**Process design decisions and project economics**
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**Module - 2**
**Flowsheet Synthesis**
**Lecture - 4**
# Input Information and Design Aspects of Batch vs. Continuous Process

Today we start module 2 of our course that is Flow Sheet Synthesis or conceptual design of a chemical process. In previous lecture I outlined the hierarchical design of a chemical process, a chemical process systematically is designed through five steps; the first step is that we decide whether we should design a batch plant or a continuous plant. The next stage is that we design the input output structure of the flow sheet, the third step is to design the recycle structure of flow sheet, where we do all the material and energy balance. The fourth stage is designing of the separation system of the process and the fifth and final stage is the energy integration of the process. Now, in this module we shall see each of these steps in process design in greater detail.

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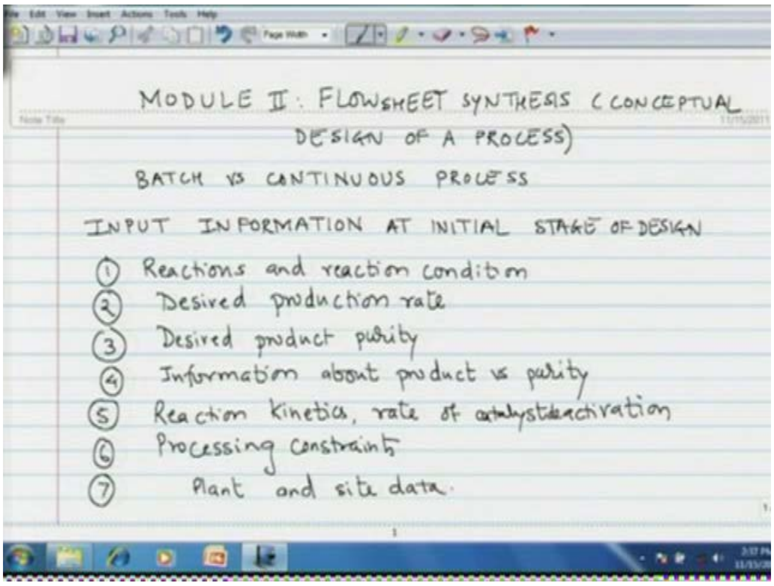


Now, the first step that is deciding whether we have to go for a batch process or continuous process. As I mentioned in previous lecture the design problems are different than other problems that we encounter in that they are always under defined that very little of the input information is available. So, we gather the remaining information or missing information either through literature survey or through experience gathered from other projects, many times some thumb rules, huristics are also used for designing of a process. However, when we start designing a new reaction scheme for a particular product, we have to design not only the reaction scheme that is invented by our own RND, but also the other processes that are already existing in the market with different process licensor. In that we will ensure the profitability and sustainability of our process.

The input information that is normally required at the initial stage of a design problem is as follows. The first information is that we know the chemistry of the process that is the reactions and reaction conditions, then the next information that we need is the desired production rate. The third information is desired product purity, the fourth information is information about product versus purity. Then the next information that is required is the reaction kinetics or rate of reaction the phases of reaction whether it is a single phase reaction, two phase reaction, three phase reaction.

And then in case of catalytic reactions we also need to know the rate of catalyst deactivation, catalyst in an expensive component of the process; so the knowledge of catalyst deactivation is essential. The next is processing constraints what are the factors that limit the reaction conditions, the temperature, pressure of the process or the reactor types so on and so forth. The seventh information is the plant and site data.

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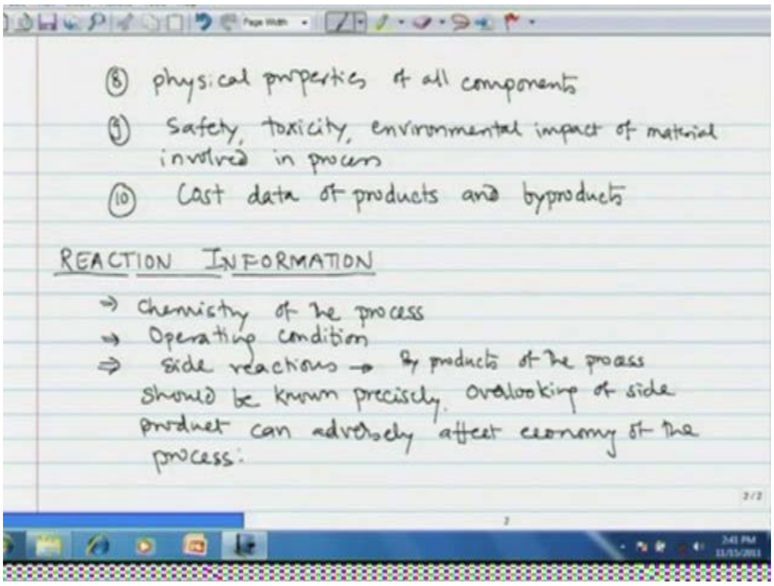

The next is the physical properties of all component and then the information about safety, toxicity and environmental impact of the material involved in the process. And finally the cost data of product and byproduct, now we shall discuss each of these ten factors in somewhat greater detail. The first is the reaction information reaction, now as I said we need to know the chemistry of the reaction very well, the chemistry of the process then next in the operating conditions, temperature pressure so on and so forth; then the information about side reactions. Now, side reactions may not be detected in a laboratory experiments, laboratory experiment is carried out on small scale. Therefore, it is it may not be possible for a chemist who is doing experiment to list all the side reactions; however, one must be careful to know these reactions and the extent of these reactions.

