Chemical Reaction Engineering

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Lecture No. # 01

Introduction and Overview

Friends, I am Jayant Modak faculty of department of chemical engineering at Indian Institute of Science. And we are here to learn about chemical reaction engineering. This course is advanced undergraduate course; what it means is I expect some background knowledge in the form of at least one course in reaction engineering that you would have done in your sixth semester or fifth semester depending on your college. Today’s class, will be basically about giving you the introduction to the subject, and what we are going to cover; and why we need to study, what we are going to study.

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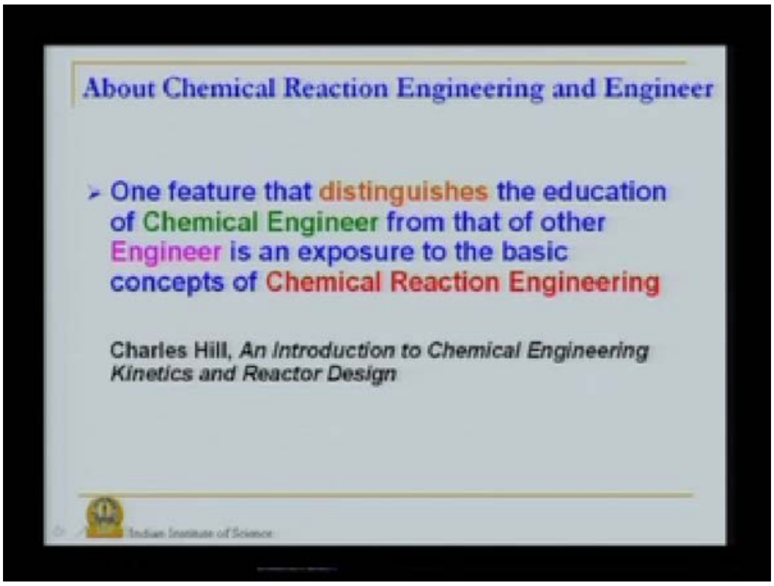

About Chemical Reaction Engineering and Engineer

- One feature that distinguishes the education of Chemical Engineer from that of other Engineer is an exposure to the basic concepts of Chemical Reaction Engineering

Charles Hill, *An Introduction to Chemical Engineering Kinetics and Reactor Design*

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So let us start with, what is chemical engineering. Charles hills in his book on introduction to chemical engineering kinetics, says that one feature that distinguishes the education of a chemical engineer from, that of other engineers is an exposure to the basic concept of chemical reaction engineering. You would have done several courses such as, mass transfer, momentum transfer, heat transfer which your friend in mechanical would have also done a similar course, friend in aerospace engineering would have done. But reaction engineering is one course, which uniquely characterizes the feature of a chemical engineer. So, this is one course that other engineering disciplines normally do not do.

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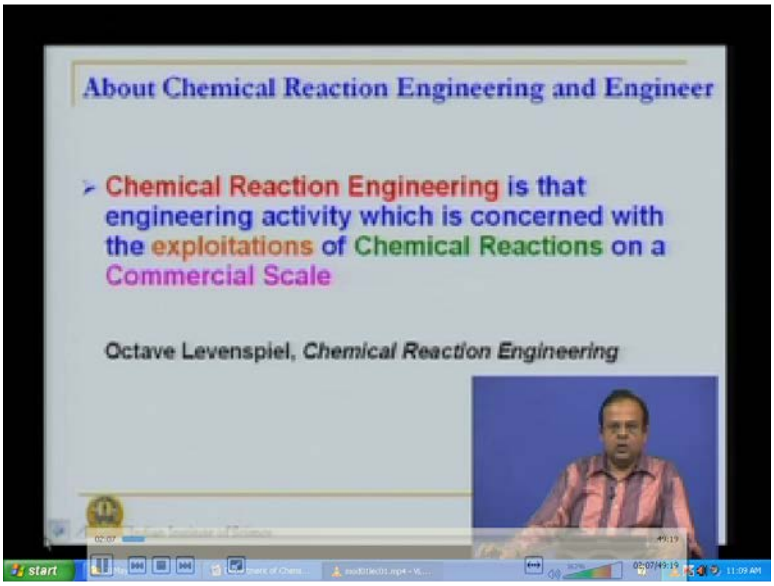

About Chemical Reaction Engineering and Engineer

- Chemical Reaction Engineering is that engineering activity which is concerned with the exploitations of Chemical Reactions on a Commercial Scale

Octave Levenspiel, *Chemical Reaction Engineering*

So what is it that we study in chemical reaction engineering. So Levenspiel in his classical book of chemical reaction engineering, characterizes chemical reaction engineering, as that engineering activity which is concerned with exploitation of chemical reactions on a commercial scale.

So, point to be noted here is chemical reactions at a commercial scale, which means that we are no longer interested only in looking at reactions, in the laboratories into 100 m l flask, 200 m l beakers or one liter reactors and so on, but we want to bring in the large scale operations of chemical reactions into our domain. This brings in lot of interesting aspects, about scale dependent processes such as, transport processes; and we will talk about those in this in this class.

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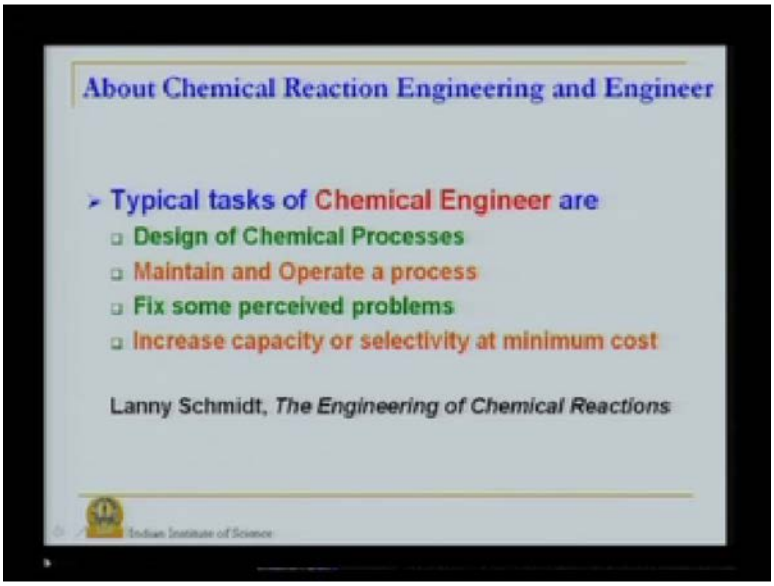

About Chemical Reaction Engineering and Engineer

- Typical tasks of Chemical Engineer are
  - Design of Chemical Processes
  - Maintain and Operate a process
  - Fix some perceived problems
  - Increase capacity or selectivity at minimum cost

Lanny Schmidt, *The Engineering of Chemical Reactions*

So what does a typical chemical engineer do, as as as far as reaction engineering is concern. The first and foremost is of course, is you can think of the design of chemical processes. That is you have a reaction, somebody has worked it out at a lab scale. So, you now want to design the complete process for making the desired chemical. Other scenario is, there is a process plant which is operating. So, you want to maintain that process going continuously or operate the reactors and so on.

