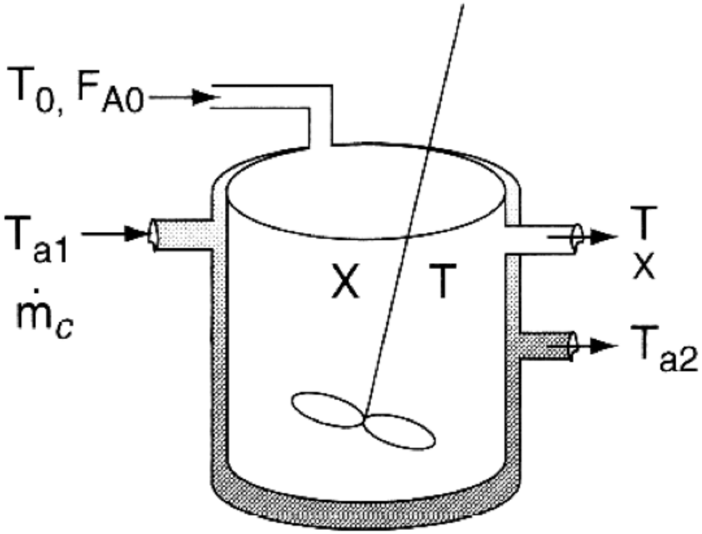
- - Understand heat effects in CSTR operation.
- - Analyze unsteady-state and steady-state energy balances.
- - Identify and evaluate multiple steady states in CSTRs.
- - Apply ignition and extinction concepts to reactor design.

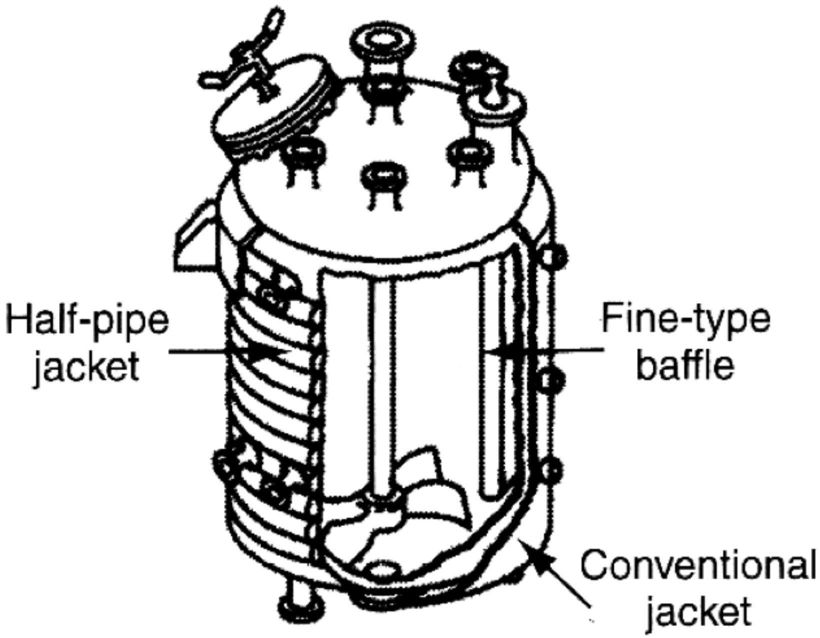
Introduction

- Understanding the relationship between heat generation and removal is crucial for predicting reactor stability.

- This session delves into steady-state and unsteady-state energy balances, multiple steady states, and the associated temperature profiles.

CSTR with Heat Effects





Courtesy of Pfaudler, Inc.

Unsteady State Energy Balance

$$\boxed{\dot{Q} - \dot{W}_S + \sum_{i=1}^{n} F_{i0} H_{i0} - \sum_{i=1}^{n} F_i H_i = \frac{d\hat{E}_{sys}}{dt}}$$

Neglect

Using $\hat{E}_{sys} = \sum N_i E_i = \sum N_i (H_i - PV_i) = \sum N_i H_i - \cancel{PV}$

$$\frac{dE_{sys}}{dt} = \frac{d\sum N_i H_i}{dt} = \sum N_i \frac{dH_i}{dt} = \sum H_i \frac{dN_i}{dt}$$

