Chemical Reaction Engineering 1

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Lecture 29 - RTD in Ideal Reactors

Welcome to the third lecture of non-ideal reactor and residence time distribution function. So before going to this lecture let us have brief recap on our previous lecture.

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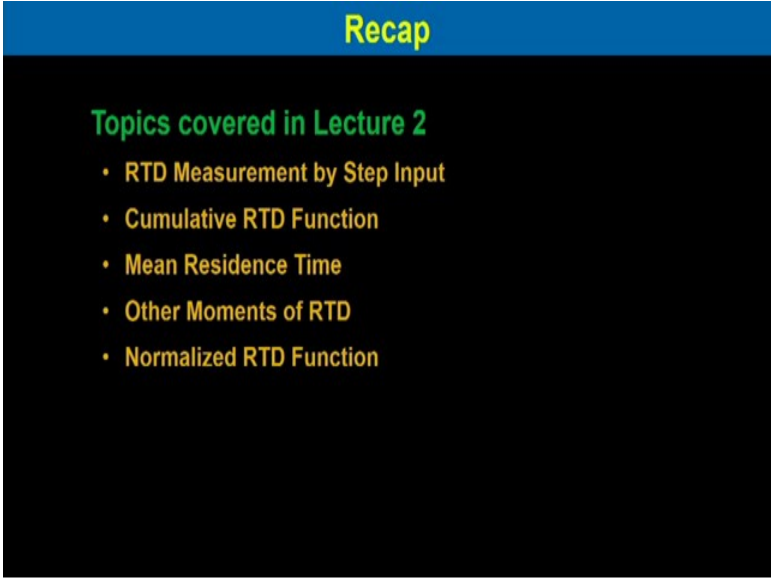

Recap

Topics covered in Lecture 2

- RTD Measurement by Step Input
- Cumulative RTD Function
- Mean Residence Time
- Other Moments of RTD
- Normalized RTD Function

In our previous lecture we have mainly covered the RTD measurement by step input method and we have seen that if we use step input method then for a tracer which are very costly it is very difficult to use step input because there is continuous injection of the tracer into the reactor and there are certain advantage and disadvantage we have discussed while discussing the RTD measurements by step input method. Then we have discussed the cumulative RTD distribution function, how to calculate the cumulative RTD distribution function and how it look like.

Then we have seen mean residence time and the other moments of residence time distribution particularly variance and skewness. Then we have seen there are certain advantage to normalise the RTD distribution function that is Et and we can write Et as a normalised function as e theta, where theta is equal to t by tau which is the dimensionless quantities.

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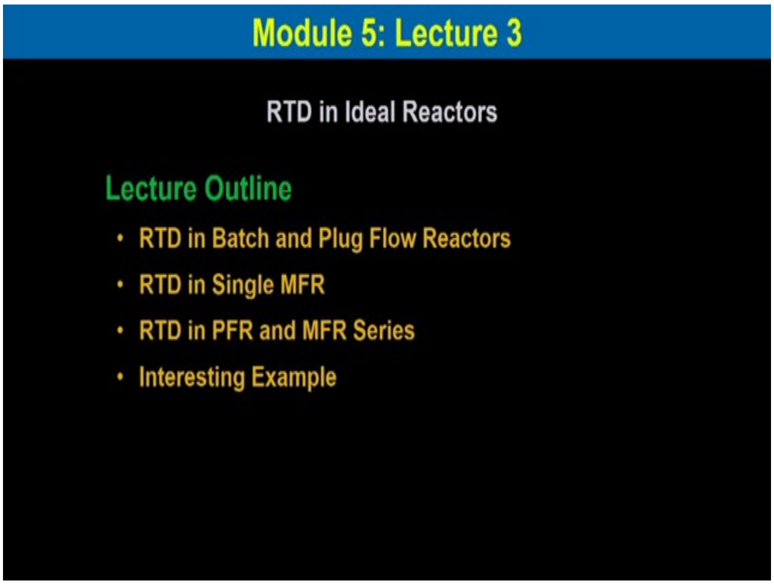

Module 5: Lecture 3

RTD in Ideal Reactors

Lecture Outline

- RTD in Batch and Plug Flow Reactors
- RTD in Single MFR
- RTD in PFR and MFR Series
- Interesting Example

Now in this lecture we will consider residence time distribution in ideal reactor. The major topic we will cover over here the RTD in batch and plug flow reactors, how the residence time distribution function look like, and what is their mathematical form. Then we will consider RTD in single mixed flow reactor or the continuous stirred tank reactor. Then if we have combination of the mixed flow reactor and the plug flow reactor and if they connected in series, how the residence time distribution changes? And, finally we will see one interesting example to see whether the only RTD can be sufficient to design the real reactor.

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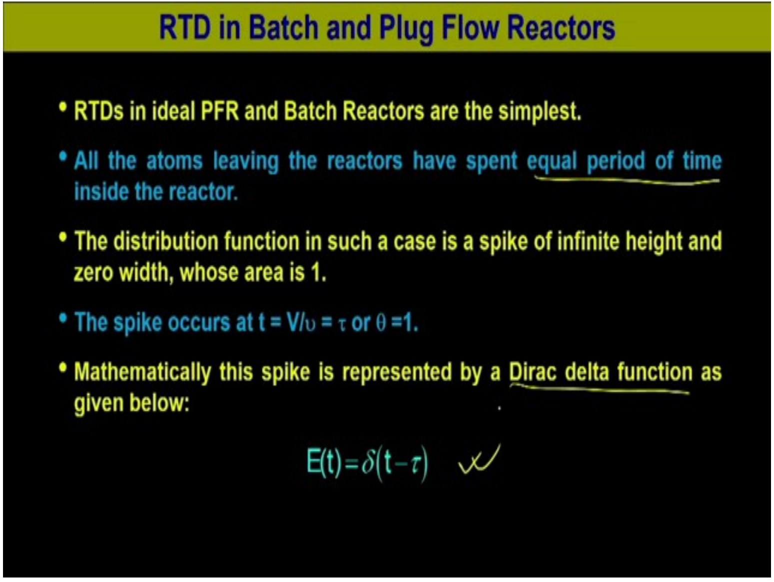

RTD in Batch and Plug Flow Reactors

- RTDs in ideal PFR and Batch Reactors are the simplest.
- All the atoms leaving the reactors have spent equal period of time inside the reactor.
- The distribution function in such a case is a spike of infinite height and zero width, whose area is 1.
- The spike occurs at $t = V/\upsilon = \tau$ or $\theta = 1$.
- Mathematically this spike is represented by a Dirac delta function as given below:

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

So let us consider RTD in batch and plug flow reactors. RTD in ideal plug flow reactor and the batch reactor are the simplest one to mathematically represents as all the atoms leaving the reactor have spent equal period of time inside the reactor. So the distribution function is such a case is a spike of infinite height and 0 width whose area is 1. So the spike occurs at t is equal to v by volumetric flow rate($t = \frac{V}{v}$), capital V is the volume of the reactor and small v is the volumetric flow rate. So which is equal to t tau or theta is equal to 1. So mathematically this spike is represented by a dirac delta function as given below. So where $E(t) = \delta(t - \tau)$, so this is the residence time distribution function in case of ideal PFR or batch reactors.