Occasionally, there will be some troubleshooting that is required in the plant, and so you have to fix those problems that arise. Although these three activities are important; increasingly you will be focusing on the last task that I have listed over here; that is increase the capacity of the plant at the minimum cost. And area what is now known as process intensification, this is precisely what you do in that. That is you already have a plant, there is a process which is running; let us say it is making 1000 tons per annum of certain chemical, you want to increase that capacity to 1500, 2000. To, whatever maximum that you can you can achieve; and that to at a minimum minimum cost.

As you are all aware, that we are now concerned with the environment around us, and any adverse impact that our chemical process industries industries may leave or on on this environment. And therefore, we are worried about no discharge or zero discharge from your chemical plant. Increasingly legal requirements are being put in place which says that, you should not discharge anything into air or water that is that is going out from your plant into the neighboring environment. What it means, is that while you want to increase the capacity of your reactor or capacity of your plant, you also want to increase the desirable product product that is being made, to that of undesirable product. That is you want now only specific product that is which is desirable.

In other words, the selectivity of the desired product over that of an undesired product is is very important, and we need to focus on increasing those selectivity. So, all these activities come under a broad umbrella process intensification; and there are various ways of doing it, as the course progresses we will see some of them.

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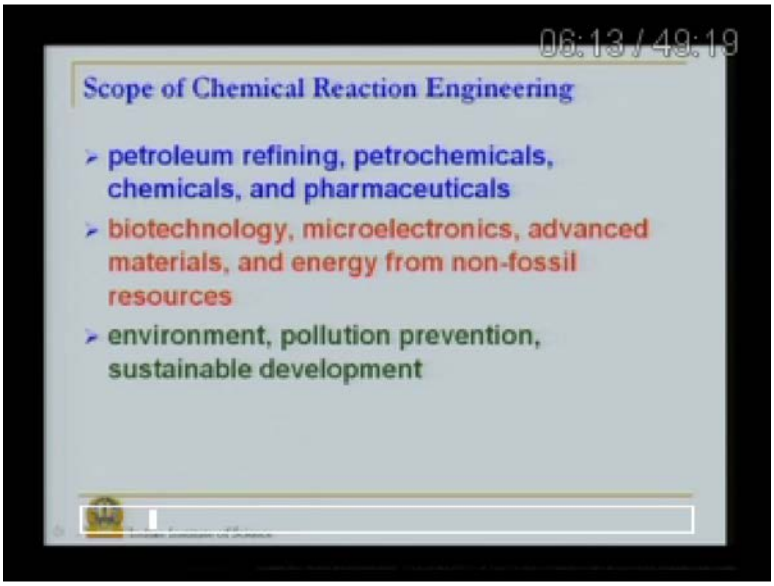

Scope of Chemical Reaction Engineering

- petroleum refining, petrochemicals, chemicals, and pharmaceuticals
- biotechnology, microelectronics, advanced materials, and energy from non-fossil resources
- environment, pollution prevention, sustainable development

Now, let us ask ourselves what does chemical reaction engineering intended for or what is the scope of chemical reaction engineering? And there are several aspects of chemical processes or products that we are familiar with some which, we are already familiar some which, we will become familiar as we move along. For example, traditionally people are used to thinking of chemical processes, concerning only with fossil fuels. So, anything and everything that has to do with petroleum refining, petrochemicals, several other chemicals, pharmaceuticals and so on. So that has been the traditional concept of chemical reaction engineering or chemical processes. But because of the training that we get as a chemical engineer, we are no longer just restricted to this traditional areas, but we are expanding into variety of different different fields.

And why is that that possible. That is possible, because you take example of chemical reaction engineering. You would have done little bit of kinetics of the processes or reactions, you would have learnt about different types of reactors and so on. You have, highly learned about any particular product that is being made in these reactors. Traditionally, we always talk of reactions as a plus b going to c plus d; without worrying what these a, b, c, d are. Now, what this has done to us is that we are focusing on basic fundamentals of chemical reactions, its kinetics, its rate and so on.

These basic fundamentals can be applied to variety of different fields. So, for example, take biological processes or bioprocesses or biochemical engineering as as we are now referring to. So, these are essentially processes involving living cells, and we are getting certain useful products from them, antibiotics and so on. Now, it turns out that even these living cells, there are lot of reactions that take place inside these cells. And the same physical, and chemical characteristic that ordinary reactions, let us say in a petrochemical industry are are are subjected to; the reactions inside the living cells, are also subjected to same same conditions or same physical and chemical conditions.

Now as a result of this, whatever we have learnt in chemical kinetics, we can easily extend it for living systems, and hence our foray into biotechnology. The same thing can be said about microelectronics, making of various kinds of devices - semiconductor devices, advanced materials, nano materials, energy from non-fossil resources and so on. So, we are slowly expanding our scope into variety of different fields, I mean the list does not end here; environment, pollution prevention, sustainable development these are all areas or fields of activities in which, our knowledge about chemical reaction engineering is going to be extremely useful.

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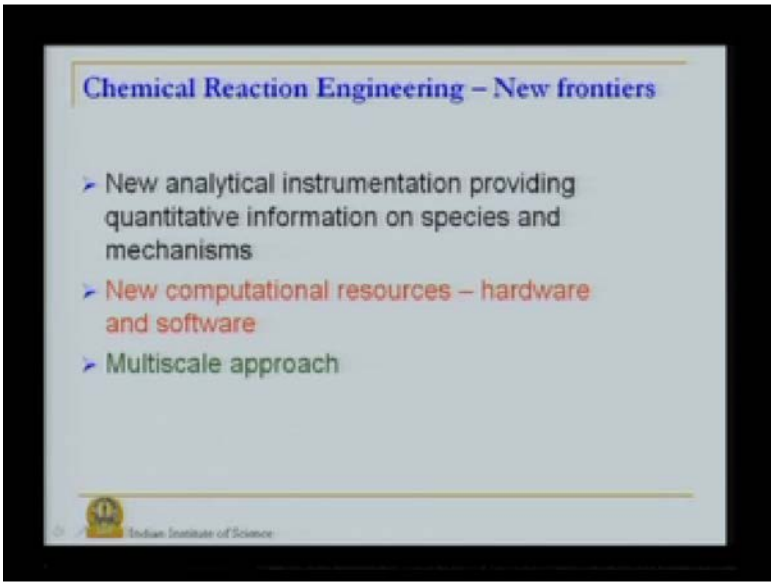

Chemical Reaction Engineering – New frontiers

- New analytical instrumentation providing quantitative information on species and mechanisms
- New computational resources – hardware and software
- Multiscale approach

Before we turn on to our chemical reaction engineering, I would just like to briefly point out to you. What are some of the new frontiers or new developments that are happening in the field of science and technology, which are influencing or which are having an impact on chemical reaction engineering discipline. The first and foremost among these is new analytical instrumentation that is being made available to us. All kinds of spectroscopic methods, enamors and different measurement tools which are providing us, not only the qualitative understanding, but quantitative understanding of how reactions proceed. And as a result, we are now able to prove these reactions, at a very wide variety of variety of skills.

