BT209

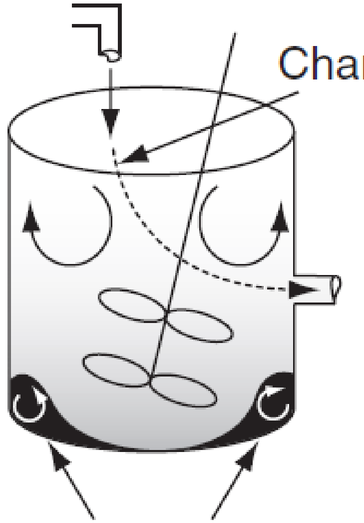
Bioreaction Engineering

24/04/2023

Non ideal flow reactor
(RTD)

Non-ideal reactors

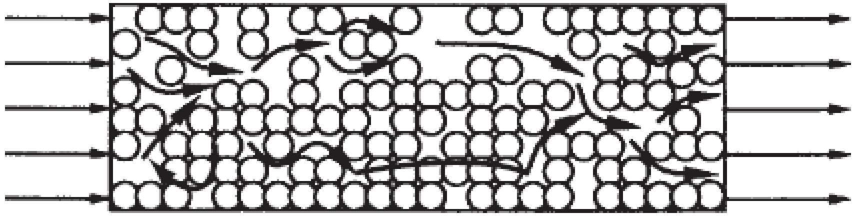
- So far **perfectly mixed batch**, **Plug-flow** tubular, and the **perfectly mixed** continuou tank reactors—have been modeled as **ideal reactors**



- Unfortunately, **In real world** often observe behavior very different from that expected (from ideal). and performance deviates from the ideal.

- Deviation from the two ideal flow patterns can be caused
  - by channeling of fluid,
  - by recycling of fluid, or
  - by creation of stagnant regions (dead zone) in the vessel.

 # Residence times (RT) is not same for all molecules in the real reactor



Channeling of fluid in packed bed reactor

- Therefore the **predicted conversion /distribution of product /size of reactors deviates** from the ideal.

✓ **Conversion or size of reactors In real reactor depends on i) residence time distribution (RTD) , ii) kinetics and iii) mixing pattern**

Measurement of Residence time distribution (RTD)

- The RTD is determined experimentally by **injecting a tracer into the reactor** and then measuring the tracer concentration in the effluent stream as a function of time.

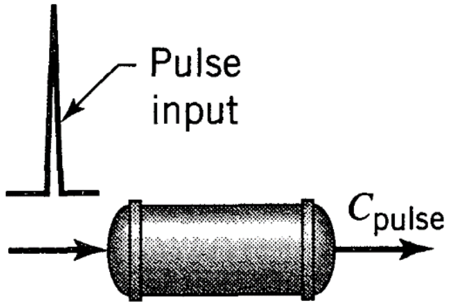
Physical properties of tracer

- ✓ Nonreactive species
- ✓ Easily detectable,
- ✓ Physical properties similar to reacting mixture
- ✓ Completely soluble in the mixture.
- ✓ It also should not adsorb on the walls or other surfaces in the reactor.

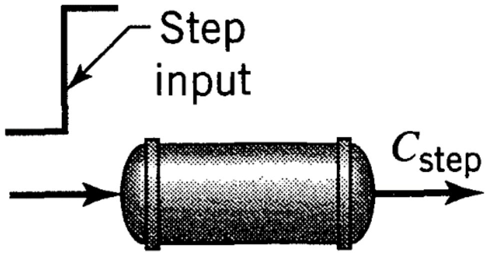
- ➢ Colored and radioactive materials are the most common types of tracers.

Method of injection

- Pulse input
  - ➢ Instantaneously introduce of tracer into the fluid entering the vessel
  - ➢ Ideal pulse input (shot) is a spike of infinite height and zero width

