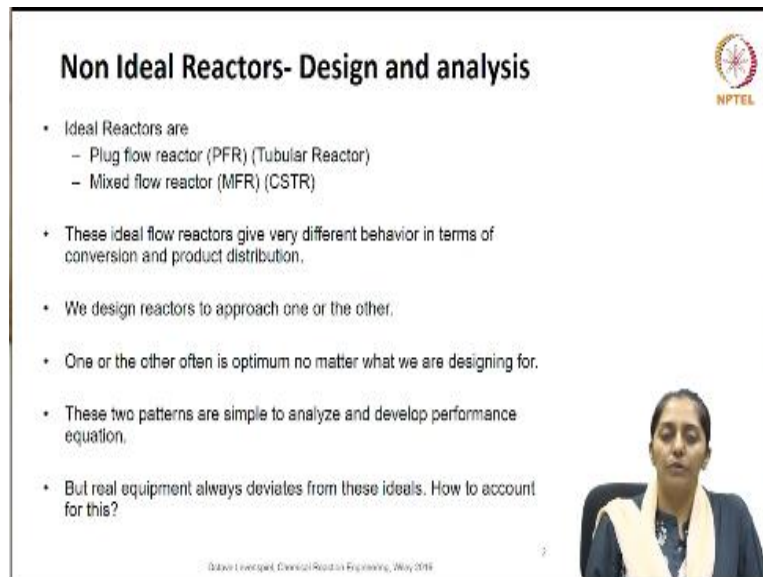


Bioreactor Design and Analysis
Dr. Smita Srivastava
Department of Biotechnology
Indian Institute of Technology – Madras


Lecture - 38
Non-Ideal Reactors: Design and Analysis – Part 1


(Refer Slide Time: 00:16)



Non Ideal Reactors- Design and analysis

- Ideal Reactors are
 - Plug flow reactor (PFR) (Tubular Reactor)
 - Mixed flow reactor (MFR) (CSTR)
- These ideal flow reactors give very different behavior in terms of conversion and product distribution.
- We design reactors to approach one or the other.
- One or the other often is optimum no matter what we are designing for.
- These two patterns are simple to analyze and develop performance equation.
- But real equipment always deviates from these ideals. How to account for this?





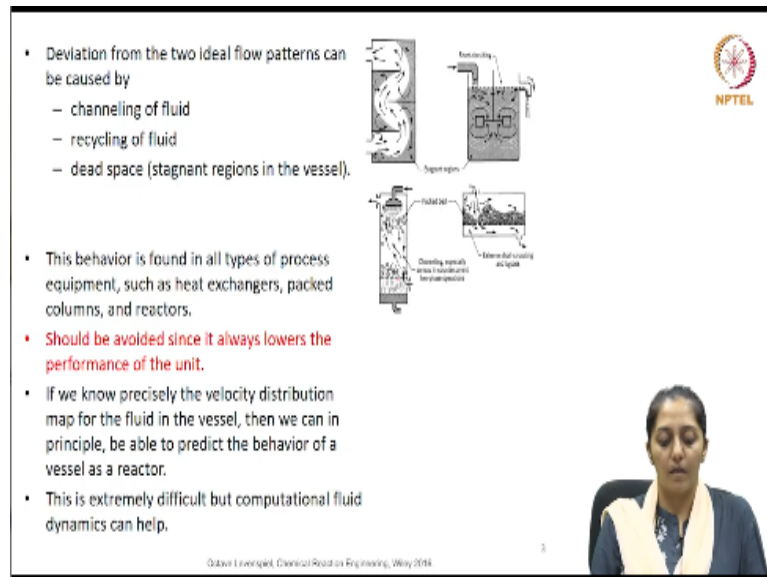
©2016 Lecturer, Chemical Reaction Engineering, May 2016

Welcome back students. Now, we are going to talk about non-ideality in reactors. To understand first, what are non-ideal reactors, their design and then analysis? So, ideal reactors, we know now, we have come across plug flow reactors, where kinetics is like a batch reactor and mix flow reactors, where we have come across continuous stirred tank reactors in as one of them mix flow reactors.

And plug flow reactors was nothing but a tubular reactor with batch kinetics. These ideal flow reactors, they give very different behaviour in terms of conversion or the product distribution. So, generally when we are designing reactors, we are trying to approach to any one of such kinetics, either of the mix flow type or the plug flow type. One or the other is always found to be often found to be optimum, no matter what we are designing for.

So, these 2 patterns, they are pretty simple to analyse and develop the performance equation. This is what we have done in the past. But practically speaking, there is always deviation from ideality. So, how to account for this deviation?