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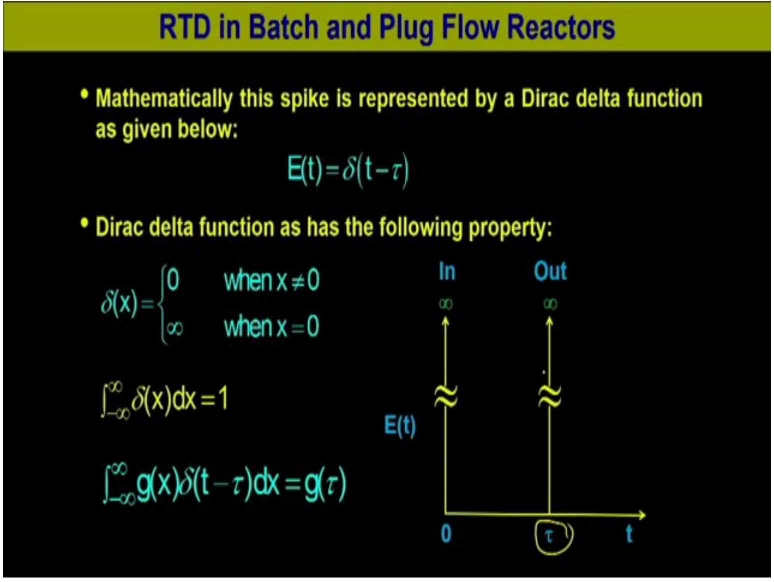

RTD in Batch and Plug Flow Reactors

- Mathematically this spike is represented by a Dirac delta function as given below:

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

- Dirac delta function as has the following property:

$$\delta(x)=\begin{cases}0 & \text{when } x\neq 0\\ \infty & \text{when } x=0\end{cases}$$

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

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

Now as we have seen, this is the mathematical form of the dirac delta function, the direct delta function has certain properties, what are they? Δx would be equal to 0 when x not equal to 0 and it should be infinity when x is equal to 0. So $\int_{-\infty}^{\infty} \delta(x)dx = 1$ and $\int_{-\infty}^{\infty} g(x)\delta(t - \tau)dx = g(\tau)$. So we can see this direct delta function graphically, so this is the y axis and this is x axis, and y axis if we plot $E(t)$ versus the t then if we have in at this location which is over here the out would be at tau, so which is at τ because all the materials have spent exactly same length of time inside the reactor. So we will get a spike of infinite height and 0 width whose area would be unity or 1.

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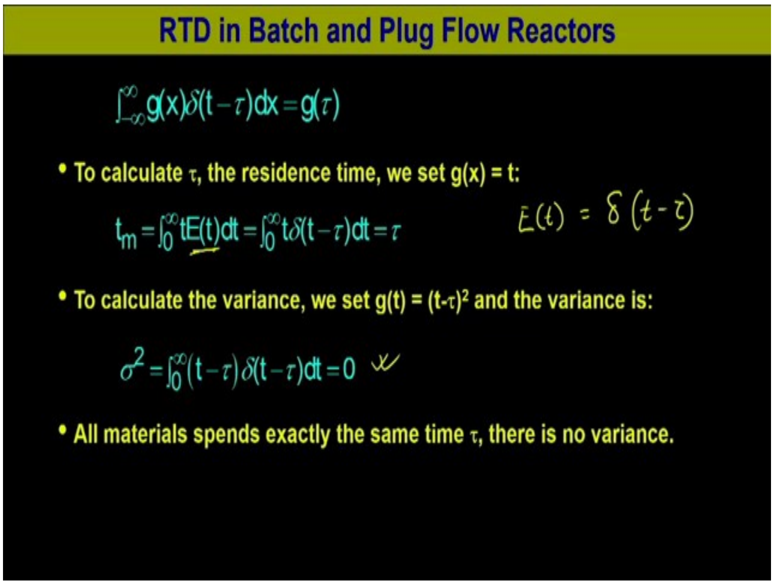

RTD in Batch and Plug Flow Reactors

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

- To calculate τ, the residence time, we set g(x) = t:

$$t_m = \int_0^{\infty} t\underline{E(t)}dt = \int_0^{\infty} t\delta(t-\tau)dt = \tau \qquad E(t) = \delta(t-\tau)$$

- To calculate the variance, we set g(t) = $(t-\tau)^2$ and the variance is:

$$\sigma^2 = \int_0^{\infty} (t-\tau)\delta(t-\tau)dt = 0 \checkmark$$

- All materials spends exactly the same time τ, there is no variance.

Now to calculate τ, the residence time we set $g(x)$ is equal to t, if we put that then our t_m as we know from the definition the mean residence time would be equal to $\int_0^{\infty} tE(t)dt$. So now if we substitute $E(t)$ for the dirac delta function this $E(t) = \delta(t-\tau)$, so if we substitute $E(t)$ over here at this location, so we will obtain $\int_0^{\infty} t\delta(t-\tau)dt = \tau$. Now to calculate the variance that is the delta square that is σ^2, we said gt is equal to t minus tau square $g(t) = (t-\tau)^2$ and the variance would be $\sigma^2 = \int_0^{\infty} (t-\tau)\delta(t-\tau)dt = 0$.

So we can see that the variance for the ideal PFR or batch reactor because each molecules spent or each atom spent exactly same length of time, so there is no variation of their residence time, so we get sigma square is equal to 0 (σ^2=0), that means all materials spent exactly the same time τ, there is no variance.

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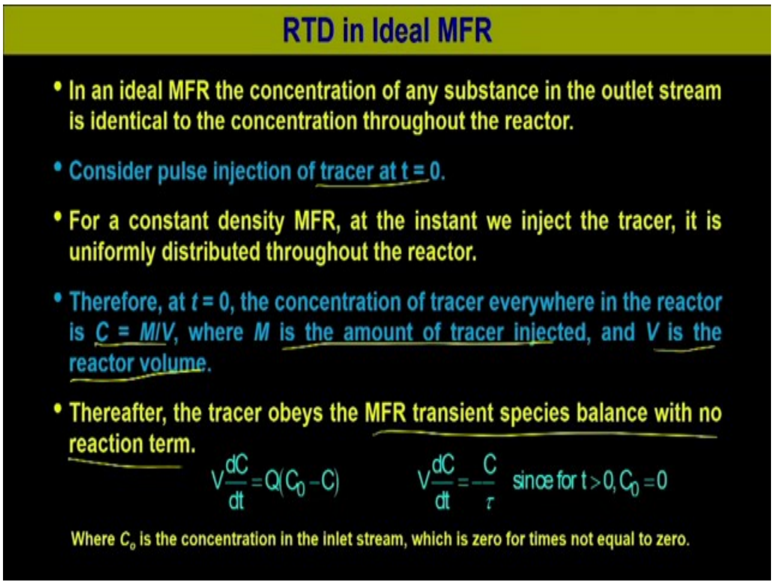

RTD in Ideal MFR

- In an ideal MFR the concentration of any substance in the outlet stream is identical to the concentration throughout the reactor.
- Consider pulse injection of tracer at t = 0.
- For a constant density MFR, at the instant we inject the tracer, it is uniformly distributed throughout the reactor.
- Therefore, at $t = 0$, the concentration of tracer everywhere in the reactor is $C = M/V$, where M is the amount of tracer injected, and V is the reactor volume.
- Thereafter, the tracer obeys the MFR transient species balance with no reaction term.

$$V\frac{dC}{dt}=Q(C_0-C) \qquad V\frac{dC}{dt}=-\frac{C}{\tau} \quad \text{since for } t>0, C_0=0$$

Where C_0 is the concentration in the inlet stream, which is zero for times not equal to zero.