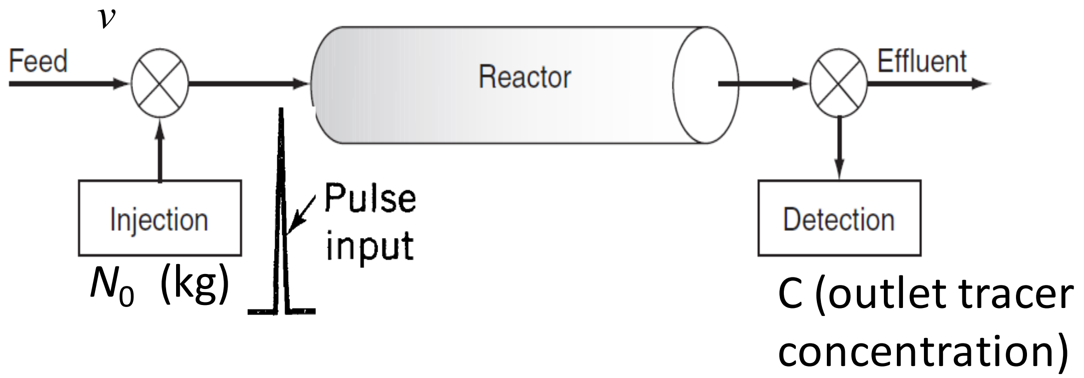


- Step input
  - ➢ **Step input:** Switch from ordinary fluid to fluid with tracer of concentration

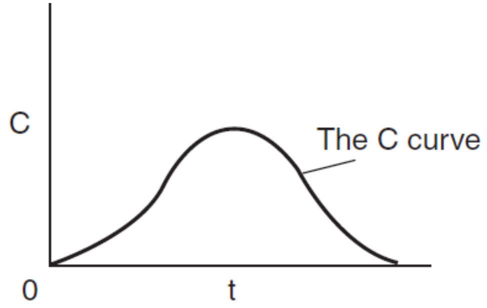


RTD by pulse injection of tracer

- An amount of tracer N_0 (kg) is suddenly injected in one shot into the feed stream entering the reactor in as short a time as possible.
- The outlet concentration of tracer (C) is then measured as a function of time.



- let Δt sufficiently small that the concentration of tracer, $C(t)$, exiting between time t and $t+\Delta t$ is essentially the same.



- The amount of tracer material, ΔN, leaving the reactor between time t and $t+\Delta t$ is then

$$\Delta N = C(t)v\ \Delta t$$

(v is the effluent volumetric flow rate).

C curve: The effluent concentration–time curve is referred to as the **C curve** in RTD analysis.

- Therefore, ΔN is the amount of material exiting the reactor that has spent an amount of time between t and $t + \Delta t$ in the reactor. Therefore,

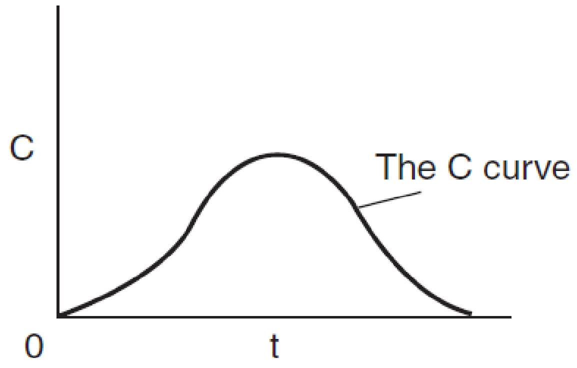
$$\frac{\Delta N}{N_0} = \frac{vC(t)}{N_0}\Delta t$$

which represents the fraction of material that has a residence time in the reactor between time t and $t + \Delta t$.

Cont.

For pulse injection it is defined, $$E(t) = \frac{vC(t)}{N_0}$$

$$\frac{\Delta N}{N_0} = E(t)\,\Delta t$$



The quantity ***E(t)*** is called the ***residence-time distribution function***.

- It is the function that describes in a quantitative manner **how much time different fluid elements have spent in the reactor**

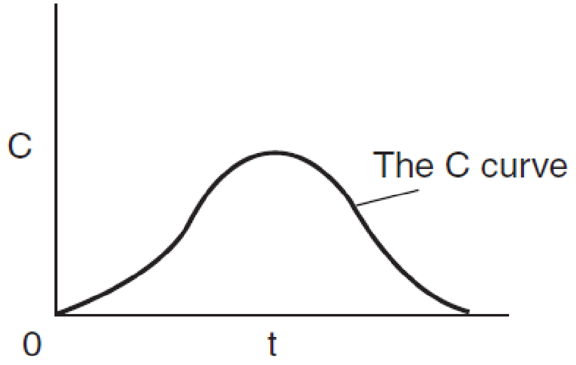
- ***E*(*t*) is also called** the ***exit-age distribution function***. "age" of an atom as the time it has resided in the reaction environment, then *E*(*t*) concerns the age distribution of the effluent stream. It characterizes the lengths of time various atoms spend at reaction conditions.

