

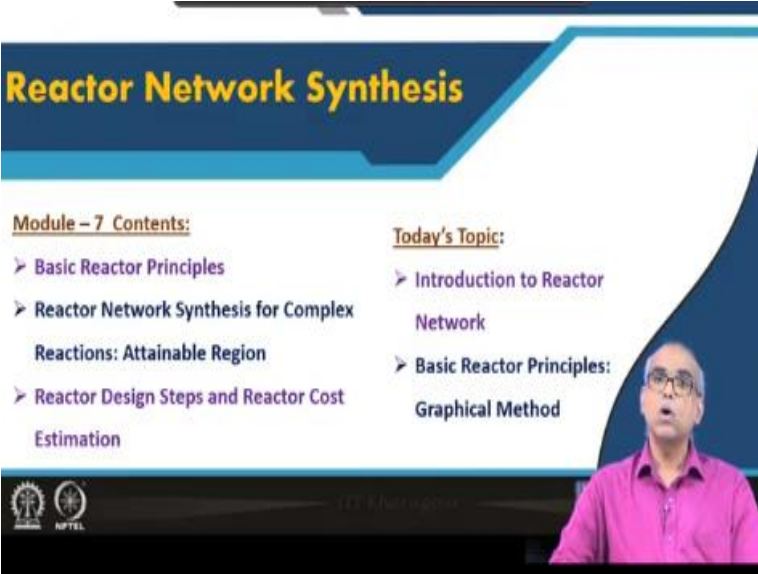
Plant Design and Economics
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Lecture No -31
Basic Reactor Principles

Welcome to lecture 31 of plant design and economics. In this module, we will discuss reactor network synthesis. In many chemical processes, the chemical reactor is the heart of the process. We have seen in our previous module that the process synthesis or process flow sheet synthesis starts with the consideration of the reactor because the consideration at the reactors level influence several other operations downstream.

For example, reactors have tremendous influence on the separation systems. Often times it may be more economical to use more than one reactor compared to a single reactor. Now what should be the optimal configuration of those reactors will be the subject of this module.

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The slide is titled "Reactor Network Synthesis" in yellow text on a dark blue background. Below the title, there are two columns of text. The left column is under the heading "Module – 7 Contents:" and lists four items: "Basic Reactor Principles", "Reactor Network Synthesis for Complex Reactions: Attainable Region", "Reactor Design Steps and Reactor Cost Estimation", and "Reactor Design Steps and Reactor Cost Estimation". The right column is under the heading "Today's Topic:" and lists two items: "Introduction to Reactor Network" and "Basic Reactor Principles: Graphical Method". In the bottom right corner of the slide, there is a small video inset showing a man in a pink shirt speaking. At the bottom left of the slide, there are logos for IIT Kharagpur and NPTEL.

So, the contents of this module is basic reactor principles, reactor network synthesis for complex reactions by attainable region and reactor design steps and reactor cost estimation. So most of the time in this module we will spend on understanding a geometric method known as attainable region for synthesis of complex reactions. You are already familiar with what should be the size of PFR or CSTR for a simple single reactions.

So in this module we will mostly focus on reactor network synthesis for complex reactions using attainable region. So today we will start with the brief introduction to reactor network. And then we will review basic reactor principles to graphical methods and most of you are already familiar with these graphical methods.

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What is Chemical Reactor Network?

The design of chemical reactors aims at achieving the optimal performance for given chemical reactions. There are various performance measures to characterize chemical reactors, such as the yield of a certain product, or the cost for a certain production rate.

A number of connected reactors are often more economical than any single reactor for achieving the same conversion. How to establish which reactor combinations and/or arrangements are optimal for a prescribed product specification?

The slide contains two flow diagrams. The first diagram shows a parallel arrangement where a single input stream splits into two paths, each passing through a reactor (Reactor 2 and Reactor 3), which then recombine. The second diagram shows a series arrangement where the output of Reactor 1 goes into Reactor 2, and the output of Reactor 2 goes into Reactor 3. A small inset image shows a man in a pink shirt speaking.

So let us start with what is the chemical reactor network? The design of chemical reactors aims at achieving the optimal performance for given chemical reaction. There are various performance measures to characterize chemical reactors such as yield of a certain product or the cost of certain production rate. A number of connected reactors are more often economical than any single reactor for achieving the same conversion.

Now when you use more than one reactors, how to establish which reactor combination and the arrangements among these reactors are optimal for a given product specification? For example, what should be the reactor combinations and the interconnections among these reactors to maximize say the product of my desired or target product?

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What is Chemical Reactor Network?

Large-scale industrial reactions are almost invariably carried out on a continuous basis, with reactants entering at one end of the reactor network and products leaving at the other.

Large scale industrial reactions are almost invariably carried out in continuous basis with reactants entering at one end of the reactor network and exiting from the other end. What you see is the various combinations of CSTRs. Which combination is optimal for your particular case?

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What is Chemical Reactor Network?

The choice of reactors and their arrangement is based on the same criteria used for single reactor selection, with the added complexity of determining the optimal reactor arrangement.

The choice of reactors and their arrangement is based on the same criteria used for single reactor selection. However, there is an added complexity here that is, the complexity of determining the optimal reactor arrangement.

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Chemical Reactor Synthesis Problem: Define

Given:

1. A reaction mechanism and its kinetics (e.g., arbitrary nonlinear kinetics)
2. Different types of reactors (e.g., CSTRs, PFRs), and
3. A performance index (e.g., yield, selectivity)

Determine a reactor network that optimizes the prescribed performance index and provides information on

1. The number and type of reactors
2. The volumes of each reactor
3. The feeding, recycling and by-passing, and
4. The topology of the reactor network and the optimal values of the flow-rates and compositions of each stream

The slide features a blue and white background with faint chemical symbols and a network diagram. A small inset video in the bottom right corner shows a man in a pink shirt speaking. Logos for institutions are visible in the bottom left corner.

So let us formally define the reactor synthesis problem. Given: A reaction mechanism and its kinetics, it may be arbitrary non-linear kinetics, different types of reactors, we will restrict ourselves to ideal reactors such as CSTRs, PFRs and a performance index such as maximization of yield or maximization of selectivity. We need to determine a reactor network that optimizes the prescribed performance index.

And also provides information on the number of reactors, the type of reactors, the volume of each reactor, the feeding, recycling and bypassing, the topology of the reactor network and the optimal values of the flow rates and compositions of each stream. So from the reactor synthesis problem, we seek to get solutions to all these questions.

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Reactor Network Synthesis: Approaches

The most notable methods can be classified into:

- Heuristics (based on experience)
- Attainable region ←
- Rigorous mathematical optimization

Hybrid methods also exist, such as the combination of attainable region with rigorous optimization.

