Process Control and Instrumentation

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Lecture - 3
Mathematical Modeling (Contd.)

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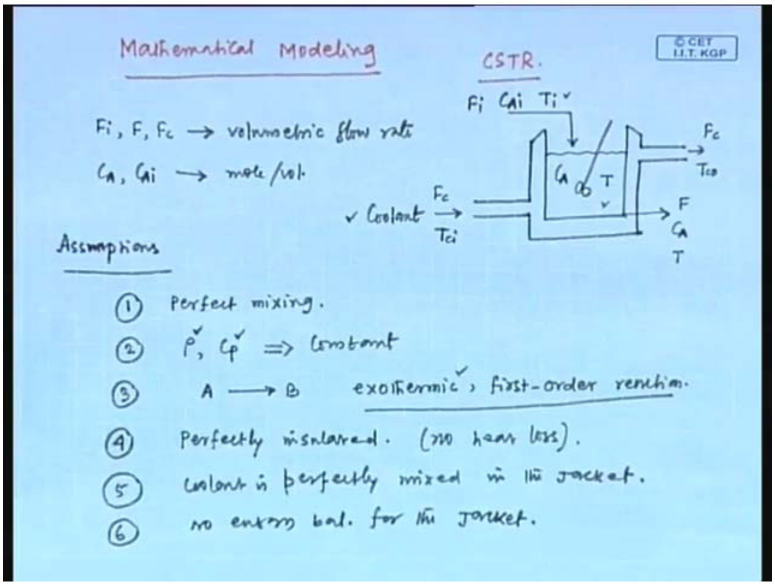

We will continue the topic Mathematical Modeling. In the last class, we have discussed about the state variables and state impressions and in this class, we will develop the mathematical model, first for a CSTR, Continuously Stirred Tank Reactor. So, you will take CSTR example and will derive the mathematical model, this is if jacketed CSTR, this is a tank, this is a jacket. Now, one medium is introduced here and that medium is coming out here, first of all the feed which is entering to the reactor has the flow rate of F i, concentration of the feed is C A i and temperature is T i.

The suffix i indicates the input, A is a component, I mean C A i is the input concentration of component i and T i is a input temperature. The product steam which is coming out from this CSTR has the flow rate of F, concentration in terms of component A is C A and temperature is T. Now, before deriving the mathematical model for this CSTR, first we will know the units of different flows like F i and F along with the coolant medium flow rate kept F c.

So, all these flow rates are basically volumetric flow rate, here temperature is T c i, outlet flow rate is F c and outlet coolant temperature is T c naught. Concentration C A and inlet concentration C A i, both are molal concentration I mean, unit is say mole per unit volume. C A and C A i both are molal concentration for example, they are in mole per unit volume. Next, you will consider the assumptions, so first assumption is perfect mixing that means, the temperature of this outlet steam T and compositions C A, they are same with that of the reaction mixture.

The perfect mixing indicates, everywhere in this tank temperature and concentration, they are identical and the outlet temperature composition also identical with the temperature and concentration of reacting mixture. Second assumption is liquid density rho and the heat capacity C p they are constant, third assumption is we are considering a simple exothermic first order reaction. And to remove this exothermic heat, the coolant steam is introduced in this jacket, this is the coolant steam.

Fourth assumption is, the reactor is perfectly insulated that means, there is no heat loss from the reactor to the surroundings it means, no heat loss from the system to the surroundings. Fifth one is, coolant is perfectly mixed in the jacket and last assumption is, we will not consider any energy balance for the jacket, there is no energy balance for the jacket. These are the assumptions adopted for this CSTR system and based on these assumptions, we will derive the modeling equations, now first we will go for the overall mass balance.

