Module - 3
Reactor Design and Cost Estimation
Lecture - 13
Algorithm and Basic Principles of Reactor Design

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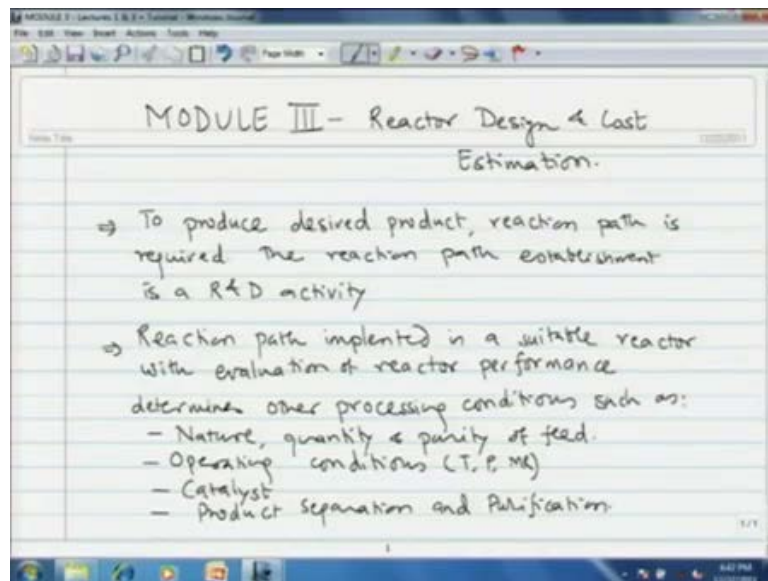
Welcome, we have completed the first two modules of our course. Now, we start the third module of our course, that is the reactor design and cost estimation. As I mentioned in the previous module to produce a desired product first we need reaction path or a process. There could be many reaction paths leading to the same product. However, the most suitable reaction path is determined by several other conditions as the availability of the raw material and a cost of raw material, sustainability parameters, profitability parameters so on and so forth. But let us say that the particular desired product is a patented product and then the reaction path establishment for that particular product is an R and D activity of that particular company.

Once, the reaction path is established the reaction path is implemented in a suitable reactor with evaluation of reactor performance. Reactions initially are carried out in laboratory on smaller scale may be in a round bottom flask or similar type of small reactors. And then depending on the success levels and the performance of the process

on that scale, larger scale equipment are designed such as the bench scale, then pilot scale and finally, the commercial scale.

At each stage we have to evaluate the performance of the reactor and that particular evaluation determines several other processing conditions such as the nature quantity and purity of the feed streams. Then second the most optimum operating conditions. Now, these could be temperature, pressure or molar ratio of the reactants. Then if it is catalytic process then the most suitable catalyst for that particular process and next the product separation and purification which essentially is the basis of design of the separation system as we have seen in the flow sheet synthesis algorithm in the previous module.

First the reactor type to be evaluated must be established and then the reaction mixture or the catalyst volume is determined by solving appropriate design equations using kinetic and thermo dynamic data. Initially kinetic data may not be available because when a chemist does experiments on small scale he or she may not be able to give you the exact kinetic expression, but what is usually available is the product distribution as a function of conversion and also the conditions that give the maximum yield of a particular product. So, based on this we have to start the reactor design. So, the reactor design procedure can be shown in an algorithmic chart.

