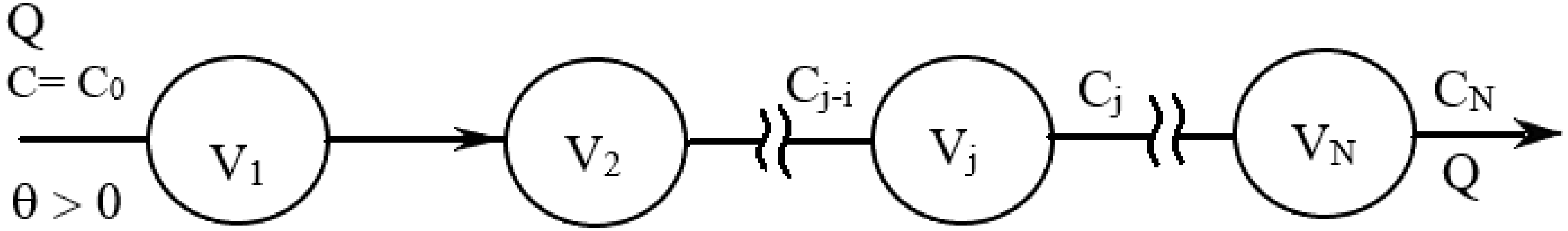
Series of Stirred –Tanks Model

If N number of tanks are connected in series. All tanks are of same size.



$$V_1 = V_2 \ldots\ldots.. = V_j = V_N$$

$$\bar{\theta}_t = \frac{NV_j}{Q} = \frac{V_t}{Q}$$

$Mole\ balance\ in\ jth\ tank:$

$$C_{j-1}Q - C_jQ = V_j\frac{dC_j}{d\theta}$$

For 1st tank

$$C_{j-1}Q - C_jQ = V_j \frac{dC_j}{d\theta}$$

$$(C_{j-1} - C_j)\frac{N}{\bar{\theta}_t} = \frac{dC_j}{d\theta} \quad it\ is\ a\ first\ order\ differential\ equation$$

For I.C. $\theta = 0,\ C_j = 0,$

$the\ solution\ is\ \frac{C_j}{C_0} = 1 - e^{-n\theta/\bar{\theta}_t}$

For 2nd tank

$$\frac{C_j}{C_0} = 1 - e^{-n\theta/\bar{\theta}_t}\left(1 + \frac{N\theta}{\bar{\theta}_t}\right)$$

For Nth tank

$$\frac{C_N}{C_0} = 1 - e^{-n\theta/\bar{\theta}_t}\left(1 + \frac{N\theta}{\bar{\theta}_t} + \frac{1}{2!}\left(\frac{N\theta}{\bar{\theta}_t}\right)^2 + \cdots + \frac{1}{(N-1)!}\left(\frac{N\theta}{\bar{\theta}_t}\right)^{N-1}\right)$$

$$\left(1 - \frac{C_N}{C_0}\right) = X_N = 1 - \frac{1}{\left(1 + \frac{k\bar{\theta}_t}{N}\right)^N}$$

For N= 1,2,3,4….N

$The\ J(\theta) = \frac{C_N}{C_0}$ can be plotted with the different number of tanks in series(N) to get various F-plot. Then experimental F-plot is compared to get ‘N’. Conversion can be calculated.

Experimental RTD

- If a pulse input is added and response from the exit is measured. We get C-plot.
- From C-plot, the E-plot is determined by the equation
- $E = \frac{C}{\int_0^\infty Cdt}, \quad where \int_0^\infty Cdt = \sum C\,\Delta t\ (for\ value\ of\ C$ $measured\ for\ descrete\ time\ at\ equal\ interval\ of\ time\ \Delta t)$

$$E = \frac{C}{\int_0^\infty Cdt} = \frac{C}{\sum C\,\Delta t}$$

E vs t plot is called RTD, residence time distribution

$$\bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt} \cong \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} \cong \sum t_i E_i \Delta t_i$$

