Continuum Mechanics And Transport Phenomena
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Lecture - 01
Measurement and Prediction Part 1

Welcome to this online course on Continuum Mechanics and Transport Phenomena. This lecture is about the introduction to the course.

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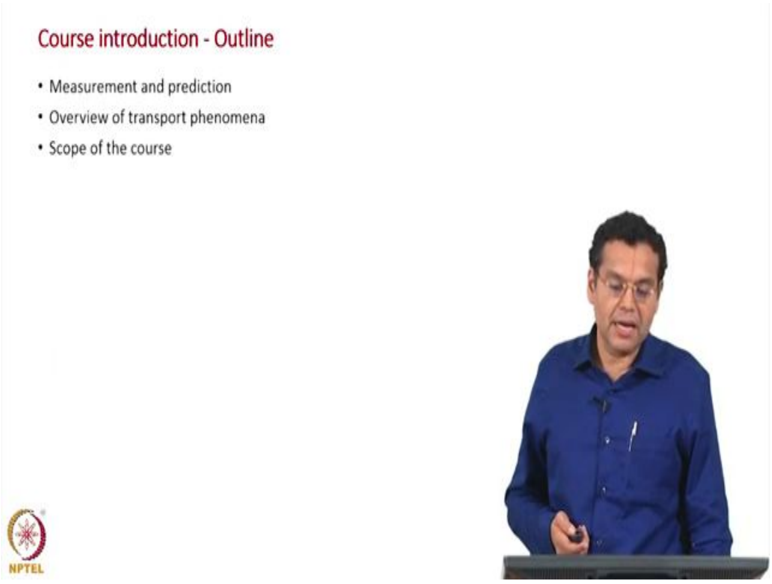

This course introduction has been split into three parts. The first part is on measurement and prediction, the second part is on overview of transport phenomena, and in the third part, we look at the scope of the course. The outline of the first part on Measurement and Prediction is shown in the refer slide below.

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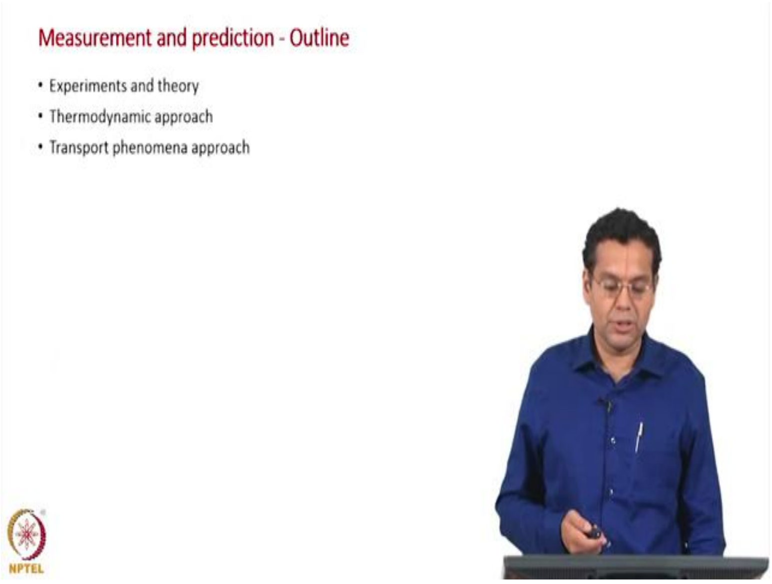

First, we discuss two different ways of analyzing a process namely the experimental method and the theoretical method. In the theoretical method, two different approaches are possible; one is the thermodynamic approach and then the transfer phenomena approach.

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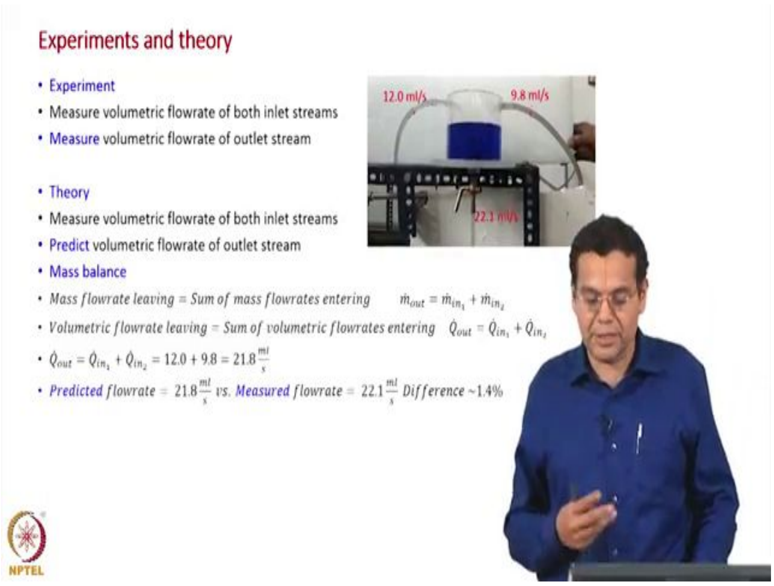

So, let us start with a simple experiment. What we have here is a small tank, it has two inlets and then an outlet. Water flows in through the two inlets and then flows out through the outlet and we maintain a steady-state condition which means the liquid level and the tank is constant. So, just two flows coming in and then flow leaving the tank.