- The quantity *E*(*t*)*dt* is the fraction of fluid exiting the reactor that has spent between time *t* and *t* + *dt* inside the reactor.

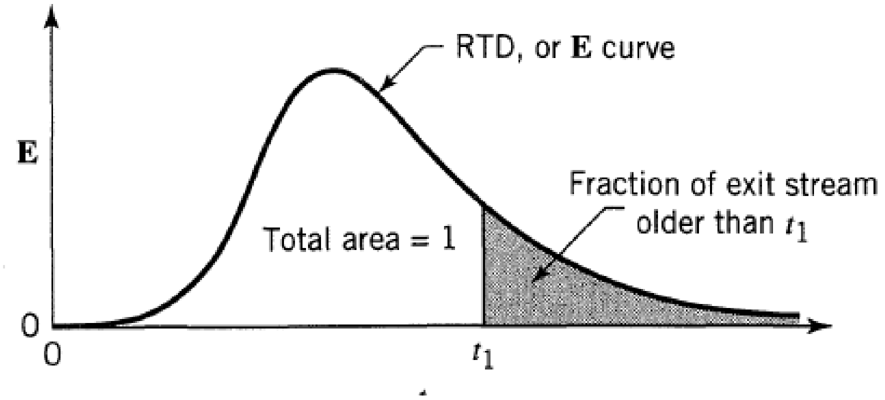
$$N_0 = \int_0^\infty vC(t)\,dt$$

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

Cont.

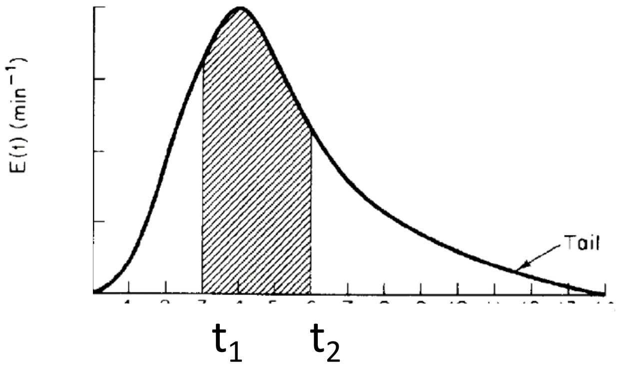


$$E(t) = \frac{C(t)}{\int_0^{\infty} C(t)\,dt}$$



- Fraction of all the material that has resided for a time *t* in the reactor between *t*=0 and *t*=t_1 *is* $\int_0^{t_1} E(t)dt$
- Fraction of all the material that has resided for a time older than t_1 *is* $\int_{t_1}^{\infty} E(t)dt$

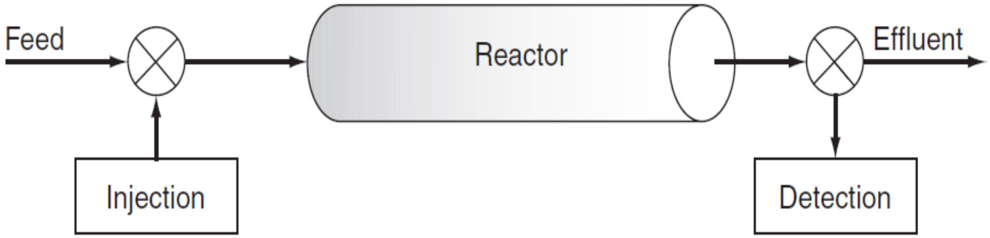
$$\left[\begin{array}{c}\text{Fraction of material leaving the reactor}\\ \text{that has resided in the reactor}\\ \text{for times between } t_1 \text{ and } t_2\end{array}\right] = \int_{t_1}^{t_2} E(t)\,dt$$