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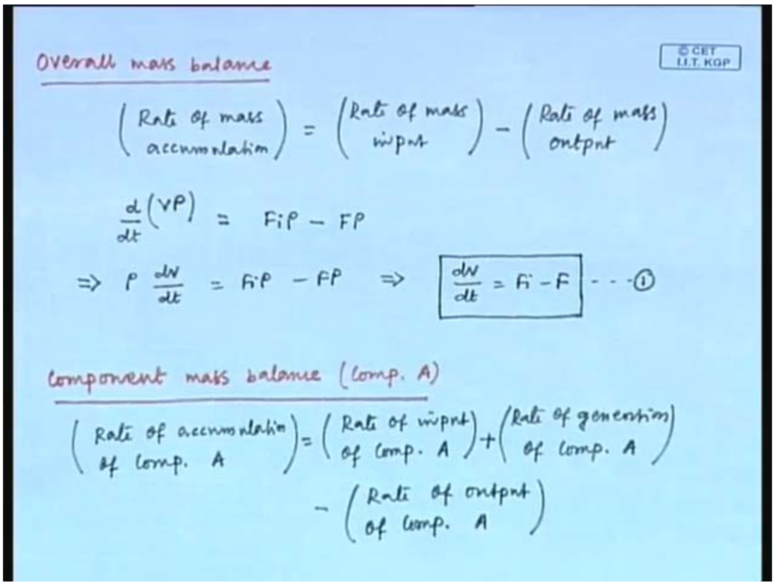

First, we will go for overall mass balance so, to develop the overall mass balance of the CSTR system, we need the conservation of mass. What is that? Conservation of mass is rate of mass accumulation equals to rate of mass input minus rate of mass output, this is the conservation of mass. Now, for this CSTR system, what is this term I mean, how we can represent the mass of accumulation see in this reactor system, you consider the volume of the liquid is v.

The volume of the liquid in the reactor is v now, if v is the volume, if we multiply with density so, this whole terms becomes mass. Now, differentiation of this is the mass flow rate d d t v rho, that is the rate of mass accumulation. Now, rate of mass input, input to the system is basically F i but, we know that, F i is the volume at the flow rate so, we have to multiply with rho. So, F i multiplied by rho that is the input mass rate similarly, what will be the output, output flow rate I mean, the volumetric flow rate that is, F.

So, if we multiply with rho then, this is the output rate now, we have assume that, rho and C p both are constant. If rho is constant then, we can write this rho d v d t equals to F i rho minus F rho that means, d v d t equals to F i minus F. Suppose, this is equation number 1 so, this is a mass balance equation similarly, we can go for mass balance of component A or you can say, that component mass balance. So, we will consider in the next, mass balance or component mass balance and the component is here component A.

So, what is the conservation principle for this rate of accumulation of component A, this is a accumulation term. Then, rate of input of component A then, rate of generation of component A minus rate of output of component A, this is a conservation principle for component mass balance. Now, we have to write all these individual term accumulation, input, output and generation now, for this CSTR system, what is the accumulation term.

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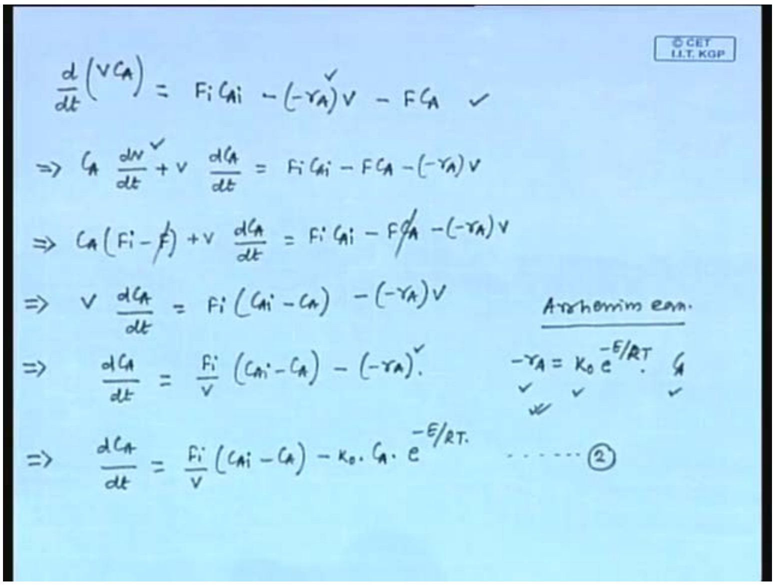

Volume multiplied by C A now, if we one to represent in terms of rate then, d d t of v C A this is mole per unit volume C A and v is volume so, mole per unit time overall. So, what is the input, F i is a flow rate of input stream and concentration is C A i so, F i multiplied by C A i, that is the rate of input of component A. Now, what is a generation, minus r A into v see, minus r A is the rate of disappearance of A. If we multiply with minus sign then, we get the generation, minus r A is the rate of disappearance of A so, if we multiply with minus then, that becomes generation.