Now, we measure the flow rate of both the inlet streams and the measurement values were 12 milliliters per second and 9.8 milliliters per second. So, we measure the volumetric flow rate of both the inlet streams. Now, coming to the outlet stream we also measure the volumetric flow rate of the outlet stream which turns out to be 22.1 milliliters per second. So, we measure the volumetric flow rate of the outlet stream. The keyword is the measure because we are measuring both the inlet streams and the volumetric flow rate to the outlet stream as well. So, we had an experiment where you measure all three flow rates.

So, alternatively let us look at the theoretical approach wherein, We once again measure the inlet flow rates of both the streams which of course, 12 and 9.8, but now we wish to predict the outlet flow rate instead of measuring the outlet flow rate. So, in the first case, we measured it, in the second case we want to predict it. So, now to predict it we will use a simple mass balance and for the simple tank with two inlets and one outlet, the mass balance is very simple, just says that the mass flow rate leaving through the outlet stream is equal to the sum of mass flow rates entering to the two inlet streams. So, if you want to express in terms of the algebraic equation it says

$$\dot{m}_{out} = \dot{m}_1 + \dot{m}_2$$

Where, $\dot{m}_{out}$; $\dot{m}$ represents the rate of mass flow rate and out represent that is leaving and $\dot{m}_1$, $\dot{m}_2$ are the mass flow rates of the inlet streams.

Now, what we have in this particular case is just water entering and then leaving. So, the densities are same or almost same. So, just becomes balance of volumetric flow rates. So, in this case it just becomes volumetric flow rate leaving is equal to some of the volumetric flow rates entering.

$$\dot{Q}_{out} = \dot{Q}_{in,1} + \dot{Q}_{in,2}$$

The densities are same so it cancels out and just becomes a balance of volumetric flow rate. We use the measured values of the volumetric flow rates of both the inlet streams and then substitute in this equation, and then get the volumetric flow rate of the outlet stream. So, substitute 12.0 and 9.8 and predict the value of the volumetric flow rate of outlet stream as 21.8 milliliters per second.

So, the second case we have measured or met only two measurements and predicted the value of the outlet flow rate using a mass balance in which this case becomes a volumetric balance.

So, to summarize what we have done, we have predicted flow rate of 21.8 milliliter per second which compares with the measured flow rate of 22.1 with small difference about 1.4 percent, which can be attributed to several reasons measurement error, as variation in flow rate and so on.

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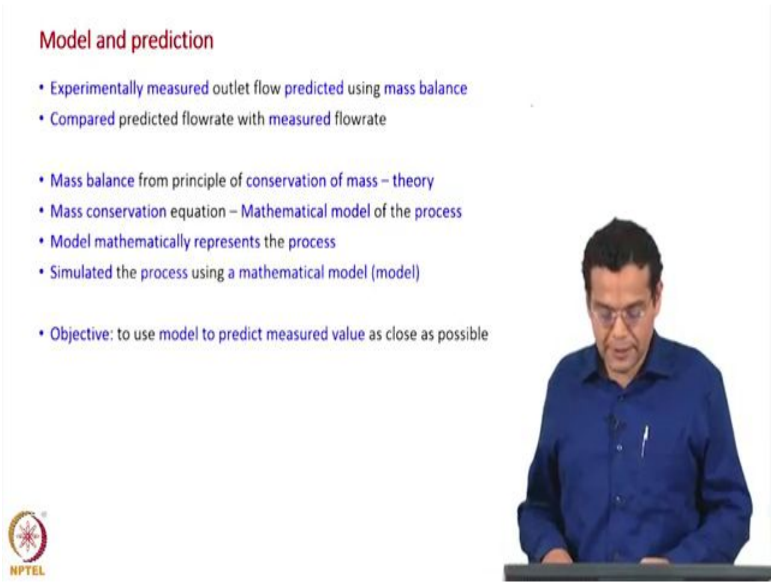

So, we have experimentally measured outlet flow rate and predicted using mass balance. then, of course, we compared this predicted flow rate with the measured flow rate.

