Lecture # 27 CHE331A

Non-ideal Reactors

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- Non-isothermal reactors
- Energy balance for ideal reactors
- Non-adiabatic PFR
- Reversible reactions in adiabatic reactors
- CSTR with heat effects
- Batch reactors

Principles behind Non-ideal reactors and their analysis

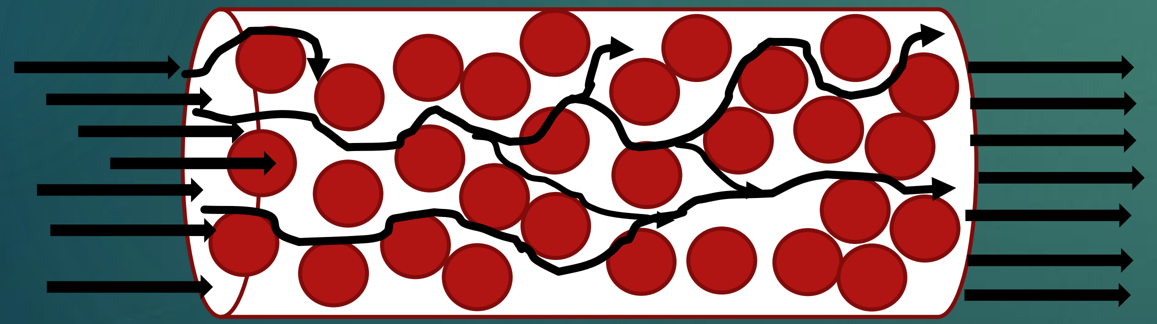
- Residence time distribution
- Tank-in-series model
- Dispersion model (will not include)
- Applications to design

Industrial Reactors are rarely ideal

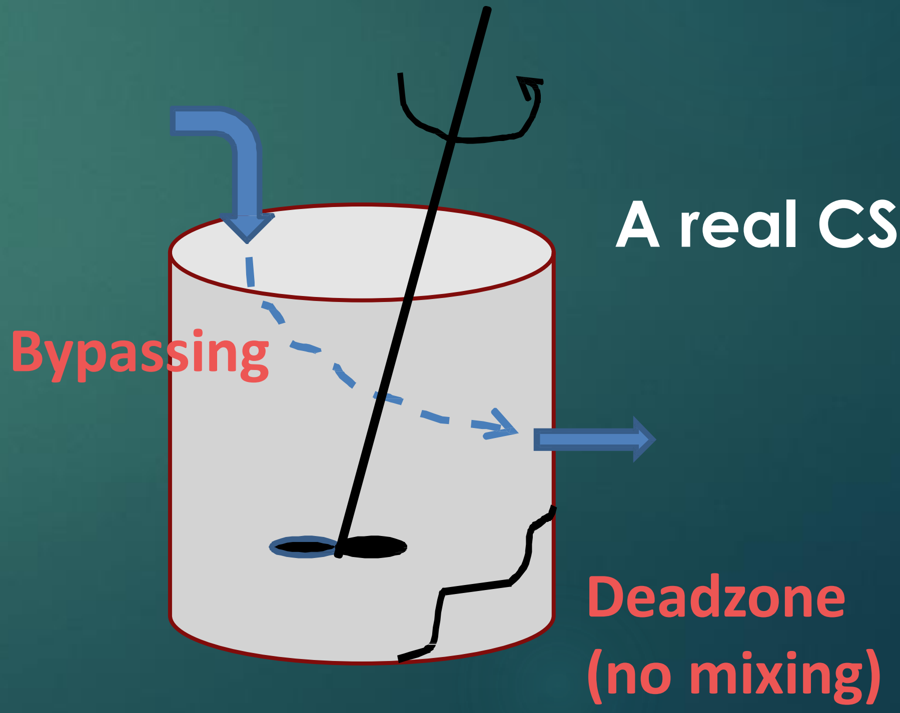
- Ideal reactors: Batch, CSTR, PFR and PBR
- Flow in these reactors are idealized and are rarely experienced
- Real flow-reactors lie between the extremes of
  - Completely mixed (no spatial variation) for CSTR (for example, no dead-zone)
  - No radial variation or axial mixing for PFR (entering fluid moves as a plug from entry to exit)

In non-ideal reactors the flows between these two extremes characterize the system

- Reasons for non-ideality in real reactors
  - Channelling, Recycle of fluid, stagnant regions, axial mixing, and velocity profile
- Time spent by fluid elements are different $\rightarrow$ $residence\ time\ distribution$

