Lecture # 29 CHE331A

Residence time distribution

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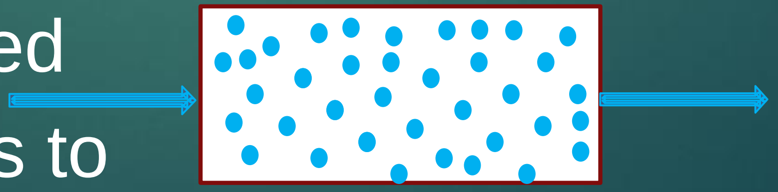
- Residence time distribution
  - Construction of C(t) and E(t)
  - Convolution integral
  - Step-input
- Some more on RTD
  - t_m and τ and other moments
  - RTD of Ideal reactors
  - RTD of LFR

Space time and mean residence time are related

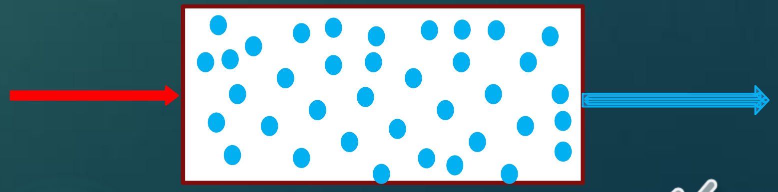
- Space time (τ) was defined as V/v and it signified the average residence time the fluid spent in the reactor
- Based on the RTD function, the mean residence time is defined as:

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

- This is the first moment of the RTD curve
- The total reactor volume can be determined from the cumulative distribution function F(t) of the reactor
  - At time t < 0 the reactor is completely filled with blue fluid elements
  - At time t = 0 red dye is injected
- Amount of blue dye corresponds to Reactor volume

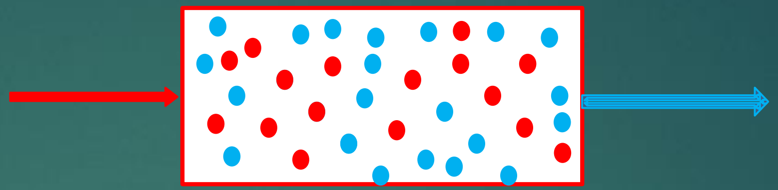


t < 0



t = 0

Calculation of reactor volume from cumulative distribution function



t > 0

- At time t = t' (> 0)
- Fraction of dye molecules in the effluent that have been in the reactor for *t ≥ t' is 1-F(t')*
- Volume of molecules leaving in a time dt is vdt
- Fraction of these molecules that have spent greater than equal to t is [1-F(t)] – only blue molecules have spent time more than t in the reactor
- Volume of blue molecules leaving the reactor in dt is

  $dV = v[1 - F(t)]dt$, which can be integrated from 0 to ∞ to give V
- Thus, $V = \int_0^\infty v[1 - F(t)]dt$ and for constant volumetric flow rate

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

The relationship between the mean residence time and the space time

- Previously, $V = v\int_0^\infty [1 - F(t)]dt$ integrating by parts
- Integrating by parts we have: $\frac{V}{v} = \int_0^\infty [1 - F(t)]dt = [t(1 - F(t)]_0^\infty + \int_0^1 t dF$
- At *t = 0, F(t) = 0* and $t \to \infty$, then *[1-F(t)] = 0*. Thus, first term is zero
- And, $\frac{V}{v} = \int_0^1 t dF = \tau$ However, $dF = E(t)dt$
- Thus, $\tau = \int_0^\infty tE(t)dt = t_m$ True when $v = v_0$ and for isobaric and isothermal operations and no change in number of moles
- Further, this is true for a closed system, i.e., no dispersion across boundaries

The RTD and its three moments

- First moment of the distribution is the mean residence time:

$$t_m = \int_0^\infty tE(t)dt$$

- Second moment is the variance, σ^2 :

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

  - indicates the “spread” of the distribution
- Third moment is also taken about the mean and is related to “skewness”

$$s^3 = \frac{1}{\sigma^{3/2}} \int_0^\infty (t - t_m)^3 E(t)dt$$

  - Magnitude indicates if the distribution is skewed in one direction or the other related to the mean
- Other moments exist too

