Inorganic Chemical Technology Prof. Nanda Kishore Department of Chemical Engineering Indian Institute of Technology, Guwahati

Lecture - 04 General Principles and Chemical Plant Design

Welcome to the MOOCs course Inorganic Chemical Technology, the title of today's lecture is General Principles and Chemical Plant Design. Before going into the details of today's lecture what we will do, we will have a kind of recapitulation what we have seen in last couple of lectures.

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We have seen a few statistics about Indian chemical industries. Then we have seen pictures different pictures like raw materials picture, energy picture and then transportation picture for India especially with respect to the chemical plants those things we have seen. Then what we have seen, how to group different sections of a chemical plant as a combination of different unit operations and then unit processes.

So, that is unit processes are nothing but the chemical reactions that are occurring in chemical plants and then unit operations are nothing but the all those operations where other than chemical only physical and or mechanical changes are occurring right. So, we have seen a few basics introductions about unit processes and in some applications etcetera where they occur those things we have seen.

Then we have also seen some commonly occurring unit operations and then what are their basic principle working principle etcetera, applications etcetera those things we have seen. Then we have seen a few general principles of chemical engineering that are applied in chemical industry those things are also we have seen under which category what we have seen a few things about the chemistry.

How they are related to the chemical plants, thermodynamics how it is related to the chemical plants and then chemical equilibrium what is chemical equilibrium, how it is related to the chemical plant those things we have seen.

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However, we again start with the general principles of chemical engineering that are essential from the industry point of view. We know that the chemical industry is very vast and then so many different types of industries are included it is not only petroleum industry, polymer industry, but also food industry, textile industry, metallurgical industry and then ceramic industries etcetera and then hydrocarbon industries so many different types of industries are there. So, all of them you know are a part of chemical engineering.

And then surprisingly you are going to see some details production details of majority of the components of these industries in this course as well as the other course inorganic chemical technology right. In this course we will be discussing about the production of a inorganic chemicals only. So, what we see that you know so many different types of industries in one particular discipline. Then; obviously, it is expected that so many courses should be there and then one has to remembering all those courses are presenting in one particular lecture or one course is not possible right. So, what we can see, we can see a few basics which are much relevant with respect to the current course content of inorganic chemical technology ok. Large number of principles of science and engineering are being used in any chemical industry and; obviously, discussing all such principles is out of scope.

So, but many complicated interrelated aspects that are essential to any chemical in industries would be there, what are they that is what we are going to see. First of all any industry the market and sales is very much essential. So, the market and sales provides justification for the industry installation or renovation or you know enhancement, whatever you wanted to do for any industry you know market and sales are very much essential right.

If there is no market so, whatever efficiently you do plant design, installation of industry etcetera it is of no use ok. Then methods of production, so many issues may be associated with the methods of production like chemical reactions, what are the chemical reactions, endothermic reaction, exothermic reaction, catalytic reaction, non catalytic reaction, heterogeneous, homogeneous reaction, you know molecular reactions, initiated reactions etcetera those many different types of reactions are there.

So, you know having so much knowledge about the chemistry is also required ok. Then process flow diagram process flow diagram in the sense it is nothing but sequential presentation description of process what is happening in a chemical plant in order to get a certain product from a given individual raw material or set of raw materials.

So, that sequential operations whatever happening in chemical plant that we present in a flow diagram process, in a process flow diagram manner and the those things are known as the flow sheets, different types of flow sheets etcetera are there, those things also we are going to see in today's lecture.

Then most important thing is materials requirement it is not just materials like which are involved in the reaction right. It may be a plus b giving rise to c plus d products is simple reaction, but a and b in order to get reacted there may be other materials also required like something like steam etcetera, something like you know process energy etcetera, those kind of thing many things should may be required. So, all those things are also very essential.

And then; obviously, chemical engineering problems where manufacturing and economics one has to think about. All of them are see now you can see market and sales is a very different thing, chemical engineering is very different and then manufacturing process, different process are may be there which one you want to select that is a very different thing.

And then see economics all together nowhere related to the engineering, but still you have to learn, this is the only engineering discipline that is chemical engineering discipline where not only chemical engineering aspects you may also be needed to look into the some economics details.

Plus not only economics the mechanical design part of you also you have to study a course right. So, these many things are interrelated especially with respect to the chemical engineering and chemical plants right. So, but obviously, when these many things are interrelated and complicated you cannot handle them as a set together.

So, what you can do? You can group them and then divide into certain kind of categories like let us say first I you study about unit operations, then you study about unit process, then you study about heat transfer, mass transfer individually. And then fluid mechanics, transport phenomena like this, individually you can study including the process design, you know chemical plant design, economics etcetera.

These things you individually study and then whatever the knowledge that you have you pour in while designing a plant before the installation or before you know commissioning of the plant etcetera. So, that way step by step one can go forward ok.

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So, inter relating complexities of such aspects can be reduced to problems which can be solved on basis of principles of science and engineering right. Again as long as it is related to the chemical plants or chemical industries there are so many basic principles from the science point of view as well as the engineering point of view.

So, again covering all of them even their short description is not possible or is out of this course right. So, what we do, only with respect to the production of any inorganic chemical what kind of a you know basic principle in general you may need to know before starting the course those things are only we are going to study. I am not saying that these are the only subject that you are going to study in chemical engineering discipline which are useful for installation or commissioning of any plant.

But I am saying these are the things are very essential to understand the course contents of the present subject inorganic chemical technology ok. So, what are they? Chemistry if you talk about chemical engineering there are reactions. So, then definitely you need to know what is the chemistry, how many types of chemistries are there, how they are related to the chemical plants etcetera.

