Plant Design and Economics
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Lecture No -33
Reactor Synthesis for Complex Reactions by Attainable Region: Example - 1

Welcome to lecture 33 of plant design and economics, we will continue our discussion on attainable region for chemical reactor networks synthesis for complex reactions. In the previous lecture, we have introduced some general properties and general characteristics of attainable region. In today's lecture, we will first consider only the PFR and CSTR and see how to construct attainable region for these reactors.

And, then we will consider a simple example to demonstrate the applications of attainable region.

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Reactor Network Synthesis

Today's Topic:

- Attainable Region for only PFR
- Attainable Region for only CSTR
- Attainable Region Example: Manufacture of Maleic Anhydride

So this will be our today's topic will first talk about attainable region for only PFR then for only CSTR and an example on a manufacturer of Maleic Anhydride will be taken last as an example of application of attainable region.

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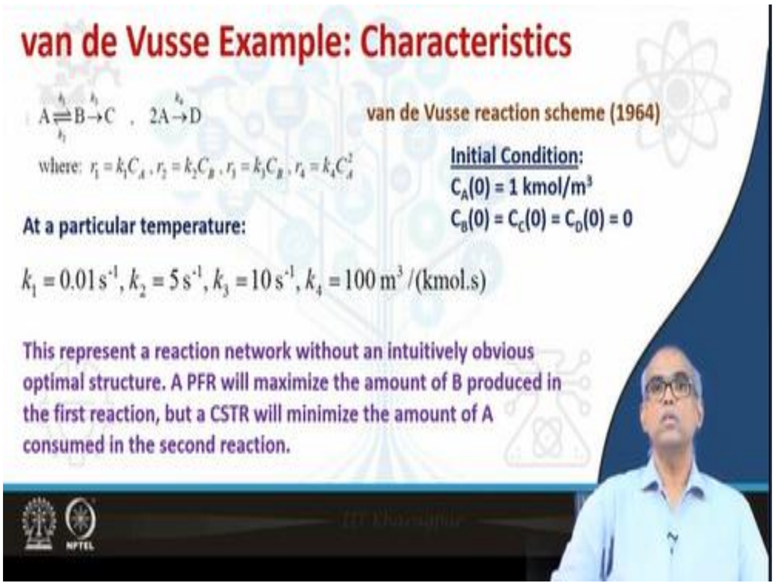

van de Vusse Example: Characteristics

$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_3} C \ , \ 2A \xrightarrow{k_4} D$

van de Vusse reaction scheme (1964)

where: $r_1 = k_1 C_A$, $r_2 = k_2 C_B$, $r_3 = k_3 C_B$, $r_4 = k_4 C_A^2$

Initial Condition:

$C_A(0) = 1$ kmol/m^3

$C_B(0) = C_C(0) = C_D(0) = 0$

At a particular temperature:

$k_1 = 0.01\,s^{-1}, k_2 = 5\,s^{-1}, k_3 = 10\,s^{-1}, k_4 = 100\,m^3/(kmol.s)$

This represent a reaction network without an intuitively obvious optimal structure. A PFR will maximize the amount of B produced in the first reaction, but a CSTR will minimize the amount of A consumed in the second reaction.

So we will consider van de Vusse reaction scheme to demonstrate the application of attainable region. Now, this is a well studied reaction mechanism and this represents a reaction network for which is not easily possible to find out what will be the optimal structure for this reaction, because a plug flow reactor will maximize the amount of B produced in the first reaction whereas, a CSTR will minimize the amount of A consumed in the second reaction.

So, we will consider this reaction to demonstrate the application of attainable region. So the reaction scheme is given basically a parallel decomposition note that A to B reaction is reversible, the rate expressions are given and also at a particular temperatures the values of rate constants, k1, k2, k3, k4 are given.

Initial conditions are given where you see that the starting mole of A is 1 kilo mole per meter cube and initially no amount of B, C and B are present.

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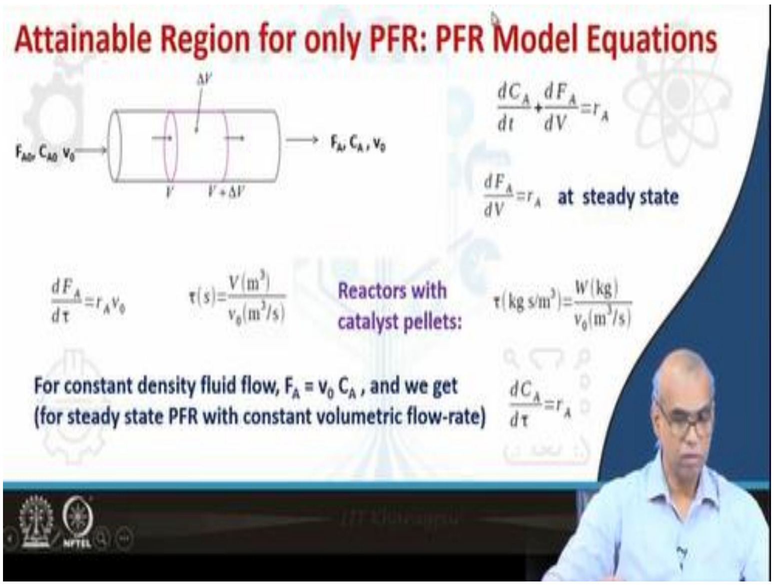

Attainable Region for only PFR: PFR Model Equations

$$\frac{dC_A}{dt} + \frac{dF_A}{dV} = r_A$$

$$\frac{dF_A}{dV} = r_A$$ at steady state

$$\frac{dF_A}{d\tau} = r_A v_0 \qquad \tau(s) = \frac{V(m^3)}{v_0(m^3/s)}$$

Reactors with catalyst pellets: $\tau(kg\ s/m^3) = \frac{W(kg)}{v_0(m^3/s)}$

For constant density fluid flow, $F_A = v_0 C_A$, and we get (for steady state PFR with constant volumetric flow-rate) $\frac{dC_A}{d\tau} = r_A$

Now, we will first consider the case of plug flow reactor. So, let us first try to model equation of plug flow reactor. The mass balance equation for plug flow reactor a trans steady state can be written as this, note that at this stage it is basically a partial differential equation as there is dependence of two variables both time and volume. So at steady state we can draw the dCA dt term, so this becomes my steady state differential equation representing a plug flow reactor.

Now, let us introduce the definition of space time which is reactor volume divided by the volumetric flow rate. So introducing the definition of space time this differential equation can now be written as this dFA d tau equal to rA into V0, note that for constant density fluid flow the FA will be equal to V0 into CA and then for steady state plug flow reactor with constant volumetric flow rate.

