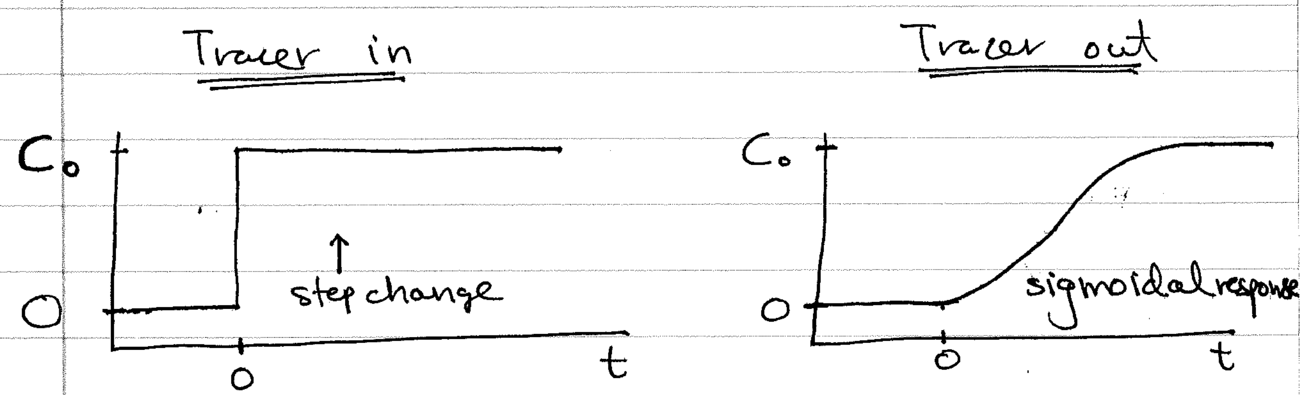
Variations in tracer input to CSTR

(1) In the example considered earlier, we merely added a drop of ink. Once that was done, we did not add any more ink.

This experiment was a <u>pulse input expt.</u>

(2) In the second case, let's vary the tracer input. Consider the following case:



The tracer concentration in the inlet is given by:

$$\left.\begin{aligned} C(t) &= 0 \qquad t < 0 \\ &= C_0 \qquad t \geq 0 \end{aligned}\right\} \text{ def}^{n}\text{. of step change}$$

Recollect:

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

& $$\int_{t_1}^{t_2} E(t)\,dt = \text{Fraction of tracer leaving between } t_1 \,\&\, t_2$$

→ (a)

At any given moment of time, the exit concentration of tracer is a fraction of the inlet concentration. After a given time, the inlet & outlet concentrations become equal.

$$\therefore\ C_{out} = C_0 \times \left\{ \begin{array}{c}\text{some}\\ \text{fraction}\end{array} \right\}$$

From (a), if $t_1 = 0$ & $t_2 = t$

$$\int_0^t E(t)\,dt = \text{fraction of tracer leaving after } t$$

can be interpreted as fraction of tracer that has been inside reactor for $\leq t$

$$\therefore \quad C_{out} = C_o \times \left(\begin{array}{l} \text{fraction of} \\ \text{tracer that} \\ \text{leaves after } t \end{array} \right)$$

$$\therefore \quad C_{out} = C_o \int_0^t E(t)\,dt$$

$$\therefore \quad \frac{C_{out}}{C_o} = \int_0^t E(t)\,dt$$

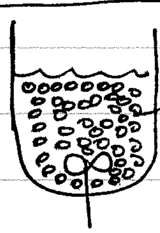
also defined as $F(t)$

$$\boxed{\therefore \quad \int_t^\infty E(t)\,dt = 1 - F(t)}$$

$F(t) \equiv$ fraction that leaves after t
(or fraction that has been inside reactor for $\leq t$)