Now in an ideal mixed flow reactor the concentration of any substance in the outlet stream is identical to the concentration throughout the reactor. So if we consider the pulse injection of tracer at t is equal to 0 for a constant density mixed flow reactor, at the instant we inject the tracer, it is uniformly distributed throughout the reactor. So since for ideal flow reactor it is the content of the reactor is mixed homogenously at each point, so there is no change of concentration inside the reactor at any location with the outlet concentration of the reactor. So it will be distributed uniformly throughout the reactor if we inject any tracer material with the reactants.

Therefore at t is equal to 0, the concentration of tracer everywhere in the reactor would be $C = {}^{M}\!/_{V}$ where M is the amount of tracer injected and V is the reactor volume. So the concentration would be the amount of tracer divided by the reactor volume, so C would be equal to M by V ($C = {}^{M}\!/_{V}$.)

Now thereafter the tracer obeys the mixed flow reactor transient species balance with no reaction term in it. So we can write $V\frac{dC}{dt} = Q(C_0 - C)$ where Q is the volumetric flow rate and C_0 is the concentration in the inlet stream which is 0 for times naught equal to 0. So for, we have given the pulse injection of the tracer, so the C_0 at t is equal to 0 for all other times above $t \quad 0$ or t <= 0 it should be, the tracer concentration would be 0. So this we can write since for $t \quad 0$, C naught is equal to 0, $V\frac{dC}{dt} = \frac{C}{r}$.

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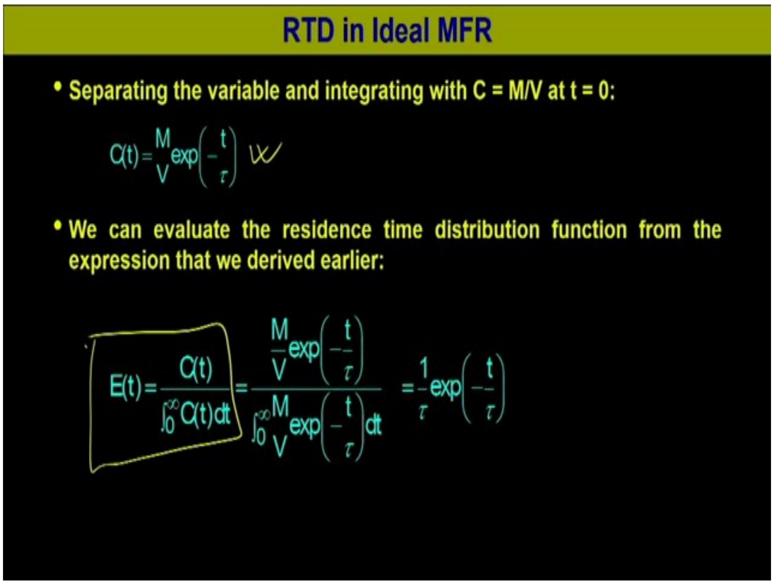

RTD in Ideal MFR

- Separating the variable and integrating with C = M/V at t = 0:

$$C(t)=\frac{M}{V}\exp\left(-\frac{t}{\tau}\right)$$ ✓

- We can evaluate the residence time distribution function from the expression that we derived earlier:

$$\boxed{E(t)=\frac{C(t)}{\int_0^\infty C(t)dt}}=\frac{\frac{M}{V}\exp\left(-\frac{t}{\tau}\right)}{\int_0^\infty \frac{M}{V}\exp\left(-\frac{t}{\tau}\right)dt}=\frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right)$$

Now if we separate the variable and integrating with C is equal to M by V at t is equal to 0, so we can get the concentration profile of the tracer, $C(t)=\frac{M}{V}\exp\left(\frac{-t}{\tau}\right)$, so this is the concentration profile. Now we can evaluate the residence time distribution function from the expression that we have derived earlier. So $E(t)=\frac{C(t)}{\int\limits_0^\infty C(t)dt}$ that is the definition of the residence time distribution function. Now if we substitute $C(t)=\frac{M}{V}\exp\left(\frac{-t}{\tau}\right)$ over here and at the denominator it is $\int\limits_0^\infty \frac{M}{V}\exp\left(\frac{-t}{\tau}\right)dt$. So if we solve it, it will give $E(t)=\frac{1}{\tau}\exp\left(\frac{-t}{\tau}\right)$

So this way we can evaluate the residence time distribution function from the expression which we have derived earlier for the ideal mixed flow reactor.

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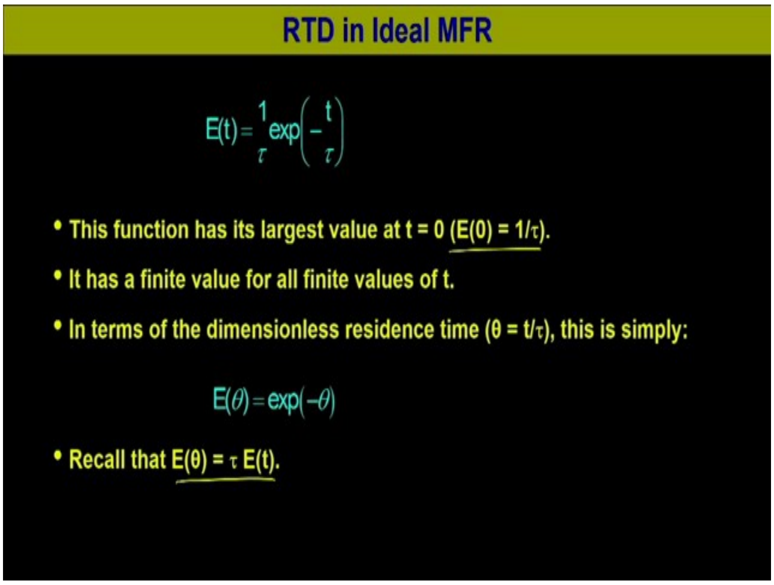

RTD in Ideal MFR

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

- This function has its largest value at t = 0 (E(0) = 1/τ).
- It has a finite value for all finite values of t.
- In terms of the dimensionless residence time (θ = t/τ), this is simply:

$$E(\theta) = \exp(-\theta)$$

- Recall that E(θ) = τ E(t).

Now this is the exit age distribution function E t which we have derived is equal to $E(t) = \frac{1}{\tau}\exp\left(\frac{-t}{\tau}\right)$. So this function has its largest value at t is equal to 0, so when t is equal to 0, $(E(0) = 1/\tau)$. So this part would be 1, so $E(t) = \frac{1}{\tau}$. It has a finite value for all finite values of t, so it should have certain values, and if we have a finite time. In terms of the dimensionless residence time, $\theta = t/\tau$ and then we can simply write $E(\theta) = \exp(-\theta)$. So as we know, we have set earlier $E(\theta) = \tau E(t)$, so we can simply relate $E(\theta) = \exp(-\theta)$.

