

**Advanced Chemical Reaction Engineering**  
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**Lecture - 17**  
**Illustrative Example: Energy Balance in Stirred Vessels**

We are looking at practice problems in energy balance in stirred vessels in this lecture. Now, let me explain what the problem we want to learn to look at today.

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Semi batch operation of a stirred vessel.

$C_{A0}$   $NH_3$  (A)  
 $T_{A0} = 0$

$T_i$   
 $HCHO$

$4NH_3 + 6HCHO = N_4(CH_2)_6 + 6H_2O$   
 (A) (B)

Reaction is instantaneous  
 $C_p = 1000 \text{ Cal/L.c for mixture}$   
 $\Delta H = -74 \text{ kcal/mol HMT.}$

$V_i = 2000 \text{ Lit}$   
 $C_{Bi} = 15 \text{ gmol/L}$   
 $C_{A0} = 15 \text{ gmol/L}$   
 $T_i = 0$

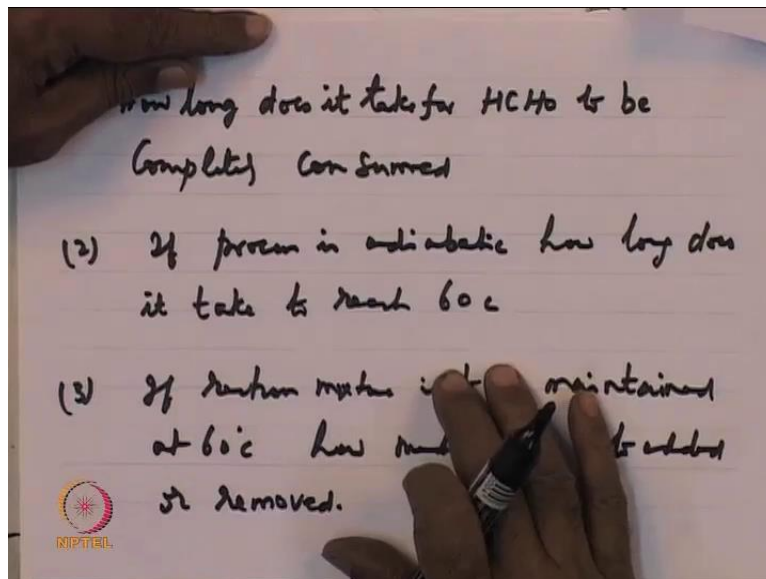
We want to look at a semi batch, semi batch operation of a stirred vessel. This is the exercise that we want to look at. What we have is a vessel, which is well stirred. Reaction that takes place is  $4 NH_3$  plus  $6 HCHO$ , giving you  $N_4 CH_2_6$  plus  $6 H_2 O$ . So, this is hexa-methylene tetramine, which is made from ammonia and formaldehyde. What we have is, we have ammonia coming in and you have here formaldehyde. So, you have an initial charge of formaldehyde in the equipment in the vessel into which you add ammonia. The reaction is instantaneous, which means, as soon as ammonia contacts formaldehyde, the reaction and the ammonia is completely consumed.

The initial composition of the vessel is, all the data is given, just put down all the numbers, I call this is as A, I call this as B. So, what is in the equipment is, that let me write here,  $V_i$  equal to 2000 litres, it is given.  $C_{Bi}$ , which is the initial formaldehyde

present here is 15g mole per litre. Now, the concentration, this is component A,  $C_{A0}$ ,  $C_{A0}$  is given as 15 gram moles per litre, per litre. Now, this temperature  $T_A$  is,  $T_{A0}$  is 0 and then,  $T_i$ , this, this temperature  $T_i$ , this  $T_i$ , is given as 0.  $C_p$ , specific heat,  $C_p$  is given as, volumetric specific heat is 1000 calories per liter  $C$  for the mixture, for mixture. It does not change, assumption is it does not change as here, the reaction is given as minus 74 kilocal per mole HMT. For every mole, which HMT formed, so much of reaction is taking place.