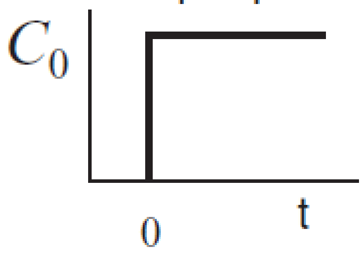
- fraction of all the material that has resided for a time *t* in the reactor between *t*=0 and *t=infinite* is 1; therefore,

$$\boxed{\int_0^{\infty} E(t)\,dt = 1}$$

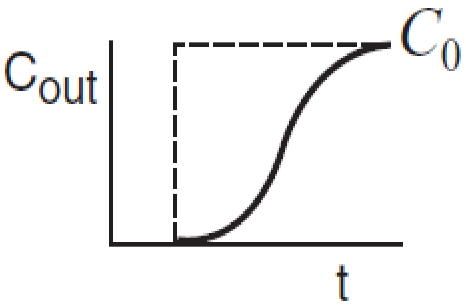
RTD using step injection of tracer



Step Input

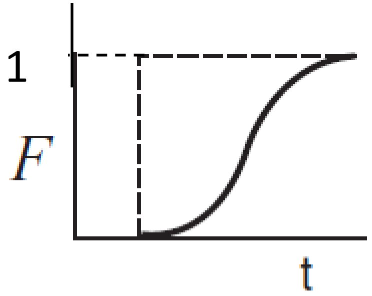


$$C_0(t) = \begin{cases} 0 & t < 0 \\ (C_0)\ \text{constant} & t \geq 0 \end{cases}$$



C_{out} (outlet tracer concentration)

$$F(t) = \left[\frac{C_{out}}{C_0}\right]_{step}$$



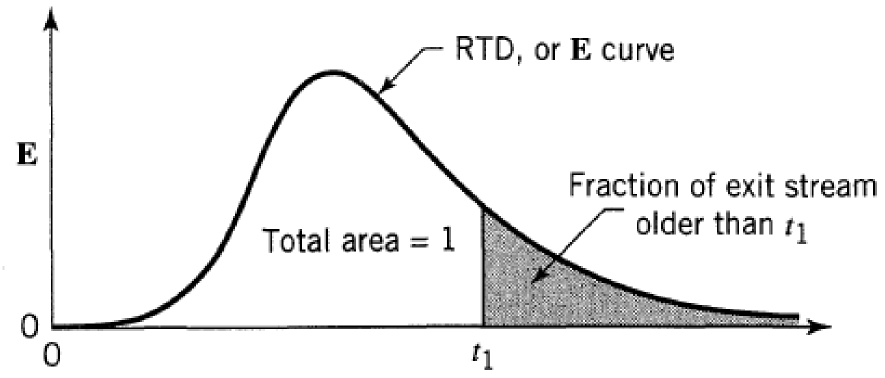
F-curve: cumulative distribution

$$\int_0^t E(t)\,dt = \left[\begin{array}{c}\text{Fraction of effluent}\\ \text{that has been in reactor}\\ \text{for less than time } t\end{array}\right] = F(t)$$

$$\int_t^\infty E(t)\,dt = \left[\begin{array}{c}\text{Fraction of effluent}\\ \text{that has been in reactor}\\ \text{for longer than time } t\end{array}\right] = 1 - F(t)$$

Mean residence time (t_m) and variance (σ^2)

$$\boxed{t_m = \frac{\int_0^\infty tE(t)\,dt}{\int_0^\infty E(t)\,dt} = \int_0^\infty tE(t)\,dt}$$



$$\boxed{\sigma^2 = \int_0^\infty (t - t_m)^2 E(t)\,dt}$$

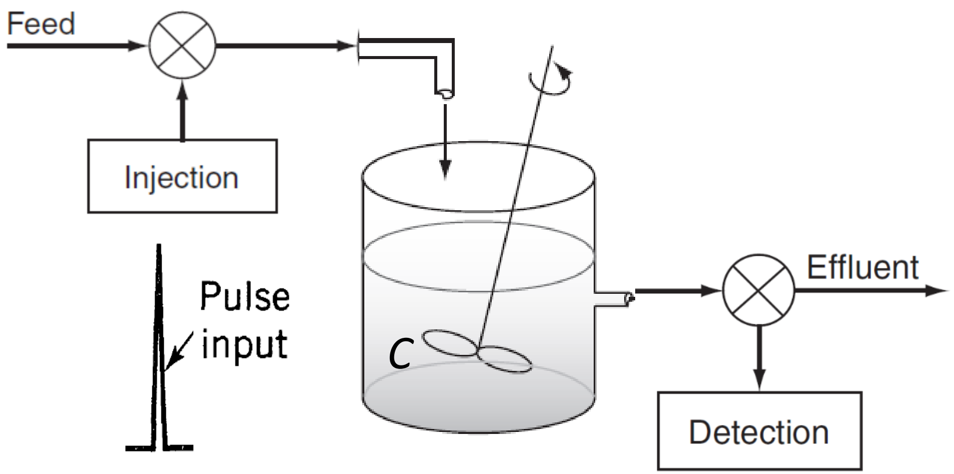
$$\sigma^2 = \int_0^\infty t^2 E(t)dt - 2t_m \int_0^\infty tE(t)dt + t_m^2 \int_0^\infty E(t)dt$$