Now, this mass balance comes from the principle of conservation of mass which we call as theory, and this mass conservation equation, we call as a mathematical model for this simple process. This process is extremely simple, we have just two inlets and one outlet operating under steady state condition, no second component is present, all temperatures are the same, the density is also happened to be the same.

So, very simple process and for this case, the mass conservative equation or the mass balance we wrote is called the mathematical model for this process. why is it a model? This model mathematically mimics the process or represents a process. Experimentally we had two flow rates they got summed up and result in an outlet flow rate. Similarly, the equation also sums up both the inlet flow rates and gives you an outlet flow rate, that is why this model mathematically mimics the process represents the process.

Now, other way of telling this is we have simulated the process using a mathematical model, in the short model in this course represents a mathematical model. The moment we say model represents the term mathematical model. So we have simulated the process using the mathematical model.

So, the whole objective is to use this model to predict the measured value, not just predict we want to be as close as possible. So, the summary of these is that we want to use a model and then predict the measured value, in this case outlet flow rate and also as close as possible.

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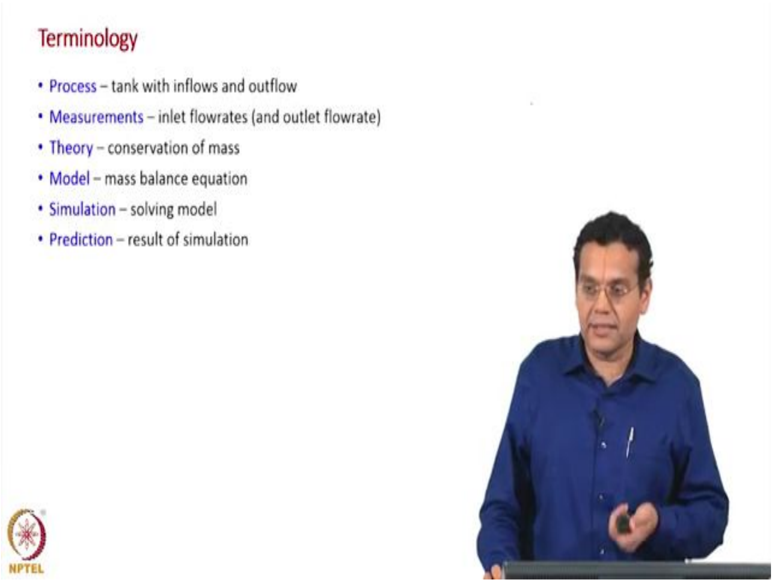

Now, let us look at some terminology which we have used, process in this case is the tank with the inflows and outflows that have a process and the measurements to inlet flow rates and outlet flow rate also. If you want to experimentally analyze this process, you measure the outlet flow rate. Suppose you want to check your model, you once again measure the outlet flow rate. In both the cases, you need to measure the outlet flow rate.

The theory in this case, the conservation of mass and then the model is the mass balance equation which we have used and then simulation is the solving of the model and the prediction is the result of the simulation in which this case, it is the outlet flow rate. Theory, the conservation of mass, the models are mass balance equation and simulation the solution of the model solving the model, prediction is a final result this a result of simulation.

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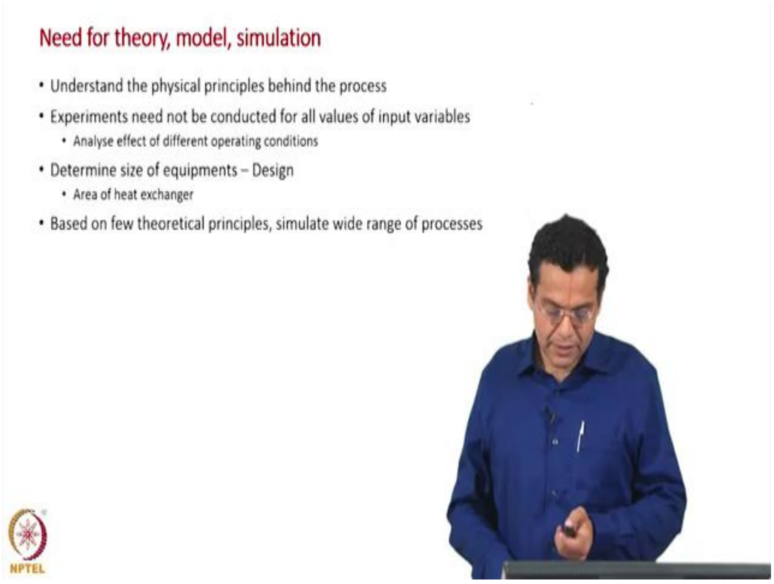

So, what is the need for theory, model, simulation? Why is it required?, first thing is to understand the physical principles behind the process in this case, understand that a simple mass balance takes place. So, helps us to understand the physical principles behind the process.