Now, the question that we have to address is the following, is, is now the temperature initially 0, calculate the time required for complete consumption of, first part is calculate the time required for complete consumption of formaldehyde, that is point one. And second part, is the time required for the temperature to reach 60. We start with 0, how long does it takes to go to 60. Third part is, how much heat is added or removed to maintain the temperature at 60 henceforth.

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So, let me state the problem once again. We have, one, first part is, how long, how long does it take, does it take for HCHO to be completely consumed. This is the first question we want to answer. Second question we want to answer is, if process is adiabatic, that is, we do not allow any heat loss, adiabatic, how long does it take, to reach 60c, that is second part.

Third part, if reactor, reaction mixture, mixture is to be maintained, maintained at 60 c, how much heat, heat is to be added or removed. So, these are the three questions that we need to answer. How long does it take for HCHO to completely get consumed? If you operated adiabatically, how long does it take to reach 60? And then, if it want to be maintained at 60, how much heat must add or remove. This is the three points that we want to address. Let us look at this one by one.

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$$(V)(r_A) = (-r_1 V)(-4) = F_{A0} = \frac{10 \text{ L}}{\text{min}} \times \frac{15 \text{ gm}}{\text{L}}$$

$$4 \text{ NH}_3 + 6 \text{ HCHO} = \text{N}_4(\text{CH}_2)_6 + 6 \text{ H}_2\text{O}$$

$$r_1 V = 150 / 4 = 37.5 \text{ gmol/min}$$

Below B

$$\frac{F_{B0}}{V} - \frac{F_{B1}}{V} + r_B V = \frac{dN_B}{dt} \quad \left| \quad t = \frac{N_{B1}}{(37.5)6} = \frac{15 \times 2000}{6 \times 37.5} = 133 \text{ min}$$

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First is, reaction is instantaneous. Therefore, what shall we say, that if volume of the equipment is V and r A is rated, which component A is getting consumed. So, our reaction is NH 3 plus, NH 3 plus, 4 NH 3 plus 6 CHO giving you N 4 CH 2 6 plus 6 H 2 O. So, this is hexamethylene tetraamine.

Now, V times r A, now what is V times r A equal to? By definition, we say, that is, minus of r 1 times V times minus 4, that is equal to, which is equal to F A is 0 equal to 10 liters per minute multiplied by 15 gram moles per liter. What is 10 liters per minute? The 10 liter per minute is the ((Refer Time: 07:15)) mentioned here. ((Refer Slide Time: 00:35)) This v not is, v not is 10 liters per minute.

So, what are we saying here? What we are saying is, that this ammonia is entering at 10 litres per minute multiplied by 15, that is, 150 moles per minute is entering and that must be equal to what, the rated, which you know, if V is the volume of the equipment and then r A is the rate of the chemical reaction, we know r A is minus of r 1 multiplied by 4

and all that. Therefore, this gives us  $r_1$  times equal to 150 divided by 4 equal to 37.5 gram moles per minute.

Now, we write a balance for B. What is balance for B? Input, output plus generation, which is  $r_B$  times  $V$  equal to  $dN_B/dt$ . What is  $r_B$ ?  $r_B$  is the, is the moles of B, which is... Now, we know there is, there is no continuous input, there is no continuous output, sorry output of A is there, therefore  $r_B$  is what?  $r_1$  with the minus sign into 6 times  $V$  equal to  $dN_B/dt$ . Is this clear? And this is constant because... Is this clear?

Therefore, what is the time shall we say? Time required equal to, so this, this whole thing becomes total amount of  $N_B$  is  $N_{B_i}$  divided by  $r_1$ .  $r_1$  is 37 point, 37.5 multiplied by 6. So,  $r_1 N_{B_i}$  is 15 multiplied by 2000 divided by 6 multiplied by 37.5. So, that gives you the time that is taken to completely consume the formaldehyde, which is present in the equipment.