Heuristics:

- Select suitable reactor type for the given reaction based on experience.
- Next optimize reactor parameters and operating conditions.
- Easy method, but may not always be applicable for any arbitrary reaction.

The slide features a background with a stylized molecular structure and a blue wave on the right. A presenter in a pink shirt is visible in the bottom right corner. Logos for IIT Bombay and NPTEL are in the bottom left.

Now, broadly there are three approaches for addressing reactor network synthesis problem. Heuristics which is based on experience, method of attainable region and rigorous mathematical optimization. Hybrid methods also exist such as a method which combines both attainable region as well as rigorous mathematical optimization technique. Now, heuristic methods are essentially based on your experience. So what you do is, you select a suitable reactor for the given reaction based on your experience.

Next you optimize reactor parameters and the operating conditions that will maximize your performance index that is, your target; maximization of yield, maximization of selectivity etcetera. This method is easy but may not always be applicable for any arbitrary reaction, also it is not guaranteed that this will lead to an optimal solution to a reactor synthesis problem. So in this module we will mostly discuss attainable region.

In today's lecture we will review the graphical methods which are mostly your familiar with, so we will very quickly go through these concepts and then finally towards end we will discuss certain heuristics which can be used for simple reactions as well as complex reactions such as series, parallel or series parallel reactions.

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Three Idealized Reactor Models

Industrial PFR

Reactants → Products

We will talk about only these three idealized reactor models; batch reactor, CSTR reactor and plug flow reactor.

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Three Idealized Reactors: General Comparison

	Batch	CSTR	Plug-Flow
Reactor size for similar conversion	A	D	A
Simplicity and cost	A	A	D
Continuous operation	D	A	A
Ability to handle large throughputs	D	A	A
Instrumentation	A	D	D
Flexibility	A	D	D

A: Advantage
D: Disadvantage

There are several advantages, disadvantages associated with all of these reactors based on various considerations. For example, reactor size for similar conversion is the advantageous for batch and plug flow reactor, but it is disadvantage with CSTR. Batch and CSTR are simpler and cost effective compared to plug flow reactor. Continuous operation is not possible with batch. Ability to large throughputs is possible with CSTR and plug flow but it is disadvantage with batch.

Instrumentation, easy instrumentation for batch but not so for CSTR and plug flow. Batch is more flexible compared to CSTR and plug flow which are responsible for essentially continuous operations, but batch is flexible and it is possible to use batch process for formation of multiple products.

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Chemical Reactors Principles: Mole Balance

The material and energy balances can be developed from the fundamental conservation equations based on a differential volume of the reacting system.

(Rate of accumulation of species i in the volume element, mol/time) = (Rate of inflow of species i into volume element, mol/time) - (Rate of outflow of species i from volume element, mol/time) + (Rate of generation of species i in the volume element, mol/time)

System Volume

F_{i0} F_i R_i

$$\frac{dN_i}{dt} = F_{i0} - F_i + \int_V R_i dV$$

N_i = Number of moles of species i in the system at time t

Now, the design equations for the ideal reactors are based on the mole balance. So we consider a system volume, we define F_{i0} as the rate of inflow of species i into the volume element in the unit of moles per time. Similarly F_i is the rate of outflow species i from the volume element in unit of mole per time. So I can write down the mass balance equation, which is rate of accumulation of species i in the volume element in unit of mole per time;

$\frac{dN_i}{dt}$ will be equal to rate of inflow of species - rate of outflow of species + rate of generations of species i in the volume element, all in unit of mole per time. Note that here N_i is the number of moles of species i in the system at time t . So this is the nomenclature will be following. So N_{i0} will be the number of moles of species a at time t equal to 0. So on and so forth. Now this mole balance equation is used to get the design equations for batch, CSTR and plug flow reactor and your familiar with this.

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Idealized Batch Reactor: Design Equation

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V}$$

If density remains constant =>

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)} = - \int_{C_A}^{C_{A0}} \frac{dC_A}{(-r_A)}$$

Levenspiel Plots

Area = t/N_{A0}

General Case

Area = t/C_{A0}

Constant Density Only

So let us quickly look at those design equations and with this these are equations what we have plotting is known as Levenspiel plots. So for general case this is the equation which gives the time required for achieving a given conversion. So if you look at this equation, t by energy NA_0 is nothing but the value of this integral. So we make a plot of 1 by $-r_A V$ versus conversion and the area under the curve from 0 to X_A , the given conversion is a measure of the time required.

So these area is basically t by NA_0 , so looking at the area you find out the time required for the given conversion. The same plot or similar plot can also be drawn in terms of concentration on the assumptions of density remains constant, you have these blocks.

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Idealized Mixed-Flow Reactor (CSTR): Design Equation

CSTR

For constant density system,

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{(-r_A)}$$

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0}(-r_A)}$$

$$\tau = \frac{V}{v} = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A}$$

Levenspiel Plots

Area = $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}}$

General Case

Area = $\tau = \frac{VC_{A0}}{F_{A0}}$

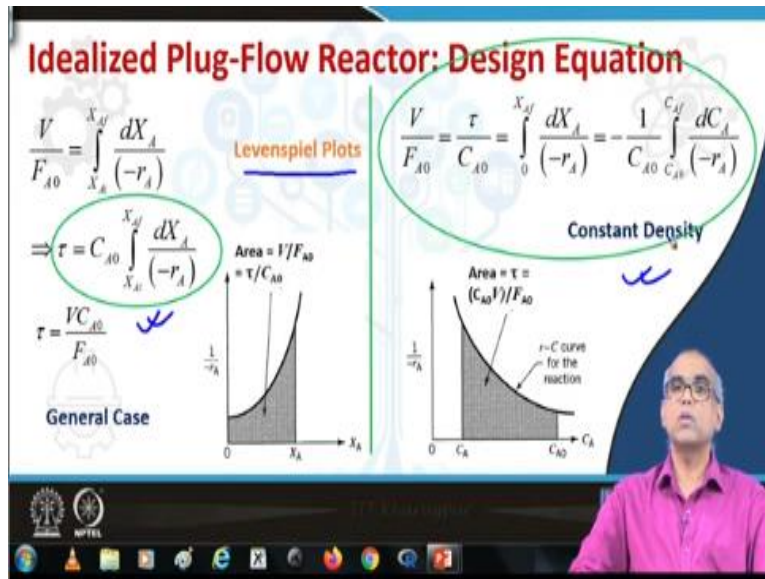
Constant Density Only

The design equations interrelate (r_A , X , F , V). Find any one if other 3 are known.