Simultaneously, we also have lot of computational resources both in the form of hardware and software, which are available to us. And we are making full use of it. To give you an example, as we speak chemical plant in Spain for example, is being monitored and controlled by people sitting in Bangalore; that is possible, because the entire operation has been networked; the sensors, the controllers have all been networked. And once you do that, once the information is available as as the say at speed of light or even faster; it is easy to do job what you would, you would normally do sitting next to the process plant, you could you could as well sit thousands of miles away and carry out the same same operations.

There is also an fundamental difference in approach, that is entering into our field of chemical reaction engineering. Namely, multi scale - multi scale approach; as you would as you would have seen for example, chemical plants are typically big in sizes, You can measure their dimensions in meters and so on. However, the processes which take place inside these reactors are happening at a atomic, and molecular level. That means, we are spanning the entire lengths scale for example, if you if you like to speak from mike (( )) meters or nano meters to meters, several meters tends of meters and so on. So, very large or 10 raise to 9, 10 raise to 10th order of magnitude difference in scales. This is about special variation. The same thing can be said about time.

For example, in a chemical plant, we generally talk about residence time; which could be in order of minutes or hours or in some cases even days. However, once again the processes are taking place at atomic level or molecular level which are occurring at the time intervals of femto seconds, nano seconds, and so on. So, both in terms of time, and length; we are dealing with processes which are multi scale. And various computational tools that are being available to us, have enabled us to carry out these studies by incorporating phenomena occurring at all levels, and thereby making analysis of reactors more meaningful.

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Top Global Players in 2008

Rank	Company	Sales $ bn
1	BASF (Germany)	70.5
2	DOW (U.S.)	57.5
3	Ineos (UK)	36
4	LyondalBasell	38.4
5	ExxonMobile Chemicals (USA)	38.4
27	Reliance Industries (India)	12.6

Chemical & Engineering News, August 2009

Indian Institute of Science

Now, before we go into go into the subject matter, it is always nice to know what is happening in outside world, outside industry. And I typically start my lectures these; these lectures series by telling who are the global players in the in the field. And this list is taken from chemical and engineering news august 2009, tells us about what who who are the players or companies in the market for top ranking, top ranking chemical companies. And here I have not included pharmaceuticals or biotech companies and so on. I am I am referring to purely chemical companies.

There you see, BASF having occupied number one position for last several years now, at global sales of about 70 billion. Dow from united state comes in the second place, and then at number 3 and 4 are two companies which probably you would not have heard, even I had not heard them till couple of years back. Ineos and Lyondalbasell - these are actually companies which are conglomerates or which have grown in volume by taking over smaller companies, by acquisitions mergers and so on. The fifth one is of course, Exxon Exxon mobile, and the last in the least that you see is our own homegrown company reliance industries, and that occupies 27 th rank in the global global scenario of having sales of about 12.6 billion dollar annually.

Now, there is something else also happening in the in the market, which is which is shown in in in the next slide.

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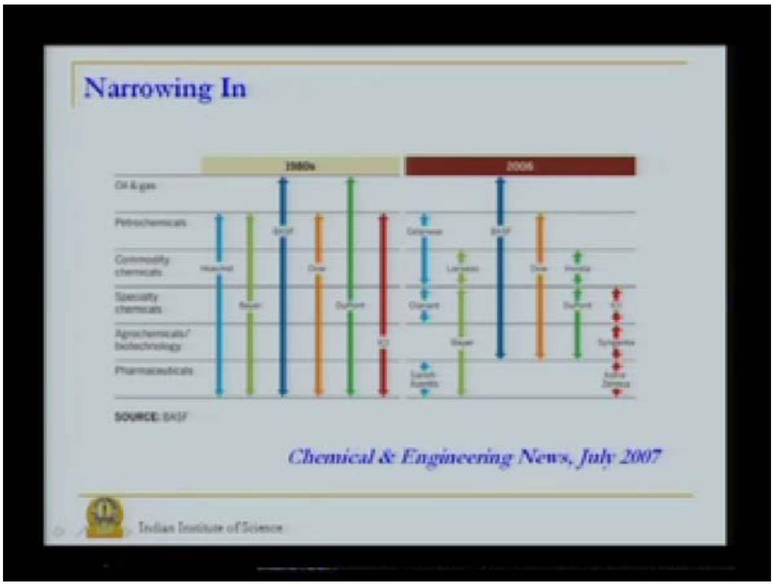

Narrowing In

SOURCE: BASF

Chemical & Engineering News, July 2007

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That how is chemical industry functioning. Now, you may not be able to able to read this clearly, but what what what is being shown is what was the status in 1980’s. And what is the current status; 1970’s and 80’s saw companies expanding their operations across the board of various different activities. For example BASF was involved in right from oil, and gas to agrochemicals to pharmaceuticals; same was the story with dupont. Over a period of time, they realized that such diversification in today’s world, is not giving the returns that they any anybody would expect. And therefore, the focus is now, focusing on core competency of the of the company, and getting rid of the other businesses where it may not be on the mains core area of the company.

For example BASF has given away their pharmaceuticals. So, is the case with dupont which have come out of petrochemicals, oil and gas, and so on. So, we are now looking at a industry which is which is narrowing in or becoming focusing more on the key sector, rather than doing everything under the under the sun.

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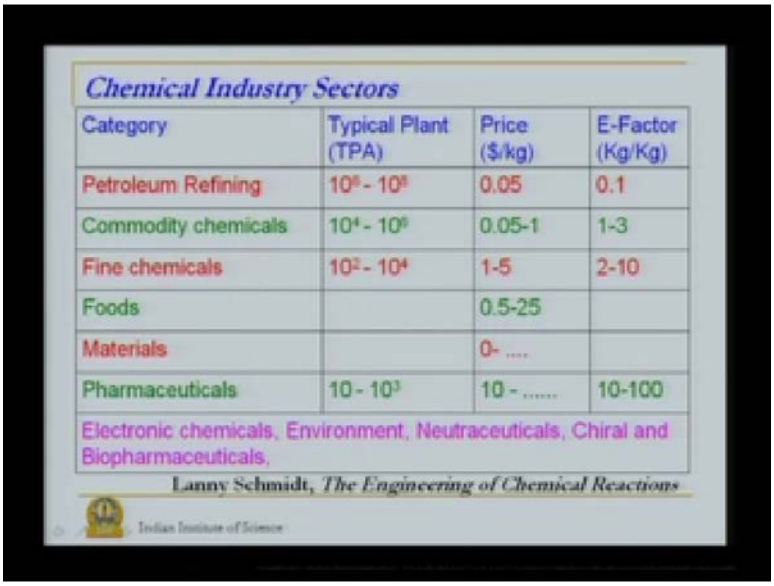

Chemical Industry Sectors

Category	Typical Plant (TPA)	Price ($/kg)	E-Factor (Kg/Kg)
Petroleum Refining	$10^6 - 10^8$	0.05	0.1
Commodity chemicals	$10^4 - 10^6$	0.05-1	1-3
Fine chemicals	$10^2 - 10^4$	1-5	2-10
Foods		0.5-25	
Materials		0-	
Pharmaceuticals	$10 - 10^3$	10 -	10-100
Electronic chemicals, Environment, Neutraceuticals, Chiral and Biopharmaceuticals.			