Because, any side product that is formed may be on a trace level in a laboratory experiment can be detrimental on large scale. Because, it is produced on much larger scale and then it can trigger many other side reaction or it can spoil the yield of the process so on and so forth; so that point we need to know. That side products or byproducts of the process should be known precisely. Overlooking of side products can adversely affect the economy of the process.

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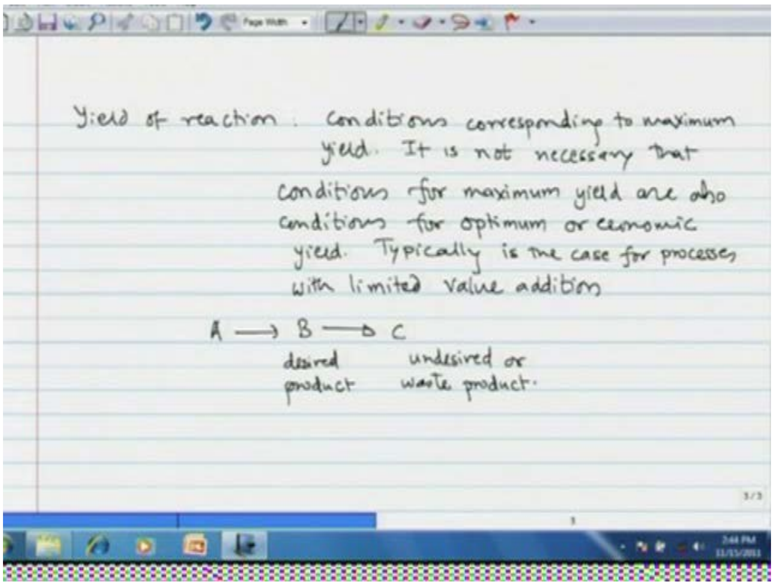


The next aspect of reaction information is the yield of reaction, under what circumstances you will get the maximum yield conditions corresponding to maximum yield. Now, when a chemist conducts an experiment he would try to get those conditions under which the yield is maximum. However it is often observed that the conditions for maximum yield may not be the most economic conditions or optimum conditions for operation of the reactor.

And that point we should note it is not necessary that conditions for maximum yield or also the conditions for optimum or economic yield. And this is typically the case for processes in which the value addition is limited, that point we also note typically is the case for processes with limited value addition, which means the difference between the cost of raw material and the product that we produce is not much; may be typically 50, 60 at the most 100 percent. Now, let me demonstrate this thing with an example, now let us say we are carrying out a reaction in which A goes to B and there is a side reaction, where B goes to C. B is the desired product of the process, while C is the undesired or waste product of the process.

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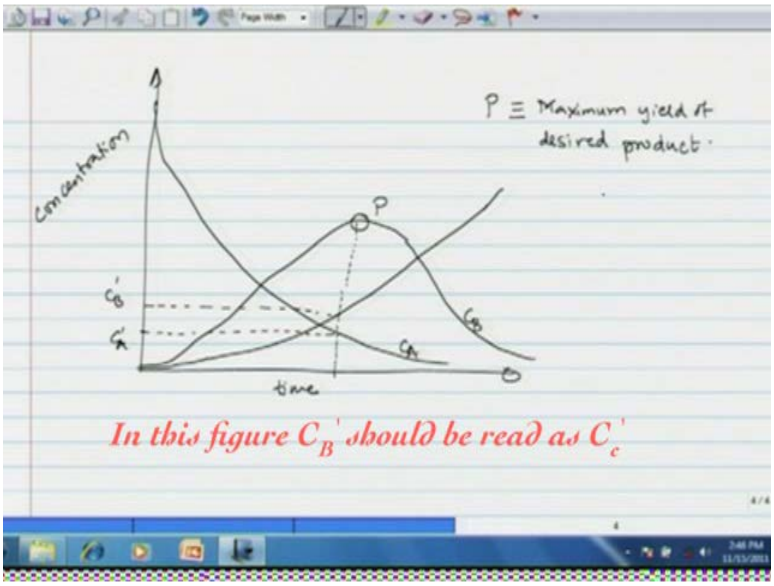


Now, the typical progress of reaction can be shown as follows with respect to time in a batch process or with respect to space time velocity in a continuous process. So, what we are plotting now is concentration versus time. The concentration of A which is the reactant main reactant falls continuously with time. The concentration of B which is an intermediate product shows a maxima, somewhere in the time course and the concentration of C which is undesired product rises continuously.

Now, a chemist will always try to give conditions at the point of maximum yield of the desired product. So, let us say point P which corresponds to maximum yield of desired product. Now, if you project this point downward and see what are the concentrations of the other two products that corresponds to maximum yield of the desired product we see that almost 70 to 80 percent of a has been converted by the time maximum yield of the desired product is reached. And in addition the concentration of the undesired product is also significantly high.

Therefore, by the time we reach condition of maximum yield of desired product a significant quantity of the reactant has been converted into waste product. Now, this is affordable if the value addition from A to B is quite high; however, if the value addition from A to B is low; that means, we are dealing with valuable raw material we cannot afford to lose thus significant amount of raw material in the form of waste product. Therefore, the point of optimum yield may not be the point of economic yield and under these concentrations or under these criteria.