Then thermodynamics because it is about the science which talks about the different forms of energy and then no plant can sustain, no chemical plant can sustain without energy. So, energy is associated involved so then you have to know the thermodynamics as well. Then reaction kinetics, it is not about the just chemistry analytical chemistry, physical chemistry, inorganic chemistry and all that, for a given plant there may be a reaction you need to know the kinetics of that reaction in detail. So, at a UG level you cannot specify that you are going to learn only this particular reaction and then associate kinetics only. So, you have to study as many as possible. So, then reaction kinetics in general are also very essential from chemical plant viewpoint.

Then process and mechanical design process design and mechanical design are two different things right, let us say we have been discussing different types of unit operations simple example of fluidized bed the combustion reactor. So, you know what we have seen we have a column in packed in fluidized bed right or even packed bed also we can take an example like any example we can take, I am taking one example of a fluidized bed.

So, here we have a column right, in this column at the bottom we have a perforated plate on this plate we have a packing material right, catalyst particles or glass beads or whatever as per the process requirement they are here right and whichever the fluid stream that has to pass through if it is a reaction there may be some gases or liquids flowing through.

If there is a heat transfer requirement then bed may be at different temperature and then entering fluid may be at different temperature those things are there so, those are different things. So, now, what should be the size of the particles, packings that you should know, what is the size of column right, what is the voidage at given flow conditions etcetera those things you should know.

What is the minimum fluidization velocity, etcetera these kind of so many aspects are there from the chemical engineering point of view all those things comes under the process design part right. Let us say if you have mass transfer operations some kind of distillation is occurring, how many stages are required, what is the energy requirement for the re boiler, what is the duty requirement for condensation section, all these things one has to do from chemical engineering point of view and these calculations are all make part of process design chemical process design.

What is mechanical design? Mechanical design let us say if you do this particular operation using these kinds of material and under these conditions. So, what you need to

have? You need to have a material of construction by which material should you construct this fluidized bed right ok. Then let us say you have to support it, what supporting material should be there, columns beams etcetera all these things comes under the so called mechanical design. So, we are going to see those things also.

So, not only from process design chemical process design point of view where heat transfer, mass transfer, fluid mechanics transport phenomena, even process control etcetera these the information the knowledge that you gain in these kind of courses mechanical unit operation etcetera these kind of courses all that knowledge that will be useful in the process designing.

But in addition to that you also need to do one or two courses on this mechanical design for example, drawing; first year engineering drawing that you are doing that is related to the mechanical design, in some universities 7th or 8th semester of UG course there is a chemical plant design course is there.

So, that is also mostly consisting of drawing. So, there you will be drawing the different types of these equipments that all come under mechanical design part so, but still you have to do under chemical engineering point view point right. So, then economics also there is a course that you have to understand minimum basics of the economics otherwise you cannot judge as a engineer whether the plant that you are going to commissioning is going to be profitable or not.

And then if there is no profit, there is no point of doing engineering, chemical engineering, you know plant installation at all ok. And then; obviously, concepts of unit operations and then unit processes are anyway most essential ok. So, out of which this part we have already seen concepts of unit operations in unit processes we have completed in our previous two to three lectures ok.

Now, what we do? We see a few basics not details I am as I am saying these are the minimum requirements that you wanted to understand the contents of this course that is going to start from the next week. This is the first week all about the introduction of the course, what are the requirements or you know minimum things that you should know before learning the true contents of the course. So, this first week is entirely dedicated for such kind of introductory things. So, these four classes this is 4th class.

So, in the 4th class we are going to see about a few basics about some other principles of science and engineering which are useful to understand the contents of this course. So, all types of chemistry are usually involved in chemical industries; obviously if reaction is there. So, then you cannot say only analytical chemistry or inorganic chemistry or organic chemistry would only be useful for your plants.

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You cannot say that when all of them are important right, what are the analytical chemistry, physical chemistry, inorganic chemistry, organic chemistry and then chemical reactions are very important for the conversion and then yield data. This data is essential this data usually you get from the lab and then you try to do it in the pilot plant and then you put it in the industry to get to cross check ok.

So, any chemical reaction is the most essential part of that chemical reaction from chemical plant viewpoint the conversion and yield data that you are going to get from the such reactions. Then analytical chemistry it is used for process control, controlling the process, determination of yield and then optimization etcetera, how you do, this some kind of analysis you do.

Let us say product you are having some liquid component right, you are producing the stream product stream is having only that component or not that if you wanted to know you can know through GCMS something like that. Such kind of things are there and then

those equipments are NMR you may use some other locations to determine about the component and then functional groups etcetera all those things.

So, all those things comes under the analytical chemistry part ok. So, that is the reason it is essential it is required. So, modern and electronic instruments such as vapor phase chromatography or gas phase chromatography or GC something like that infrared FDR etcetera, NMR etcetera. These kinds of things are you know very essential and all these operate based on the analytical chemistry principles. So, some knowledge about analytical chemistry is also required.

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Then physical chemistry it is integrated with chemical engineering operations; obviously, and then in phase diagrams, especially for separation processes this physical chemistry is useful, it involves use of chemical kinetics and catalysis etcetera. Then inorganic chemistry it involves one or more reactions which do not contain combinations of C, H and O.

If these combinations are not there with or without other non-metallic elements then such chemistry we call inorganic chemistry, if any reaction that contain combinations of C, H and O then we call it organic chemistry ok. Large portion of commercial organic chemicals derived from aliphatic and aromatic components of petroleum, from petroleum industry from the crude petroleum crude we get n number of components not only individual components we even get the some you know polymers also from such crudes right it is just for example, for mentioning it is given ok.



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Then thermodynamics, it is science which deals with relationships amongst various forms of energy in any chemical engineering plant you take there is no aspect there is no section without energy. So, energy is associated with almost all unit operations including pipe connections and then unit processes almost all if not all at least almost all we can say. So, then; obviously, we need to know different aspects of thermodynamics ok.