Conversion directly from tracer information

$$\begin{pmatrix} Mean\ concentration \\ of\ reactant\ in\ exit \\ stream \end{pmatrix} = \sum_{\substack{all\ elements \\ of\ exit \\ stream}} \begin{pmatrix} concentration\ of\ reactant \\ remaining\ in\ an\ element\ of\ age \\ between\ t\ and\ t+dt \end{pmatrix} \begin{pmatrix} fraction\ of\ exit \\ streamof\ age\ between \\ t\ and\ t+dt \end{pmatrix}$$

$$\bar{C}_A = \int_{t=0}^{\infty} C_{A,element}\ E\ dt$$

For irreversible-first order reaction with constant density, the concentration in any element changes with time as follows:

$$ln \frac{C_{A,element}}{C_{A0}} = -kt \quad or \quad C_{A,element} = C_{A0} e^{-kt}$$

$$\frac{\bar{C}_A}{C_{A0}} = \sum e^{-kt} E \Delta t$$

For other reactions, prediction by RTD

For reversible first-order reaction with no product in feed:

$$\bar{C}_A = C_{A0} \int_0^\infty [1 - X_{Ae} + X_{Ae} e^{-kt/X_{Ae}}] \mathbf{E}\, dt$$

For successive first-order reaction with R as intermediate product.

$$\bar{C}_R = \frac{C_{A0} k_1}{k_2 - k_1} \int_0^\infty [e^{-k_1 t} - e^{-k_2 t}] \mathbf{E}\, dt$$

Spread of distribution

- Spread of distribution will describe the variance σ^2, defined as

$$\sigma^2 = \frac{\int_0^\infty (t-\bar{t})^2 C dt}{\int_0^\infty C dt} = \frac{\int_0^\infty t^2 C dt}{\int_0^\infty C dt} - \bar{t}^2$$

$$\sigma^2 \cong \frac{\sum t_i^2 C_i \Delta t_i}{\sum C_i \Delta t_i} - \bar{t}^2$$

$$\sigma^2 \cong \sum t_i^2 E_i \Delta t - \bar{t}^2$$

- For closed vessel Dispersion number is calculated from normalized variance $\sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2}$

$$\sigma_\theta^2 = 2\frac{D}{uL} - 2\left(\frac{D}{uL}\right)^2 \left(1 - e^{-uL/D}\right), \qquad D\ is\ same\ as D_L$$

$$No.of\ tanks = N \cong \frac{1}{\sigma_\theta^2}$$

Conversion by dispersion model(Ref: O. Levenspiel)

$$\frac{C_A}{C_{A0}} = 1 - X_A = \frac{4a \exp\left(\frac{1}{2}\frac{uL}{D}\right)}{(1+a)^2 \exp\left(\frac{a}{2}\frac{uL}{D}\right) - (1-a)^2 \exp\left(-\frac{a}{2}\frac{uL}{D}\right)}$$