$$= \int_0^\infty t^2 E(t)dt - 2t_m^2 + t_m^2$$

$$\boxed{\sigma^2 = \int_0^\infty t^2 E(t)dt - t_m^2}$$

RTD of ideal CSTR

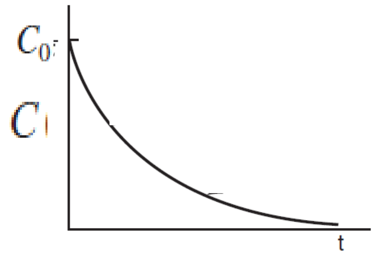
- In an ideal CSTR (perfectly mixed) the concentration of any substance in the effluent stream is identical to the concentration throughout the reactor.



A material balance on an **inert tracer** that has been injected **as a pulse** at time ***t*=0 into a CSTR yields for *t* > 0**

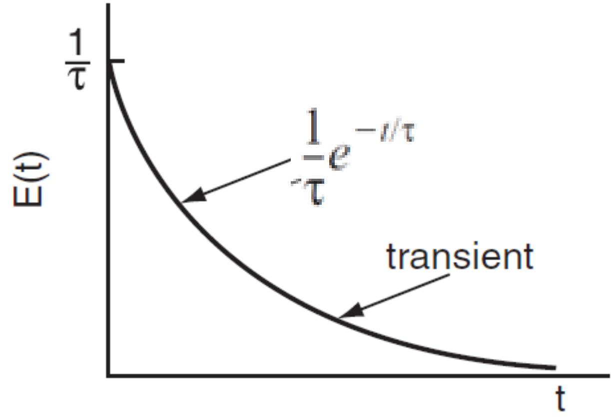
$$\text{In} - \text{Out} = \text{Accumulation}$$

$$\overbrace{0} - \overbrace{vC} = \overbrace{V\frac{dC}{dt}}$$



$$C(t) = C_0 e^{-t/\tau}$$

$$\boxed{E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt} = \frac{C_0 e^{-t/\tau}}{\int_0^\infty C_0 e^{-t/\tau}\,dt} = \frac{e^{-t/\tau}}{\tau}}$$



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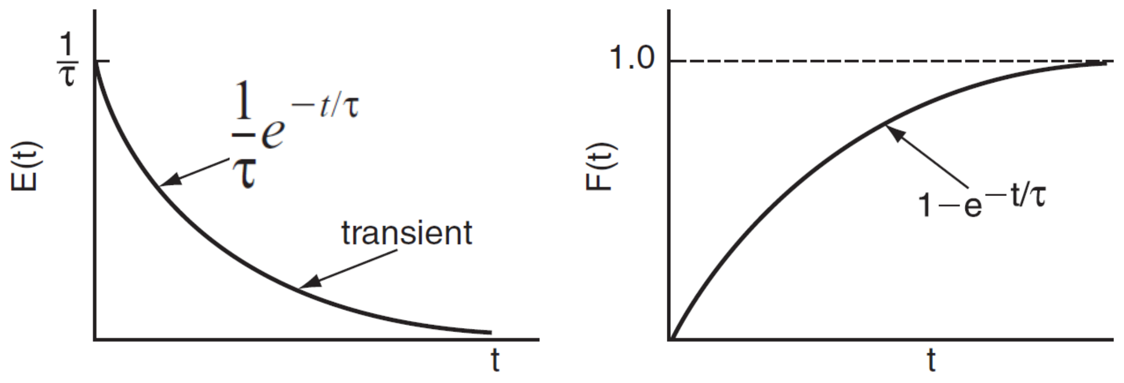
F-curve of ideal CSTR: $$F(t) = \int_0^t E(t)dt = 1 - e^{-t/\tau}$$



Mean residence time of ideal CSTR: $$t_m = \int_0^\infty tE(t)\,dt = \int_0^\infty \frac{t}{\tau}\,e^{-t/\tau}\,dt = \tau$$