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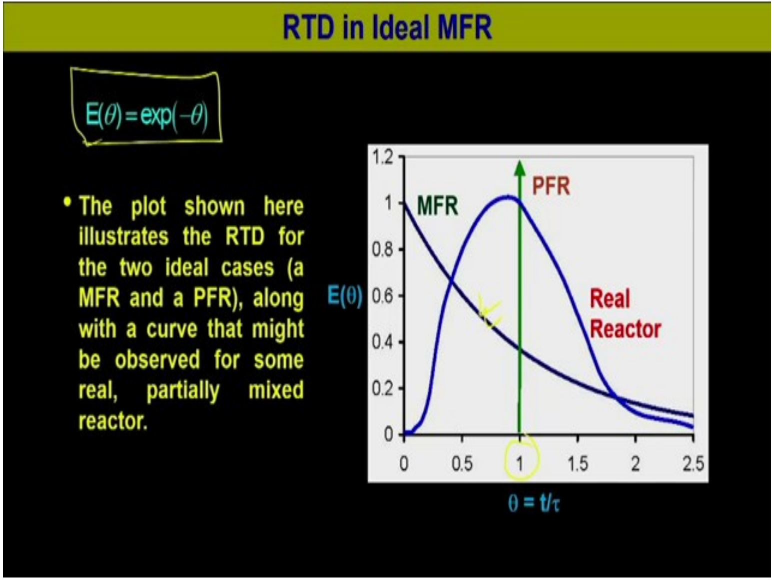

RTD in Ideal MFR

$$\boxed{E(\theta) = \exp(-\theta)}$$

- The plot shown here illustrates the RTD for the two ideal cases (a MFR and a PFR), along with a curve that might be observed for some real, partially mixed reactor.

Now look into this plot where it shows the RTD for two ideal cases, one is for mixed flow reactor and then the plug flow reactor and then what we actually observe in case of the real reactor or partially mixed reactor. So this is θ on the x axis which is t/τ and this is $E(\theta)$. So, if we plot $E(\theta)$ versus θ we would obtain for the mixed flow reactor this is the curve, for mixed flow reactor. So the residence time distribution function, the dimensionless residence time distribution function will be this, that is the exponential decay as per this relation.

In case of ideal PFR which is shown over here and that will be $\theta = t/\tau$, so all t should be equal to τ so θ would be equal to 1, so which is shown over here. At θ is equal to 1, it will give all elements of the reactants will have the same residence time and so it will give a spike of infinite height with 0 height with 0 width.

So that is what it is shown with a vertical line for the ideal PFR. Now actually for the partially mixed reactor or any real reactor where the mixing is not the ideal mixed flow reactor or the ideal plug flow reactor as we say it, these two will set the two extremes of the mixing pattern. So, in real reactor we would see this blue line which is the residence time distribution function for the real reactor.

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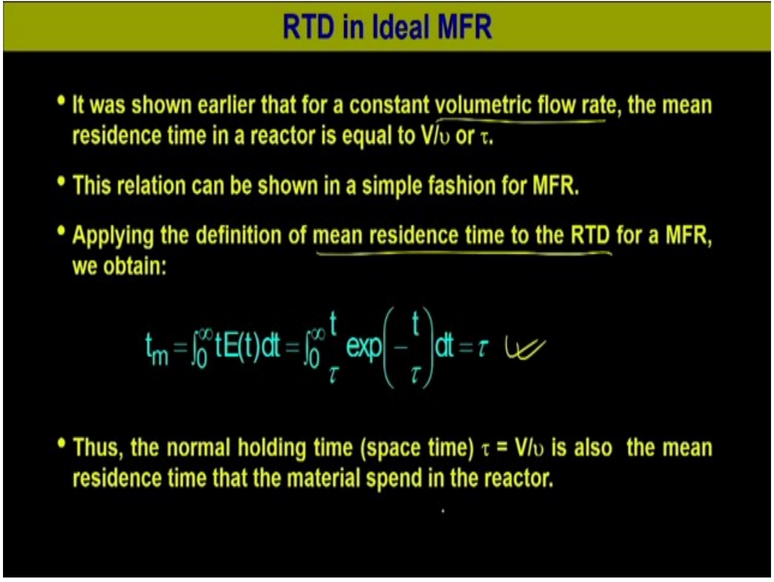

RTD in Ideal MFR

- It was shown earlier that for a constant volumetric flow rate, the mean residence time in a reactor is equal to V/υ or τ.
- This relation can be shown in a simple fashion for MFR.
- Applying the definition of mean residence time to the RTD for a MFR, we obtain:

$$t_m = \int_0^\infty tE(t)dt = \int_0^\infty \frac{t}{\tau}\exp\left(-\frac{t}{\tau}\right)dt = \tau \checkmark$$

- Thus, the normal holding time (space time) τ = V/υ is also the mean residence time that the material spend in the reactor.

Now it was already shown earlier that for constant volumetric flow rate the mean residence time in a reactor is equal to V by volumetric flow rate or τ. This relation can be shown in a simple fashion for mixed flow reactor, applying the definition of the mean residence time for

RTD, for MFR, we obtain. $t_m = \int_0^\infty tE(t)dt = \int_0^\infty \frac{t}{\tau}\exp\left(\frac{-t}{\tau}\right)dt = \tau$. Thus the normal holding time or space time tau would be V by volumetric flow rate is also the mean residence time that the materials spend in the reactor.

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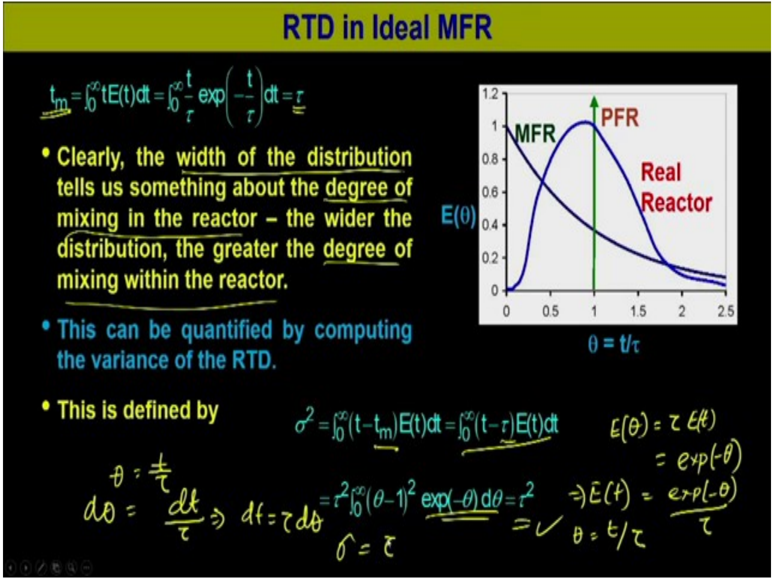

RTD in Ideal MFR

$t_m = \int_0^\infty tE(t)dt = \int_0^\infty \frac{t}{\tau}\exp\left(-\frac{t}{\tau}\right)dt = \underline{\underline{\tau}}$

- Clearly, the width of the distribution tells us something about the degree of mixing in the reactor – the wider the distribution, the greater the degree of mixing within the reactor.
- This can be quantified by computing the variance of the RTD.
- This is defined by $\sigma^2 = \int_0^\infty (t-t_m)E(t)dt = \int_0^\infty (t-\tau)E(t)dt$

$\theta = \frac{t}{\tau}$

$d\theta = \frac{dt}{\tau} \Rightarrow dt = \tau d\theta$

$= \tau^2 \int_0^\infty (\theta-1)^2 \exp(-\theta)d\theta = \tau^2$

$\sigma = \tau$

$= \checkmark$

$E(\theta) = \tau E(t)$

$= \exp(-\theta)$

$\Rightarrow E(t) = \frac{\exp(-\theta)}{\tau}$

$\theta = t/\tau$

Now t_m, the mean residence time is the space time, equal to the space time τ and clearly the width of this distribution as we have seen for the different reactors, the width of the distribution tells us something about the degree of mixing in the reactor. The wider the distribution, the greater the degree of mixing within the reactors, so you can see in case of ideal mixed flow reactor, the distribution is much wider compared to the real reactors. Real reactors, whereas in case of PFR there is no distribution, so we can see the real reactor falls in between. So, basically the distribution tells us about the degree of mixing inside the reactor.

