Chemical Reaction Engineering I

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Lecture 30 - Reactor Modelling using the RTD

Welcome to the fourth lecture of module 5 for Chemical Reaction Engineering I and this is the final lecture of this course. Before going to this lecture let us have brief recap on our previous lecture.

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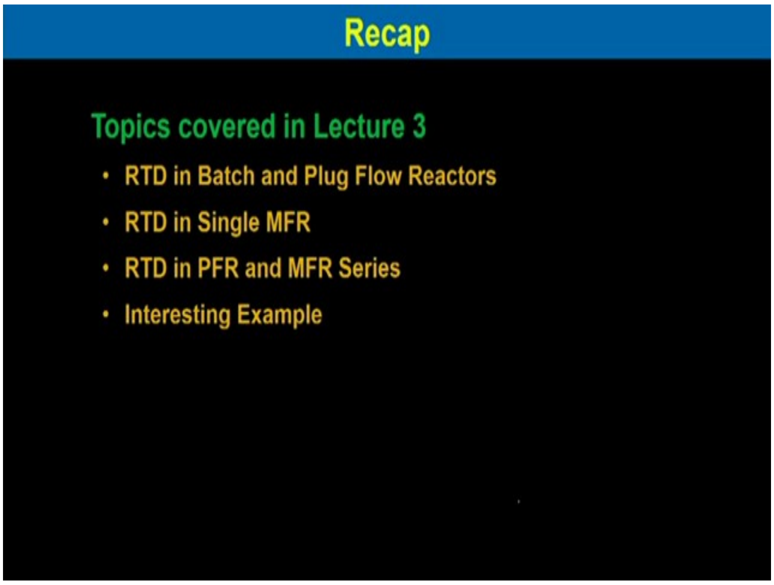

Recap

Topics covered in Lecture 3

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

In the last lecture we have covered residence time distribution in batch and plug flow reactor then RTD in single mix flow reactor. We have considered RTD in plug flow reactor and mix flow reactor in series and then we have discussed various interesting examples to see the RTD residence time distribution in the reactors.

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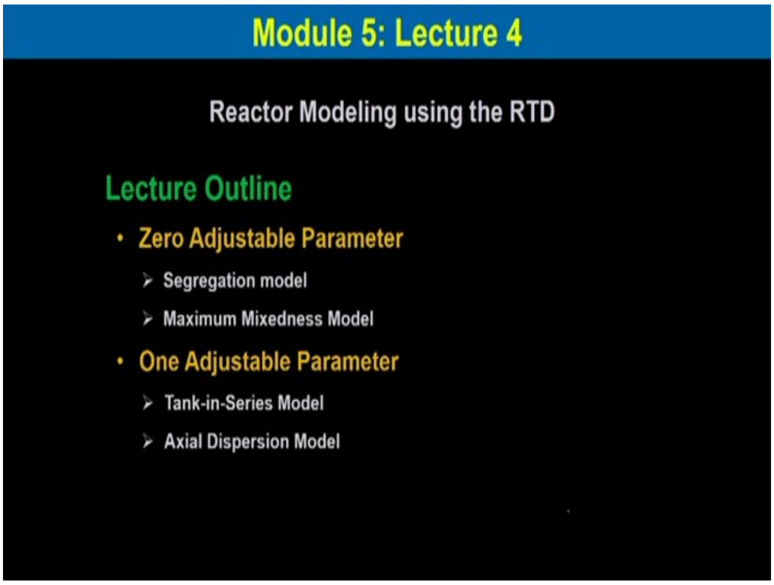

Module 5: Lecture 4

Reactor Modeling using the RTD

Lecture Outline

- Zero Adjustable Parameter
  - Segregation model
  - Maximum Mixedness Model
- One Adjustable Parameter
  - Tank-in-Series Model
  - Axial Dispersion Model

In this lecture we will consider reactor modelling using RTD. The brief outline of this lecture are zero adjustable parameter model and under which we will consider first the segregation flow model and then we will consider maximum mixedness model. We will also consider one adjustable parameter model under which we will consider tank-in-series model and axial dispersion model. There are also other models which are two parameter models and we will not consider over here for the two parameter models but for understanding of the reader or more knowledge the readers are requested to read two books, one is Levenspiel and another is Fogler’s book.

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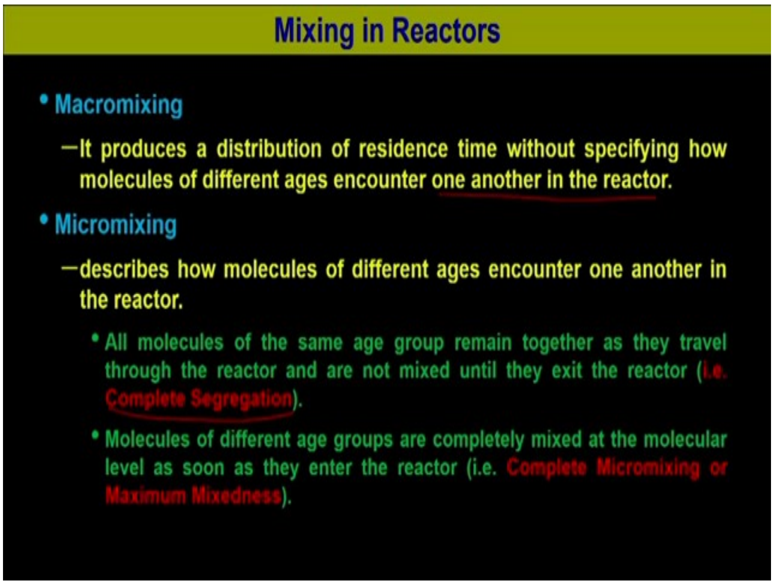

Mixing in Reactors

- Macromixing
  - It produces a distribution of residence time without specifying how molecules of different ages encounter one another in the reactor.
- Micromixing
  - describes how molecules of different ages encounter one another in the reactor.
    - All molecules of the same age group remain together as they travel through the reactor and are not mixed until they exit the reactor (i.e. Complete Segregation).
    - Molecules of different age groups are completely mixed at the molecular level as soon as they enter the reactor (i.e. Complete Micromixing or Maximum Mixedness).

So, let us start with mixing in the reactors. There are two types of mixing, one is macromixing, another is micromixing. The macromixing it produces a distribution of residence time without specifying how the molecules of different ages encounter one another in the reactor. So, the distribution of their residence time that means how long the elements of the fluid will stay inside the reactor will be obtained without specifying how molecules of different ages they collide or they encounter each other inside the reactor.

And micromixing describes the how molecules of different ages encounter one another in the reactor. So, in this case all molecules of the same age group remain together as they travel through the reactor and are not mixed until they exit through the reactor. So, we call it complete segregation. So, basically the elements of same age groups remain together and they travel through the reactor and they are not mixed until it comes out to the exit of the reactor. That means each molecules or each element of fluid remains separated from other bid of molecules as long as they are inside the reactor but as soon as they come out they are well mixed.

So, inside the reactor they are completely segregated, so that is one case. The other case molecules of different age groups are completely mixed at the molecular level as soon as they enter the reactor. So, we call complete micromixing or maximum mixedness. That means all the elements of fluid and all age groups they are homogeneously mixed.

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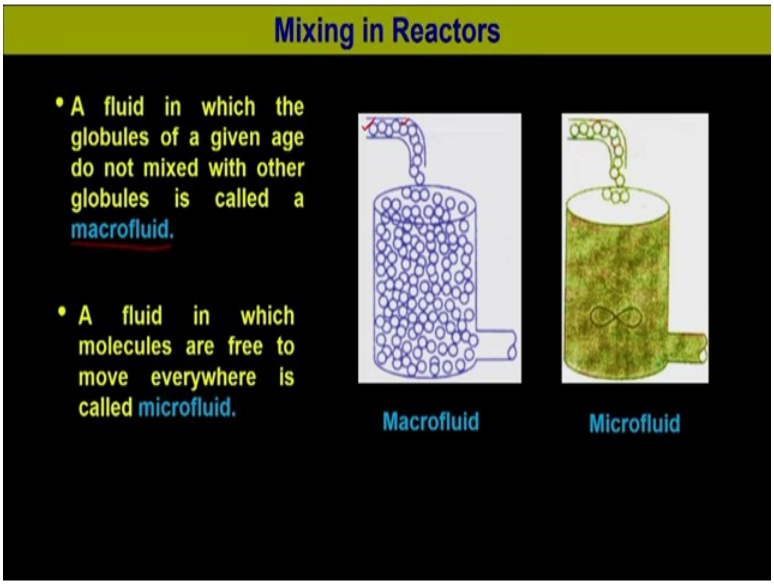

Mixing in Reactors

- A fluid in which the globules of a given age do not mixed with other globules is called a macrofluid.
- A fluid in which molecules are free to move everywhere is called microfluid.

Macrofluid

Microfluid

So, a fluid in which the globules of a given age do not mix with each other globules is called the macrofluid. So, like if we consider over here you can see the molecules which entered at different times and they are not mixed each other throughout the reactor, they remain separated. So, that is called macrofluids.

And a fluid in which molecules are free to move everywhere is called the microfluid. We can see here there are globules which entered and they are mixed. They are free to move anywhere inside the reactor, they are not separated, mixed, so it is microfluid.