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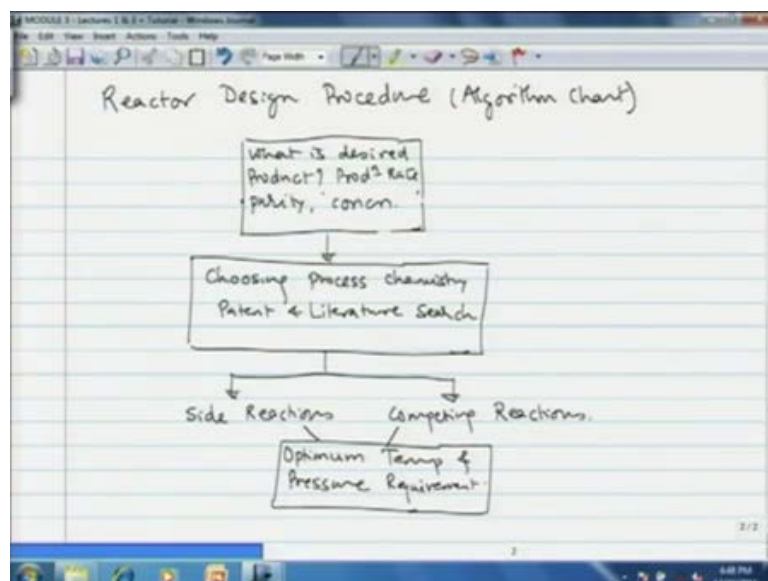
So, that we see now, reactor design procedure, algorithm chart. First we have to decide as what is the desired product? Then what is the production rate? What is the purity level or in some cases what is the concentration of that particular product? Once, we close down on this then we have to choose a particular reaction for the process, choosing process chemistry.

For that purpose we may have to do some patent and literature search, so as to find out as what are the processes that are available to produce this particular product. Then we have to account for the side reactions and competing reactions of that particular process. Now, having scanned this then we have to choose the optimum pressure and temperature of operation.

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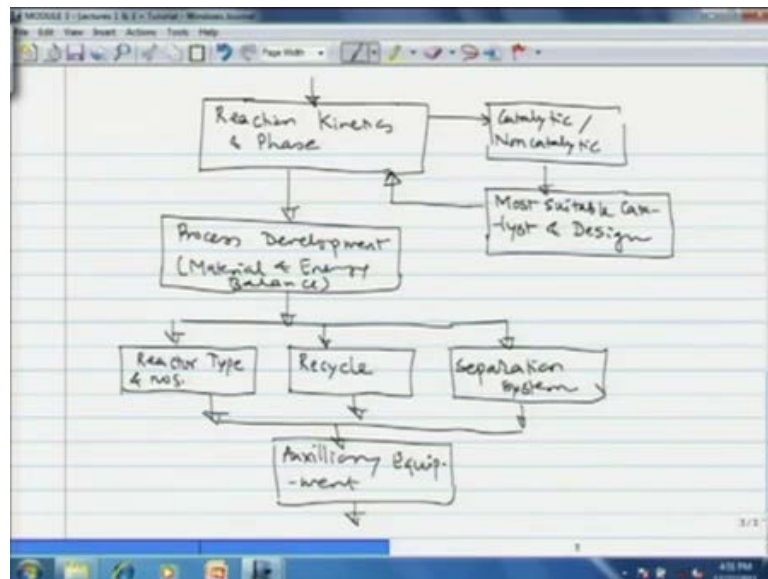
Next is we have to determine the reaction kinetics and the phase of the reaction whether it is vapor phase reaction or it is a liquid phase reaction or it is a mixed phase like gas liquid reaction or gas liquid solid reaction so on and so forth. Now, another activity here would be to see whether the reaction is catalytic or non catalytic and then what is the most suitable catalyst and a design of the catalyst. So, these are let us say, the sub components of this particular step that is the reaction kinetics and phase.

Thereafter, we have to go for actual process development and then carry out the material and energy balance. Having done this we have to decide the reactor type and the number of reactors, then which components we have to recycle or what we termed as recycle

structure of the flow sheet in the previous module and also a typical separation system that would be required. Whether we need a series of distillation columns or we need simply a flash drum or we need liquid liquid extraction or absorption or adsorption so on and so forth.

So, that is the, those are the components of the separation system. With these three components we will be able to figure out what are the auxiliary requirements of the process or auxiliary equipment like how much hot utility we need, how much cold utility we will need, what are the temperature levels, whether only steam will do the job, steam at various pressure levels or we have to go for some advance feed transfer like some dowtherm liquid or even higher may be some molten metal's or molten salt, so on and so forth. So, that gives us an idea of the auxiliary equipment. After having done this we have to go for the economic evaluation.