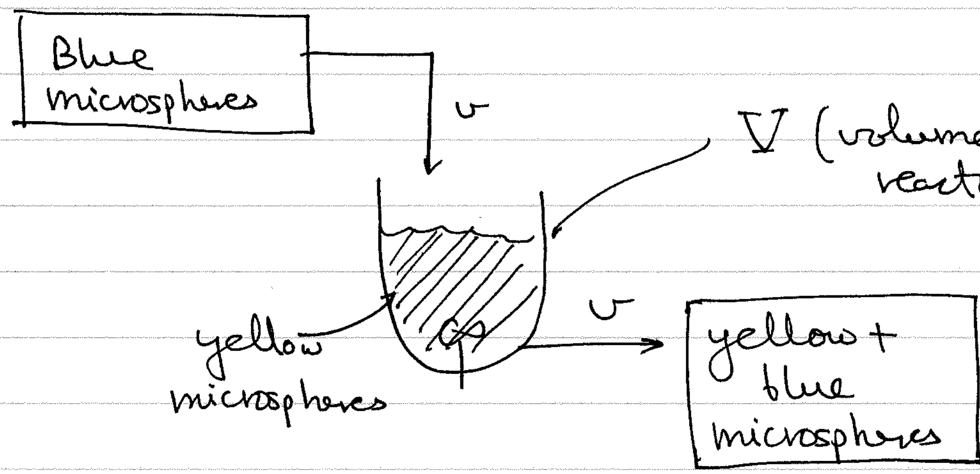
$\Rightarrow$ Consider the following thought experiment:

$\boxed{\text{Goal: prove } \tau = t_m}$



yellow microspheres @ $t = 0$

We start introducing a volumetric flowrate v that contains blue microspheres



Consider a very small time window dt

In this window, the volume of liquid that leaves the reactor is

$$v\,dt$$

Fraction of molecules in reactor for $\leq t$ $F(t)$

$> t$ $1-F(t)$

$\therefore$ Volume change of yellow molecules:

$$dV = v\,dt\left[1-F(t)\right]$$

yellow molecules are older

$$\therefore \quad V = \int_0^\infty v\,dt\,[1 - F(t)]$$

volume of all yellow molecules

At steady state, $v \equiv$ constant

$$\therefore \quad V = v \int_0^\infty [1 - F(t)]\,dt$$

keep in this form for simpler math

Remember integration by parts:

$$\int x\,dy = xy - \int y\,dx$$

$$\therefore \int \underbrace{[1 - F(t)]}_{\text{'}x\text{'}} \underbrace{dt}_{\text{'}dy\text{'}} = [1 - F(t)]\,t - \int t\,d[1 - F(t)]$$

$$d(1 - F(t)) = -\,dF(t)$$

$$\therefore \int [1 - F(t)]\,dt = [1 - F(t)]\,t + \int t\,dF(t)$$

$$\therefore \frac{V}{v} = \left[\{1 - F(t)\}t + \int t\,dF(t)\right]_0^{\infty}$$

$\nwarrow$ time limits

$$\therefore \frac{V}{v} = [1 - F(t)]t\Big|_0^{\infty} + \int_0^1 t\,dF(t)$$

F(t) limits (0 to 1)

At $t \to \infty$, fraction of molecules that are in the reactor for $\leq \infty$ is $\underline{\underline{1}}$

$$\therefore \frac{V}{v} = \int_0^1 t\,dF(t)$$

$$\therefore \tau = \int_0^1 t\,dF(t) \quad \ldots \frac{V}{v} = \tau$$

Also, $F(t) = \int_0^t E(t)\,dt$

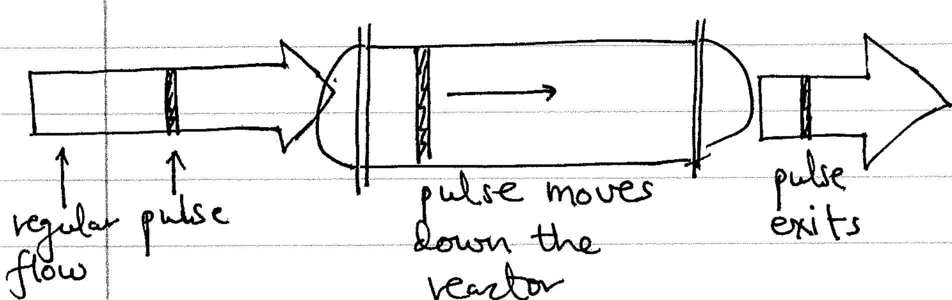
i.e. $dF(t) = E(t)\,dt$ ...{limits 0 to ∞}

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

$$\therefore \quad \tau = t_m$$

* RTDs in different reactors

(1) PFRs + pulse input



For an ideal reactor, the pulse experiment should produce a Dirac Delta fn.