(Refer Slide Time: 01:53)



The slide contains a list of bullet points on the left and two diagrams of reactor vessels on the right. The top diagram shows a vessel with 'Recirculation' and 'Stagnant regions' labeled. The bottom diagram shows a vessel with 'Channeling', 'Dead space', and 'Internal mixing' labeled. The NPTEL logo is in the top right corner. A small video inset of a woman is in the bottom right corner. At the bottom of the slide, it says 'Datta Lectures, Chemical Reaction Engineering, May 2018'.

- Deviation from the two ideal flow patterns can be caused by
 - channelling of fluid
 - recycling of fluid
 - dead space (stagnant regions in the vessel).
- This behavior is found in all types of process equipment, such as heat exchangers, packed columns, and reactors.
- **Should be avoided since it always lowers the performance of the unit.**
- If we know precisely the velocity distribution map for the fluid in the vessel, then we can in principle, be able to predict the behavior of a vessel as a reactor.
- This is extremely difficult but computational fluid dynamics can help.

First, we need to understand, what are the source of deviations? So, deviation from the 2 ideal flow patterns, it can be caused by channelling of the fluid, recycling of the fluid or presence of dead space, which is the stagnant regions in the vessel. So, if you see on the slide, various kind of flow patterns have been shown here including the stagnant regions shown above in the 2 figures, where there is effectively no mixing happening, no fluid currents are there.



And then the bottom to show the channelling and the short circuiting, not going through the entire path, but taking the shortest route or the least resistive route. Now, this behaviour is found in all types of process equipment like for example, heat exchangers, packed columns or your bioreactors. It should be avoided, since this will lower the performance of the unit.

So, if we know the velocity distribution map for a fluid in the vessel, then in principle, we should be able to predict the behaviour of the vessel as a reactor whether it will behave as a ideal reactor or there can be non-idealities. So, you see in case of non-ideal behaviour, the flow patterns or the fluid movement changes inside the reactor in terms of its velocity distribution pattern. So, this is extremely difficult, however, your computational fluid dynamics here can help.

(Refer Slide Time: 03:48)

Overall **three somewhat interrelated factors** make up the **contacting or flow pattern**:

1. The RTD or **residence time distribution** of material which is flowing through the vessel.
2. The **state of aggregation of the flowing material**, its tendency to clump and form a group of molecules to move about together.
3. The **earliness and lateness of mixing** of material in the vessel.





©2016 University of Colorado, Boulder, CO. All rights reserved. NPTEL

So, 3 somewhat interrelated factors, they make up the contacting of flow patterns. One is the residence time distribution, this is of the material which is flowing through the vessel. Then the state of aggregation of the flowing material which means, it is tendency to clump or form a group of molecules which move together. The third aspect is earliness and lateness of mixing of the material in the vessel.

(Refer Slide Time: 04:28)

The Residence Time Distribution, RTD

- For design of reactors, it is enough if we know how long the **individual molecules stay in the vessel**, or more precisely, the **distribution of residence times of the flowing fluid**.
- This information **can be determined by using tracer technique**. It is also referred to as the **stimulus-response experiment**.
- The **analysis is restricted to steady-state flow**, without reaction and without density change of a single fluid through a vessel.



©2016 University of Colorado, Boulder, CO. All rights reserved. NPTEL

So, let us talk more about residence time distribution. Now, for designing the reactors, it is enough if we know how long the individual molecules are staying in the vessel or know precisely the distribution of the residence times of the flowing fluid elements. Now, this information can be determined by using tracer techniques. It is also referred to as stimulus response experiments.

The analysis is restricted to steady flow patterns without reactions and without any density change of the fluid through the vessel.

(Refer Slide Time: 05:19)

State of Aggregation of the Flowing Stream

Microfluid
Gases and ordinary not very viscous liquids
Individual molecules are free to move about and intermix

Macrofluid
Noncoalescing droplets
Solid particles
Very viscous liquids
Molecules are kept grouped together in aggregates or packets

Single phase system- Lie between the extremes of macro and microfluids. Solids behave as macrofluid.
Two-phase system- For gas-liquid system, either phase can be macro or microfluid, depending on the contacting pattern.