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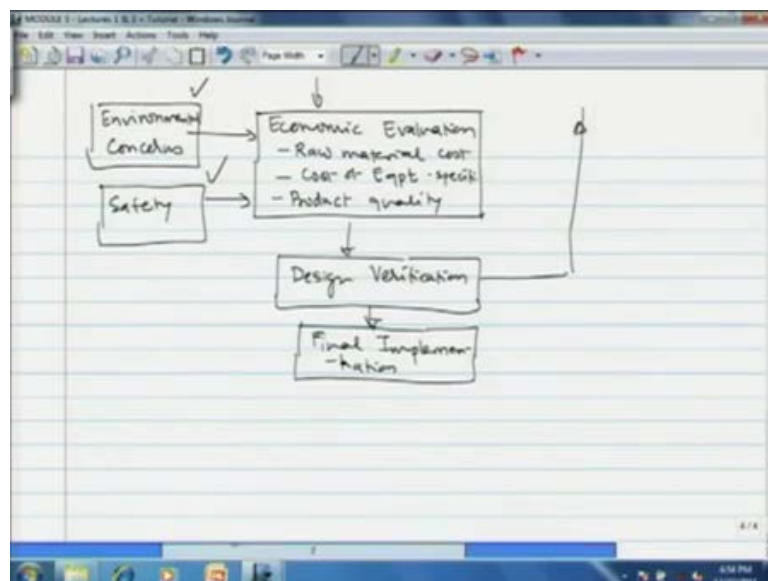
Economic evaluation will consider the cost of raw material exactly the same as we did in previous module which, where we said it was economic potential, raw material cost, then the cost of equipment, but here we have to consider only the major equipment. Cost of equipment will depend on the specification of equipment. So, that also we have to consider and then the revenue that we are likely to earn that will depend on the product quality.

Now, here we have to also consider the environmental concerns. For example, some reaction path may be very much profitable. However, if they are using hazardous and toxic chemicals we have to take that into consideration, that risk and then the safety. If the reactor operation is at excessively high temperature, excessively high pressure then even those conditions can pose potential problem for the operation. So, all these things we have to take into consideration while making economic evaluation.

Economic evaluation should not be based only on the cost, but it should also account for these other ((Refer Time: 10:46)) like sub components of that particular step. And on this basis we have to verify the design that we have arrived at. And if it is satisfactory we can go for the final implementation of the process. In case this is not satisfactory then we may go back to the step of process development which is this.

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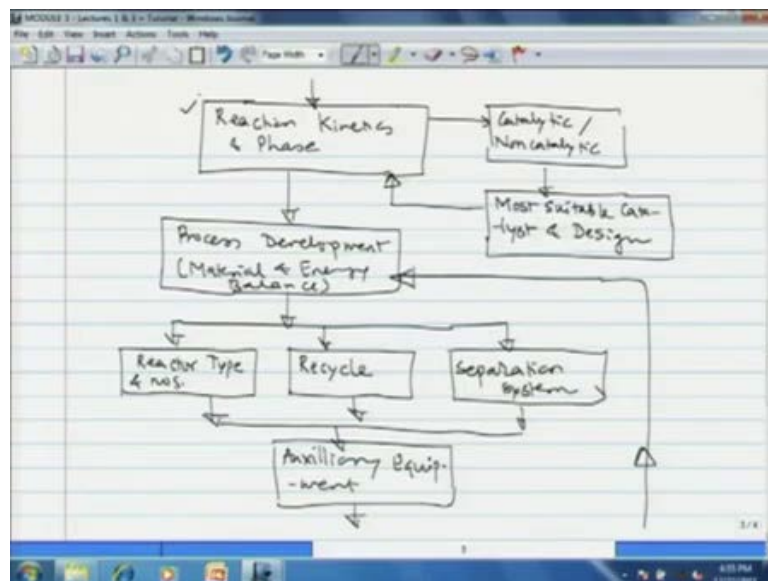
And then repeat the whole calculations again. The material energy balance, reactor type and numbers, so on and so forth. However, there is no need to change the chemistry as such. Chemistry may remain the same. So, this is how we go for the reactor design and cost estimation. So, this is the basic algorithm of it. Now, having said this we shall now see some basic reactor principles.