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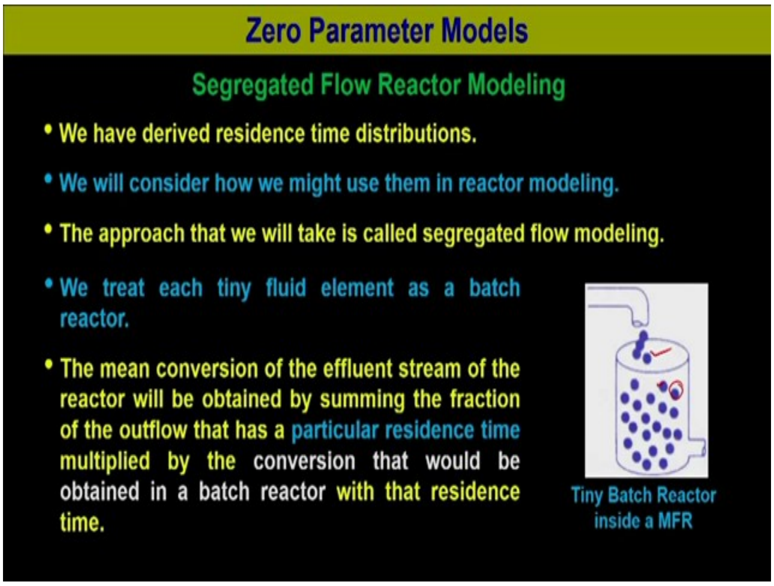

Zero Parameter Models

Segregated Flow Reactor Modeling

- We have derived residence time distributions.
- We will consider how we might use them in reactor modeling.
- The approach that we will take is called segregated flow modeling.
- We treat each tiny fluid element as a batch reactor.
- The mean conversion of the effluent stream of the reactor will be obtained by summing the fraction of the outflow that has a particular residence time multiplied by the conversion that would be obtained in a batch reactor with that residence time.

Tiny Batch Reactor inside a MFR

Now, we will consider zero parameter model. One of them is segregated flow reactor modelling and we have derived residence time distributions earlier. We will consider how we might use this residence time distribution in the reactor modelling. The approach that we take is called the segregated flow modelling and we treat each tiny fluid element as a batch reactor. As we have seen earlier say if you consider a continuous stirred tank reactor or mixed flow reactor you can see different globules entered inside and each tiny bit of globules is considered a batch reactor.

So, here each globule is considered as a batch reactor inside a mixed flow reactor. So this is continuous mixed flow reactor and inside that whatever the fluid element enters they are in a small globules and they remains intact until that come out to the reactor. So, basically the mixed flow reactor contains large number of batch reactor inside.

So, the mean conversion or the mean concentration of the effluent stream of the reactor will be obtained by summing the fraction of the outflow that has a particular residence time multiplied by the conversion that would be obtained in a batch reactor with that residence time. We can see not all globules from a mixed flow reactor will come out at the same time.

So, each globules will spend certain period of time inside the reactor and that is the residence time of that globules. So, in that globules or in that tiny bit of elements the fluid inside that is well mixed and the conversion will obtain as per the batch reactor kinetics. So, the conversion which we obtain in each tiny bit of element is the batch reactor conversion and we sum up all the conversion of the tiny bit of elements then we will get the conversion in a mixed flow reactor. That is the concept.

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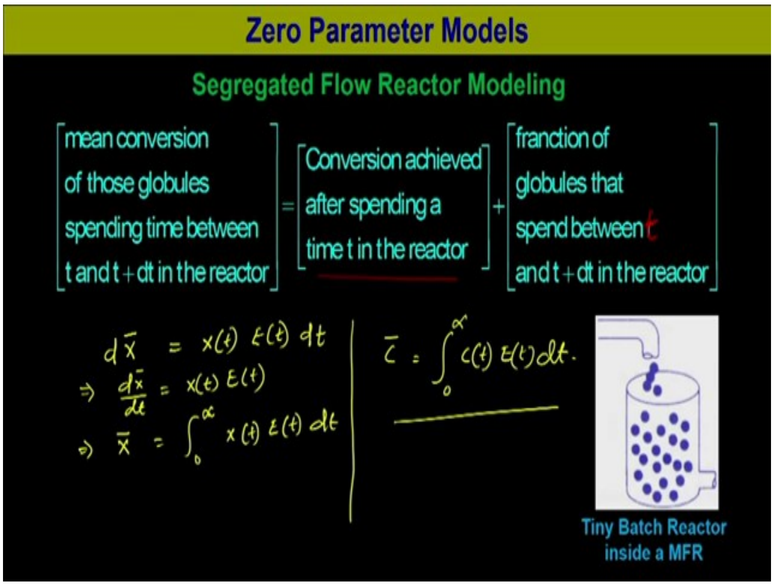

Zero Parameter Models

Segregated Flow Reactor Modeling

[mean conversion of those globules spending time between t and t+dt in the reactor] = [Conversion achieved after spending a time t in the reactor] + [frantion of globules that spend between t and t+dt in the reactor]

$d\bar{x} = x(t)\,E(t)\,dt$

$\Rightarrow \frac{d\bar{x}}{dt} = x(t)\,E(t)$

$\Rightarrow \bar{x} = \int_0^{\infty} x(t)\,E(t)\,dt$

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

So, the mean conversion of those globules spending time between t and t+ dt in the reactor would be equal to conversion achieved after spending a time in the reactor plus the fraction of globules that spend between t and t + dt in the reactor. So, we can write $d\overline{X} = X(t)E(t)dt$.. So, x bar is the main conversion and xt is the conversion which obtain in a batch reactor and E t is the residence time distribution function. So, here we are using the residence time distribution function for a particular reactor to calculate the mean conversion using the segregated flow model. So, RTD is used in conjunction with the segregated flow model to obtain the conversion for a particular non-ideal reactors.

So, we can write from here $\frac{d\overline{X}}{dt} = X(t)E(t)$ or $\overline{X} = \int_0^{\infty} X(t)E(t)dt$. So, if we considered in terms of the mean concentration we can write $\overline{C} = \int_0^{\infty} C(t)E(t)dt$. So, we can either calculate the mean conversion or the mean concentration.

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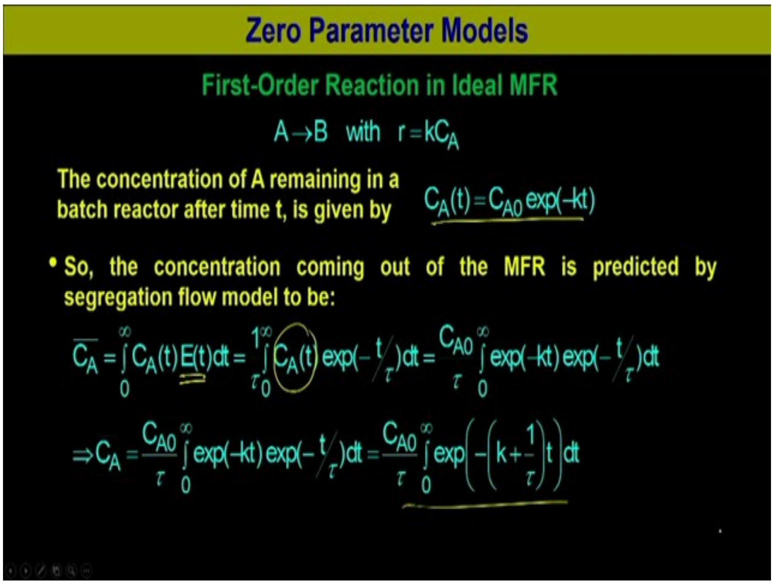

Zero Parameter Models

First-Order Reaction in Ideal MFR

$A \rightarrow B$ with $r = kC_A$

The concentration of A remaining in a batch reactor after time t, is given by $C_A(t) = C_{A0}\exp(-kt)$

- So, the concentration coming out of the MFR is predicted by segregation flow model to be:

$$\overline{C_A} = \int_0^\infty C_A(t)E(t)dt = \frac{1}{\tau}\int_0^\infty C_A(t)\exp(-t/\tau)dt = \frac{C_{A0}}{\tau}\int_0^\infty \exp(-kt)\exp(-t/\tau)dt$$

$$\Rightarrow C_A = \frac{C_{A0}}{\tau}\int_0^\infty \exp(-kt)\exp(-t/\tau)dt = \frac{C_{A0}}{\tau}\int_0^\infty \exp\left(-\left(k+\frac{1}{\tau}\right)t\right)dt$$

Now, let us consider first order reaction in ideal mixed flow reactor. So, if we consider the reactions $A \rightarrow B$ with $r = kC_A$, we will try to see how we can calculate the mean concentration using the ideal CSTR model and using the segregated flow model in conjunction with the residence time distribution function. So, the concentration of A remaining in a batch reactor after time t is given by $C_A(t) = C_{A0}\exp(-kt)$. So, this is the batch reactor concentration profile for a first order reaction.

Now, the concentration coming out of the mixed flow reactor is predicted by segregation flow model is $\overline{C_A} = \int_0^\infty C_A(t)E(t)dt$. So $\overline{C_A} = \frac{1}{\tau}\int_0^\infty C_A(t)\exp(-t/\tau)dt$. Now, this CA t we can substitute the concentration profile from here. So, if we substitute this would be

$$= \frac{C_{A0}}{\tau}\int_0^\infty \exp(-kt)\exp(-t/\tau)dt$$

So, from here we can write the average concentration of A would be

$$C_A = \frac{C_{A0}}{\tau}\int_0^\infty \exp(-(k + 1/\tau)t)dt$$

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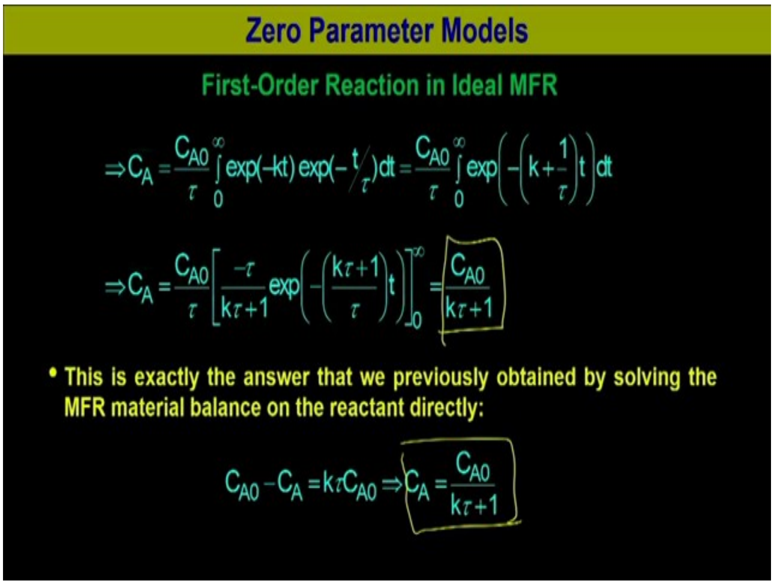