Conditions within reactor and at exit represents lowest rate

Again, this is the Levenspiel plot for CSTR, the mixed flow reactor. So again I make a Levenspiel plot -1 by r_A versus X_A and from this equation you see that this area, the shaded area is basically a measure of the volume of the reactor. The shaded area is equal to V by F_{A0} or same as the residence time τ by C_{A0} . The plot can also be drawn for constant density case between $1/r_A$ versus concentration C_A and the shaded area is the residence time τ which is $V C_{A0}$ by F_{A0} .

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Finally, this is the design equation and the Levenspiel plot for the plug flow reactors. So everywhere we are making a plot of reciprocal of rate versus concentration or conversion and we can get the information, volume information for CSTR and plug flow reactor looking at this area, either area under the curve for the plug flow reactor or the entire shaded area for CSTR. For batch reactor, you get the information on time required for achieving a given conversion.

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Comparing Idealized Batch and Plug-Flow Reactor

The Batch Reactor is well suited to produce small amounts of material and to produce many different products from one piece of equipment. On the other hand, the continuous process is nearly always found to be more economical for the chemical treatment of materials in large amounts.


An element of fluid reacts for the same length of time in the batch and in the plug flow reactor. Thus, the same volume of these reactors is needed to do a given job.

For long-term production, correction required for shutdown time (empty, clean-out, refill) in Batch Reactor.

Batch Reactor:

$$t = C_{A0} \int_0^{X_f} \frac{dX_A}{(-r_A)} = - \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{(-r_A)}$$

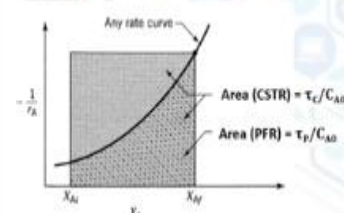
PFR:

$$\tau = C_{A0} \int_0^{X_f} \frac{dX_A}{(-r_A)} = - \int_{C_{A0}}^{C_{Af}} \frac{dC_A}{(-r_A)}$$


Now if we compare idealized batch reactor and idealized plug flow reactors, both the reactors will require same volume for achieving the specified degree of conversion. This is because an element of fluid reacts for the same length of time in batch and plug flow reactor.

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Comparing CSTR and PFR (or Batch Reactor) Sizes



The Figure compares the profiles for a CSTR and PFR between the same inlet and outlet concentrations. CSTR requires a larger volume than a PFR for same job.

The rate of reaction in a CSTR is uniformly low as the reactant is instantly diluted by the product that has already been formed.

In a PFR or Ideal-Batch reactor, the rate of reaction is high initially and decreases as the concentration of reactant decreases (or conversion increases).

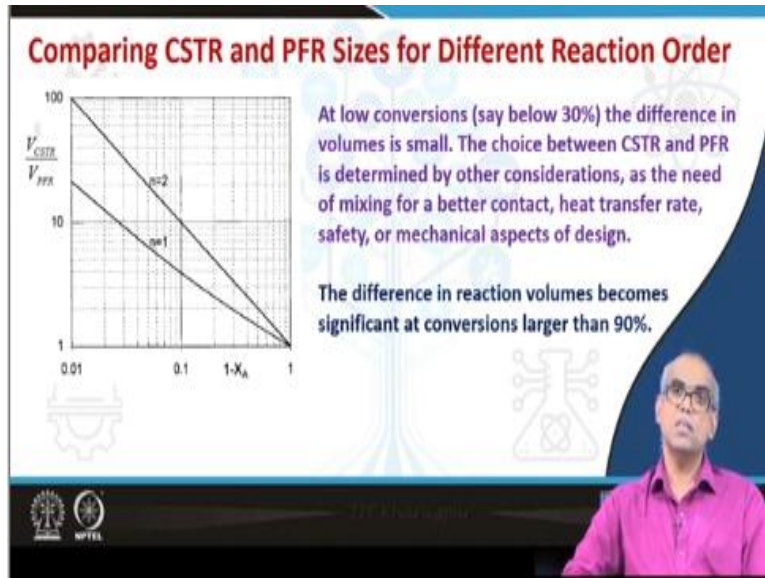


If you compare CSTR and plug flow reactor, the figure will tell you that the CSTR will require always a larger volume than a plug flow reactor for achieving the given conversion. Look at this figure, the area under the rate curve is a measure of area for plug flow reactor, whereas the entire shaded area is a measure of CSTR volume. So CSTR volume is always higher than the PFR volume for a given conversion.

The rate of reaction in CSTR is uniformly low, whereas for PFR the rate of the reaction is high

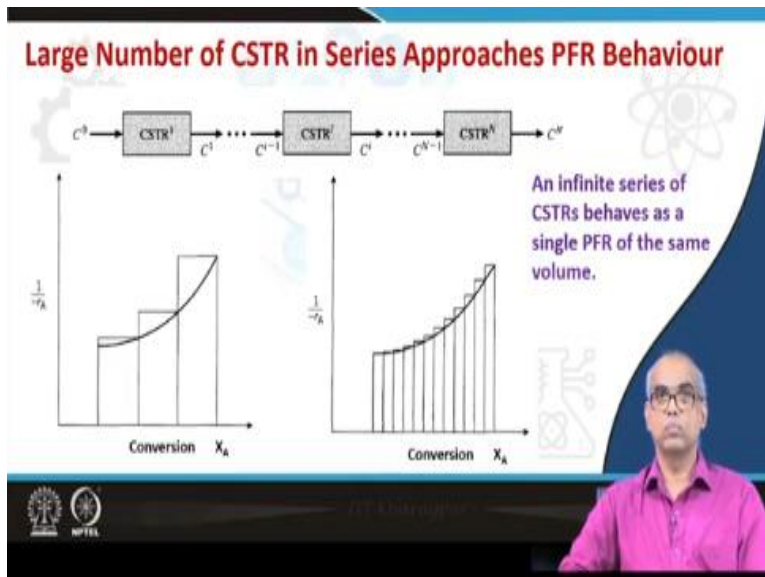
initially and decreases as the concentration of the reactant decreases or as the conversion increases.

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Now, at low conversions the difference in the CSTR volume and the plug flow volume is small. But as the conversion increases, the difference increases. The difference also increases with increase in reaction order.

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So how to decrease this difference? We can use multiple CSTRs in series and infinite series of CSTRs behaves as a single plug flow reactor of the same volume.

