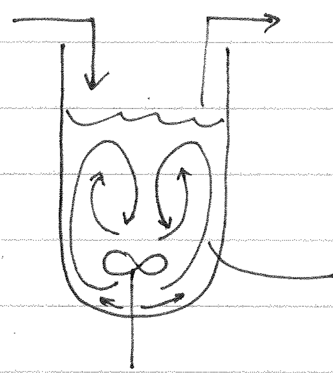
Non-ideality part 2: Mixing

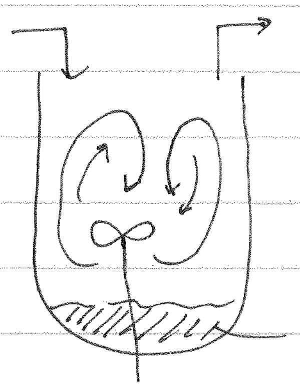
* Nothing in real life is ideal

* Far from it, really!



Ideal CSTR

concentration uniform
no dead zones



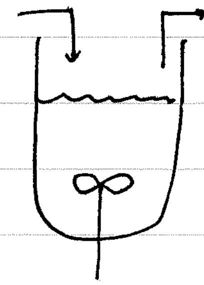
dead zones

possibly due to impeller geometry

NON-IDEAL MIXING

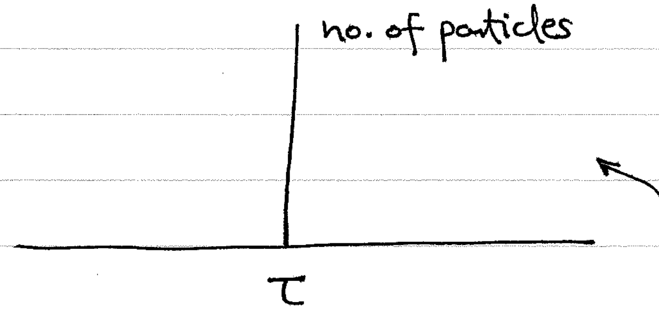
Residence Time Distribution

Ideal reactor :
CSTR



What is the amount of time spent by a reactant molecule in the reactor?

residence time = $\tau = \frac{V}{v}$

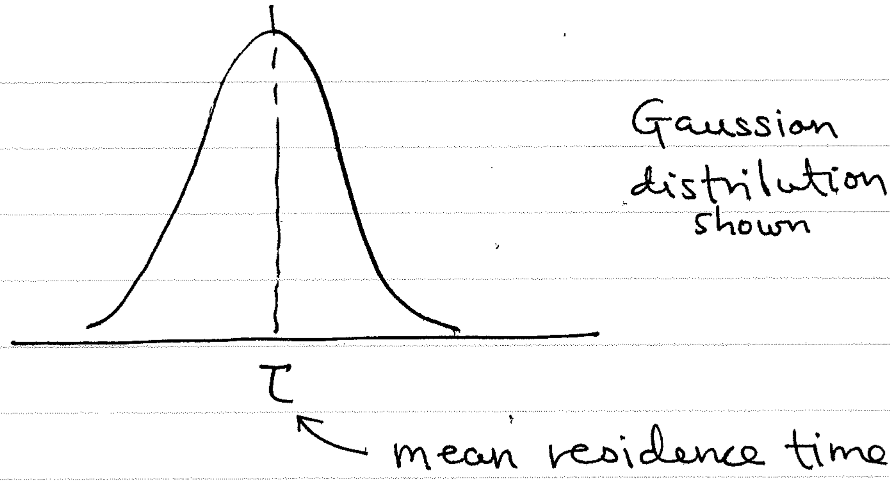


this is what the distribution looks like

What happens if there are non-idealities?

* some molecules exit very quickly (by-pass)

* some stay within the reactor a bit too long

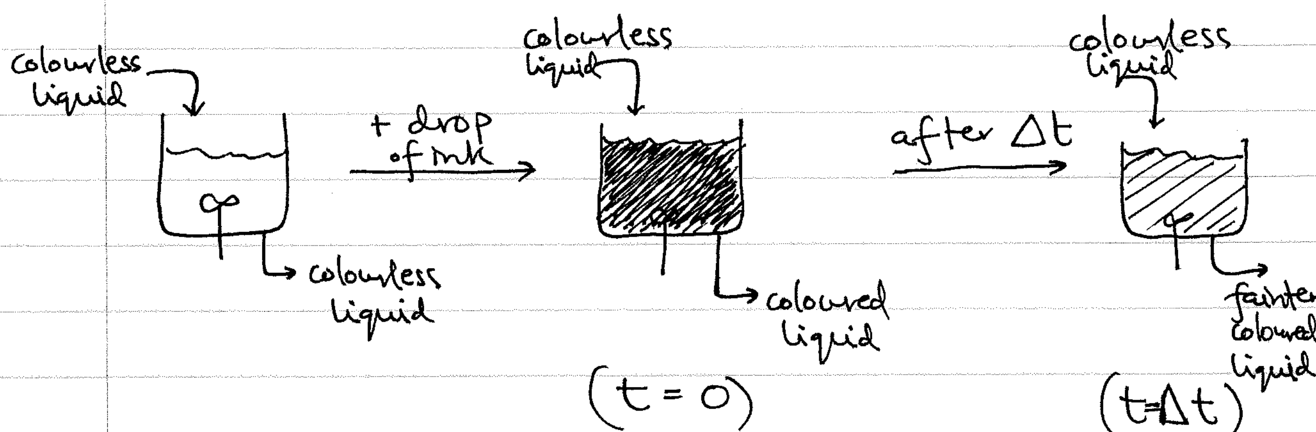


* Like everything in life, molecules too exhibit a distribution

* By studying the distribution, one can make very good assumptions regarding the source of the non-ideality