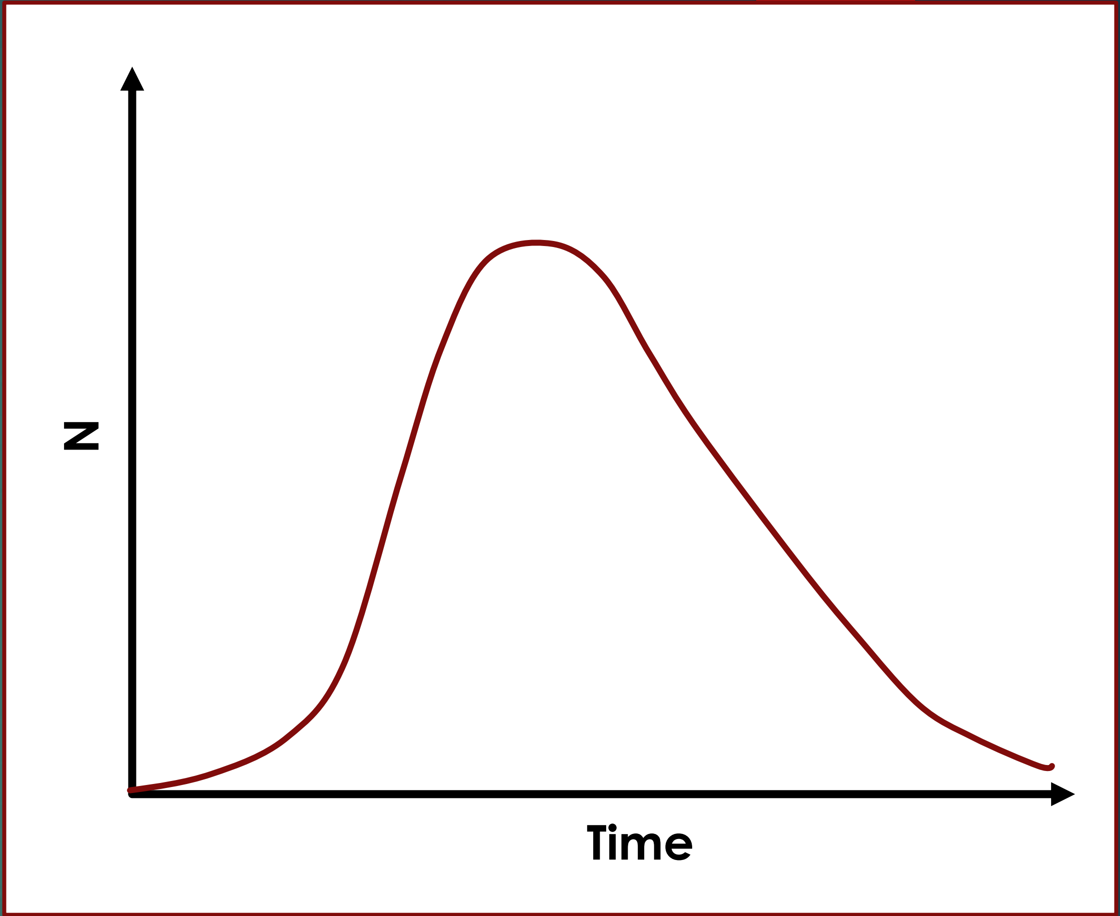


A real Packed Bed Reactor



Ways to account for non-ideality

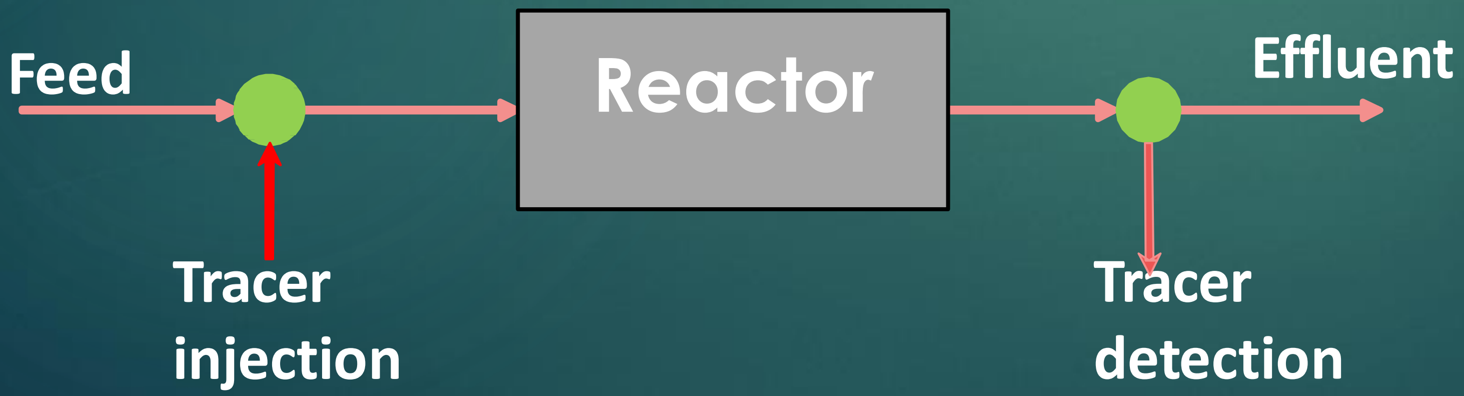
- Three concepts used to describe non-ideal reactors:
  - Residence time distribution
  - Quality of mixing
  - Model used to describe the system
- For example, in an ideal PFR reactor all atoms of material have been in the reactor for the same "residence" time