Second, experiments need not be conducted for different values of input variables in the example which we have seen. So, the flow rates were some set values suppose you change the inlet flow rates and then you measure the outlet flow rate, you need not do this experiment several times if you have a model for this process it is enough if you know the inlet flow rates you can predict the outlet flow rate.

You can also determine the size of equipments in a chemical engineering plan which we call as design. Usually when you find size the terminology becomes a design, and for example, if you have a heat exchanger in a chemical engineering plant, you find the area of the heat exchanger using model it becomes a design and because of the advantage of model and theory is that based on few theoretical principles, you can simulate a wide range of processes. The theoretical principles governing different processes are same, a small set. So, if we understand them we can simulate a wide range of process that is a advantage of theory and model.

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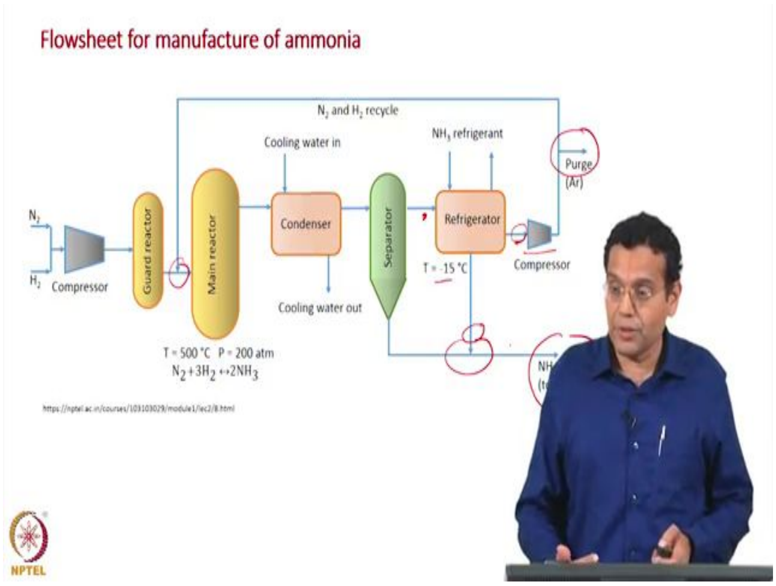

So, now what we will do is, extend what we have discussed for a simple process namely the tank to a entire flow sheet. What we are seeing here is flow sheet for the manufacture of ammonia. We have nitrogen, hydrogen entering and it may have some impurities as well and based on thermodynamics, the nitrogen hydrogen reaction giving ammonia has to be conducted at a high pressure and for increasing the rate of reaction, we need to conduct at high temperature.

So, it is a high temperature, high pressure reaction. So, we need to compress the inlet gas to the high pressure of let us say 200 atmosphere. So, we need a compressor which compresses from let us say atmospheric pressure to a high pressure of 200 atmospheres. And that stream enters a guard reactor which remove some impurities which will impair the activity of the catalyst; it is a catalytic reaction and iron is used as catalyst and so we remove those impurities in the guard reactor.

It is a catalytic reactor using iron as a catalyst, conditions as we mentioned of 500 degrees and 200 atmospheres. This reversible reaction between nitrogen, hydrogen giving ammonia takes place, and it should be noted the conversion is usually very low order of just 20 percent per pass and the stream leaving the reactor has ammonia, unreacted nitrogen hydrogen and some impurities as well let us say argon.

Now we need to separate ammonia from this stream, we do the first condensation using cooling water and where part of the ammonia condenses out as a liquid. So, you send it to a gas liquid separator, simple gas liquid separator where separation takes place by gravity, and so liquid ammonia comes out, that is also part of the product stream and the remaining stream goes through the refrigerator.

Based on the high pressure of 200 atmosphere, you need a temperature of about minus 15 degrees centigrade. So, that the ammonia going in this stream is as minimum as possible. If you cool maintain at a higher temperature let us say more than minus 15 degree centigrade then there will be enough amount of ammonia in the stream which you do not want to happen. You want most of the ammonia to be in the stream. So, you maintain a very low temperature of minus 15 degree centigrade that is why require a refrigeration.

So, now ammonia condenses out from the refrigeration unit also and these two ammonia streams are mixed and that is our product ammonia. Now, the recycle stream is argon in it so, which we do not want to accumulate. So, we have a purge which avoids accumulation of argon and this cycle and then of course, unreacted nitrogen hydrogen is recycled back to the main reactor.

Because there is some loss of pressure during the process, we have a small compressor which makes up for this difference in pressure. So, whatever let us say 200 bar comes down, let us say 190 bar it adds up to 10 bar extra and brings it back 200 bar or 200 atmosphere. So, let us say we want to set up this ammonia plant and we want to design this plant, we want to simulate this plant. Now, how do we go about it?.