Consider the following experiment:

What happens if you introduce a drop of ink (non-reacting) into the CSTR ?



or 'tracer' (in technical parlance)

The ink is gradually washed out.

* If I introduce N_0 moles of ink at $t=0$

↳ the amount of ink leaving the reactor in a short time Δt is:

conc. of tracer

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

small enough so that $C(t)$ is approx. const. & we can discretize

Why func. of t?
mixing may or may not be ideal

$$\therefore \quad \frac{\Delta N}{N_0} = \frac{C(t)\, v\, \Delta t}{N_0}$$

fraction of tracer that has exited the reactor

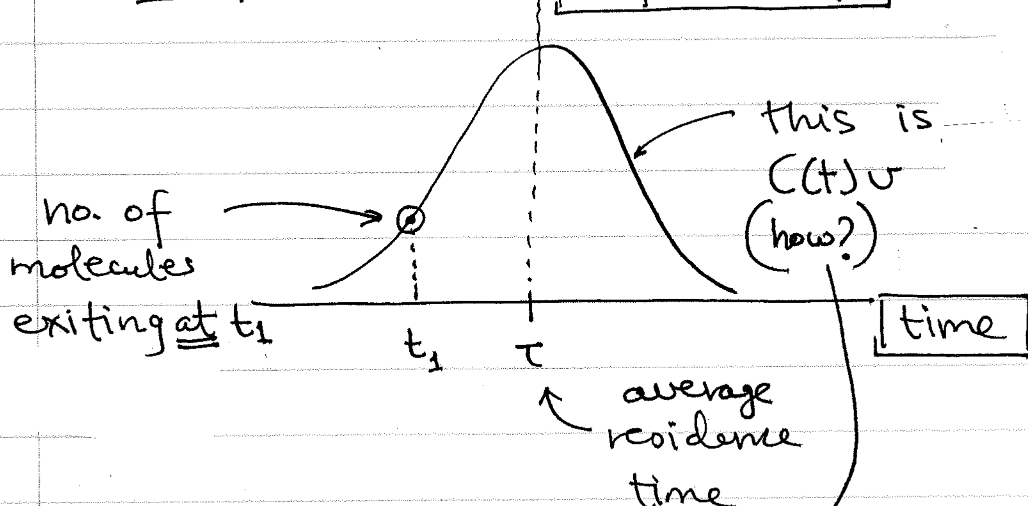
$$\therefore \quad \frac{\Delta N}{N_0} = \left[\frac{C(t)\, v}{N_0}\right] \Delta t$$