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

$$\frac{dN_i}{dt} = -\upsilon_i r_A V + F_{i0} - F_i$$

We obtain after some manipulation:

$$\frac{dT}{dt}=\frac{\dot{Q}-\dot{W}_S-\sum F_{i0}C_{Pi}\left(T-T_{i0}\right)+\left[-\Delta H_{Rx}(T)\right]\left(-r_A V\right)}{\sum N_i C_{Pi}}$$

Collecting terms with $\dot{Q}=UA\left(T_a-T\right)$ and $\dot{W}_S=0$ high coolant flow rates, and $F_{i0}=F_{A0}\Theta_i$

Unsteady State Energy Balance

$$\frac{dT}{dt}=\frac{(\Delta H_{Rx})(r_A V)-\left[F_{A0}\overbrace{\sum \Theta_i C_{P_i}}^{C_{P_0}}(T-T_0)+(UA(T-T_a))\right]}{\sum N_i C_{P_i}}$$

$$=\frac{F_{A0}}{\sum N_i C_{P_i}}\left[\overbrace{\Delta H_R \frac{r_A V}{F_{A0}}}^{\boldsymbol{G}(\boldsymbol{T})}-\overbrace{\left[C_{P_0}\left[T-T_0+\frac{UA}{\underbrace{F_{A0}C_{P_S}}_{\kappa}}(T-T_a)\right]\right]}^{\boldsymbol{R}(\boldsymbol{T})}\right]$$

Unsteady State Energy Balance

$$\frac{dT}{dt} = \frac{F_{A0}}{\sum N_i C_{P_i}}\left[\boldsymbol{G}(\boldsymbol{T}) - \boldsymbol{R}(\boldsymbol{T})\right]$$

$$G(T) = (r_A V)\left[\Delta H_{Rx}\right]$$

$$R(T) = C_{P_0}\left[(1+\kappa)T - (T_0 + \kappa T_a)\right]$$

$$R(T) = C_{P_0}(1+\kappa)\left(T - \frac{T_0 + \kappa T_a}{1+\kappa}\right) = C_{P_0}(1+\kappa)(T - T_C)$$

$$\kappa = \frac{UA}{F_{A0}C_{P0}} \qquad T_C = \frac{T_0 + \kappa T_a}{1+\kappa}$$

$$\frac{dT}{dt} = \boldsymbol{G}(\boldsymbol{T}) - \boldsymbol{R}(\boldsymbol{T})$$

If G(T) > R(T) Temperature Increases

If R(T) > G(T) Temperature Decreases

Steady State Energy Balance for CSTRs

At Steady State

$$\frac{dT}{dt} = \frac{dN_A}{dt} = 0$$

$$-r_A V = F_{A0} X$$

$$\boldsymbol{G(T) - R(T) = 0}$$

$$(-\Delta H_{Rx}) F_{A0} X - F_{A0} \sum \Theta_i C_{P_i} (T - T_0) - UA(T - T_a) = 0$$

Solving for X.

Solving for X:

$$X = \frac{\sum \Theta_i C_{P_i}(T - T_0) + \frac{UA}{F_{A0}}(T - T_a)}{-\Delta H^\circ_{Rx}} = X_{EB}$$

Solving for T:

$$T = \frac{F_{A0} X(-\Delta H_{Rx}) + UAT_a + F_{A0} \sum \Theta_i C_{P_i} T_0}{UA + F_{A0} \sum \Theta_i C_{P_i}}$$

Steady State Energy Balance for CSTRs

$$X\left(-\Delta H_{Rx}\right) = C_{P_0}\left[T - T_0 + \frac{UA}{F_{A0}C_{P_0}}\left(T - T_a\right)\right]$$

$$\text{Let } \kappa = \frac{UA}{F_{A0}C_{P_0}}$$

$$X\left(-\Delta H_{Rx}\right) = C_{P_0}\left(T + \kappa T - T_0 - \kappa T_a\right) = C_{P_0}\left(1+\kappa\right)\left(T - \frac{T_0 + \kappa T_a}{1+\kappa}\right)$$