Zero Parameter Models

First-Order Reaction in Ideal MFR

$$\Rightarrow C_A = \frac{C_{A0}}{\tau}\int_0^\infty \exp(-kt)\exp(-t/\tau)dt = \frac{C_{A0}}{\tau}\int_0^\infty \exp\left(-\left(k+\frac{1}{\tau}\right)t\right)dt$$

$$\Rightarrow C_A = \frac{C_{A0}}{\tau}\left[\frac{-\tau}{k\tau+1}\exp\left(-\left(\frac{k\tau+1}{\tau}\right)t\right)\right]_0^\infty = \boxed{\frac{C_{A0}}{k\tau+1}}$$

- This is exactly the answer that we previously obtained by solving the MFR material balance on the reactant directly:

$$C_{A0} - C_A = k\tau C_{A0} \Rightarrow \boxed{C_A = \frac{C_{A0}}{k\tau+1}}$$

So, now if we integrate this, so we would obtain $C_A = \frac{C_{A0}}{\tau}\left[\frac{-\tau}{k\tau+1}\exp(-(k+1/\tau)t)\right]_0^\infty$. So, after putting this limit we would obtain $\frac{C_{A0}}{k\tau+1}$. So, this is our prediction of the mean concentration using RTD and segregation flow model for first order reaction.

Now, if we use the ideal CSTR model to calculate the conversion or concentration, mean concentration this is exactly the same thing which we obtain from the material balance of the CSTR or mixed flow reactor. So, here we can write $C_{A0} - C_A = k\tau C_A \Rightarrow C_A = \frac{C_{A0}}{k\tau+1}$ which is exactly same as we obtained from the segregated flow model.

So, for the first order system as we can see the concentration or average concentration or mean concentration predicted by the segregation flow model is exactly same as that obtained from the concentration profile from the ideal CSTR model. So, with this encouraging result if we start to look into the second order system, how that behave or how that prediction we can get?

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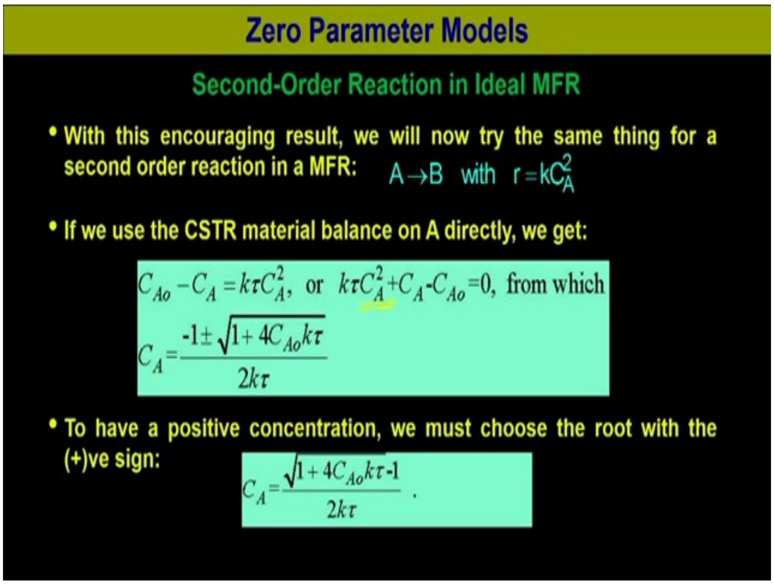

Zero Parameter Models

Second-Order Reaction in Ideal MFR

- With this encouraging result, we will now try the same thing for a second order reaction in a MFR: $A \rightarrow B$ with $r = kC_A^2$
- If we use the CSTR material balance on A directly, we get:

$C_{Ao} - C_A = k\tau C_A^2$, or $k\tau C_A^2 + C_A - C_{Ao} = 0$, from which

$$C_A = \frac{-1 \pm \sqrt{1 + 4C_{Ao}k\tau}}{2k\tau}$$

- To have a positive concentration, we must choose the root with the (+)ve sign:

$$C_A = \frac{\sqrt{1 + 4C_{Ao}k\tau} - 1}{2k\tau} .$$

So, now second order system and if we write this is $A \rightarrow B$ with $r = kC_A^2$ and we will obtain the CSTR or mixed flow reactor material balance on A directly we get, $C_{A0} - C_A = k\tau C_A^2$ and from here we can rearrange it $k\tau C_A^2 + C_A - C_{A0} = 0$ and calculate the concentration CA. So, $C_A = \frac{-1 \pm \sqrt{1 + 4C_{A0}k\tau}}{2k\tau}$. So, to have a positive concentration, so concentration cannot be negative, so we must choose the root with the positive sign.

So, our concentration is equal to CA would be $C_A = \frac{\sqrt{1 + 4C_{A0}k\tau} - 1}{2k\tau}$. So, this minus 1 is outside the square root. So, this is the concentration which we can obtain for the second order reaction in an ideal mixed flow reactor or CSTR. So, this is using the ideal mixed flow reactor model. Now, we will apply the segregation flow model for the second order system and see how we can get the concentration profile.

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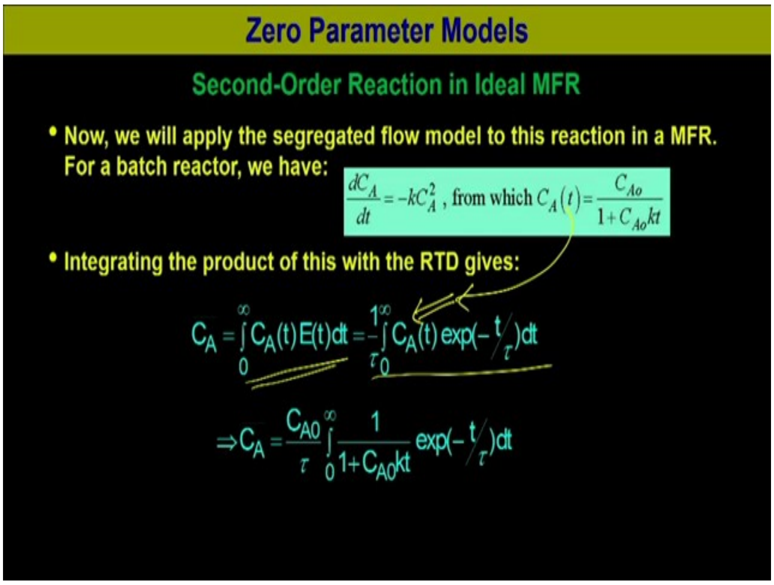


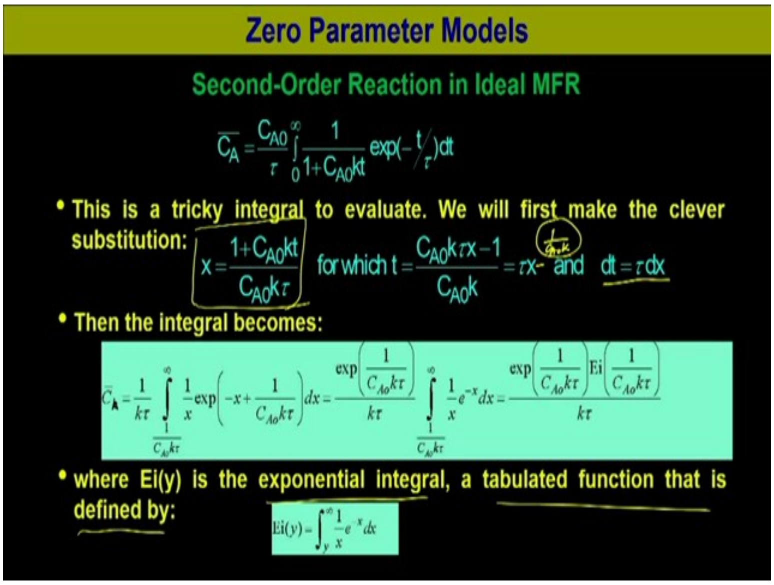
Zero Parameter Models

Second-Order Reaction in Ideal MFR

- Now, we will apply the segregated flow model to this reaction in a MFR. For a batch reactor, we have: $\frac{dC_A}{dt}=-kC_A^2$, from which $C_A(t)=\frac{C_{Ao}}{1+C_{Ao}kt}$
- Integrating the product of this with the RTD gives:

$$C_A=\int_0^\infty C_A(t)E(t)dt=\frac{1}{\tau}\int_0^\infty C_A(t)\exp(-t/\tau)dt$$

$$\Rightarrow C_A=\frac{C_{A0}}{\tau}\int_0^\infty \frac{1}{1+C_{A0}kt}\exp(-t/\tau)dt$$



Zero Parameter Models

Second-Order Reaction in Ideal MFR

$$\overline{C_A}=\frac{C_{A0}}{\tau}\int_0^\infty \frac{1}{1+C_{A0}kt}\exp(-t/\tau)dt$$

- This is a tricky integral to evaluate. We will first make the clever substitution: $x=\frac{1+C_{A0}kt}{C_{A0}k\tau}$ for which $t=\frac{C_{A0}k\tau x-1}{C_{A0}k}=\tau x-\frac{1}{C_{A0}k}$ and $dt=\tau dx$
- Then the integral becomes:

$$\bar{C}_A=\frac{1}{k\tau}\int_{\frac{1}{C_{Ao}k\tau}}^{\infty}\frac{1}{x}\exp\left(-x+\frac{1}{C_{Ao}k\tau}\right)dx=\frac{\exp\left(\frac{1}{C_{Ao}k\tau}\right)}{k\tau}\int_{\frac{1}{C_{Ao}k\tau}}^{\infty}\frac{1}{x}e^{-x}dx=\frac{\exp\left(\frac{1}{C_{Ao}k\tau}\right)\mathrm{Ei}\left(\frac{1}{C_{Ao}k\tau}\right)}{k\tau}$$

- where Ei(y) is the exponential integral, a tabulated function that is defined by: $\mathrm{Ei}(y)=\int_y^\infty \frac{1}{x}e^{-x}dx$

So, in case of segregated flow model for the second order reaction the conversion or the concentration which we obtain is the concentration as per the batch reactor concentration profile. So, $\frac{dC_A}{dt}=-kC_A^2$ so from which we can get concentration profile, $C_A(t)=\frac{C_{A0}}{1+C_{A0}kt}$.