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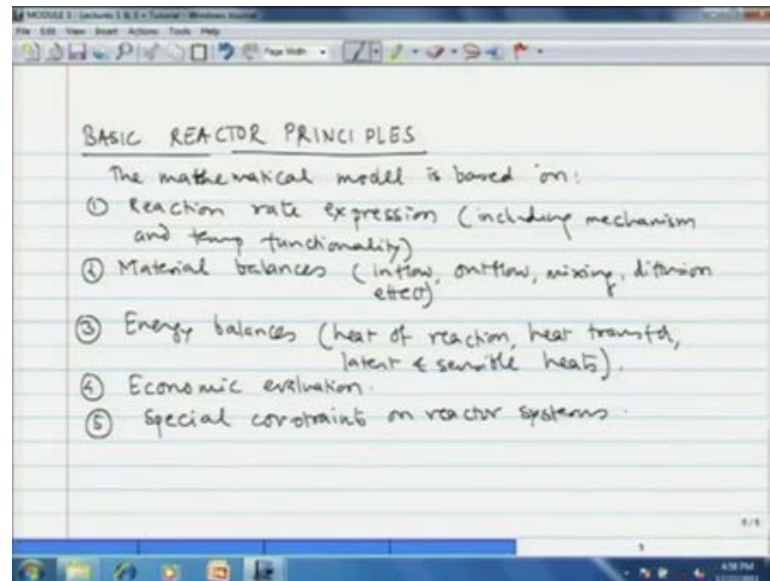
Basic mathematical model for the reactor is developed using following considerations. The mathematical model is based on first the reaction rate expressions which should include the mechanism definition and also the temperature functionality. Then second is the material balances including inflow, outflow, reaction rate, mixing effect and diffusion effect.

Basically, the transport phenomena or transport properties of that particular reactor. Then the energy balance, that should include the heat of reaction, then the heat transfer, then the latent and sensible heats of component, then the economic evaluation and finally, the special constraints on the reactor or the design system. So, this is how we should proceed for developing the mathematical model, we have to account for all these factors.

The first step for that will be the material balance. In the previous module we have seen several algorithm for material balance and then we developed material balance for several processes in terms of the design variable. The general material balance, general form of material balance would be that rate of accumulation of species, we denote it by i, species i in the volume element of reactor is equal to the rate of inward flow of that species minus the rate of outward flow plus the rate of generation or consumption. The energy balance can also be written in a similar way. The general form of energy balance would be rate of energy accumulation in volume element is equal to the rate of inward energy flow minus the rate of outward flow plus the rate of energy generation or consumption in the reactor or the volume element of the reactor.

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As far as the energy balance is concerned we can write a general expression or overall form of expression based on the conservation of species. So, the summation for all species i m i C p i into d T by d theta where d T by d theta is the rate of change of temperature is equal to summation overall species m i dot where m dot indicates the flow rate, integral of C p i d T from T i in to T i out where T i in is the inlet temperature of the species, T i out is the outlet temperature plus the rate sorry the energy that is generated or absorbed in the reaction.

Now, we are denoting it as V R into minus delta H r x n into r i. r i is the rate of reaction, minus delta H r x n is the specific heat of the reaction, heat liberated or absorbed per mole of reactant. And V R is the volume of the reactor plus if there is any external power input to the reactor then that comes into picture. This is general form of the energy balance in a particular reactor. Can we write a similar general form for mass value? Many types of reactor operate at various conditions such as batch flow, your batch or flow or homogeneous or heterogeneous.