Now this can be quantified by computing the variance of the RTDs, and the variance is defined by sigma square for ideal mixed flow reactor, we can write, $\sigma^2 = \int_0^\infty (t-t_m)^2 E(t)dt$

Now this t_m for the ideal mixed flow reactor we have calculated as τ, so if we substitute t m with τ this would be $\int_0^\infty (t-t_m)^2 E(t)dt$. So, as we know $E(\theta) = \tau E(t)$ which is equal to

$E(\theta) = \exp(-\theta)$, so E(t) from here we can write, $E(t) = \dfrac{\exp(-\theta)}{\tau}$. So if we simplify this one this would be $\tau^2 \ (\theta - 1)^2$ whole square and in place of E(t)we can write $\exp(-\theta)$ by τ.

And $\sigma_\theta^2 = \dfrac{\sigma^2}{\tau^2}$, d theta would be dt by tau($\Delta\theta = t / \tau$). From here we can write $dt = \tau \times d\theta$. So if we substitute E t and dt so it would be $\exp(-\theta) \ \ d\theta$. If we integrate it, we will get τ^2, that means σ would be equal to τ.

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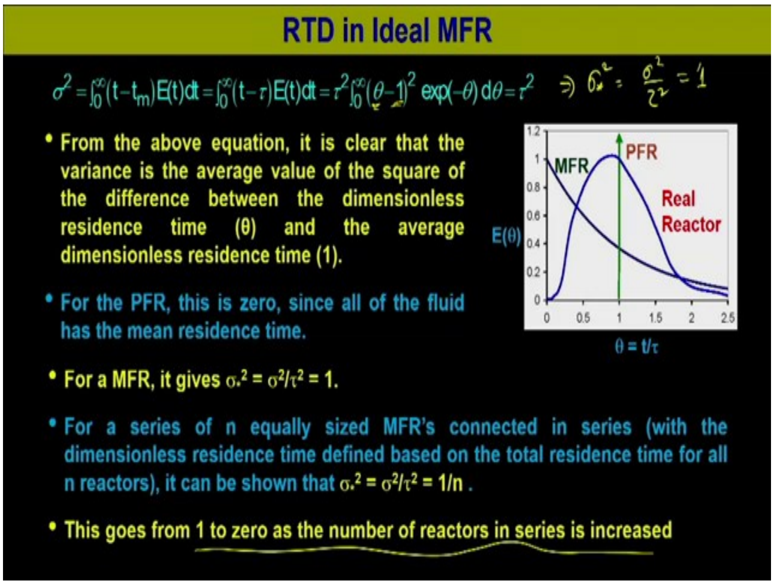

RTD in Ideal MFR

$$\sigma^2=\int_0^\infty (t-t_m)E(t)dt=\int_0^\infty (t-\tau)E(t)dt=\tau^2\int_0^\infty (\theta-1)^2\exp(-\theta)\,d\theta=\tau^2 \Rightarrow \sigma_*^2=\frac{\sigma^2}{\tau^2}=1$$

- From the above equation, it is clear that the variance is the average value of the square of the difference between the dimensionless residence time (θ) and the average dimensionless residence time (1).
- For the PFR, this is zero, since all of the fluid has the mean residence time.
- For a MFR, it gives $\sigma_*^2 = \sigma^2/\tau^2 = 1$.
- For a series of n equally sized MFR's connected in series (with the dimensionless residence time defined based on the total residence time for all n reactors), it can be shown that $\sigma_*^2 = \sigma^2/\tau^2 = 1/n$.
- This goes from 1 to zero as the number of reactors in series is increased

Now from the above equations which we have derived it is clear that the variance is the average value of the square of the difference between the dimensionless residence time. So square of the difference of the dimensionless residence time theta and the average dimensionless residence time which is 1. For the PFR, this is zero since all of the fluid has the mean residence time which we have already discussed earlier. In case of ideal PFR sigma square is equal to 0, we have derived.

So from here also we can see for PFR, the sigma would be 0 since there is no difference in their mean residence time. So for a mixed flow reactor, it gives sigma star square which we can define sigma square by tau square which is equal to 1, so from here we can write sigma star square would be $\frac{\sigma^2}{\tau^2}=1$. So for a series of n equally sized mixed flow reactor connected in series with the dimensionless residence time defined based on the total residence time for all the n reactors, it can be shown that $\sigma_\theta^2=\frac{\sigma^2}{\tau^2}=\frac{1}{n}$.

So if we connect n number of CSTR in series we can calculate σ_θ^2 would be equal to 1 by n where n is the number of reactors connected in series. So we could see that this goes from, this value σ_θ^2 goes from 1 to 0 as the number of reactor in series increased. So when n is equal to infinity so it will be, sigma star square would be equal to 0. When n is equal to 1, then σ_θ^2 is equal to 1.

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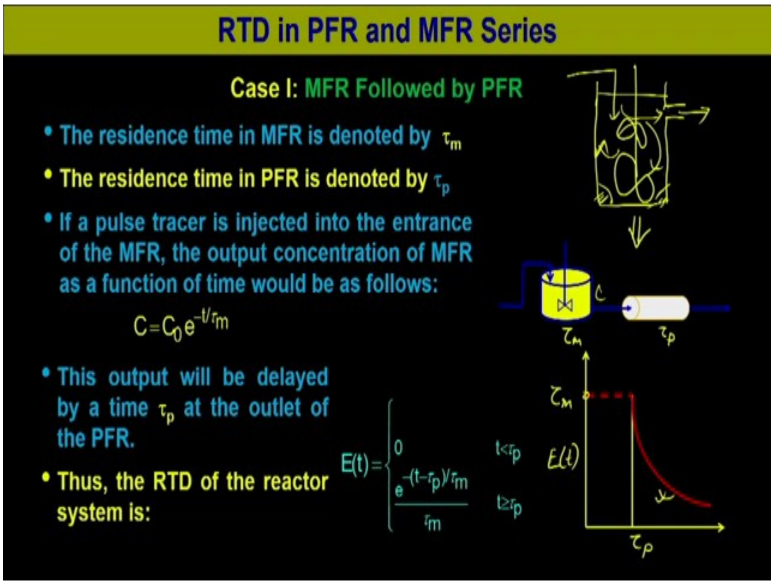
RTD in PFR and MFR Series

Case I: MFR Followed by PFR

- The residence time in MFR is denoted by τ_m
- The residence time in PFR is denoted by τ_p
- If a pulse tracer is injected into the entrance of the MFR, the output concentration of MFR as a function of time would be as follows:

$$C=C_0 e^{-t/\tau_m}$$

- This output will be delayed by a time τ_p at the outlet of the PFR.
- Thus, the RTD of the reactor system is:

$$E(t)=\begin{cases}0 & t<\tau_p\\ \dfrac{e^{-(t-\tau_p)/\tau_m}}{\tau_m} & t\geq\tau_p\end{cases}$$

Now let us consider RTD in PFR and mixed flow reactor connected in series. So we will first, case we will consider mixed flow reactor followed by PFR and how the RTD is look like. Basically if we have a real reactor, so there is mixing inside and there should be, there is also some dead zone and there is also some short circuiting. So this real reactor we can assume as it is a combination of CSTR and the plug flow reactor connected in series.