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Comparing CSTR and PFR Sizes: Rules

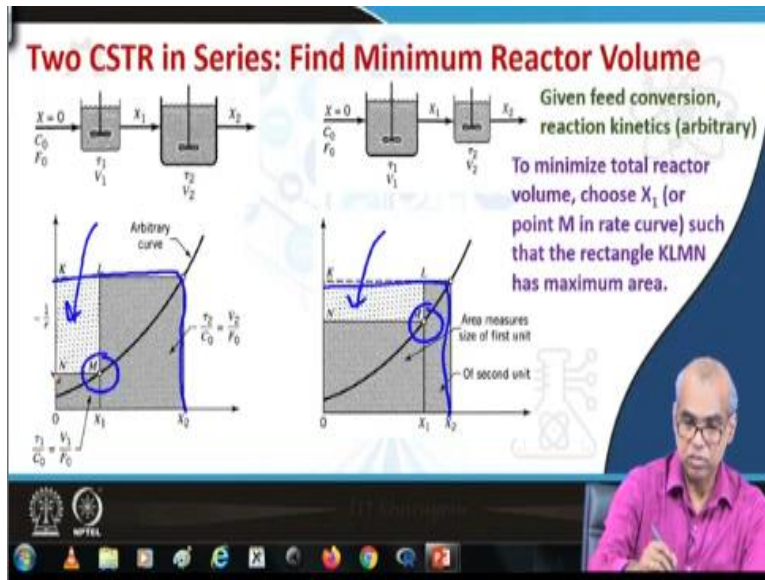
1. If the reaction order is positive, the CSTR is larger than the PFR at all conversion levels.
2. The higher the fraction conversion involved, the greater the disparity between the sizes of the CSTR and the PFR.
3. The higher the order of the reaction, the greater the ratio of sizes at a fixed conversion level. For zero-order reactions, reactor size is independent of reactor type.
4. Variations in fluid density on reaction can have significant effects on the size ratio, but the effects are secondary compared to the variations in reaction order.

Logos for IIT Bombay and NPTEL are visible in the bottom left corner of the slide.

So, comparison of CSTR and plug flow reactor gives a certain rules. So let us follow these heuristics. If the reaction order is positive, the CSTR is larger than the plug flow reactor at all conversion levels. The higher the fraction conversion involved, the greater the disparity between the sizes of the CSTR and the plug flow reactor. The higher the order of the reaction, the greater the ratio of the sizes at a fixed conversion level.

For zero order reactions, reactor size is independent of the reactor type. Variation in fluid density on reaction can have significant effects on the size, on the size ratio. But the effects the secondary when this is compared against the variations in reaction order. So the changes in reaction order has much more stronger effect than the variations in fluid density. So these are the rules which we should remember while comparing CSTR and PFR sizes.

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Now let us consider 2 CSTR in series. So this figure shows 2 CSTRs in series, the first one is smaller in volume compared to the second one. So the focus you are attention on this inter stage conversion X_1 which is at the effluent coming out of the first CSTR. So, the plot of reciprocal rate versus conversion will look like this. Note that the conversion achieved in the first reactor is 0 to X_1 . So, this is the rectangle which is a measure of the volume of the first reactor, that is V_1 .

So from X_1 to X_2 is achieved in the second CSTR. So this volume, this area is a measure of the volume of the second CSTR. And note that these conversion X_1 is indicated by point M on the rate curve. Now, if I just reverse the order of these 2 reactors, so this shaded area OX1MN is a measure of V_1 and this one is a measure of V_2 . Now let us say we have to find out the minimum reactor volume. So this can be done by suitably choosing what will be the interstage conversion x_1 .

So given feed conversion, the final conversions X_2 , reaction kinetics, we can minimize the total volume by appropriately selecting X_1 such that this rectangle KLMN has maximum area. Why so? Because note that in both the cases these area is identical. So to get the minimum total volume we have to subtract a rectangle KLMN with maximum possible area. So question now is select point M1 on the rate curve such that the area KLMN is maximum. And that is the conversion that we must achieve in the first reactor.

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Two CSTR in Series: Find Minimum Reactor Volume

For reaction rate expressions of the nth-order form it can be shown that there is always one and only one point that minimizes the total volume when $n > 0$. This situation is obtained when the intermediate fraction conversion X_1 is selected so that the slope of the curve representing the reaction rate expression at this conversion level is equal to the slope of the diagonal of rectangle KLMN.

For cascades of multiple equal-sized CSTRs, the problem of determining the reactor sizes necessary to achieve a specified degree of conversion can be solved by a trial-and-error procedure.

Now, it has been shown that this can be done by selecting M1 on the rate curve such that the slope of the rate curve at point M is equal to the diagonal of the rectangle KLMN. Under this condition, the KLMN will have maximum area and the reactor will have minimum volume. Now, this discussion is for 2 CSTRs in series. For cascade of multiple equal size CSTR, the problem of determining the reactor size is necessary to achieve a specified degree of conversion is more involved and this can be done by trial and error procedure.

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Minimum Reactor Volume: Example

We wish to treat 10 L/min of liquid feed containing 1 mol A / L to 99% conversion. The stoichiometry and kinetics of the reaction are given by

$$A \rightarrow R, \quad -r_A = \frac{C_A \text{ mol}}{0.2 + C_A \text{ liter} \cdot \text{min}}$$

Suggest a good arrangement for doing this using two mixed flow reactors, and find the size of the two units needed.

Solution Steps:

From $-r_A = \frac{C_A \text{ mol}}{0.2 + C_A \text{ liter} \cdot \text{min}}$

Plot $1/r$ vs concentration.

Find optimum C_1 graphically:
 $V_1 = 27 \text{ L}$
 $V_2 = 19 \text{ L}$

Let us take a quick example on finding minimum reactor volume. We wish to treat 10 litre per minute of liquid feed containing one mole A per litre to 99% conversion. The stoichiometry and kinetics of the reactions are given by A to R and that expression is given. Suggest a good

arrangement for doing this using 2 mixed flow reactors and find the size of the 2 units needed. So we have to perform this using 2 CSTRs in series. So you just follow whatever we have discussed in the previous 2 slides.

So I will just show you the solution steps. We have 2 CSTRs in series. So the kinetics of the reactions is given. So you can plot $1/r_A$ versus concentration. What we have shown in previous slides is $1/r$ versus conversion, but you can also make a plot of reciprocal of rate versus concentration and you find the optimum C_1 , optimum inter stage concentration graphically such that the total volume is minimum.

Solve with graphically and the result will approximately we say 27 litre for the volume V_1 and 19 litre for volume V_2 . So 2 CSTRs connected in series, the first one is larger than the second one.