©2006 University of California, Berkeley, Chemical Reaction Engineering, Wiley 2018

NPTEL

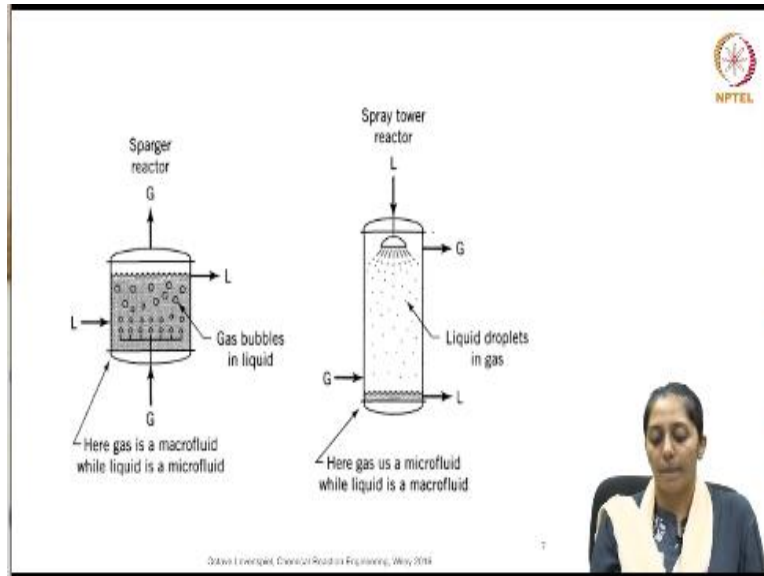
6

So, state of aggregation of the flowing stream. If you see the picture on the slide, this is a mixing where they have shown gas, mixing with not very viscous liquid. So, individual molecules, they are free to move about and intermix in case of micro fluids. Non coalescing droplets or solid particles are very, very viscous liquids. These are some examples of macro fluids.

So, you can see here in the picture, the molecules, they are grouped together as aggregates or as packets. So, this is the way the 2 fluids can behave differently. One is the micro fluid and the other is macro fluid. So, single phase system, it will lie between the extremes of the 2 macro and micro fluids. The solids, they behave as a macro fluid, while the gases will come under micro fluids.

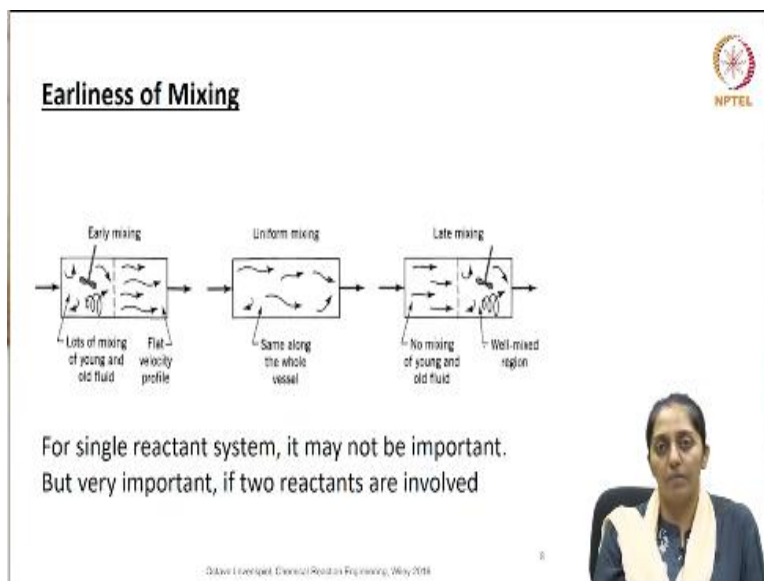
Now, for a 2 phase system like for example, gas liquid system, either phase can be a macro or micro fluid depending on the contacting pattern, which means that either gas can be dispersed in the liquid phase or the liquid can be the dispersed phase in the gas.

(Refer Slide Time: 06:56)



So, like the picture shown here, this is a sparged reactor. So, here the gas is the macro fluid while the liquid is the micro fluid. So, the gas bubbles are moving up. Now, if you see triple bed reactor or a spray reactor, tower reactor, then the liquid becomes the macro fluid and the gas is the micro fluid. The liquid is being dispersed in the gas phase.

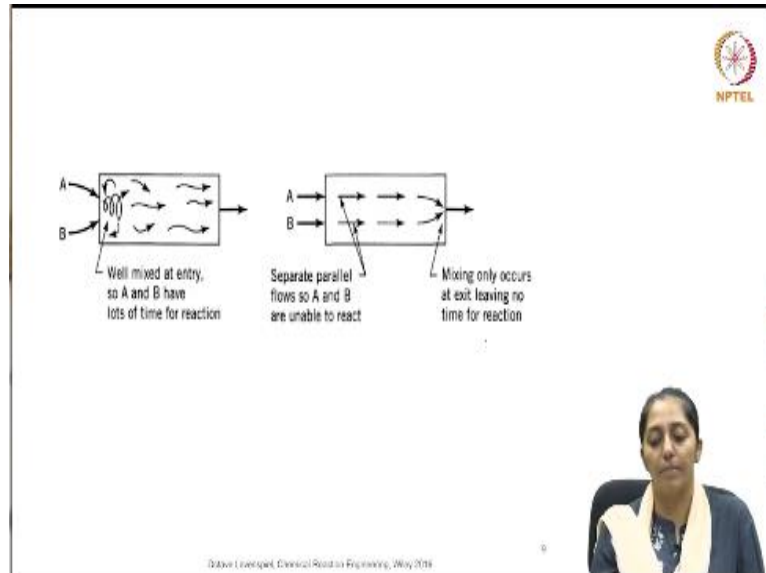
(Refer Slide Time: 07:30)