If it so happen, the first case we consider mixed flow reactor followed by the Plug Flow Reactor. So the residence time in mixed flow reactor is denoted by the τ_m, so over here. And the residence time for PFR is τ_p. If a pulse tracer is injected into the entrance of the MFR, the output concentration of MFR as a function of time would be as follows: $C = C_0 e^{-t/\tau_m}$. So this output will be delayed by time τ_p at the outlet of the PFR because this is the concentration which is at the exit of the CSTR that is C and this concentration would be delayed by time τ_p

So the RTD of the reactor system would be represented $E(t)=\begin{cases}0t<\tau_p\\ \dfrac{e^{-(t-\tau_p)/\tau_m}}{\tau_m}t \quad \tau_p\end{cases}$.

So under these two conditions we can see the RTD distribution function. Now if we represent graphically for this, this is $E(t)$ and this is τ_p and this is the locations where tau CSTR or tau mixed flow reactor τ_m at this locations. After that the profile would look like this. So this is for the case where mixed flow reactor is connected before the plug flow reactor, so they are connected in series.

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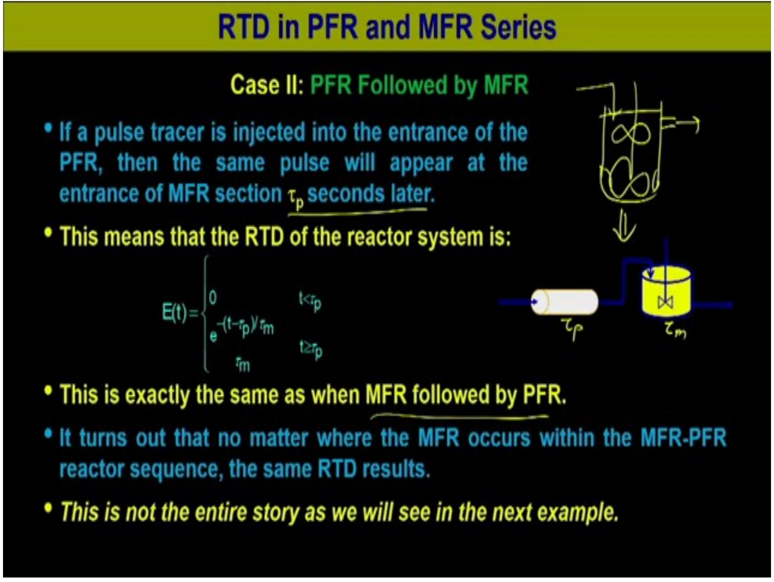

RTD in PFR and MFR Series

Case II: PFR Followed by MFR

- If a pulse tracer is injected into the entrance of the PFR, then the same pulse will appear at the entrance of MFR section τ_p seconds later.
- This means that the RTD of the reactor system is:

$$E(t)=\begin{cases} 0 & t<\tau_p \\ \dfrac{e^{-(t-\tau_p)/\tau_m}}{\tau_m} & t\geq\tau_p \end{cases}$$

- This is exactly the same as when MFR followed by PFR.
- It turns out that no matter where the MFR occurs within the MFR-PFR reactor sequence, the same RTD results.
- *This is not the entire story as we will see in the next example.*

Now let us see the other case of modelling this reactor in the second case where PFR is connected earlier than the mixed flow reactor or the mixed flow reactor is preceded by Plug Flow Reactor. So in this case, so we have same reactor system. And we have inlet, so we have dead zone so this is real reactor and this we can model in the second method where we have connected first the plug flow reactor and then CSTR and we know the residence time τ_p and this is for mixed flow reactor τ_m.

Now if a pulse tracer is injected into the entrance of the PFR then the same pulse will appear at the entrance of the mixed flow section that is τ_p seconds later. That means as for ideal plug flow reactor, the tracer which will be injected over here that has to be delayed for τ_p time to enter into the CSTR. So the residence time, distribution of this reactor system would be same as we obtain for the earlier case. So, this is exactly the same one when MFR followed by PFR. This turns out that no matter where the MFR occurs within the MFR-PFR reactor sequence, the same RTD results.

So whether the MFR is connected first than the PFR or PFR is connected first than the CSTR, the RTD distribution function or the residence time distribution function for these series reactors are the same. So this is not the entire story as we will see in the next examples. Although their RTDs are same, they may not generate the same conversion level as we desire.

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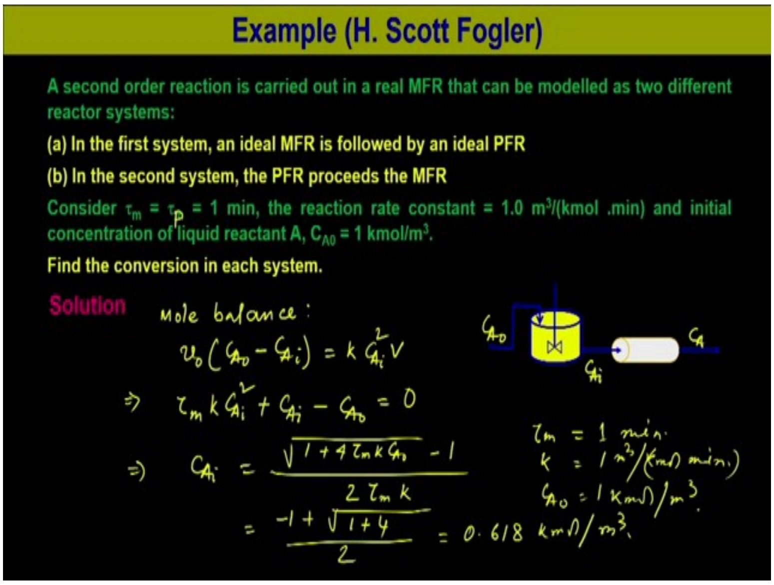


Example (H. Scott Fogler)

A second order reaction is carried out in a real MFR that can be modelled as two different reactor systems:

(a) In the first system, an ideal MFR is followed by an ideal PFR

(b) In the second system, the PFR proceeds the MFR

Consider $\tau_m = \tau_p = 1$ min, the reaction rate constant = 1.0 $m^3/(kmol\ .min)$ and initial concentration of liquid reactant A, $C_{A0} = 1\ kmol/m^3$.

Find the conversion in each system.