Dimensionless RTD function is used instead of function E(t), which depends on reactor size and flows

- Dimentionless time, θ, defined as: $\theta = \frac{t}{\tau}$
- Dimensionless RTD function, E(θ), is defined as: $E(\theta) = \tau E(t)$
- Thus, $E(\theta)\ vs\ \theta$ is identical for all ideal PFRs and CSTRs
  - $E(t)\ vs\ t$ would vary depending on the space-time, i.e., the value of τ
- By normalizing different reactors can be compared directly
  - Numerical values may be otherwise different
- It can be easily shown that $\int_0^\infty E(\theta)d\theta\ = 1$
- Similar to E(t) (exit-age distribution function) the internal-age distribution, $I(\alpha)$, is also sometimes used: $I(\alpha) = (1 - F(\alpha))/\tau$

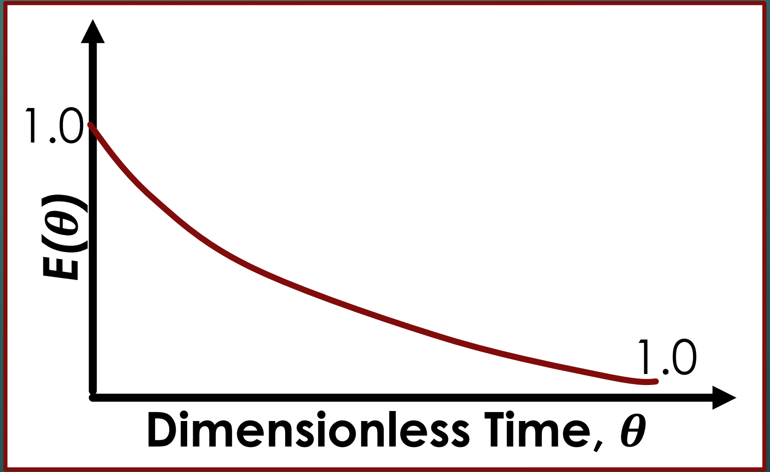
RTD function can be defined for ideal reactors

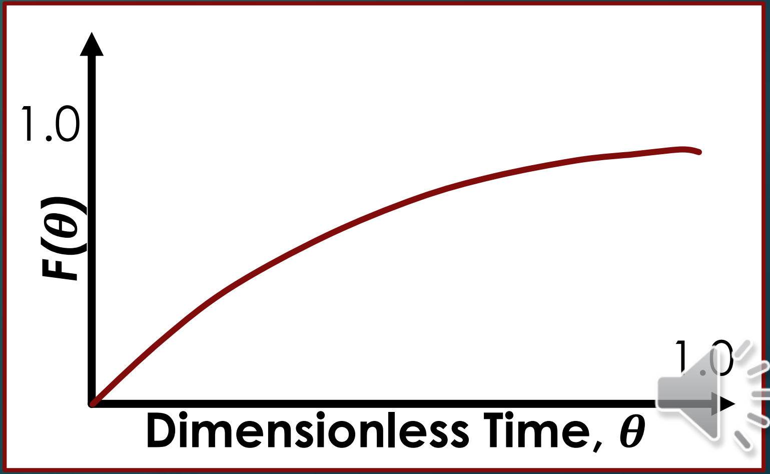
- RTD function for PFR/PBR and Batch are simple
  - All atoms leaving the reactor (PFR/PBR) or in the reactor (Batch) have spent the same amount of time within the reactor
  - The RTD function is a spike of infinite height, zero width and area of 1
  - Spike occurs at $t = \tau$ or $\theta = 1 \rightarrow$ represented by the Dirac delta function
  - $E(t) = \delta(t - \tau)$ where $\delta(x) = 0\ at\ x \neq 0\ and\ \delta(x) = \infty\ at\ x = 0$
  - Further, $\int_{-\infty}^{\infty} \delta(x)dx = 1$ and $\int_{-\infty}^{\infty} g(x)\delta(x - \tau)\, dx = g(\tau)$
- Mean residence time is: $t_m = \int_0^{\infty} tE(t)dt = \int_0^{\infty} t\delta(t - \tau)dt = \tau$
- Variance $\sigma^2 = \int_0^{\infty} (t - \tau)^2\delta(t - \tau)dt = 0 \rightarrow$ No variance!
- Cumulative distribution function F(t) is: $F(t) = \int_0^t E(t)dt = \int_0^t \delta(t - \tau)dt$