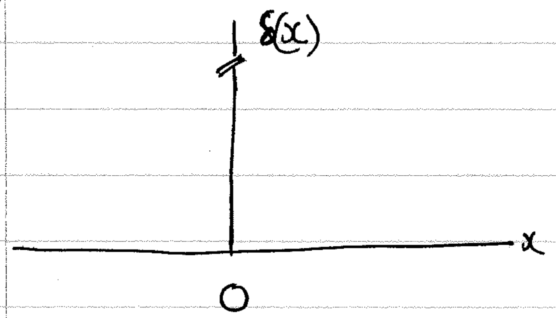
Dirac Delta fn: $\delta(x) = 0$ when $x \neq 0$

$= \infty$ when $x = 0$

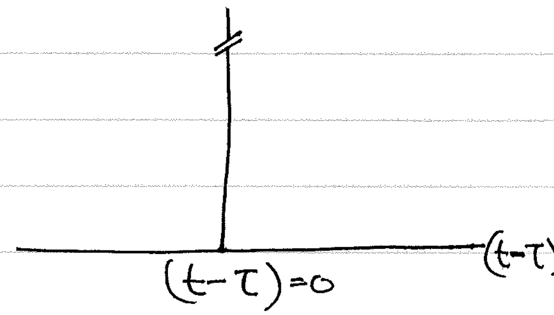
Also $$\int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

$$\int_{-\infty}^{\infty} g(x)\,\delta(x-\tau)\,dx = g(\tau)$$

For the PFR :



Dirac delta $\delta(x)$



PFR

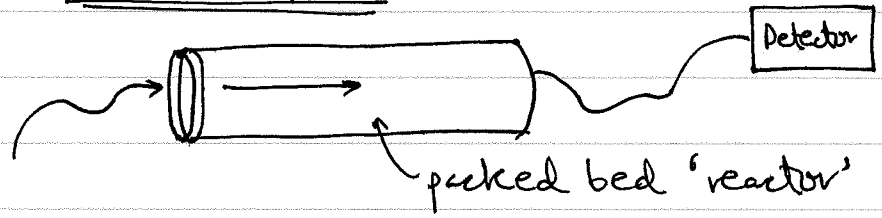
$\therefore$ The tracer RTD, $\boxed{E(t) = \delta(t-\tau)}$

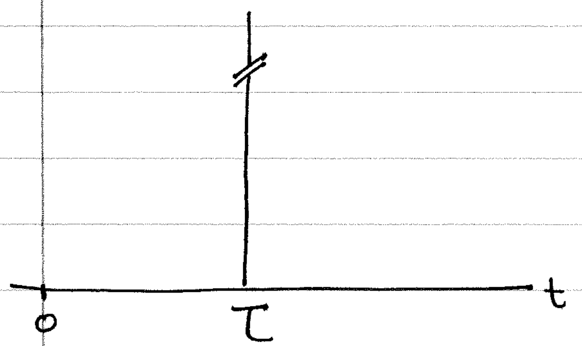
If $g(t) = t$

$$t_m = \int_0^{\infty} g(t)\,\delta(t-\tau)\,dt = g(\tau)$$

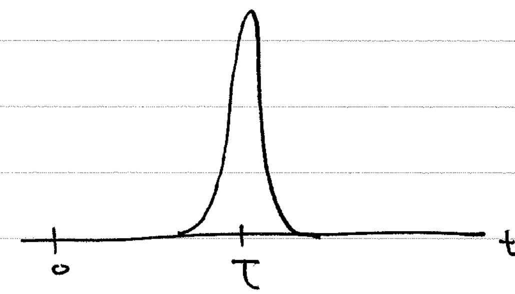
$\therefore \quad t_m = \tau \Longrightarrow$ ideal PFR

② Non-ideal PFR : e.g. chromatography
+ pulse input





Ideal PBR



Real PBR

(band separation due to interaction with column & column heterogeneity)

3 Ideal CSTR + pulse input

Let's revisit the problem with mole balances.