Now, if we take the average concentration and if we use the segregated flow model, this is the model equations, so what we need to do? We need to submit this CA t from here and if we substitute and then if we integrate this then we would obtain the concentration profile. But this evaluation of this integral is no simple, it is little tricky to evaluate.

So, we must have a clever substitution on it. So, let us have $x = \frac{1+C_{A0}kt}{C_{A0}k\tau}$ and if we rearrange this relation so this is we have assumed, x is this and now if we rearrange, we can write $t = \frac{C_{A0}k\tau x - 1}{C_{A0}k} = \tau x$ but if we differentiate, $dt = \tau dx$ because this part is constant. So $dt = \tau dx$ Now, if we substitute that over here, so we would obtain the integration $\overline{C_A} = \frac{1}{k\tau}\int_{\frac{1}{C_{A0}k\tau}}^{\infty}\frac{1}{x}\exp(-x - \frac{1}{C_{A0}k\tau})dx =$. So, after integration you will get

$\frac{\exp(\frac{1}{C_{A0}k\tau})}{k\tau}\int_{\frac{1}{C_{A0}k\tau}}^{\infty}\frac{1}{x}e^{-x}\,dx =$ and then you will obtain $\frac{\exp(\frac{1}{C_{A0}k\tau})Ei(\frac{1}{C_{A0}k\tau})}{k\tau}$ This E i 1 by this, it is a function E i and parameter of this is a function of this, so E i is the exponential integral and is a tabulated function that is defined $Ei(y) = \int_{y}^{\infty}\frac{1}{x}e^{-x}\,dx$. So, if we use the tabulated function we can obtain the results of concentration profile.

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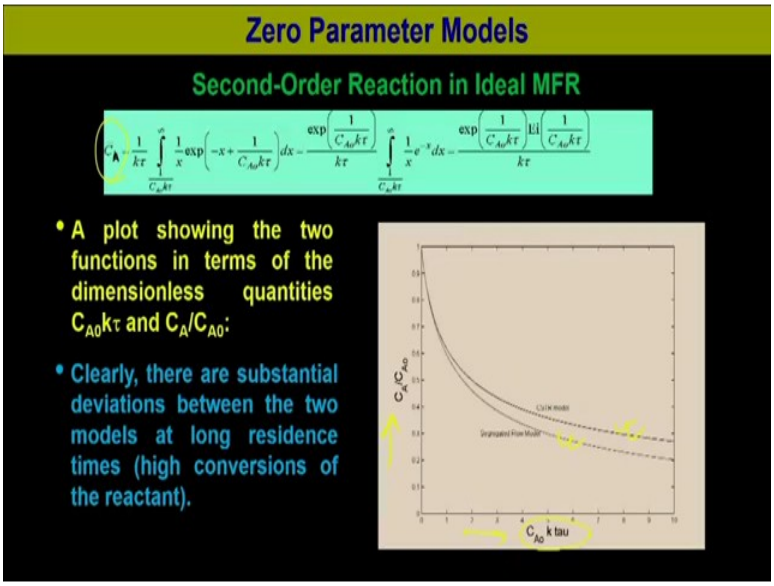

Zero Parameter Models

Second-Order Reaction in Ideal MFR

$$C_A = \frac{1}{k\tau}\int_{\frac{1}{C_{A0}k\tau}}^{\infty}\frac{1}{x}\exp\left(-x+\frac{1}{C_{A0}k\tau}\right)dx = \frac{\exp\left(\frac{1}{C_{A0}k\tau}\right)}{k\tau}\int_{\frac{1}{C_{A0}k\tau}}^{\infty}\frac{1}{x}e^{-x}dx = \frac{\exp\left(\frac{1}{C_{A0}k\tau}\right)\mathrm{Ei}\left(\frac{1}{C_{A0}k\tau}\right)}{k\tau}$$

- A plot showing the two functions in terms of the dimensionless quantities $C_{A0}k\tau$ and C_A/C_{A0}:
- Clearly, there are substantial deviations between the two models at long residence times (high conversions of the reactant).

Now, if we plot the concentration profile obtained using the segregated flow model and the concentration profile which we obtain for the ideal CSTR model, we can see this this curve is using the ideal CSTR or mixed flow reactor model and this curve represents the concentration profile obtained using this relation that is the segregation flow model.

So, we could see that this is the plot of two functions in terms of the dimensionless quantities CA0 k tau vs CA by CA0. What we can observe, there are substantial deviations between the two models at long residence time that is at high conversion. When the conversion becomes more then there is a substantial deviation for the prediction of the average concentration using the ideal CSTR model and the segregated flow models.

So, we can see also for other reaction order and it would be seen that for except the first order reactions for all other order of the reactions there is a deviation of prediction of concentration profile or average concentration or the average conversion between the segregated flow model and the ideal CSTR or mixed flow reactor model.

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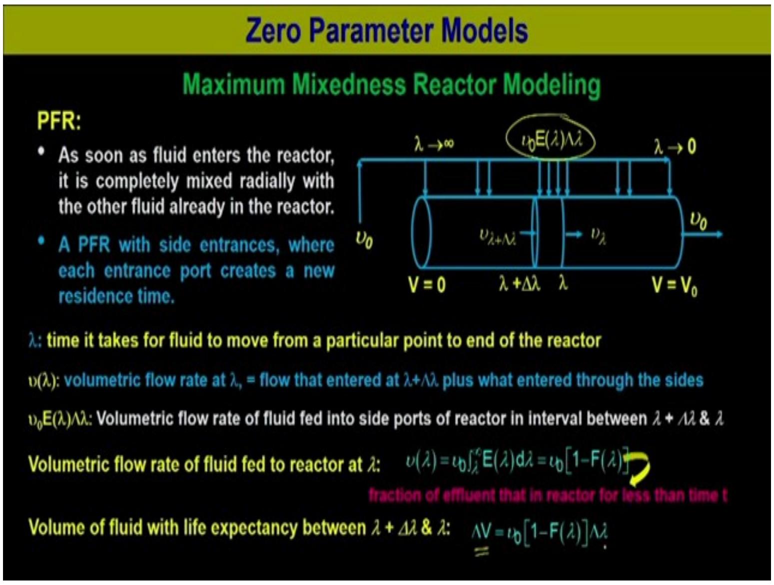

Zero Parameter Models

Maximum Mixedness Reactor Modeling

PFR:

- As soon as fluid enters the reactor, it is completely mixed radially with the other fluid already in the reactor.
- A PFR with side entrances, where each entrance port creates a new residence time.

λ: time it takes for fluid to move from a particular point to end of the reactor

$\upsilon(\lambda)$: volumetric flow rate at λ, = flow that entered at $\lambda+\Delta\lambda$ plus what entered through the sides

$\upsilon_0 E(\lambda)\Delta\lambda$: Volumetric flow rate of fluid fed into side ports of reactor in interval between $\lambda + \Delta\lambda$ & λ

Volumetric flow rate of fluid fed to reactor at λ: $\upsilon(\lambda) = \upsilon_0 \int_\lambda^\infty E(\lambda) d\lambda = \upsilon_0 [1 - F(\lambda)]$

fraction of effluent that in reactor for less than time t

Volume of fluid with life expectancy between $\lambda + \Delta\lambda$ & λ: $\Delta V = \upsilon_0 [1 - F(\lambda)] \Delta\lambda$

Now, we will consider another model under zero parameter models which is known as Maximum Mixedness Reactor Modelling and basically using the plug flow reactor with side stream, we can also obtain the complete mixing in a plug flow reactor. That also we have discussed earlier. So, as soon as fluid enters the reactor it is completely mixed radially with the other fluid already in the reactor. So, a PFR with side streams where each entrance port creates a new residence time. So, the fluid which enters at different locations in the side stream will have a different residence time because there is no backflow over here.

λ is the time it takes for fluid to move from a particular point to the end of the reactor. So, the λ is maximum where it starts and the fluid which enters at the ends its time or its pain inside the reactor is the minimum. So, $\upsilon(\lambda)$ is the volumetric flow rate at λ which is equal to flow that entered at $\lambda+\Delta\lambda$ plus what entered through the sides. So, $\upsilon_0 E(\lambda)\Delta\lambda$ is the volumetric flow rate that is here is the volumetric flow rate of the fluid fed into the side port of the reactor in interval $\lambda+\Delta\lambda$ and λ.

