Chemical Reaction Engineering 1
Professor Bishnupada Mandal
Department of Chemical Engineering
Indian Institute of Technology Guwahati
Lecture 27 - Non-Ideal Reactors and Residence Time Distribution

Welcome to the first lecture of module 5. In this module, we will consider the non-ideal reactors and the residence time distribution. So, before going to this lecture let us have brief recap on our previous lecture.

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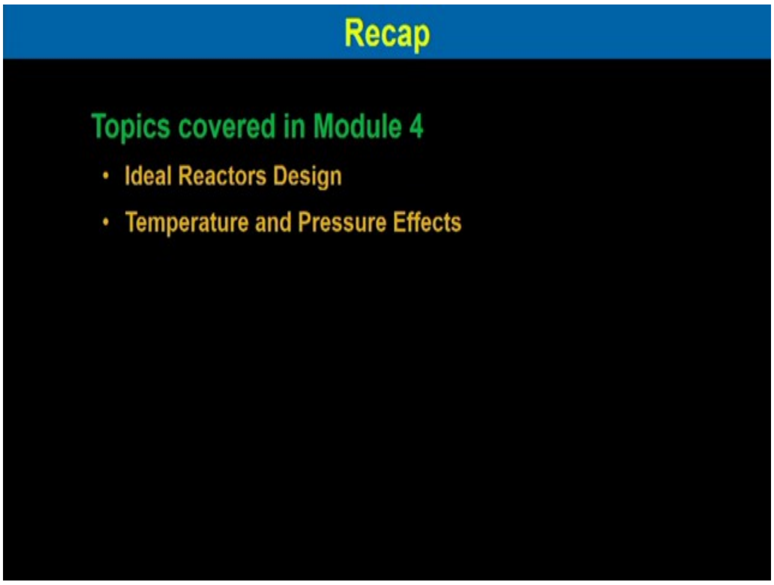

Recap

Topics covered in Module 4

- Ideal Reactors Design
- Temperature and Pressure Effects

In particular for module 4, the last module, we have considered two things: one is ideal reactor design, and then we consider temperature and pressure effects in case of ideal reactors. So, basically we have considered three idealized reactors; one is ideal batch reactor, ideal plug flow reactor and ideal continuous stirred tank reactor or mixed flow reactor. So, in this ID3 idealized reactor, we have seen how to calculate the volume of the reactors for a particular job, and then we compared the different reactors and we see which one is most effective in terms of the volume required for a particular job among the three idealized reactors.

We have considered several cases, one case we have considered single reaction is happening and then we have considered multiple reactions where initially we consider parallel reactions and finally we have considered series and series parallel combinations. And then for all these designs we have mainly considered the overall mass balance as well as the species mole balance to calculate the volume required.

But when the reactions in general, they are either endothermic or exothermic in nature, so that there is a change in temperature or enthalpy into the overall reaction systems. So, then we consider for the energy balance equation where it maybe adiabatic reactors or it may be non-adiabatic reactors. Both case we have considered and we have considered from this energy balance equations.

We have seen that if there is exothermic reactions, for a single reactions we can find out the optimum temperature particularly in case of the reversible exothermic reactions. And we have considered critically three ideal reactors and they compared their heat effects in case of or optimum temperature progressions. And when we consider the ideal continuous stirred tank reactor or the mixed flow reactor, we have seen that the mixed flow reactors gives three steady states and we call the multiplicity of the CSTR, steady state multiplicity of the CSTR.

And then out of them there are two stable steady states, whereas the one middle one steady state was the unstable steady states. So, with this we have completed our reactor design for the ideal reactors in module 4. In this module we will consider the non-ideal reactors and the residence time distribution.

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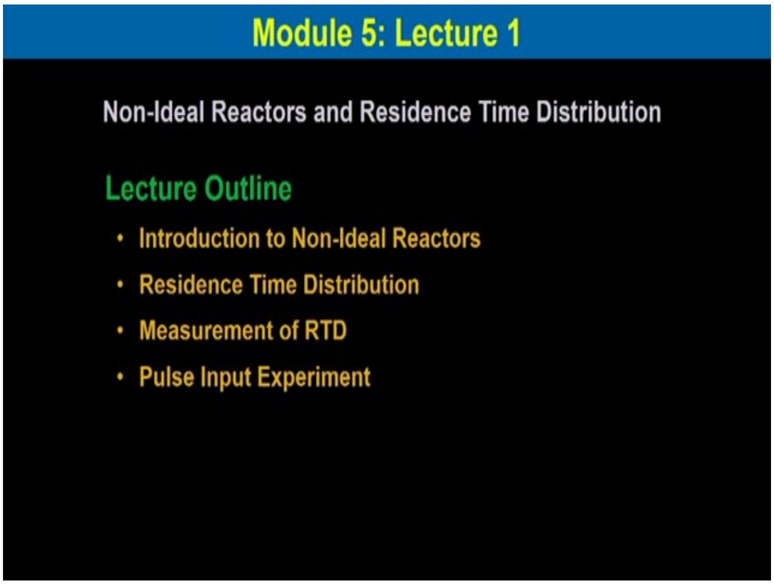

Module 5: Lecture 1

Non-Ideal Reactors and Residence Time Distribution

Lecture Outline

- Introduction to Non-Ideal Reactors
- Residence Time Distribution
- Measurement of RTD
- Pulse Input Experiment

So, in the first lecture we will cover mainly introduction to non-ideal reactors and then we consider residence time distribution. We will see how to measure the residence time and there are two methods to measure the residence time, the pulse tracer input method and another one is stiff tracer input method and from then, in this lecture we will consider the pulse input experiments.

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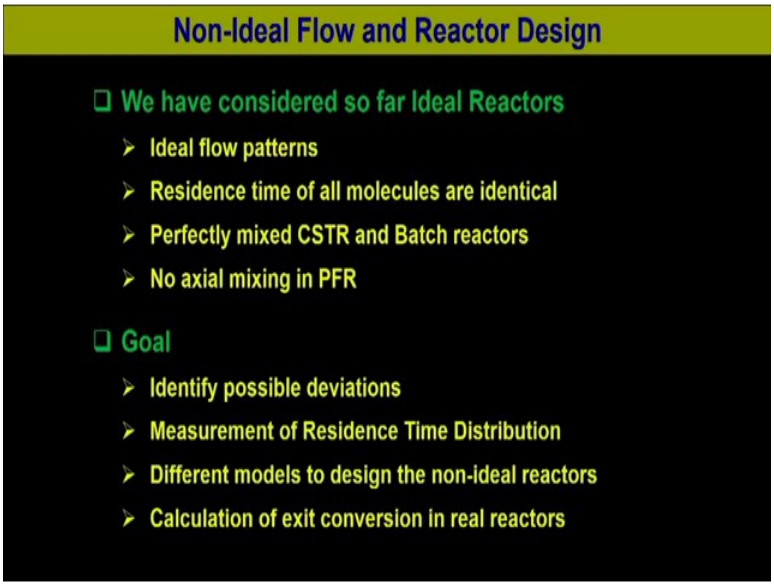

Non-Ideal Flow and Reactor Design

❑ We have considered so far Ideal Reactors

- Ideal flow patterns
- Residence time of all molecules are identical
- Perfectly mixed CSTR and Batch reactors
- No axial mixing in PFR

❑ Goal

- Identify possible deviations
- Measurement of Residence Time Distribution
- Different models to design the non-ideal reactors
- Calculation of exit conversion in real reactors

So, non-ideal reactors. As we have said we have considered so far ideal reactors and we have seen the ideal flow patterns. The residence time of all molecules are identical. And we have seen perfectly mixed CSTR and batch reactors. So, the content inside these reactors are perfectly mixed. And we have seen for PFR, ideal plug flow reactor there is no axial mixing among the fluid elements.

In this case we can see the reactor behaviour, if we consider the two flow reactors, one is ideal plug flow reactors and the other one is ideal stirred tank reactors or mixed flow reactor. In these two reactors, in one case we have considered the complete back mixing happens, that is the ideal continuous stirred tank reactors, that means the whole content is completely mixed, homogenously mixed, so the mixing in the reactor is complete.

In other case if we consider ideal plug flow reactor where there is no axial mixing or there is no back mixing, that means no mixing, so these two reactors set the two extreme limits of the reactor mixing inside the reactor, how the reactant mix, or the reactant and product mix with each other. So, the ideal plug flow reactor, there is no mixing whereas in case of continuous stirred tank reactors that is complete mixing.

So, these reactors pose the two extremes of the reactor mixing conditions. In reality or the real reactors, they are actually non, either no-mixing or complete mixing. They lie in between these two, so which we call the partially mixing reactors. So, ideal reactors is basically partially mixed reactors and that will be between these two reactor conditions. Although, we assume certain reactors, which will be closely the mixing, based on the mixing conditions we can assume closely to either of these ideal reactors.

But actually the mixing pattern will be in between these two reactors. The most prominent example for the partially mixed reactor is the fluidized bed reactor. Because in the fluidized bed reactor, it may be solid gas or the gas liquid in case of the fluidized reactor, which is generally used in case of catalytic reactions and all. So, in that case behaviour of the fluid flow or the mixing behaviour are drastically changed or they change, as it size of the particles and the fluid elements which we put.