$$= C_{P_0}\left(1+\kappa\right)\left(T - T_C\right)$$

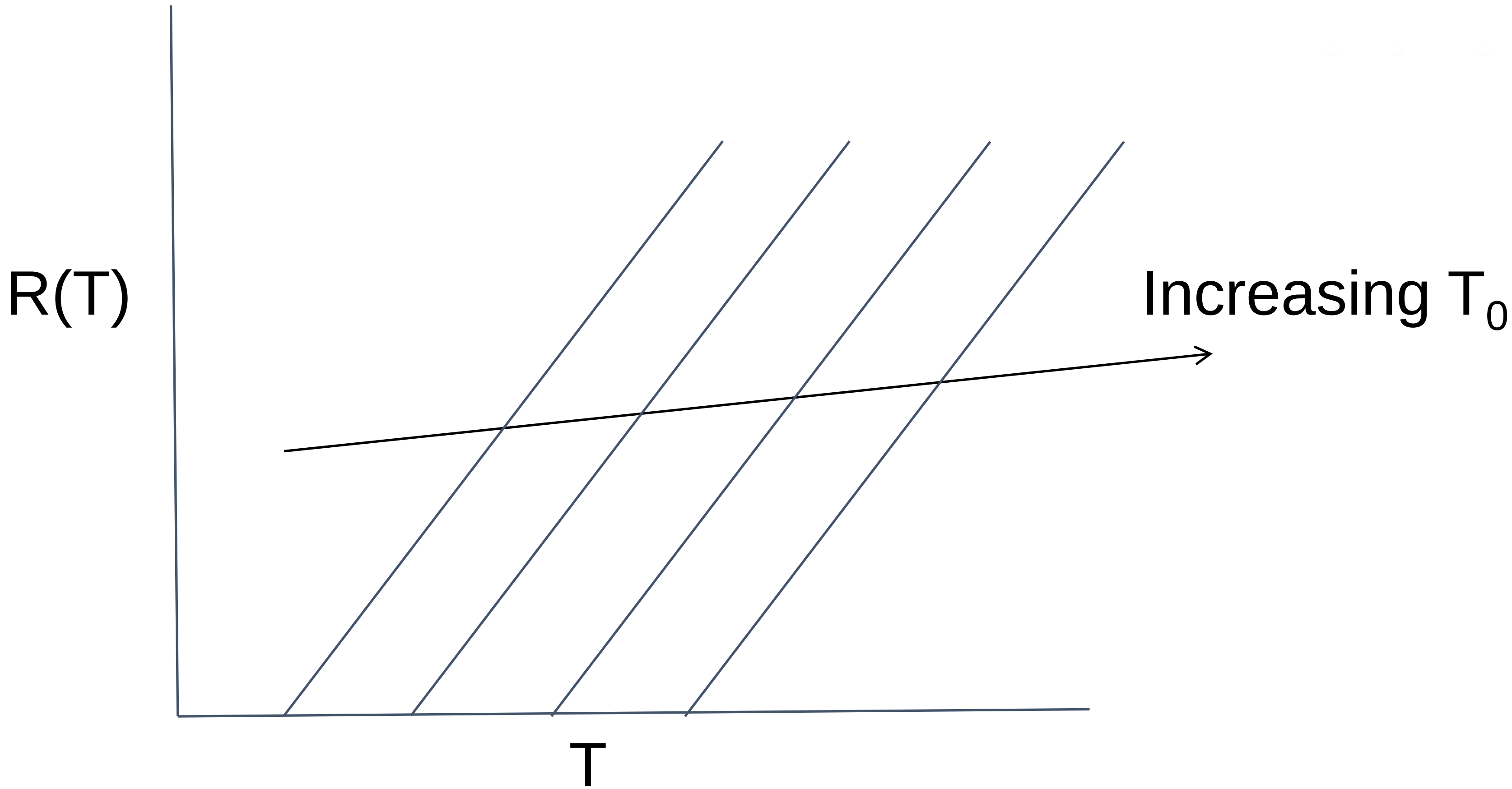
$$T_C = \frac{T_0 + \kappa T_a}{1+\kappa}$$