Lanny Schmidt, *The Engineering of Chemical Reactions*

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Now, let us look at chemical industry different sectors, and how are they how are they comparable, compared with each other. For example, what I have shown here, is different types of, different category of sectors. Their typical operating operating size; the price per kg, price is in dollars, per kilogram that these products command. And then the last factor, environmental factor or e factor, that is the amount of waste generated that is kilogram of waste generated, per kilogram of product desirable product that is produced. And you see there is a wide variation between different chemical chemical sectors.

For example, typical size of petroleum refining is nothing less than 10 raise to 6 or one million to hundreds of million tons per annum. That is the typical size, the price that it fetches is about 5 cents a kg, and the waste is generate is about 0.1 kilogram per kilogram of product that is that is generated. Now, you can then look at other different categories; for example, commodity chemicals, fine chemicals, foods, materials, pharmaceuticals and all the remaining remaining other.

Now, what you see here, is the size of a typical plant is decreasing, as we are going down the list. But the price that the finish product gives us is is increasing, as the size is decreasing. And so is the waste that is undesirable materials, that is generated; you for example, you take pharmaceuticals. Is not unrealistic to see, that you actually generate 100 kilogram of waste per kilogram of kilogram of material that you produce. And the reason reason for this, is that pharmaceuticals pharmaceuticals or specialty chemicals are typically produced in very dilute quantities. There concentrations could be ppm, if not ppb. And therefore, to get a kilogram of desired chemical, you have to separate out 10s of 100 of kg's of undesired material. So that, you get that final final product.

The reason for showing this kind of comparison is is also for the fact, that because of these variations in different different sectors. The focus of process improvement or process intensification, could also change when you go from one sector to one sector to other. For example, in pharmaceuticals or bio chemicals; since, they are they are produced in such a dilute concentrations. The focus is mostly on separating or separation processes rather than worrying about how to improve the reactor and so on. But that is not the case for example, with petroleum refining, and so on. So, depending on the process or the product that one is looking at, we have to, we have to decide on what activity will eventually lead to improve profitability and so on.

Now, as I said, this is an undergraduate or advanced undergraduate or graduate level course. So, you would have done reaction engineering, one at least one course of reaction engineering. How do we how do we now move forward or what are some of the interesting aspects of chemical reactions that we need to know, before we start with our with our course that is from the next next lecture.

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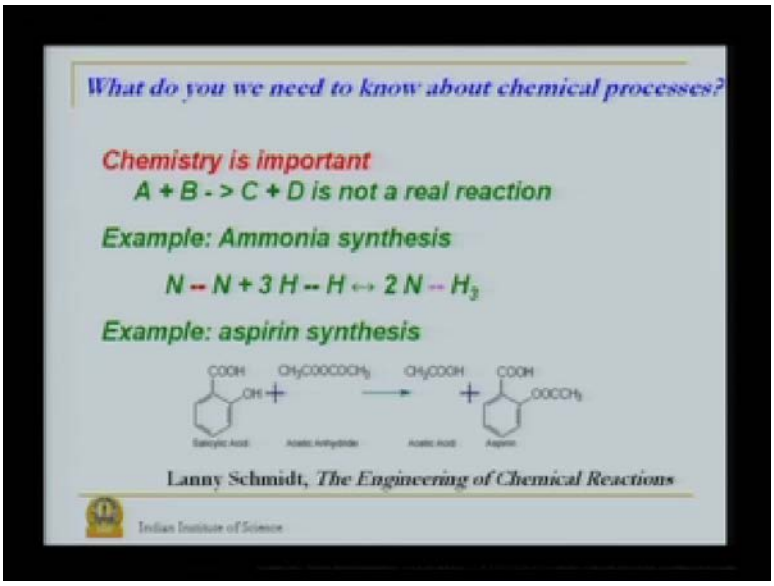

What do you we need to know about chemical processes?

Chemistry is important

A + B - > C + D is not a real reaction

Example: Ammonia synthesis

$N - N + 3 H - H \leftrightarrow 2 N - H_3$

Example: aspirin synthesis

Lanny Schmidt, *The Engineering of Chemical Reactions*

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So, what do we need to know about chemical chemical processes. The first, and foremost most important thing is chemistry is important. As I said few minutes back that typically we have been used to studying reactions as A plus B goes to C plus d. Now, we should realize that A plus B going to C plus D is not a real reaction - there is some species A, there is some definite species B, and so on.

So take for example, Ammonia synthesis; it is nitrogen plus 3 moles of hydrogen giving rise to two moles of NH 3. Now, it may appear to be simple enough, to just say it that one can represent these reactions as A plus 3 B going to C, but notice what has to have has to happen for ammonia to be formed. For example, the bond between two nitrogen atoms has to be broken; so, is the bond between the two hydrogen atoms, and after that the bond between nitrogen and hydrogen has to be form. In the case of, in the case of ammonia; so, it is not just the just A plus 3 B, there are lot of things happening at a molecular, and atomic level which are equally important, which makes up how the reaction will proceed and so on. And, we should never lose sight of this this aspect.

Another example is this aspirin. You know when you get headache, we all run to our medical cabinet, and take aspirin or its equivalent. Now, the reaction of aspirin synthesis is actually a reaction between salicylic acid, and acidic anhydrate giving raise to acidic acid, and this wonderful compound, there is aspirin. So, there is lot of chemical rearrangement for breaking up bonds, formation of bonds, and we we should we should keep focus of of this aspect. That is chemistry is chemistry is important. So, that is first thing that we should we should worry worry about. Now, I should also tell you that we are not going to focus on chemistry, and mechanisms of reactions, except may be few examples during this course. But I want to emphasize again, that chemistry is at the heart of chemical engineering or chemical reaction reaction engineering.

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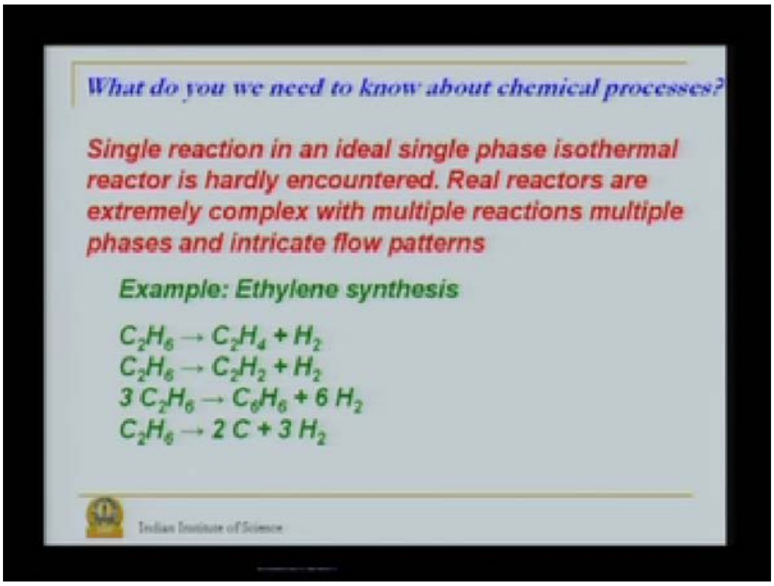

What do you we need to know about chemical processes?