So, we can calculate the volumetric flow rate of the fluid fed to the reactor at λ which is $\upsilon(\lambda)$ which would be $\upsilon(\lambda)=\upsilon_0\int_{\lambda}^{\infty}E(\lambda)d\lambda$. So, if we put over here $E(\lambda)$ we will obtain $\upsilon_0\left[1-F(\lambda)\right]$. So, that is $F(\lambda)$ is the fraction of the effluent that in the reactor for less than time t or λ. Now, volume of fluid with life expectancy between $\lambda+\Delta\lambda$ and λ that is ΔV, so that is the volume of the fluid which is $\Delta V=\upsilon_0\left[1-F(\lambda)\right]\Delta\lambda$

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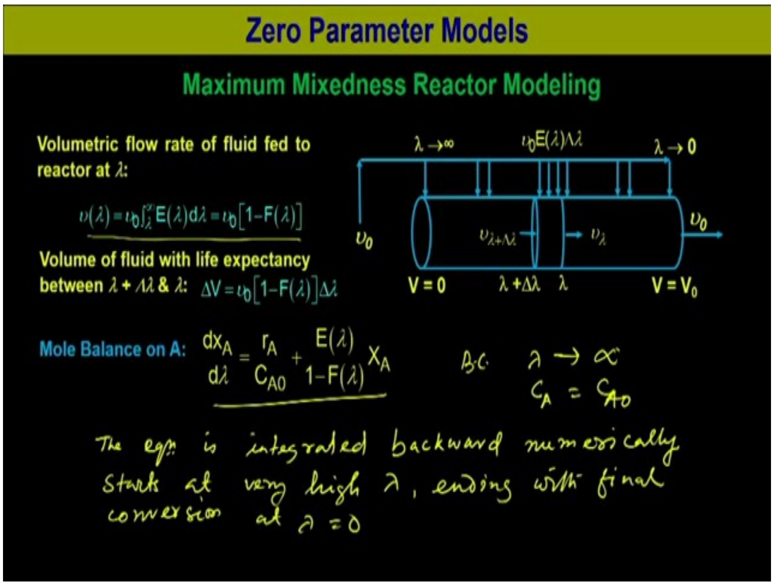

Zero Parameter Models

Maximum Mixedness Reactor Modeling

Volumetric flow rate of fluid fed to reactor at λ:

$$\upsilon(\lambda)=\upsilon_0\int_{\lambda}^{\infty}E(\lambda)d\lambda=\upsilon_0[1-F(\lambda)]$$

Volume of fluid with life expectancy between $\lambda+\Delta\lambda$ & λ: $\Delta V=\upsilon_0[1-F(\lambda)]\Delta\lambda$

Mole Balance on A: $\dfrac{dX_A}{d\lambda}=\dfrac{r_A}{C_{A0}}+\dfrac{E(\lambda)}{1-F(\lambda)}X_A$

B.C. $\lambda\to\infty$
$C_A = C_{A0}$

The eqn is integrated backward numerically
Start at very high λ, ending with final
conversion at $\lambda = 0$

Now, the volumetric flow rate of fluid fed to the reactor at λ would be $\upsilon(\lambda)$ which we have obtained earlier and the volume of fluid which life expectancy between this is this one. So, if we do the mole balance on A for this particular section which is taken over here, so if we do so we would obtain $\dfrac{dx_A}{d\lambda}=\dfrac{r_A}{C_{A0}}+\dfrac{E(\lambda)}{1-F(\lambda)}X_A$

So, for this the boundary condition would be $\lambda \rightarrow \infty$ then $C_A = C_{A0}$ or so to obtain the solutions of this the equation is integrated backward numerically. So, which starts at very high λ and ending with final conversion at $\lambda = 0$.

So, for a given RTDs and the reaction order greater than 1 this maximum mixedness model give the lower bound on the conversion. So, the examples for the segregation flow models and the maximum mixedness model and their comparison is given in the Fogler's book. So, I request all the readers to go through that book for the examples on the better understanding for the solution using the these two models.

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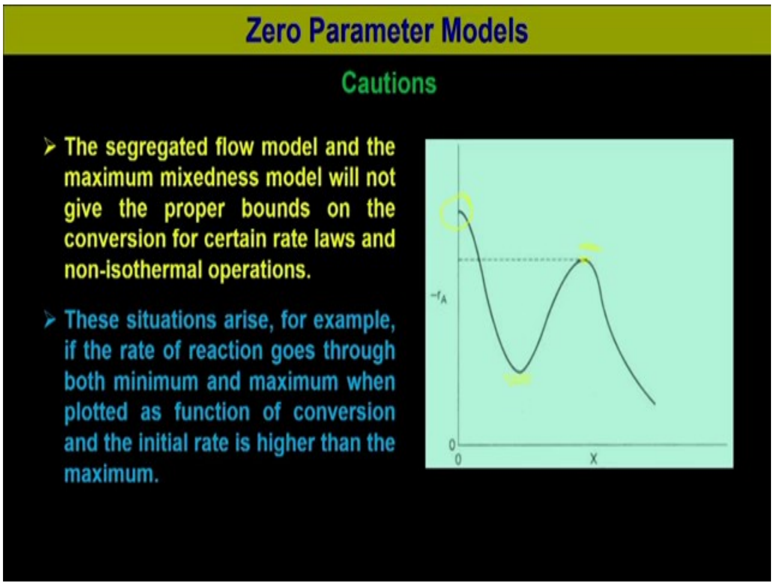

Zero Parameter Models

Cautions

- The segregated flow model and the maximum mixedness model will not give the proper bounds on the conversion for certain rate laws and non-isothermal operations.
- These situations arise, for example, if the rate of reaction goes through both minimum and maximum when plotted as function of conversion and the initial rate is higher than the maximum.

The segregated flow model and the maximum mixedness model will not give the proper bounds on the conversion for certain rate laws and the segregated flow model and the maximum mixedness model will not give the proper bound on the certain conversion on the conversion for certain rate laws and the non-isothermal operations.

For example, if the rate versus conversion curve as you can see over here goes through both maxima and minima, so when plotted with respect to the conversion, the initial rate is higher than the maximum. So, you can see the initial rate over here is higher than the maxima it can obtain. So, the maxima which is lower than the initial rate, so we cannot use the segregated flow models or the maximum mixedness model to calculate the conversion. So, these are the precautions which we need to take care while using this model.

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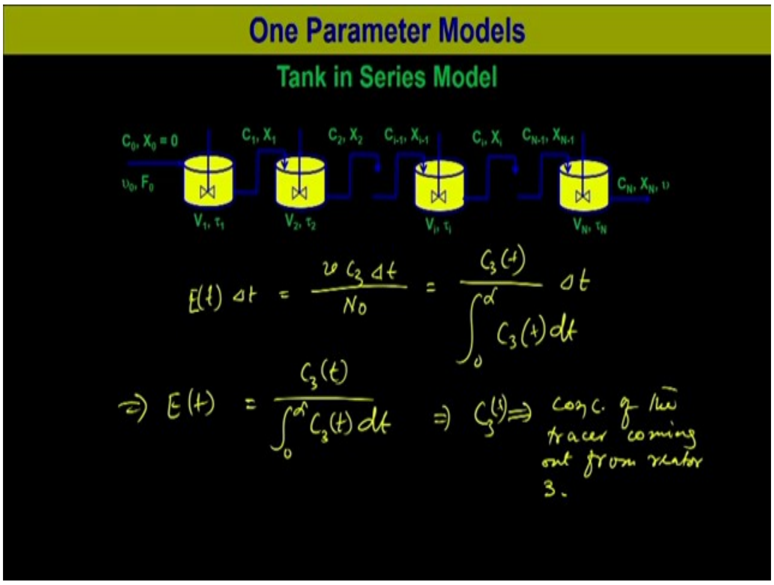

One Parameter Models

Tank in Series Model

$$E(t)\,\Delta t = \frac{\upsilon C_3 \Delta t}{N_0} = \frac{C_3(t)}{\int_0^\infty C_3(t)\,dt}\,\Delta t$$

$$\Rightarrow E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)\,dt} \Rightarrow C_3(t) \Rightarrow$$ conc. of the tracer coming out from reactor 3.

Now, in one parameter model we will consider tank in series model first. In the tank in series model basically equal sized CSTR they are connected in series and you can see if you have n number of CSTR connected in series so you have the inlet concentration is equal to X_0 would be equal to 0, conversion would be 0 and you have volumetric flow rate and the molar flow rate given for the exit of the reactor 1 will goes to the reactor 2 and so on and it will carry on till the nth reactor and the volume and the residence time for each reactor is given and essentially for equal size and equal volumetric flow rate they are same.

So, we know $E(t)\Delta t$ would be equal to V, say if you take 3 reactors connected in series so we can write the exit concentration which is coming out from reactor 3 would be $E(t)\Delta t = \frac{\upsilon C_3 \Delta t}{N_0} = \frac{C_3(t)}{\int_0^\infty C_3(t)dt}\Delta t$. So, from here we can write $E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)dt}$. So, here c3 t is the concentration of the tracer coming out from reactor 3.

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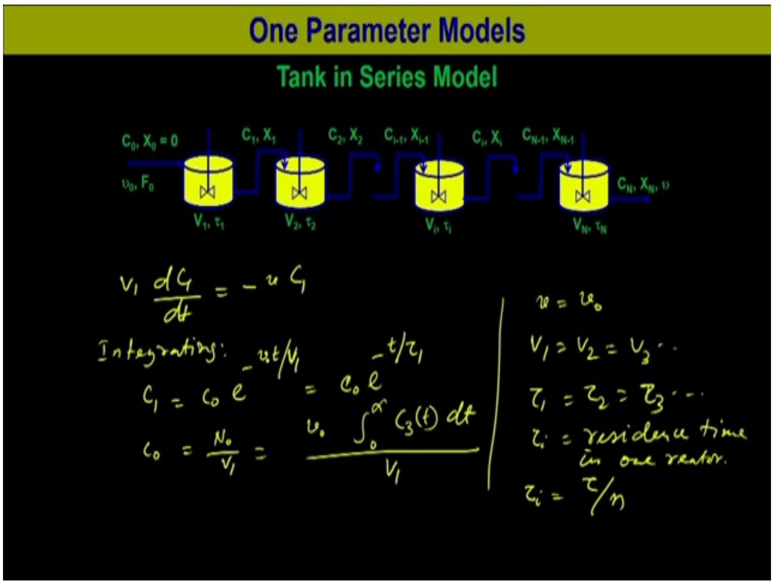

One Parameter Models

Tank in Series Model

$$V_1 \frac{dC_1}{dt} = -\upsilon C_1$$

Integrating:

$$C_1 = C_0 e^{-\upsilon t/V_1} = C_0 e^{-t/\tau_1}$$

$$C_0 = \frac{N_0}{V_1} = \frac{\upsilon_0 \int_0^\infty C_3(t)\,dt}{V_1}$$

$\upsilon = \upsilon_0$

$V_1 = V_2 = V_3 \cdots$

$\tau_1 = \tau_2 = \tau_3 \cdots$

τ_i = residence time in one reactor.