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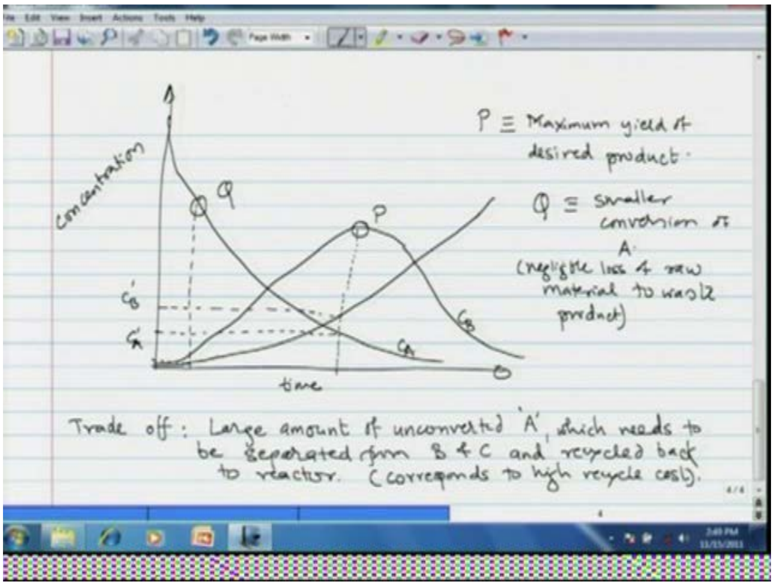


We would find that it may be economic to design the reactor for a smaller conversion of A which corresponds to point Q. Now, we are encountering an economic trade off at point Q the conversion A is small. However as you will see the conversion of A into C is negligibly small you can see that concentration of C a corresponding to concentration of

Q is very small. That means, at point Q we have negligible loss of raw material to waste product; however, we have a large amount of unconverted A at the reactor outlet.

And then the cost of separation of A from B and C and then recycling it back to the reactor is an additional cost. So, that point we note, we are having a trade off for large amount of unconverted A, which is the reactant which needs to be separated. And separated from B and C and recycled back to the reactor, this means that the recycle cost is high corresponds to high recycle cost.

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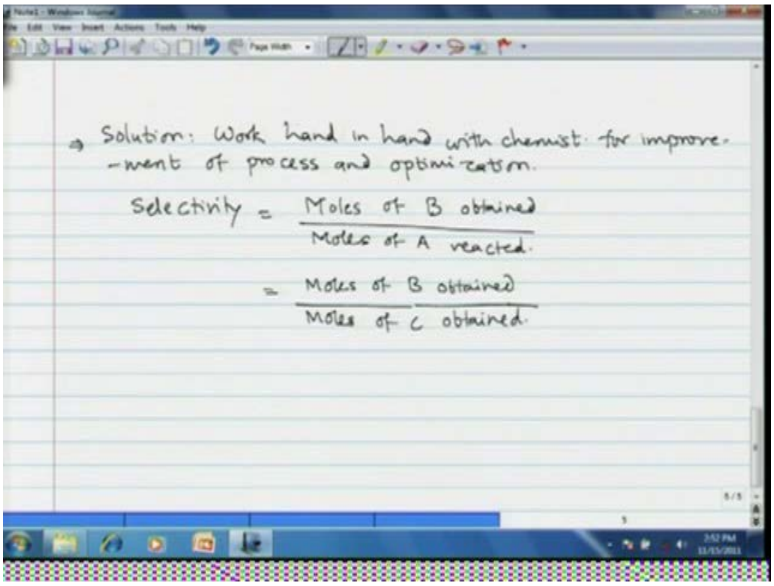


Now, a better approach for optimization of a process under such condition is to work hand in hand with a chemist. Once we determine that point Q is the economic point or optimum point of reactor operation we need to know more about the reactor outlet at point Q as the kinetics of the reaction, the side products at point Q and so on and so forth. Therefore, an engineer should give an input to the chemist and then the study of the chemist on that particular point could be a good input for improving the process design.

So, that is what the solution is for a better process design, work hand in hand with chemist for improvement of process and optimization. Now, the concept of selectivity whenever we have more than one product from a process we always need to define the selectivity the selectivity for the desired product, now in the example that just that we just saw B was the desired product. So, we define selectivity as moles of B obtained per mole of or moles of A, reacted this is one of the common definitions of selectivity that is used. Some engineers used the definition of moles of B obtained that is the desired product divided by moles of C obtained both definitions are correct there is no hard and fast rule that you use any of the definitions. However, when we use literature data for designing of a process we need to check which definition of the selectivity the authors have used.

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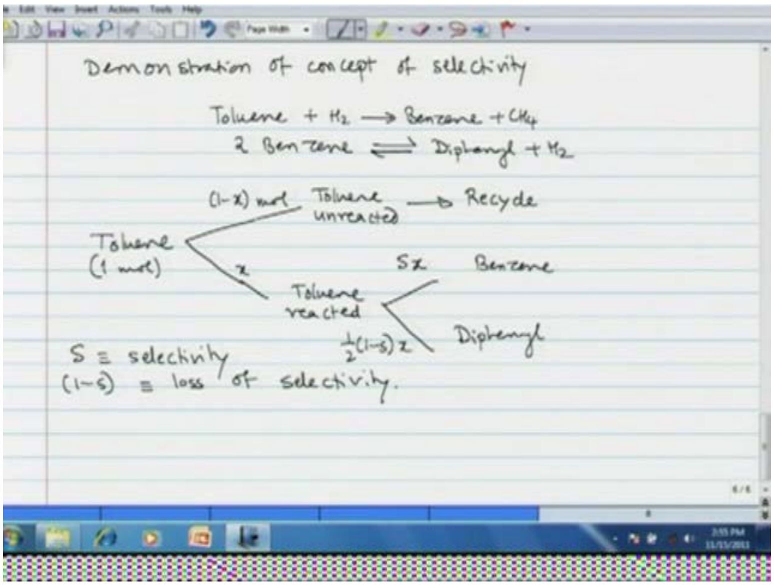