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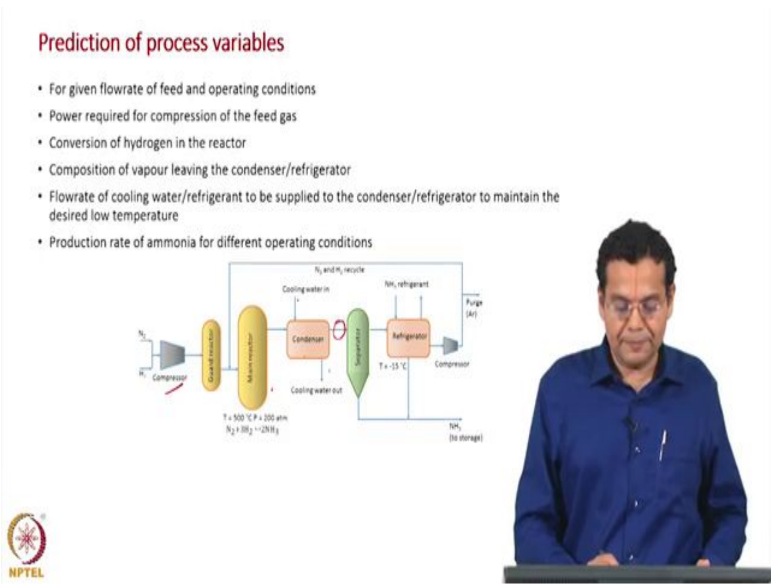

As I say, simulate look is equivalent to prediction of variables. Now, what are the variables which we like to predict in this particular flow sheet. First, for a given flow rate of the feed and operating conditions, let us say the feed and the operating conditions are given. We have the compressor unit. So, we like to predict the power required for compression of the feed gas, we are going from a atmospheric pressure let us say to a very high pressure. So, lot of power is required, what is the power required on the compressor.

Now, we have the main reactor, what is the conversion of hydrogen in this reactor we like to know that as well, and that determines quantity of ammonia produced and we have separation of ammonia from the unreacted reactants, some separation takes place in the condenser, some separation takes place in the refrigerator. Those are we also like to find out. What is the composition of the stream leaving the condenser, leaving the refrigerator.

And of course, finally, we also require the flow rate of cooling water, we have cooling water here, cooling water entering and leaving, you also send in ammonia refrigerant here. So, we like to find out what is the flow rate of cooling water, what is the flow rate of refrigerant required in these two units.

We also wish to find out what is the production rate of ammonia for different operating conditions. So, we like to predict the power for the compressor, the conversion and the reactor and then the composition of vapour leaving and the flow rate of the coolants required and the production rate of ammonium.

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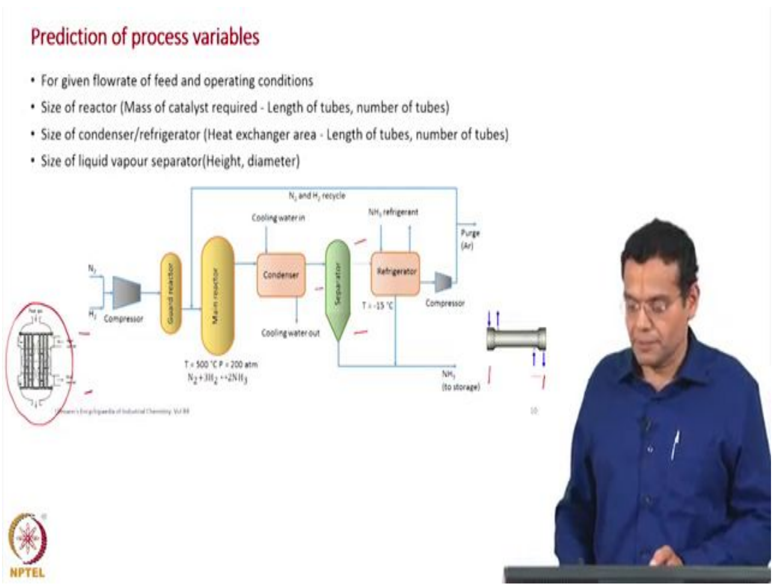

Now, what other variables we like to predict. Now, these variables which we will discuss next, fall in the category of something do with size, area etcetera of the equipment. So, we want to predict or we now want to know the size of the reactor, what do you mean the size of the reactor? As we discussed sometime back, we have used a catalytic reactor, we use a multi tubular catalytic reactor shown here.

So, when we say size, it mean mass of catalyst required which is equivalent to finding out what is the length of the tubes required, number of tubes required. So, mass of catalyst required can be explained in terms of length and number of tubes that gives the size of the reactor.