Talking about the earliness of mixing, if you see the picture on the slide, where the incoming stream, it is mixed early on. So, there is a lot of mixing of the old and the young fluid elements and then in the later half, it is almost flat velocity profile. In a uniform mixing through the entire vessel, the fluid patterns will be similar. Now, in the late mixing in the early phase, there is no mixing of the young and the old fluid while in the later half, this becomes a well mixed region where the mixing is happening.

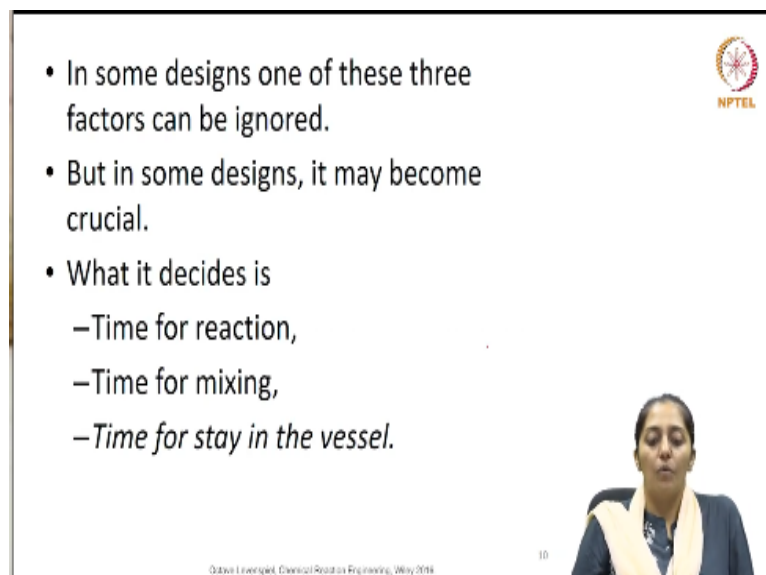
Now, for a single reactant system, this may not be of that importance, but it becomes very important when there are 2 separate reactant streams and they are supposed to react to give the product.

(Refer Slide Time: 08:36)




Like, as shown in the picture on the slide. So, A and B, they have to be well mixed at the entry. So, that they have enough time for reaction. If A and B have late mixing, then there are separate parallel flows of A and B, they are unable to react and only at the end, the mixing is happening. So, giving no time for reaction.

(Refer Slide Time: 09:08)



So, in most designs, one of these 3 factors, they can be ignored. But in few designs, it may become crucial. Why? Because it decides the time for the reaction, the time for the mixing and the time for stay in the vessel. So, all these 3 things are governed.

(Refer Slide Time: 09:35)




E, THE EXIT AGE DISTRIBUTION OF FLUID, THE RTD

- When fluid taking different routes through the reactor, they take different lengths of time to pass the vessel.
- The distribution of these times for the stream of fluid leaving the vessel is called the exit age distribution E , or the Residence Time Distribution (RTD) of fluid.

©2016 NPTEL, Chemical Reaction Engineering, Wiley 2016

11



So, in order to find the residence time distribution, which is also called as the exit age distribution of the fluid, we use make use of the tracer experiments. Now, when the fluid is taking different routes through the reactor, they can take different lengths of time to pass the vessel. Is not it? Now, if we consider all these different fluid elements entering the reactor going through different time spans inside the reactor before they pass the vessel.

This distribution of times for which the stream of fluid leaving the vessel is called the exit age distribution, denoted as capital E or the residence time distribution of the fluid. So, I will repeat. The distribution of these times for the stream of the fluid is called a exit age distribution, denoted as capital E which is same as the residence time distribution, we generally call it as RTD of the fluid.

(Refer Slide Time: 10:59)

- It is convenient to represent RTD in such a way that area under the curve is unity. It is normalization of the distribution. The units for E is time⁻¹.

$$\int_0^{\infty} E dt = 1$$

The graph shows a bell-shaped curve representing the Residence Time Distribution (RTD) or E curve. The vertical axis is labeled 'E' and the horizontal axis is labeled 't'. The area under the curve is shaded in light grey and labeled 'Total area = 1'. A vertical line is drawn at time t_1 on the horizontal axis. The area under the curve to the right of t_1 is shaded in dark grey and labeled 'Fraction of exit stream older than t_1 '. The curve is labeled 'RTD, or E curve'.