So, examples of applications of chemical engineering thermodynamics because chemical engineering thermodynamics is also one separate course in a semester ok. So, what we have there we try to understand chemical equilibria, what is chemical equilibria actually you know, in industry or in chemical engineering often what happens more than one phase when they come into contact with each other often it happens that they form two immiscible phases.

So, there is a equilibrium amongst those phases so, that equilibrium relations one has to understand. So, that to know the composition of a given particular component in each of the phase etcetera those things one has to understand or calculate a priori before going to the lab or before starting the industry right. So, that such kind of information you can get from the chemical equilibrium thermodynamics. Then some energy applications also there wherever the energy associated like you know expansion combustion etcetera compression of gases or expansion of gases etcetera those kind of things are there. So, then energy definitely comes into the pictures and then also we need to know these thermodynamic principles.

Under chemical equilibrium system is at low pressure then we call that system ideal system right, if the system is at high pressure then we call such systems are non-ideal systems right temperature may be variable. What happens at low pressure, why the system is called ideal because if it is a gaseous system and then pressure is low the molecules are far away from each other and then there may not be intermolecular interactions amongst them right.

But when the pressure increases you know molecules come close to each other and then interactions increases and then intermolecular interactions especially from the chemical different types of chemical substances these interactions are going to play huge role on this equilibrium thermodynamics or chemical equilibrium aspects so, they known as the non-ideal systems.

So, all these things we study in chemical equilibrium thermodynamics. Under the energy application like heat of reaction is very essential, whether it is endothermic reaction or exothermic reaction definitely heat is involved right. So, how it is involved whether it is liberating or absorbing based on that one you have to calculate the heat of reaction. So, then you may need to know thermodynamics for that purpose.

Similarly, work of compression and expansion of real gases etcetera often takes place in chemical plants. So, then; obviously, you need to know thermodynamic principles in order to handle such kind of issue in order to handle such kind of situations ok. So, these are a few mentioning only I am not saying that these are the only thing that you are going to be important from chemical engineering thermodynamics point of view ok.

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• Thermo	dynamic functions and relations of energy
terms:	H = Enthalpy
	G = Free Energy TS
	Unavailable Energy
	A = Total Useful Work TS PV
	External work

Then thermodynamic functions and relations of energy terms different energies are there. So, that we pictorially see right, rather showing in a equation form in a pictorial form we will see ok. So, let us say enthalpy is the total energy of the system, from that enthalpy whatever the unavailable energy S delta T is there or T multiplied by S that if you subtract then you get the Gibbs free energy.

TS T multiplied by S, S stands for the entropy, T stands for the temperature, the multiplication of two whatever energy is there that is the energy of the system actually that is unavailable for any work to be done ok. So, from enthalpy if you subtract that energy then you get Gibbs free energy that is the free energy available. Can we make use of that entire energy if to do some kind of work? No.

From that also if you subtract P multiplied by V that is external work then whatever the remaining thing is there that is only available for total useful work right. If you wanted to know the internal energy of the system from the enthalpy if you remove or subtract this P multiplied by V then you get internal energy ok. This all these things different forms different relations etcetera all those details are there you might have studied or you might be studying in your thermodynamics courses of chemical engineering discipline.

Then chemical equilibrium, equilibrium exists if the process moves either sides let us say from reactants to products not only from reactants to product from products to reactants also some chemical changes are occurring then only equilibrium exists for a chemical reaction ok.

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So, let us say if you take a reversible reaction mM plus nN reversibility giving rise to xX plus zZ, here small m n x z indicating the stoichiometric coefficient whereas, the capital M, capital N, capital X, capital Z indicate the components, like component M, component N etcetera those two are reacting and then giving product X and product Z.

Enthalpy of the reaction, if you wanted to find out what you have to do, you have to find out what is the enthalpy of the product and then what is the enthalpy of the reactants and then from the enthalpy of products if you subtract enthalpy of the reactants whatever the difference is that we call enthalpy of the reaction that is often indicated by delta H R.

Now, let us say the enthalpy of the reactants is higher than the enthalpy of the products then what happens in order to reaction occur, we do not need to give energy because reactants are already at higher energy or enthalpy of the reactants is already at higher end. So, products when the products are forming from these reactants, it liberates the energy it liberates the energy. So; obviously, sigma delta H product minus sigma delta H reactants is nothing but the negative right.

So, when this delta H R is negative such reactions we call exothermic reaction when the system liberates the energy because the reactant enthalpy of the reactants is already at the

higher end compared to the enthalpy of the products. So, when the reaction takes place from reactants to products it liberates the energy.

Whereas the reverse is that let us say enthalpy of the reactants is smaller compared to the enthalpy of the products; obviously, reaction will not take place until and unless you give additional energy to the reactants; that means, it absorbs the energy so that two reaction takes place and products to form.

So, any reaction where delta HR is positive that is products enthalpy is higher than the reactants enthalpy then when the reaction occurs the system absorbs the heat and then such kind of reactions are known as the endothermic reactions right. So, if you wanted to know this whether the reaction is endothermic or exothermic then you have to know the thermodynamics and then apply thermodynamic principles here ok.

Then delta G f naught is standard free energy of formation of a component, if you take the difference of this G f naught from product to the reactants then whatever difference is there that is nothing but delta G f naught in the equation form mathematical form representation. This is related to the rate constant of the reaction, how it is related that is minus delta G f naught is equals to RT ln k or delta G is equals to RT d ln k that is what you might have studied.

So, that is minus delta G f naught is equals to RT ln k, this k is nothing but equilibrium constant based on forward reaction for this one. So, rate constant is very much essential now here this is reversible reaction. So, then we call it equilibrium constant equilibrium rate constant ok. Equilibrium constant based on the forward reaction that we are representing ok.