And what is the output, output is F multiplied by concentration of output steam that is, C A so, from the conservation principle, we got this equation. Now, we can write this equation in this form C A d v d t plus v d C A d t equals to F i C A i minus F C A minus, minus of r A into v. Now, we know the d v d t term I mean, if we substitute equation 1 then, this equations becomes C A F i minus F plus v d C A d t equals to F i C A i minus F C A minus, minus of r A into v.

Now, this F multiplied by C A and this F C A will be canceled out then, we can rearrange this equation to v d C A d t equals to F i C A i minus C A minus, minus of r A into v. If we divide again both sides by v, we will finally get d C A d t equals to F i divided by v, C A i minus C A minus, minus of r A, minus of r A is the rate of disappearance of A. Now, if we consider Arrhenius equation then accordingly, we can write minus of r A equals to k naught exponential of minus of E divided by R T into C A.

According to the Arrhenius principle, the reactions rate equals to pre exponential factor then, exponential of minus E divided by R T, C A is the activation energy and R is the universal gas constant. If we substitute this reaction rate expression here then finally, we get d C A d t equals to F i divided by v, C A i minus C A minus k naught C A exponential of minus of E divided by R T. So, this is the final form of component mass balance equation so, these two equations we have derived based on the conservation of mass in the next, we will consider the energy balance equation.

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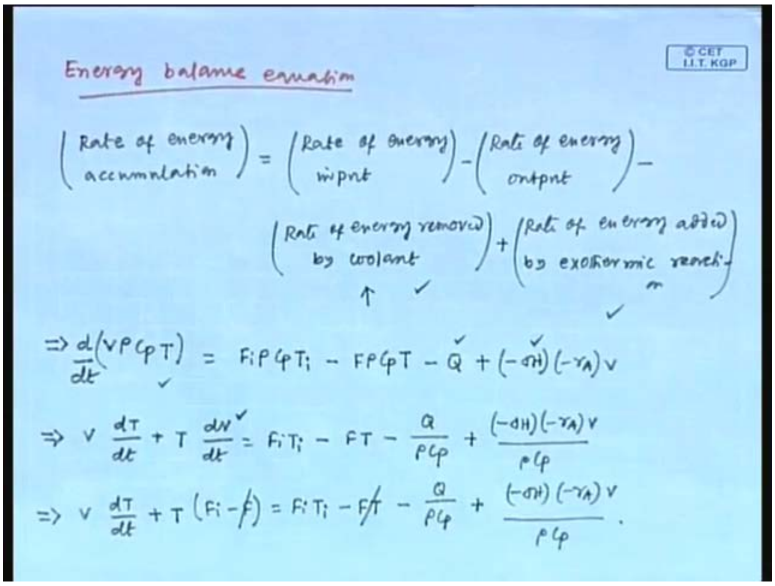

Energy balance equation for the example CSTR system, what is the conservation principle of energy, conservation principle we can write in this form, rate of energy accumulation equals to rate of energy input minus rate of energy output minus rate of energy removed by the coolant plus rate of energy added by exothermic reaction. So, here 4 terms are involved accumulation, input, output, energy removable and energy added by the exothermic reaction.

So, next we have to representation all these terms using term mathematical terms I mean, variables. So, what is the energy accumulation say, volume in the tank is represented by v and if we multiply with rho, this becomes m then C p, then d t, energy term we can write in terms of m C p d t. Now, here we are considering reference temperature equals 0 now, if we write here d d t of v rho C p T then, this becomes rate of accumulation of energy.

Now, next we will consider the rate of energy input, volumetric flow rate of input steam that is, F i if we multiply with rho then, that becomes mass flow rate. Similarly, C p then, d t I mean, T i minus T reference here, reference temperature we are assuming 0. So, T i and you recall, we have consider the C p that is constant, what will be the output rate of energy output. The flow rate of outlet steam I mean, the volumetric flow rate that is, F similarly, if we multiply rho, this becomes mass C p and outlet temperature is T.

Now, rate of energy removed by the coolant this one, this will represent by Q, energy removed by the coolant is represented by here Q. What is Q, how we can calculate Q, we know flow rate F c, rho c, C p c and then, temperature difference is outlet temperature of coolant minus inlet temperature of coolant. What is the last term I mean, how we can represent the last term, last term we have to consider in this way, minus del H that is, heat of reaction then, minus r A multiplied by v.