Now, let us demonstrate the concept of selectivity with the example of HDA process that we saw in previous lecture demonstration of concept of selectivity. HDA process I would write again briefly toluene reacts with hydrogen to give benzene and methane and two moles of benzene combine reversibly to give diphenyl and hydrogen benzene is a desired product and diphenyl is the side product or waste product. Now, if for a given reaction conversion, let us say the conversion is x then per mole of toluene fed to the reactor 1 minus x moles of toluene are unreacted and x moles of toluene react.

Now, the unreacted toluene is separated and recycled out of the reacted toluene some toluene forms benzene and some forms diphenyl. If we use the first definition of selectivity that is moles of desired product divided by the moles of the reactant reacted, then the moles of benzene that are formed S into x where, S is the selectivity. Now, stoichiometry from toluene to benzene conversion is 1, but from benzene to diphenyl conversion is 2. Therefore the moles of diphenyl that form are half into 1 minus s into x, so 1 minus S is a loss of selectivity.

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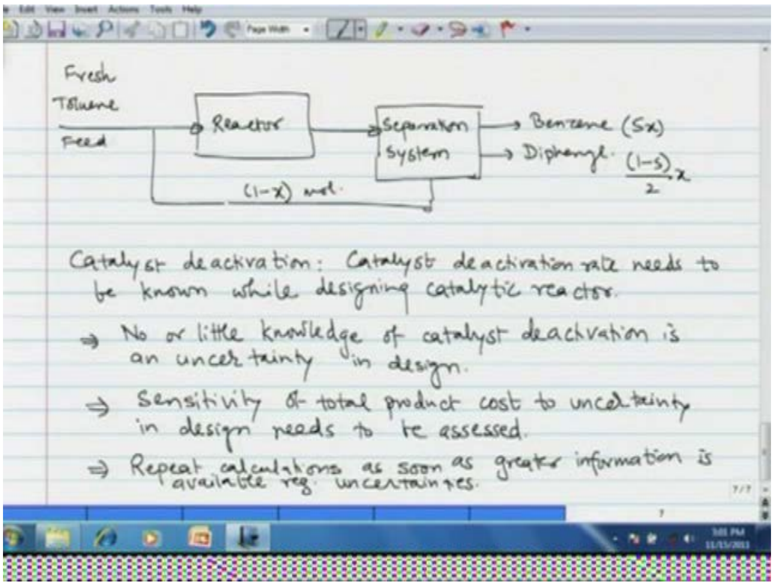


Now, using this definition we can alter the flow sheet of the process that we had seen earlier. We see a reactor and then the toluene feed, toluene is of two types one is fresh toluene and second is the recycle toluene. The reactor affluent goes into a separation system where benzene and diphenyl are produced and un reacted toluene is sent back to the process, the benzene produced is S into x while dihpenyl produced is 1 minus S by 2 into x. So, we can write the process flows in a simple flow sheet using selectivity as shown. The next parameter is set off the catalyst deactivation, now a chemist tries to design a catalyst that has not only high yield, but also high selectivity. However, an important factor in the operation of a plant over long for a long term is the catalyst sustainability is catalyst able to give same performers for a prolong period without getting deactivated.

Therefore, catalyst deactivation rate needs to be known while designing the reactor, if the catalyst deactivation rate is not known then that is an uncertainty in the process design. Of course, when we are designing the process for the first time there could be many uncertainties in the design. And therefore, we need to check the profitability or the sensitivity of total product cost to the uncertainties and designs needs to be known.

Now, as the design proceeds the resurgent development section of the company may carry out simultaneous experiments and maybe in later stage or stages of design greater knowledge of these uncertainties is available. In that case one need to repeat the calculation for a better process design, repeat calculations as soon as greater information is available regarding the uncertainties.

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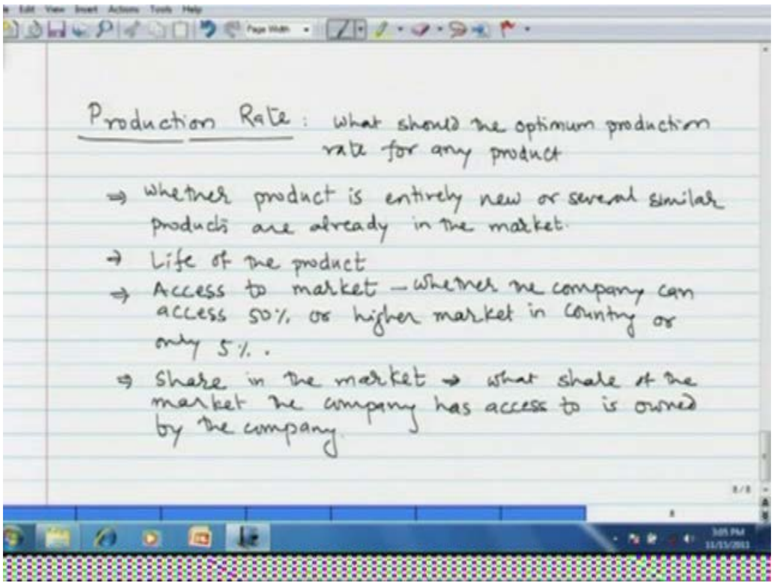


