Lecture 15 Non-Ideal Reactors and RTD Models

Goal of the lecture: To study the behavior of non-ideal reactors and understand the use of residence time distribution (RTD) analysis to describe deviations from ideal reactor models.

Brief lecture notes: This lecture explores the nature of non-ideal flow patterns in chemical reactors and their impact on reaction performance. We will examine how deviations from ideal plug flow (PFR) and perfectly mixed (CSTR) models arise due to dispersion, channeling, and dead zones. The lecture introduces the concept of residence time distribution (RTD) and its key functions — E(t) and F(t) — along with experimental methods to determine RTD using tracer techniques. We will also discuss mathematical models that describe non-ideal behavior, such as the tanks-in-series model and the axial dispersion model. Understanding RTD is crucial for accurately modeling real reactors, predicting conversion and selectivity, and improving reactor design and scale-up.

Main part

In real reactors, fluid flow rarely follows the ideal assumptions of plug flow or complete mixing. Deviations occur due to:

- velocity gradients and turbulence,
- molecular diffusion and axial dispersion,
- stagnant or dead zones, and channeling effects.

These factors cause fluid elements to spend different times inside the reactor, leading to changes in conversion, selectivity, or yield compared to the predictions of ideal reactor models.

Residence Time Distribution (RTD)

The RTD describes the time distribution of fluid elements (or tracer particles) within a reactor. It provides insight into how long different portions of fluid remain inside before exiting.
The exit age distribution function, *E(t)*, is defined as:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt}$$

where *C(t)* is the tracer concentration measured at the reactor outlet after a pulse input.
The cumulative distribution function, *F(t)*, represents the fraction of material that has left the reactor by time *t*:

$$F(t) = \int_0^t E(t')\,dt'$$

These functions characterize the hydrodynamic behavior of the reactor independently of reaction kinetics.

Experimental Determination of RTD

RTD is determined experimentally using tracer studies, in which an inert tracer (e.g., dye, gas, ion) is introduced at the reactor inlet. Its concentration is measured at the outlet over time.

The shape of the *E(t)* curve provides insight into flow characteristics:

- Narrow, sharp peak: flow close to plug flow (PFR behavior).
- Broad peak: strong back-mixing, approaching CSTR behavior.
- Multiple peaks: presence of parallel flow paths or recirculation zones.

Tracer experiments can be conducted in pulse or step mode, depending on whether the tracer is injected instantaneously or continuously.

Models of Non-Ideal Reactors

To describe deviations from ideal flow, simplified hydrodynamic models are used. These models help in predicting reactor performance and designing scale-up processes.

Model	Description	Key Parameter(s)	Typical Application
Axial Dispersion Model	Considers longitudinal mixing due to diffusion and turbulence	Peclet number (*Pe*)	Gas and liquid flow in tubular reactors
Tanks-in-Series Model	Reactor represented as *N* perfectly mixed tanks in sequence	Number of tanks (*N*)	Liquid-phase systems, biochemical reactors
Dead-Zone Model	Includes stagnant regions with limited mass exchange	Fraction of dead volume	Large industrial reactors, slurry systems
Bypass Flow Model	A portion of fluid bypasses the main reaction volume	Bypass fraction	Maldistributed flow systems

These models provide simplified yet effective ways to represent complex hydrodynamic phenomena.

RTD and Reactor Performance

Once RTD is known, it can be linked to reactor performance through the macro-mixing approach. The overall conversion of a first-order reaction can be expressed as:

$$X = 1 - \int_0^\infty E(t) e^{-kt}\, dt$$

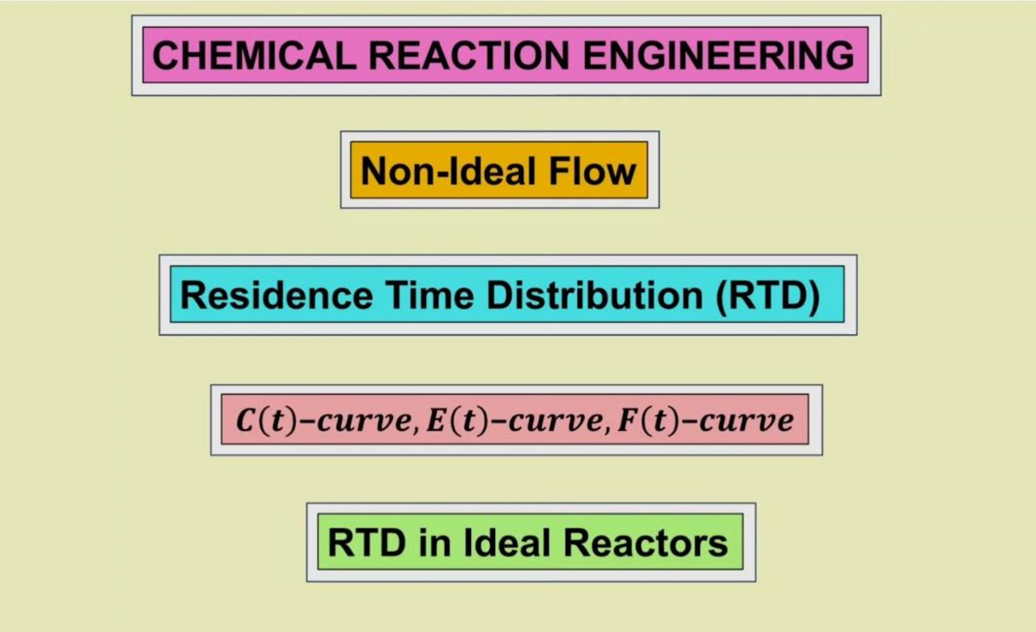
where k is the reaction rate constant.
This relationship connects flow non-ideality to chemical conversion and helps in predicting real reactor efficiency compared to ideal models.

(Figure 1: Typical RTD curves for ideal and non-ideal reactors)

A conceptual plot shows:

- PFR: sharp peak at mean residence time (τ),

- CSTR: exponential decay curve,
- Non-ideal reactor: intermediate, broadened distribution.



Questions for Self-Control

1. What physical factors cause deviations from ideal flow patterns in reactors?
2. How is the residence time distribution (RTD) experimentally determined?
3. What is the difference between *E(t)* and *F(t)* functions?
4. Describe the main assumptions and parameters of the tanks-in-series model.
5. How can RTD be used to predict reactor conversion for a first-order reaction?

Literature

1. Levenspiel, O. Chemical Reaction Engineering, 3rd Ed., Wiley, 1999.
2. Froment, G.F., Bischoff, K.B., & De Wilde, J. Chemical Reactor Analysis and Design, 3rd Ed., Wiley, 2010.
3. Fogler, H.S. Elements of Chemical Reaction Engineering, 5th Ed., Prentice Hall, 2016.
4. Nauman, E.B. *Residence Time Distributions and Micromixing*, Wiley-Interscience, 2008.
5. Hill, C.G. Jr. *An Introduction to Chemical Engineering Kinetics and Reactor Design*, Wiley, 1977.