RTD function for the CSTR is not the same

- In a CSTR the conc. inside is the same as the conc at the exit
- For an inert tracer pulsed at t = 0 into a CSTR then at t > 0 we can do a material balance for the tracer, i.e., in – out = accumulation (no reaction)
- $0 - v.C = V\frac{dC}{dt}$ Further, C = C_0 at t = 0. Then $C(t) = C_0 \exp(-{}^{t}/_{\tau})$
- The C(t) for the CSTR can be used to determine E(t)
- Thus, $E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} = \frac{C_0 \exp(-{}^{t}/_{\tau})}{\int_0^\infty C_0 \exp(-{}^{t}/_{\tau})\ dt}$ and $E(t) = \frac{\exp(-{}^{t}/_{\tau})}{\tau}$
- Further, $E(\theta) = \exp(-\theta)$ and
- $F(\theta) = \int_0^\theta E(\theta)\, d\theta$

$F(\theta) = 1 - \exp(-\theta)$





The moments of the RTD for a CSTR

- The first moment, the mean residence time, is given by: $t_m = \int_0^\infty tE(t)dt$
- Thus, $t_m = \int_0^\infty \frac{t}{\tau} \exp(-{}^t/_\tau)\, dt = \tau$ and
- The mean residence time is the space time, $\tau = V/v$
- The second moment, which is a measure of spread: $\sigma^2 = \int_0^\infty (t - t_m)^2 E(t)dt$
- $\sigma^2 = \int_0^\infty \frac{(t-\tau^2)}{\tau} \exp(-{}^t/_\tau)\, dt = \tau^2$
  - Standard deviation is the square root of variance, and
  - For a CSTR, the standard deviation of the RTD function is as large as the mean

Laminar flow tubular reactor is an non-ideal reactor

- Before applying the RTD function to estimate conversions we can look into the flow behavior for a tubular reactor where there is laminar flow
- For laminar flow the velocity profile is parabolic, $U(r)$ – not ideal
- Velocity profile: $U(r) = U_{max}\left[1-\left(\frac{r}{R}\right)^2\right] = 2\left(\frac{v_0}{\pi R^2}\right)\left[1-\left(\frac{r}{R}\right)^2\right]$
  - Where $\frac{v_0}{\pi R^2}$ is the average fluid velocity through the tube
- The time required for a fluid element, t(r), to flow through the tube of length L

$$t(r) = \frac{L}{U(r)} = \frac{\pi R^2 L}{v_0}\frac{1}{2\left[1-\left(\frac{r}{R}\right)^2\right]} = \frac{\tau}{2\left[1-\left(\frac{r}{R}\right)^2\right]}$$

- The volumetric flow rate of fluid element between r and $r+dr$, dv, is
- $dv = U(r)2\pi r dr$ and the fraction of fluid passing is: $\frac{dv}{v_0} = \frac{U(r)2\pi r dr}{v_0}$

The E(t) curve for a laminar flow reactor

- The fraction of fluid between $r\ and\ r + dr$ is dv/v_0, which is $\frac{dv}{v_0} = \frac{U(r)2\pi r dr}{v_0}$
- This fraction of fluid between $r\ and\ r + dr$ and has a flow between between $v\ and\ v + dv$ spends time between $t\ and\ t + dt$ in the reactor
- Thus, $E(t)dt = \frac{dv}{v_0} = \frac{U(r)2\pi r dr}{v_0}$
- This fluid fraction between $r\ and\ r + dr$ is to be related to the fluid spending between $t\ and\ t + dt$ in the reactor
  - The time required to flow through the reactor of length L: $t(r) = \frac{\tau}{2\left[1-\left(\frac{r}{R}\right)^2\right]}$
  - Thus, $\frac{dt}{dr} = \frac{d}{dr}\left[\frac{\tau}{2\left[1-\left(\frac{r}{R}\right)^2\right]}\right] = \frac{4t^2}{\tau R^2} r$ Thus, $r dr = \frac{\tau R^2}{4t^2} dt$

