Lecture 5 Isothermal Design of Chemical Reactors (Batch, CSTR, PFR)

Goal of the lecture: To study the fundamental principles and equations governing the isothermal design of chemical reactors, including batch, continuous stirred-tank (CSTR), and plug flow (PFR) reactors.

Brief lecture notes: In this lecture, we will explore the theoretical and practical foundations of isothermal reactor design, focusing on how reaction kinetics, residence time, and conversion determine reactor performance. The discussion will cover the derivation of design equations for different reactor types, the relationship between space time and conversion, and the comparison of reactor efficiencies under isothermal conditions. Special attention will be given to graphical methods for design evaluation and to the role of reactor type in chemical process optimization.

Main part

The isothermal reactor design assumes that the temperature of the reacting system remains constant throughout the reaction process. This condition is particularly important for reactions where heat effects are either negligible or effectively controlled through heat exchange. The three main reactor types used in chemical engineering — Batch Reactors, Continuous Stirred-Tank Reactors (CSTRs), and Plug Flow Reactors (PFRs) — can all be analyzed under isothermal operation.

Batch Reactor Design

A batch reactor operates without inflow or outflow of material during the reaction. It is typically used for small-scale production, laboratory studies, and slow reactions. The mass balance for a batch reactor under isothermal conditions is given by:

$$\frac{dN_A}{dt} = -r_A V$$

or, in terms of conversion X_A:

$$t = \int_0^{X_A} \frac{dX_A}{-r_A(1 - X_A)}$$

Here, $r_A$is the rate of reaction, $V$the reactor volume, and $N_A$the moles of reactant A. For first-order reactions ($r_A = kC_A$), the solution provides a direct relation between time and conversion, which is useful for estimating batch times.

Continuous Stirred-Tank Reactor (CSTR)

A CSTR operates continuously with steady inflow and outflow, maintaining uniform composition and temperature throughout the reactor. The steady-state design equation for a single CSTR is:

$$\tau = \frac{C_{A0} - C_A}{-r_A}$$

where $\tau = \frac{V}{v_0}$is the residence time, $C_{A0}$and $C_A$are the inlet and outlet concentrations, respectively. The CSTR provides complete mixing, leading to lower conversion per unit volume compared to PFRs for the same kinetics and conditions, but it is easier to control and operate.

3. Plug Flow Reactor (PFR)

A PFR is characterized by a continuous flow without axial mixing, where concentration changes along the reactor length. The design equation is obtained from the differential mole balance:

$$\tau = \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

or equivalently in terms of conversion:

$$\tau = \int_{0}^{X_A} \frac{dX_A}{-r_A(1 - X_A)}$$

For first-order reactions, PFRs achieve higher conversions than CSTRs for the same space time due to the gradient in reactant concentration.

Comparison of Reactor Performance

The performance of reactors under isothermal conditions can be summarized by comparing conversion at equal residence times. For a given reaction order, the ranking is typically:

$$X_{\text{Batch}} \approx X_{\text{PFR}} > X_{\text{CSTR}}$$

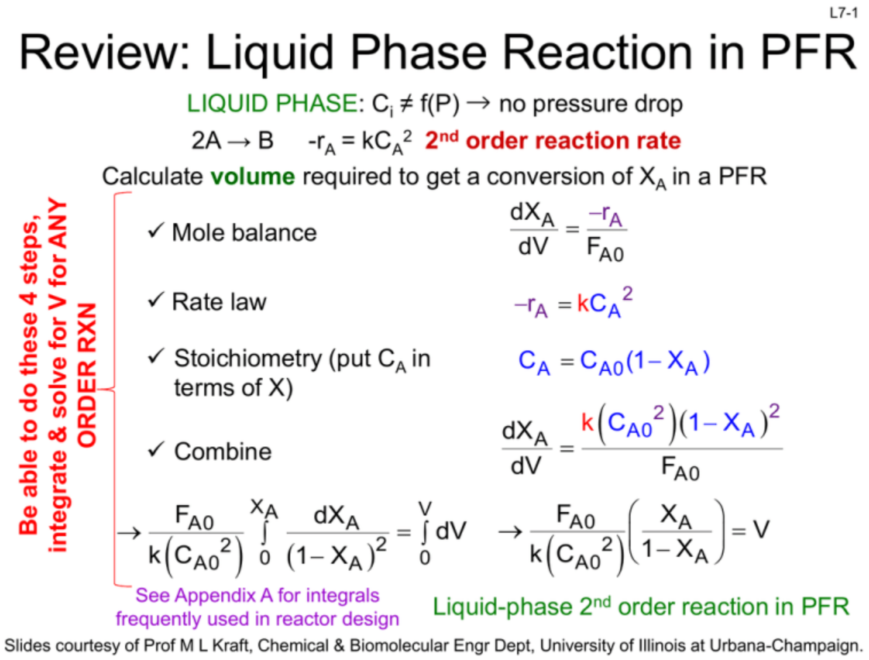
This difference arises from concentration profiles within each reactor type. PFRs maintain higher reactant concentrations throughout, promoting faster overall reaction rates.