- Assumption: no eddies, no diffusion at the vessel boundaries. It is assumed to be a closed vessel boundary

©2006 J. Lee, NPTEL, Chemical Reaction Engineering, Wiley 2016

Now, it is convenient to represent the RTD in such a way that the area under the curve of E versus time which is nearly unity. So, in a sense, we are trying to normalise the distribution. So, if you make a plot of exit age versus time, then the area under the curve is unity, where E versus t plot is what is called as residence time distribution and this is also called as E curve.

So, if in this picture which is shown on the slide at time t_1 , if you see the fraction of the exit stream which is older than time t_1 is what is represented in that dark grey colour. Here, we are assuming that there are no Eddies, no diffusion at the vessel boundaries and it is assumed to be a closed vessel boundary. So, using the E curve, one can determine the fraction of the exit stream older than a particular time or age.

(Refer Slide Time: 12:25)

The graph shows the same RTD or E curve as in the previous slide. The area under the curve to the left of t_1 is shaded in light grey and labeled 'the fraction younger than age t_1 is'. The area to the right of t_1 is shaded in dark grey and labeled 'Fraction of exit stream older than t_1 '. The curve is labeled 'RTD, or E curve'.

the fraction younger than age t_1 is

$$= \int_0^{t_1} E dt$$

whereas the fraction of material older than t_1 ,

$$\int_{t_1}^{\infty} E dt = 1 - \int_0^{t_1} E dt \quad [-]$$

The E curve is the distribution needed to account for nonideal flow.

How to find it for a vessel? Experimental methods are available

©2006 J. Lee, NPTEL, Chemical Reaction Engineering, Wiley 2016

So, the fraction younger than age t_1 can be given in terms of integral 0 to $t_1 E dt$, the portion shown in white colour here. So, the older than t_1 would be $1 - \int_0^{t_1} E dt$ which is same as integral of $E dt$ with the time limits of t_1 to infinity. So, E curve is the distribution needed to account for the non-ideal flow. Now, how to find it for a vessel?

(Refer Slide Time: 13:05)

• Simplest method is to use a non reactive tracer for finding E Curve.

• Pulse and step input are easy to analyze.

NPTEL

© 2013 NPTEL. Chemical Reaction Engineering, May 2018

The simplest method is use, is to use a non reactive tracer for finding the E curve. So, where you can make use of a pulse input or a step input or a random input or periodic inputs, mostly pulse and step inputs are used because they are easy to analyse as shown on the picture here.

(Refer Slide Time: 13:35)

The Pulse Experiment

- Let vessel volume be $V \text{ m}^3$
- Fluid Flow is $v \text{ m}^3/\text{s}$
- To the fluid entering the vessel, instantaneously introduce M units of tracer (kg or moles).
- Record the concentration-time of tracer leaving the vessel.
- This is the C_{Pulse} curve.

NPTEL

© 2013 NPTEL. Chemical Reaction Engineering, May 2018

Let us take first, the pulse input. So, in the pulse tracer experiment, please make note of the notations to be used here. Let the vessel volume V metre cube, the fluid flow is being represented by small v and the vessel volume was capital V . So, the fluid entering the vessel

instantaneously they introduce M units of tracers, which is in kgs or moles. So, this is a pulse experiment.

So, suddenly, we introduced M units to the entering fluid. And then at the same time, we begin recording the concentration versus time profile of the tracer leaving the vessel.. on the other end. Here, we are giving the pulse input and here, we begin recording concentration versus time of the element. Now, this concentration versus time profile of the tracer in the vessel will be called as C pulse curve.

(Refer Slide Time: 14:55)

• From the material balance for the vessel we find,

(Area under the C_{pulse} curve): $A = \int_0^{\infty} C dt \cong \sum_i C_i \Delta t_i = \frac{M}{v} \left[\frac{\text{kg} \cdot \text{s}}{\text{m}^3} \right]$

(Mean of the C_{pulse} curve): $\bar{t} = \frac{\int_0^{\infty} tC dt}{\int_0^{\infty} C dt} = \frac{\sum_i t_i C_i \Delta t_i}{\sum_i C_i \Delta t_i} = \frac{V}{v} [\text{s}] =$