We get the well known differential equation dCA d tau equal to rA representing plug flow reactor operation, note that if you have catalyst pellets in the reactor, for example a packed bed reactor can be modelled as a plug flow reactor. So, we can write the space time tau as weight of catalyst divided by the volumetric flow rate. So, let us now focus your attention on this equation dCA d tau equal to r A, so we will make use of this equation.

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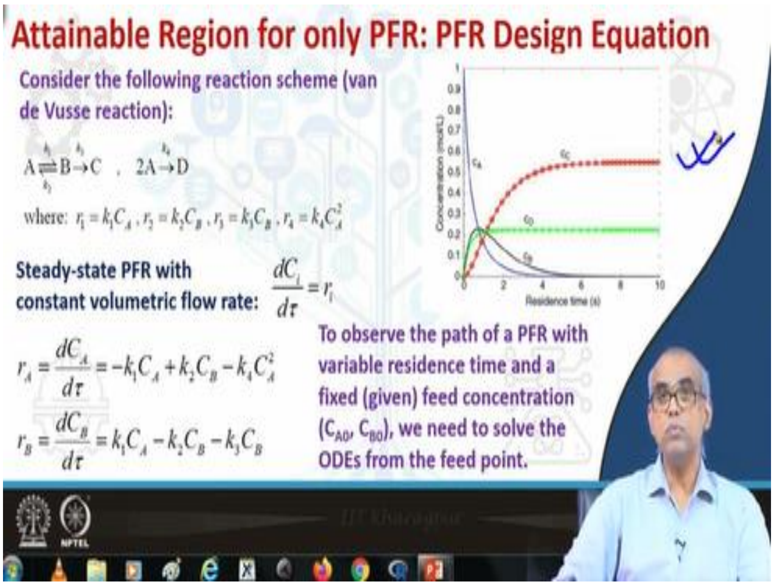

Attainable Region for only PFR: PFR Design Equation

Consider the following reaction scheme (van de Vusse reaction):

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_3} C \quad , \quad 2A \xrightarrow{k_4} D$$

where: $r_1 = k_1C_A, r_2 = k_2C_B, r_3 = k_3C_B, r_4 = k_4C_A^2$

Steady-state PFR with constant volumetric flow rate: $\frac{dC_i}{d\tau} = r_i$

$$r_A = \frac{dC_A}{d\tau} = -k_1C_A + k_2C_B - k_4C_A^2$$

$$r_B = \frac{dC_B}{d\tau} = k_1C_A - k_2C_B - k_3C_B$$

To observe the path of a PFR with variable residence time and a fixed (given) feed concentration (C_{A0}, C_{B0}), we need to solve the ODEs from the feed point.

So consider the when there was van reaction scheme again we have just seen that the steady state plug flow reactor with constant volumetric flow rate, we can write dCi d tau equal to ri, for any higher species. So, now look at the van de Vusse equations we have four species A, B, C and D. Let us now consider my objective is to maximize the amount of B, now write equation dCA d tau equal to r A and dCB d tau equal to rB.

So I get these two expressions from my rate expressions given. Now, if you look at this, two equations in the equations for dCA d tau and dCB d tau the species concentration of C and D they do not appear. So it is possible for me to represent these systems in two dimensions, that is on the concentration species CA versus CB. So to observe the path of a plug flow reactor with variable residence time for a given feed concentration all you need to do is we have to solve these two differential equations.

And, if we do that let us say I have obtained these profiles for all the components A, B, C and D for this you also have to write the differential equations for species C and species D, but now let us focus your attention only the profile for A and B. Now these two trajectories represent how the concentration of A and B vary with respect to tau. So, these two trajectories will allow me to pick CA, CB values corresponding to various residence times and, can and make a plot on CA versus CB concentration space.

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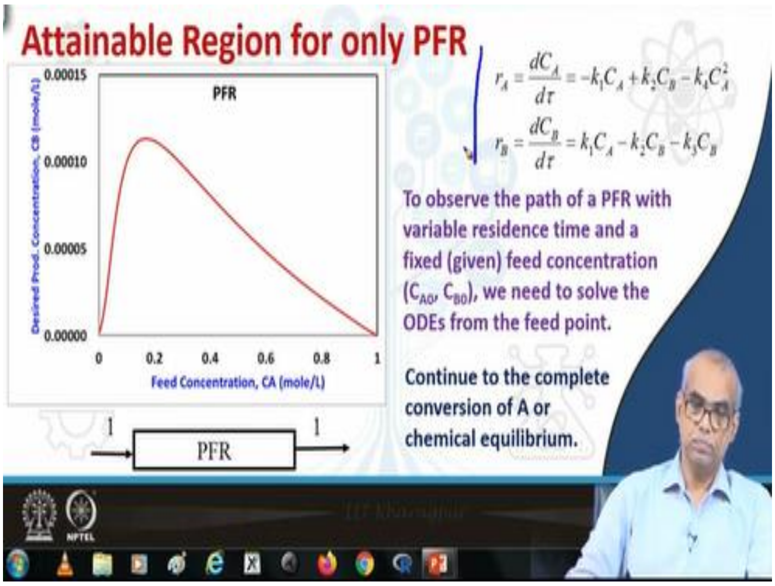

Attainable Region for only PFR

$$r_A = \frac{dC_A}{d\tau} = -k_1C_A + k_2C_B - k_4C_A^2$$

$$r_B = \frac{dC_B}{d\tau} = k_1C_A - k_2C_B - k_3C_B$$

To observe the path of a PFR with variable residence time and a fixed (given) feed concentration (C_{A0}, C_{B0}), we need to solve the ODEs from the feed point.

Continue to the complete conversion of A or chemical equilibrium.

So, this is what we have done here, to observe the path of this plug flow reactor with variable tau and a fixed feed concentration CA0, CB0, we have solved the ordinary differential equations from the feed point. So the initial condition here is CA0 equal to 1 kilo mole per meter cube and CB0 = 0, you can continue your integration of this differential equations up to the point where complete conversion of 8 x space or up to the point of equilibrium, then we make this CA, CB plot.