Single reaction in an ideal single phase isothermal reactor is hardly encountered. Real reactors are extremely complex with multiple reactions multiple phases and intricate flow patterns

Example: Ethylene synthesis

$C_2H_6 \rightarrow C_2H_4 + H_2$

$C_2H_6 \rightarrow C_2H_2 + H_2$

$3\,C_2H_6 \rightarrow C_6H_6 + 6\,H_2$

$C_2H_6 \rightarrow 2\,C + 3\,H_2$

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The second thing, that we need to we need to worry about, when we talk about real reactions or reactions in the real world is that single reaction, I will read this out, single reaction in an ideal single phase, isothermal reaction is hardly encountered. For example, in a in a typical four standard graduate course, one talks about single phase reaction, isothermal reactor in a single single CSTR or plug flow reactors and and so on.

However in reality, reactions are hardly as simple or they are carried out in this simplistic manner. The real reactors are extremely complex with multiple reactions taking place in different phases, that are present in the reactor, and various intricate intricate flow patterns. And I will illustrate this one by one by giving some suitable suitable example

We are all using the product polyethylene or in many product made form this, the monomer for this polyethylene is ethylene. So, the simplest way of making ethylene is dehydrogenation of ethane. So we have ethane, getting dehydrogenated giving raise to ethylene. However, in a real reactor this would not be the only reaction that is that is taking place. For example, ethane can give raise to give raise to ethylene or as well ethylene, as well as acetylene or ethane can give raise to cyclohexane or ethane can give raise to simple carbon, and hydrogen.

All these reactions are producing producing hydrogen. The point is that even though your product of interest is ethane, when you have these reactions which are possible, which can occur simultaneously unless you do not, unless you do not control your reactions properly. There is a every possibility that you can have, not only ethylene in your reactor, but also acetylene, cyclohexane, carbon, and so on. Or in other words, it is important that when you design your reactors, the selectivity for the first desired product has to be improved in comparison to all the other products that are likely, in this in this process.

So, this is where the selectivity comes into picture, because if you do not, then not only you are wasting your precious resource namely ethane, in making all undesirable products. It may turn out that this undesirable products are toxic. And unfortunately that is the case in many many such examples. That it is always undesirable products which cause problems, not the desirable product. Or in other words, we have to we have to ensure that while we promote this first reaction which is a desired reaction, we make sure that these other reactions do not do not take place. So, we have not just to deal with single reaction, but multiple reactions involving various different different chemical species. So, our understanding or our study of reaction engineering or reactors must start with with such with such realization.

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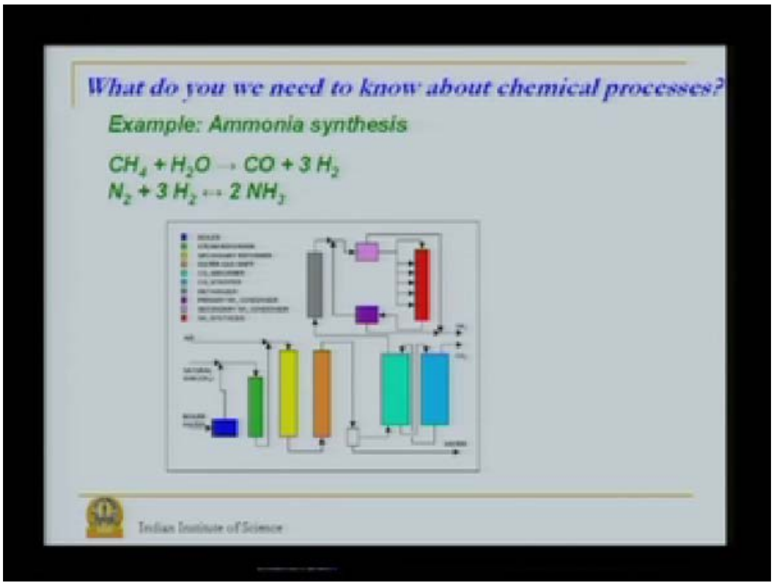

What do you we need to know about chemical processes?

Example: Ammonia synthesis

$CH_4 + H_2O \rightarrow CO + 3H_2$

$N_2 + 3H_2 \leftrightarrow 2NH_3$

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The next thing that we need to know is that, chemical reactors are never designed in its isolation. For example, take take ammonia synthesis, we took this example earlier. So, we have one mole of nitrogen, 3 moles of 3 moles of hydrogen giving raise to two moles of ammonia. Now, in the classroom, when you deal with your design problems, you may actually just design the reactor for ammonia synthesis, saying that I will focus on nitrogen and hydrogen as my input material, ammonia as my as my output material. But in reality, the problem is much more complex. And what you actually see here by way of this flow diagram is the entire setup or the plant consist which which is which is representing the ammonia synthesis, synthesis process.

So, you may be wondering what are all these other units other units doing. So, this is for the following fine. Even though, we can say that our raw material is nitrogen and hydrogen, where do we get these raw material. Nitrogen of course, we can get it from here, that is plenty of it; provided you remove oxygen. But what about hydrogen - where do we get this hydrogen. We get this hydrogen from this first force reaction; that is methane plus water giving raise to carbon monoxide plus hydrogen. So, hydrogen which is to be used for ammonia synthesis is to be generated in C 2, because you cannot generate gas in one place and transport it, it is not easy to transport gas.

So, this reaction has to occur simultaneously. So, what we see now is actually a apart from apart from main reactors, you see all these other reactors that are that are involved in making of making of hydrogen for example. The problem does not does not end here; so, we have for example, natural gas that is methane coming in with boiler water, and you are ammonia the hydrogen generation, that hydrogen goes to our ammonia synthesis and so on.

Now, problem does not end there, because it turns out that the catalyst which is required for synthesis of ammonia, is inhibited strongly by presence of even trace quantities of carbon monoxide. So, while we are generating hydrogen, we cannot just pass this product mixture to the ammonia synthesis reactor, but before we do that, we have to ensure that this carbon monoxide is completely removed. So that, no trace quantity is there; and therefore, we we we we can then pass this hydrogen into the reactor. So, not only are there reactors here, there are absorber for removal of carbon monoxide. So, we must remove this carbon monoxide from the, from the reacting reacting system.

So now, my ammonia synthesis design process involves the synthesis of hydrogen, removal of carbon monoxide, ammonia synthesis and finally, you would not you do not get 100 percent conversion - 100 percent conversion is only in in the in the dream, it is not in the real world. So, you have lot of unreacted nitrogen, and hydrogen which you do not want to just bleed off, but you want to recycle. So, you have a recycle stream. So, the entire chemical design or process design for the chemical reaction, will now involve all these sub units. And remember, these sub units are all linked to each other. So, any improvement that you try to do in one process, is going to influence the performance of other process.

So, process intensification for example, we will have to consider all this together. So, we have multiple reactions taking place in our reactors, not only that in a chemical plant per say, there are multiple reactors which are which are operating, which have to be suitably suitably designed.