Please let us understand this once again. What are we saying? What we are saying is, that if you write a material balance for component B, there is no input of component B, there is no output of component B. Whatever is the material is present inside it, is undergoing reaction as per this rate function  $r_B$ .  $r_B$  is what? By definition is  $r_1$  multiplied by ((Refer Time: 09:44)) matrix coefficient, that is what I have written here. So it is  $r_1$  is ((Refer Time: 09:48)), I should have put the minus sign here. So, it is minus sign should have been put here, minus 6. So, this is,  $r_1$  is 37.5 multiplied by 6, 15 into 2000, 2000 is the initial volume. So, 133 minutes is what it takes for the material to be completely consumed.

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$$\sum N_i \frac{dH_i}{dt} = \sum_{i=1}^{n \text{ species}} F_{i0} (H_{i0} - H_i) + \sum_{l=1}^{p \text{ rxns}} r_l V (-\Delta H_l^*) + Q - W_s$$

$$V C_p \frac{dT}{dt} = v_0 C_p (T_0 - T) + r_1 V (-\Delta H_1^*)$$

$$(V_i + v_0 t) \frac{dT}{dt} = (10)(10)(0 - T) + (37.5)(-74.6)$$

$$(2000 + 10t) \frac{dT}{dt} = -10T + (37.5 \times 74.6)$$

$$= -10T + 2797.5$$

Now, the next part of the question is, how long does it take for it to reach 60 degree C? What are we saying now? Now, as this reaction proceeds, heat is generated and therefore, whole thing gets heated up from initial temperature T of 0 degree C. And then, we want to know how long it takes to reach the 60 C? For which what we have to do is to write the energy balance.

What is the energy balance? Let me write the energy balance in the most general form.  $\sum N_i \frac{dH_i}{dt}$ . We have, we have derived all this at an earlier stage. So, I am not doing it again,  $\sum F_{i0} (H_{i0} - H_i)$ , we have derived this also, plus  $\sum r_l V (-\Delta H_l^*)$ , we have done this also minus of  $\Delta H$ , then plus  $Q$  minus of  $W_s$ , that we have removed now,  $\sum N_i \frac{dH_i}{dt}$ .

Now, what is  $N_i$ ? Adiabatic operation, therefore,  $B$ , this is not there. So, we have, on the left hand side is written as  $V C_p \frac{dT}{dt}$ . And then, this, this term,  $i=1$  to  $n$  species. So, this term I write as  $V C_p \frac{dT}{dt}$ , some another volumetric specific heat, times  $T$  naught minus of  $T$ .

And this term, there is this reaction, I write as  $r_1 V (-\Delta H_1^*)$ . Is this clear? So, the left hand side is volume... So, notice this volume  $V$  is actually  $V_i + v_0 t$  and  $dT/dt$  equal to, right hand side is  $10$  multiplied by  $C_p$  is  $1.0$  times  $0$  minus of  $T$  plus,  $r_1$  is  $37.5$ ,  $r_1 v$ , multiplied by this delta is minus of  $74.6$ . So, this, notice here, this  $v$  naught is  $2000$ , this is  $10 t$  times  $dT/dt$  equal to  $10$  with minus minus

10 T plus 37.5 times. So, this is minus minus plus because exothermic, this is the exothermic, so it is plus only, multiplied by 74.6. So, I can also write minus 10 plus 2797.5. So, this is, we have to only integrate this to find out how temperature changes its time.

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Handwritten mathematical derivation on a whiteboard:

$$(2000 + 10t) \frac{dT}{dt} = -10T + (37.5 \times 74.6)$$

$$= -10T + 2797.5$$

$$\frac{dT}{dt} + \frac{T}{200 + 10t} = \frac{279.7}{200 + t}$$

after integration ✓

$$T(200 + t) = (279.7) t$$

↑

$$t = \frac{12000}{219.7} = 54.6 \text{ min.}$$

NPTEL logo is visible in the bottom left corner of the whiteboard image.