They actually changes the mixing pattern inside the reactors and that is why if you could see in last three to four decades, there are almost 4,000 patents which are issued with the name fluidized bed reactor. So, our goal in this module would be identify the possible deviation from the ideal reactors. Then to measure the residence time distribution in a reactor, and then we will choose different models to design or to predict the non-ideal reactors performances.

And finally we need to calculate the exit conversion in real reactors. So, to measure quantitatively the degree of mixing in real reactors, we use function called residence time distribution function. And then we will see how to calculate the residence time distribution function and then we will see how to calculate the mean residence time and then cumulative distribution function and the variance for the distribution.

So, all these parameters will tell us or will characterize the real reactors. We will also try to find out these parameters in case of the ideal reactors and if we know the ideal reactor behaviour parameters, we can compare these parameters with the real reactors and we can see how much they deviate from the ideal reactors.

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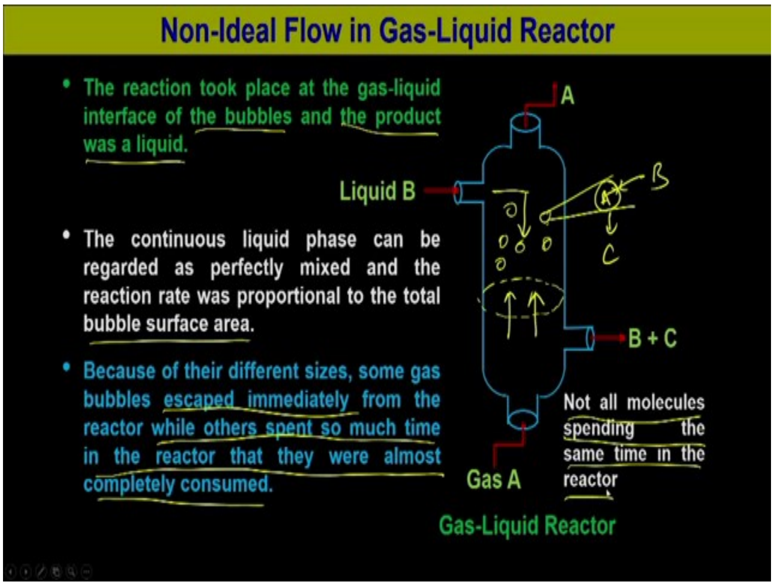

Non-Ideal Flow in Gas-Liquid Reactor

- The reaction took place at the gas-liquid interface of the bubbles and the product was a liquid.
- The continuous liquid phase can be regarded as perfectly mixed and the reaction rate was proportional to the total bubble surface area.
- Because of their different sizes, some gas bubbles escaped immediately from the reactor while others spent so much time in the reactor that they were almost completely consumed.

Not all molecules spending the same time in the reactor

Gas-Liquid Reactor

So, now if we consider gas liquid reactors and where fluid or liquid B which is fed at the top, over here, and then a gas which is fed at the bottom. So, the gas is, comes at the top and there is a gas is bubbled through the liquid which is coming down. So the reactions which happens on the gas liquid interface that is on the surface on the bubble and the product is a liquid which comes out at the exit, at the bottom over here. So, the reaction took place at a gas liquid interface of the bubble and the product is a liquid.

The continuous liquid phase can be regarded as a perfectly mixed and the reaction rate was proportional to the total bubble surface area. So, the reactions which is happening between A and B, so if we consider, this is the bubble, so basically this is A which is bubbling and it is reacting at the surface with the B (moli) and the product which is forming is basically C, which is coming down with it and forming.

So, outlet, you will get some unconverted B and C, so the unconverted gas will go up from here at the top. Because of their different sizes, as the gas will bubble through the liquid, the size of the bubble will vary as it travels to the liquid. There will be different size of bubbles from bigger to the smaller. So, gas bubbles escaped immediately from the reactor while the others spent so much time in the reactor that they are were almost consumed.

So, this way the reactions which happens in a gas liquid reactors, the bubbles or the fluid elements, they spent different length of time inside the reactor. So, there is a distribution of their ages inside the reactor. So, in this case the time the bubble stays inside the reactor, we can call it the bubble residence time. But in this case we are not more concerned about the mean residence time that means the average residence time of all the bubbles. We are more interested in the distribution of their residence time of different bubbles.

That means how much is bubble spent the inside the reactor, how much time they spent. So, the total reaction rate can be obtained by summing up the rates, individual rates of each bubble which is happened inside the reactor so that we can get the total rate of the reaction. So, an understanding of their residence time distribution and relate with the reaction as well as the conversion is more important particularly in case of the non-ideal reactors. So, we can see that not all molecules spending the same time in the reactor.

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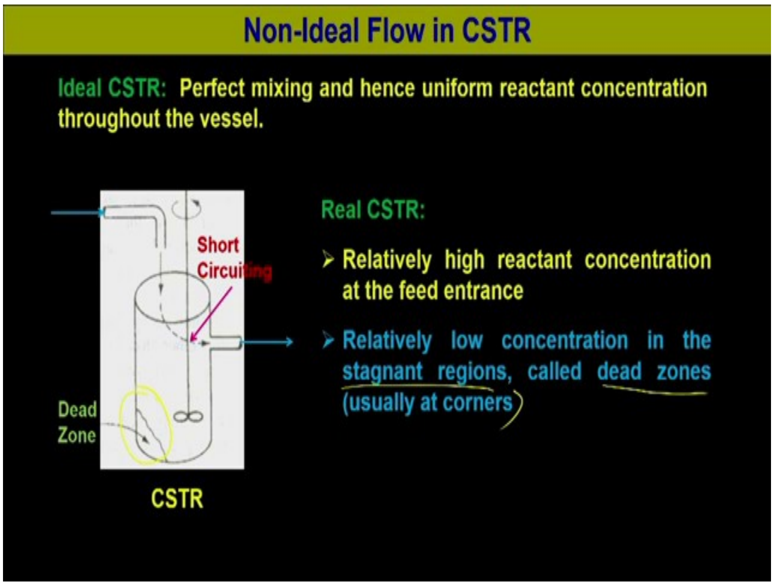

Non-Ideal Flow in CSTR

Ideal CSTR: Perfect mixing and hence uniform reactant concentration throughout the vessel.

Real CSTR:

- Relatively high reactant concentration at the feed entrance
- Relatively low concentration in the stagnant regions, called dead zones (usually at corners)

Now, another example of non-ideal reactor is the CSTR. If we consider ideal CSTR, we consider perfect mixing and hence uniform reactant concentration throughout the vessel. So, if we look into this CSTR, we have fluid which is entered over here that is feed and which is coming out over here. So, we could see there is certain zone over here there the mixing at this zone is rare or very less, so if mixing is less at this location as the reactant enters over here, it filled that corner and it stays for longer time without mixing.

So, we call it dead zone that means the fluid element over here spent longest time. In some cases if the outlet is very close to the inlet, in that case what will happen, the first reactant which will enter into the reactor they will immediately some of the fluid elements, some of the reactants they will come out through the out lid, so we call it short circuiting, that means those fluid elements spent very less time inside the reactor.

So, we can see there is dead zone and short circuiting, so the mixing in this case if we consider the non-idealized CSTR over here, we have dead zone as well as short circuiting because of that the age of the fluid elements are vastly different and hence this creates the non-ideality in CSTR. So, real CSTR we could see relatively high reactant concentration at the feed entrance.

And relatively low concentration in the stagnant zone and called the dead zone and usually at the corners. So, in case of ideal CSTR we have uniform concentration throughout, so from the entrance to the exit and at all locations of the reactor, in case of ideal CSTR having uniform concentration. But because of this short circuiting and the dead zone, the reactant concentrations markedly varied inside the reactor because that changes the degree of mixing inside the real reactors.

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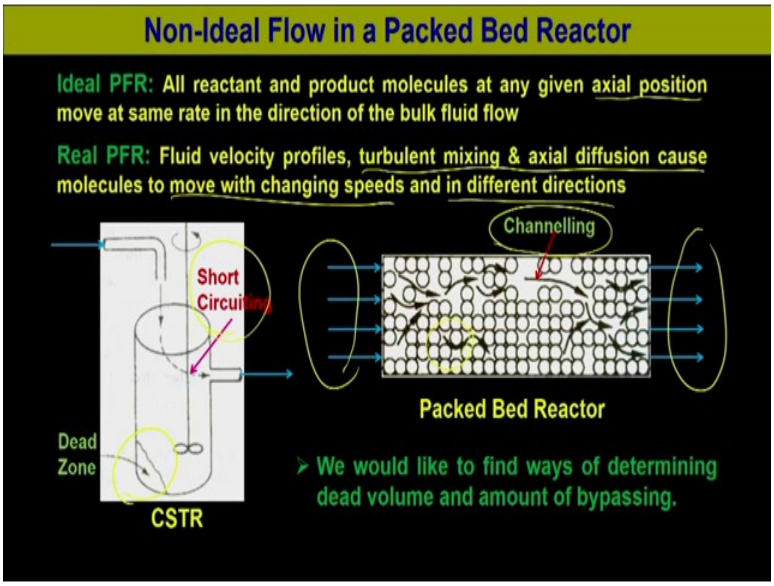

Non-Ideal Flow in a Packed Bed Reactor

Ideal PFR: All reactant and product molecules at any given axial position move at same rate in the direction of the bulk fluid flow

Real PFR: Fluid velocity profiles, turbulent mixing & axial diffusion cause molecules to move with changing speeds and in different directions

- We would like to find ways of determining dead volume and amount of bypassing.