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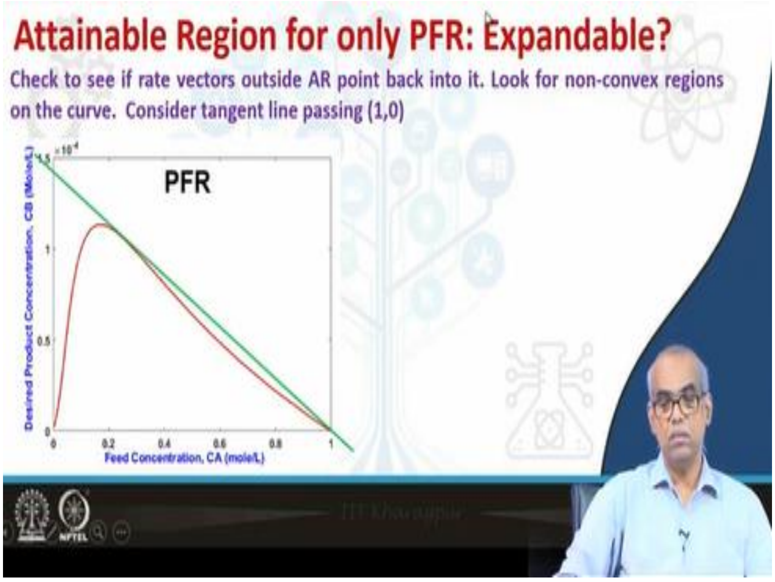

Attainable Region for only PFR: Expandable?

Check to see if rate vectors outside AR point back into it. Look for non-convex regions on the curve. Consider tangent line passing (1,0)

Now, let us examine if rate vectors outside the attainable region point back to in. So we look for non-convex regions on the curve that I have obtained for the plug flow reactor, for the given figure we consider the tangent line passing through the feed point 1, 0; we clearly see the presence of non-convex region. So I can extend the obtained region by mixing.

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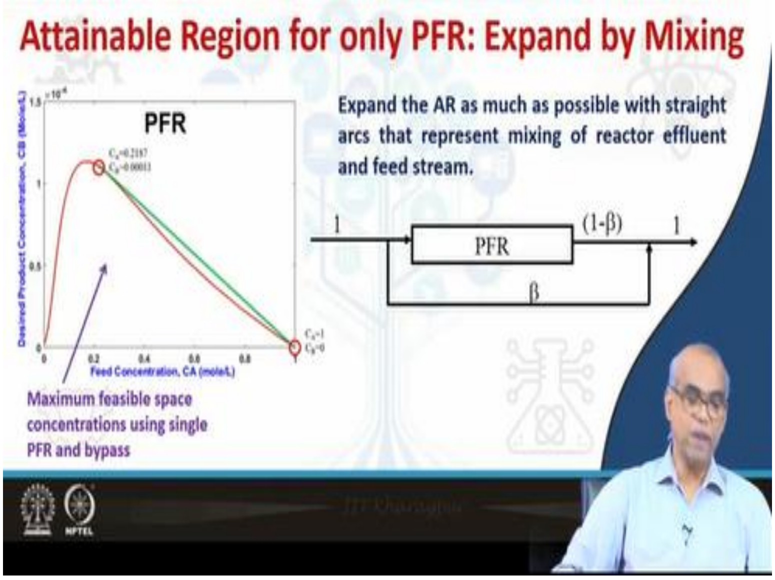

Attainable Region for only PFR: Expand by Mixing

Expand the AR as much as possible with straight arcs that represent mixing of reactor effluent and feed stream.

Maximum feasible space concentrations using single PFR and bypass

So, we expand that attainable region as much as possible with straight line arcs that represent mixing of reactor effluent and the fixed streams. So, you consider this point and draw a straight line up to the feed point such that you can extend or expand the previous attainable region or the candidate for the attainable region to the maximum extent that is possible. So, now we get after joining these straight arc maximum feasible space concentrations using plug flow reactor and a bypass.

Because any point on the straight line arc can be obtained by mixing these condition and the feed point. So effluent represented here with the fixed term, so maximum feasible space is now obtained using plug flow reactor with a bypass. So, we take the mixing fraction.

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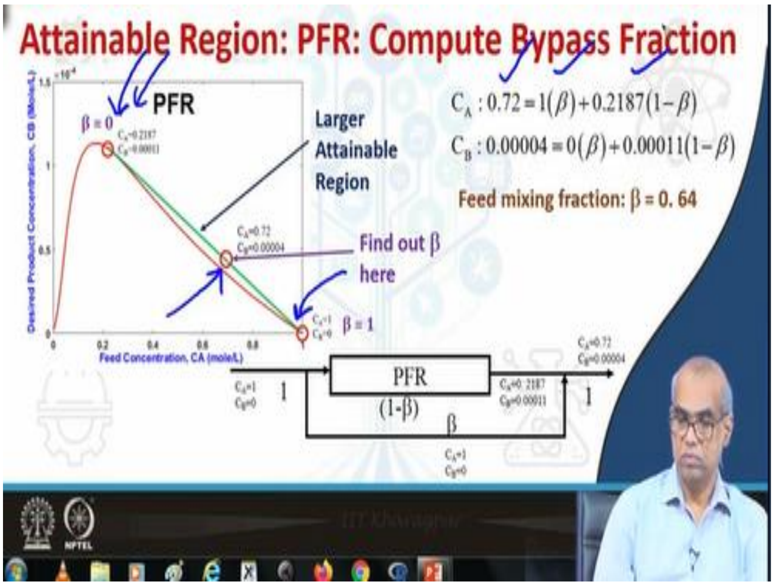

Attainable Region: PFR: Compute Bypass Fraction

$$C_A : 0.72 = 1(\beta) + 0.2187(1-\beta)$$

$$C_B : 0.00004 = 0(\beta) + 0.00011(1-\beta)$$

Feed mixing fraction: β = 0. 64

Larger Attainable Region

Find out β here

So how do i obtain the bypass fraction beta? This can be obtained by writing down simple mass balance equation, my feed point is pure A, so concentration at feed point SCA = 1. Let us consider this point representing plug flow reactor effluent where CA = 0.2187. Now consider this point which has CA = 0.72, so how do I obtain this point? What should what is the corresponding mixing fraction beta?

So we can write 0.72 equal to beta into 1 + beta into + 1 - beta into 0.2187, you can solve this equation and we will obtain beta equal to 0.64. Similar equation you can also write for concentration of B.