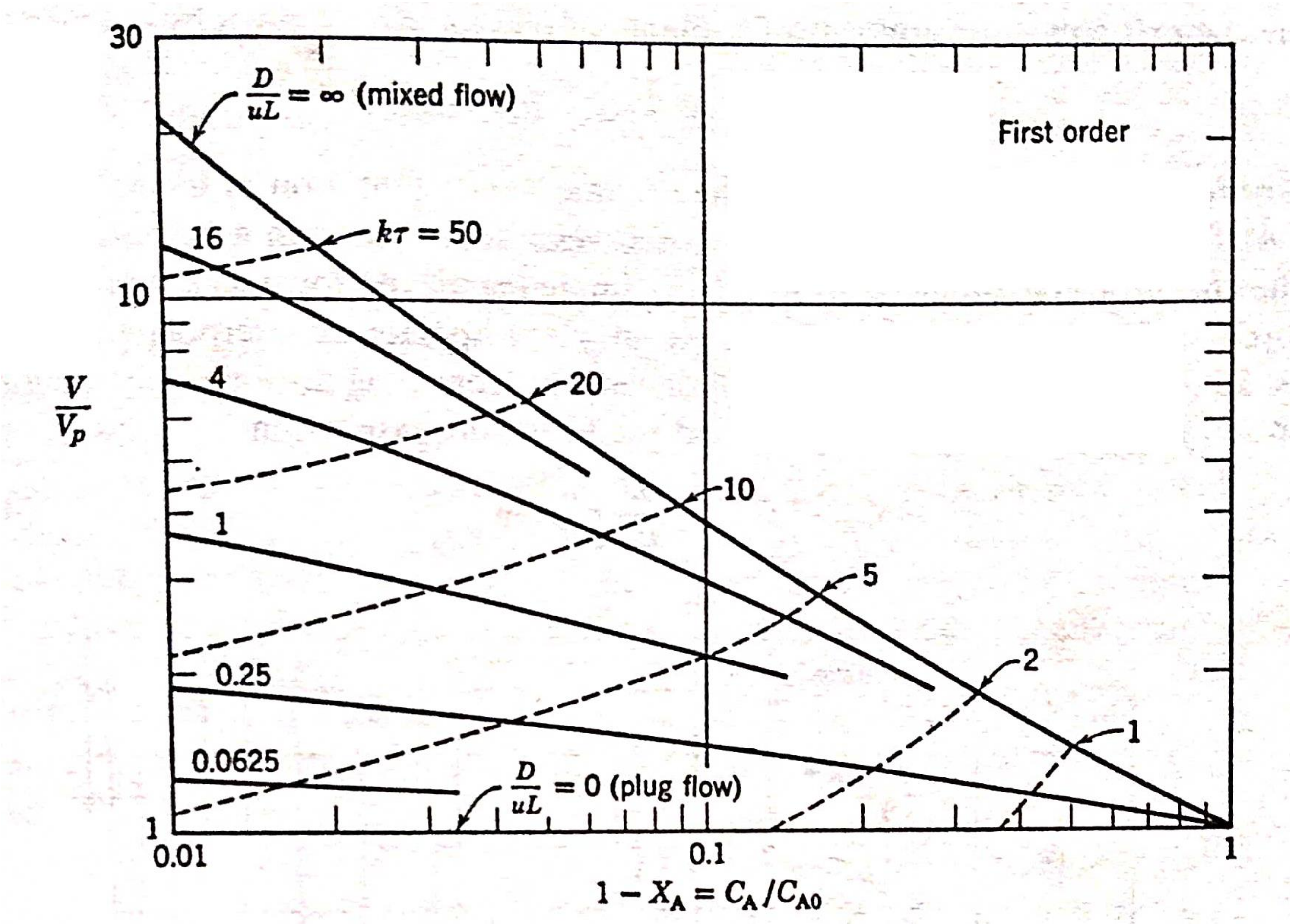
$$a = \sqrt{1 + 4k\tau(D/uL)}$$

For *small deviations from plug flow* D/uL becomes small, the **E** curve approaches gaussian, hence on expanding the exponentials and dropping higher order terms reduces to

$$\frac{C_A}{C_{A0}} = \exp\left[-k\tau + (k\tau)^2 \frac{D}{uL}\right]$$

$$= \exp\left[-k\tau + \frac{k^2\sigma^2}{2}\right]$$

Comparison real and plug flow reactor



Q.1 The response data to a pulse input in a closed vessel is given below, Construct the E-Curve and determine mean residence time.