Design Applications and Industrial Relevance

In industrial practice, combinations of reactors (e.g., CSTRs in series, or hybrid CSTR–PFR systems) are used to optimize yield, cost, and control. Isothermal conditions are often maintained through cooling jackets, heat exchangers, or external temperature control systems. Such designs are vital in processes like polymerization, hydrogenation, oxidation, and biochemical fermentation.

Table 1. Comparison of Isothermal Reactor Types

Reactor Type	Flow Pattern	Mixing Characteristics	Design Equation	Typical Use
Batch Reactor	None (closed system)	Perfectly mixed	dNA=−rAV	Laboratory, small-batch production
CSTR	Continuous, complete mixing	Uniform composition	τ=−rACA0 −CA	Continuous processes, exothermic reactions
PFR	Continuous, plug flow	No axial mixing	τ=∫CA0CA −rAdCA	Large-scale continuous production



L7-1

Review: Liquid Phase Reaction in PFR

LIQUID PHASE: $C_i \neq f(P)$ → no pressure drop

$2A \rightarrow B$ $-r_A = kC_A^2$ **2nd order reaction rate**

Calculate **volume** required to get a conversion of X_A in a PFR

Be able to do these 4 steps, integrate & solve for V for ANY ORDER RXN

✓ Mole balance $\frac{dX_A}{dV} = \frac{-r_A}{F_{A0}}$

✓ Rate law $-r_A = kC_A^2$

✓ Stoichiometry (put C_A in terms of X) $C_A = C_{A0}(1-X_A)$

✓ Combine $\frac{dX_A}{dV} = \frac{k(C_{A0}^2)(1-X_A)^2}{F_{A0}}$

$$\rightarrow \frac{F_{A0}}{k(C_{A0}^2)} \int_0^{X_A} \frac{dX_A}{(1-X_A)^2} = \int_0^V dV \rightarrow \frac{F_{A0}}{k(C_{A0}^2)}\left(\frac{X_A}{1-X_A}\right) = V$$

See Appendix A for integrals frequently used in reactor design

Liquid-phase 2nd order reaction in PFR

Slides courtesy of Prof M L Kraft, Chemical & Biomolecular Engr Dept, University of Illinois at Urbana-Champaign.

Figure 1. Reaction in PFR

Questions for Self-Control

1. What are the main assumptions underlying the isothermal reactor model?
2. How do conversion and residence time differ between CSTR and PFR?
3. Why does a PFR achieve higher conversion than a CSTR for the same reaction kinetics?
4. What are the advantages and disadvantages of batch reactors?
5. How can reactor combinations improve process efficiency?

Literature

1. Fogler, H. S. Elements of Chemical Reaction Engineering, 5th Ed., Prentice Hall, 2016.
2. Levenspiel, O. Chemical Reaction Engineering, 3rd Ed., Wiley, 1999.
3. Smith, J. M. Chemical Engineering Kinetics, 3rd Ed., McGraw-Hill, 1981.
4. Froment, G. F., Bischoff, K. B., & De Wilde, J. Chemical Reactor Analysis and Design, Wiley, 2011.
5. Hill, C. G. An Introduction to Chemical Engineering Kinetics & Reactor Design, Wiley, 1977.