- In real reactors some material leave quicker than the rest
  - There is a residence time distribution (RTD) or exit age distribution for a stream of fluid

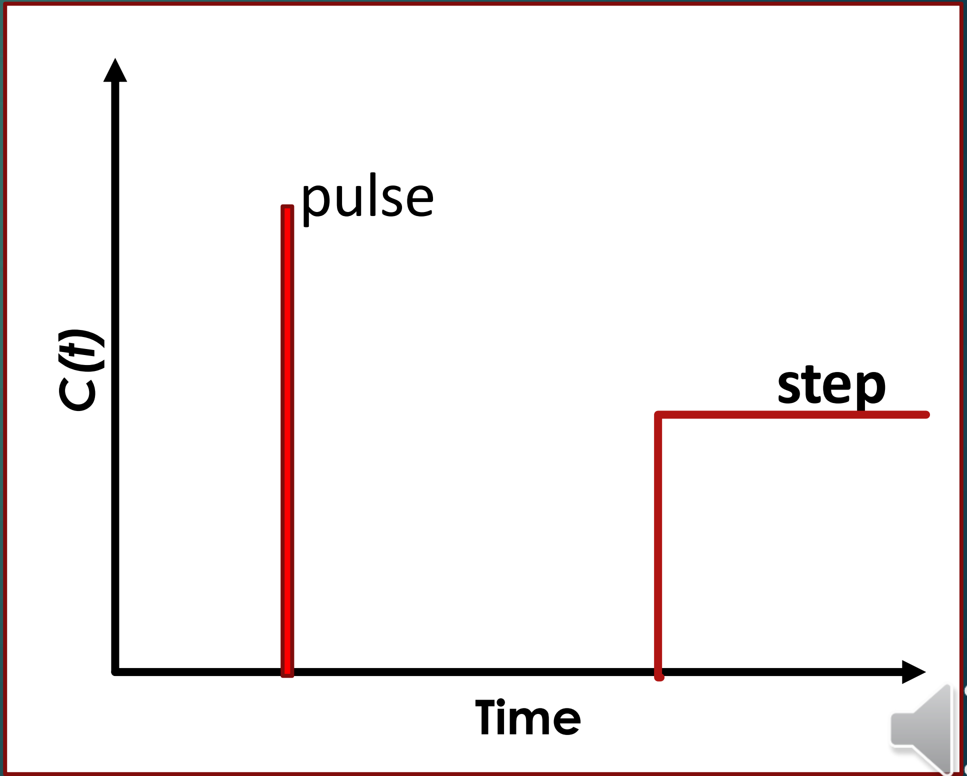


- **In PFR/PBR and Batch are the only reactors in which each fluid element spends the same amount time in the reactor**
- **In a CSTR there is a distribution**