Now, if we consider ideal plug flow reactor, all reactants and product molecules at a any given axial positions move at the same rate in the direction of the bulk fluid flow. That means, if we have a plug flow reactor, ideal plug flow reactor, the fluid which enters at a particular locations of the tube or the reactors, it proceeds through the length of the reactors and exit at the other end and there is no overtaking of the fluids which is behind one fluid elements.

That means there is no axial mixing of the fluid in an ideal plug flow reactor. So, each and every element of the fluid spent same length of time inside the reactor. But if we consider real PFR – Plug flow reactor: Fluid velocity profile, the velocity of the each fluid elements will change. So if that has changed then there will be back mixing. So, we will get turbulent mixing and axial mixing or axial diffusion cause the molecules to move with changing speeds and in different directions.

So, the degree of mixing in the reactor would change or would change compared to the ideal plug flow reactor. Now, if we consider a packed bed reactor, so here packing materials are packed inside and in general if we do a random packing in a packed bed, so the porosity inside the bed may not be same at every locations or they form some places is very compact with the solid packing compared to some other locations.

So, when the fluid passes through the packed bed, if it enters over here, the fluid elements and it comes out on the other side, we could see there is some zones, which are less resistant to the fluid to move. So, fluid will always try to move in that directions where resistance is comparably low. So, we call this as channelling. So, channelling would happen, so that these fluids elements which are going through that channel will have spent less amount of time or less time inside the reactor compared to the fluid which is flowing to the more resistive path.

So, we could get different mixing or the flow residence time of the fluid elements in a packed bed. So, now, what we want to do? We would like to find ways of determining the deal volume as we have seen over here in case of CSTR and the amount of bypassing or the channelling, which is happens in case of, in this case the short circuiting in case of the CSTR and channelling in case of the packed bed reactors. So, those things we need to quantitatively determine from this for the non-ideal reactors. So, that is our target.

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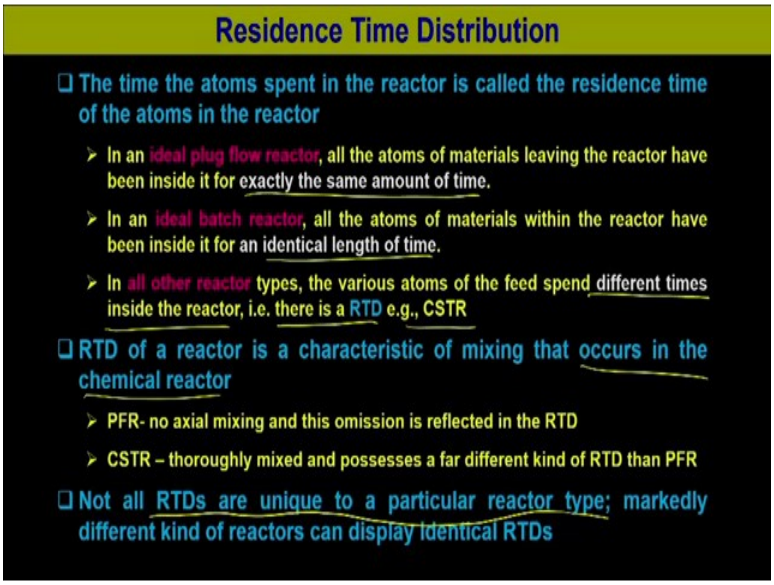

Residence Time Distribution

- The time the atoms spent in the reactor is called the residence time of the atoms in the reactor
  - In an ideal plug flow reactor, all the atoms of materials leaving the reactor have been inside it for exactly the same amount of time.
  - In an ideal batch reactor, all the atoms of materials within the reactor have been inside it for an identical length of time.
  - In all other reactor types, the various atoms of the feed spend different times inside the reactor, i.e. there is a RTD e.g., CSTR
- RTD of a reactor is a characteristic of mixing that occurs in the chemical reactor
  - PFR- no axial mixing and this omission is reflected in the RTD
  - CSTR – thoroughly mixed and possesses a far different kind of RTD than PFR
- Not all RTDs are unique to a particular reactor type; markedly different kind of reactors can display identical RTDs

So, the residence time distribution, so the time the atoms spent in the reactor is called the residence time distribution of the atoms in the reactor. If we consider ideal plug flow reactor, all atoms of the materials leaving the reactor have been inside it for exactly the same amount of time. So, in case of the ideal plug flow reactor, the residence time of all the fluid elements is same. In case of the batch reactor, what we do?

We put some reactors in a container which is continuously stirred and there is no exist which close it and run for a particular length of time and then we take out, that means each material which is fed to the ideal batch reactor is spent exactly the same length of time inside the reactor. So, the residence time is identical to all the elements. But in all other reactor types, even considering the ideal CSTR, the time they spent inside the reactor is fluid elements are not same, they are different and there is element of the fluid spend different length of time.

So, there is a distribution of their residence time of each fluid elements and we call it residence time distribution, that is what we also get in case of the CSTR or mixed flow reactor. So, RTD of a reactor is a characteristic of mixing that occurs in the chemical reactor. Residence time distribution which is one of the characteristics and that represents the degree of mixing in that reactor and which occurs in most of the chemical reactors.

PFR – no axial mixing, so ideal PFR if we consider, so no axial mixing so there is no distribution of the residence time. So, this is omitted and which is reflected in their RTD distribution. In case of CSTR thoroughly mixed and possesses a far different kind of RTD than PFR. So, we could see that not all RTDs are unique to a particular reactor type. So, residence time distribution is not unique for a particular reactor type.

Markedly different kind of reactors can display identical RTDs. So, if we take a CSTR and we have a plug flow reactor depending on the degree of mixing in both the reactors, they are different reactors, one is CSTR another is plug flow reactor. If we consider ideal, they are markedly different from each other. One is giving the mixing level is 0, there is no axial mixing, the other one is, the mixing is complete, so complete mixing in the CSTR.

But if there is a partial degree of mixing, we can change and which has happened in case of the real reactors, so even if plug flow reactor can give same RTD as we get from the CSTR as well.

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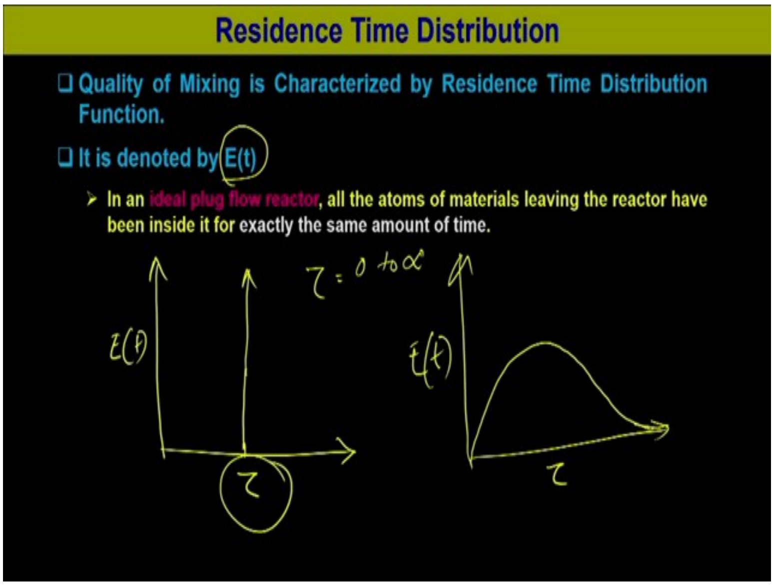

Residence Time Distribution

- ❑ Quality of Mixing is Characterized by Residence Time Distribution Function.
- ❑ It is denoted by E(t)
  - ➢ In an ideal plug flow reactor, all the atoms of materials leaving the reactor have been inside it for exactly the same amount of time.

So, quality of mixing is characterized by the residence time distributions function and this represented of denoted by $E(t)$. So, $E(t)$ is the residence time distribution function which will tell us the how much degree of mixing inside the reactor or how their residence time distribution each. So, ideal plug flow reactors, all the atoms of the materials leaving the reactor have been inside it for exactly the same length of time. So, when we consider ideal CSTR and if we now look into the residence time distribution for this.

We will later in more detail mathematically, so if we plot $E(t)$ that residence time distribution function versus tau, we could see the residence time ideal plug flow reactor is a same, for all elements is same so there is no residence time distribution. All are tau for all fluid elements. So, we get $E(t)$ versus τ plot and we see that is the infinite length of the 0 width, which we call direct delta function, so which we will discuss later.

In case of ideal CSTR we can see that there the residence time of the elements can vary from 0 to infinity, so τ can vary from 0 to infinity, so there would be residence time distribution would be like this. So, in case of $E(t)$ versus τ for ideal CSTR. So, the degree of quality of mixing or the degree of mixing that can be characterized with the help of a function called residence time distribution function. Now, we will discuss how to calculate the residence time distribution function.