Let us do that, let us do that, so we get, so please notice here, this is equation we have. So, 2000 plus 10 t dT dt minus of 10 T plus 2797. So, we can integrate this, we can integrate this, I have done this like this. So, dT, let me see whether I can do like this, plus T divided by 2000 plus 10 t equal to 279.7 divided by plus t. Is this ok? Let me see how it how it shapes up. I will put it here. So, dT dt, I am dividing T divided by 2000 plus 10t. 200 plus, this is not 2000, this is 200, alright.

Now, the integrated form, the solution looks like this. So, after integration, after you can, you can do all this, not very, not very difficult to do integration, we get 200 plus t multiplied by 200 plus t multiplied by 60 equal to 279.7 times t. This is the solution. Therefore, sorry, plus T, T is here, turns over the t equal to 12000, 12000 T divided by 219.7, that is about 54 minutes.

Now, what is that we know is, that what is the time, that is needed when this become 60, that is what is. So, you will have to put T equal to 60 here and find time here. Now, next part of the question is, I hope, I hope this is clear. We are just integrating it, this is the solution to the integral and then, we want to find out what is the time corresponding T

equal to 60, what is the time? You put T equal to 60 and find time and this that is what I find to be about 54 minutes.

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Maintain  $T = 60\text{ C}$

Energy Balance

$$v_0 C_p (T_0 - T) + r_1 V (-\Delta H_1^*) + Q = 0$$

$$= V C_p \frac{dT}{dt}$$

$$(10)(1.0)(0-60) + (37.5)(74.6) + Q = 0$$

$$Q = -2197 \text{ kcal/min. [heat has to be removed.]}$$

Third part of the question is, maintain, maintain T equal to 60. ((Refer Slide Time: 13:15)) Here what we have done, for, for T equal to 60 C, what is the time? What is the, what is T? This is what, what we have found out, now we want to maintain T. At 60 how much heat is to be added or removed? So, for that energy balance. What is the energy balance?

In our form we write, the energy balance as  $V \text{ naught } C_p T \text{ naught minus of } T \text{ plus } r_1 V \text{ times of minus } \Delta H_1^* \text{ This is plus } Q \text{ minus } W S \text{, that is equal to } V C_p dT dt \text{. This is our energy balance and we want this to be and we, so we want } Q \text{. This is what we want, so we can put all the numbers. Let me see. Therefore, I am putting all the numbers, } 10 C_p \text{ is } 1 \text{ kilocal per minute and then, temperature is going from } 0 \text{ to } 60 \text{, alright, plus plus } r_1 V \text{ is } 37.5 \text{ multiplied by } 74.6 \text{ plus } Q \text{. Is this clear? Therefore, } Q \text{ equal to, it turns out to be } 2197 \text{ kilocal per minute.}$

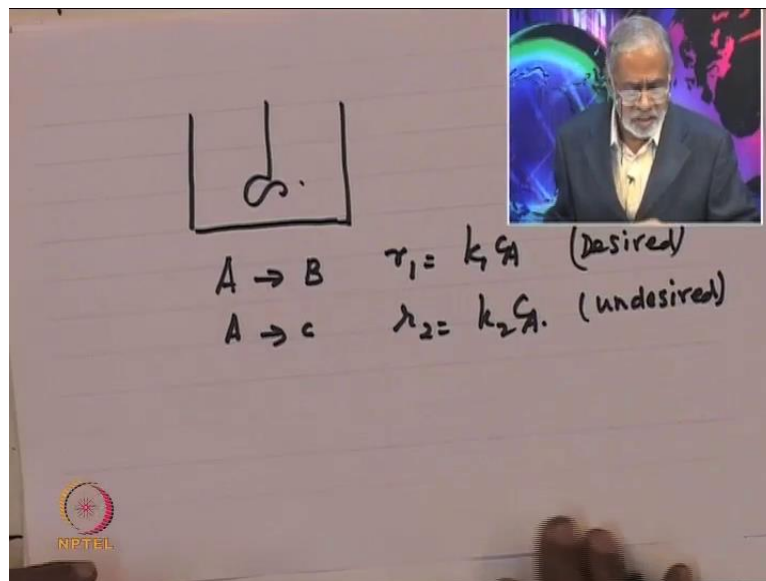
So, what we are saying is, that in order to maintain the temperature at 60 we have to, so much of heat has to be. So, what is this?  $T \text{ naught}$ ,  $T \text{ naught}$  is the temperature at which material is coming in and this is, 60 is temperature to which it must be heated, therefore this much heat has to be continuously supplied. This is the heated, which heat is