$\tau_i = \tau/n$

Now, if we want to calculate the $C_3(t)$ as a function of time, we would start with the first reactor where we can do the material balance for this reactor and which is $V_1 \frac{dC_1}{dt} = -\upsilon C_1$ and now if we integrate, we can obtain $C_1 = C_0 e^{-\upsilon_0 t/V_1} = C_0 e^{-t/\tau_1}$. So, $C_0 = \frac{N_0}{V_1} = \frac{\upsilon_0 \int_0^\infty C_3(t)dt}{V_1}$ So, here we assumed that the volumetric flow rate $\upsilon = \upsilon_0$ that is constant, all reactor volumes are identical $V_1 = V_2 = V_3 \ldots\ldots$, $\tau_1 = \tau_2 = \tau_3 \ldots\ldots$. So, we can if τ_i is the residence time in one reactor then we can write $\tau_i = \tau/n$ so if we have n number of reactors.

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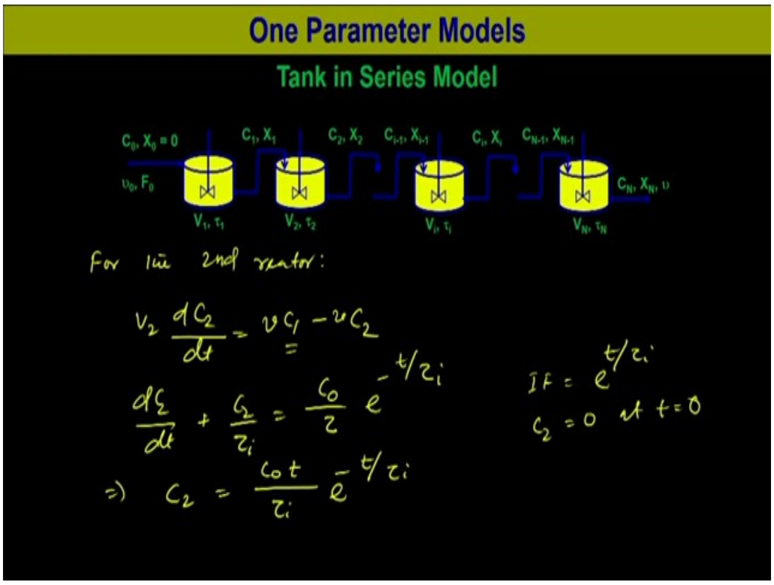


One Parameter Models

Tank in Series Model

For the 2nd reactor:

$$V_2 \frac{dC_2}{dt} = \upsilon C_1 - \upsilon C_2$$

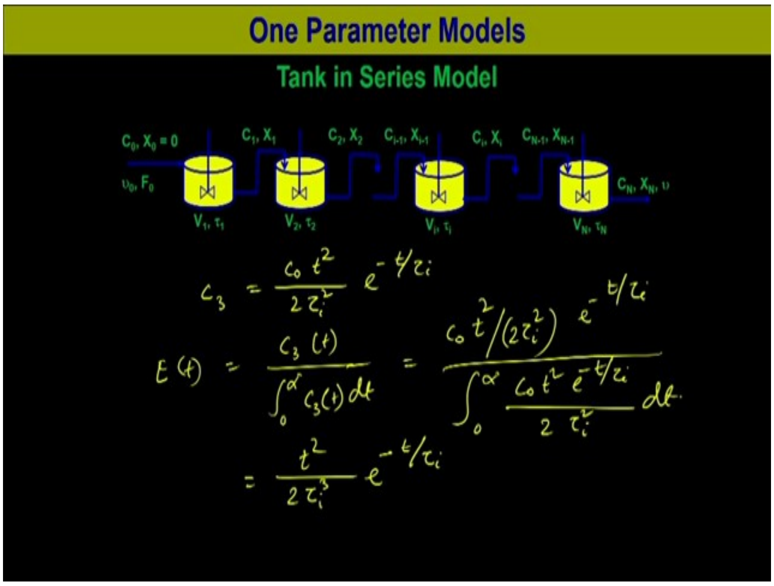
$$\frac{dC_2}{dt} + \frac{C_2}{\tau_i} = \frac{C_0}{\tau} e^{-t/\tau_i}$$

$IF = e^{t/\tau_i}$

$C_2 = 0$ at $t = 0$

$$\Rightarrow C_2 = \frac{C_0 t}{\tau_i} e^{-t/\tau_i}$$

Now, if we do the material balance for the second reactor, for the second reactor $V_2 \frac{dC_2}{dt} = \upsilon C_1 - \upsilon C_2$. Now, if we substitute c1 which we obtained earlier we would obtain $\frac{dC_2}{dt} + \frac{C_2}{\tau_i} = \frac{C_0}{\tau} e^{-t/\tau_i}$. So, which can be solved using the $IF = e^{t/\tau_i}$ and with initial conditions $C_0 = 0, t = 0$, so we can obtain the concentration profile $C_2 = \frac{C_0 t}{\tau_i} e^{-t/\tau_i}$ (Refer Slide Time: 35:01)



One Parameter Models

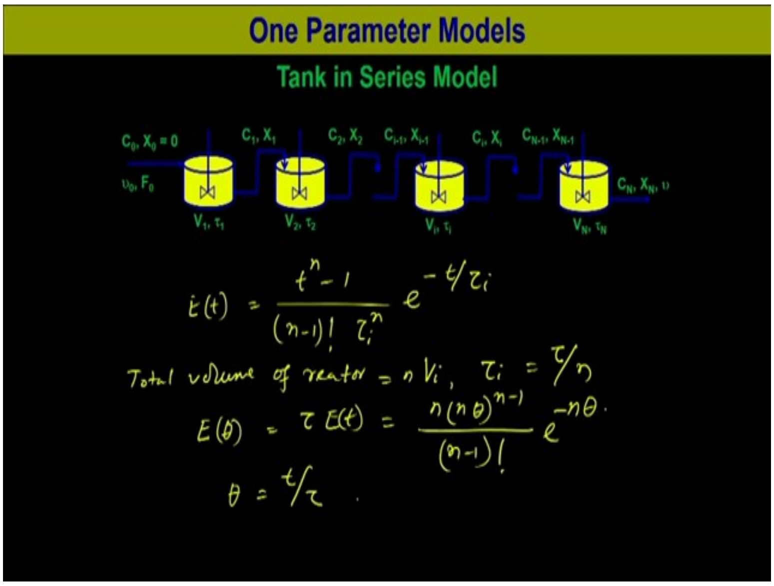
Tank in Series Model

$$C_3 = \frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i}$$

$$E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)\,dt} = \frac{C_0 t^2/(2\tau_i^2)\, e^{-t/\tau_i}}{\int_0^\infty \frac{C_0 t^2 e^{-t/\tau_i}}{2\tau_i^2}\,dt}$$

$$= \frac{t^2}{2\tau_i^3} e^{-t/\tau_i}$$

Now, similarly for the third reactor if we substitute this we were to obtain for third reactor $C_3 = \frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i}$. Now, if we substitute this concentration c3 in the RTD equations E t would be $E(t) = \frac{C_3(t)}{\int_0^\infty C_3(t)dt} = \frac{\frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i}}{\int_0^\infty \frac{C_0 t^2}{2\tau_i^2} e^{-t/\tau_i} dt}$ So, if we solve it, it would be $= \frac{t^2}{2\tau_i^3} e^{-t/\tau_i}$ (Refer Slide Time: 36:50)



One Parameter Models

Tank in Series Model

$$E(t) = \frac{t^n - 1}{(n-1)!\, \tau_i^n} e^{-t/\tau_i}$$

Total volume of reactor $= n V_i$, $\tau_i = \tau/n$

$$E(\theta) = \tau E(t) = \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta}.$$

$$\theta = t/\tau.$$

Now, if we use this expression for the n number of CSTR connected in series we can write $E(t) = \frac{t^n - 1}{(n-1)!\tau_i^n} e^{-t/\tau_i}$. Now, since the total volume of the reactor is equal to nV_i, $\tau_i = \tau/n$ then we can write $E(\theta) = \tau E(t) = \frac{n(n\theta)^{n-1}}{(n-1)!\tau_i^n} e^{-n\theta}$. So this is in dimensionless residence time distribution function where $\theta = t/\tau$

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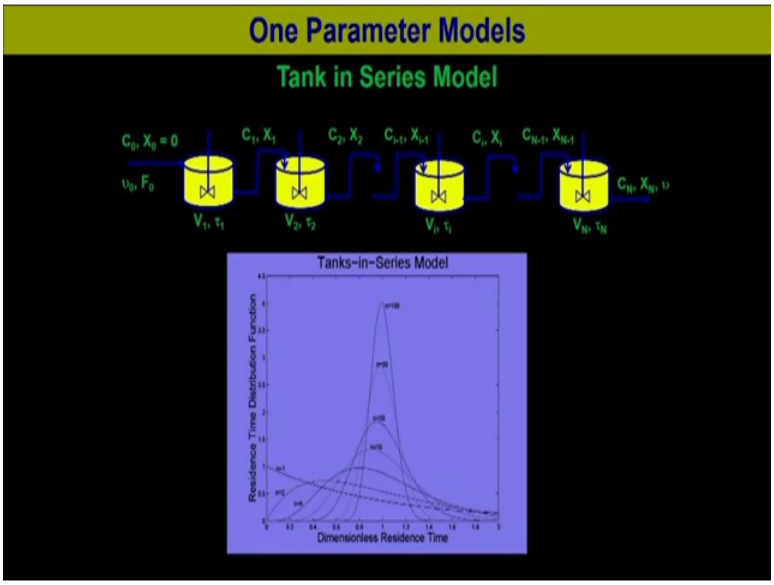

One Parameter Models

Tank in Series Model

Now, if we plot theta versus dimensionless residence time the plot would look like this, you can get for n is equal to 1 this is the residence time distribution function. As the number of CSTR increases your distribution is close to the plug flow reactor models.