Now, we also want to know the size of the condenser in the refrigerator which are heat exchangers. So, what do we mean by size of heat exchanger? it mean the length of the tubes let say some multi tubular heat exchanger, shell and tube heat exchanger then we need to know the length of the tubes and all the number of tubes in the heat exchanger. And also we like to know the size of the liquid vapour separator, what you mean by size here? it is the height of the separator and the diameter of the separator.

So, as I told you these are also process variables which I like to predict, but these fall into the category of sizes of these equipment size of reactor, condenser, or liquid vapour separator ok, you will shortly know why distinguish these two kind of process variables.

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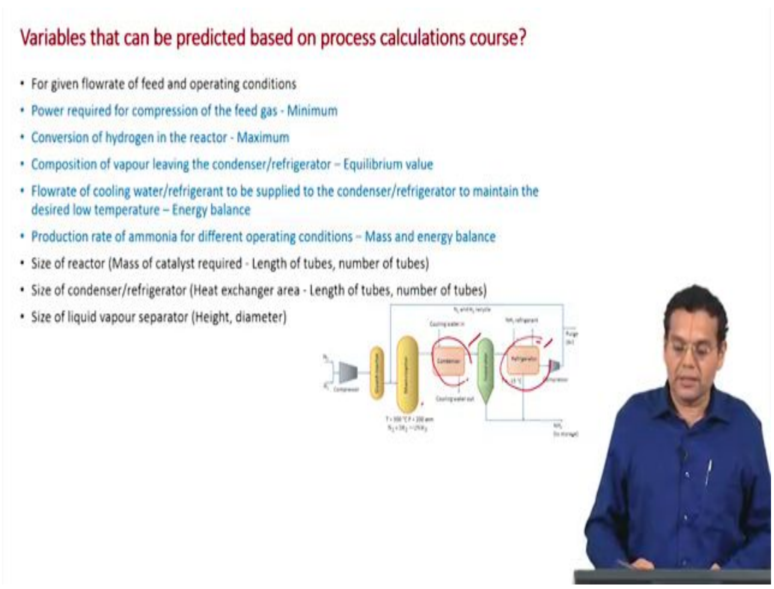

Now, having taken a process calculation course, what are the variables which we can predict among this list. First, once again of course, for given flow rate of feed and operating conditions, we can calculate the power required for a compression of the feed gas and of course, we can find out the process calculation requires a mini thermodynamics course. So, based on principles of thermodynamics, you can calculate the minimum power required for compression.

Now, we can find out the conversion of hydrogen in the reactor and we can find out what is the maximum possible conversion let say using a law of mass action, you can find out the maximum conversion of hydrogen in the reactor. Now, we can also find out the composition of vapour leaving the condenser, leaving the refrigerator and that we assume equilibrium and find out the equilibrium value of composition of the vapour leaving the condenser and refrigerator.

Now, we can also do a simple energy balance around the condenser and then around the refrigerator and find out what is the flow rate of cooling water, what is the flow rate of ammonia refrigerant required.

Of course, doing a mass balance and energy balance for the entire plant, we can find out what is the production rate of ammonia. So, based on the knowledge gained from a process calculation course, you can solve for different variables in the plant namely power required for compression, conversion of hydrogen in the reactor, composition of vapour leaving the condenser and refrigerator, cooling water required in them and the production rate of ammonia.

Now, what are the variables which we cannot predict based on a process calculation course. Whatever variables we classified as size; falls in the category of size, they cannot be predicted using a process calculation course knowledge. For example, the size of reactor cannot be predicted, the size of the condenser, refrigerator, heat exchanger that cannot be predicted and then of course, size of the liquid vapour separator can also not be predicted.

So, all other variables like power etcetera could be predicted, but whatever has to do with size cannot be predicted using the knowledge gained from process calculation course. Now, what are the assumptions made in process calculation course ok.

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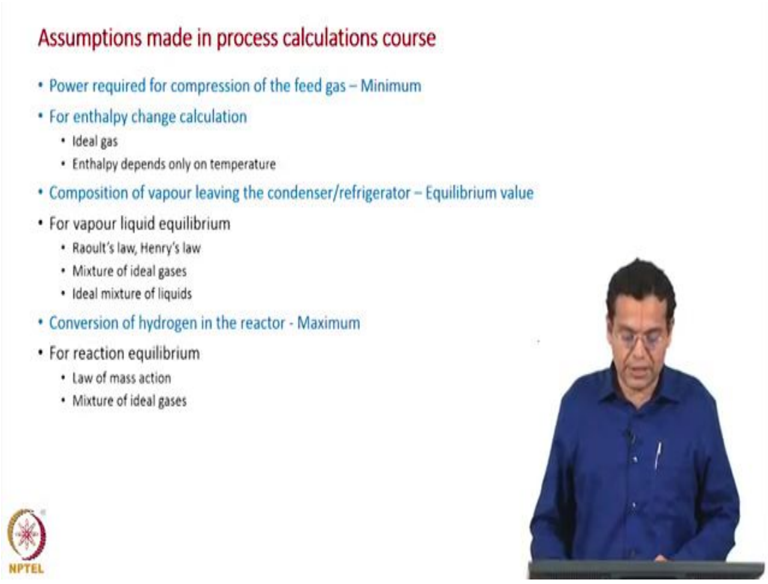