generated, therefore this  $Q$ . And then,  $Q$  is positive and negative  $Q$  is to be negative. So, in that so much of heat has to be removed heat, has to be removed.

So, what is it, that we have tried to learn from this exercise is, that when we are dealing with very explosive reactions, we find it more convenient to do semi batch operations, so that the concentration of ammonia in solution is kept 0. So, it is very safe, that is number one. Number two, since the heat is generated, heat is generated, we were able to use that heat to heat up the flow. It is able to achieve some amount of energy conservation and then, subsequent to reaching the appropriate temperature we are able to remove the heat or in other words, we are able to adjust the rate of ammonia addition, so that the heat removal that we are able to achieve without causing any explosion. So, this kind of semi batch operation and useful in our dealing with very explosive reactions.

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Now, let us go on to the next exercise. Second exercise of interest was, now we have finished one, we go to the next one. The second exercise that we want to look at is the following.

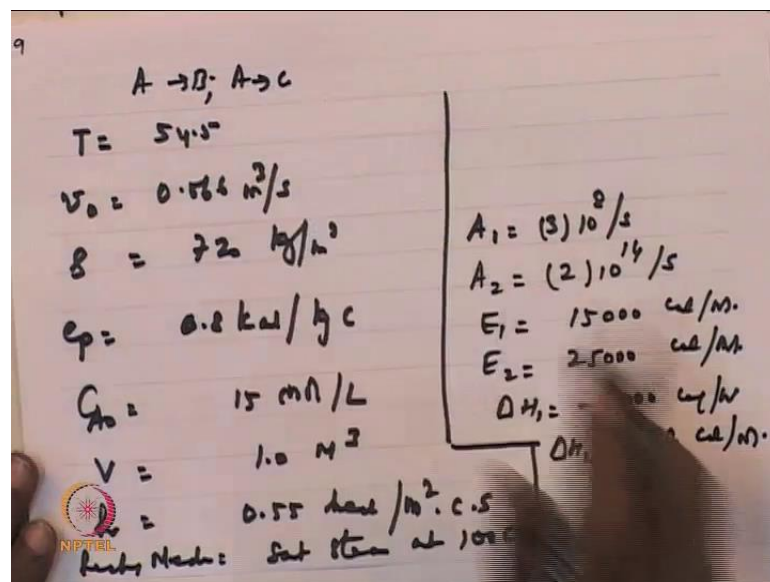
Here, we have a stirred tank. Reaction A goes to B and then reaction A goes to C, and this  $r_1$  equal to  $k_1 C A$  and  $r_2$  equal to  $k_2 C A$ . In other words, we are conducting a reaction and then, what as we call the data is given here, let me write down all the data: temperature, volumetric flow, density, heat capacity, heat concentration, coolant heating



medium, all the data is given, and all the data of the reactions, lot of data is given. Let me explain all that in a minute.

So, the important point, that we want to convey in this is, that when you have a reaction where you have, let us say this is desired and this is undesired, undesired. So, our interest is, of course, to operate the equipment and the conditions where the desired reaction is favored or the product B is the preferred product that we would like to see and therefore, you should like keep product C as small as possible under conditions of reaction. How do you achieve this? What kind of process operation should choose? Etcetera, is the point of interest in this exercise.