Steady State Energy Balance for CSTRs

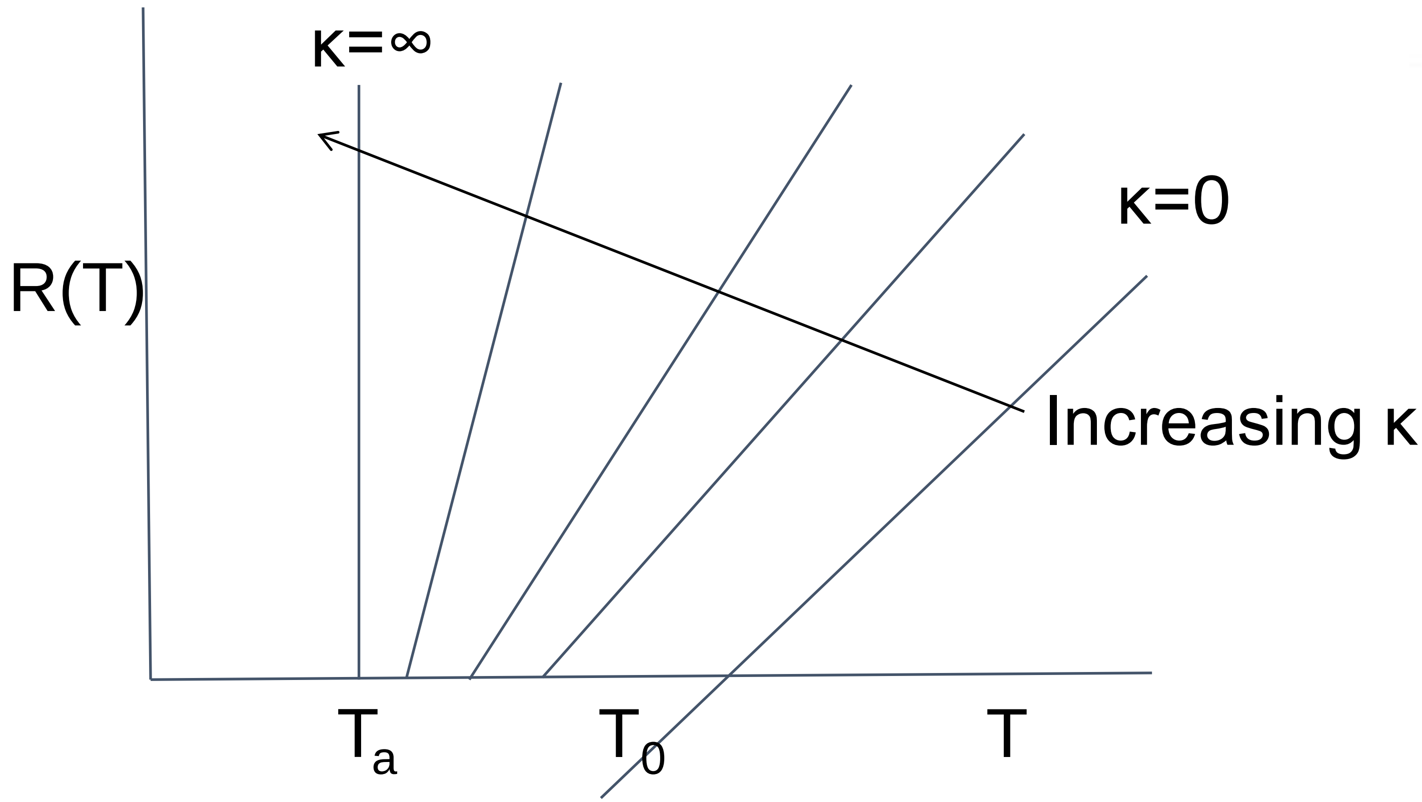
$$\overbrace{-X\,\Delta H^{o}_{Rx}}^{G(T)} = \overbrace{C_{P0}(1+\kappa)(T-T_C)}^{R(T)}$$

$$\boxed{X = \frac{C_{P0}(1+\kappa)(T-T_C)}{-\Delta H^{o}_{Rx}}}$$

$$\boxed{T = T_C + \frac{(-\Delta H^{o}_{Rx})(X)}{C_{P0}(1+\kappa)}}$$



Variation of heat removal line with inlet temperature.



Variation of heat removal line with κ ($\kappa = UA/C_{P0}F_{A0}$)

$$V = \frac{F_{A0}X}{-r_A(X,T)}$$

$$A \rightarrow B$$

1) Mole Balances:

$$V = \frac{F_{A0}X}{-r_A}$$

2) Rate Laws:

$$-r_A = kC_A$$

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

4) Combine:

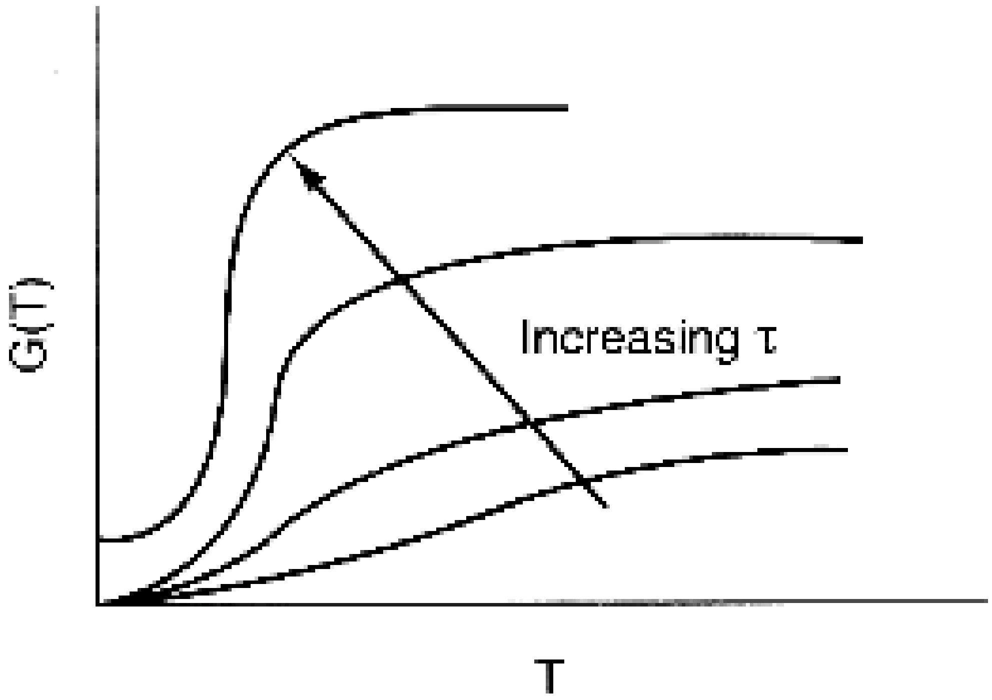
$$V = \frac{F_{A0}X}{kC_{A0}(1-X)} = \frac{C_{A0}\upsilon_0 X}{kC_{A0}(1-X)}$$

$$\tau k = \frac{X}{1-X}$$

$$X = \frac{\tau k}{1+\tau k} = \frac{\tau A e^{-E/RT}}{1+Ae^{-E/RT}}$$

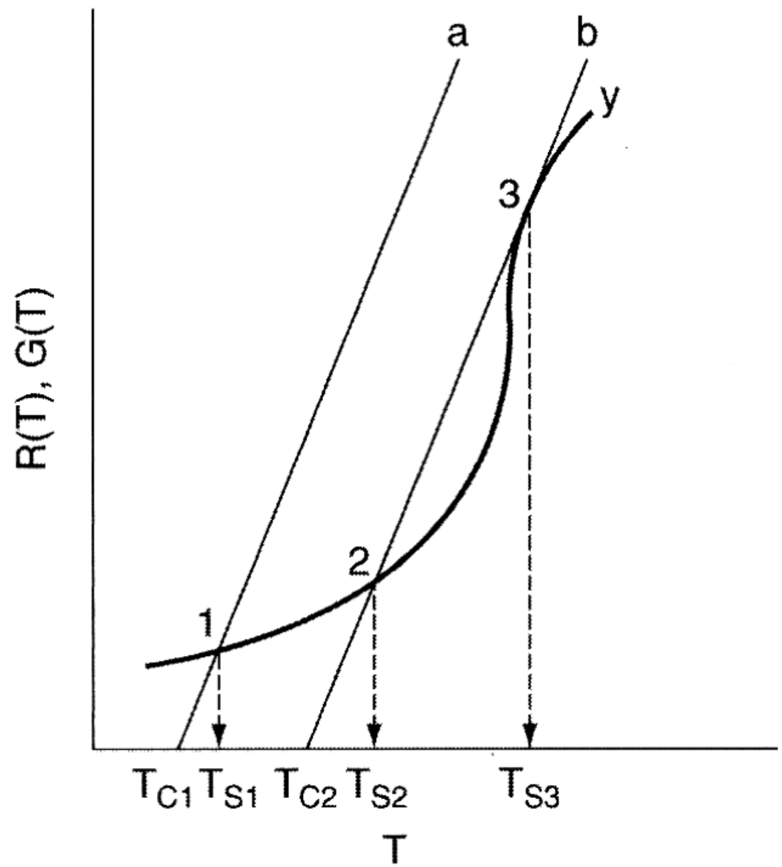
$$G(T) = X(-\Delta H_{Rx}) = \frac{\tau A e^{-E/RT}}{1+Ae^{-E/RT}}(-\Delta H_{Rx})$$