The next important factor in the process design is the production rate, what should be the optimum production rate for a product. Now, this is a crucial factor in process design which is influenced by many parameters, the first parameter is that whether the product is entirely new product or several similar products are already in the market. Whenever a company invents a process for production of a new product or a new process for production of an existing product they patented; that means, no other company or competitor can use the same process or manufacture the same product.

However, competitor companies always try to find alternate methods or ways of designing or producing the same product or a similar product which has same properties as the product introduced by this company. And therefore, the product has certain life, so the life of the product is also an important factor in designing the production rate. As soon as competiting products come into market the same of particular product goes down.

And therefore, we have to see whether we are going to access about 50 percent of the market or only 5 percent of the market access to market; whether the company can access 50 percent market or higher in country or only 5 percent. Then another factor is the share in this market, let us say for a particular product the total demand is hundred thousand tons per annum, but what share of this market my company is going to access. Therefore it matters a lot whether what share of the market, the company has access to is owned by the company.

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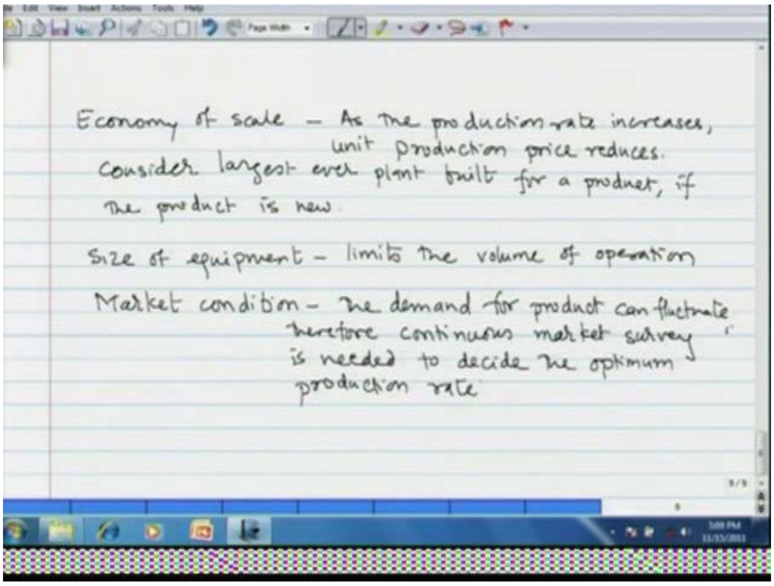


Now, there is always a economy of production or economy of scale as the production rate increases the unit production price goes down. However, there is a limit as how much product one company can manufacture, therefore whenever we are introducing new product in a market we have to consider the largest ever plant built for that particular product which will give the highest economy upscale; however, the product has to be new in this case.

Then another factor that is that governs the size of the plant is the size of the equipment that is needed for the plant if the equipment for the plant is manufactured at another site. And then it is transported to the site of the factory then there is a limit as how large a reactor could be, how large a compressor could be, if it is transported by road if it is transported by rail so on, so forth. So, size of the equipment limits the volume of operation and finally, the market conditions the demand for a product may fluctuate in time.

Therefore, the company has to keep a record or a knowledge of the demand for the product while producing a particular product the demand for product can fluctuate. Therefore, continuous market survey is needed to decide the optimum production rate, if the demand for a particular product falls then the company may have to operate the plant below the capacity.

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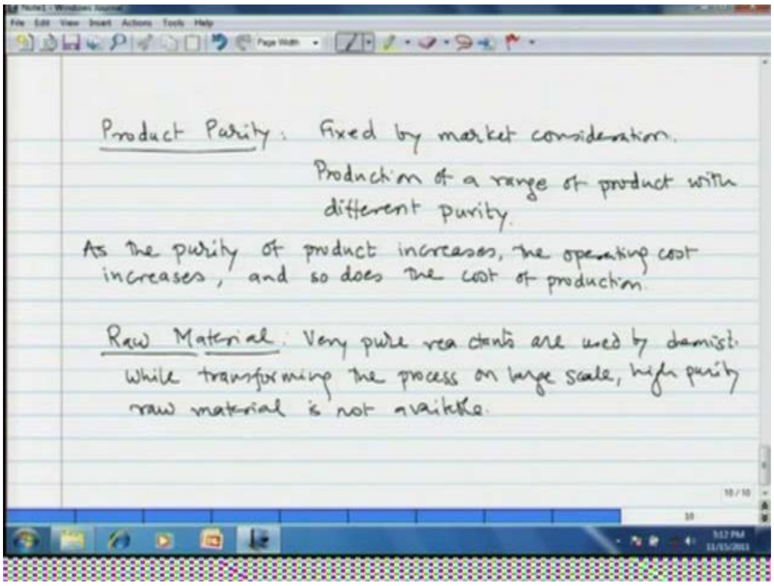


The next factor is that of product purity, now product purity is also fixed by market forces it could be possible to produce the same product with varying purity if the market, allows for it, production of a range of product with different purities. Now, typically as the purity of the product increases the operating cost increases and so does the cost of production therefore, the unit cost of a product can rise as the purity rises. So, this factor is an important factor in deciding the design of a plant.