t, min	0	5	10	15	20	25	30	35
C_{pulse} , g/L tracer output	0	3	5	5	4	2	1	0

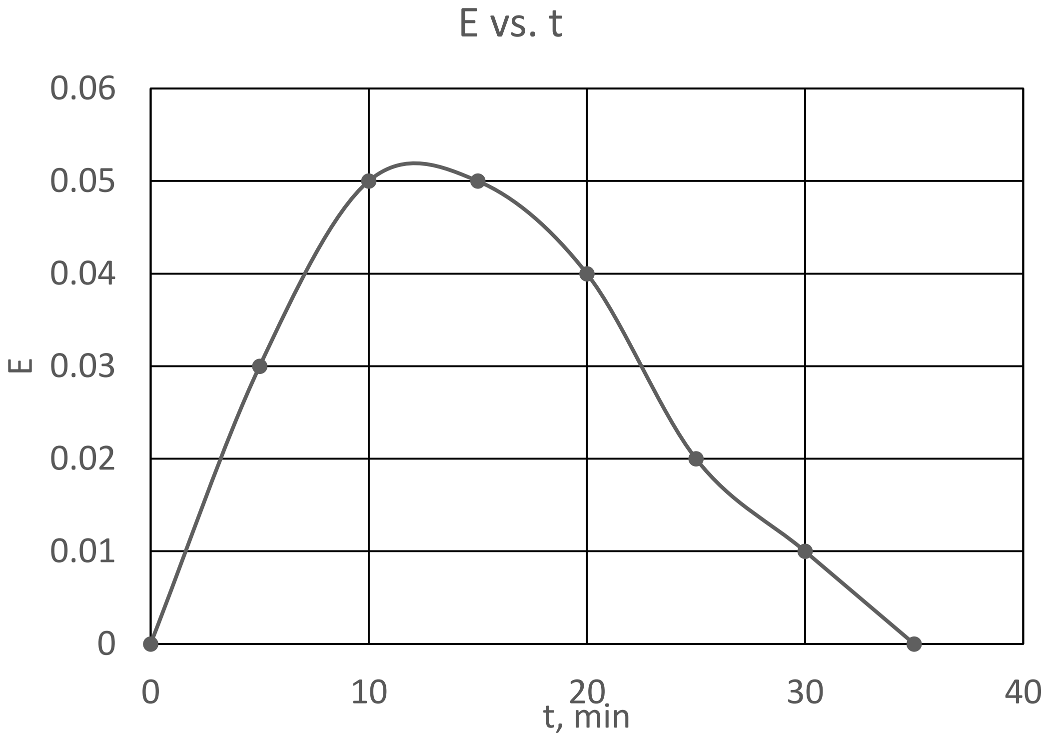
$$\bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt} \cong \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} \cong \sum t_i E_i \Delta t_i = \frac{\sum t_i C_i}{\sum C_i}$$

$$\bar{t} = \frac{\sum t_i C_i}{\sum C_i} = \frac{5 \times 3 + 10 \times 5 + 15 \times 5 + 20 \times 4 + 25 \times 2 + 30 \times 1 + 35 \times 0}{0 + 3 + 5 + 5 + 4 + 2 + 1 + 0} = 15min$$

$$\sum C_i \Delta t_i = (3 + 5 + 5 + 4 + 2 + 1) \times 5 = 100(g.min)/L$$

- $E = \frac{C}{\int_0^\infty C dt} = \frac{C}{\sum C \Delta t} = \frac{C}{100}$ at t= 5min, E=0.03
- E is determined at various t,

t, min	0	5	10	15	20	25	30	35
E, min^{-1}	0	0.03	0.05	0.05	0.04	0.02	0.01	0



Q.2 The response data to a pulse input in a closed vessel is given below, The vessel is used as a reactor to react A to produce product .

$$A \rightarrow Product, \qquad -r_A = kC_A, \qquad k = 0.307\ min^{-1}$$

(i) Estimate the fractional conversion of A in a real reactor

(ii) Estimate the fractional conversion of A in a PFR for same size or space time.

t, min	0	5	10	15	20	25	30	35
C_{pulse} , g/L tracer output	0	3	5	5	4	2	1	0

- $\bar{t} = \frac{\sum t_i C_i}{\sum C_i} = \frac{5\times3+10\times5+15\times5+20\times4+25\times2+30\times1+35\times0}{0+3+5+5+4+2+1+0} = 15min$
- In PFR $\tau = \bar{t}$= 15 min
- $\frac{\bar{C}_A}{C_{A0}} = e^{-k\tau} = e^{-0.307\times15} = 0.01$, 1% is unconverted.
- Real Reactor,
- Fraction of unconverted A is given by
- $\frac{\bar{C}_A}{C_{A0}} = \sum e^{-kt} E\Delta t$