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Now, let us put all the data because this, we need all the data to be able to solve this problem. Let me put all the data. So, we have temperature is given as 54.5; volumetric flow, which is given as 0.066 cubic square meter per second; density of reaction mixture is given as kg per cubic meter; heat capacity,  $C_p$ , is given as 0.8 kilocal per kg degree C. So, density is given and therefore, volumetric specific heat can be found out. Heat concentration is given as 15 mole per, mole per litre, reactor volume is given as 1 cubic meter, heat transfer coefficient is given as 0.55 kilocal per square meter degree C second, and heating medium is given, heating medium, heating medium is saturated steam at 100 C. This is some data, lot more data is given regarding the reaction also.

If we look at the reaction, let me just put a line here, so that we have some idea what is what. So, the reaction, so we have A.  $A \xrightarrow{k_1} B$  and  $A \xrightarrow{k_2} C$ , A goes to B, A goes to C. Rate functions are given, given C A,  $k_2 C A$ , desired and undesired, all the data, etcetera, is given. And the question in front of us is the following. What is the temperature, which maximizes the production of B is the question one.

What is the reaction? Reaction, as we have said, A goes to B and A goes to C, A goes to B, A goes to C. Rate functions are given, given C A,  $k_2 C A$ , desired and undesired, all the data, etcetera, is given. And the question in front of us is the following. What is the temperature, which maximizes the production of B is the question one.

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(1) Show that  $T$  which maximizes production of B  
 $k_2 T = \frac{E_1}{(E_2 - E_1)}$

(2) Find Conversion, Reactor Temp

(3) What is area of cooling/heating coil required.

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Let me just write down, just in to provide the context. So, we want to know. So, first part is, first part is, show, show that temperature, which maximizes, maximizes production, production of B is given as  $k_2 T = \frac{E_1}{E_2 - E_1}$ . That means, the choice of temperature should be such, that this equality is satisfied, then only we get maximum rate of production of B, that is first thing we have to show. Then, find now, that find conversion, conversion reactor temperature, reactor temperature for the conditions above. Three, what is the area of cooling heating coil required.

Now, the context is frequently we encounter problems like this where there are the desired reactions, undesired reaction and therefore, we need to choose conditions under which our objective of making the desired product. Therefore, first thing is to show what

that the temperature, which maximizes the production rate of B is given by the expression. Once we have found that, then for those conditions what is the conversion, the reactor temperature, all those conditions have to be fully specified. So, this is the question that is of interest.

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$A \rightarrow B \quad r_1 = k_1 C_A \quad (\text{Desired})$   
 $A \rightarrow c \quad r_2 = k_2 C_A \quad (\text{Undesired})$

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Let us try to go through this now. We have this problem here and there is a coil, I will show this coil like this, one coil like this, which provides the heating or cooling.

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Stoichiometric Table

A	$F_{A0} (1 - x_1 - x_2)$
B	$F_{A0} x_1 + \cancel{F_{B0}}$
C	$F_{A0} x_2 + \cancel{F_{C0}}$

Material Balance for B

$$0 - F_B + r_1 V = 0$$

$$0 - F_{A0} x_1 + k_1 C_A (1 - x_1 - x_2) V$$

$Q = \frac{F_B}{v} = \frac{F_{A0} (1 - x_1 - x_2)}{v}$   
 $= Q_{A0} (1 - x_1 - x_2)$

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So, let us write the stoichiometry, stoichiometric table, stoichiometric table. What does it say? It tells us what happens to A, B, C because of reactions. So, the reaction takes a way. So, this is and B is  $F_{A0} X_1$  and C is  $F_{A0} X_2$ , correct, plus  $F_{B0}$ . It is stricken as 0, plus  $F_{C0}$ , it is stricken as 0. So, what are we saying here, that because stoichiometry, if the reaction extends  $X_1$  and  $X_2$ , this is what it is.