Minus del H here is heat of reaction, it is well known to ask that, heat of reaction is negative I mean, this negative term is used for the case of exothermic reaction and for endothermic reaction, we use here positive sign. So, this term represents the energy added by exothermic reaction next, we need to simplify this equation. Now, dividing both sides by rho C p, v d capital T d small t plus temperature d v d t equals to F i T I, since we have we are dividing both sides by rho C p.

Next term is F multiplied by T then, Q divided by rho C p and finally, minus del H minus r A v divided by rho C p. Now, you will substitute this term d v d t, we have the equation of d v d t obtained from the total mass balance, if we substitute d v d t then, we can write it like this way, T multiplied by F i minus F equals to F i T i minus F t minus Q divided by rho C p plus minus of del H minus of r A into v divided by rho C p now, this F T and this F T we can cancel.

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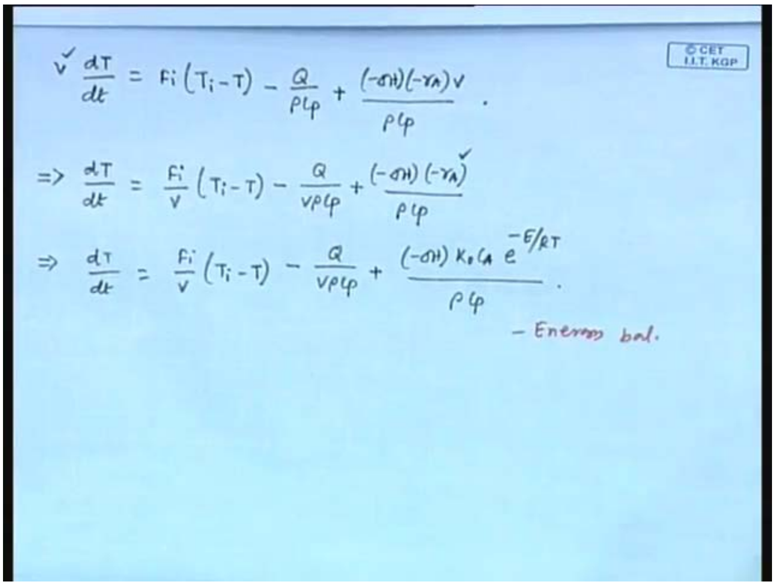

And then, we get v d T d t equals to F i T i minus T minus Q divided by rho C p plus minus of del H minus of r A into v divided by rho C p. And finally, we will divide both sides by this volume term then, we get d T d t equals to F i divided by v T i minus T minus Q divided by v rho C p plus minus of del H minus of r A divided by rho C p. Now, again we will substitute here the Arrhenius law then, d T d t equals to F i divided by v T i minus T minus Q divided by v rho C p plus minus of del H k naught C A exponential of minus E divided by R T whole divided by rho C p so, this is a energy balance equation.

So, for the example CSTR system we got three equations, one is based on total mass balance then, component mass balance and last one is based on energy balance.

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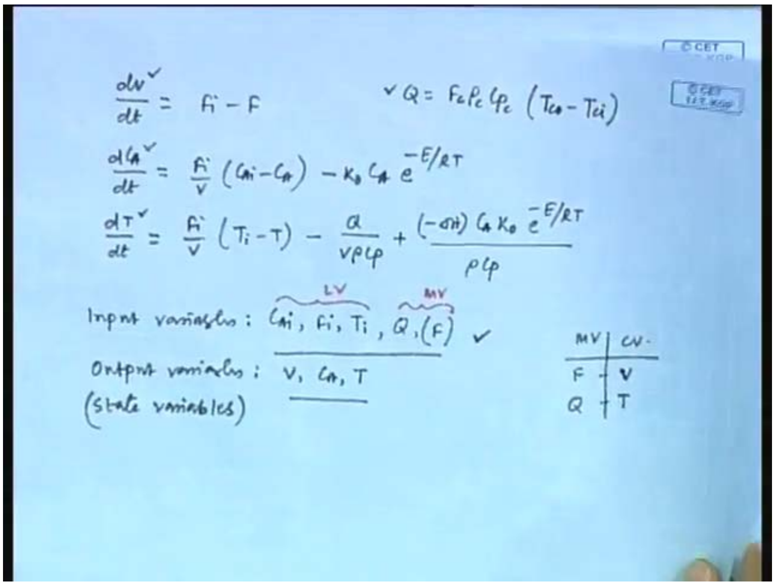

Now, the modeling equations I am writing here, one we got d v d t that is equals to F i minus F, second equation d C A d t that we got F i divided by v, C A i minus C A minus k naught C A exponential of minus E divided by R T. And energy balance equation we got that is, d T d t equals to F i minus v into T i minus T minus Q divided by v rho C p plus minus of del H C A k naught exponential of minus E divided by R T whole divided by rho C p.