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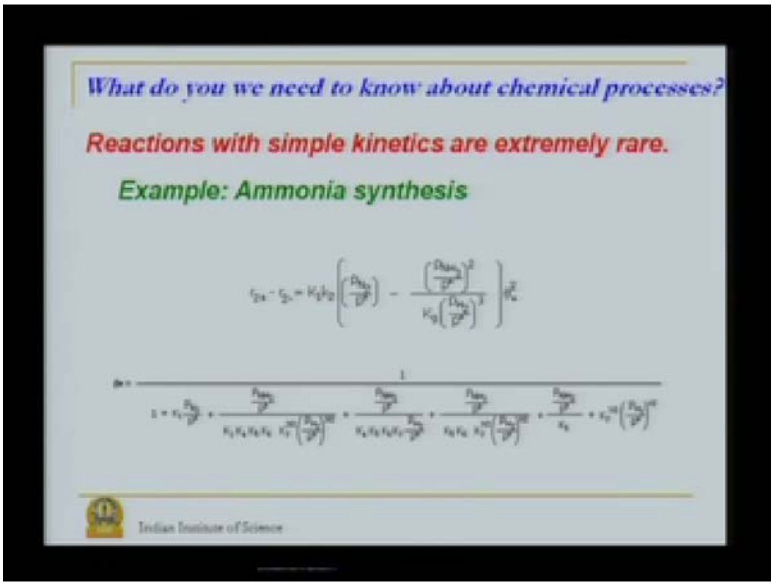

What do you we need to know about chemical processes?

Reactions with simple kinetics are extremely rare.

Example: Ammonia synthesis

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Now, let us come to the next aspect of reaction engineering. Namely, we would have done kinetics. And we always talk about first order kinetics or even better zero order kinetics; first order kinetics, second order kinetics and so on. Now, chemical reactions with simple kinetics are extremely rare. In practice, the kinetics of the processes are fairly complex. I have given here an example of ammonia synthesis, which tells us what is the rate of synthesis of ammonia. And it is it is actually a complicated equation involving nitrogen partial pressure, hydrogen total pressure, ammonia pressure and so on. And it is a complex function. Do not worry, even if you are not able to see in its detail - the details are not that important at this stage, the message I am trying to communicate to you is that, it is a fairly complex kinetics, it is not simply rate of ammonia synthesis is partial pressure of nitrogen into partial pressure of hydrogen raise to power 3. It is not as simple as simple as that.

Now, so what? You may ask, so what if it is not simple, it is a complex kinetic. The complex kinetics often lead to, very different kinds of phenomena, when you operate these reactions in the real reactors. And these can give raise to for example, run away reactions; where things are happening normally, but suddenly because of some small perturbation in the in the reactor; things just explore for example, or temperature just shoot up; the there is a there is a runaway what what we call runaway reactions.

Most of the times, the tragedies that are associated with chemical reactors or chemical plants is a result of such uncontrolled reactions. You have not designed your reactor for running for uncontrol, you are designed them perfectly well. They were indeed running perfectly well for decades, but suddenly something happens and reactions goes uncontrolled. Bhopal gas tragedy for example, which happened in 1984 was a result of one such one such behavior. The tennessee gas valley explosion which took place in united states in 70 (s) is is another example, and there are countless number of number of examples. Very often, I am not saying always, but very often the reason why reactions behave in such an sensitive manner is linked to the kind of kinetics or complex kinetics, and the results resulting behavior that we get.

And therefore, we must try to understand how does this kinetics come about; what what so, origin of this kind of crazy which may at at in present moment looks completely strange, and crazy behavior. What is what is the origin of this kind of kinetic rate expressions. We tried to spend initial part of our lectures looking at behavior behavior of such such type, because ultimately when we design reactors such kinetics has a major major role to play.

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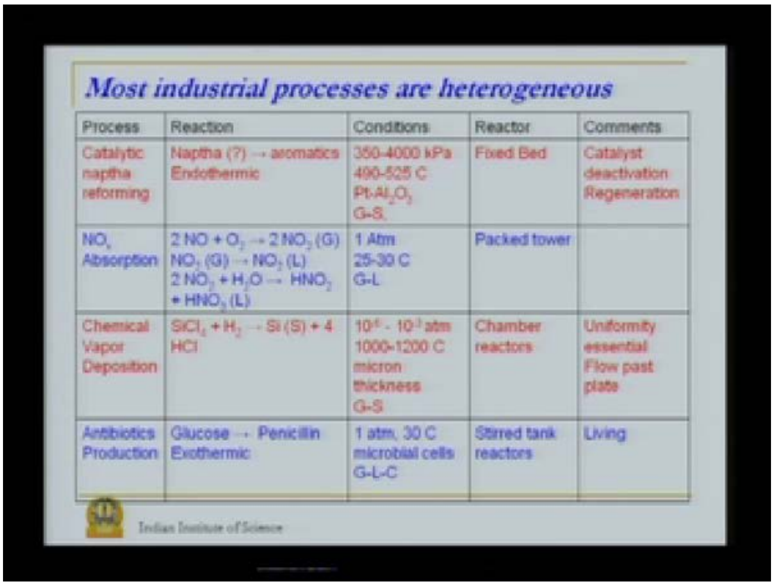

Most industrial processes are heterogeneous

Process	Reaction	Conditions	Reactor	Comments
Catalytic naptha reforming	Naptha (?) → aromatics Endothermic	350-4000 kPa 490-525 C $Pt-Al_2O_3$ G-S	Fixed Bed	Catalyst deactivation Regeneration
NO_x Absorption	$2 NO + O_2 \rightarrow 2 NO_2 (G)$ $NO_2 (G) \rightarrow NO_2 (L)$ $2 NO_2 + H_2O \rightarrow HNO_3 + HNO_2 (L)$	1 Atm 25-30 C G-L	Packed tower	
Chemical Vapor Deposition	$SiCl_4 + H_2 \rightarrow Si (S) + 4 HCl$	10[illegible] - 10[illegible] atm 1000-1200 C micron thickness G-S	Chamber reactors	Uniformity essential Flow past plate
Antibiotics Production	Glucose → Penicillin Exothermic	1 atm, 30 C microbial cells G-L-C	Stirred tank reactors	Living

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So, we started out saying that reactions are hardly ever single reactions, kinetics is never simple first order, second order kinetics. We also use we are also used to thinking that reactions are homogeneous or there is only one phase, that is that is happening, but most industrial processes are heterogeneous in nature. And what I have shown here is few examples of such heterogeneous reactions; what are the actual reaction - what are the conditions - what is the reactor that is used, and few general general comments.

For example take Catalytic naptha reforming reactions. So, this is a this is a reaction which gives from naptha we get different aromatics, and different different useful useful chemicals. Notice here, I have put naptha question mark. The firs thing that strikes when I write a reaction like this, is that this is no precise information is available, as far as my reactants are concerned, and as far as my products are concerned. I am just calling some quantity or some group of chemicals as naptha; and some other group of chemicals as aromatics.

And in reality that is the situation; that I cannot in (( )) naptha cracking process or reforming process, I do not know what is the precise composition of this of this naptha perceive. And so is what is these aromatics; so that is another problem that we encounter. That we have to design reactors, where we do not know what precisely what is our reactant - what is our product. So, but reactors have to be designed; so how do we deal with that. That we will see, it little later.