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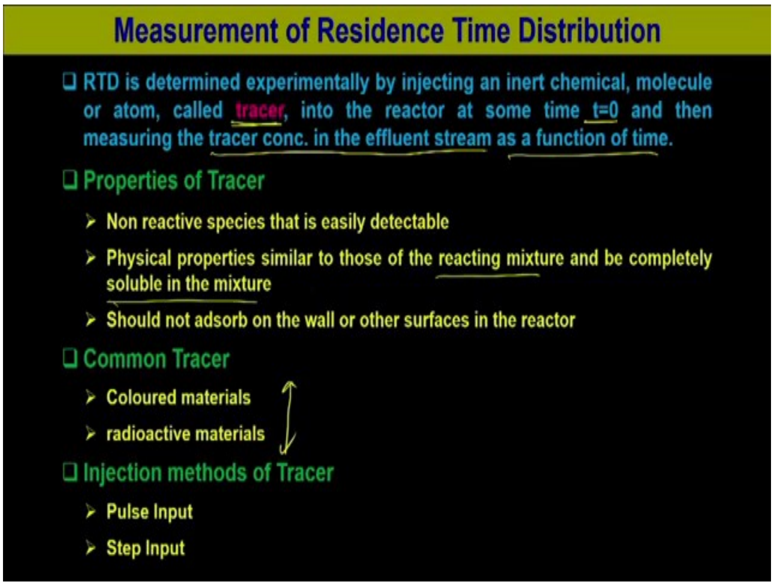

Measurement of Residence Time Distribution

- ☐ RTD is determined experimentally by injecting an inert chemical, molecule or atom, called tracer, into the reactor at some time t=0 and then measuring the tracer conc. in the effluent stream as a function of time.
- ☐ Properties of Tracer
  - Non reactive species that is easily detectable
  - Physical properties similar to those of the reacting mixture and be completely soluble in the mixture
  - Should not adsorb on the wall or other surfaces in the reactor
- ☐ Common Tracer
  - Coloured materials
  - radioactive materials
- ☐ Injection methods of Tracer
  - Pulse Input
  - Step Input

So, the residence time is determined experimentally by injecting an inert chemicals which is the molecules or atoms and we call it tracer. So, the tracer is fed into the reactor at time t = 0 and then measuring the tracer concentration in the effluent stream as a function of time, so the residence time with the reactants. To calculate the residence time, what we do, we inject some tracer materials or inert chemicals into the reactants at the inlet of reactors and then we measure the concentration of the tracer, not the product concentration or the reactor concentration.

We measure the concentration of the tracer at the reactor outlet, so it is injected at time t = 0 and measure the concentration of the effluent as a function of time. So, that we can calculate basically the distribution of the ages of the different elements. We can look this tracer measurement in another ways. Like when a reactant materials are fed into the reactors, we can distinguish the whole reactant or a reactant volume is separated as a huge number of tiny droplets or tiny fluid elements.

And each fluid element is so small compared to the total volume of the reactors, but it is large enough to contain large number of molecules so that we can consider this fluid element as continual. So, we would see how these tiny fluid elements spent inside the reactors, how long they spent. It is as if, if we can imagine we can sit in the reactor exit and ask each fluid element which is coming out, “Hey, what is your age? How long you stayed inside the reactor?”

So, each fluid element whenever it would come out from the reactor and as if you are asking their age and recording their age with respect to the time and that you can quantitatively do with respect to the measurement of the concentration of the tracer. One important thing for the trace is that it is should have certain properties to be used. So, one of them would non-reactive species that is easily detectable.

That means if it should not react with the reactants and it should be very easily detectable at the reactor exit. Physical properties should be similar to those of the reacting mixture and can be completely soluble in the mixture. It would be completely soluble but it should not react. Should not adsorb on the wall or the surface of the reactors, because we are measuring the concentration of the tracer at the exit.

If it adsorb on the wall or on the surface so that materials may not come out at the exit, so there will be a problem of the mass balance of the tracer at the outlet. So, we need to, all the tracer which would be injected should come out at the exit. The common tracer should be a coloured materials which is helpful, radioactive materials. These are the two different types of common tracers we generally use, like different dyes and different radioactive materials we use as trace experiments.

There are two injection methods for tracer experiments, one of them is pulse input where we give a small pulse of the tracer materials at a time t = 0 and then we measure its concentration at the outlet with respect to time. The other one is the pulse input where we give the other one is the step input where we give the reactants where we inject the tracer into with the reactant entrance at a particular time interval.

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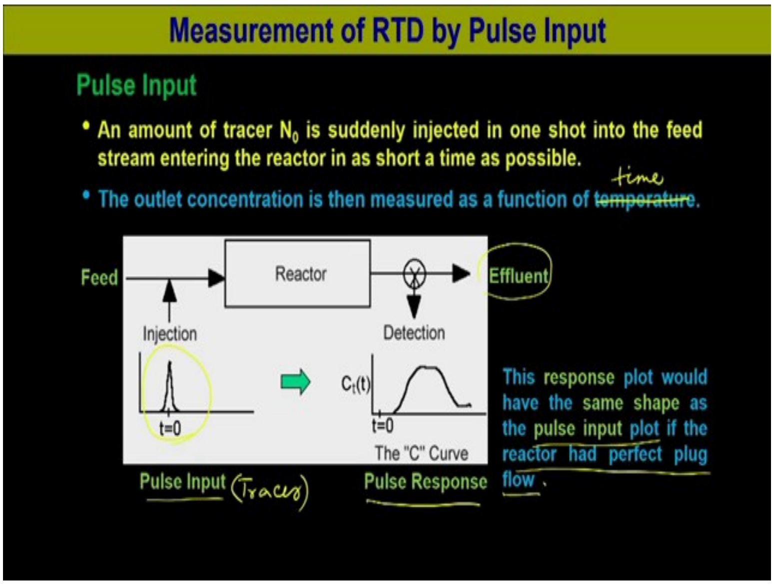

Measurement of RTD by Pulse Input

Pulse Input

- An amount of tracer N_0 is suddenly injected in one shot into the feed stream entering the reactor in as short a time as possible.
- The outlet concentration is then measured as a function of ~~temperature~~ time.

This response plot would have the same shape as the pulse input plot if the reactor had perfect plug flow.

So, we will first start with the RTD measurements using the pulse input. So, let us consider this reactor, we have an amount of tracer, N_0 is suddenly injected in one shot into the feed stream entering the reactor in as short time as possible. So, a pulse of tracer, is which is a known concentration, which is N_0 is suddenly injected at the inlet, so with the feed, with which it is given and then this is the pulse input.

So, at a time t is equal to 0 so you have given the tracer in a short time, so you can see their distribution, how it looked like, the concentration time distribution. Then it will come out with the effluent, so you are measuring the effluent concentration at the exit. The outlet concentration is then measured as a function of time. So, if the pulse input is given, if you detect at the effluent with respect to time, you could see $C(t)$ versus t curve, the distribution would be in real reactor, is like this.

So, this is called the pulse response. So, you have given pulse input over here of the tracer, so this is tracer input. And the tracer response curve concentration of the tracer with respect to time, you can see the concentration distribution. If the response plot would have the same shape as the pulse input plot, you could see over here, it would have same response in the exit as well if the reactor had a perfect plug flow.

So, if it is perfect plug flow there should not be any back mixing so the tracer which is coming out will give the same pulse input curve as we have seen. It should not be the response curve should have been similar, but however, actually in real plug flow reactor we used to see the distribution of the tracer in a different way. It shows the degree of back mixing inside the plug flow reactor.

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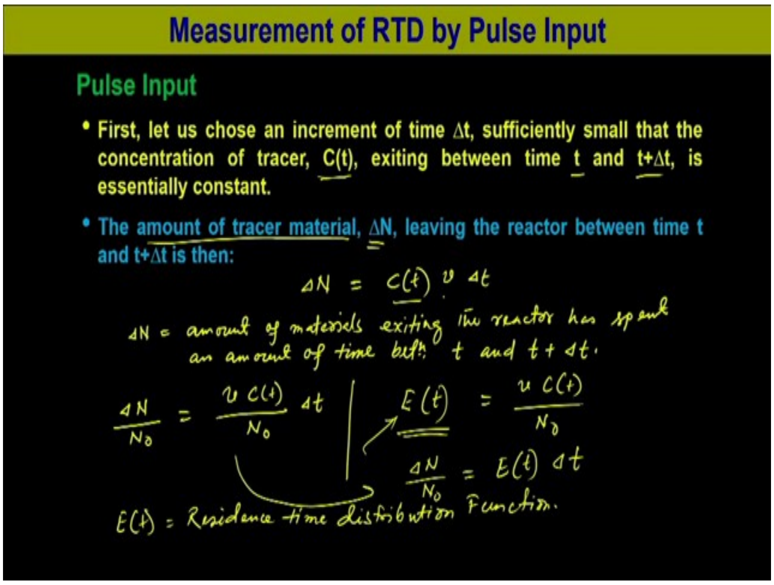

Measurement of RTD by Pulse Input

Pulse Input

- First, let us chose an increment of time Δt, sufficiently small that the concentration of tracer, C(t), exiting between time t and t+Δt, is essentially constant.
- The amount of tracer material, ΔN, leaving the reactor between time t and t+Δt is then:

$$\underline{\Delta N} = \underline{C(t)}\, v\, \Delta t$$

ΔN = amount of materials exiting the reactor has spent an amount of time betⁿ t and t + Δt.