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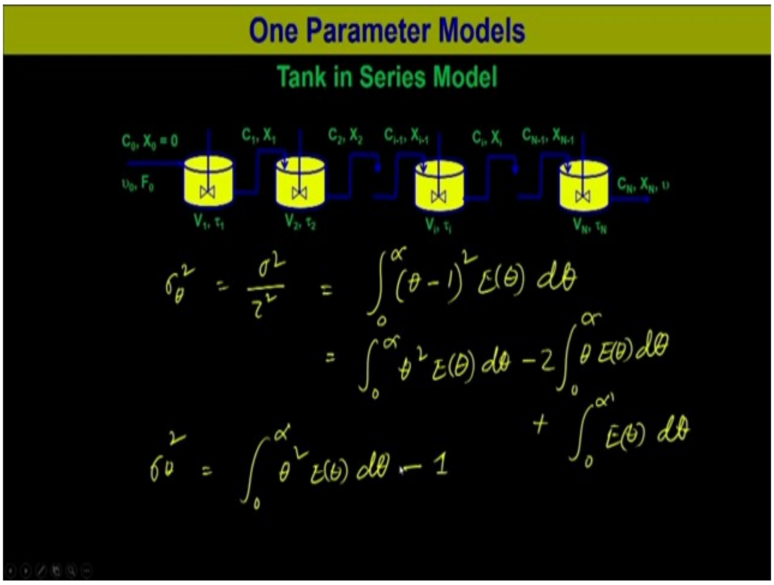

One Parameter Models

Tank in Series Model

$$\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \int_0^\infty (\theta-1)^2 E(\theta)\, d\theta$$

$$= \int_0^\infty \theta^2 E(\theta)\, d\theta - 2\int_0^\infty \theta E(\theta)\, d\theta + \int_0^\infty E(\theta)\, d\theta$$

$$\sigma_\theta^2 = \int_0^\infty \theta^2 E(\theta)\, d\theta - 1$$

So, we can see this by calculating the variance like we can evaluate $\sigma_\theta^2 = \frac{\sigma^2}{\tau^2} = \int_0^\infty (\theta-1)^2 E(\theta) d\theta = \int_0^\infty \theta^2 E(\theta) d\theta - 2\int_0^\infty \theta E(\theta) d\theta + \int_0^\infty E(\theta) d\theta$.. So if we multiply with $E(\theta)$ we can get this one. So, then we can write $\sigma_\theta^2 = \int_0^\infty \theta^2 E(\theta) d\theta - 1$.

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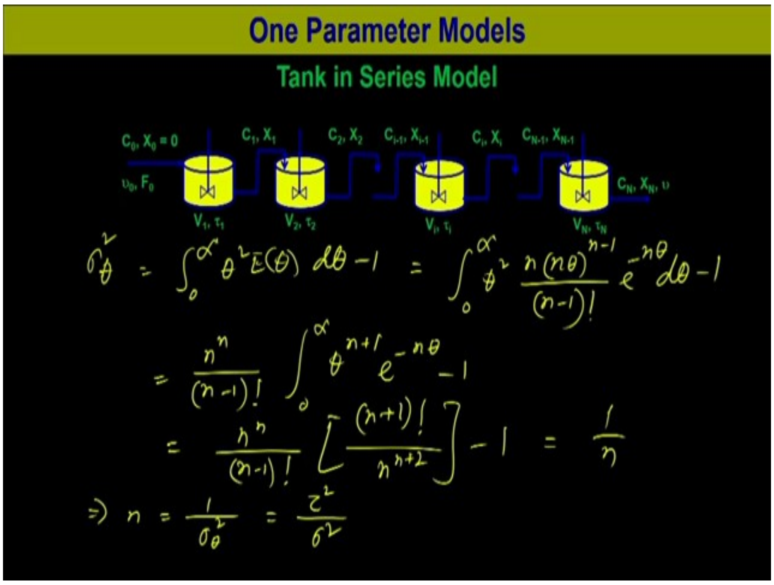

One Parameter Models

Tank in Series Model

$$\sigma_\theta^2 = \int_0^\infty \theta^2 E(\theta)\, d\theta - 1 = \int_0^\infty \theta^2 \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta} d\theta - 1$$

$$= \frac{n^n}{(n-1)!}\int_0^\infty \theta^{n+1} e^{-n\theta} - 1$$

$$= \frac{n^n}{(n-1)!}\left[\frac{(n+1)!}{n^{n+2}}\right] - 1 = \frac{1}{n}$$

$$\Rightarrow n = \frac{1}{\sigma_\theta^2} = \frac{\tau^2}{\sigma^2}$$

So, which is if we do that $\sigma_\theta^2 = \int_0^\infty \theta^2 E(\theta) d\theta - 1 = \int_0^\infty \theta^2 \frac{n(n\theta)^{n-1}}{(n-1)!} e^{-n\theta} d\theta - 1$ Now, if we solve it, it would be $\frac{n^n}{(n-1)!}\int_0^\infty \theta^{n+1} e^{-n\theta} d\theta - 1$ and hence we can write this would be equal $\frac{n^n}{(n-1)!}\left[\frac{(n+1)!}{n^{n+2}}\right] - 1$. So, from here we can write this is $\frac{1}{n}$. So, the n from here we can calculate $n = \frac{1}{\sigma_\theta^2} = \frac{\tau^2}{\sigma^2}$.

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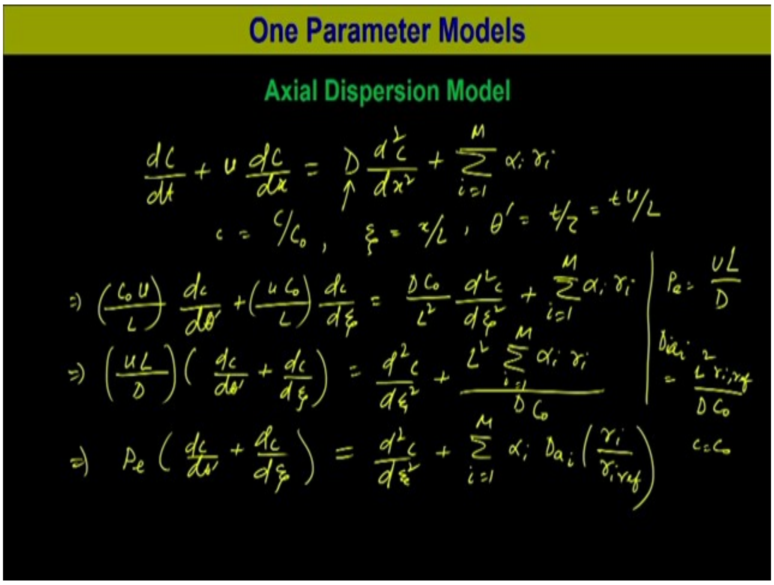

One Parameter Models

Axial Dispersion Model

$$\frac{dc}{dt} + u\frac{dc}{dx} = \underset{\uparrow}{D}\frac{d^2c}{dx^2} + \sum_{i=1}^{M}\alpha_i r_i$$

$$c = C/C_0, \quad \xi = x/L, \quad \theta' = t/\tau = tu/L$$

$$\Rightarrow \left(\frac{C_0 u}{L}\right)\frac{dc}{d\theta'} + \left(\frac{uC_0}{L}\right)\frac{dc}{d\xi} = \frac{DC_0}{L^2}\frac{d^2c}{d\xi^2} + \sum_{i=1}^{M}\alpha_i r_i \qquad Pe = \frac{uL}{D}$$

$$\Rightarrow \left(\frac{uL}{D}\right)\left(\frac{dc}{d\theta'} + \frac{dc}{d\xi}\right) = \frac{d^2c}{d\xi^2} + \frac{L^2\sum_{i=1}^{M}\alpha_i r_i}{DC_0} \qquad Da_i = \frac{L^2 r_{iref}}{DC_0}$$

$$\Rightarrow Pe\left(\frac{dc}{d\theta'} + \frac{dc}{d\xi}\right) = \frac{d^2c}{d\xi^2} + \sum_{i=1}^{M}\alpha_i Da_i\left(\frac{r_i}{r_{iref}}\right) \qquad c = C_0$$

So, now we will consider axial dispersion model that is plug flow reactor with axial dispersion and in this case if we do the mass balance where if we consider 1 species and its constant velocity of the fluid and the effective diffusion coefficient is d, so we can $\frac{dC}{dt} + u\frac{dC}{dx} = D\frac{d^2C}{dx^2} + \sum_{i=1}^{M}\alpha_i r_i$. So, if it is m number of reactions taking place so we can write this is the mass balance equation for plug flow reactor with axial dispersion, so this is the effective dispersion coefficient.