Therefore, general expression of mass balance is quite complex. Now, we will try to develop an appropriate model that will describe a specific reaction system for the reactor type under consideration. For example, if we are considering a reactor at steady state then we have to set the time term to 0. Let us see some general forms of reactor design equations, general approach to reactor design. If the reactor is of batch type then the

volume V R can be taken as constant and let us say we have a homogeneous reaction, then the convenient form of rate expression for a particular reaction in this reactor would be minus r i is equal to 1 by V R into d N i by d theta is equal to k i into C a into C b up to C i or C n.

Now, the rate expression is 1 by V R volume into d N i by d theta; the rate of change of moles of species i with time is equal to k i which is the rate constant into the concentrations of various species in the reactor at any, at that particular time theta. In case of a batch reactor since it is mixed we can assume that C a, and C b and everything means all concentrations are same throughout the reactor. There is no concentration gradient.

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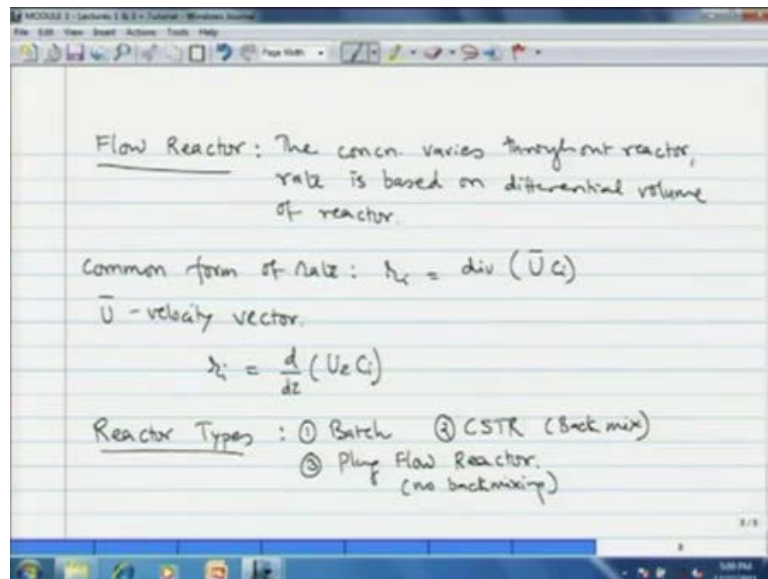
The flow reactor, in case of a flow reactor the concentration varies throughout the reactor. And the rate is based on differential volume, useful form of rate is r i is equal to divergence of velocity vector and the concentration of the species. U bar is the velocity vector. Now, if we assume that the flow is predominantly in the z direction in a plug flow reactor then we can convert the divergence into d by d z and then the same expression becomes r i is equal to d by d z into U z into C i. So, basically what we are seeing is, are some common forms of equations for the design of batch as well as flow reactor. There are mainly three reactor types.

The first is the batch reactor in which the reactants are mixed and stirred till a particular conversion is obtained. Now, that particular vessel is like a close system where there is no inflow or outflow until the reaction is completed or the desired convergence is obtained, that is called as a batch reactor. The second type of reactor is what is known as continuous stirred tank reactor, CSTR. Here the reactants are mixed in a particular vessel.

However, there is a continuous flow of reactants into the vessel and ((Refer Time: 24:46)) product from the vessel. So, CSTR is essentially a batch reactor as an open system where there is an exchange of material like reactant comes in and the product is continuously withdrawn that is, what is CSTR. It is also known as sometimes the back mix reactor and the third type of reactor is the flow reactor that is the plug flow reactor. In plug flow reactor there is no back mixing ideally. Plug flow reactors are usually developed for steady state operation and at steady state concentration as well as temperature profile does not change with time.