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

$$\underline{\underline{E(t)}} = \frac{v\,C(t)}{N_0}$$

$$\frac{\Delta N}{N_0} = E(t)\,\Delta t$$

E(t) = Residence time distribution Function.

So, first let us choose an increment of time Δt which is sufficiently small that the concentration of the tracer, $C(t)$, exiting between time t and $t+\Delta t$ is essentially constant. So, the amount of material that is ΔN, leaving the reactor between time t and $t+\Delta t$, we can write,

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

So, the ΔN that is the amount of tracer material, amount of tracer material ΔN would be

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

So, in other words we can write, ΔN is the amount of material exiting the reactor has spent an amount of time between t and $t+\Delta t$. Now, if we divide this ΔN with the total amount of tracer that was injected in the reactor, we would get

$$\frac{\Delta N}{N_0} = \frac{vC(t)}{N_0}\Delta t$$

So, this represents $\frac{\Delta N}{N_0}$, this represents the fraction of the material that has spent the time inside the reactor between t and $t + \Delta t$. So, now we can define the pulse injection, that is

$$E(t) = \frac{vC(t)}{N_0}$$

So, $E(t)$ is the exit age distribution function. So, if we define $E(t)$, then we can write this relation as

$$\frac{\Delta N}{N_0} = E(t)\,\Delta t$$

So, $E(t)$ is basically the residence time distribution function or exit age distribution function, residence time distribution function.

So, this $E(t)$ basically quantitatively describes the how much different fluid elements spent time inside the reactors and the parameters $E(t)\,\Delta t$ represents the fraction of the materials that has spent time inside the reactor between time t and $t + \Delta t$.

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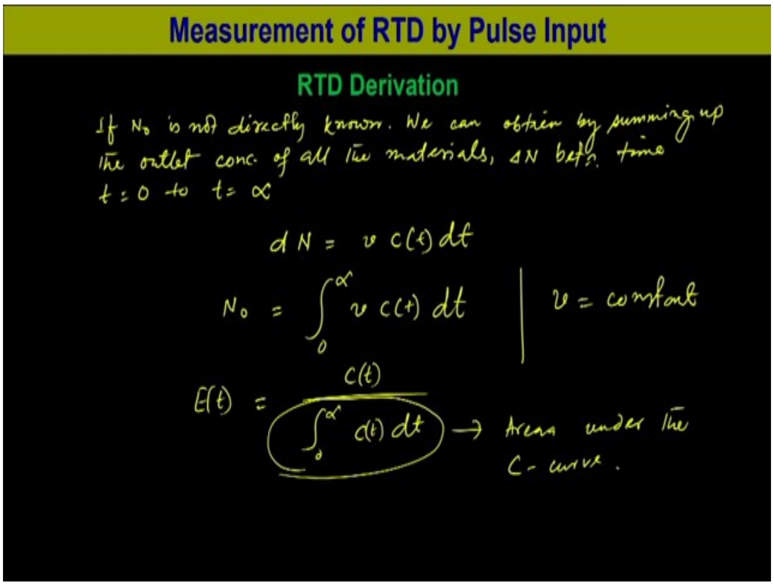

Measurement of RTD by Pulse Input

RTD Derivation

If N_0 is not directly known. We can obtain by summing up the outlet conc. of all the materials, ΔN betn. time $t = 0$ to $t = \infty$

$$dN = v\,c(t)\,dt$$

$$N_0 = \int_0^{\infty} v\,c(t)\,dt \quad \Bigg| \quad v = \text{constant}$$

$$E(t) = \frac{c(t)}{\int_0^{\infty} c(t)\,dt} \rightarrow \text{Area under the C- curve.}$$

Now, if N_0 is not directly known, if N_0 is not directly known, we can obtain by summing up the measured outlet concentration. So, we can obtain by summing up the outlet concentration of all the materials ΔN between time $t = 0$ to $t = \infty$. So, if we write the earlier equations in a differential forms, we can write

$$dN = vC(t)\,dt$$

So, if we integrate this relation, we would obtain

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

The volumetric flow rate v is usually constant. So, if this is constant we can calculate $E(t)$ or define $E(t)$ as

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

So, basically the denominator over here is the area under the C curve that is concentration time curve.

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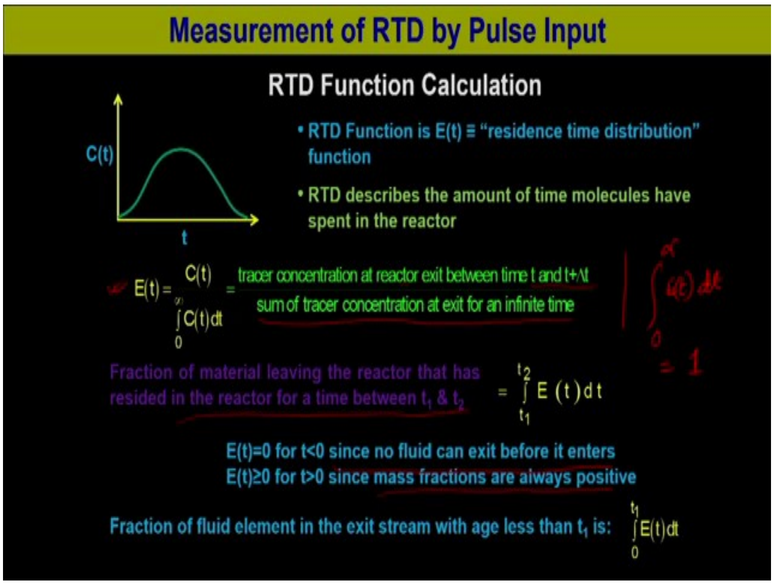

Measurement of RTD by Pulse Input

RTD Function Calculation

- RTD Function is E(t) ≡ “residence time distribution” function
- RTD describes the amount of time molecules have spent in the reactor

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} = \frac{\text{tracer concentration at reactor exit between time t and t+}\Delta t}{\text{sum of tracer concentration at exit for an infinite time}}$$

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

Fraction of material leaving the reactor that has resided in the reactor for a time between t_1 & t_2 $= \int_{t_1}^{t_2} E(t)dt$

E(t)=0 for t<0 since no fluid can exit before it enters
E(t)≥0 for t>0 since mass fractions are always positive

Fraction of fluid element in the exit stream with age less than t_1 is: $\int_0^{t_1} E(t)dt$

So, RTD function $E(t)$ is the residence time distribution function and RTD describes the amount of molecules that have spent inside the reactor. And if we consider the concentration and time curve, that is the tracer concentration and the time curve, we can calculate the residence time distribution function

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

So, residence time distribution function can be obtained if we know the concentration time history and the concentration time of the tracer if we plot and if we can calculate the area under the curve. So, that we can calculate $E(t)$. So, tracer concentration at the reactor exit between time t and t plus delta t and sum of the tracer concentration at the exit at infinite time. So, that is the exit is distribution.

We can also define in another way, the function, fraction of the material leaving the reactor that has spent or that has resided in the reactor between t_1 and t_2, we can write $\int_{t_1}^{t_2} E(t)\,dt$

And as we know the, all the materials which was resided between time $t = 0$ and $t = \infty$, so that can be normalized.

So, $\mathrm{E}(t) = 0$ for $t < 0$ since no fluid element exit before it enters.

And $\mathrm{E}(t)$ 0 for $t > 0$, since mass fraction are as always positive.

So, the fraction of the fluid element in the exit streams with age $< t_1$ is would be from $\int_0^1 E(t)\,dt$. And the residence time or $E(t)$ which is between $\int_0^\infty E(t)\,dt = 1$ which is normalized, that means all the fluid elements which has entered between 0 to infinity, all of them should come out.

So their exit is distribution should be or the fractional of the material that has spent between time 0 and infinity should be 1, the fraction should be 1 because all the fluid elements which has enters in this time period should come out, so their fraction of the material should be 1. So, we will use this relationship and see with an example from H. Scott Fogler how to calculate the residence time distribution, residence time distribution function.

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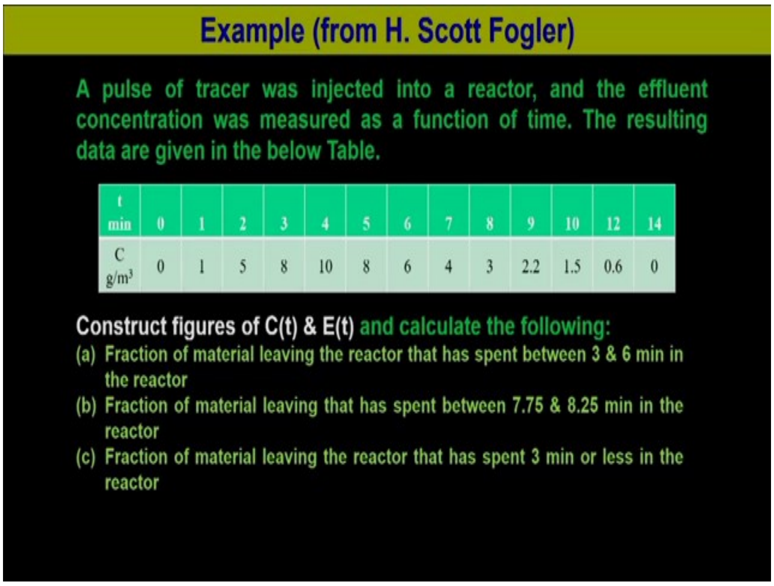

Example (from H. Scott Fogler)

A pulse of tracer was injected into a reactor, and the effluent concentration was measured as a function of time. The resulting data are given in the below Table.