The E(t) curve for the Laminar flow reactor … contd

- Previously, $E(t)dt = \frac{dv}{v_0} = \frac{U(r)2\pi rdr}{v_0} = \frac{L}{t}\left(\frac{2\pi}{v_0}\right)rdr = \frac{L}{t}\left(\frac{2\pi}{v_0}\right)\left(\frac{\tau R^2}{4t^2}\right)dt = \frac{\pi R^2 L\tau}{v_0 2t^3}dt$

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

- Minimum time (t_{min}) the fluid spend in the reactor is: $t_{min} = \frac{L}{U_{max}} = \frac{L}{2U_{avg}} = \frac{\tau}{2}$
- Thus, the RTD function is given by:

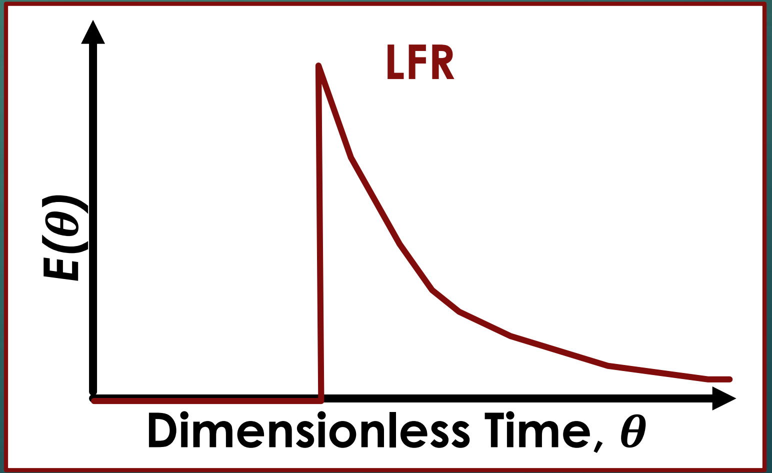
$$E(t) = 0 \; for \; t < \frac{\tau}{2}$$

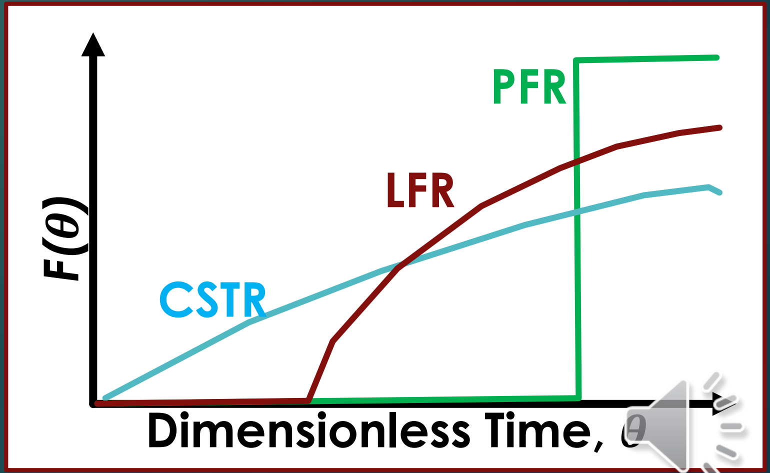
$$E(t) = \frac{\tau^2}{2t^3} \; for \; t \geq \frac{\tau}{2}$$

- Based on this above *E(t)* it can be shown:

  $t_m = \tau$ and $F(t) = 1 - \frac{\tau^2}{4t^2}$

- Further, $E(\theta) and\ F(\theta)$ can be derived





Summary

- Determination of volume of reactor from F(t) curve: $V = v\int_0^\infty [1 - F(t)]dt$
- Equivalence of space-time and mean residence time: $\tau = t_m$
- Three moments of the RTD: $t_m,\ \sigma^2,\ s^3$
- Dimensionless time and RTD function: $\theta, E(\theta)\ and\ F(\theta)$
- RTD functions for PFR/PBR and CSTR: $E(t) = \delta(t - \tau)$ $\quad E(t) = \dfrac{\exp(-{}^{t}/_{\tau})}{\tau}$
- Laminar flow reactor as an ideal reactor: $E(t) = 0\ for\ t < \dfrac{\tau}{2}$

$$E(t) = \frac{\tau^2}{2t^3}\ for\ t \geq \frac{\tau}{2}$$