Here, I have mentioned that Q, Q equals to our coolant flow rate is F c now, density is suppose rho c, heat capacity if we will consider C p c multiplied by the temperature difference. What is the outlet temperature of this, T c o minus T c i so, this is the expression for Q. Now, you will just classify, we will just see what are the different variables involved in the modeling equations here, what are the input variables. Input variables are C A i then, F i then, T i then, Q.

We are not considering F c, T c i we are considering Q and F definitely, F will be input variable. If this is considered as the manipulated variable for controlling the liquid height or liquid volume so, these are the input variables. What are the output variables, output variables are here v, C A and T see, in this three modeling equations v, C A and T, they are present within the accumulation term so, these three variables are also state variables. So, we can write here these are also state variables because, they are present within the accumulation term.

Now, among this input variables, which are the manipulated variables, for the example CSTR system, if we consider liquid volume is a first I mean, one control variable and another one is say, temperature. Now, the corresponding manipulated variables are, if we consider F as the manipulated variable for v and Q as the manipulated variable for temperature then so, Q and F, these two are basically manipulated variables.

So, these three I mean, the rest input variables are load variables or disturbance variables, among these five input variables, two are the manipulated variables and other three are the load variables. So, this is the development of model structure for the sample CSTR and we have seen the different variables, which are involved in this example CSTR. Before going to discuss another system, we will study about the degrees of freedom analysis.

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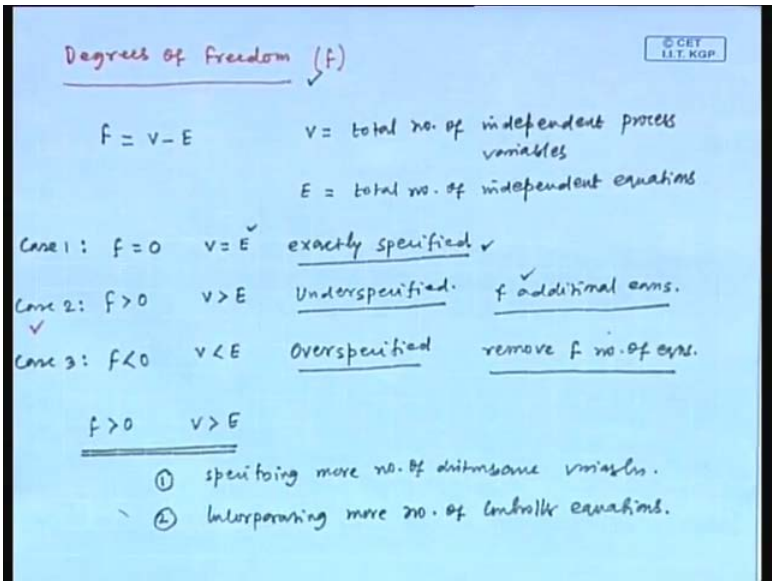

So, we will next study the degrees of freedom so, so far we have discussed about the modeling of chemical processes, after deriving the mathematical model of a process, we need to solve those modeling equations. The solution of a model structure is basically called simulation, we need to stimulate the modeling equations. Now, for the stimulation of a modeling equation, we need to describe this degrees of freedom. Degrees of freedom, which suppose is represented by F then, we can write F equals to v minus E, degrees of freedom we are representing here by F then, F equals to v minus E.

V is the total number of independent process variables and E is the total number of independent equations. So, degrees of freedom basically, total number of independent variables minus total number of equations. Now, in the analysis of degrees of freedom, we will consider three different cases, in the first case we will consider say, F equals to 0. It means, number of independent variables equals to number of independent equations that means, the system is exactly specified.

When degrees of freedom equals 0 then, we can write v equals to E that means, number of independent process variables equals the number of independent equations. In this situation, we can say the system is exactly specified I mean, there is no problem to find the solution of the modeling equations. In the second case, we will consider F is greater than 0 that means, v is greater than E so, in this case, the system is called under specified. How we can make it exactly specified system by the inclusion of F number of additional equations.