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So, this is related to the activity of component that particular component because this rate constants also or equilibrium constant also with respect to a component we define ok. So, with respect to a component we are defining, so that particular component would be having some activity.

So, the activity of a given component is nothing but the product of the activity coefficient multiplied by the concentration of that particular component in the system that is a is nothing but gamma multiplied by C. So, k equilibrium rate constant whatever k is there that if you have to write, you have to write activity of a product to the power of stoichiometry of the product.

If there is one product then a X power x, but here z is also product. So, that should be multiplied by a Z power z, a suffix capital X stands for activity of component X, power small x stands for stoichiometric coefficient of that particular product x in the reaction whatever we have taken m M plus n N giving rise to x X plus z Z right similarly it is for the z,m and n a is nothing but activity.

Now, activity is related to the concentration of that particular component C suffix capital X is nothing but the concentration of that particular component at equilibrium right and then to the power of X is nothing but stoichiometric coefficients like that C Z power z etcetera and then this and then it is multiplied by activity coefficient gamma.

Gamma suffix x transfer the activity coefficient of that particular component x. Activity coefficient would be equal to 1 if the system is ideal. If the system is non-ideal then they will be having you know depending on the non-ideality there will be having different number, system can be positively non ideal or negatively non ideal etcetera all those concepts are there, those things you will be studying in chemical engineering thermodynamics course.

Now, this is in general, but if the system is gaseous system if the system is gaseous system then concentration whatever is there that is nothing but the product of total pressure multiplied by the mole fraction of that particular component. So, total pressure we are indicating pi and then mole fraction we are indicating capital Y and then this gamma is in general for the liquid system in general.

But if it is a gaseous system then fugacity will come into the picture, fugacity it also indicate how much a gas is non-ideal that is that indication you can get from this fugacity or fugacity coefficient ok. So, for a gaseous system same equation if you write in place of C you write pi multiplied by Y and substitute and then just replace gamma by f then you have this one ok. This is for the gaseous system.

That is about the thermodynamics and then chemical equilibrium thermodynamics little bit whatever is required to understand. Next what we see reaction kinetics.



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Reaction kinetics is the most essential part of any unit process and then unit process is going to govern the success of a given plant, how much of reactant is converting into the product, all that if you wanted to know you need to know the reaction kinetics ok. It is study of chemical kinetics and their applications to the design of processes ok.

So, since chemical kinetics are so much essential so, it is also need to know are these chemical kinetics are going to be same for all kind of reaction or they going to be different all those things we need to understand. In order to understand those things what we have to see? We have to see what are the different types of chemical reactions, because these kinetics are there for the reactions chemical reactions so, different types of chemical reactions we have to see.

So, these chemical reactions may be classified broadly the way they are occurring, depending on phases, phases of reaction the reaction can be homogeneous or heterogeneous, depending on the catalyst used or not it can be catalytic or non-catalytic, depending on the mechanism like the different way they can be classified ok.

So, we see a list of a such kind of classifications, based on the reacting phases they can be homogeneous and heterogeneous reactions, based on the mechanism; molecular, chain initiated, photochemical initiated etcetera these kind of reactions possible, based on the catalysis whether catalyst involved or not so we can have catalytic, non-catalytic reactions, then based on the energy transfer also as we have seen, energy is the most essential part of any reaction, based on the energy what type of energy it is involved.

So, these reactions can be adiabatic, isothermal reactions are intermediate kind of thing, intermediate in the sense they are neither adiabatic nor isothermal kind of thing ok. Then based on the chemical equations chemical equations like you know a plus b giving rise to b a plus s giving rise to r, but again now different types of equations are possible.

So, based on the equation form chemical reaction equation form they can be simple reactions, parallel reactions, series reactions, complex reactions, reversible reactions etcetera are possible right. So, all of these reactions you know effect of variables temperature, pressure and concentration is very essential to know, how much are they important and all that and then flow patterns also, what type of reactor are you taking for the reactions to occur. So, according the flow pattern will change in the reactor right.

So, you know if you have a simple tubular plug flow reactor so, there is no inter mixing kind of thing, if you have a state tank batch reactor kind of thing so, then there is a rigorous mixing in that one. So, the flow pattern is changing. So, accordingly you know this kinetics etcetera those things are also going to be affected right.

So, flow patterns also important and then transport of properties transport properties also, transport properties like you know thermal diffusivity, momentum diffusivity, mass diffusivity etcetera all these things also play essential role in reaction kinetics ok. So, we need to know them also.

So, now, quickly what we do we cannot go all these reactions everything because all these things if you include it that will be more than a individual course rather a chapter right. So, what we are trying to do now next slide we take just you know these reactions based on the chemical equations form we see a few details about the concentration variation of a reactant and products for these different types of reactions ok.

So, let us start with simple reaction, from the chemical equation point of view simple reaction is nothing but which is having simple form of equation.



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Like A giving rise to R, A plus B giving rise to R, A is giving rise to R plus S like that they are all simple very simple. So, if you wanted to plot concentration versus time profile for such kind of reactions any reactions the reactant concentration is going to decrease with respect to time if at all there is a reaction.

Is not it, if there is a reaction; obviously, the reactant A now we are taking A as a reactant, reactant concentration gradually decrease because the reaction is occurring some of the A is being consumed chemically to form products right. So, then that concentration is going to decrease gradually anyway so, by default initially at time T 0 it is going to be maximum concentration and gradually it is going to decrease.

And in product initially product is not there at T is equals to 0 before starting of the reaction or just beginning of the reaction there is no product formation. As the time progresses the product forms and then its concentration gradually increases. So, its concentration versus time profile if you wanted to see it looks like this simple, simple understanding kind of thing.

