Lecture 13 Transient Processes in Chemical Reactors

Goal of the lecture: To study the dynamic behavior of chemical reactors during non-steady-state conditions, focusing on how concentration, temperature, and pressure change over time and how these variations affect reactor performance and control.

Brief lecture notes: This lecture explores the transient (time-dependent) behavior of chemical reactors when they deviate from steady-state operation. It discusses the governing differential equations for unsteady processes, the physical meaning of transient response, and its significance in startup, shutdown, and disturbance conditions. Students will learn how to model transient mass and energy balances for different reactor types—batch, continuous stirred-tank reactor (CSTR), and plug flow reactor (PFR)—and understand how these affect conversion, selectivity, and stability. Emphasis is placed on the transition to steady-state, response to perturbations, and the role of control systems in maintaining reactor safety and performance.

Main part

In chemical engineering, transient processes refer to situations when the reactor's operating variables—such as concentrations, temperature, and flow rates—change with time. This occurs during startup, shutdown, or any disturbance (e.g., feed composition change or cooling failure). Understanding transient behavior is essential for designing reactors that can respond safely and efficiently to such changes.

In contrast to steady-state conditions, where all variables remain constant $(\frac{dC_i}{dt} = 0)$, transient states are characterized by non-zero time derivatives, indicating system evolution toward a new equilibrium or steady-state.

For a general reacting system, the mass balance under unsteady conditions can be written as:

$$\frac{dN_i}{dt} = F_{i,in} - F_{i,out} + r_i V$$

where:

 N_i —number of moles of component i,

 $F_{i,in}$ and $F_{i,out}$ —inlet and outlet molar flow rates,

 r_i —rate of formation (positive) or consumption (negative) of component i,

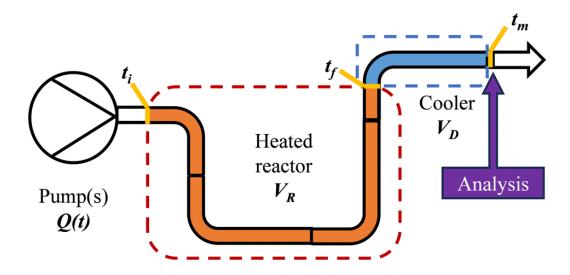
V— reactor volume.

For a CSTR, assuming constant density and volume, the dynamic mass balance simplifies to:

$$V\frac{dC_A}{dt} = F(C_{A0} - C_A) - Vr_A$$

This first-order differential equation describes how the concentration of reactant A evolves with time before reaching steady-state ($\frac{dc_A}{dt} = 0$). The transient solution depends on the system's time constant, which indicates how quickly the reactor responds to changes.

Figure 1 shows a typical transient response of concentration in a CSTR after a step change in feed concentration—initially deviating from steady-state and gradually stabilizing.



Thermal Transients

Thermal behavior often accompanies concentration transients. In exothermic systems, a small perturbation in feed or cooling rate can cause significant temperature deviations. The unsteady-state energy balance is expressed as:

$$\rho C_p V \frac{dT}{dt} = F \rho C_p (T_{in} - T) + (-\Delta H_r) V r_A - U A (T - T_c)$$

where ρ is density, C_p heat capacity, ΔH_r reaction enthalpy, U overall heat transfer coefficient, Aheat transfer area, and T_c coolant temperature.

Such systems may exhibit thermal runaway or oscillatory behavior if heat generation exceeds removal, highlighting the need for dynamic analysis and control.

Table 1 summarizes typical characteristics of transient behavior in different reactor types.

Reactor Type	Key Dynamic Feature	Response Time	Typical Use Case
Batch Reactor	Natural transient (no steady-state)	Long	Laboratory or small-scale production
CSTR	Approaches steady-state exponentially	Moderate	Continuous industrial systems
PFR	Spatially dependent transients	Short	Large-scale production and flow processes

In reactor design and control, understanding transient dynamics allows engineers to prevent unsafe conditions and optimize operational efficiency. During startup, the reactor must safely pass through non-steady conditions before achieving desired temperature and conversion. Similarly, during disturbances, the rate of return to steady-state—known as dynamic stability—is a critical performance criterion.

Dynamic modeling and simulation tools such as MATLAB, Aspen Dynamics, or COMSOL Multiphysics are often used to predict transient responses and design appropriate control systems. These models help in tuning control loops, selecting safety interlocks, and improving energy efficiency.

Questions for self-control

- 1. What distinguishes transient processes from steady-state operation in chemical reactors?
- 2. How are unsteady-state mass and energy balances formulated?
- 3. What is the physical meaning of the time constant in reactor dynamics?
- 4. Why can thermal transients lead to reactor instability?
- 5. How do computational models assist in analyzing transient reactor behavior?

Literature

- 1. Levenspiel, O. Chemical Reaction Engineering, 3rd ed., Wiley, 1999.
- 2. Fogler, H. S. Elements of Chemical Reaction Engineering, 5th ed., Prentice Hall, 2016.
- 3. Froment, G. F., Bischoff, K. B. Chemical Reactor Analysis and Design, 3rd ed., Wiley, 2010.
- 4. Bequette, B. W. Process Control: Modeling, Design, and Simulation, Prentice Hall, 2003.
- 5. Nauman, E. B. Chemical Reactor Design, Optimization, and Scaleup, 2nd ed., Wiley, 2008.