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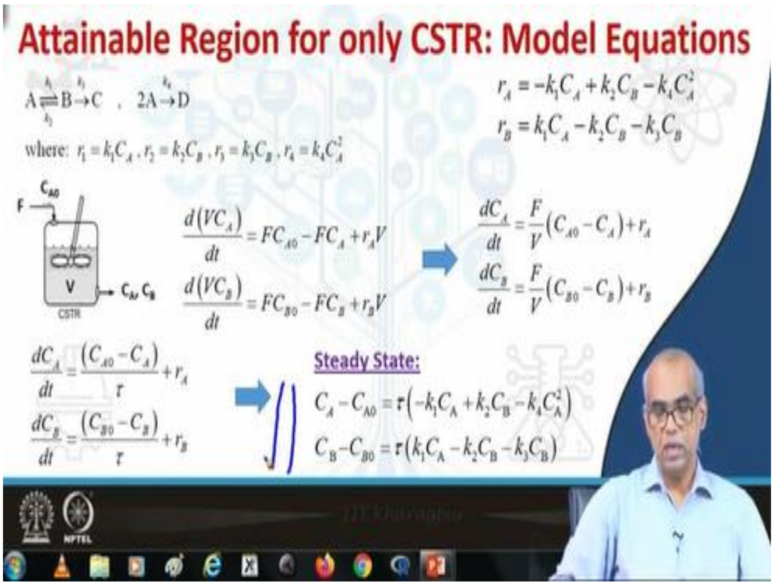

Attainable Region for only CSTR: Model Equations

$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_3} C \quad , \quad 2A \xrightarrow{k_4} D$

where: $r_1 = k_1 C_A, r_2 = k_2 C_B, r_3 = k_3 C_B, r_4 = k_4 C_A^2$

$r_A = -k_1 C_A + k_2 C_B - k_4 C_A^2$

$r_B = k_1 C_A - k_2 C_B - k_3 C_B$

$$\frac{d(VC_A)}{dt} = FC_{A0} - FC_A + r_A V$$
$$\frac{d(VC_B)}{dt} = FC_{B0} - FC_B + r_B V$$

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) + r_A$$
$$\frac{dC_B}{dt} = \frac{F}{V}(C_{B0} - C_B) + r_B$$

$$\frac{dC_A}{dt} = \frac{(C_{A0} - C_A)}{\tau} + r_A$$
$$\frac{dC_B}{dt} = \frac{(C_{B0} - C_B)}{\tau} + r_B$$

Steady State:

$$C_A - C_{A0} = \tau(-k_1 C_A + k_2 C_B - k_4 C_A^2)$$
$$C_B - C_{B0} = \tau(k_1 C_A - k_2 C_B - k_3 C_B)$$

Now, let us consider a similar situation with only CSTR. So, what is the attainable region for only CSTR? Again we will start with model equations for CSTR, so let us first write down the differential equations for CSTR where this van de Vusse reaction is taking place. So, consider the schematic of the CSTR as shown and then let us write down the mass balance equations.

So, which is the rate of change of concentration of A is equal to the term which indicates the amount of A entering to the reactor FCA0, the term representing the A leaving the CSTR and then the reaction term. Similarly equation you write also for species B concentration, so you can rearrange this equation assuming constant volume, the volume can be taken out from the integral and you can divide both the differential equation throughout by volume v.

So these allow me to introduce the definition of the space time tau and now I can write these two equations. Now, I apply this for steady state, so I draw the dCA dt and dCB dt and obtain the two algebraic equations for CSTR at steady state. So this two equations will tell me for a given value of space time tau what will be the concentration of A and concentration of B given the feed concentration CA0, CB0. I have pure feed so CA0 = 1 and CB 0 = 0.

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Attainable Region for only CSTR: CSTR Locus

Upon specification of a feed point (C_{A0}, C_{B0}) and CSTR residence time τ, a CSTR effluent concentration C = [C_A, C_B] can be obtained. Specification of a different feed point or τ results in a different value for C.

PFR operates over a range of achievable concentrations, but the CSTR operates at distinct concentrations for a fixed feed point and τ.

Specify a range of CSTR residence times for a common feed concentration and solve for the corresponding CSTR effluent concentrations C. When a collection of such CSTR solutions for a fixed feed is plotted in phase plane, each point on the profile indicates a physically different CSTR scenario corresponding to a unique residence time. The collection of CSTR points for a range of residence times is referred to as a *CSTR locus*.

So upon specification of a feed point CA0, CB0 in this particular case 1, 0 and CSTR residence time tau, a CSTR effluent concentration can be obtained. CSTR effluent concentration will be indicated by the concentration vector CA, CB specification of a different feed point or different space time will result in a different value of the concentration vector C.

Note that the concentration vector is a vector with two components CA and CB. Plug flow reactor operates over a range of achievable concentrations, but the CSTR operates at distinct concentrations for a fixed feed point and tau, so there is a difference between the plug flow reactor trajectories and the CSTR trajectories. The CSTR operates at distinct concentrations for a given feed point and tau.

So specify a range of CSTR residence times for a common feed concentrations and solve for the corresponding CSTR effluent concentration C. Recall how we obtain the PFR trajectory, we just solve the differential equations, two differential equations representing the PFR, the independent variable for this differential equation was tau. Now to obtain the similar trajectory for CSTR, we specify a range of CSTR tau for a given feed concentrations and solve the two equations algebraic equations to find out CA, CB which represents a CSTR effluent concentration.

So when a collection of such CSTR solutions for a fixed weight is plotted in a phase plane CA, CB each point on the profile indicates of physically different CSTR scenario corresponding to a unique resistance time tau. The collection of CSTR points for a range of residence times is referred to as CSTR locus, so the collection of these CSTR points for a range of residence times tau will be known as CSTR locus.

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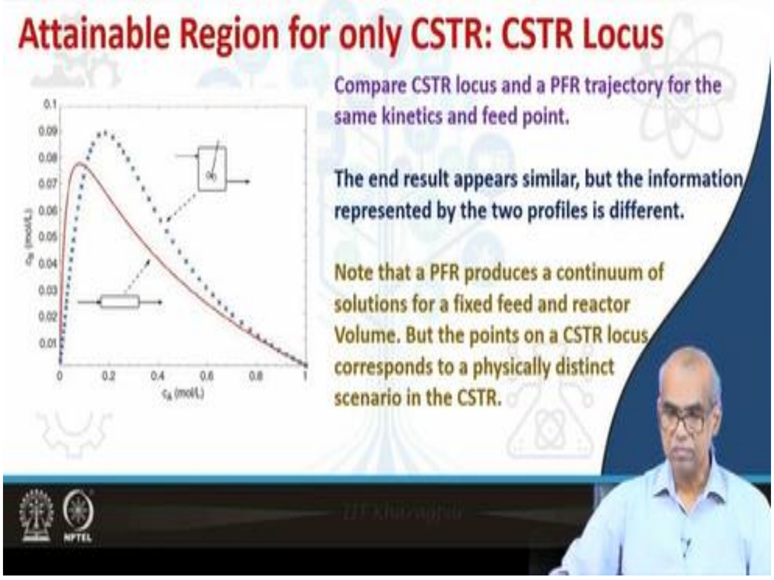

Attainable Region for only CSTR: CSTR Locus

Compare CSTR locus and a PFR trajectory for the same kinetics and feed point.

The end result appears similar, but the information represented by the two profiles is different.

Note that a PFR produces a continuum of solutions for a fixed feed and reactor Volume. But the points on a CSTR locus corresponds to a physically distinct scenario in the CSTR.