Then parallel reaction in the sense parallelly reactions occur like A is giving rise to R it is also giving rise to S. A and B giving rise to r and then they are also giving rise to S and they are also giving rise to T. So, they are occurring parallelly. So, when such kind of reactions are there again if you see concentration profile versus time plot. So, for the reactants; obviously, concentration decreases with time whatever the type of reaction it is because it is being consumed during the reaction and then products are forming.

Since, it is being consumed its concentration is going to decrease with time and then whatever are the products forms their concentration initially 0 at time T is equals to 0 they are 0 and then as the time progresses their product formation gradually increases and then they their concentration is going to increase. Now here in this particular picture the concentration of R is S and then T is low and then S is in between. So, that is just indication only it is not like that always R concentration is going to be higher ok.

Then series reaction what does it mean by, you have a reaction like A is giving rise to R and then reaction is not stopping there right, it is further forming S it is not that A is giving another product S, no A is giving product R, now which is a reactant for, product S right. So, they are in series a giving rise to R and then that product of first reaction is becoming reactant to form product S. So, that is the second reaction. So, these two reactions are occurring in series like this ok.

So, now, whether parallel reaction, simple reaction or series reaction whatever it is reactant now initial reactant is A. So, its concentration is going to be maximum when time T is equal to 0 and then since it is being consumed, its concentration is gradually going to decrease with respect to time. And now about R, R what happens initially R is the product actually.

So, there is no product initially at T is equals to 0. So, then as the time progresses what happens R formation takes place. So, its concentration increases up to that it is fine. But what happens after certain time of reaction that R is being converted into the S that is reacting to give product S.

So, after certain time what happens is concentration will decrease because now it started reacting and then forming component S product S; that means, after certain time initial time it is not being consumed, it is forming initial sometime after certain concentration reaches then only that a start forming another product from R.

So, then from that time onwards its concentration will decrease as A concentration decreasing because after this time R is also behaving as a kind of a reactant ok, but S is the final product, S is the final product it is not consumed further right, it is gradually forming initially it is also 0, but as the time progresses its concentration is increasing, its formation increasing and then its concentration increasing.

So, it is not going to fall anywhere because it is a final product. So, this is series reaction like that you know they are simple, parallel series even series reaction all of them are simple actually right. So, these profiles they are going to change what is the order of reaction from A to R and R to S all those things you are going to learn in your chemical reaction engineering course that is not part of the course here.

Just for understanding you need to know such kind of reactions are possible. Now complex reactions let us say here now A and B forming R and this R is reacting with reactant A again to give S and this S again reacting with A and then forming T right. So, this S may reacting with B or R also it is possible and then giving some other products may also be possible it is all complicated you cannot generalize or simplify it right.

For that case let us say if you wanted to plot the concentration versus time profile. So, A is the initial reactant, B is also initial reactant. So, initially they are having some

maximum concentration and their concentration is gradually going to decrease right. So, there is no doubt about because as the time progress the reaction takes place and then A and B are being consumed.

Now, this R is the initial product first product. So, initially its concentration is 0, but gradually as time progresses its concentration increases to certain time. Now, after certain amount of R has formed this R is again reacting with A and then forming S. So, then the R's concentration is going to decrease because after certain time it is also started reacting so, then its concentration versus time profile having a declining path like this right.

Then S, S also is a product, but it is initially 0. So, initially it is not there, but as sufficient amount of R has formed that is reacting with A and then forming S. So, then gradually to some extent of time its concentration is going to increase, but again it is reacting with A after certain time, after what time it is depends on the process, reaction, rate of reaction and all that is it those calculations are not required now.

But definitely after certain time this S is again reacting with A and then forming T. So, then S concentration would start decreasing after certain time because it is being consumed along with A to form T, but this T is final product which is not being consumed further it is not reacting with any or combining with any other component.

So, initially its concentration is; obviously 0 because its product initially at T is equal to 0 there is no product, but as time progresses reaction progresses its concentration gradually increases like this right. So, now, let us say reversible reaction aA reversibly giving rise to rR. So, A is the reactant forward direction we are taking. So, now, forward direction we take a initially A component is pure and maximum and then as time progresses its concentration decreases like this with time.

And then product initially it is 0, but as time progresses its concentration increases like this, but there is an equilibrium. So, after that there will not be any change in whatever the once the equilibrium is established, what is the difference between this profile and then first profile of simple reaction? Here you know after certain time whatever this time I have drawn here, after this time whatever the time you allow for the reaction to occur their concentration is not going to change. Because equilibrium has established and the transfer is taking either place, equilibrium established does not mean that ceases it means that transfer occurs either direction at whatever rate A is forming R at the same rate R is forming A that is what it means by after this time it is this profile is going to be flat it will not change anymore whatever time you allow for the reaction to occur ok. This is about the concentration versus time profile for the reversible reactions.

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Now, we see classification of chemical reactors different types of reactors are possible batch reactors, semi-batch reactor, continuous reactor like this ok. Simple batch homogeneous reactors are the ones where no addition or removal of contents during the reaction time occurs. So, no addition or removal, if you are not adding or not removing anything during the reaction then that we call simple batch homogeneous reactors.

If you are adding or removing one or more constituents from the reactor during the reaction then we call them semi-batch reactors, continuous homogeneous reactors are the other ones and then continuous heterogeneous reactors are the other types possible ok.

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Now, next what we see design criteria for reactors, if you wanted to understand the design criteria for the reactors you need to know something about the economics, something about the equipment, what kind of equipment should you use for such kind of reactors and then something about equations ok.

So, economic considerations are very much essential, why they are essential, whether you need to use continuous or batch reactor if you wanted to decide. So, then you know you have to decide based on the economic consideration. Because one reaction may be carried out in either of the continuous or batch reactors, but if you do in batch reactor if it is profitable then you have to go for a batch reactor.

So, such kind of economic consideration should be taken when you define design criteria for the reactors right. So, use continuous systems for large scale high production rate. If you need to have large scale and high production rate plant then you better to go for a continuous systems.