Multiple Steady States (MSS)



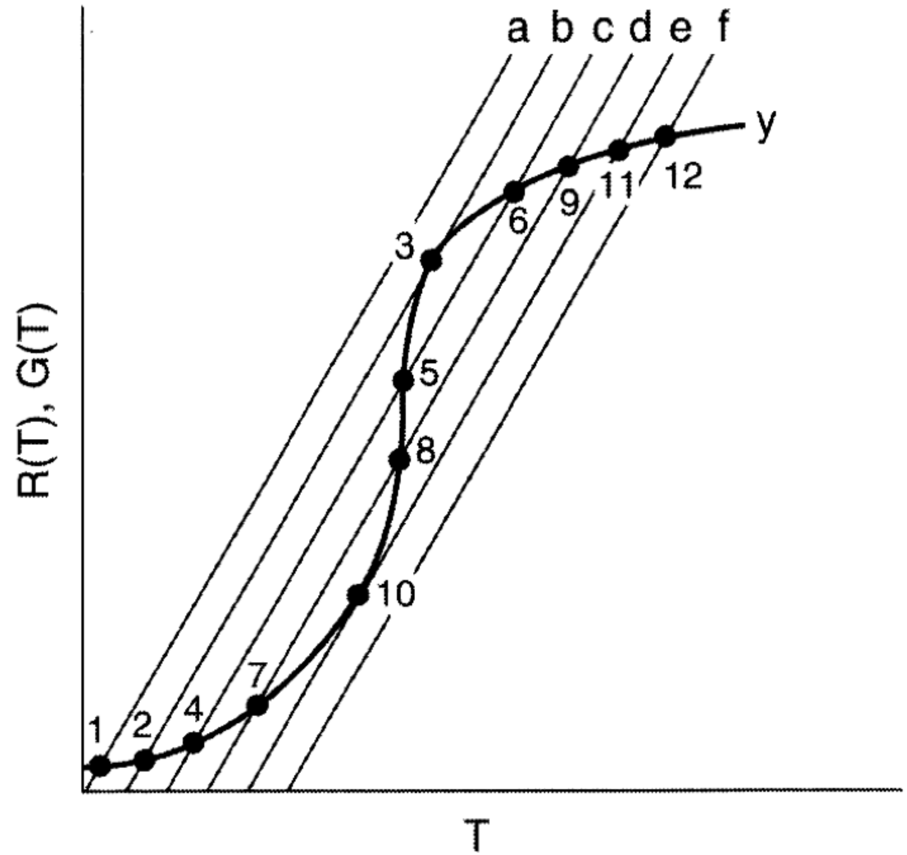
Variation of heat generation curve with space-time.

Multiple Steady States (MSS)



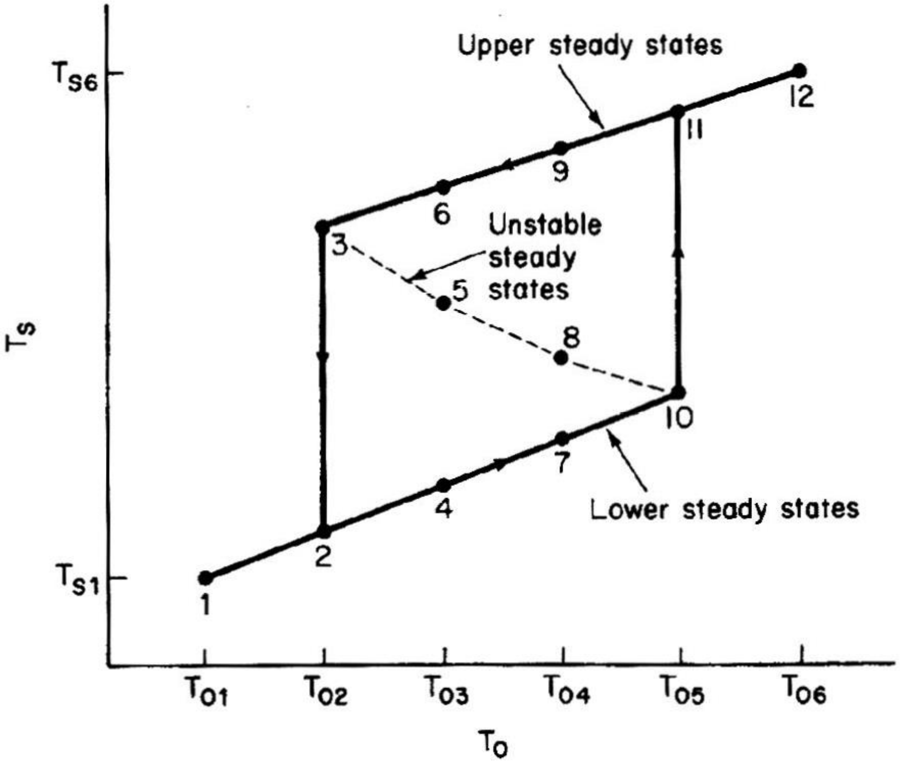
Finding Multiple Steady States with T_0 varied