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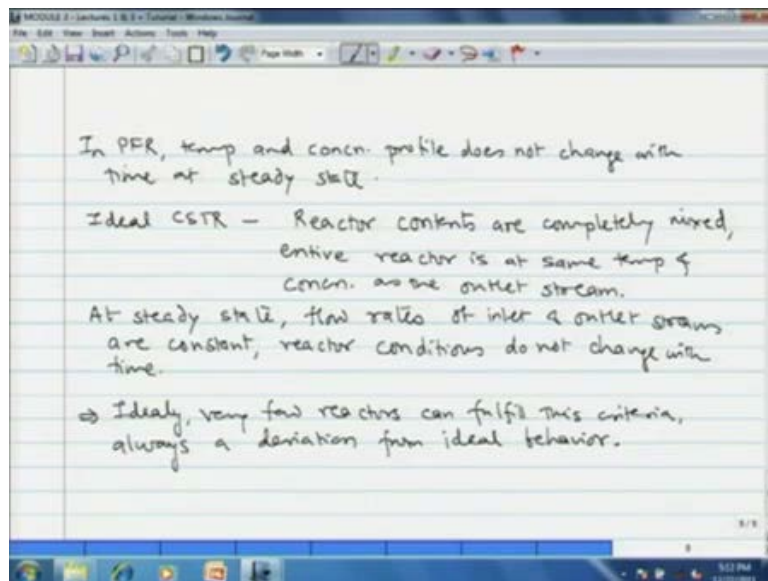
That point we note that in PFR, temperature and concentration profile does not change with time at steady state. Similarly, in an ideal CSTR the reactor contents are completely mixed and the entire reactor is at same temperature and concentration. Now, this temperature and concentration is same as the outlet stream from the reactor. Now, idealized CSTR is also designed for steady state operation. So, at steady state the flow

rate of inlet and outlet stream remain constant and reactor conditions remain unchanged with time. Now, ideally very few reactors can fulfill these criteria and there is always a deviation from ideality. Now, reactor performance can be improved by using recycling of some of the reactants and products and that we have already seen in the previous module.

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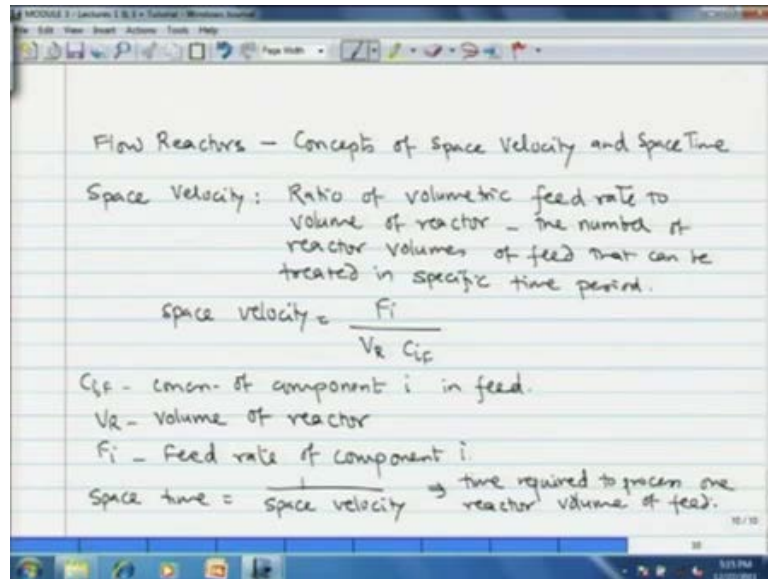
Now, as far as flow reactors are concerned whether CSTR or PFR, there are two concepts that are used for analyzing them and these are the concept of space velocity and space time. Space velocity is defined as the ratio of volumetric feed rate to the volume of the reactor or in other words the number of reactor volumes of the feed that can be treated in a specific time period. So, mathematically the space velocity is F i where the F i is the feed rate of component i divided by V R the reactor volume into C i F where C i F is the concentration of component i in feed. Now, space time is essentially the inverse of space velocity. This is the time required to process one reactor volume of the feed.