Use batch system for small quantities, intermediate demand, very long holding times, if the reaction holding time is very long and then only small quantities are sufficient. One or two tons is a kind of small quantity only, 100s of tons per day then it is a large quantity right. Most of the pharmaceuticals are small quantity industries. So, then most of the pharmaceutical reactors are batch type reactors. Then equipment selection what equipment should you use that is also very important design criteria for the reactors right. So, whether should you go for the continuous reactors or should you go for the batch reactors where closed stirred tank and tank with outside circulations, recirculation are there. So, those things let us say you have a this thing and then you are putting contents and then mixing them and then closing them.

So, this is a batch reactor, sometimes what happens. So, some of the things may be removed and then put them back here those kind of circulation is also possible. So, then they are you know with or without outside circulation that is what we call, but they are batch process they are coming to the same system.

Continuous processes are single pipe for homogeneous system with low reaction time. So, let us say low reaction time; that means, they can quickly react you have a simple pipe what you do you allow these components A and B because they are quickly reacting. So, then you do not need to do you just allow to pass through a simple pipe and then other side if the C and D products you can collect right.

So, these are the simple plug flow reactor they are called so, those things you study in chemical reaction in the courses. So, that is single pipe for homogeneous system with low reaction time right, system is homogeneous. What are the criteria to use the single pipe plug flow kind of reactors? The system has to be homogeneous that is very first point and then low reaction time that is quickly they have to react, they should not take hours to complete the reaction.

Then packed or baffled towers for homogeneous systems with high holdup like packed bed, fluidized beds etcetera such kind of reactors. Then, stirred tank for high degree of agitation, low holding time and no detrimental effects on back mixing right. So, this reactor stirred tank reactor is something similar to this thing like you know batch reactor by appearance, but they are not similar.

So, here a container is there the reactants A and B are continuously coming and then products C and D etcetera are also continuously drawn, drawn out through the output right. So, here if your holding time is required holding time is low and then you need high degree of agitation for this reaction to occur then you go for this kind of continuous stirred tank reactor etcetera.

This is PFR plug flow reactor etcetera this is batch reactor. So, like this you have to decide, as it is not like that you know you have only batch reactor and everything you try to do it in that one. So, you are not going to make economic benefit out of it. So, that is the reason economic consideration is one of the important for listing out the design criteria for the reactors.

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	• Design equations
	Homogeneous systems
	Batch reactors:
	For $A \rightarrow R$ first order reaction, $-\frac{dC_A}{dt} = kC_A \Rightarrow ln\left(\frac{C_A}{C_{AO}}\right) = -kt$
	Similarly for other order and other type of reactions, one has to
	find and utilize for design purpose
100	Flow reactors:
	$\frac{V_R}{F} = \int_0^x \frac{dx}{r} = \theta$ where x is fraction of conversion desired, V _R is
	reactor volume, F is volumetric feed rate and θ is holding time

Then design equations, for homogeneous systems batch reactors, let us say batch reactor then A is giving rise to R and then reaction is first order reaction. So, then the rate of the reaction this is what you get minus dC A by dt is equal to kC A this is differential form how are you getting up to this one. This you get simply by doing a material balance on A, you take a particular element in the system and then what is A is going in, what is the A is going out right.

And then what is the rate of generation or rate of disappearance and then what is the rate of accumulation these quantities you list out and then put them in a balance equation then you apply the limiting conditions for a small delta t time then you can get minus dC A by dt is equals to kC A this is true for only first order reaction, second order reaction different one you may get ok like that ok this is how you get.

Now, this equation if you integrate then you get this form. So, this is nothing but the rate equation for the first order reaction A going to R right here C A naught is nothing but initial concentration of component A, from C A naught to C A it is forming and then at

what rate at this rate, this k is the rate constant, t is the reaction time ok like that different types of reactions different types of reactors you can get it.

Similarly, for other order and other type of reactions one has to find and utilize for design purpose accordingly you have to develop, this is only for this kind of reaction first order reaction, but may be reversible reaction. So, then you get different equations right. So, those things one has to see.

Then flow reactors if you have flow reactors similar balance you can get this is what you can get the equation V R is the reactor volume, F is the volumetric feed rate, theta is the holding time.

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If you have heterogeneous systems mostly for catalytic systems or catalytic reactions such kind of heterogeneous reactors are used. So, then equation is this one where W by F is nothing but kg of catalyst per kg moles of feed per time. Here rate equation r for catalytic systems are mostly empirical whatever the previous slide that equation rate equation that has been shown for the first order irreversible reaction a goes to r that is for homogeneous reaction only, that is for the homogeneous reaction homogeneous system occurring in batch reactor ok. So, space velocity, reactor designs are frequently based on the space velocity, it is nothing but for homogeneous reactors 1 by theta are F by V R, V R is the reactor volume and then F is nothing but feed rate.



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SV for heterogeneous reactor design that is space velocity different way it is defined two ways we are presenting here. One way is that VHSV that is volume hourly space velocity which is nothing but gas volume specified whether inlet or outlet at STP per hour, per void volume of the reactor ok, this is one of the definitions.

Then, WHSV weight hourly space velocity which is nothing but feed rate feed mass rate of the feed per mass of the catalyst is nothing but WHSV, space velocities if you see the units are time inverse units ok. So, till now this is all about some basics about the basic principles of science and engineering which may be essential to know from the chemical plant view point right.

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Now, quickly what we see chemical plant design right few details ok. Process and mechanical design, design of commercial chemical plant requires synthesis details or combinations of unit operations and unit processes that we understand. Any plant unit you have a combination of different types of unit operations and unit processes they are presented in systematic way in order to get a chemical production to take place.