So, to make it exactly specified, we need F additional equations, to make the under specified system exactly specified, we need F number of additional equations then, we can only get the solutions of the modeling equations. Last case is, F is less than 0 that means, total number of independent process variables is less than total number of independent equations and in this case, the system is called over specified. So, to make this over specified system exactly specified, we need to remove F number of equations.

Usually in practice, the case 2 is the common I mean, F greater than 0 is the common case in practice, F greater than 0 that means, v greater than 0. Now, thing is that, if this is the situation F greater than 0, how we can make it exactly specified basically, there are 2 options, first option is we can specify more number of disturbance variables. So, by specifying more number of disturbance variable, if we can specify more number of disturbance variables then, number of unknown variables is reduced.

So, this is one option and in the second option, by incorporating more number of controller equations. This is a second option, either we have to reduce the number of unknown variables or we have to increase the number of equations to make the F equals 0. Anyway, we will discuss this degrees of freedom with taking one simple example, we will consider the stirred tank heater.

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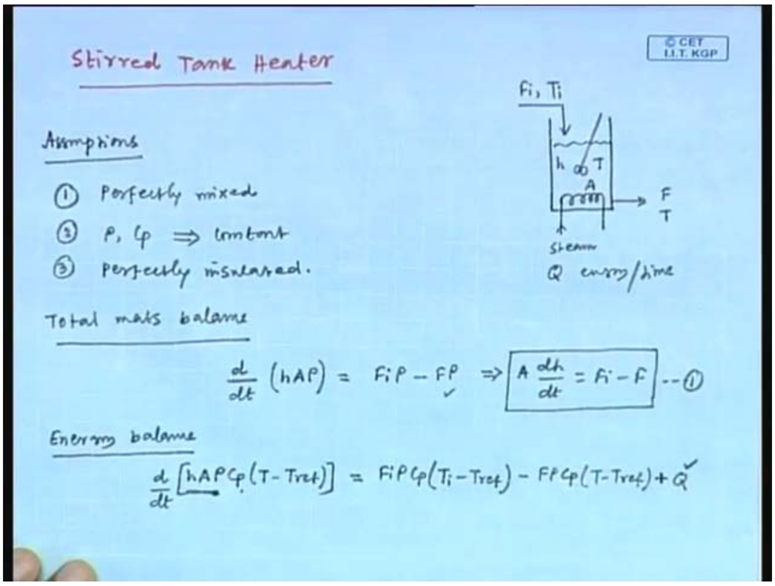

To describe this degrees of freedom analysis, stirred tank heater example for degrees of freedom analysis. So, before going to analyze the degrees of freedom, we need the model so, first we will develop the model for the system and then, we will go for the degrees of freedom analysis. The schematic of this system, we have to draw we have to develop first so, this is F i and temperature is T i. Now, steam is introduced here through the coil for heating purpose, this is steam suppose, flow rate is Q, outlet flow rate is F and temperature is T.

Now, liquid in the tank has the height of h, temperature here also T, cross sectional area of this tank is A. Now, before going to develop the model, we need to consider some assumptions so, what are these assumptions, first assumption is, the tank is perfectly mixed. Second assumption is rho and C p both are constant, third assumption is the tank is perfectly insulated that means, there is no heat loss from the tank to the surroundings. So, first we will develop the total mass balance equation so, what is the accumulation of mass d d t liquid height multiplied by cross sectional area that is, volume.

Volume multiplied by density that is mass, h is the liquid height multiplied by cross sectional area, this is volume. Now, volume multiplied by density that is mass so, this is mass flow rate I mean, this is the rate of accumulation. What is the inflow rate, F i rho minus F rho, this is a outflow rate so, we can write this equation A d h d t equals to F i minus F. This is the total mass balance equations since rho is constant so, we can get this from this equation, you give some equation number for this suppose, this is equation number 1.

In the next, you will go for energy balance, what is the accumulation term, height multiplied by area that is volume, volume multiplied by rho, mass. Mass, C p, temperature difference is T minus suppose, T reference so, d d t of this is the accumulation term, h multiplied by rho that is volume, multiplied by rho, h multiplied by A that is volume, multiplied by rho that is mass. So, if this is the mass C p and this is temperature difference, what is the energy input rate, F i rho this is mass flow rate, C p T i minus T reference this is the energy input rate.

What will be the energy output rate, F rho C p T minus T reference and another term is energy supplied by steam per unit time. Energy supplied by steam per unit time that is, Q basically, the unit of Q is here, energy per unit time say for example, ((Refer Time: 47:47)) thermal unit per minute, the unit of this is energy per unit time. So, this is the energy added or energy supplied by steam per unit time.

