Lecture 14 Modelling of Non-Ideal Reactors: Residence Time Distribution (RTD)

Goal of the lecture: To understand how real chemical reactors deviate from ideal flow behavior and how residence time distribution (RTD) can be used to model and analyze non-ideal reactor performance.

Brief lecture notes: In this lecture, we study the concept of *residence time distribution* (RTD) as a tool for characterizing real flow behavior in chemical reactors. The discussion covers the theoretical foundations of RTD, methods of experimental determination, and its connection to reactor performance. Students will learn about deviations from ideal plug flow and perfectly mixed flow, causes of non-ideality such as channeling and dead zones, and how RTD functions—E(t) and F(t)—are used to describe flow patterns. Mathematical models such as the tanks-in-series model and dispersion model are also introduced, illustrating how real reactors can be approximated based on measured RTD data.

Main part

In real industrial systems, chemical reactors rarely behave as ideal reactors. The two idealized flow types—Plug Flow Reactor (PFR) and Continuous Stirred-Tank Reactor (CSTR)—serve as theoretical limits. Real reactors often exhibit non-ideal flow, where mixing is incomplete, or flow patterns are irregular due to design, operation, or hydrodynamic effects.

To describe these deviations, chemical engineers use the concept of Residence Time Distribution (RTD), which quantifies how long individual fluid elements spend inside the reactor. RTD analysis helps identify back-mixing, dead zones, bypassing, and channeling—factors that significantly affect conversion and selectivity.

1. Concept of RTD

When a tracer (e.g., a dye or a radioactive isotope) is injected into a reactor at the inlet, its concentration is measured over time at the outlet. The resulting curve represents how long different fluid elements have stayed inside the reactor.

The E(t) function defines the probability density of residence times:

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

where $C(t)$is the tracer concentration at the outlet at time t. The area under $E(t)$is always equal to 1, representing the total fluid volume that has passed through.

The mean residence time ($\bar{t}$) is calculated as:

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

Ideally, for a PFR all fluid elements have the same residence time (a sharp pulse), while for a CSTR the distribution is exponential, indicating full mixing.

RTD Functions and Reactor Models

Figure 1 shows typical RTD curves for ideal and non-ideal reactors. In real systems, RTD curves are broader and asymmetric, showing delayed flow or short-circuiting.

- ***Residence time distribution (RTD)*** *function* (*E function*) *is* proposed to describe residence time presented bv different reaction elements inside a reactor, therefore: $$\int_0^{\infty} E dt = 1$$

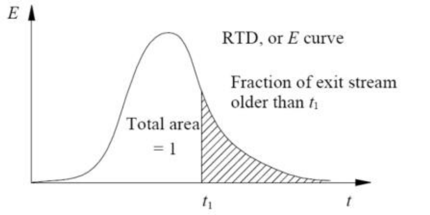

Figure 11.1 Residence Time Distribution (RTD) Function

The fraction of exit stream of age between t and $t + dt$ is Edt, and the fraction younger than age t_1 is:

$$\int_0^{t_1} E dt$$

whereas the fraction of material older than t_1 is:

$$\int_{t_1}^{\infty} E dt = 1 - \int_0^{t_1} E dt$$

- The direct reason responsible for RTD is mixing within a reactor, thus, RTD can be used to describe all kinds of non-ideal flow presented within real reactors mathematically.

Table 1 summarizes RTD characteristics for common reactor types.

Reactor Type	RTD Function	Curve Shape	Mixing Characteristics
PFR	$E(t) = \delta(t - \bar{t})$	Sharp peak	No mixing along flow
CSTR	$E(t) = \frac{1}{\bar{t}} e^{-t/\bar{t}}$	Exponential decay	Perfect mixing
Non-Ideal Reactor	Measured experimentally	Broad/asymmetric	Partial mixing

Models of Non-Ideal Flow

To describe non-ideal reactors, several theoretical models are used:

- Tanks-in-Series Model — The reactor is modeled as a series of *N* CSTRs connected in sequence. The RTD becomes narrower as *N* increases, approaching plug flow.

$$E(t) = \frac{(t/\bar{t})^{N-1} e^{-Nt/\bar{t}} N^N}{(N-1)!}$$

- Dispersion Model — Based on diffusion analogy, it assumes axial mixing due to molecular diffusion and turbulence, characterized by the Peclet number (Pe):

$$Pe = \frac{uL}{D}$$

where u is flow velocity, L reactor length, and D axial dispersion coefficient. Large Pe values indicate near-plug flow, while small values approach complete mixing.

Experimental Determination

RTD is determined experimentally by introducing a non-reactive tracer pulse or step input and monitoring the output concentration over time. Analysis of the resulting curve reveals important features of flow, such as:

- Dead zones: regions where fluid movement is slow.
- Short-circuiting: some fluid leaves the reactor too quickly.
- Recirculation: backward mixing of fluid elements.

These deviations affect the effective conversion of reactants. For instance, excessive back-mixing reduces selectivity in parallel reactions, while dead zones decrease overall reactor utilization.

Applications and Interpretation

RTD is a powerful diagnostic tool for:

- Evaluating reactor performance and scale-up.
- Troubleshooting industrial reactors for flow maldistribution.
- Designing reactors with desired flow patterns.
- Developing correlations between mixing and conversion.

Combining RTD data with kinetic information allows simulation of real reactor behavior and prediction of conversion under actual flow conditions.

Questions for self-control

1. What is the physical meaning of residence time distribution (RTD)?
2. How are the E(t) and F(t) functions defined and interpreted?
3. What are the key differences in RTD between plug flow and mixed flow reactors?
4. How does the tanks-in-series model describe non-ideal reactors?
5. What operational problems can RTD analysis help identify in industrial reactors?

Literature

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