Multiple Steady States (MSS)



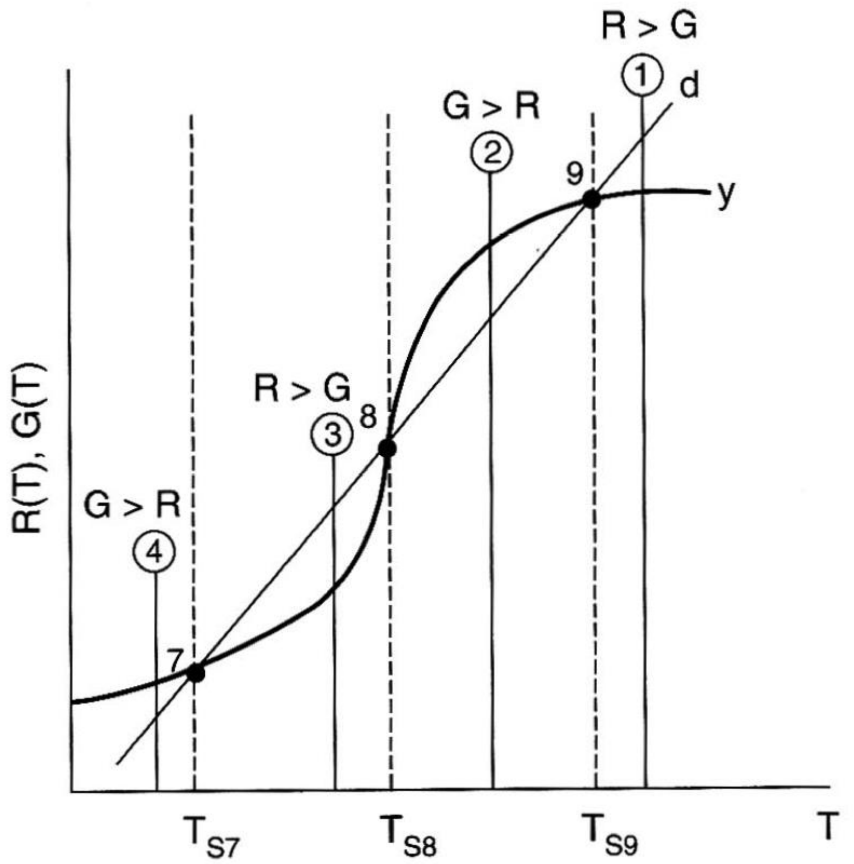
Finding Multiple Steady States with T_0 varied

Multiple Steady States (MSS)



Temperature ignition-extinction curve

Multiple Steady States (MSS)



Stability of multiple state temperatures

MSS - Generating G(T) and R(T)

$$\frac{dT}{dt} = 1$$

$$G(T) = X \cdot (-\Delta H_{Rx})$$

$$R = C_{P_0} \cdot (1+\kappa) \cdot (T - T_C)$$

Need to solve for X after combining **mole balance**, **rate law,** and **stoichiometry.**

MSS - Generating G(T) and R(T)

For a first order irreversible reaction

$$X = \frac{tau \cdot k}{(1 + tau \cdot k)}$$

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

<u>Parameters</u>

$$Tau, (-\Delta H_{Rx}), k_1, E, R, T_1, T_C, kappa, C_{P_0}$$

Then plot G and R as a function of T.

Are you ready?

Summary

- In this lecture, we covered:

- - Heat effects and energy balance fundamentals for CSTRs.
- - Analysis of multiple steady states and their stability.
- - Concepts of ignition and extinction temperatures.
- - Practical examples to reinforce theoretical concepts.

- Understanding these principles is critical for designing stable and efficient reactor systems.