So this is the figure which shows you the PFR trajectory as well as the CSTR locus, so they obtain for the same reactions van de Vusse reaction scheme same kinetics and also the same peak point 1, 0; CA equal to 1, CB = 0, the end result appears similar but the information represented by the two profiles is quite different. What is the difference? The PFR produces a continuum of solutions for a fixed speed and reactor volume but the points on a CSTR locus corresponds to a physically distinct scenario in the CSTR.

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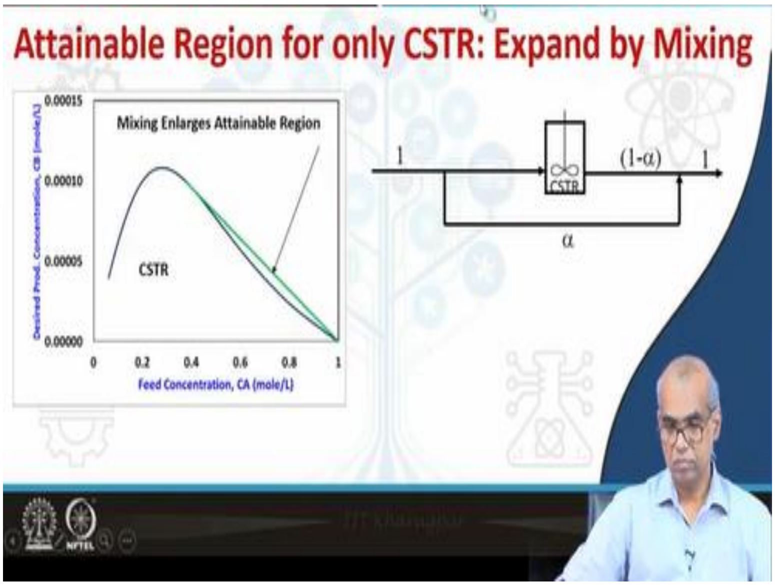

Attainable Region for only CSTR: Expand by Mixing

So, to obtain the CSTR locus, we solve these two CSTR steady state equations for range of values of tau and where plot CA, CB values on the concentration space CA versus CB and we approximate this feasible region. So, this is the candidate region for attainable region for only CSTR. So again we have to check whether this region can be enlarged upon mixing or not, so is their presences of non-convex region, yes it is.

So there is non-convex regions and mixing can enlarge that enable region, so we join the feed point we say this point with this state line are and this clearly indicates that mixing enlarges the attainable region, again the mixing fraction alpha can be obtained using simple mass balance equations lever arm rules.

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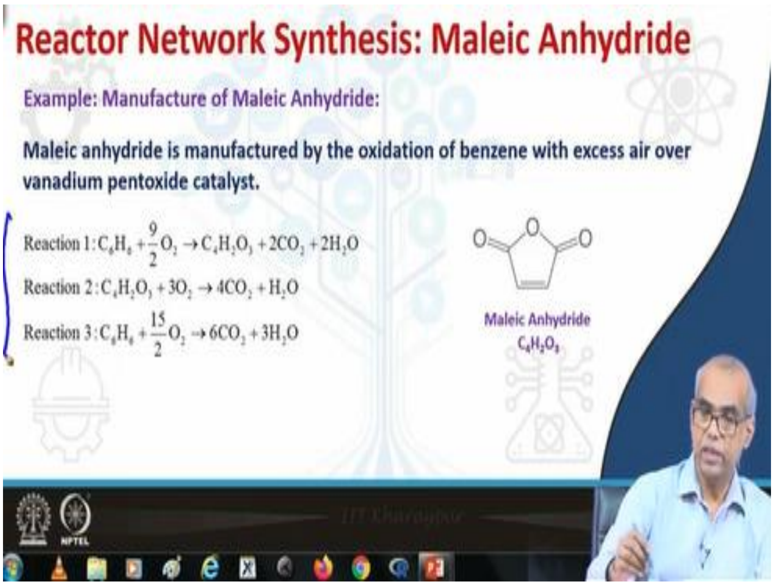

Reactor Network Synthesis: Maleic Anhydride

Example: Manufacture of Maleic Anhydride:

Maleic anhydride is manufactured by the oxidation of benzene with excess air over vanadium pentoxide catalyst.

Reaction 1: $C_6H_6 + \frac{9}{2}O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O$

Reaction 2: $C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$

Reaction 3: $C_6H_6 + \frac{15}{2}O_2 \rightarrow 6CO_2 + 3H_2O$

Now, we will consider the reactor network synthesis for manufacture of Maleic Anhydride. Maleic Anhydride is manufactured by the oxidation of benzene with excess air over vanadium pentoxide catalyst. The reaction scheme is shown here as a collection of three reactions; in reaction one benzene reacts with oxygen to produce Maleic Anhydride, carbon dioxide and H2O.

Reaction two; Maleic Anhydride reacts with oxygen to give CO2 and H2O, reaction three; benzene react with oxygen to produce carbon dioxide and H2O.

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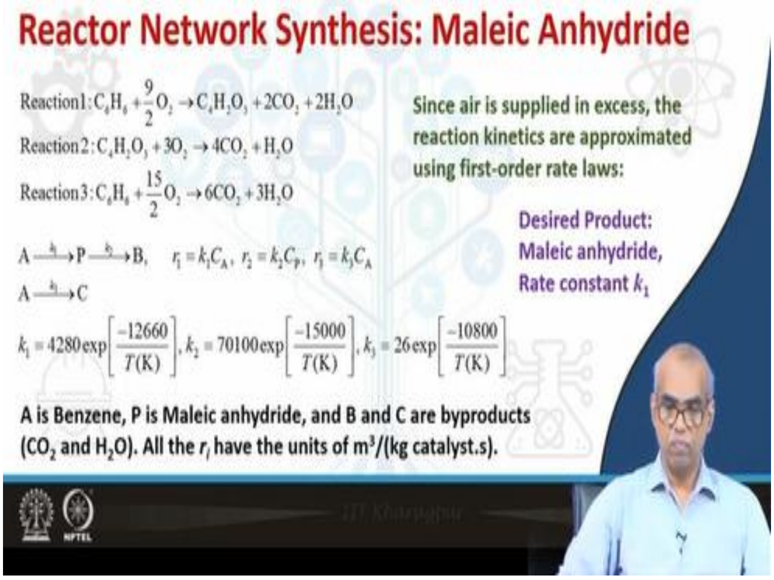