This is the most broad and important endeavor of chemical engineer whatever that you learned, whatever you learnt in your UG Chemical Engineering curriculum all the principles are going to be useful when you design a plant. When you design a plant and then plant design is two ways, one is the chemical process design, another one is the mechanical design as I mentioned.

So, everything that you learned in the UG Chemical Engineering course everything is going to be useful in process design of any particular plant that you are going to start designing or installing or improvisation whatever you are trying to do. These principles chemical engineering heat transfer, mass transfer, fluid mechanics, process control, transport phenomena, reaction engineering, mass transfer 1, mass transfer 2, mass transfer operations different courses all those you know knowledge is going to be useful in this process design. Chemical plant design is divided into two as I mentioned one is the chemical process design, another one is the mechanical design, what are they, I have already mentioned, but again we see.

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Process design deals with design aspects of unit operations and unit processes, then mechanical design deals with construction details of equipment, foundations, buildings, process auxiliaries, installation, operation and maintenance. So, all these things comes in the mechanical design.

Some plants you know what they have, they have designated mechanical engineers to take care about the such kind of mechanical design, but; however, it is expected chemical engineers should know all these things in addition to the process design calculations they should also know the mechanical design calculations also, that is the reason we have engineering drawing and then chemical plant drawing courses separately.

Because of chemical engineers having major role in solving design problems, there is a considerable overlapping between two sections of design in general ok.

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Now, we see little more about the process design role of R and D on chemical process is said to be completed when sufficient information is available to prepare a series of flow diagrams or flow sheets which incorporates unit operations and unit processes to achieve desired production ok. That all that if you have then we can say that whatever the research and development requirement from the plant viewpoint are complete right.

So, usually process design includes several things one is the flow sheets, flow sheets as I mentioned it is a description of a sequential operation that is occurring in the plant in a pictorial manner right. So, how do you report? That you know what details you give based on that one again then flow sheets are different ways different categories are there those things we see subsequently.

Other thing is the process steps what are the steps involved that also one should know as a part of process design calculations and then design steps when you design a let us say froth flotation cell. So, what are the calculations, if you going to design a thickener or sedimentation what are the flow rates, what are the thickness and then what is the outlet flow rates etcetera all those things you have to get through ok.

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Now, as I mentioned depending on what type of how many different types of details are you providing in flow sheets these flow sheets are again different types, one is the block diagrams, another one is the simplified engineering flow sheets, another one is the other design flow sheets ok.

We will see individually what are they, block diagrams and simplified engineering flow sheets used to understand process design aspects of chemical technology and they are simple rectangular box diagrams which may graphic layout of various steps in a process ok. Example heat exchangers for optimum heat recovery are not usually shown arrow points out the start of the process and the products are underlined.

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Let us say if we wanted to put it pictorial form it will be easy to understand, if you wanted to show a flow sheet in terms of a black diagram how does it look like that is what we see by taking an example of sulfuric acid and oleum production by contact process. So, this is all the flow process that we do not understand that we do not want to go, what we see that the end of the arrow is there that is what going into the process unit operation or whatever it is there.

So, this is the entering and then all the details like sulfur burner we are just showing as a box, heat exchanger then also we are showing as a box, but you know they have different forms to show different details are also there, but all those things we are not showing and then here products are usually underlined.

So, this product should be underlined here. So, this is what called a block diagram representation of the flow sheet right, some of the reactions associated with this process are given here, but; however, not required to know.

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Now, simplified engineering flow sheets; visualization of process in terms of possible equipment to carry out operations is very essential in formulating a process design. Thus simplified engineering flow sheets fulfill such requirements and include all degrees of complexity giving details such as, stream quantities, specifications, material and energy balance and then instrumentation details and process auxiliary requirements.

What does it mean by the same contact process for production of sulfuric acid that we will see here, then what you can see here?

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Now, rather showing just reactor you are showing the proper representation of the reactor and then you are also giving the conditions like this right. You are also giving material and energy balance etcetera also in general separately or within the flow sheets also possible.

Compared to the previous block box type of representation compared to that one this simplified engineering flow sheet is better one it gives more details compared to that one, but still simplified if you include all the engineering details; that means, all of your chemical engineering knowledge you are putting here. So, then that will become much more complicated rather making it for understanding it will become more complicated.

So, that is the reason it is called as simplified engineering flow sheet, most of the details would be there to understand for a process engineer if not for the non-chemical engineering person, for a chemical engineering person such kind of representation is more than sufficient to understand what is about this particular plant like that, that is the reason it is known as simplified engineering flow sheet.

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Other design flow sheets are a complete plant design requires vast number of intricate and detailed flow sheets for such things such as, piping layout, electrical layout, instrumentation details, plant layout etcetera are also included, but it is not required to know them. (Refer Slide Time: 57:04)



Now, process steps if you see following broad steps can be considered as elementary approach for most of the chemical processes like, prepare reactants, react them, separate the products, then purify the products, all these kind of things are the process steps, is not it.

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Now, design steps what are the steps that are involved in the design it is a kind of summary of what we have discussed till now. So, in the design what are the steps that you follow collect laboratory and process development information, then prepare flow

sheets, choose conventional design procedures for equipment designated on flow sheets as unit operations oriented right, this is like you know like a checklist that one you can have when you are designing a plant.

So, you can have the design steps and then you put a checklist tick mark when it is done like this then design the reactors it is one of the major problems of the plant design job and then optimum design is very critical. So, one has to be very careful while designing the reactors for a chemical plants not only from the economics point of view, but also from the safety point of view as well.

Select control instrumentation for process monitoring and analysis it is also very essential, why it is essential let us say if you wanted to maintain the reaction temperature 300 degree centigrade and then there is a controller you have to use right. If that controller is not properly working or if it is not located at proper place in the plant or in the reactor then it is not going to show the true picture or true temperature so, then it is going to be disastrous from the reaction point of view is not it or it may not be giving the desired results ok.