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The batch reactors, we can write a simple expression for design of batch reactors that is integral 0 to theta d theta where theta is a time of the batch is equal to integral d N i divided by V R into r i where r i is the reaction rate with respect to component i, V R is the volume of reactor and the limits for the right hand side are N i o and N i e where N i o is the number of moles of species i in feed and N i e is the same number of moles of species i at exit. Now, we can rewrite this expression in terms of conversion. The conversion X i of species i can be written as N i is equal to N i naught which are the initial moles minus N i naught into X i which can be rearranged as N i is equal to N i naught into 1 minus X i.

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And after differentiation you get minus or sorry the d N i is equal to minus N i naught into d X i. So, after substituting this for d N i in previous expression the batch time theta is N i naught integral d X i divided by minus V R into r i where conversion goes from 0 to X i e where X i is the conversion at the exit of the reactor. If the reactor volume is constant which is the case most of the time then we can rearrange the above equation to get the volume of the reactor for a particular batch time to achieve a certain conversion.

I am simply rewriting the same expression in another form. So, these are the some simple design expressions for the reactor. We can develop a similar expression for tubular reactor. Here we assume that the predominant flow is in z direction and there is steady state operation. Then we can rearrange the equation that we wrote earlier for the this thing, for the tubular reactor integral d z from 0 to z is equal to integral U z C i at reactor inlet and U z C i at reactor exit into d U z C i divided by r i. I have simply changed the variables or the separation of variables. So, it is what I have done.
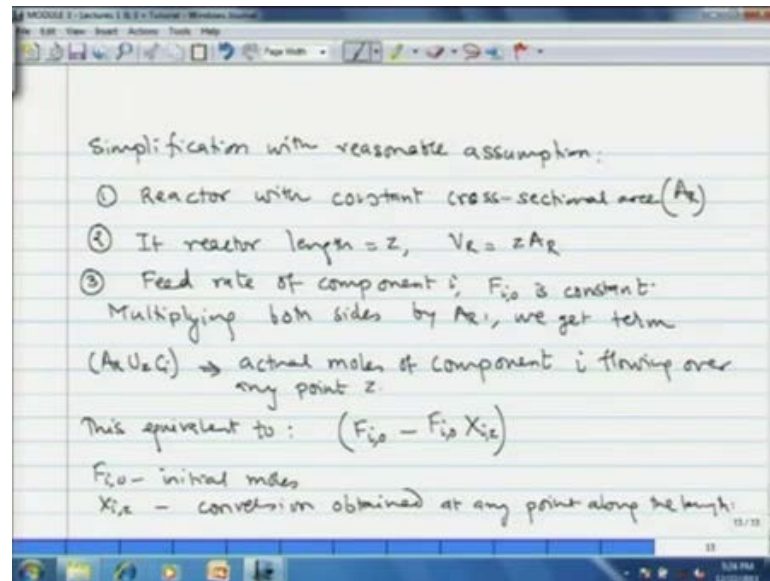
Now, this expression can be simplified with several assumptions which are reasonable. The first assumption that we make is that the reactor has constant cross sectional area that we denote by A R. Then next is if the total length of the reactor is z then we can calculate V R directly. V R is equal to z into A R. We can also assume that the feed rate of component i that is F i naught is constant. Now, with this assumption if you multiply both sides of the equation by A R we get the term A R into U z into C i which is nothing but the actual moles of component i flowing over any point z.

Now, this is equivalent to the number of moles flowing over any point z are equivalent to the number of moles that enter minus the number of moles that react till point z. And this is what we note by this F i naught minus F i naught into X i z. F i naught are the initial moles of species i and X i z is the conversion obtained at any point along the length of the reactor.