Reactor Network Synthesis: Maleic Anhydride

$$\text{Reaction1}: C_6H_6 + \frac{9}{2}O_2 \rightarrow C_4H_2O_3 + 2CO_2 + 2H_2O$$

$$\text{Reaction2}: C_4H_2O_3 + 3O_2 \rightarrow 4CO_2 + H_2O$$

$$\text{Reaction3}: C_6H_6 + \frac{15}{2}O_2 \rightarrow 6CO_2 + 3H_2O$$

Since air is supplied in excess, the reaction kinetics are approximated using first-order rate laws:

$$A \xrightarrow{k_1} P \xrightarrow{k_2} B, \quad r_1 = k_1 C_A,\ r_2 = k_2 C_P,\ r_3 = k_3 C_A$$

$$A \xrightarrow{k_3} C$$

$$k_1 = 4280 \exp\left[\frac{-12660}{T(\text{K})}\right],\ k_2 = 70100 \exp\left[\frac{-15000}{T(\text{K})}\right],\ k_3 = 26 \exp\left[\frac{-10800}{T(\text{K})}\right]$$

Desired Product:
Maleic anhydride,
Rate constant k_1

A is Benzene, P is Maleic anhydride, and B and C are byproducts (CO_2 and H_2O). All the r_i have the units of $m^3/(\text{kg catalyst.s})$.

Now air is supplied in excess, so this reaction scheme can be approximated using first order rate laws. So this reaction scheme as shown in reaction 1, reaction 2 and reaction 3 can be represented approximately by first order rate laws. A to P to B and A to C, the rate expressions are given r1 = k1 into CA, r2 = k2 into CP and r3 = k3 into CA. The rate constants are given as a function of temperature my desired product is maleic anhydride.

A represents benzene, the reactant P is Maleic anhydride and B and C are by-products CO2 and H2O. Note that oxygen is present in excess all the rates have the units of meter cube per kg catalyst second. So desired product maleic anhydride the corresponding rate constant is k 1.

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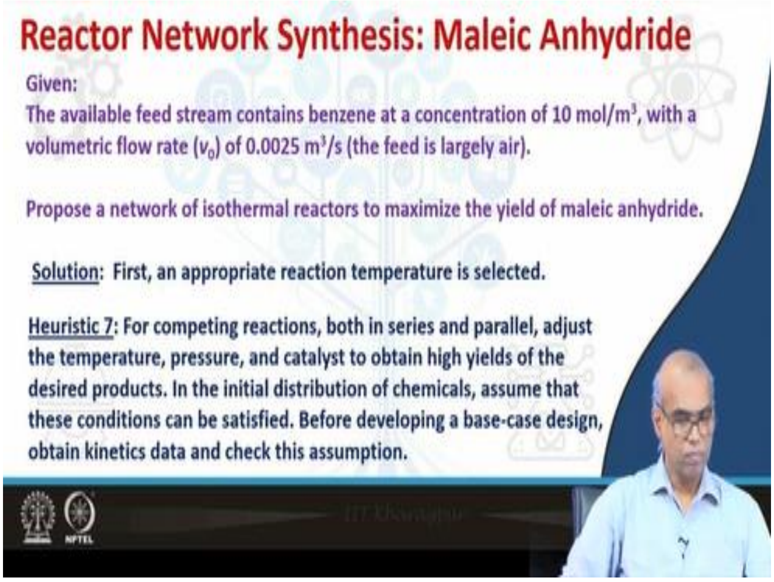

Reactor Network Synthesis: Maleic Anhydride

Given:

The available feed stream contains benzene at a concentration of 10 mol/m^3, with a volumetric flow rate (v_0) of 0.0025 m^3/s (the feed is largely air).

Propose a network of isothermal reactors to maximize the yield of maleic anhydride.

Solution: First, an appropriate reaction temperature is selected.

Heuristic 7: For competing reactions, both in series and parallel, adjust the temperature, pressure, and catalyst to obtain high yields of the desired products. In the initial distribution of chemicals, assume that these conditions can be satisfied. Before developing a base-case design, obtain kinetics data and check this assumption.

So the definition of the problem is as follows; given the available feed stream containing benzene at concentration of 10 mole per meter cube with the volumetric flow rate of 0.0025 meter cube per second propose reactor network of isothermal reactors to maximize the yield of maleic anhydride, you can note that feed is largely air. So to solve this first we need to fix an appropriate reaction temperature.

We make use of one heuristic that we talked about in our old very early lectures for competing reactions both in series and parallel adjust the temperature pressure and catalyst to obtain high yields of the desired product. In the initial distribution of chemicals, assume that these conditions can be satisfied. Before developing a base case design obtain kinetics data and check this assumption.

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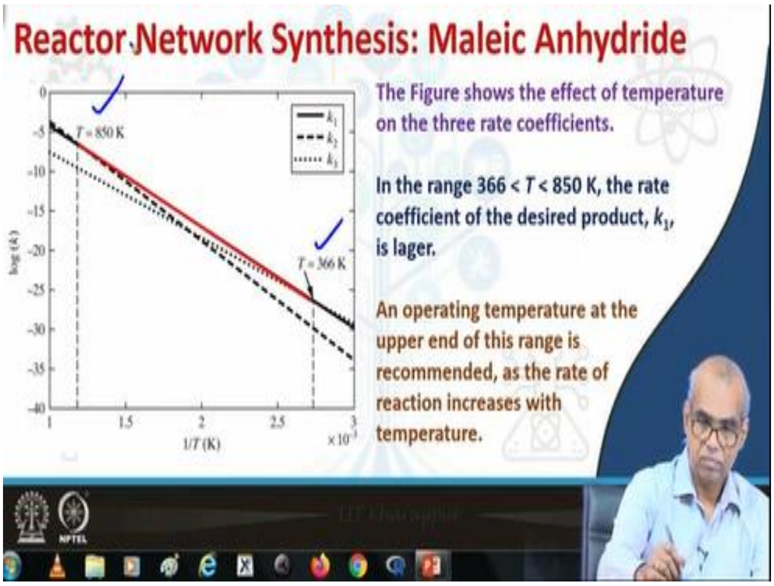

Reactor Network Synthesis: Maleic Anhydride

The Figure shows the effect of temperature on the three rate coefficients.

In the range 366 < T < 850 K, the rate coefficient of the desired product, k_1, is lager.

An operating temperature at the upper end of this range is recommended, as the rate of reaction increases with temperature.

So for various values of temperature I plot, how the rate constants k1, k2, k3 vary? We are interested in the desired product maleic anhydride and the corresponding rate constant k1, the plot is 1 by t in kelvin versus log of rate constants, k1, k2, k3. So, we see that in the range of 366 kelvin to 850 kelvin the rate coefficient of the desired product, k 1 is larger compared to other rate constants, k 2 and k 3.

So an operating temperature at the upper end of this range is recommended, as the rate of reaction increases with increasing temperature.