So, rather 300 if it is showing 250 and then 350 so, the such kind of differences are going to make process uneconomical. So, control system also control instrumentation is also very much essential from the design point of view. Then select and size materials handling equipment like pump, piping, conveyors etcetera, then design all process auxiliaries, then make plant layouts, then itemize all designs for cost estimating etcetera.

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Finally, economics that we see before winding up today's class. So, profitability analysis of a projected chemical process venture is very much essential that one can do if you have some basic knowledge about economics. Then principles of economic balance is also required so, under this category individually if you see, there are other things like you know choice between alternative processes right.

All these three things are essential from the economics point of view. Let us say production of acetylene that can be produced by n number of ways; you have to select one which is better one from the economics point of view. So, that is choice between alternative processes is also very much important ok.

So, under the profitability analysis of projected chemical process venture what you have to worry about you have to worry about the capital cost, you have to worry about total product cost, you have to worry about economical analysis, we are going to see a few basics about them in the next slides.

Anyway under the capital costs or capital investment you have "fixed capital for plant facilities" and "working capital". So, working capital and then fixed capitals comes under capital investment. So, what are they, we are going to see next. Then total product cost is nothing but manufacturing cost and then general expenses what are included in this such kind of cost that we are going to see anyway, then economical analysis like "selling price" and "profitability" etcetera.

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So, now we see what are the things involved in capital investment like fixed capital for plant facilities include site, building, utilities plants, process equipment, storage facilities, etcetera all those things. And then working capitals include raw materials inventory, inprocess inventory, product inventory, maintenance and repair inventory, accounts receivable, credit carryover and minimum cash reserve etcetera are comes under the working capital.

So, capital investment two things are there fixed capital and then working capital, what kind of things are included under these things are mentioned here ok.

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Likewise total product cost we have manufacturing cost which includes you know raw materials, shipping, containers, operating cost, labour cost, supervision, supplies, water, fuel etcetera. Then overhead cost like employee benefits, medical services to the people associated with the plants, cafeteria, purchasing, shops, property protection, general plant supervision etcetera.

And then depreciation, property taxes and insurances all those things comes under the manufacturing cost which comes under total product cost. And then general expenses which are also comes under total products cost include freight and delivery, administrative expenses, sales expenses, research expenses etcetera.

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About the economic analysis selling price, profitability are important. Under the selling price market analysis one has to do, application of products and competition etcetera one has to do, income taxes details one has to see and then net and new earnings one has to list out. Under the profitability return on investment, cost and profit charts and other methods of economic analysis, payout time, interest rate of turn return on discounted cash flow method, project present worth etcetera all these things comes under you know profitability.

So, all these things again as I mentioned there are different subjects. So, we cannot go in detail if at all of them.

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So, finally, principles of economic balance selection of conditions which will yield a maximum return on investment for the plant should be one of the important concern of the engineer ok accordingly one has to select ok. Why a set of variables chosen in a given process or one process favored over another is based on optimizing the economic balance.

We will see one example also what does it mean by taking heat exchangers example. Example; optimum design of a heat exchanger for a given capacity is a familiar equipment sizing problem in most of the if not all in most of the chemical plants. So; obviously, we understand if you increase the fluid velocity that heat transfer coefficient will increase.

If you have done the heat transfer coefficient that you can understand and reduces the size of heat exchanger, but this reduces the annual charges on fixed investment of heat exchangers, but; however, increased velocity will increase the pumping cost. So, you have to make a tradeoff between two, whether should you go for increasing the fluid velocity or capital fixed investment you have to see ok.

So, a minimum operating cost is found which fixes the conditions for the design of HE as shown below here in the picture.

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Now, hourly operating cost versus fluid velocity if you do, heat exchanger fixed charges decreases with the fluid velocity, but the pumping cost increases with the fluid velocity increasing fluid velocity. So, we have a kind of optimum when you consider both of them then you can have a kind of trend like this which is optimum.

And then corresponding to the minimum one, so that velocity you have to take optimum one accordingly you have to do the designing of heat exchanger and then operating of the heat exchanger ok. This is such kind of economic analysis also one should do. Same principle applies to selection of alternative for a complete plan and economic operation of plants as well as equipment and process design. And computational knowledge is in general is very useful in decision making of such problems.

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Now finally, choice between alternative processes we conclude with three examples let us say for many major chemical products, variety of alternative routes available depending on cost and availability of raw materials etcetera. You may be having one process in a plant, but the raw material required for that process may be coming far away or you know getting them is expensive.

So, one has to make a tradeoff between these two like that one has to analyze. For example, acetaldehyde production from following routes you know these many different reactions you can have to get the acetaldehyde, which one you have to use that you have to see especially from raw materials LPG, how much it is available ethyl, alcohol, how much cheaper it is available or how closely it is available near the plant all those things one has to see ok.

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Similarly, acetone productions also there are different routes as shown here. So, one has to see raw material availability, economics and all those things whatever we have seen and then we have to choose a process which is economically feasible ok.

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Similarly, butadiene also I am just mentioning there are n number of methods are there you have to choose the one which is economically more favorable, when you talk about economically you have to do the profit analysis, economic analysis for each and every unit operation and then each and every raw material or streams are associated. So, that to make a entire plant as a economically feasible ok.



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Now, see glycerol are all see, so many are there. So, accordingly one has to choose.

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Now, summary of week one lecture what we have seen in this week that I have presented here. Common and basic unit processes we have seen and in common unit operations of plant we have seen, we have also seen basic principles of science and engineering useful in chemical plants. We have also seen chemical plant design aspects from both process and mechanical design viewpoint, we also seen basic economics of chemical plants and importance of alternative process in general by taking a few examples ok.



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The references for this lecture are provided here you can go through any of these books such kind of details are available, but; however, this reference book is better for this week lectures.

Thank you.