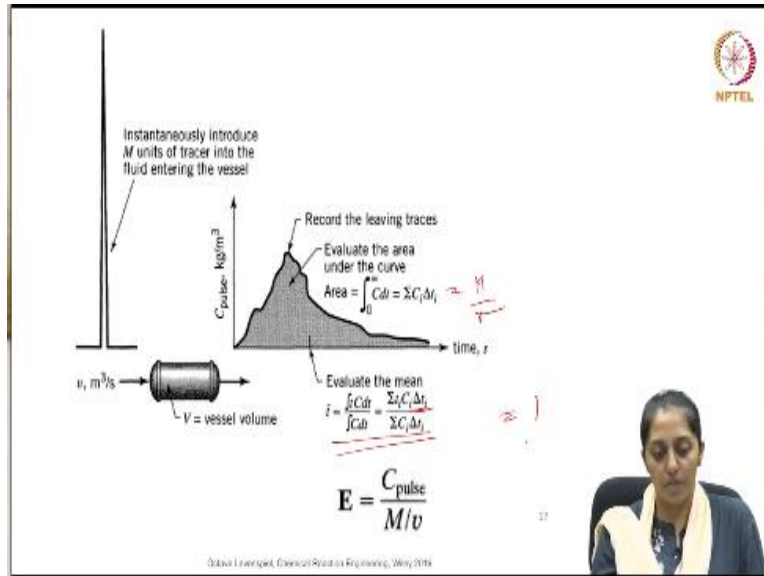
Handwritten notes on the slide:
 $= \frac{\int_0^{\infty} tC dt}{\int_0^{\infty} C dt}$
 $= \frac{\int_0^{\infty} C dt}{\int_0^{\infty} C dt}$
 $= \frac{M}{v} \frac{\text{kg} \cdot \text{s}}{\text{m}^3}$
 $= \sum_i C_i \Delta t_i$

©2014 IIT Bombay, Chemical Reaction Engineering, May 2014

So, if we do the material balance for the vessel, we find that area under the C pulse curve can be called as 0 to infinity C dt. So, this will be the entire area under the curve which is 0 to infinity C dt. Now, in terms of small time distributions delta t equally distributed, we can further reduce it in the form of summation C i delta t i, which is nothing but total amount of tracer which was added divided by the volumetric flow rate which is metre cube per second.

So, this is the area under the curve. Now, mean of this curve can be determined by using statistics as shown here. So, your mean residence time or mean time can be obtained, we now know, it is F by V inverse, so, which is V by F. So, volume and small v, volumetric flow rate.

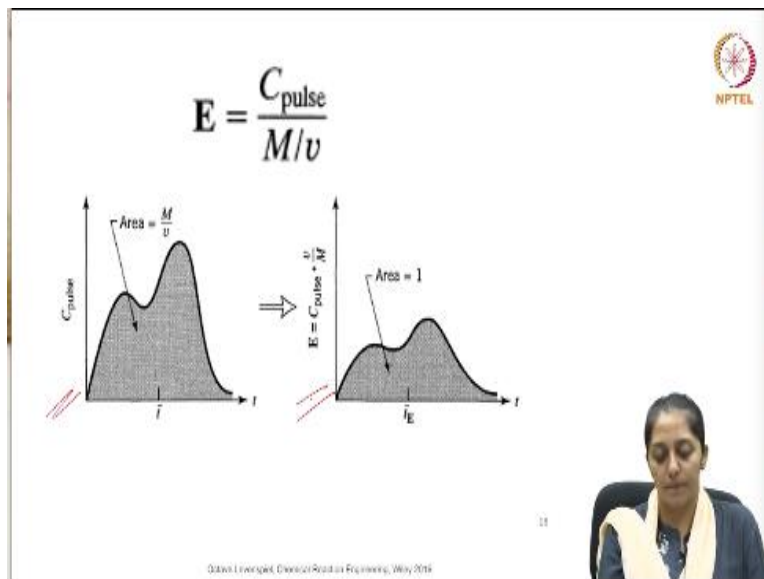
(Refer Slide Time: 16:47)



Now, as the M amount of tracer is instantaneously introduced into the fluid entering the vessel as shown here. When we start noting down the concentration, it will rise to a value and then it starts decreasing because of the subsequent dilution of the incoming stream. So, this area under the curve is nothing but your M by small v and your residence time or mean residence time can be given as $\Delta t_i C_i \Delta t_i$ by $C_i \Delta t_i$.

So, your E curve can be obtained from C pulse curve. Now, the area under the curve is equal to 1 for an E curve. So, if we divide the C pulse values by M by V , then we should be able to get E values.

(Refer Slide Time: 17:57)



So, this is what is done to convert C pulse curve to an E curve.

(Refer Slide Time: 18:08)

- Another RTD function is E_θ , which is measured in terms of mean residence time.
- $\theta = t/\bar{\tau}$.

$$E_\theta = \bar{\tau} E = \frac{V}{v} \cdot \frac{C_{\text{pulse}}}{M/v} = \frac{V}{M} C_{\text{pulse}}$$

- The relationship between C_{pulse} and the E curves only holds exactly for vessels with closed boundary conditions.