Now, look at the conditions. So, this is a this is a high pressure process, moderate temperature a catalyst, and essentially a gas-solid system. NO X absorption, again an environmental problem; where you want to you want to adsorb this obnoxious gases into water, and gas-liquid reaction fairly mild conditions. Actually atmospheric pressure and ambient conditions, but gives raise to various interesting phenomena. Again an example from semi-conductor industry, chemical vapor deposition; so, you want to get pure silica in the form of plates or whatever. It is done by silicon tetra chloride reduction of it, so it is a gas phase chemical reactants, resulting into solid product; and so gas-solid reactions occurring at extremely high temperatures, but extremely low pressures.

So, wide variety in terms of in terms of operating conditions, and the last example is of course, antibiotic production, where you have glucose, penicillin giving that is starting with sugar, you get antibiotic again using living cells. So, we will talk about this. So, the point is these are all heterogeneous heterogenous reactions; so this, there are more than one phase present. So, you have gas phase, and you have liquid phase.

Now, the moment you have two phases - there is a interphase between the two. So, the moment that is a interphase between two phases; there is a resistance to transfer from one phase to another phase. Or in other words, we are now coming into domain, where transport phenomena becomes an important aspect of your chemical reaction engineering. So, not just the kinetics, but transport phenomena is is is important.

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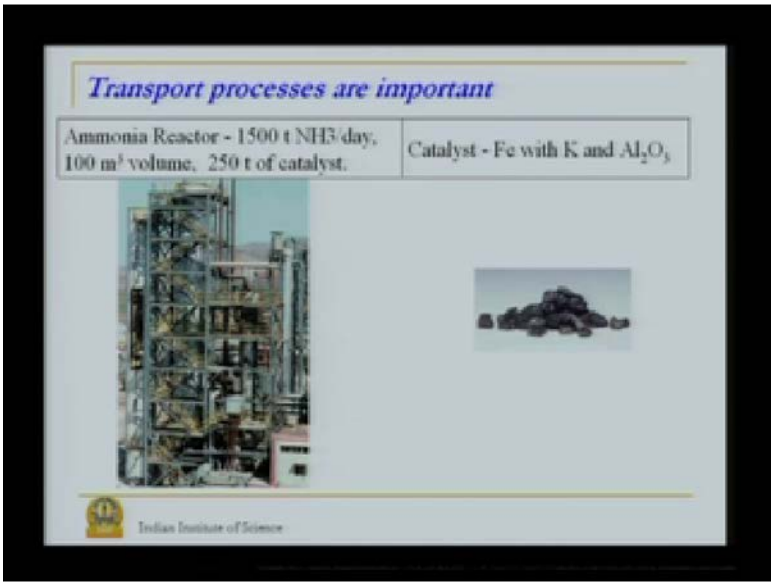

Transport processes are important

Ammonia Reactor - 1500 t NH3/day, 100 m^3 volume, 250 t of catalyst.	Catalyst - Fe with K and Al_2O_3

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Here is an illustration of what do I mean by transport phenomena is important from a different different aspect. What you see on the left hand side, is again once again the ammonia synthesis reactor which is roughly 100 meter cube in volume, contains about 250 tones of catalyst in this whole whole reactor; and it produces about 1500 tons of ammonia per day. Now, this so you can imagine the lengths scale here, in terms of meters and so on. But the actual conversion of nitrogen, and hydrogen to ammonia is brought about by this catalyst, namely ion with potassium and alumina which is in the form of pellets of few millimeter. So, on one side you have process occurring at meter scale length, by a catalyst which is in few millimeters, but its outer size is few meters, the actually where the reactions is taking place is in micron sizes, and so on. So, we have to study about transport processes occurring at all these levels; from micron level to millimeters to meters and so on. So, these processes become become important.

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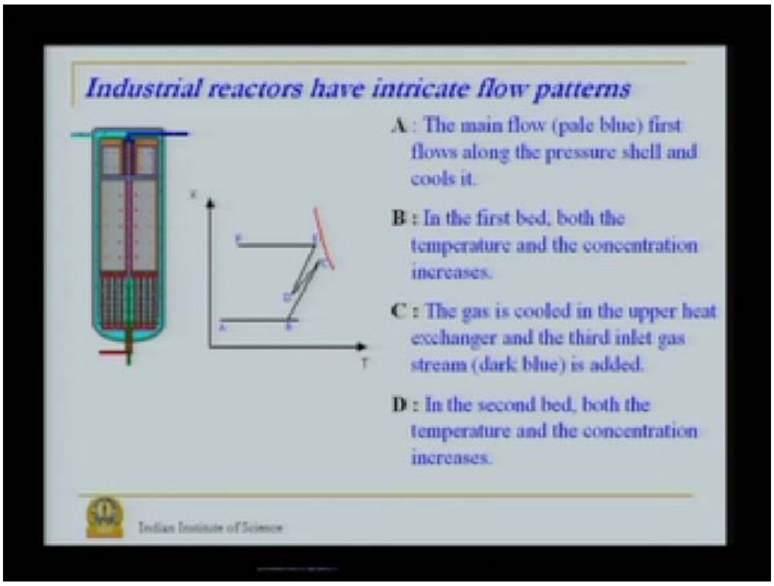

Industrial reactors have intricate flow patterns

A : The main flow (pale blue) first flows along the pressure shell and cools it.

B : In the first bed, both the temperature and the concentration increases.

C : The gas is cooled in the upper heat exchanger and the third inlet gas stream (dark blue) is added.

D : In the second bed, both the temperature and the concentration increases.

So these are some of the aspects of of reactors, that we need to we need to study. Now, last point when we talk about let us say, chemical reactor, a tubular reactor we are always used to thinking a tube, material comes in from one side reacts and goes from another side. Now, actual reactors are hardly of of that nature. What you see here is a tubular reactor for again ammonia synthesis kind of situation, where the reactants are actually coming in from the top, going all the way to the end, then again flowing upwards and so on. That is the flow patterns are quite intrinsic. They are not straight one way entry, one way exit. But there are all kinds of loopings and so on. And this is, because of the reaction - properties of these reactions, and we will study little bit about this as time progresses.

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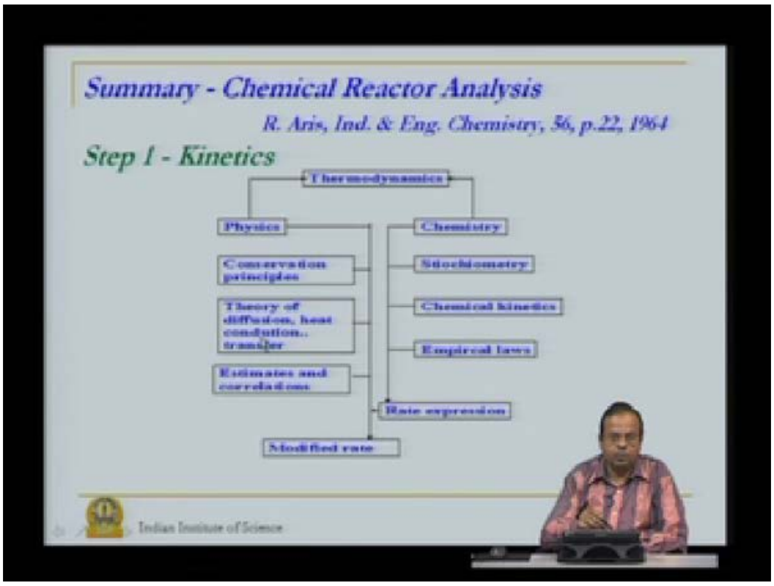

Summary - Chemical Reactor Analysis

R. Aris, Ind. & Eng. Chemistry, 56, p.22, 1964

Step I - Kinetics

Thermodynamics

Physics

Conservation principles

Theory of diffusion, heat condution., transfer

Estimates and correlations

Chemistry

Stiochiometry

Chemical kinetics

Empirical laws

Rate expression

Modified rate

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Now, I will conclude today's class by giving you, and brief overview of how we analyze chemical reactors. And this classic frame framework was given by Aris, in way back in 1960's middle 60's, and it is very much applicable even today. So, we study chemical reactors at two levels. Step one is the kinetics of the kinetics of the process - and this kinetics in turn is we use thermodynamic information, both chemistry as well as physics of the problem is important. So, we have thermodynamics, the chemistry of the reaction, stoichiometry of the reaction, kinetics of the reaction, and some empirical laws. So this is the chemistry of the reaction.