Now, if we make it non-dimensional equations we can introduce $c = C/C_0$, $\xi = x/L$, $\theta' = t/\tau = tu/L$, L is the length of the reactor then we can write this relation

$\left(\frac{C_0 u}{L}\right)\frac{dC}{d\theta} + \left(\frac{uC_0}{L}\right)\frac{dC}{d\xi} = \frac{DC_0}{L^2}\frac{d^2C}{d\xi^2} + \sum_{i=1}^{M}\alpha_i r_i$ Now, if we simplify this, this would be

$\left(\frac{uL}{D}\right)\left(\frac{dC}{d\theta} + \frac{dC}{d\xi}\right) = \frac{d^2C}{d\xi^2} + L^2\sum_{i=1}^{M}\alpha_i r_i$ and this term here is the peclet number $Pe = \frac{uL}{D}$ that is velocity into length divided by effective diffusivity is the peclet number

$Pe\left(\frac{dC}{d\theta} + \frac{dC}{d\xi}\right) = \frac{d^2C}{d\xi^2} + \sum_{i=1}^{M}\alpha_i D_{ai}\left(\frac{r_i}{r_{iref}}\right)$ So, pe is the peclet number which we have defined,

$Pe = \frac{uL}{D}$ and da i is the Damköhler number which is $D_{ai} = \frac{L^2 r_{iref}}{DC_0}$, reaction rate at standard conditions usually at $C = C_0$. So, this relation to see how the degree of mixing or axial mixing varies with the peclet number we will consider the residence time distribution predicted by this model where we can do the partial differentiation of this.

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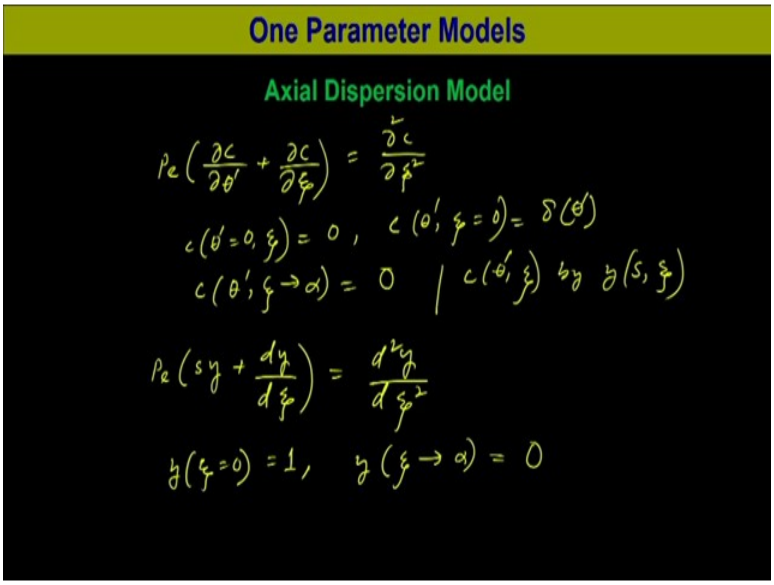

One Parameter Models

Axial Dispersion Model

$$Pe\left(\frac{\partial c}{\partial \theta'} + \frac{\partial c}{\partial \xi}\right) = \frac{\partial^2 c}{\partial \xi^2}$$

$c(\theta'=0, \xi) = 0$, $c(\theta', \xi=0) = \delta(\theta')$

$c(\theta', \xi \to \infty) = 0$ | $c(\theta', \xi)$ by $y(s, \xi)$

$$Pe\left(sy + \frac{dy}{d\xi}\right) = \frac{d^2 y}{d\xi^2}$$

$y(\xi=0) = 1$, $y(\xi \to \infty) = 0$

We can write $Pe\left(\frac{dC}{d\theta'} + \frac{dC}{d\xi}\right) = \frac{d^2C}{d\xi^2}$ and if we use the boundary conditions, initial and boundary conditions, that $C(\theta' = 0, \xi) = 0, C(\theta', \xi = 0) = \delta(\theta')$, $C(\theta', \xi \to \infty) = 0$ So, with this initial and boundary conditions if we use this and solve this differential equations we would obtain pe sy so the transform if we define the $C(\theta', \xi) = 0y(s, \xi)$ we can write

$Pe\left(sy + \frac{dy}{d\xi}\right) = \frac{d^2y}{d\xi^2}$. And here $y(\xi = 0) = 1$ and $y(\xi \to \infty) = 0$

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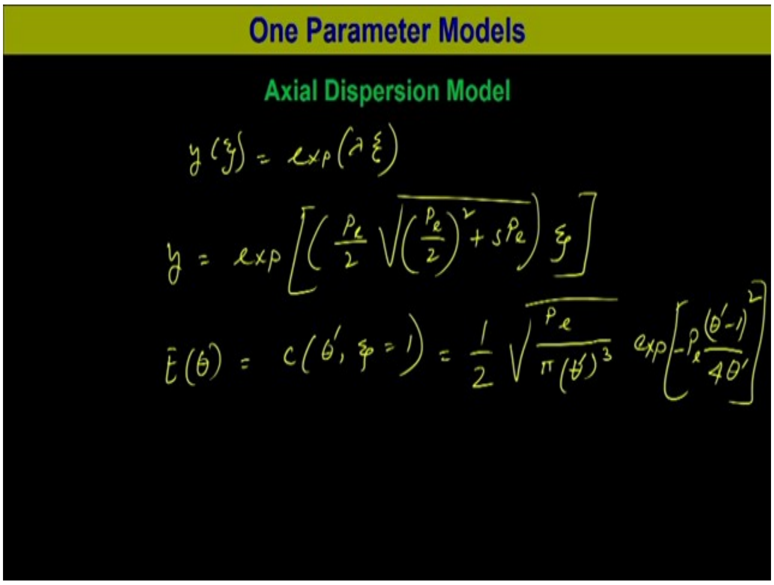

One Parameter Models

Axial Dispersion Model

$$y(\xi) = \exp(\lambda \xi)$$

$$y = \exp\left[\left(\frac{P_e}{2}\sqrt{\left(\frac{P_e}{2}\right)^2 + sP_e}\right)\xi\right]$$

$$E(\theta) = c(\theta', \xi = 1) = \frac{1}{2}\sqrt{\frac{P_e}{\pi(\theta')^3}}\exp\left[-P_e\frac{(\theta'-1)^2}{4\theta'}\right]$$

So, this transformation for one dimensional boundary value problem to a semi-infinite domain we can solve it by assuming the form $y(\xi) = \exp(\lambda\xi)$ and solving this you would obtain $y = \exp\left[\left(\frac{Pe}{2}\sqrt{\left(\frac{Pe}{2}\right)^2 + sPe}\right)\xi\right]$. So, finally you would obtain $E(\theta) = C(\theta', \xi = 1) = \frac{1}{2}\sqrt{\frac{Pe}{\pi(\theta')^3}}\exp\left[-Pe\frac{(\theta'-1)^2}{4\theta'}\right]$. So, I have written this directly to the solutions, you can look into the literature to solve these differential equations.

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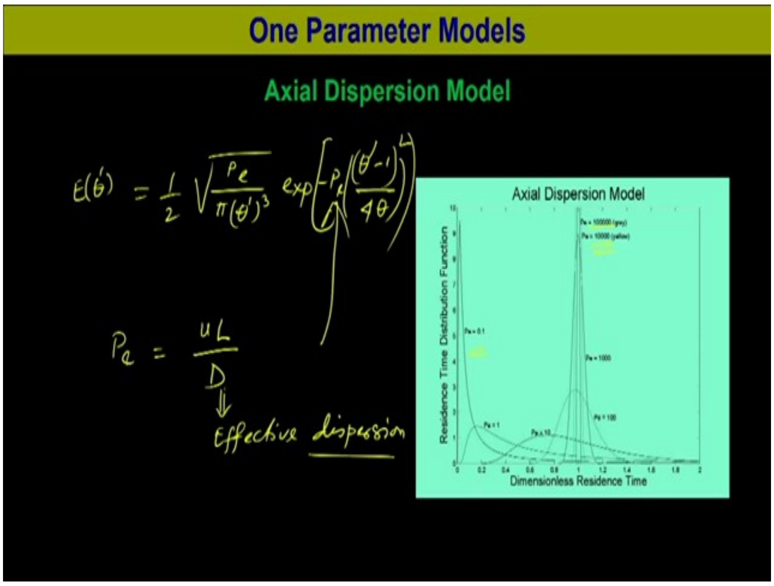

One Parameter Models

Axial Dispersion Model

$$E(\theta') = \frac{1}{2}\sqrt{\frac{P_e}{\pi(\theta')^3}}\exp\left[-P_e\frac{(\theta'-1)^2}{4\theta'}\right]$$

$$P_e = \frac{uL}{D}$$

$$\Downarrow$$

Effective dispersion

And if you look into the variations of the peclet number using this relation that is $E(\theta')=\frac{1}{2}\sqrt{\frac{Pe}{\pi(\theta')^3}}\exp\left[-Pe\frac{(\theta'-1)^2}{4\theta'}\right]$. So, if we plot residence time distribution versus the dimensionless residence time at various peclet number p e, so you will get the distribution function like this. As you can see when your peclet number is very high that means your D as peclet number we have defined $Pe=\frac{uL}{D}$, so D is the effective dispersion.

So, when D is very small the axial dispersion or the effective dispersion is very small then peclet number is very high. So, we could see that when peclet number is very high in that case the distribution will give the close to the ideal plug flow reactor model. And when the peclet number is less that means there is a significant axial dispersion or axial mixing and hence it will give the distribution like the CSTR. So, that is what we can see at very low peclet number the distribution is behave like a mixed flow reactor models.

I hope you have enjoyed the lectures and we will have discussions if you have any queries over the YouTube, you know discussion as well as if you wanted know more about this particularly the reactor modelling parts, you can go to the Levenspiel book as well as the book of H. Scott Fogler where you will get many more examples to use and solve the reactor model equations. I suggest for two parameter models you should also consider the book of Fogler. So, thank you very much for attending this lecture as well as the whole course.