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PFR in Series and Parallel

PFR in Series:

$$\frac{V}{F_0} = \sum_{i=1}^N \frac{V_i}{F_0} = \frac{V_1 + V_2 + \dots + V_N}{F_0}$$

$$= \int_{X_0=0}^{X_1} \frac{dX}{-r} + \int_{X_1}^{X_2} \frac{dX}{-r} + \dots + \int_{X_{N-1}}^{X_N} \frac{dX}{-r} = \int_0^{X_N} \frac{dX}{-r}$$

N plug flow reactors in series with a total volume V gives the same conversion as a single plug flow reactor of volume V.

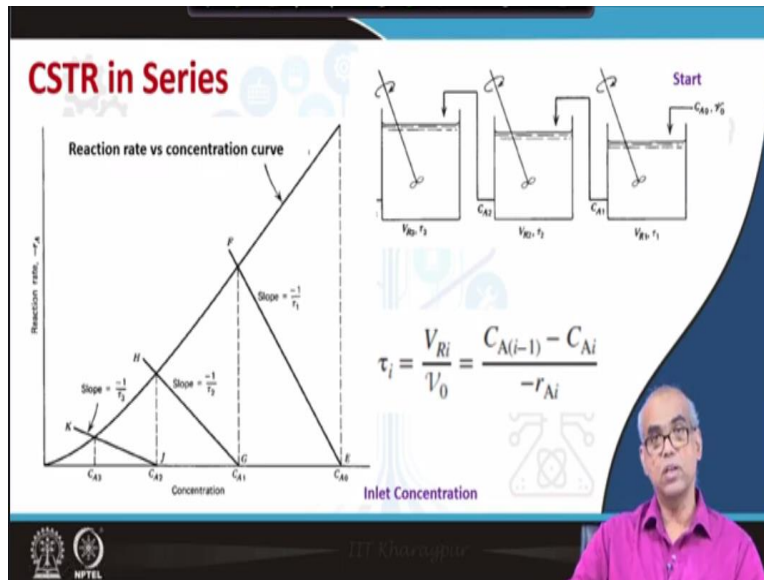
PFR in Parallel:

When plug flow reactors are connected in parallel, the most efficient utilization of the total reactor volume occurs when mixing of streams of differing compositions does not occur. For this case, too, the network acts as if it were a single plug flow reactor with a volume equal to the sum of the constituent reactor volumes.

NPTEL

When PFRs are connected in series, say N plug flow reactors are connected in series with the total volume V that will give the same conversion as a single plug flow reactor of same volume V. When plug flow reactors are connected in parallel for this course also the network acts as if it were a single plug flow reactor with the volume equal to the sum of the constituent reactor volumes.

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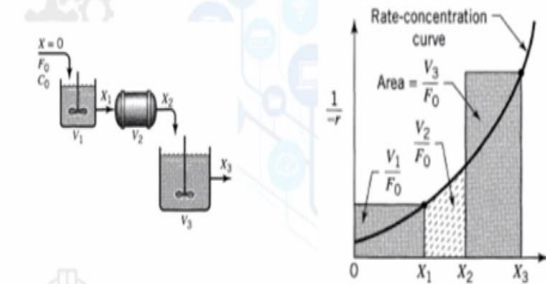
Let us consider several CSTR connected in series, for example, in this case, we have connected 3 CSTR in series - CSTR 1, CSTR2, CSTR 3. They may be all of different sizes. The resistances are tau 1, tau 2 and tau 3. Then let concentration of A is CA0. So how do I find out the concentration C1, C2, C3 etcetera? So let us draw the reaction rate versus concentration curve. Find out tau1, tau2, tau3 for all 3 reactors.

Locate the inlet concentration on the concentration axis. From this point you draw a straight line with slope minus 1 by tau1. The line intersects the rate curve at point F. So draw perpendicular line on concentration from point F. That gives you CA1. That means the outlet concentration of the CSTR1. Again from CA1, you draw a straight line with slope minus 1 by tau 2. And you get CA2.

Similarly, you also get CA3. So this way graphically you can solve for concentrations for a cascade of CSTRs in series.

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Two CSTR and One PFR in Series



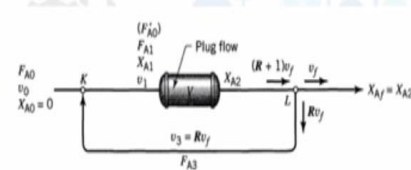
We can predict the overall conversions for such systems, or conversions at intermediate points between the individual reactors. Intermediate conversions determines the heat duty of interstage heat exchangers.

What you see in a figure is 2 CSTRs and 1 plug flow reactor, they are connected in series. So you can very conveniently find out the overall conversions represents the reactors on the levels 3 plots of reciprocal rate versus conversion. So this represents these area is a measure of volume V_1 of first reactor. Shaded area under the curve is a measure of volume of the plug flow reactor. And this shaded area is a measure of area of V_3 for the second CSTR.

So you can predict the overall conversion of such systems or conversions at intermediate points between the individual reactors. Intermediate conversions is useful to find out the heat duty of inter stage heat exchangers.

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Recycle Reactors



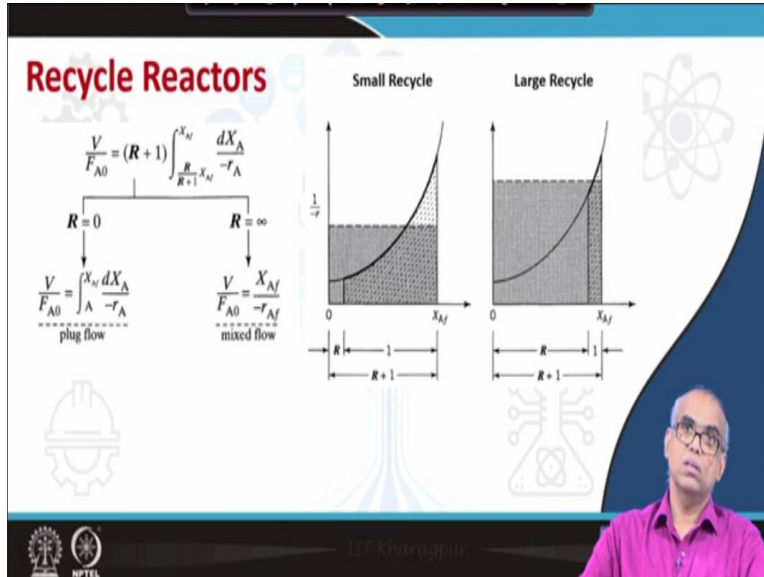
In certain situations it is advantageous to divide the product stream from a plug flow reactor and return a portion of it to the entrance of the reactor.