For the tracer:

Accumulation = Input − Output

$$\therefore \; V \frac{dC}{dt} = \underset{\substack{\uparrow \\ \text{post-pulse}}}{0} - v C$$

$$\therefore \; V \frac{dC}{dt} = - v C$$

$$\therefore \frac{dC}{dt} = -\frac{C}{\tau}$$

$$\therefore \ln C = -\frac{t}{\tau} + \gamma$$

$$\gamma = \ln C_0 \quad \cdots\cdot \quad C(0) = C_0$$

$$\therefore \ln\left(\frac{C}{C_0}\right) = -\frac{t}{\tau}$$

$$\boxed{\therefore \frac{C}{C_0} = \exp\left(-\frac{t}{\tau}\right)} \quad \text{..... Ideal CSTR}$$

For an ideal CSTR, $E(t)$ is:

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

$$\therefore E(t) = \frac{\exp(-t/\tau)}{\int_0^\infty \exp(-t/\tau)\,dt}$$

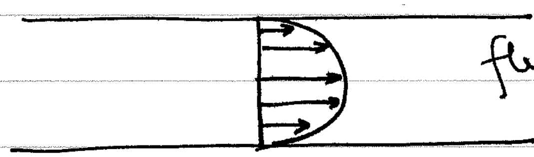
$$\therefore E(t) = \frac{\exp(-t/\tau)}{\left[\exp(-t/\tau) \times -\tau\right]_0^\infty}$$

$$\therefore E(t) = \frac{\exp(-t/\tau)}{\tau}$$

$$\boxed{\therefore E(t) = \frac{1}{\tau} \exp(-t/\tau)}$$

(4) Laminar flow reactor (LFR)

(anti-thesis of a PFR!)



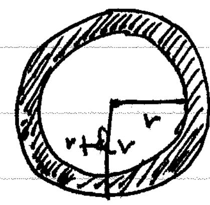
fluid velocity is a fn. of the radius of the reactor

$$U = \underbrace{U_{max}}_{\text{centre line velocity}} \left[1 - \left(\frac{r}{R}\right)^2\right]$$

But $U_{max} = 2 \underbrace{U_{avg}}_{\text{average velocity in the reactor (related to } v_0)}$

$$\therefore U = 2 U_{avg} \left[1 - \left(\frac{r}{R}\right)^2\right]$$

$$\therefore \quad u = \frac{2v_0}{\pi R^2}\left[1 - \left(\frac{r}{R}\right)^2\right]$$



the volume of fluid passing through this annular cross section is given by:

$$dv = U(r)\,\underbrace{2\pi r\,dr}$$

$$\Downarrow$$

$$= \pi(r+dr)^2 - \pi r^2$$

$$\therefore \underbrace{\frac{dv}{v_0}}_{\text{fraction of total fluid passing through annulus}} = \frac{U(r)\,2\pi r\,dr}{v_0}$$

↳ if I were to introduce a tracer pulse, the amount of tracer molecules passing through in a time interval dt would be related to $\underline{dv/v_0}$.

In fact, the fraction of tracer leaving the annulus in dt would be equal to the fraction of the total fluid passing through the annulus.

$$\therefore \quad E(t)\,dt = \frac{dv}{v_0} = \frac{U(r)\,2\pi r\,dr}{v_0}$$

$$\therefore \quad E(t)\,dt = \frac{2U_{avg}}{v_0}\left[1-\left(\frac{r}{R}\right)^2\right] 2\pi r\,dr$$

$$\therefore \quad E(t)\,dt = \frac{2\cancel{v_0}}{\cancel{\pi}R^2\cancel{v_0}}\left[\frac{R^2-r^2}{R^2}\right] 2\cancel{\pi}r\,dr$$

$$\therefore \quad E(t)\,dt = \frac{2}{R^4}\left(R^2-r^2\right) 2r\,dr$$

$$\boxed{\therefore \quad E(t)\,dt = \frac{4}{R^4}\left(R^2-r^2\right) r\,dr} \rightarrow (1)$$

If the reactor is of length L,

$$\underset{\substack{\uparrow \\ \text{residence} \\ \text{time}}}{t(r)} = \underset{\left\{\frac{\text{length}}{\text{speed}}\right\}}{\frac{L}{U(r)}} = \frac{L}{\frac{2v_0}{\pi R^2}\left(1-\frac{r^2}{R^2}\right)}$$

$$t(r) = \frac{L}{\frac{2v_0}{\pi R^2}\left(\frac{R^2-r^2}{R^2}\right)} = \frac{\pi L R^4}{2v_0(R^2-r^2)}$$