Next is the raw material, now when a particular reaction is carried out in laboratory, chemist uses very pure reactants which may not be available commercially, very pure reactants are used by chemist and when we try to transform the same process on large scale that purity of raw material may not be available. Now, in case in pure raw material rise are available we have to assess the level of impurity, we have to assess the sensitivity of overall operation of the process that is the reactor the catalyst towards this impurity.

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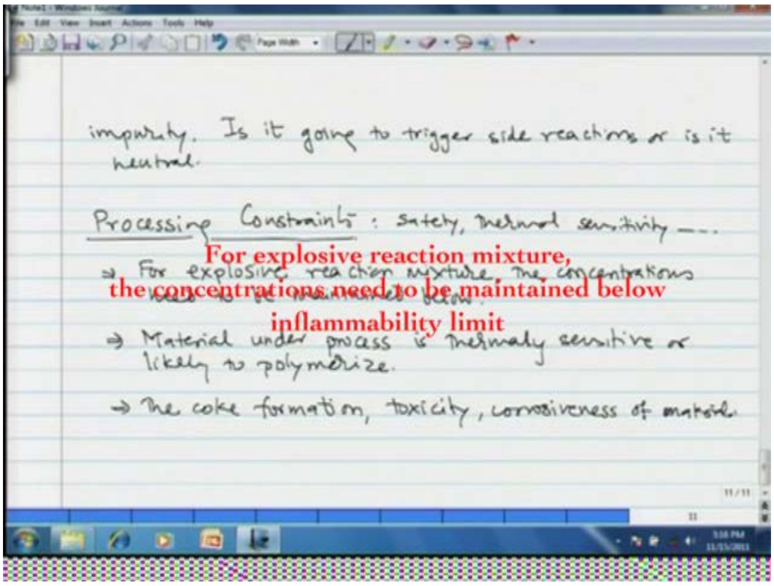


Is this impurity going to trigger side reactions or is it in neutral impurity. So, depending on these factors, we have to decide whether we need to purify raw material or not that is all. Then is the factor of processing constraints, now processing constraints are mainly due to safety or thermal sensitivity of the material and so on and so forth. Now, if the reaction mixture is explosive then we need to keep the concentrations of reactant below the explosive limit.

If the material that is under a process either the reactant or the product is thermally sensitive or is likely to polymerize, we need to restrict our processing conditions. For example, for thermally sensitive material we cannot go for very high temperature because the reactant may decompose before it is converted into product. Similarly, for reactant set polymerize we may have to add inhibitors to prevent polymerization. In some cases the coke formation is a processing constraint, then toxicity of the material corrosiveness all these factors affect the design of the process and they also put constraints on the processing.

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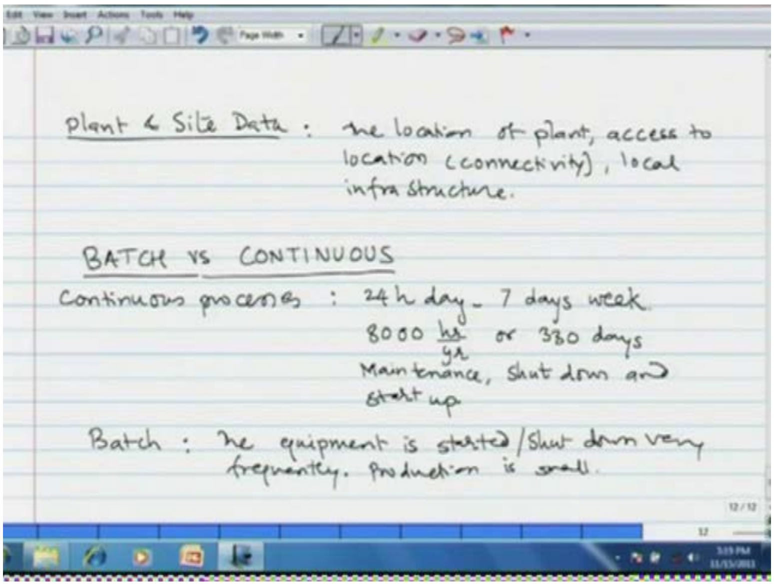


Then is the factor of plant and site data where we are going to build the plant, what is the source of raw material at that particular location, what is the infrastructure that is available in terms of electricity, in terms of water, in terms of sanitation for disposal of the liquid waste solid waste and so on and so forth. So, all these factors come into picture, the location of the plant access to the location, whether it is connected by road, rail, air then the local infrastructure these all factors come into picture. So, this is typically the general information that is needed at the beginning of process design.

Now, when we want to decide whether we want to go for batch process or continuous process, we need to take into consideration some more factors. Now, continuous processes are typically 24 by 7 that they operate 24 hour a day and 7 days a week. The typical working hours of continuous process are taken as 8000 hour per year or in some cases it is something like 330 per year. The rest of the time is for maintenance and shutdown and startup, now batch processes are where the equipment is started and shutdown very frequently the production is small.