Residence time distribution is determined experimentally

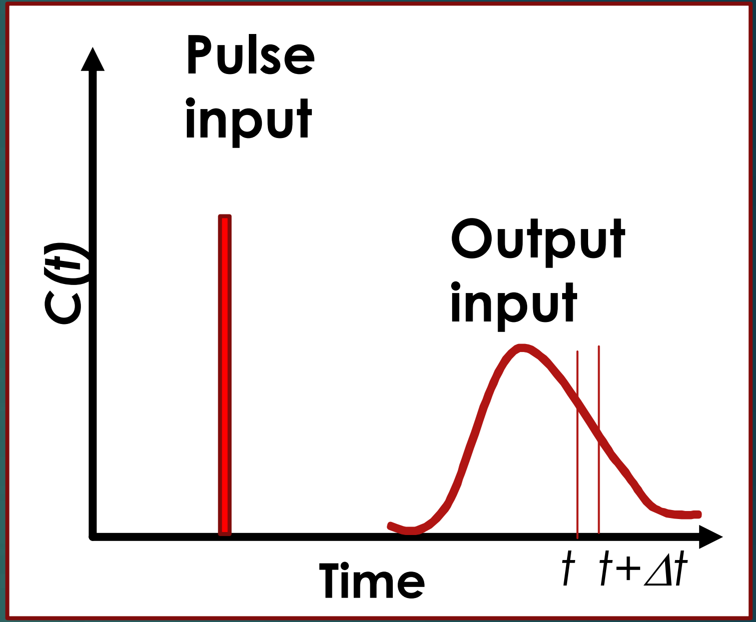
- Injecting tracer at some time and measuring outlet concentration of tracer
  - Tracer is an inert chemical molecule that can be detected in the feed
- Reactors give responses to different types of tracer input
- Tracer input primarily of two types
  - Pulse input and step input
  - Other types exist





A known amount of tracer material injected in one shot in a pulse input to determine the RTD

- Outlet concentration in a real reactor is measured as a function of time, C-curve. For example,



- Amount of tracer leaving between $t \; and \; t + dt$ is

$$\Delta N = C(t).\nu.\Delta t$$

Where, ν is the volumetric flowrate

- To make this independent of the amount of tracer
- Fraction of material spending between $t \; and \; t + dt$ in the reactor is ${}^{\Delta N}/_{N_0}$ where N_0 is the total amount of material injected
- For a pulse injection the residence time distribution function, $E(t)$, is defined as $E(t) = (C(t).\nu)/N_0$ so that $\frac{\Delta N}{N_0} = E(t).\Delta t$

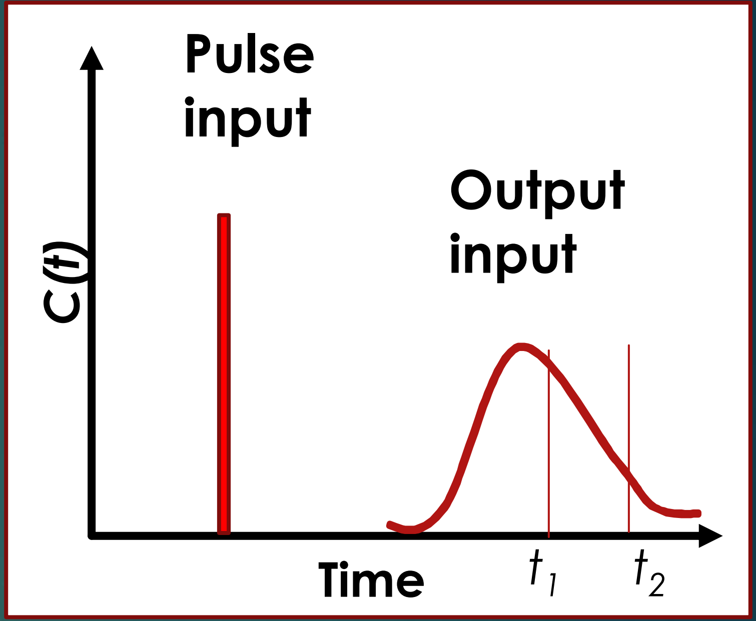
The residence time distribution function, $E(t)$

- $E(t)$, is defined as $E(t) = (C(t).v)/N_0$ so that $\frac{\Delta N}{N_0} = E(t).\Delta t$
  - describes quantitatively how much time different fluid elements spend in the reactor
  - $E(t).dt$ is the fraction of fluid exiting the reactor that has spent between $t\ and\ t + dt$ time inside the reactor
- If N_0 is not known it can be determined by integrated the outlet concentration vs time curve
  - $dN = C(t).v.dt \quad \rightarrow \quad \int_0^{\infty} dN = N_0 = \int_0^{\infty} C(t).v.dt$ and

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

Residence time distribution function is also expressed in its integral form

$$\int_{t_1}^{t_2} E(t)dt =$$ The fraction of material leaving the reactor that has resided in the reactor between t_1 and t_2



Furthermore, $\int_0^\infty E(t)dt = 1$

- Sometimes there are difficulties with the pulse technique, such as:
  - injection must take place in a short time compared to the residence time,
  - negligible dispersion between point of injection and entrance to the reactor, and
  - the $C(t)$ vs t curve has a long tail