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Construct figures of C(t) & E(t) and calculate the following:

(a) Fraction of material leaving the reactor that has spent between 3 & 6 min in the reactor

(b) Fraction of material leaving that has spent between 7.75 & 8.25 min in the reactor

(c) Fraction of material leaving the reactor that has spent 3 min or less in the reactor

A pulse of tracer was injected into a reactor and the effluent concentration was measured as a function of time. The resulting data are given in the below table. So, where the tracer concentrations are measured time and the concentration of the tracer is given at different times. So, we need to construct the concentration curve C curve and E curve.

And then calculate the fraction of the materials leaving the reactor that has spent between 3 and 6 minute in the reactor. The second problem is to calculate the fraction of the material leaving that has spent between 7.75 and 8.25 minute in the reactor. The third problem is to calculate the fraction of the material leaving the reactor that has spent 3 minute or less in the reactor.

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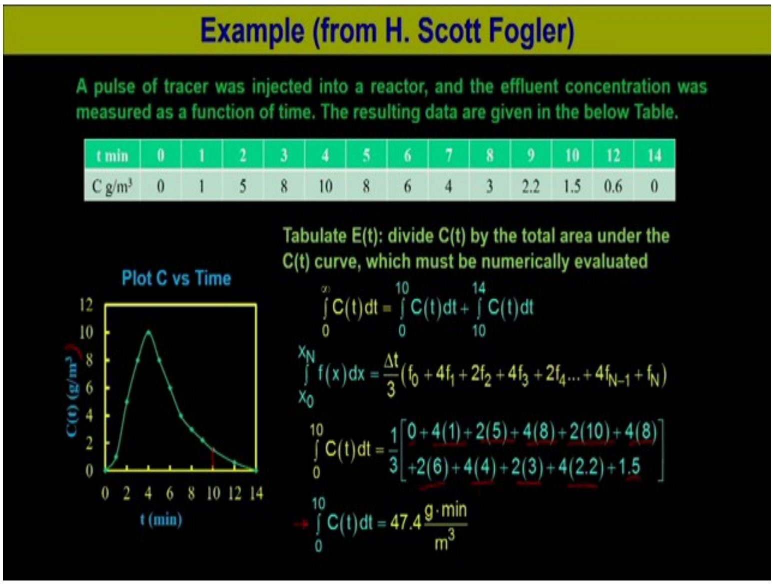

Example (from H. Scott Fogler)

A pulse of tracer was injected into a reactor, and the effluent concentration was measured as a function of time. The resulting data are given in the below Table.

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Tabulate E(t): divide C(t) by the total area under the C(t) curve, which must be numerically evaluated

Plot C vs Time

$$\int_0^{\infty} C(t)dt = \int_0^{10} C(t)dt + \int_{10}^{14} C(t)dt$$

$$\int_{X_0}^{X_N} f(x)dx = \frac{\Delta t}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 ... + 4f_{N-1} + f_N)$$

$$\int_0^{10} C(t)dt = \frac{1}{3}\begin{bmatrix} 0 + 4(1) + 2(5) + 4(8) + 2(10) + 4(8) \\ +2(6) + 4(4) + 2(3) + 4(2.2) + 1.5 \end{bmatrix}$$

$$\rightarrow \int_0^{10} C(t)dt = 47.4 \frac{g \cdot min}{m^3}$$

So, let us start with this concentration and time data and if we plot the concentration and time data, so we will get this C curve, so the time varies from 0 to 12 and then we could see the time is varied from 0 to 14 and tracer concentration in gm m^{-3} is from 0 to 12. So, what we need to do, tabulate, to calculate $E(t)$ divide $C(t)$ by the total area under the C curve which must be numerically evaluated.

So, we need to obtain $E(t)$ curve, so to obtain $E(t)$ curve, what we need, we need to calculate the area under the curve $\int_0^{\infty} C(t)\,dt$. So, this area under the curve between the time frame it is given, we need to calculate. So, we can use this different formula which are given in the Fogler's book, in the appendix you could see, either you can use Simpson's one third rule or we can use Simpson's one third rule and there are different other methods given in that book, you can follow it.

So, the area under the curve, we can calculate from

$$\int_{X_0}^{X_N} f(x)\,dx = \frac{\Delta t}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + ...4f_{N-1} + 2f_N\right)$$

So, if we use this formula in this time, time frame that means that is between 0 to 10 minutes. So, after this period we can calculate using this Simpson's one third formula and where we can calculate the different terms over here which is given over here.

So, we can calculate the using Simpson's one third rule we can calculate area up to this portion from 0 to 10 minute.

$$\int_0^{10} C(t)\,dt = \frac{1}{3}\begin{bmatrix} 0+4(1)+2(5)+4(8)+2(10)+4(8)+2(6)+4(4) \\ +2(3)+4(2.2)+1.5 \end{bmatrix}$$

Then which you will get is about

$$\int_0^{10} C(t)\,dt = 47.4\ gm\ m^{-3}$$

So, this is the area under the curve. Now, we need to calculate the other part which is

$$\int_{10}^{14} C(t)\,dt$$

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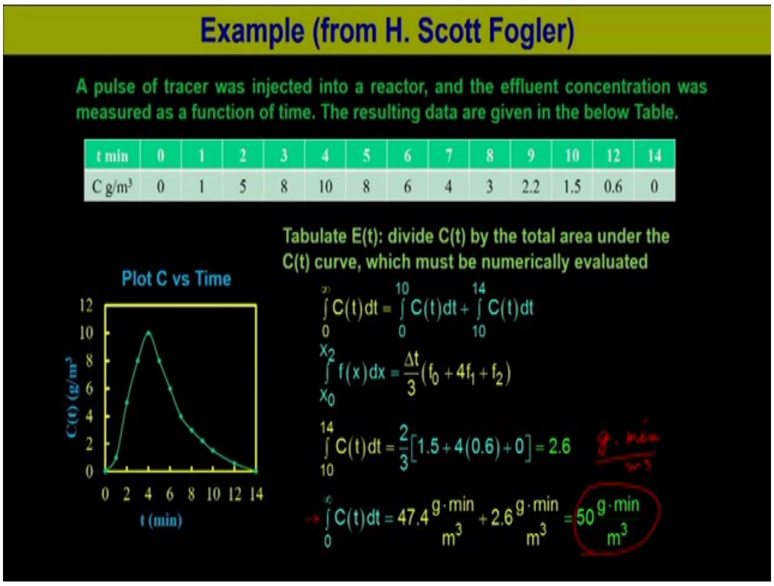

Example (from H. Scott Fogler)

A pulse of tracer was injected into a reactor, and the effluent concentration was measured as a function of time. The resulting data are given in the below Table.

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Tabulate E(t): divide C(t) by the total area under the C(t) curve, which must be numerically evaluated

$$\int_0^{\infty} C(t)dt = \int_0^{10} C(t)dt + \int_{10}^{14} C(t)dt$$

$$\int_{X_0}^{X_2} f(x)dx = \frac{\Delta t}{3}(f_0 + 4f_1 + f_2)$$

$$\int_{10}^{14} C(t)dt = \frac{2}{3}[1.5 + 4(0.6) + 0] = 2.6 \quad \frac{g\cdot min}{m^3}$$

$$\rightarrow \int_0^{\infty} C(t)dt = 47.4\frac{g\cdot min}{m^3} + 2.6\frac{g\cdot min}{m^3} = \boxed{50\frac{g\cdot min}{m^3}}$$

Plot C vs Time

So, we can calculate the other part which is also you can use, the same formula from the other part from X naught to X 2 fx dx which would be equal to delta t by 3 into f naught plus 4 f1 plus f2.

$$\int_{X_0}^{X_2} f(x)\,dx = \frac{\Delta t}{3}\left(f_0 + 4f_1 + f_2\right)$$

Now if we substitute the values so it would be

$$\int_{10}^{14} C(t)\,dt = \frac{2}{3}\left[1.5 + 4(0.6) + 0\right]$$

so if we calculate the total, so this is

$$\int_{10}^{14} C(t)\,dt = 2.6$$

So, the area under the curve which we can calculate the total area is

$$\int_{0}^{\infty} C(t)\,dt = 47.4\frac{g.\text{min}}{m} + 2.6\frac{g.\text{min}}{m} = 50\frac{g.\text{min}}{m}$$

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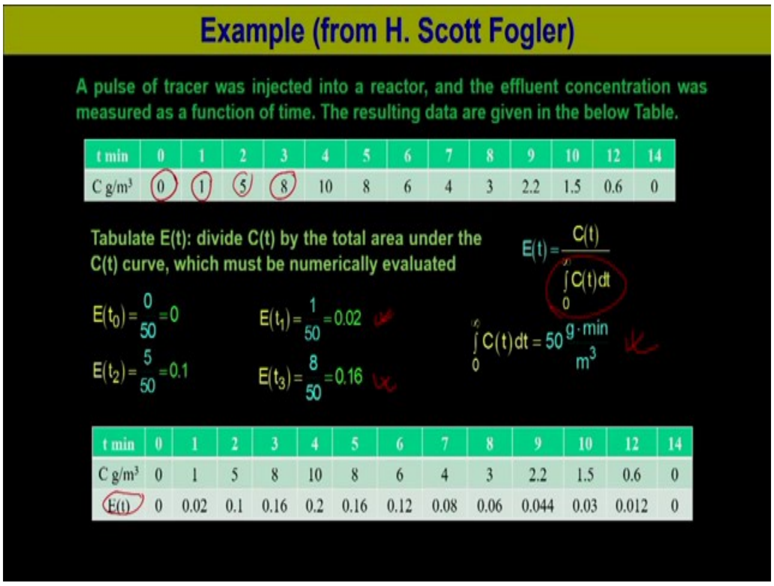

Example (from H. Scott Fogler)

A pulse of tracer was injected into a reactor, and the effluent concentration was measured as a function of time. The resulting data are given in the below Table.