NPTEL

21

©2014 University of Texas at Austin, Fall 2014

Now, another RTD function is called E_θ which is measured in terms of the mean residence time. So, here, E_θ is mean residence time multiplied by the E values. So, residence time is nothing but V by F , so, which is capital D by small v and E was given as C_{pulse} by capital M by small v . So, effectively E_θ can be obtained, values can be obtained from the C_{pulse} curve, if we divide the corresponding C values by M and multiply by the volume.

So, now, we have correlation between the C_{pulse} and the E curves and E_θ which is true for the vessels with closed boundary conditions.

(Refer Slide Time: 19:15)

The Step input Experiment

- Let $v \text{ m}^3/\text{s}$ of fluid flow through a vessel of volume V .
- At time $t = 0$ switch from ordinary fluid to fluid with tracer of concentration $C_{\text{max}} = \text{Kg or mol}/\text{m}^3$
- Measure the outlet tracer concentration C_{step} vs t ,

NPTEL

22

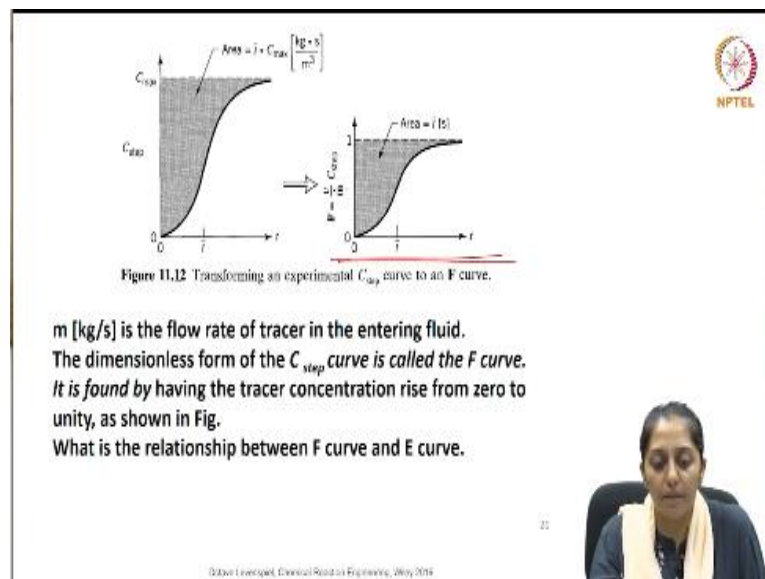
©2014 University of Texas at Austin, Fall 2014

Now, if we use a step input rather than using a pulse input, then how does it change? How to determine the E curve? Now, when we use a step input, this is how it can be demonstrated. At

time t is equals to 0, there is no tracer or less than 0, no tracer and at time t greater than 0, let us assume this the amount of tracer being dropped in is $m \dot{}$ which is nothing but in terms of kg per second.

Small v again is your volumetric flow rate; capital V is the volume of the reactor. So, once we start sending in the step input, we start determining the concentration of the exit of the tracer. Being a step input, the profile would look like as shown here. We will call now the concentration profile as C step versus time profile and it will take a form as shown here. So, gradually the new fluid is going to take over the old fluid.

(Refer Slide Time: 20:34)



So, for your C step, it is converted in order to normalise into the area one, it is converted into an F value such that its value is ranging from 0 to 1. Now, $m \dot{}$ is the flow rate of the tracer in the entering fluid. So, the dimensionless form of C step curve is called the F curve as shown here. So, it is found by having the tracer concentration rise from 0 to unity as shown here in the figure.



So, now, let us see, how we can relate F and E values? So, your F value in order to change it to C max, it will become C step divided by $m \dot{}$ by v .

(Refer Slide Time: 21:40)

- How to relate E with F ?
- Imagine a steady flow of white fluid. Then at time $t = 0$ switch to red and record the rising concentration of red fluid in the exit stream, i.e., obtain F curve.
- At any time $t > 0$ red fluid and only red fluid in the exit stream is younger than age t.
- This means,

**(fraction of red fluid in the exit stream) =
(fraction of stream younger than age t)**

- The first term is simply the F value, while the second is given by

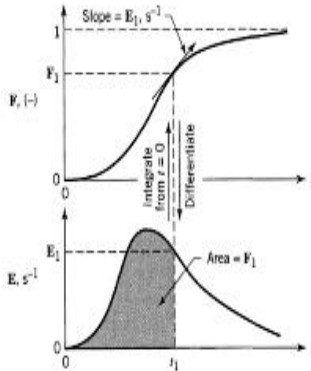





22

© 2011 University of Central Florida, Orlando, FL, USA

So, how do we relate E with the F values? Imagine a steady flow of the white fluid, then at time t which is equal to 0, we switch to a red and record the rising concentration of the red fluid in the exit stream and then we obtain the F curve. At any time t greater than 0, the red fluid and only the red fluid in the exit stream would then be younger than the age t. This means what? This means that if you see on the screen, the fraction of the red fluid in the exit stream is equal to the fraction of the stream younger than age t.