$$R = \frac{\text{volume of fluid returned to the reactor entrance}}{\text{volume leaving the system}}$$



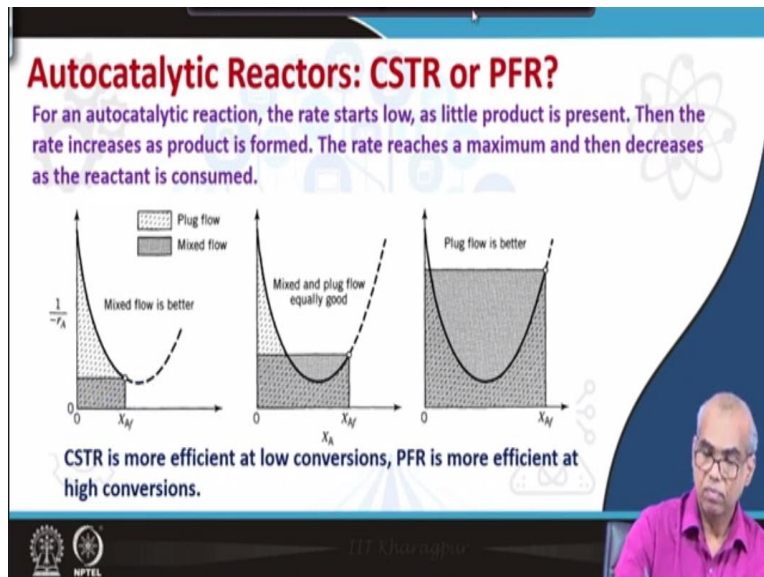
Recycle reactors. In certain situations it is advantages to divide the product stream from a plug flow reactor and return a portion of it to the entrance of the reactor as recycle. Now the recycle rate is defined as volume of fluid return to the reactor entrance divided by volume leaving the system.

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Now, if you analyze this recycle reactor you will see that when your amount of recycle is small in the limiting situation when recycle rate is 0, the reactor will behave like a plug flow reactor. So for small recycle the reactor will behave like a plug flow reactor whereas when the recycle rate is extremely high, very high, large recycle the reactor will tend to behave like a CSTR.

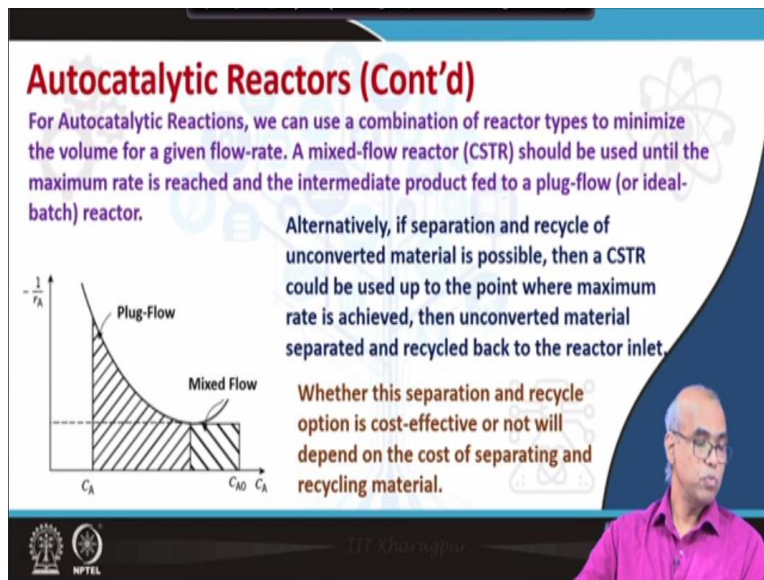
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Let us consider now autocatalytic reactors. Which should I use for auto catalytic reactors; CSTR or PFR or a combination of both? For an autocatalytic reaction, the rate starts low as little product is present. Then the rate increases as product is formed. The rate reaches a maximum and then decreases as the reactant is consumed. So look at this figures for different scenarios. So this corresponds to plug flow reactor and this corresponds to CSTR.

Now CSTR is more efficient at low conversions. Look at the rate curve it passes through a maximum here. So here we are talking about low conversion, does not reach maximum. If you consider the areas are you see that CSTR is more efficient at low conversion. Now this is a scenario at much higher conversion. Now area under the rate curve is smaller than the entire shaded area. So PFR is more efficient at higher conversions, but may be at intermediate conversions both CSTR and plug flow reactor may be equally good.

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Now, how do I optimize the reactor volume for autocatalytic reactors? For auto catalytic reactions, we can use the combination of reactor types to minimize the volume for a given flow rate. A mixed flow reactor should be used until the maximum rate is reached and the intermediate product fed to a plug flow reactor to minimize the total volume requirement. So look at the level spill plot. So low conversion, CSTR is efficient.

If you look at the shaded area and the shaded area that would have got if we have drawn the area

under the curve for this portion. You see that CSTR is more efficient. So I take CSTR up to the point where rate is maximum. And then the remaining part, I use PFR. So that way I can minimize the total volume requirement. Alternately if separation and recycle of unconverted material is possible then a CSTR could be used up to the point where maximum rate is achieved.

And then the unconverted material separated and recycle back to the reactor inlet. But whether this separation and recycle option is cost effective or not will depend on the cost of separating and recycling material. So you need to perform a detailed economic analysis for evaluating these 2 options.

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Autocatalytic Reaction: Example

We wish to explore various reactor setups for the transformation of A into R. The feed contains 99% A, 1% R; the desired product is to consist of 10% A, 90% R. The transformation takes place by means of the elementary reaction $A + R \rightarrow R + R$

The rate constant $k = 1 \text{ L/mol-min}$. The concentration of active materials throughout is $C_{A0} + C_{R0} = C_A + C_R = C_0 = 1 \text{ mol/liter}$

What reactor holding time will yield a product in which $C_R = 0.9 \text{ mol/L}$?

- in a plug flow reactor
- in a mixed flow reactor,
- in a minimum-size setup without recycle?

Let us take a quick example of autocatalytic reactions. Wish to explore various reactor setups for the transformation of A into R. The feed contains 99% A, 1% R. The desired product is to consist of 10% A, 90% R. The transformation takes place by means of the elementary reaction $A + R \rightarrow R + R$. The rate constant K equal to 1 litre per mole minute. The concentration of active materials throughout is $C_{A0} + C_{R0}$ equal to $C_A + C_R$ equal to C_0 equal to 1 mol per litre.

What reactor holding time will yield a product in which C_R equal to 0.9 mole per litre - plug flow reactor or a mixed flow reactor or a minimum size set up of PFR and CSTR without recycle.