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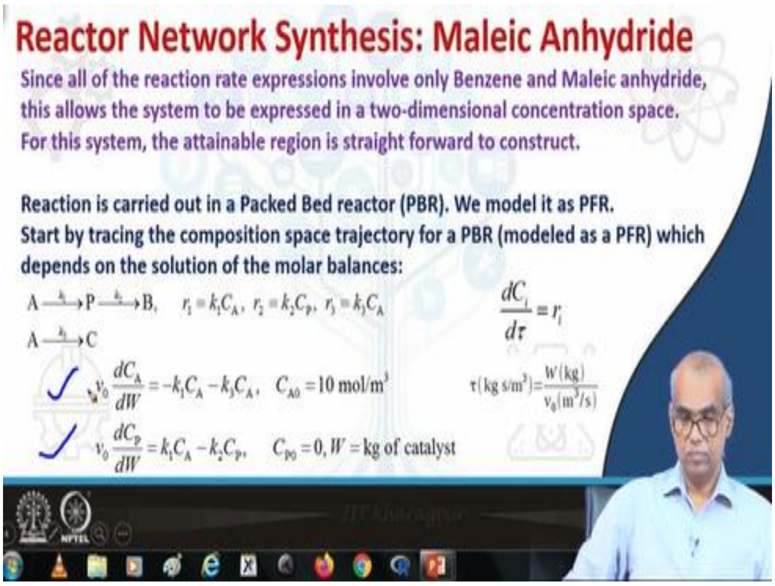

Reactor Network Synthesis: Maleic Anhydride

Since all of the reaction rate expressions involve only Benzene and Maleic anhydride, this allows the system to be expressed in a two-dimensional concentration space. For this system, the attainable region is straight forward to construct.

Reaction is carried out in a Packed Bed reactor (PBR). We model it as PFR.
Start by tracing the composition space trajectory for a PBR (modeled as a PFR) which depends on the solution of the molar balances:

$A \xrightarrow{k_1} P \xrightarrow{k_2} B, \quad r_1 = k_1 C_A, \ r_2 = k_2 C_P, \ r_3 = k_3 C_A$

$A \xrightarrow{k_3} C$

$$\frac{dC_i}{d\tau} = r_i$$

✓ $v_0 \frac{dC_A}{dW} = -k_1 C_A - k_3 C_A, \quad C_{A0} = 10 \text{ mol/m}^3$

$$\tau(\text{kg s/m}^3) = \frac{W(\text{kg})}{v_0(\text{m}^3/\text{s})}$$

✓ $v_0 \frac{dC_P}{dW} = k_1 C_A - k_2 C_P, \quad C_{P0} = 0, W = \text{kg of catalyst}$

Now, you look at the reaction scheme all of the rate all of the reaction rate expressions involve only benzene and maleic anhydride, CA and CP. So this allows us to represent the system on a two-dimensional concentration space of CA versus CP concentration of benzene versus concentration of maleic anhydride. Reaction is carried out in a packed bed reactor and we have catalyst will model it as plug flow reactor.

So, we start by pressing the composition space trajectory for a packed bed reactor, which is modelled here as plug flow reactor which depends on the solutions of the molar balances. So we have to write down the differential equations representing the pack bed reactor, which is being modelled here as plug flow reactor. We discuss that dCi data equal to ri, is obtained for plug flow reactor this is catalyzed reactor. So the space time tau we can write as W by V0.

So then note that this can be written as V0 into dCi dW. So, let us write those differential equations for CA and CP, so basically, we are writing V0 d CA, dW = r A and V0 d CP, dW

= rP. So, to obtain the PFR trajectories we just have to solve these 2 differential equations with initial conditions for CA and CP.

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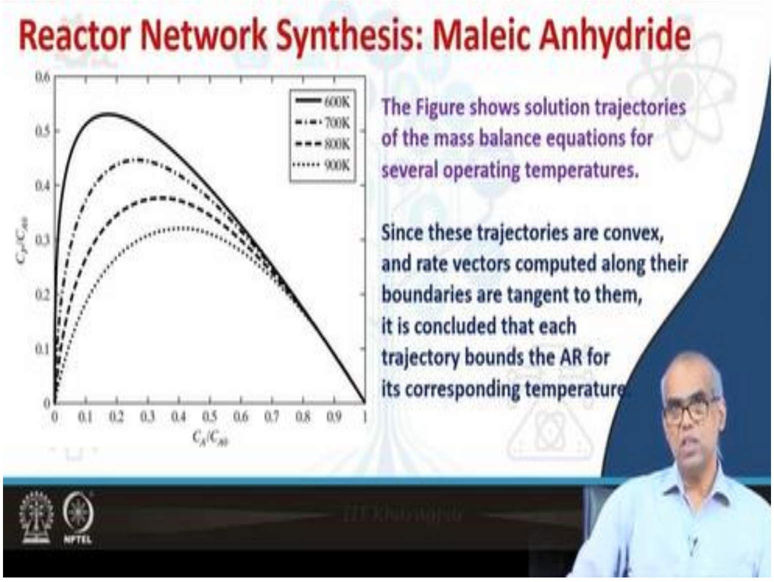

Reactor Network Synthesis: Maleic Anhydride

The Figure shows solution trajectories of the mass balance equations for several operating temperatures.

Since these trajectories are convex, and rate vectors computed along their boundaries are tangent to them, it is concluded that each trajectory bounds the AR for its corresponding temperature

Now you obtain the trajectories by solving the mass balance equations for various operating temperatures. For example, 600, 700, 800, and 900 these trajectories are convex and the rate vectors computed along their boundaries are tangent to them. So, we can conclude that each trajectory bounds the attainable region for its corresponding temperature, so we have obtained our attainable region these cannot be further expanded.

So we have obtained for individual temperatures the attainable region for the pack bed reactor which is being modelled here as plug flow reactor.

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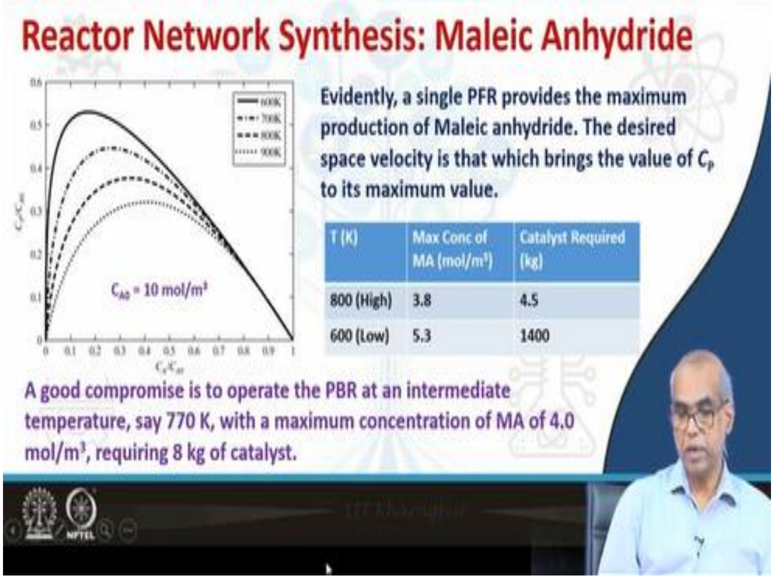

Reactor Network Synthesis: Maleic Anhydride

Evidently, a single PFR provides the maximum production of Maleic anhydride. The desired space velocity is that which brings the value of C_P to its maximum value.