But $V = \pi R^2 L$ & $\frac{V}{v_0} = \tau$ ← res. time of ideal reactor

$$\boxed{\therefore \quad t(r) = \frac{\tau R^2}{2(R^2-r^2)}} \longrightarrow (2)$$

$$\therefore \quad \frac{dt}{dr} = \frac{\tau R^2}{2}\left[-1\left(R^2-r^2\right)^{-2} \times (-2r)\right]$$

$$\therefore \quad \frac{dt}{dr} = \frac{\tau R^2}{2}\left[\frac{2r}{(R^2-r^2)^2}\right]$$

$$\therefore \quad \frac{dt}{dr} = \frac{\tau r R^2}{(R^2-r^2)^2}$$

$$\therefore \quad dt = \frac{\tau r R^2}{(R^2-r^2)^2}\, dr$$

But $t = \frac{\tau R^2}{2(R^2-r^2)}$ i.e. $t^2 = \frac{\tau^2 R^4}{4(R^2-r^2)^2}$

$$\therefore \; dt = \frac{\tau R^2}{(R^2 - r^2)} \left[\frac{r}{(R^2 - r^2)} \right] dr$$

$$\boxed{\therefore \; dt = \frac{2t}{R^2 - r^2} \, r \, dr} \longrightarrow (3)$$

$$\boxed{\text{Also,} \quad t^2 = \frac{\tau^2 R^4}{4 (R^2 - r^2)^2}} \longrightarrow (4)$$

Subst. (3) in (1) :

$$E(t) \, dt = \frac{4}{R^4} (R^2 - r^2) \frac{(R^2 - r^2) \, dt}{2t}$$

$$\therefore \quad E(t) = \frac{4 (R^2 - r^2)^2}{R^4} \left(\frac{1}{2t} \right)$$

Subst. (4) into

$$\therefore \; E(t) = \frac{\tau^2}{t^2} \left(\frac{1}{2t} \right)$$

$$\boxed{\therefore \; E(t) = \frac{\tau^2}{2t^3}}$$

Least amount of time a fluid particle spends inside the reactor is:

$$t_{min} = \frac{L}{u_{max}} = \frac{L}{2u_{avg}} = \frac{L}{2\left(\frac{v_o}{\pi R^2}\right)}$$

$$\therefore \quad t_{min} = \frac{L\pi R^2}{2v_o} = \frac{\tau}{2}$$

$$\boxed{\begin{aligned} \therefore \quad E(t) &= 0 \quad \text{for} \quad t < \frac{\tau}{2} \\ \& \quad E(t) &= \frac{\tau^2}{2t^3} \quad \text{for} \quad t \geq \frac{\tau}{2} \end{aligned}}$$

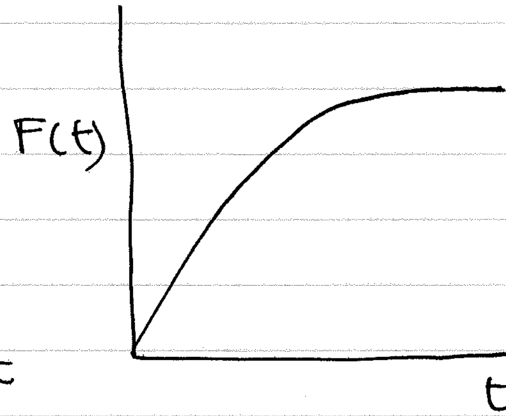
Diagnostics

1) CSTR : Ideal CSTR

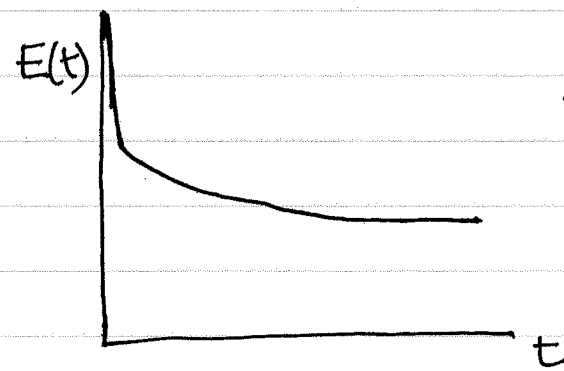
$$E(t) = \frac{1}{\tau}\exp\left(\frac{-t}{\tau}\right)$$