Solution

Mole balance :

$$v_0 (C_{A0} - C_{Ai}) = k C_{Ai}^2 V$$

$$\Rightarrow \tau_m k C_{Ai}^2 + C_{Ai} - C_{A0} = 0$$

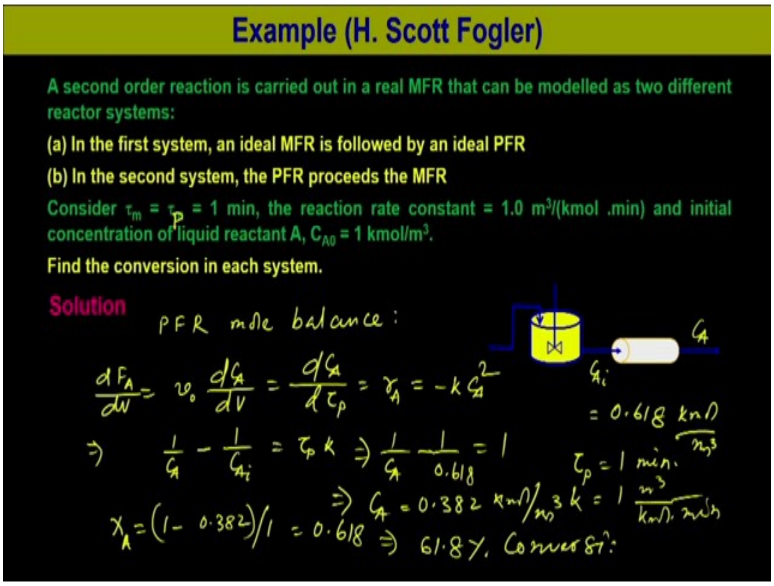
$$\Rightarrow C_{Ai} = \frac{\sqrt{1 + 4\tau_m k C_{A0}} - 1}{2\tau_m k}$$

$$= \frac{-1 + \sqrt{1+4}}{2} = 0.618\ kmol/m^3.$$

$\tau_m = 1$ min.

$k = 1\ m^3/(kmol\ min.)$

$C_{A0} = 1\ kmol/m^3.$



Example (H. Scott Fogler)

A second order reaction is carried out in a real MFR that can be modelled as two different reactor systems:

(a) In the first system, an ideal MFR is followed by an ideal PFR

(b) In the second system, the PFR proceeds the MFR

Consider $\tau_m = \tau_p = 1$ min, the reaction rate constant = 1.0 $m^3/(kmol\ .min)$ and initial concentration of liquid reactant A, $C_{A0} = 1\ kmol/m^3$.

Find the conversion in each system.

Solution

PFR mole balance :

$$\frac{dF_A}{dW} = v_0 \frac{dC_A}{dV} = \frac{dC_A}{d\tau_p} = r_A = -kC_A^2$$

$$\Rightarrow \frac{1}{C_A} - \frac{1}{C_{Ai}} = \tau_p k \Rightarrow \frac{1}{C_A} - \frac{1}{0.618} = 1$$

$$\Rightarrow C_A = 0.382\ kmol/m^3$$

$$X_A = (1 - 0.382)/1 = 0.618 \Rightarrow 61.8\%\ \text{Conversion}$$

$C_{Ai} = 0.618\ kmol/m^3$

$\tau_p = 1$ min.

$k = 1\ \frac{m^3}{kmol.\ min}$

So let us take an example which is taken from the Fogler’s book and a second order reaction is carried out in a real mixed flow rector that can be modelled out as two different systems as we have discussed before. So in the first system, an ideal mixed flow reactor is followed by an ideal PFR and in the second system the PFR proceeds the mixed flow reactor. Now let us consider τ_m would be equal to this is τ_p would be equal to 1 minute, the reaction rate constant $k = 1 m^3/(kmol \min)$ and the initial concentration of the liquid reactant that is $C_{A0} = 1 kmol/m^3$.

So we need to find out the conversion in each system as stated in a and b. So let us consider the first system, this is t p, τ_p. So if we do the mole balance for the CSTR, so we will get, this is MFR, so for MFR mole balance, so we can write $\upsilon_0(C_{A0} - C_{Ai})$. So consider we have inlet concentration over here, C_{A0} and outlet over here is C_{Ai} and this is C_A. So for the MFR, this would be equal to $kC_{Ai}{}^2V$

Now if we rearrange, we can write $\tau_m kC_{Ai}{}^2 + C_{Ai} - C_{A0} = 0$.And now if we solve for $C_{Ai} = \dfrac{\sqrt{1+4\tau_m kC_{A0}} - 1}{2\tau_m k}$. So now if we substitute the values, it would be

$$C_{Ai} = \frac{-1+\sqrt{1+4}}{2} = 0.618\, kmol/m^3 \cdot$$

Now let us consider mole balance in case of the MFR, in case of the PFR. So PFR mole balance we can write $\dfrac{dF_A}{dV} = \upsilon_0 \dfrac{dC_A}{dV} = \dfrac{dC_A}{d\tau_p} = r_A = -kC_A{}^2$. So this will give $\dfrac{1}{C_A} - \dfrac{1}{C_{Ai}} = \tau_p k$

Now if substitute C_{Ai}, which we have obtained over here, which is equal to $0.618\, kmol/m^3$. Now if we substitute over here, we will obtain, so C_{A0} is this, C_{Ai} is this and

$$\begin{aligned}\tau_m &= 1\min \\ k &= 1 m^3/(kmol\min)\end{aligned}$$

. So substituting these values, this would be $\dfrac{1}{C_A} - \dfrac{1}{0.618} = 1$

And from here we can get $C_A = 0.382\, kmol/m^3$ .So, the concentration of the reactant in the effluent of the reactor systems which is C_A, that is over here, so we have calculated which is coming out. So, it is basically the conversion is $X_A = (1-0.382)/1 = 0.618 \Rightarrow 61.8\%$

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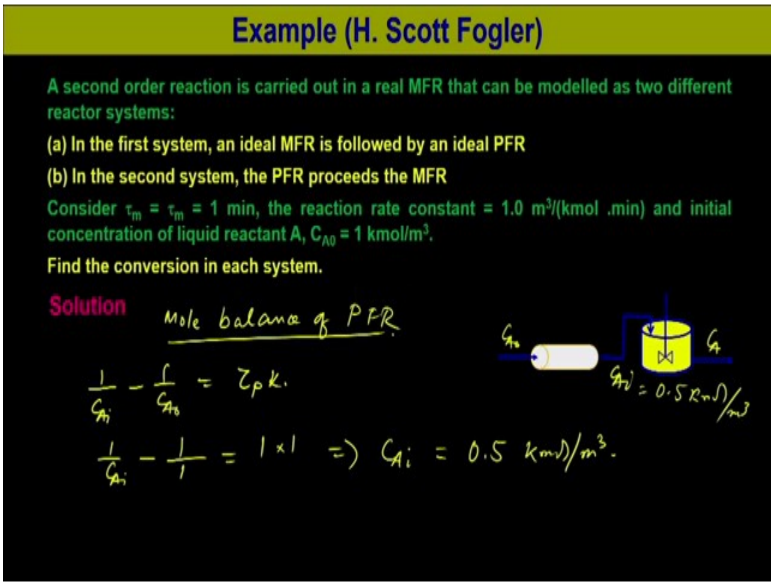


Example (H. Scott Fogler)

A second order reaction is carried out in a real MFR that can be modelled as two different reactor systems:

(a) In the first system, an ideal MFR is followed by an ideal PFR

(b) In the second system, the PFR proceeds the MFR

Consider $\tau_m = \tau_m = 1$ min, the reaction rate constant = 1.0 m³/(kmol .min) and initial concentration of liquid reactant A, $C_{A0} = 1$ kmol/m³.