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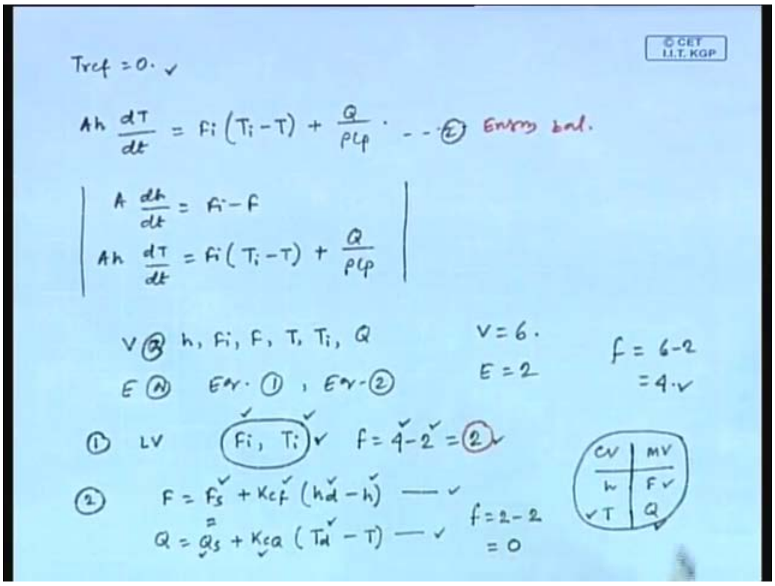

Now, if we simplified this considering T reference equals to 0 and if we simplify the energy balance equation, we will get A h d T d t equals to F i T i minus T plus Q divided by rho C p, this is a energy balance equation. If we consider T reference equals to 0 and if we simplify finally, we will get this energy balance equation. So, there are basically 2 equations, one is based on total mass balance and another one is based on energy balance.

So, these two equations are, first one is A d h d t equals to F i minus F and this is A h d T d t equals to F i T i minus T plus Q divided by rho C p, you give some equation number to this suppose, this is equation number 2 so, this is the model structure. Now, you will go for the degrees of freedom analysis, how many variables are involved in this equation h, F i, F, T, T i and Q so, these are the variables. We can write v equals to 6 agree or not, agree so, there are 6 unknown variables then, how many equations are involved there, one is equation 1 and another one is equation 2.

So, we can write E equals to 2 so, what is F, 6 minus 2 that is equals to 4 so, degrees of freedom for the example system is 4. We have discussed, there are two ways to reduce the degrees of freedom, first option is we can specifies some load variables, what are the lowered variables in this system, one is F i, another load variables is T i. So, if we can specify these two load variables then, the degrees of freedom reduces to 4 minus 2 that is, 2 initially it was 4.

Now, two lowered variables we are specifying, how we can specify, by the direct measurement. We can measure this flow rate, we can measure this temperature then, we can get the information of flow rate and temperature that means, F i and T i are known that means, degrees of freedom we can write 4 minus 2 that is, 2. Another option, I told by including some controlled equations, for the example liquid heating tank system, what are the controlled variable and manipulated variable pairs to be considered, one is height, another one is temperature.

So, we can manipulate this height, we can control this height by the manipulation of suppose F, we can control this temperature by the manipulation of Q. So, we can develop two control equations, although we did not study the control equations, I am just mentioning the simplest control equations for these two control pairs. If F is the manipulated variable, the control equation we can write like this, F equals to F s plus k c F multiplied by h d minus h.

F s is the steady state value of F, k c F is one tuning parameter, which the value of that tuning parameter we need to determine, that is constant k c F basically, h d is the desired value and h is the liquid height. So, this is one additional equation similarly, if we consider another control scheme for temperature, in which Q is the manipulated variable, we can add another equation Q equals to Q s plus k c Q T d minus T. Here, Q s is the steady state value of Q, k c Q is the control at tuning parameter, that is a constant term then, this is desired temperature.

So, additionally, we are getting two equations, we had F equals to 2 now, if we can add two equations then, the degrees of freedom becomes 0. So, we had basically degrees of freedom 4 additionally, we have specified two load variables through direct measurement. Then, we have just paired control variable manipulated variable then, we got to additional equations. And finally, the degrees of freedom becomes 0 that means, the system is exactly specified.

Thank you.