Now, for calculating the power required for compression of the feed gas, we said we will get the minimum power required. This power required is calculated from enthalpy change. So, in a process calculation course, we assume that the gas is ideal and hence we assume the enthalpy to depend on the temperature only. So, based on the assumption that it is an ideal gas and the enthalpy depends on temperature only we will find out what is the power required.

Now, regarding the composition of vapour leaving the condenser and refrigerator, we will assume vapour liquid equilibrium and we will use Raoult's law or Henry's law depending on the case and then we will also assume it is a mixture of ideal gases, we will also assume it is a ideal mixture of liquids. So, based on all these assumptions mixture of ideal gases, ideal mixture of liquids, we will assume the vapour liquid under equilibrium and find out the composition of vapour leaving the condenser refrigerator.

Now, coming to the conversion of hydrogen in the reactor, for reaction equilibrium we assume the law of mass action. We use the law of mass action and then we assume to be a mixture of ideal gases and find out the conversion of hydrogen in the reactor. Of course, we get the minimum power required; the equilibrium value of composition and the maximum conversion in the reactor.

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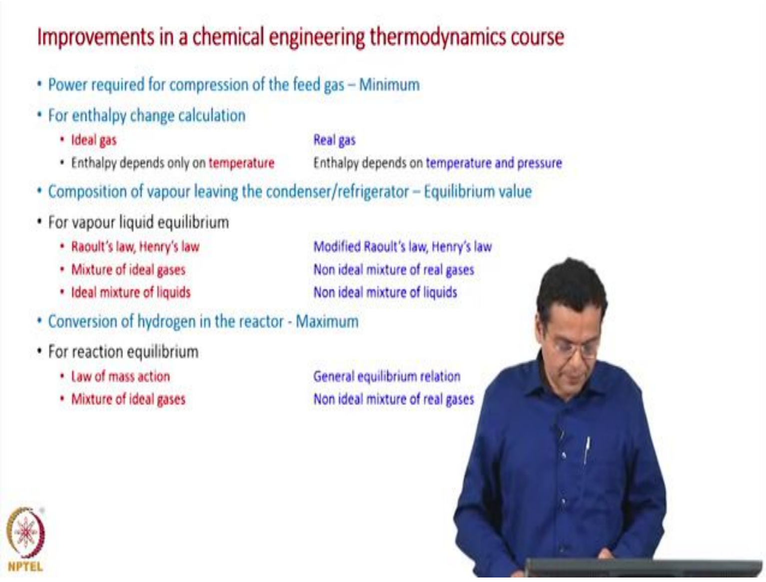

Now, as we have been discussing, the process calculations course a mini thermodynamics course. So, now, if you take a full-fledged chemical engineering thermodynamics course, what are the improvements possible in this prediction values. So, let us start with the power required for compression of the feed gas. For enthalpy change calculation in the earlier case, we assumed the gas to be ideal, but now we will assume the gas to be here as a real gas, what is the implication? The enthalpy which was assumed to depend only on temperature, will us take the dependency of enthalpy both on temperature and pressure which makes it a better value.

Now, coming to the composition of vapour leaving the condenser and refrigerator, for vapour equilibrium we assumed all ideal conditions Raoults law, Henry's law etcetera. Now, we will assume a modified Raoults law, modified Henry's law, how do we modify? In the earlier case we took mixture of ideal gases, but now we will say it is a non ideal mixture of real gases. So, we take into account the non-ideality in the gas phase.

Also for the liquid phase, we assume ideal mixture of liquids, but now we will take it as non ideal mixture of liquids. So, we take into account the non ideality both in the vapour phase and the liquid phase and make better prediction of the equilibrium value, when we say better prediction as we have seen in the beginning, better prediction means closer to reality.

Now, coming to the conversion of hydrogen in the reactor, we assume of course, reaction equilibrium. We assume law of mass action, but we will use a more general expression based on general equilibrium relationship.

Now, again we will assume non ideal mixture of real gases. So, here we take into account the non ideal behaviour of the gases. So, the improvements in the chemical and thermodynamics course is that, we take into account a non ideality and the predicted values are going to be closer to experimental values because we take into account non ideality.