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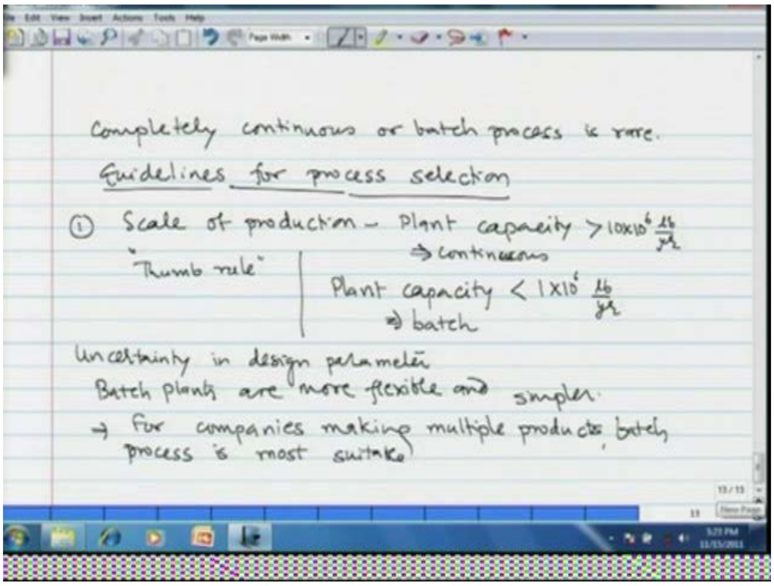


But, rarely you will find a process which is completely continuous or completely batch, you will always find a process that has some units operating in batch mode and some units in continuous mode. Like for example, if there is a distillation column in batch process, then the material to be distilled is stored in tank from different batches and a distillation column operates continuously, so that is a sort of hybrid design. However, when we say a batch process, then majority of the equipment in that a process operate in batch mode.

Now, what are the guidelines for selection of a batch or continuous process the first and foremost is of course, the scale of production, typically if the plant capacity is greater than 10 million pounds per year, we use the continuous process. And for plant capacity less than 1 million pound a year we use a batch process, but remember these are thumb rules, these are not hard and fast laws. Now, uncertainty in design is also a factor like I just said that the catalyst deactivation rate is a parameter, which cannot be determined with accuracy, so that is an uncertainty in design.

So, if a process design for a new product has several uncertainties then it is a good idea to carry out that process in batch mode, where you can startup and shutdown equipment and do all the process changes more frequently. So, batch plants are more flexible and simpler and due to this for companies making multiple products or plants making multiple products batch process is the most suitable.

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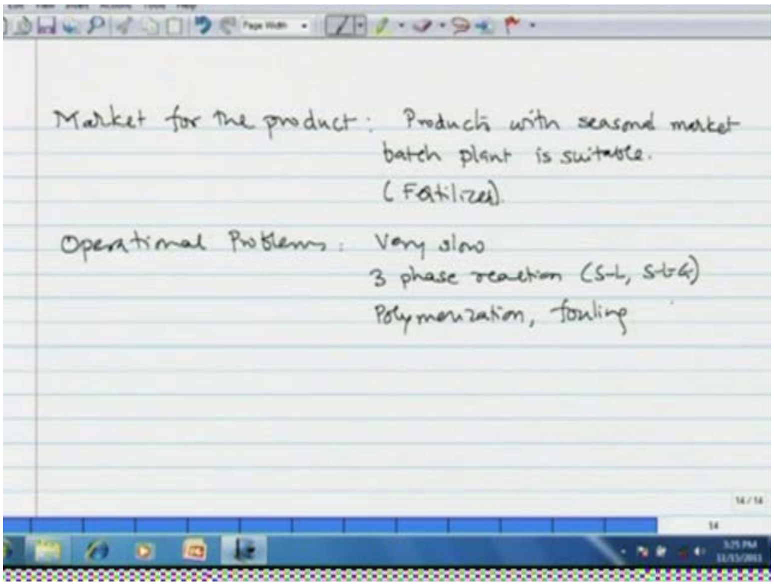


The next factor is the market for the product that some that the plant is making, for products with seasonal market batch plant is more suitable. And an example of this category is fertilizer, if the fertilizer is produced throughout the year, then we have to store for that fertilizer till the next season, which may increase the operating cost. Therefore, it is it is preferred to produce the seasonal product in a batch plant, then the operational problems some reactions might be very slow.

And therefore, if they are carried out in continuous reactors the volume of the reactor becomes very large, some reactors may use three phase reactions or two phase reactions solid liquid or solid liquid or gas type of reactions. Now, in this if the kinetics is small, then you have to pump the slurry with solid suspending liquid at a very small rate and that may cause settling of the solids. Now, in some cases where polymerization of the reactions, polymerization of the product occurs or fouling takes place frequently. Then also you cannot carry out the reaction in continuous mode, because you will have to shut down and clean up very often, which is not very practical.