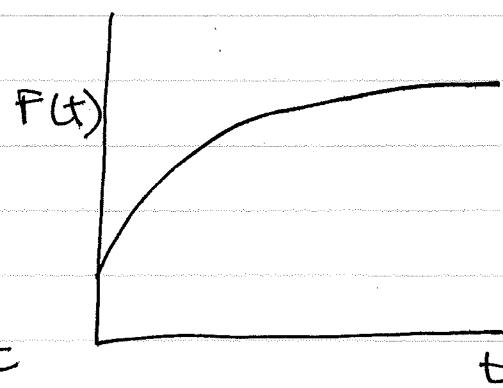
By-pass & dead volume : 2 most common problems

Regulor :

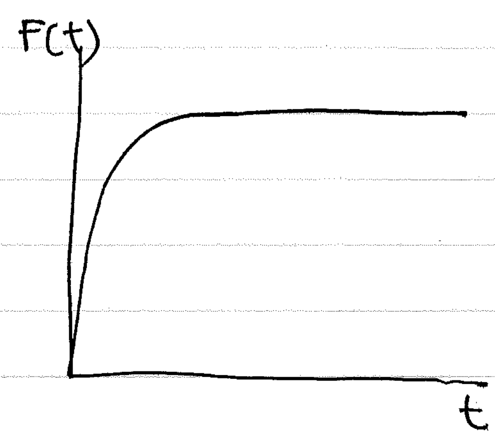


By-pass :

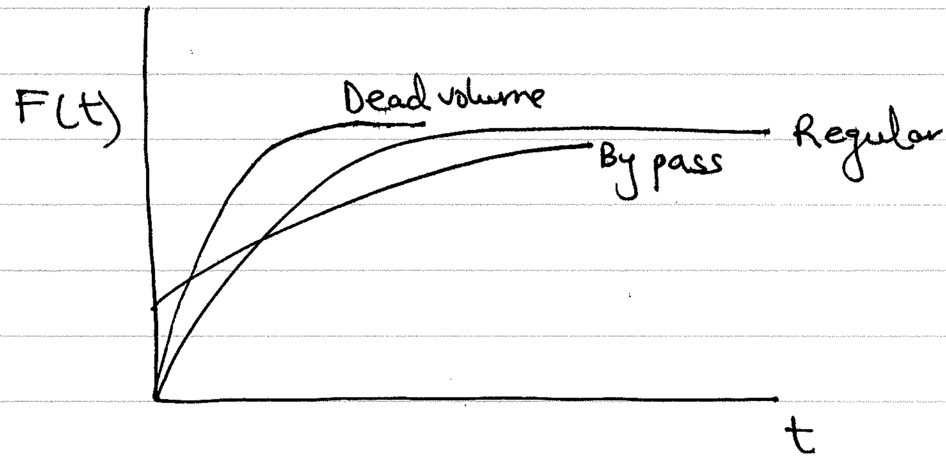




Dead volume :

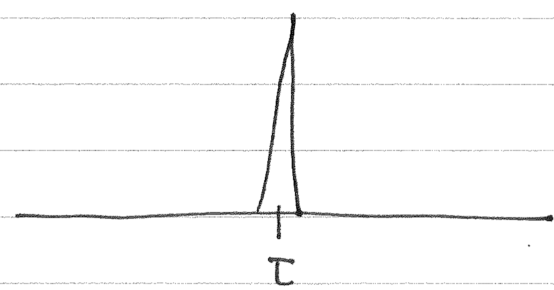


Summary:



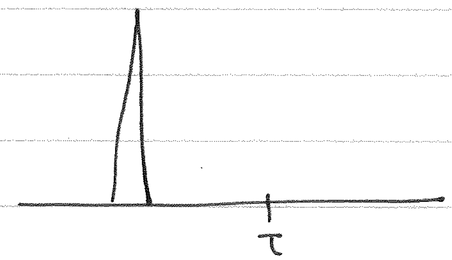
PFR: $E(t) = \delta(t-\tau)$

Regular:



By-pass:

Dead volume :



Modeling methologies for non-ideal reactors

The general approach is to describe the reactor as a combination of ideal reactors or similar assumptions.

There are 5 major ways to do this:

1. Segregation model
2. Maximum mixedness model
3. Tanks-in-series model
4. Dispersion model
5. Combination of ideal reactors

We will look at segregation model, tanks-in-series & combination of reactors.