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Now, if you differentiate this we get an expression in terms of conversion of the component which we can use in place of the concentration in the previous expression. So, that we do now. 0 to z A R d z A R that is what we have done, multiplied throughout by A R equal to integral 0 to V R d V R is equal to V R is equal to F i naught integral 0 to X i z into d X i z by r i. Now, this is simple expression that applies for any reaction provided a rate expression available carried out in an idealized tubular plug flow reactor.

That point we note here. Many reactions are heterogeneous; these are carried out over a catalyst. For such reactions where the reaction is occurring on the surface of a catalyst the reaction rate is based on the mass of catalyst rather than the volume of the reactor. So, that point we treat now, heterogeneous or in other words catalytic reactions. The reaction rate is based on mass of catalyst rather than the volume of reactor because reaction occurs essentially over the surface of catalyst. Now, here we substitute r i by r i c where c is for the catalyst. And the above expression gets transformed into a simple form.

W c divided by F i naught equal to integral 0 to X i z d X i z divided by minus r i c where r i c, this important r i c is the rate of reaction expressed as moles of component i converted per unit time per unit weight of or mass of catalyst. Let us see a similar expression for back mix or CSTR type of reactor. Now, here the general steady state operation is characterized by this expression the rate of accumulation of species i in the volume element is equal to the inflow rate minus the outflow rate plus the rate of generation of the species. We substitute all variables.

F i naught again is the flow rate of component i at the inlet. Now, the outward flow rate of species i would be the unconverted component of F i, F i naught into 1 minus X i e where X i e is the conversion obtained till exit plus the fraction that reacts. So, this is the inflow minus outflow plus the reaction. Now, if you rearrange this particular equation you get a simple design equation for CSTR which you have seen in the course of reaction engineering as V R by F i naught is equal to X i e divided by r i.

We have designed or we have derived general rate expressions for the three types of reactors. Now, as I said that in reality the performance of reactor deviates from ideality. Now, what are the major causes of this non ideal behavior? The first cause is the imperfect distribution of material and energy within reactor, due to transport limitation, due to limited mass and energy transport. If there is a imperfect transport then there is reduced reaction rate, increase in the undesired reaction and many cases fowling of the reactor, kinetic variation due to the temperature variation if temperature is not uniform at you know throughout the reactor.

Then in some cases the kinetic fluctuations could be disastrous for exothermic or autocatalytic reaction. In some cases temperature variation can lead to occurrence of un-forcing reaction that could be harmful or dangerous or it can cause loss of the valuable reactant. Mass and energy transport limitation on the molecular level cannot be easily removed like for example, if we characterize the mass and energy transport limitation of a particular reactor.

These are either on the molecular level or in the microscopic level like for example, in a CSTR if the rate of stirring is not high then there is concentration gradient in the reactor. There is temperature gradient in the reactor which could cause all side effects as we just mentioned. Now, this is an imperfection over a microscopic level which can be cured by making better designs of the mixers giving for, going for higher mixing rates or you can provide adequate heating or cooling, so that temperature gradients are killed.

So, these microscopic level imperfections can be controlled to large extent using modifications in the design. However, molecular level transport issues like for example, adsorption of a reactant species over the catalyst surface. This is an example of molecular level transport limitation. Now, these issues cannot be rectified by simple

changes in improvement in mechanical design of the reactor because these occur on very small scale.

These type of transport issues can be spared by better design of a particular catalyst or particular adsorbent. These issues are mainly encountered in case of fluid solid or liquid liquid invisible systems and these need to handled on that scale like for example, if you have a catalyst, catalytic limitation like the surface of the catalyst is small then we have to go for suitable support that we are going to deal in the next lecture. We can go for a porous support catalyst where the surface area is enhanced.

So, those issues are handled on another level. Simple changes in the mechanical design of the reactor, is not a solution for these issues. So, this concludes our discussion for in this lecture. In the next lecture we shall see topics of residence time distribution, the type of chemical reaction and then non ideal reactor immolation like the non ideality in the reactor can be immolated by simple analysis of stacking of ideal reactors in which the flow limitations are taken into consideration. So, these things we shall see in the next lecture.