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Autocatalytic Reaction: Example (Cont'd)

Solution Steps:

Prepare $(-1/r_A)$ vs C_A curve.

$$-r_A = kC_A C_R$$

$$C_{A0} + C_{R0} = C_A + C_R = C_0 = 1 \text{ mol/liter}$$

Vary C_A (say 0.10 to 0.99), compute C_R as $1 - C_A$, find r_A

Now find holding time graphically:
 PFR = 6.8 min, CSTR = 9.9 min,
 Optimum combination of PFR + CSTR = 4.2 min

So the solution steps will be as follows. You prepare the levels will plot. Note that rate of reaction minus r_A equal to $kC_A C_R$. Now you know that $C_{A0} + C_{R0}$ equal to $C_A + C_R$ equal to C_0 equal to 1 mole per litre. So let us vary C_A , let us say from 0.1 to 0.99 and then compute C_R as $1 - C_A$ and then you can find out reaction rate r_A . So now we can make a plot, levels will plot. We can make a plot. This plot we can make $1/r_A$ versus C_A .

Then we find the holding time graphically as in this case. And also this case for the minimum size set up. So if you do this, the PFR will give around 6.8 minutes, CSTR will give around 9.9 minute and the optimum combination of PFR CSTR will give around 4.2 minute.

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Economic Optimum

While considering the relative size requirements for CSTR cascades and plug flow reactors, the relative economics of the two alternative reactor network configurations must be evaluated.

When few reactors are employed, the volume requirement is high.

The cost associated with volume requirement decreases as cascade of large number of reactors is considered, but the cost associated with engineering, fabrication, installation, and maintenance increases.

Number of CSTR	Total Cost (Relative)
1	Very High
2	High
3	Medium-High
4	Minimum
5	Low-Medium
6	Low
7	Low-Medium

Now while we were considering the relative size requirement for CSTR cascades and plug flow reactors, the relative economics of the 2 alternative reactor network configuration must be evaluated. What we mean is as follows. When we are using few reactors in the cascade, the volume requirement is high. So the cost associated with volume requirement will decrease as the cascade of larger number of reactors is considered.

But then as we consider more and more number of reactors in the cascade the cost associated with engineering, fabrication, installation and maintenance will also increase. So if we make a plot of total cost versus number of CSTR, this that may look like this which will decrease with number of CSTR. That is fine because of volume requirement, but that will increase again due to increase in the engineering, fabrication, installation and maintenance cost.

So for this example, the most the optimum may be around 5 number of CSTR. So this we must consider as a practical approach.

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Heuristics for Simple Reactions: Single Reactions

Consider: $A \rightarrow \text{Products}$, $-r_A = kC_A^n$

Guidelines for optimum utilization of a given set of ideal reactors operating as an isothermal reactor network:

Levenspiel

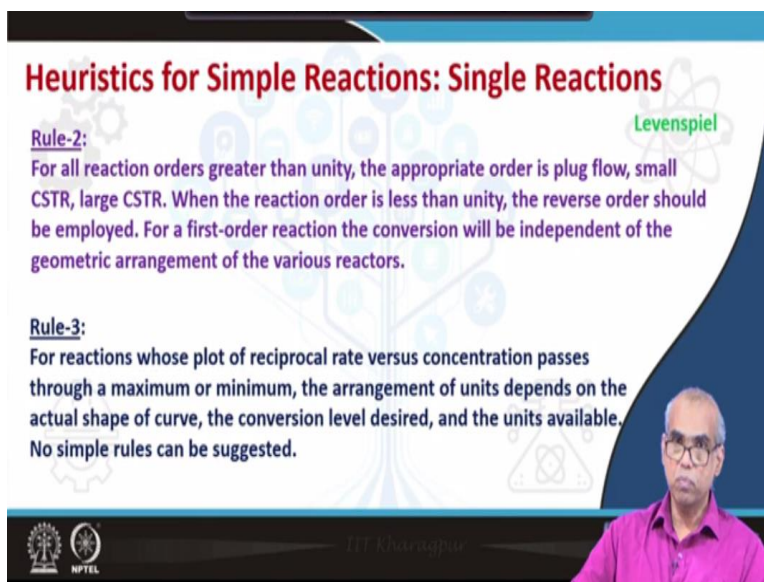
Rule-1:
For a reaction whose reciprocal rate-concentration curve rises monotonically (any positive n-th order reaction) the reactors should be connected in series. They should be ordered so as to keep the concentration of reactant as high as possible if the curve is concave ($n > 1$), and as low as possible if the curve is convex ($n < 1$).

The slide features a background with faint icons of a reactor, a tree, and a gear. At the bottom left, there are logos for IIT Bombay and NPTEL. A presenter in a pink shirt is visible in the bottom right corner.

Now we will quickly talk about certain heuristics. Heuristics for simple reactions single reaction. These all heuristics are taken from Levenspiel. Guidelines for optimum utilization of a given set of ideal reactors operating as an isothermal reactor network. Rule 1: for a reaction whose reciprocal rate concentration curve rises monotonically, any positive nth order reaction, the reactors should be connected in series.

They should be ordered so as to keep the concentration of reactants as high as possible if the curve is concave, that is n is greater than 1, and as low as possible if the curve is convex, that is n is less than 1. So here we are considering a simple single reaction $A \rightarrow 2$ products. Reaction rate is given as $-r_A$ equal to kC_A to the power n .

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The slide is titled "Heuristics for Simple Reactions: Single Reactions" in red text. It features a background with faint chemical symbols and a blue and white color scheme. A presenter in a pink shirt is visible in the bottom right corner. The slide contains two rules:

Rule-2:
For all reaction orders greater than unity, the appropriate order is plug flow, small CSTR, large CSTR. When the reaction order is less than unity, the reverse order should be employed. For a first-order reaction the conversion will be independent of the geometric arrangement of the various reactors.

Rule-3:
For reactions whose plot of reciprocal rate versus concentration passes through a maximum or minimum, the arrangement of units depends on the actual shape of curve, the conversion level desired, and the units available. No simple rules can be suggested.

Logos for IIT Bombay and NPTEL are visible at the bottom left of the slide.

Rule 2: for all reaction orders greater than unity, the appropriate order is plug flow, small CSTR, large CSTR. When the reaction order is less than unity, the reverse order should be employed. For a first order reaction, the conversion will be independent of the geometric arrangement of the various reactors. Rule 3: for reactions whose plot over reciprocal rate versus concentration passes through a maximum or minimum, the arrangement of units depends on actual shape of curve, the conversion level desired and the units available.

No simple rules can be suggested. You actually have to follow detailed economic evaluations or optimization technique.