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Tabulate E(t): divide C(t) by the total area under the C(t) curve, which must be numerically evaluated

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

$$E(t_0) = \frac{0}{50} = 0 \qquad E(t_1) = \frac{1}{50} = 0.02$$

$$\int_0^\infty C(t)dt = 50\,\frac{g\cdot\text{min}}{m^3}$$

$$E(t_2) = \frac{5}{50} = 0.1 \qquad E(t_3) = \frac{8}{50} = 0.16$$

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

So, now we need to calculate the values for $E(t)$ at different times. So, $C(t)$ is known at different times, $C(t)$ is given and the area under this curve, this part we have calculated. So now, if we calculate for the first one that is

$$E(t_0) = \frac{0}{50} = 0$$

Similarly, so that is for the second one.

$$E(t_1) = \frac{1}{50} = 0.02$$

so that is for the second one.

For the third one, your $C(t)$ values is 5, and

$$E(t_2) = \frac{5}{50} = 0.1$$

Similarly, we can calculate E t 3 which is

$$E(t_3) = \frac{8}{50} = 0.16$$

So, this way we can calculate the $E(t)$ values at different time because at different time we know the $C(t)$ values, that is the concentration of tracer at different times. So, we can obtain this table, to calculate $E(t)$ at different times. Now, we can plot from here $E(t)$ versus t, so $E(t)$ plot we can calculate with respect to time, that means the residence time distribution with respect to time.

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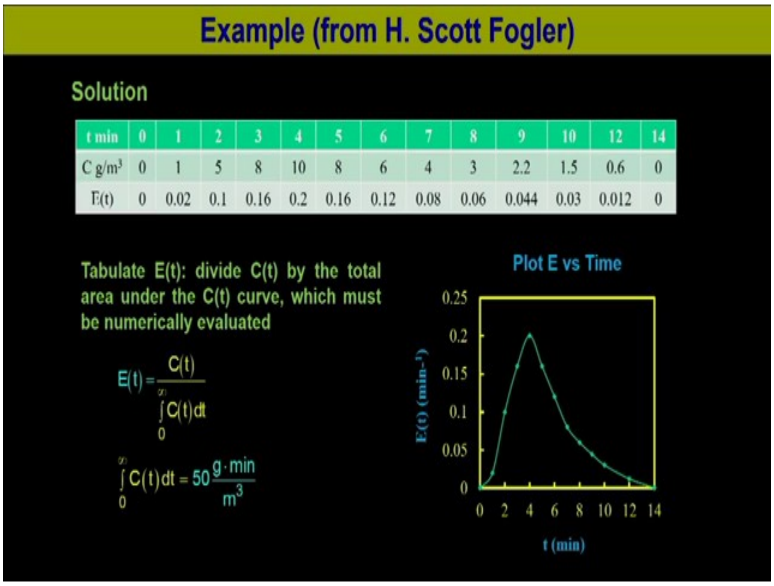

Example (from H. Scott Fogler)

Solution

t min	0	1	2	3	4	5	6	7	8	9	10	12	14
C g/m³	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0
E(t)	0	0.02	0.1	0.16	0.2	0.16	0.12	0.08	0.06	0.044	0.03	0.012	0

Tabulate E(t): divide C(t) by the total area under the C(t) curve, which must be numerically evaluated

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

$$\int_0^\infty C(t)dt = 50\frac{g \cdot min}{m^3}$$

Plot E vs Time

So, plot $E(t)$ versus time, so we could get $E(t)$ which is, unit is minute inverse versus time t, so the curve will look like this and which varies, the time is varies between 0 to 14 and the $E(t)$ values varies between 0 to 0.2.

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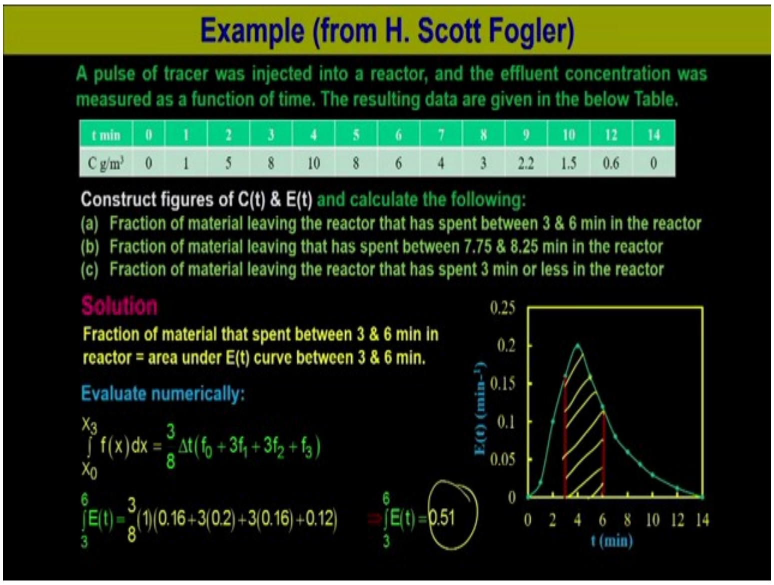

Example (from H. Scott Fogler)

A pulse of tracer was injected into a reactor, and the effluent concentration was measured as a function of time. The resulting data are given in the below Table.

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Construct figures of C(t) & E(t) and calculate the following:

(a) Fraction of material leaving the reactor that has spent between 3 & 6 min in the reactor

(b) Fraction of material leaving that has spent between 7.75 & 8.25 min in the reactor

(c) Fraction of material leaving the reactor that has spent 3 min or less in the reactor

Solution

Fraction of material that spent between 3 & 6 min in reactor = area under E(t) curve between 3 & 6 min.

Evaluate numerically:

$$\int_{X_0}^{X_3} f(x)dx = \frac{3}{8}\Delta t(f_0 + 3f_1 + 3f_2 + f_3)$$

$$\int_3^6 E(t) = \frac{3}{8}(1)(0.16+3(0.2)+3(0.16)+0.12) \Rightarrow \int_3^6 E(t) = \boxed{0.51}$$

So, now we have C t curve, we have $E(t)$ curve. Now, we have to calculate the fraction of the material leaving the reactor that has spent between 3 and 6 minute in the reactor. So, we can solve it, the fraction of the material that has spent between 3 and 6 minute in the reactor would be area under the curve, $E(t)$ curve between 3 and 6 minutes, that means if we have this figure $E(t)$ t curve, and the time is between 3 and 6 minute. So, the area under this curve will be the time or the fraction of the material that has been inside the reactor between time 3 and 6 minute.

So, if we calculate this area numerically, we can use the three-eighth rule,

$$\int_{X_0}^{X3} f(x)\,dx = \frac{3\Delta t}{8}(f_0 + 3f_1 + 3f_2 + f_3)$$

so if we put that, it would be in between 3 to 6 minute,

$$\int_3^6 E(t)\,dt = \frac{3}{8}1(0.16 + 3(0.2) + 3(0.16) + 0.12)$$

so it would be about 0.51. So,

$$\int_3^6 E(t)\,dt = 0.51$$

So similar procedure we can use to numerically calculate the area under this curve, so which would give 51 percent of the material that has been inside the reactor between time 3 minute and 6 minute.

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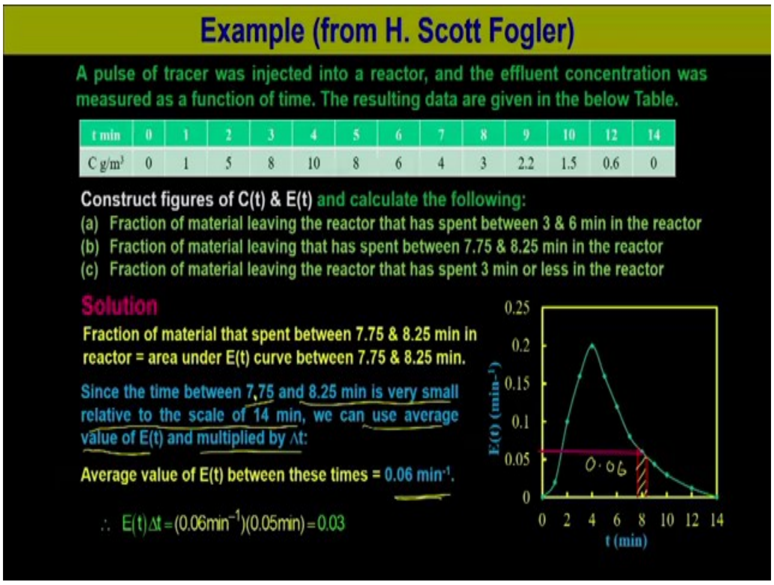

Example (from H. Scott Fogler)

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C g/m^3	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Construct figures of C(t) & E(t) and calculate the following:

(a) Fraction of material leaving the reactor that has spent between 3 & 6 min in the reactor
(b) Fraction of material leaving that has spent between 7.75 & 8.25 min in the reactor
(c) Fraction of material leaving the reactor that has spent 3 min or less in the reactor

Solution

Fraction of material that spent between 7.75 & 8.25 min in reactor = area under E(t) curve between 7.75 & 8.25 min.