The physics essentially involves conservation principles, mass has to be conserved; various transport processes that is diffusion, conduction, heat transfer processes, and so on. So, by putting this transport information as well as kinetic information, we develop rate expression or rate expression as defined by kinetics, which may get modified as as the transport phenomena takes place. Now, I want to emphasize one aspect which is which is crucial. This part of the reaction that in namely the chemical parts stoichiometry, is not dependent on scale; that is the stoichiometry of the reaction does not change, if you do reaction in 10 m l flask or 10 m l test tube or 10 meter cube reactor. So, is the case with the kinetics, so is the case the rate of reaction in general.

However, it is the transport processes which are scale dependent. So, depending on whether reaction is taking place at 10 m l level or 10 meter cube level. Theses diffusion, conduction, transfer processes will be different; and thereby making the rates of reaction sometimes different at different scales. So, pure kinetics is scale independent, transport is scale dependent, when you put together the actual reaction rate or kinetics becomes scale dependent.

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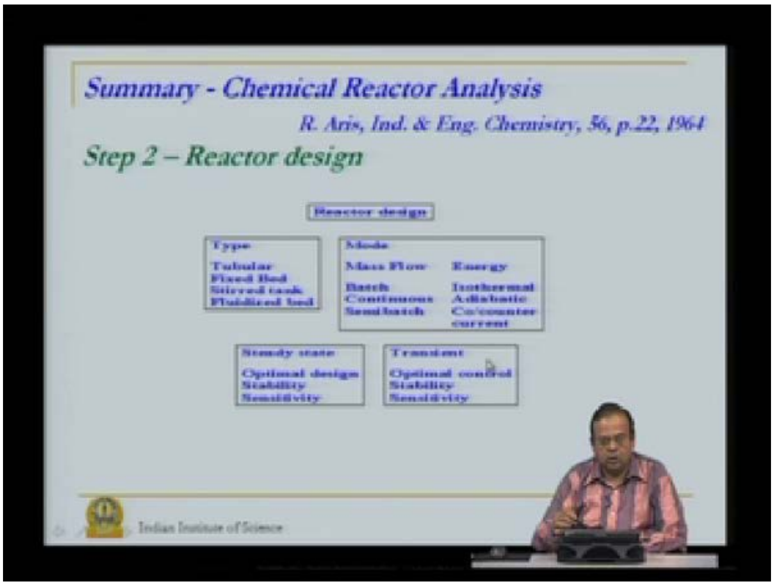

Summary - Chemical Reactor Analysis

R. Aris, Ind. & Eng. Chemistry, 56, p.22, 1964

Step 2 – Reactor design

Reactor design

Type
Tubular
Fixed Bed
Stirred tank
Fluidized bed

Mode
Mass Flow
Batch
Continuous
Semibatch

Energy
Isothermal
Adiabatic
Co/counter current

Steady state
Optimal design
Stability
Sensitivity

Transient
Optimal control
Stability
Sensitivity

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So this is at the kinetic level. Then next is the reactor design which essentially consist of, consist of looking at what kind of reactors, we we are going to use. That is the type of reactor, the mode of operation that is do we use classification, again based on mass flow or energy flow. So, do we use batch process or continuous process or semi batch process or based on energy do we use isothermal processes, adiabatic processes, co-current or countercurrent processes and so on.

So, reactor design essentially deals with deciding on the type of reactor, how to operate it. And what happens when the reactor is either operated at steady state or at transient. So, these are some of the aspects of reactor design, that we are going to focus on.

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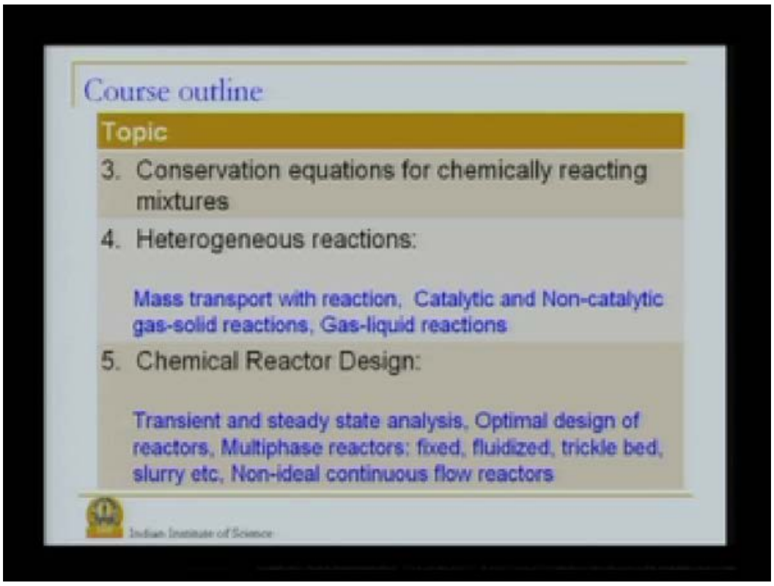

Course outline

Topic
3. Conservation equations for chemically reacting mixtures
4. Heterogeneous reactions: Mass transport with reaction, Catalytic and Non-catalytic gas-solid reactions, Gas-liquid reactions
5. Chemical Reactor Design: Transient and steady state analysis, Optimal design of reactors, Multiphase reactors: fixed, fluidized, trickle bed, slurry etc, Non-ideal continuous flow reactors

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So in summary let me let me say, this course is going to be carried over next 40 lectures actually 39, if you discount today's class. And these are the topics, that we are going to deal with. Starting with review of some undergraduate material, it is always to look back before we go forward. So, some of the things that you would have already seen, may be in a slightly different form. Coming then to the kinetics of complex reactions, I mention that there are all kinds of different kinetics that come in; so we will spend little bit of time on that. Conservation equations for chemically reacting species, and then we will spend quite a bit of time on heterogeneous reactions. That is I said there are more than one phase. So, what happens when we have more than one phase in the reactor.

So, we have to worry about not only just reactions now, but transport phenomena, and here we come across various different catalytic and non-catalytic reactions. The last portion of our course, would be about chemical reactor design, both transient and steady state operations, looking at optimal design of reactors, various multiphase reactors, some non-ideal flow conditions that come in. So, this in short is the overall introduction to the course, that we are going to look at in subsequent classes, thank you.