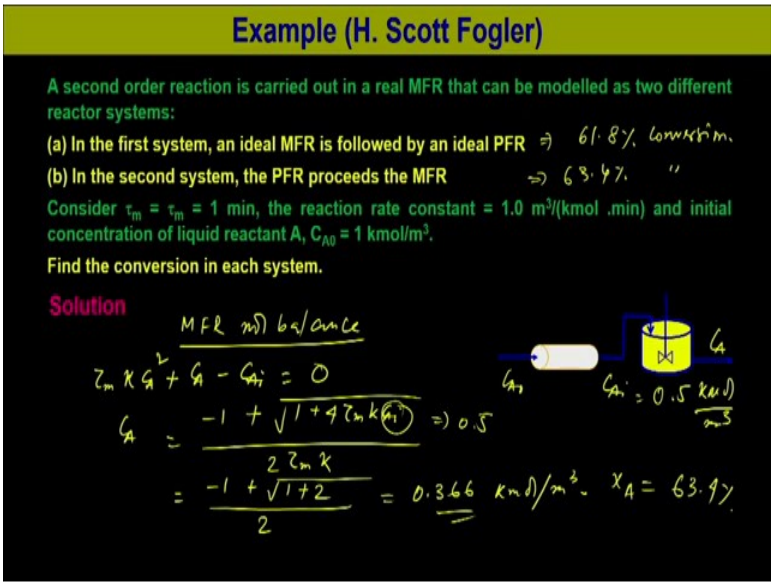
Find the conversion in each system.

Solution

Mole balance of PFR

$$\frac{1}{C_{Ai}} - \frac{1}{C_{A0}} = \tau_p k.$$

$$\frac{1}{C_{Ai}} - \frac{1}{1} = 1 \times 1 \Rightarrow C_{Ai} = 0.5 \text{ kmol/m}^3.$$



Example (H. Scott Fogler)

A second order reaction is carried out in a real MFR that can be modelled as two different reactor systems:

(a) In the first system, an ideal MFR is followed by an ideal PFR ⇒ 61.8% conversion.

(b) In the second system, the PFR proceeds the MFR ⇒ 63.4% "

Consider $\tau_m = \tau_m = 1$ min, the reaction rate constant = 1.0 m³/(kmol .min) and initial concentration of liquid reactant A, $C_{A0} = 1$ kmol/m³.

Find the conversion in each system.

Solution

MFR mol balance

$$\tau_m k C_A^2 + C_A - C_{Ai} = 0$$

$$C_A = \frac{-1 + \sqrt{1 + 4\tau_m k \boxed{C_{Ai}}}}{2\tau_m k} \Rightarrow 0.5$$

$$= \frac{-1 + \sqrt{1+2}}{2} = \underline{0.366} \text{ kmol/m}^3. \quad X_A = 63.4\%$$

So now we will consider the second case where first PFR is connected and then CSTR. So in this case, this is C_{A0}, this is C_{Ai} and this is C_A. So we can write from the mole balance of PFR, $\frac{1}{C_{Ai}} - \frac{1}{C_{A0}} = \tau_p k$ and $\frac{1}{C_{Ai}} - \frac{1}{1} = 1*1$. So from here we can calculate $C_{Ai} = 0.5\, kmol/m^3$

Now, this $C_{Ai} = 0.5\, kmol/m^3$ which is inlet to the CSTR and we have to do the CSTR mole balance with the inlet concentration of $0.5\, kmol/m^3$. So, to calculate CA. Now MFR mole balance, so this is C_{A0}, C_{Ai} and C_{A0} which is $0.5\,kmol/m^3$. So if we do this, this would be

$\tau_m k C_A^{\,2} + C_A - C_{Ai} = 0$. And form here we can write

$$C_A = \frac{-1+\sqrt{1+4\tau_m k C_{Ai}}}{2\tau_m k} \Rightarrow 0.5$$
$$= \frac{-1+\sqrt{1+2}}{2} = 0.366\,kmol/m^3$$

So then conversion over here, that is $X_A = 63.4\%$.

So, we could see that in these two configuration; in the first configuration, we obtain 61 point for this case, 61.8 percent conversion and in the second case we obtain 63.4 percent conversion. So, as we can see although there is a marginal difference of the conversion between these two arrangements but there is a point that there is a difference of conversion. So let us conclude from this example.

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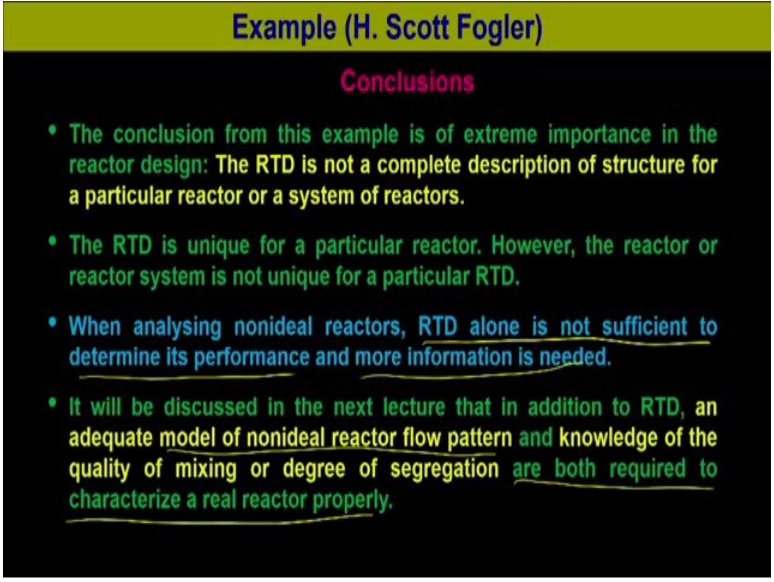

Example (H. Scott Fogler)

Conclusions

- The conclusion from this example is of extreme importance in the reactor design: The RTD is not a complete description of structure for a particular reactor or a system of reactors.
- The RTD is unique for a particular reactor. However, the reactor or reactor system is not unique for a particular RTD.
- When analysing nonideal reactors, RTD alone is not sufficient to determine its performance and more information is needed.
- It will be discussed in the next lecture that in addition to RTD, an adequate model of nonideal reactor flow pattern and knowledge of the quality of mixing or degree of segregation are both required to characterize a real reactor properly.

So the conclusion from this example is of extreme importance in the reactor design. Particularly we can see that the RTD is not the complete description of structure for a particular reactor or the reactor systems because as we have seen earlier, the RTD function is the same for both the arrangements but as we could see the conversion of these two different arrangements they are different. So the RTD is unique for a particular reactor however the reactor or reactor system is not unique for a particular RTD.

When we are analysing the non-ideal reactors, RTD alone is not sufficient to determine the performance and more information is needed. So, only RTD alone cannot be sufficient to determine the performance of the reactor. So we need to have certain other information or more information for the design of the reactor or analysing the characteristics of the real reactors. So it will be discussed in our next lecture that in addition to the RTD, an adequate model of non-ideal reactor flow pattern as well as the knowledge of the mixing, quality of the mixing or the degree of segregation inside the reactor are both required to characterise a real reactor properly.

So, we will consider these aspects of the non-ideal reactor design based on the flow pattern inside the reactor as well as the segregation inside the reactor in our next lecture. So thank you very much for attending this lecture.