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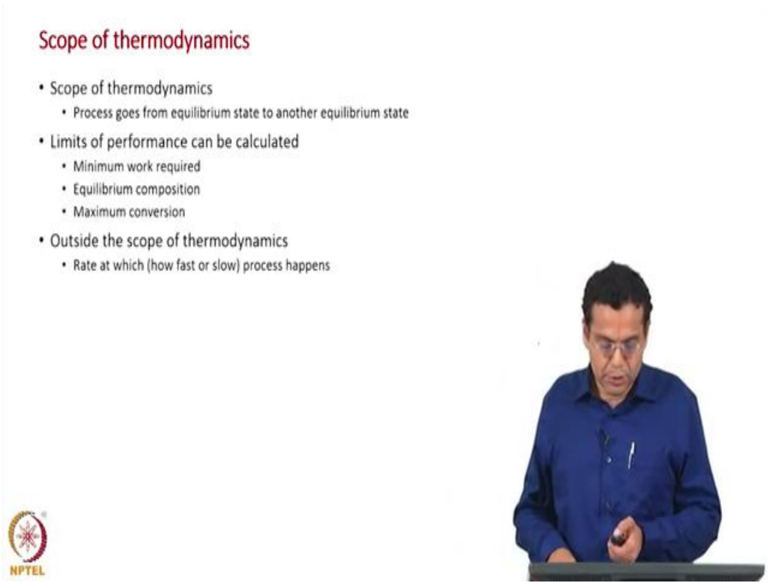

So, that gives out the scope of thermodynamics course. Now, in thermodynamics, we talk about process going from one equilibrium state to another equilibrium state and thermodynamics always gives us the limits of performance as we have seen. For example, it gives a minimum work required in the compressor, equilibrium composition which would attain if they have an contact for a very long time which has the maximum composition and the maximum conversion possible in the reactor. So, it talks about minimum, maximum, equilibrium etcetera.

Now, what is outside the scope of thermodynamics? It is the rate at which the process happens how fast it happens, how slow it happens, it is not under the scope of thermodynamics. So, it talks about limits of performance, talks about process going from one state to another, does not talk about how fast the process happens.

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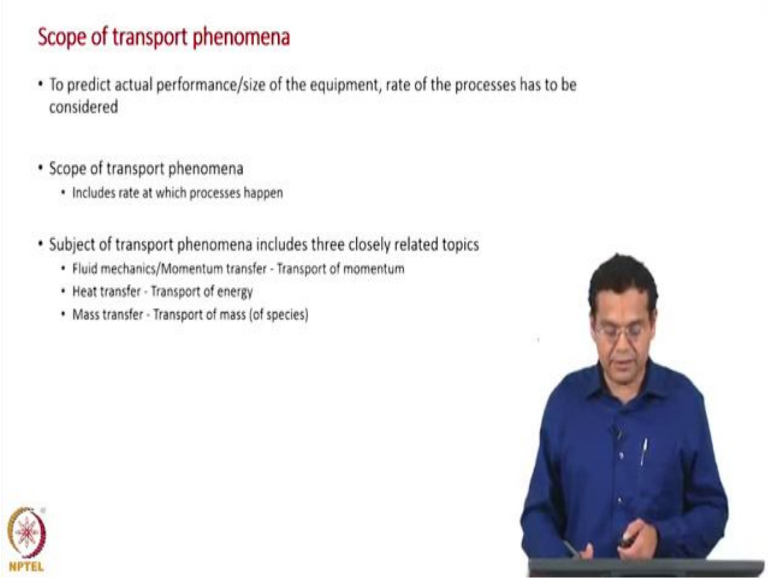

So, that brings in the scope of transport phenomena because we need to take into account the rate at which the process happens so that you can find out the size of equipments. Size of equipments is not under the scope of thermodynamics we need to predict them and that is where scope of transport phenomena comes in.

So, to predict actual performance and size of equipment, rate of the processes has to be considered that is the central theme behind the scope of transport phenomena. So, transport phenomena considers or includes the rate at which processes takes place and transport phenomena includes three closely related topics, namely fluid mechanics or momentum transfer which deals with transport of momentum.

And then heat transfer which deals with transport of energy and mass transfer which deals with transport of mass when we say mass, it mean mass of species. So, subject of transport phenomena is required to take into account the rate of processes rate which process happens how fast, how slow and it required to predict the actual performance.

We have thermodynamics limits itself to limits of performance, but we like to predict the actual performance, find out the size of equipment. So, we need to consider rate and transport phenomena and the subject of transport phenomena includes three closely related topics fluid mechanics or momentum transfer, heat transfer, mass transfer deal with transport of momentum, transport of energy, transport of mass of species.