(Refer Slide Time: 22:32)


$$F = \int_0^t E dt \qquad \frac{dF}{dt} = E$$




23

© 2011 University of Central Florida, Orlando, FL, USA

The first term simply means the F value can be given as $\int_0^t E dt$ is what is F which is the fraction younger than time t. So, if $\int_0^t E dt$ is F, then dF/dt is E, if you have the F curve at every time point, if you find the slope at that point in the F curve, you can determine the value of E. And this is how F can be changed to the E curve as shown in the picture here.

(Refer Slide Time: 23:06)



$$F = \frac{v}{m} \cdot C_{step}, \quad E = \frac{dF}{dt}$$

$$\bar{t} = \frac{V}{v}, \quad \theta = \frac{t}{\bar{t}}, \quad \bar{\theta}_E = 1, \quad E_\theta = \bar{t}E$$

$\theta, E_\theta, F \dots$ all dimensionless, $E = [\text{time}^{-1}]$


24

©2006 University of Colorado, Chemical Reaction Engineering, Wiley 2018

So, now, just to consolidate, F is related to C step where E and F are related as shown here, E equals to dF by dt. And your mean residence time is V by F, F is small v, theta is the dimensionless time factor, where the time is getting divided by the mean residence time. So, E theta is related to E by the mean residence time. So, your theta, E theta, F, they are all dimensionless entities and E is time inverse.

(Refer Slide Time: 23:54)

Finding RTD by experiment



The concentration readings in Table E11.1 represent a continuous response to a pulse input into a closed vessel which is to be used as a chemical reactor. Calculate the mean residence time of fluid in the vessel \bar{t} , and tabulate and plot the exit age distribution E .

Table E11.1

Time t , min	Tracer Output Concentration, C_{pds} gm/liter fluid
0	0
5	3
10	5
15	5
20	4
25	2
30	1
35	0

25

©2006 University of Colorado, Chemical Reaction Engineering, Wiley 2018

So, let us try to find the RTD where an experiment done using C pulse or using a pulse tracer, the data which is collected of the concentration of the tracer at the exit with respect to time is shown here in the table. Now, it is asked to determine the mean residence time of the fluid and to plot the exit age distribution, which means E versus t curve. What we have in hand is the C pulse and the unit given here is grams per litre.

(Refer Slide Time: 24:31)

Table 8.1.1

Time, t , min	Tracer Output Concentration, C , g/l
0	0
5	3
10	5
15	5
20	4
25	2
30	1
35	0

The mean residence time, from Eq. 4, is

$$\bar{t} = \frac{\sum t_i C_i \Delta t_i}{\sum C_i \Delta t_i} = \frac{\sum t_i C_i}{\sum C_i}$$

$$= \frac{5 \times 3 + 10 \times 5 + 15 \times 5 + 20 \times 4 + 25 \times 2 + 30 \times 1}{3 + 5 + 5 + 4 + 2 + 1} = 15 \text{ min}$$

The total area under the concentration-time curve:

The area under the concentration-time curve:

$$\text{Area} = \sum C_i \Delta t_i = (2 + 3 + 5 + 4 + 2 + 1) \times 5 = 100 \text{ gm-litre-min}$$

Then we have

t , min	$E = \frac{C_i}{\text{Area}}$
0	0
5	0.03
10	0.05
15	0.05
20	0.04
25	0.02
30	0.01

Osaka University, Chemical Process Engineering, May 2018

So, effectively, we can find first the C pulse by t and then the area under the curve can be divided to get the E curve E values. So, how to find the area under the curve? First, we calculate the mean residence time. So, mean residence time, you see the time intervals are equally distributed. So, we can have it as Δt_i is 5 minutes here. So, we will have $C_i \Delta t_i$ by summation C_i .

So, if we do that as shown here on the right hand side by calculating summation $C_i \Delta t_i$ by summation C_i . So, here if we do this using the table data, we find that the mean residence time is 15 minutes. If the main residence time is 15 minutes, the area under the concentration time curve can be given as addition of all concentrations multiplied by Δt_i which is 5 minutes. So, then we calculate the area as 100 grams per litre in 2 minutes.

Now, we divide all these C pulse values by this area and we get the corresponding E values which was 100. So, if you are dividing all these C values by 100, you will get your E values. So, this is your E curve, E versus t curve.