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Heuristics for Complex Reactions: Parallel Reactions

Consider:

$$A \rightarrow P, \quad r_1 = k_1 c_A^\alpha$$

$$A \rightarrow R, \quad r_2 = k_2 c_A^\beta$$


For multiple reactions, selectivity to the desired product is important. Here, P is the desired product, while R is a waste. The relative rate of formation of P to R is

$$\frac{r_P}{r_R} = \frac{k_1}{k_2} c_A^{\alpha-\beta}$$

Levenspiel

Rule-1:
If the desired reaction has a higher reaction order than the unwanted reaction ($\alpha > \beta$), a high reactant concentration is favourable; PFRs or batch reactors are suitable.

Rule-2:
If the desired reaction has lower reaction order than the unwanted reaction ($\alpha < \beta$), the reactant concentration should be kept low. Select CSTR at high conversion, although the required reaction volume is large.



Now let us consider some heuristics for complex reactions. We start with parallel reactions. So you consider reaction A to P, reaction rate is $k_1 c_A^\alpha$. Other reaction A to R, reaction rate is r_2 equal to $k_2 c_A^\beta$. For multiple reactions, selectivity to the desired product is important. Let us consider P is the desired product here and R is waste. So the relative rate of formation of P to R can be written like this.

Rule 1: If the desired reaction has a higher reaction order, then the unwanted reaction that is $\alpha > \beta$ a high reactant concentration is favourable; plug flow reactor or batch reactors are suitable for this purpose. **Rule 2:** If the desired reaction has lower reaction order, then the unwanted reaction that is $\alpha < \beta$ the reactant concentration should be kept low.

So what kind of reactor we should select? We should select CSTR at high conversion, although the reaction volume will be large.

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Heuristics for Complex Reactions: Parallel Reactions

Consider: $A \rightarrow P, r_1 = k_1 C_A^\alpha$
 $A \rightarrow R, r_2 = k_2 C_A^\beta$


$$\frac{r_P}{r_R} = \frac{k_1}{k_2} C_A^{\alpha-\beta}$$

Levenspiel

Rule-3:
 If $\alpha = \beta$, the concentration has no effect. The only way to control the product distribution is by modifying the ratio k_1/k_2 .

The activation energies of the competing reactions should be examined. If $E_1 > E_2$, the reaction temperature should be maximised.

If $E_1 < E_2$, the reaction temperature should be kept low. However, in this situation, much more efficient is to search for a suitable catalyst.



Rule 3: if alpha equal to alpha V, sorry, alpha equal to beta, then the concentration will have no effect. The only way to control the product distribution is by modifying the ratio k_1 by k_2 . The activation energy is of the competing reactions should be examined then, if the activation energy for reaction 1 is greater than the activation energy reactant 2, the reaction temperature should be maximized.

If the activation energy for reaction 1 is less than the activation energy of the reaction 2, the reaction temperature should be kept low. However, in this situation a more efficient solution will be that we research for a efficient or suitable catalyst.

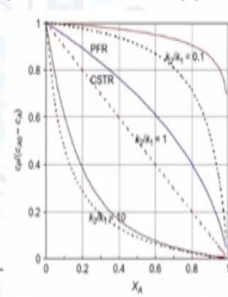
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Heuristics for Complex Reactions: Series Reactions

Consider: $A \xrightarrow{k_1} P \xrightarrow{k_2} R$ P is the main product and R is the by-product.

The formation of P or of any other intermediate is maximised when fluids of different compositions at different stages of conversion are not allowed to mix. Therefore, PFR will give a better yield of P compared to CSTR.

PFR always gives a better selectivity



$$\frac{C_{P,max}}{C_{A0}} = \left(\frac{k_1}{k_2}\right)^{k_2/(k_2-k_1)} \quad \tau_{p,opt} = \ln \frac{k_2/k_1}{k_2-k_1}$$


Now heuristics for series reactions. So you consider a reaction A to P to R. Again P is the main product and R is the by-product. The formation of P or of any other intermediate is maximized when fluids of different composition at different stages of conversion are not allowed to mix. So with these heuristics in mind we can conclude that the plug flow reactor will give a better yield compared to a CSTR, better yield for the desired product P.

So for this given reaction, we can compute what will be the CP max and the corresponding residence time. We can make a plot of CP versus CA0 minus CA versus conversion and this figure also says that the plug flow reactor will always give a better selectivity compared to CSTR.

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Heuristics for Complex Reactions: Series-Parallel Reactions

Consider: $A + B \xrightarrow{k_1} P$
 $P + B \xrightarrow{k_2} R$

Levenspiel

These reactions can be analysed in terms of their constituent reactions. The optimum contacting device for favourable product distribution is the same as for the constituent reactions.

If P is desired, the above reaction system can be analysed by analogy with the series reaction $A \rightarrow B \rightarrow P$

Then, PFR gives always a higher yield in intermediate, the feeding policy of B being irrelevant.

NPTEL

Next, heuristics for complex reactions: series parallel reactions. So you consider reactions such as A + B to P and P + B to R. This reactions can be analyzed in terms of their constituent reactions. The optimum containing, the optimum contacting device for favourable product distribution is the same as for the constituent reactions. So considering A + B to P, I can find out what will be the optimum contacting devices if my desired product is P.

So P is desired. The above reaction system can be analyzed by analogy with the series reaction A to B to P. And you have seen that for this case such scenario plug flow reactor is better.

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Heuristics for Complex Reactions: Conclusion

Selectivity is the key issue in selecting a chemical reactor for multiple reactions. Typically, high selectivity might be obtained at low conversion, but this implies a large amount of reactant to be recycled.

The design of the reactor should not be seen as isolated, but in the context of the separations with recycles. The type and the size of reactor, as well as the operating parameters, should be optimised against the cost of separations.

This is possible by taking advantage of the optimisation capabilities offered by the flow-sheeting programs.

NPTEL

The slide features a blue and white background with faint chemical symbols and a speaker in a pink shirt in the bottom right corner. The NPTEL logo is visible in the bottom left.

Now we talked about various heuristics for single simple reactions and then complexity reactions such as parallel reaction series, reaction series, parallel reaction etcetera. Selectivity is the key issue in selecting a chemical reactor for multiple reactions. Typically high selectivity might be obtained at low conversions, but this implies a large amount of reactant must be recycled. The design of the reactor should not be there, should not be seen in isolation, but it must be seen in the context of separations with recycles.

The type and size of the reactor as well as the operating parameters should be optimized against the cost of separations. This is possible by taking advantage of the optimization capabilities offered by various flow sheeting programs that are available. So with this we stop our discussion.