Since the time between 7,75 and 8.25 min is very small relative to the scale of 14 min, we can use average value of E(t) and multiplied by Δt:

Average value of E(t) between these times = 0.06 min^{-1}.

$$\therefore\ E(t)\Delta t = (0.06\text{min}^{-1})(0.05\text{min}) = 0.03$$

Now, if we consider the second problem which is the fraction of the material leaving that spent between the time 7.75 and 8.25 minute in the reactor. So, we need to calculate the area under the curve $E(t)$ curve between 7.75 and 8.25 minutes. So, we have $E(t)$ plot and our time is only 0.5 minutes. Since, the time is very small, so basically we need to calculate area under this curve.

But since the time scale is very small that is 0.5 minutes, we can approach in a different way. We what we can do, since this time 7.75 and 8.25 is very small relative to the scale of 14 minute, we can take the average value of $E(t)$ and multiply it by delta t. So, average value of E(t) over here which is at this location is 0.06. So, average value of $E(t)$ between this times 7.75 and 8.25 minute is basically 0.06 minute inverse.

So, if we multiply this with Δt is 0.5, so this

$$E(t)\,\Delta t = 0.06 \times 0.05 = 0.03$$

That means 3 percent of the material which has spent time between 7.75 and 8.25 minute, so very small percentage of the materials spent inside the reactor in this time frame.

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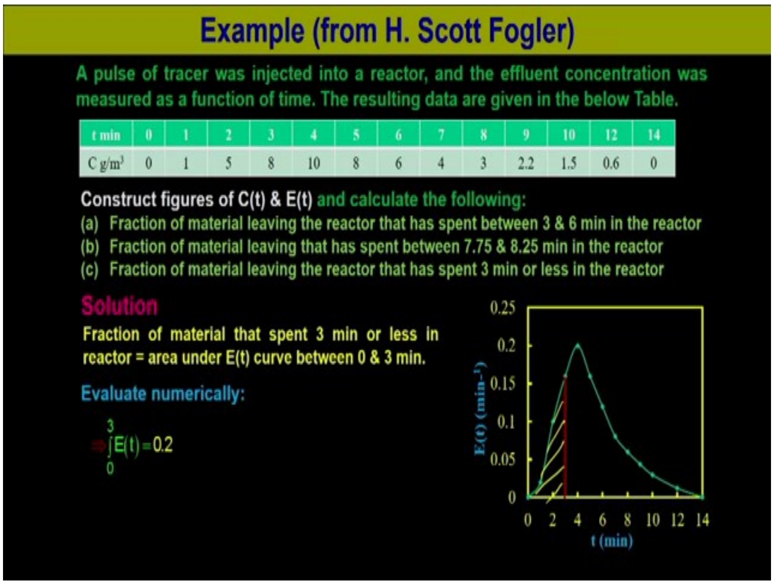

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Construct figures of C(t) & E(t) and calculate the following:

(a) Fraction of material leaving the reactor that has spent between 3 & 6 min in the reactor

(b) Fraction of material leaving that has spent between 7.75 & 8.25 min in the reactor

(c) Fraction of material leaving the reactor that has spent 3 min or less in the reactor

Solution

Fraction of material that spent 3 min or less in reactor = area under E(t) curve between 0 & 3 min.

Evaluate numerically:

$$\Rightarrow \int_0^3 E(t) = 0.2$$

The last one is the fraction of the material leaving the reactor that has spent 3 minute or less. So, what we need to calculate? We need to calculate the area under this curve. So, this is between 0 to 3 minute, so if we calculate the area under this curve numerically, we would obtain

$$\int_0^3 E(t)\, dt = 0.2$$

That means 20 percent of the material was there inside the reactor less than 3 minute time.

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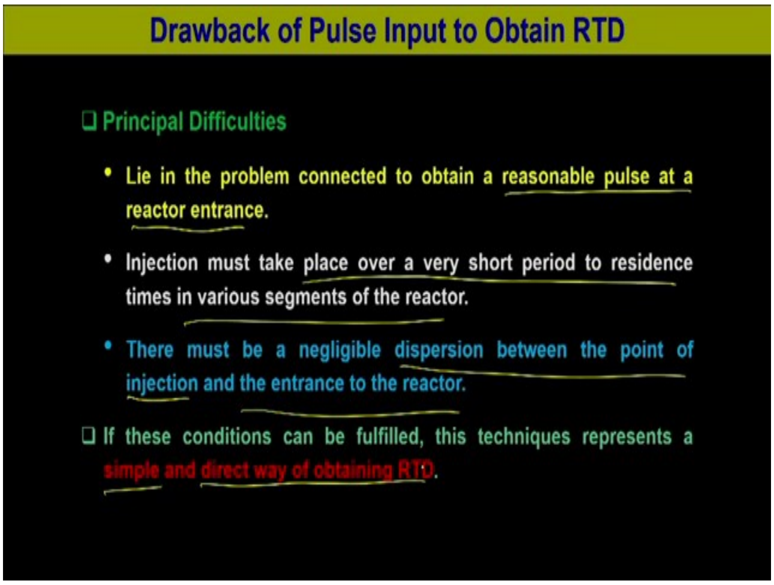

Drawback of Pulse Input to Obtain RTD

- ❑ Principal Difficulties
  - Lie in the problem connected to obtain a reasonable pulse at a reactor entrance.
  - Injection must take place over a very short period to residence times in various segments of the reactor.
  - There must be a negligible dispersion between the point of injection and the entrance to the reactor.
- ❑ If these conditions can be fulfilled, this techniques represents a simple and direct way of obtaining RTD.

So, the major drawback of the pulse input to obtain RTD is basically the difficulties we face. One difficulties lie in the problem connected to obtain the reasonable pulse at a reactor entrance. That means, to given the pulse at a very small time is very-very difficult. So, injection must take place over a very short period of time so that in various segments of the reactors.

So, there must be negligible dispersion between the point of injection and the entrance to the reactors. If these conditions can be fulfilled, this pulse injection method of measuring the residence time distribution is a simple and direct way of obtaining residence time distribution.

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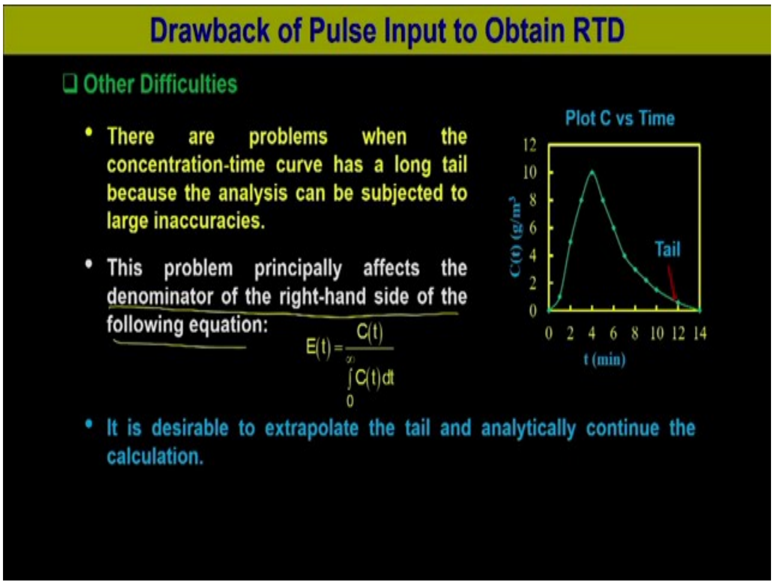

Drawback of Pulse Input to Obtain RTD

☐ Other Difficulties

- There are problems when the concentration-time curve has a long tail because the analysis can be subjected to large inaccuracies.
- This problem principally affects the denominator of the right-hand side of the following equation: $E(t)=\frac{C(t)}{\int_0^\infty C(t)dt}$
- It is desirable to extrapolate the tail and analytically continue the calculation.

The other problem lies in this method. There are problems when the concentration and time curve has a long tail because the analysis can be subjected to a large inaccuracy using the numerical truncation. So, if we look into the concentration and time curve, and this is the region when there is a long tail, so this is the tail region and we have to make the numerical truncation

Because this problem affects the denominator of the right hand side of the following equation. So, if we look into this $E(t)$,

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

We have to make the (trunc), a numerical truncation. So, because of this truncation there will be error in this method. It is desirable to extrapolate the tail and analytically continue the calculations. So, and the inaccurate which would obtain that may be less.

So, these are the principle difficulties and this is how we can measure the residence time distribution in case using the pulse injection technique. In the next lecture we will consider the step input of the tracer to find out the residence time distribution. So, thank you very much for attending this lecture and we will continue our discussion of non-ideal reactor characterizations by step input method in the next lecture.