Find E for each t

- Real Reactor,
- Fraction of unconverted A is given by
- $\frac{\bar{C}_A}{C_{A0}} = \sum e^{-kt} E\Delta t$

t, min	0	5	10	15	20	25	30	35
E, min^{-1}	0	0.03	0.05	0.05	0.04	0.02	0.01	0

t, min	0	5	10	15	20	25	30	35
e^{-kt}	0	0.2165	0.0464	0.01	0.00215	0.00462	0.0001	0
e^{-kt} E Δt	0	0.0325	0.0116	0.0025	0.00043	0.000462	5×10^{-6}	0

$$\sum e^{-kt} E\Delta t = 0.0475$$

Unconverted A= 4.75% in real reactor by RTD method

Q3. A reactor giving responses for pulse input is as follows:

t, min	0	10	20	30	40	50	60	70
C_{pulse}	35	38	40	40	39	37	36	35

Reaction is $A \rightarrow R,\qquad -r_A = 0.05C_A \;\; mol/(l.min)$

Calculate the conversion (i) assuming plug flow, (ii) assuming the tanks –in-series model and (ii) Assuming mixed flow

$$\bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt}$$

$$\int_0^\infty tCdt = 91750$$

$$\int_0^\infty Cdt = 2651$$

$$\bar{t} = \frac{\int_0^\infty tCdt}{\int_0^\infty Cdt} = \frac{91750}{2651} = 34.61min$$

t	0	10	20	30	40	50	60	70
E	0.013	0.014	0.015	0.015	0.015	0.014	0.0136	0.013
$t-\bar{t}$	-34.61	-24.61	-14.61	-4.61	5.39	15.39	25.39	35.39
$(t-\bar{t})^2.E$	15.57	8.48	3.2	0.32	0.43	3.31	8.75	16.28

$$\sigma^2 = \int_0^\infty (t-\bar{t})^2 . E\, dt = 390.33\, min^2$$

$$N = \frac{1}{\sigma_\theta^2} = \frac{1}{0.3259} = 3.068 \qquad \sigma_\theta^2 = \frac{\sigma^2}{\bar{t}^2} = \frac{390.33}{34.61^2} = 0.3259$$

Conversion in tank-in-series model:

$$X_A = 1 - \frac{1}{\left(1+\frac{k\bar{t}}{N}\right)^N} = 1 - \frac{1}{\left(1+\frac{0.05 \times 34.61}{3}\right)^3} = 0.746 = 0.75$$

Conversion by plug flow reactor:

$$X_A = 1 - \frac{\bar{C}_A}{C_{A0}} = 1 - \ e^{-k\tau} = 1 - e^{-0.05\times 34.61} = 0.823, i.e\ \ 82.3\%$$

Conversion by Mixed flow reactor:

$$X_A = \frac{\tau k}{1+\tau k} = \frac{\bar{t}k}{1+\bar{t}k} = \frac{0.05\times 34.61}{1+0.05\times 34.61} = 0.634, i.e\ 63.4\%$$

Conversion by Dispersion Model:
Determine the Dispersion number by

$$\sigma_\theta^2 = 2\frac{D}{uL} - 2\left(\frac{D}{uL}\right)^2\left(1 - e^{-uL/D}\right)$$

Neglecting the second term, $\sigma_\theta^2 = 2\frac{D}{uL}$

$$\frac{D}{uL} = \frac{\sigma_\theta^2}{2} = \frac{0.3259}{2} = 0.1629$$

$$\frac{C_A}{C_{A0}} = 1 - X_A = \frac{4a \exp\left(\frac{1}{2}\frac{uL}{D}\right)}{(1+a)^2 \exp\left(\frac{a}{2}\frac{uL}{D}\right) - (1-a)^2 \exp\left(-\frac{a}{2}\frac{uL}{D}\right)}$$

$$a = \sqrt{1 + 4k\tau(D/uL)}$$