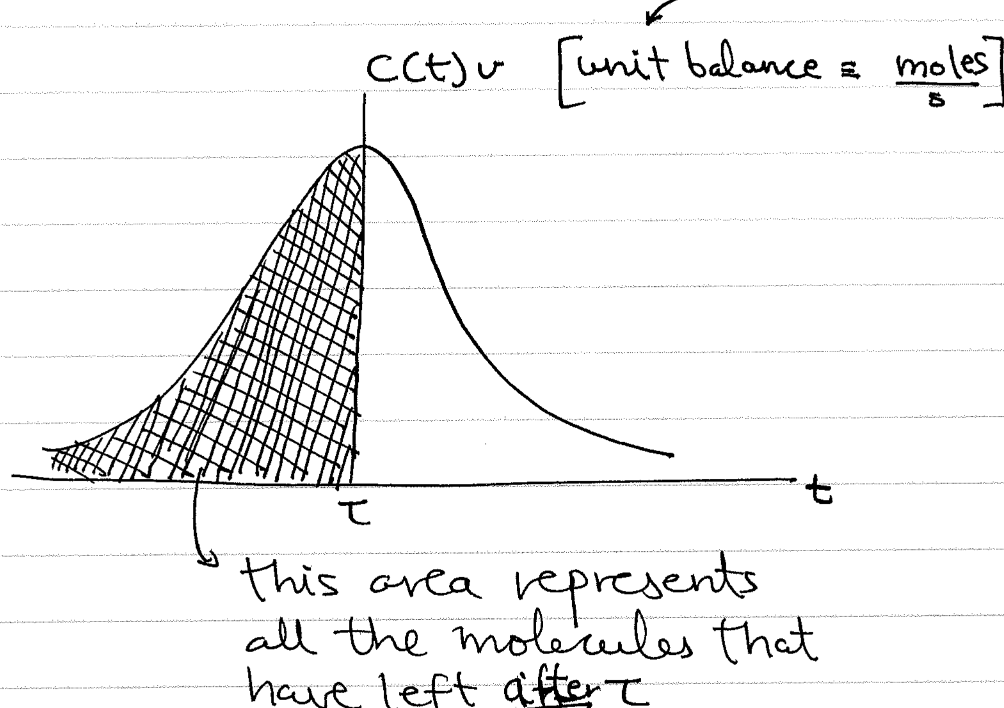
$\Downarrow$

$E(t)$ or the residence time distribution

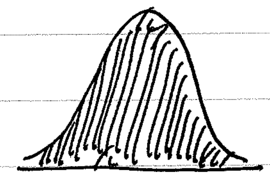
$$\therefore \quad \boxed{\frac{\Delta N}{N_0} = E(t)\,\Delta t \qquad \& \qquad E(t) = \frac{C(t)\,v}{N_0}} \Rightarrow 1$$

<u>Interpretation:</u>





$\therefore$ Area under the whole curve is the total # of molecules leaving in the entire duration of the study i.e. $\underline{\underline{N_0}}$.



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

Back to our definition:

$$\frac{\Delta N}{N_0} = E(t)\Delta t = \left[\frac{C(t)v}{N_0}\right]\Delta t$$

But $\quad \Delta N = C(t) v \Delta t \quad$ ... discretized form

$\therefore \quad dN = C(t) v\, dt \quad$ ... differential form

Therefore,

$$\frac{dN}{N_0} = E(t)\, dt$$

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

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

Based on this definition,

$$\left\{\begin{array}{l}\text{Fraction of material}\\ \text{that has resided}\\ \text{in the reactor}\\ \text{between } t_1 \;\&\; t_2\end{array}\right\} = \int_{t_1}^{t_2} E(t)\,dt$$

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

So what is needed to estimate $E(t)$?

* Just a measure of the tracer concentration in the exit stream at multiple time pts.

If you can collect data in the form:

t	- - - - - - -
C	- - - - - -

* you can use numerical integration to solve $E(t)$

Numerical integration recap:

Trapezoidal rule (2 pts.)

		Area of slice
X_0	Y_0	$\frac{(X_1 - X_0)}{2}\left[Y_0 + Y_1\right]$
X_1	Y_1	
X_2	Y_2	$\frac{(X_3 - X_2)}{2}\left[Y_2 + Y_3\right]$
X_3	Y_3	
X_4	Y_4	

Total area $= \sum$ slices

Simpson's 1/3rd rule (3 pts.)

X_0	Y_0	$\frac{(X_2 - X_0)}{6}\left[Y_0 + 4Y_1 + Y_2\right]$
X_1	Y_1	
X_2	Y_2	

Total area $= \sum$ slices

Simpson's 3/8th rule (4 pts.)

$$\left.\begin{array}{c|c|} X_0 & Y_0 \\ X_1 & Y_1 \\ X_2 & Y_2 \\ X_3 & Y_3 \end{array}\right\} \quad \frac{X_3 - X_0}{8}\left[Y_0 + 3Y_1 + 3Y_2 + Y_3\right]$$

Total area = $\sum$ slices

$\therefore$ For a typical RTD problem

2 questions → find $E(t)$ {standard}

→ what fraction of material left between t_1 & t_2 {easy, but longer}

Let's look @ the typical workflow

Major formulas: $E(t) = \dfrac{C(t)}{\int_0^\infty C(t)\,dt}$

$$\text{fraction} = \int_{t_1}^{t_2} E(t)\,dt$$

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

each data point

total area (i.e. $\sum$ slices)

time	Conc. tracer	Area of slice	$E(t)$
t_0	C_0	$\left(\frac{t_3 - t_0}{8}\right)\left[C_0 + 3C_1 + 3C_2 + C_3\right]$	C_0/α
t_1	C_1		C_1/α
t_2	C_2		C_2/α
t_3	C_3		C_3/α
t_4	C_4	$\left(\frac{t_7 - t_4}{8}\right)\left[C_4 + 3C_5 + 3C_6 + C_7\right]$	C_4/α
t_5	C_5		C_5/α
t_6	C_6		C_6/α
t_7	C_7		C_7/α

Total area $= \sum$ areas $= \alpha$

To find the fraction of material leaving between t_7 & t_4:

$$\text{fraction} = \int_{t_4}^{t_7} E(t)\,dt = \left[\frac{t_7 - t_4}{8}\right]\left\{E(t_4) + 3E(t_5) + 3E(t_6) + E(t_7)\right]$$

Mean residence time

Like any statistical distribution, the mean is calculated using the following formula:

$$\mu = \frac{\int_0^\infty x\, f(x)\, dx}{\int_0^\infty f(x)\, dx}$$ .... definition of mean using functions

$$\left\{ \mu = \int x\, P(x)\, dx \right.$$ .... using probability density fn. }

Why the difference?

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

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

$$\boxed{\therefore \quad t_m = \int_0^\infty t\, E(t)\, dt}$$ .... E(t) is likea probability density fn.