T (K)	Max Conc of MA (mol/m³)	Catalyst Required (kg)
800 (High)	3.8	4.5
600 (Low)	5.3	1400

A good compromise is to operate the PBR at an intermediate temperature, say 770 K, with a maximum concentration of MA of 4.0 mol/m³, requiring 8 kg of catalyst.

So a single plug flow reactor provides the maximum production of maleic anhydride here, so what will be the desired space velocity the desired space velocity is that which brings the value of CP to its maximum value. So you have to obtain tau corresponding to these maximum values of CP. Now, let us look at the two trajectories corresponding to 800 degree Kelvin and 600 degree Kelvin.

For 800 degree Kelvin the maximum concentration of maleic anhydride is 3.8 molar meter cube and catalyst required is 4.5 kg, whereas at 600 degree kelvin the maximum concentration of maleic anhydride is 5.3 mole per meter cube, but catalyst required is very high 1400 kg. So with increase in temperature the catalyst required is less but the maximum concentration of maleic anhydride decreases.

So a compromise is required and a good compromise is to operate the packed bed reactor then intermediate temperature, let say 770 degree kelvin which will correspond to a maximum concentration of maleic anhydride of 4 mole per meter cube and this will required 8 kg of catalyst.

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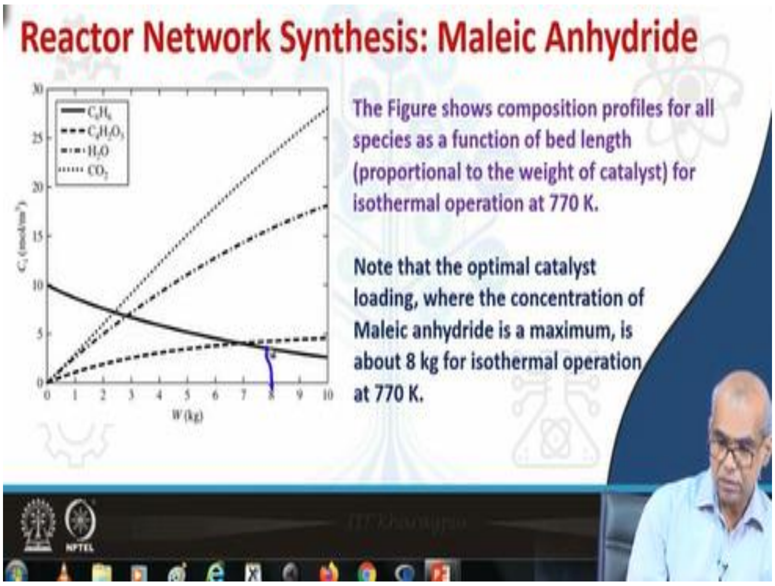

Reactor Network Synthesis: Maleic Anhydride

The Figure shows composition profiles for all species as a function of bed length (proportional to the weight of catalyst) for isothermal operation at 770 K.

Note that the optimal catalyst loading, where the concentration of Maleic anhydride is a maximum, is about 8 kg for isothermal operation at 770 K.

This figure shows composition profiles for all species as a function of weight or catalyst, which is also basically proportional to the bed length and these figure corresponds to the temperature 770 kelvin which we considered as a paste compromise temperature. Now, you can note that the optimum catalyst loading where the concentration of maleic anhydride is maximum is about 800 sorry is about 8 kg for this isothermal operation at 770 kelvin.

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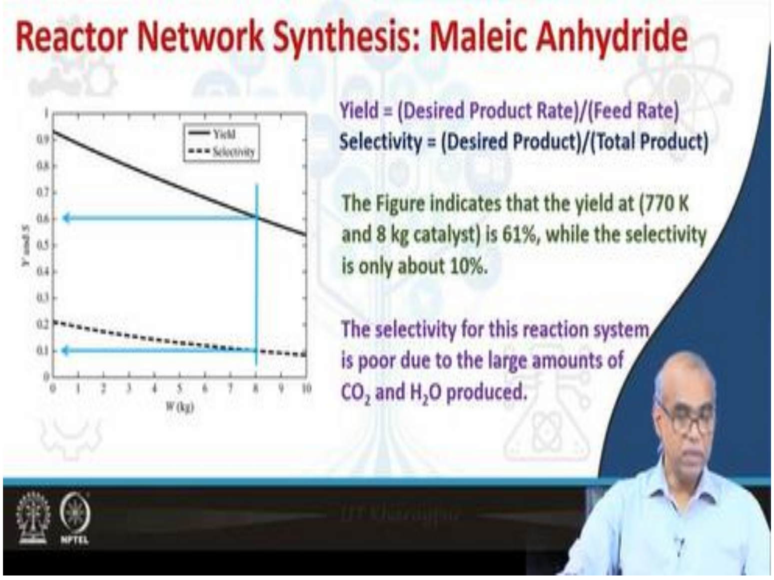
Reactor Network Synthesis: Maleic Anhydride

Yield = (Desired Product Rate)/(Feed Rate)
Selectivity = (Desired Product)/(Total Product)

The Figure indicates that the yield at (770 K and 8 kg catalyst) is 61%, while the selectivity is only about 10%.

The selectivity for this reaction system is poor due to the large amounts of CO_2 and H_2O produced.

Finally, we make a plot here of yield versus yield and selectivity versus weight of catalyst. Yield is defined as desired product rate divided by feed rate, whereas selectivity is defined as desired product divided by total product. Look at the figure the yield at 770 Kelvin and 8 kg catalyst that is the condition that you have chosen is 61% while the selectivity is only 10% why the selectivity is so low here.

The selectivity is so low, because the production of the large amount of bi- product CO2 and H2O. So, here we learn how to obtain that attainable region for a simple example of production of manufacturing production of a maleic anhydride, it was possible to obtain that attainable region with a single plug flow reactor. In the next class, we will look at a more involved example where the attainable region will be obtained by combinations of plug flow reactors CSTR and mixing of steps; with this we stop our discussion here.