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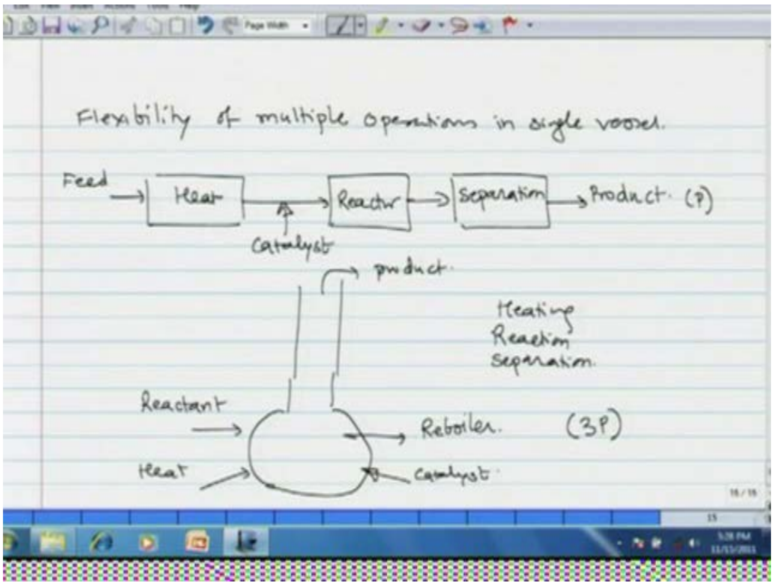


Finally the batch process offer flexibility of carrying out multiple reactions or multiple processes in a single vessel. Like consider a case where the feed is heated and then admitted in the reactor after addition of catalyst and then the product is separated with some process like distillation. Now, in a continuous process you will need three different vessels for heating of the feed, reaction and separation. However in a batch process you can carry out the same operation in a single vessel, which could be the reboiler of a distillation column.

You can take the reactant and then heat it, then add catalyst, let the reaction proceed and the product is simultaneously distilled off. Now, here the heating reaction and separation takes place in a single vessel. Now, cost of three separate vessels and cost of a single vessel is much different, there you achieve the economy of scale. However, if the production rate in a continuous process is P then to achieve the same production rate you will have to take a larger vessel which is of capacity 3 P.

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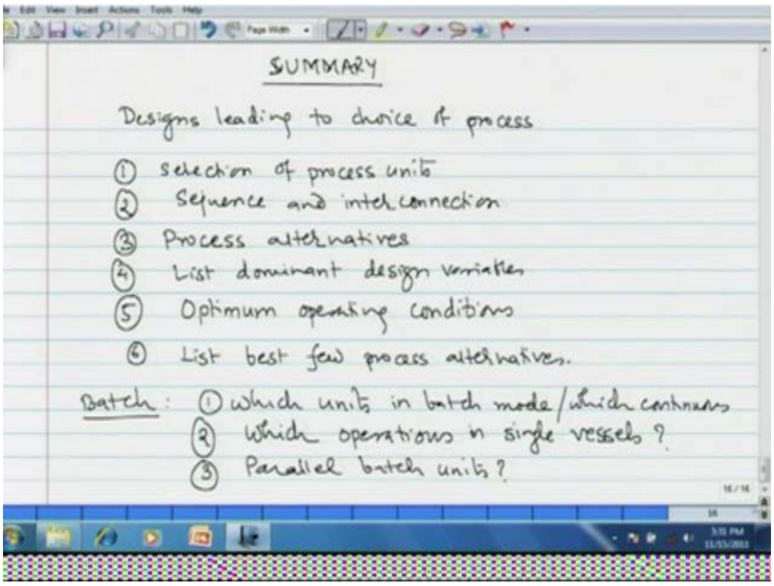


So, now we list the decisions that we need to the decision that we lead to choice of process whether continuous or batch. The first is selection of process units then optimum inter connection or sequence an inter connection, then the process alternatives that we need to consider. Then we need to list the design the dominant design variables, then the optimum operating conditions and on the basis of these criteria, we have to assist the profitability of the process and list the best few process alternatives.

However, in case of batch process we need to consider some more factors like for example, which units should be batch and which unit should be continuous. Then which operations can be coupled as we just saw like heating reaction and separation could be coupled. So, which operations to be carried out in a single vessel and for which operations you need separate vessels or can we use individual vessels in parallel steps.

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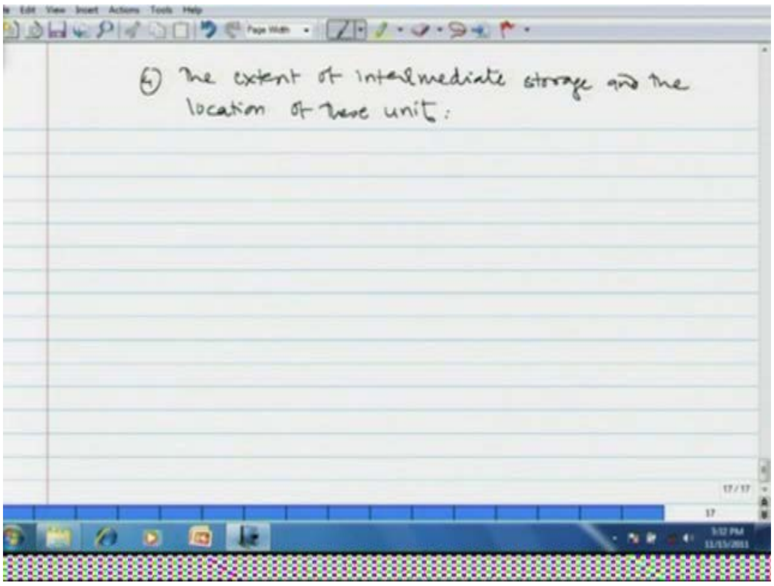


Then the extent of intermediate storage and the location. So, today we have seen the first stage in process synthesis that is decision, whether we have to go for continuous process and batch process. And we have also discussed in detail the factors that lead to this decision, in the next lecture we shall see the input output structure of the flow sheet in greater detail.