Therefore, material balance, to do a material balance, balance for B, for B, we get what? Input minus output, which is  $F_B$ ,  $F_B$ ,  $F_B$ , which is plus  $r_B$  times  $V$  equal to 0. So, 0 minus of  $F_B$  is what?  $F_{A0}$  times  $X_1$ . What is  $r_B$  is  $k_1$  plus  $k_2$  times  $C_{A0}$ ,  $C_{A0}$  times  $1 - X_1 - X_2$ . Notice, here  $C_A$  is  $F_A$  by  $V$ , therefore it is  $F_{A0}$  times  $1 - X_1 - X_2$ . Notice, here it is  $C_A$  is  $F_A$  by  $V$ , therefore it is  $F_{A0}$  times  $1 - X_1 - X_2$ . So, that is equal to  $C_{A0}$ ,  $C_{A0}$  times  $1 - X_1 - X_2$ . So, that is what is written here, multiplied by  $V$ .

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Material Balance for Comp B

$$0 = F_{A0} X_2 + k_2 C_A (1 - X_1 - X_2) V \quad (2)$$

From (1) and (2)

$$\frac{X_1}{X_2} = \frac{k_1}{k_2} \quad (3)$$

Put eq (3) in eqn (1)

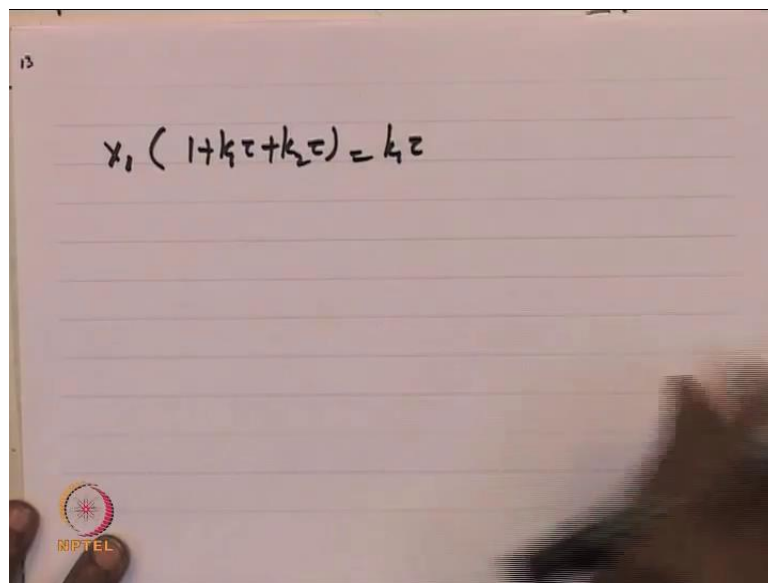
$$-F_{A0} X_1 + k_1 C_A (1 - X_1 - \frac{k_2}{k_1} X_1) = 0$$

Similarly, we can write a material balance for component C. Let me write material balance for component C, material balance, balance for component C. What does it say? 0 minus of  $F_{A0}$  input output and then, what is  $k_2$   $C_{A0}$  times  $1 - X_1 - X_2$  times  $V$  equal to 0. This is material balance. So, if I call this equation 2, if you call this as equation 1, simply by 1 divided by 2 gives you, from 1 and 2, 1 and 2 what do we get?  $X_1$  divided by  $X_2$  equal to  $k_1$  divided by  $k_2$ , straight forward. In this just look at this,

this is  $X$ , ok, just look at these two, it is quite obvious, that you know,  $x_1$ ,  $x_1$  divided by  $x$ , it is very obvious, you can see here. So,  $x_1$  divided by  $x_2$  is equal to  $k_1$  by  $k_2$ . So, we can call this is equation 3.

Now, you can substitute for this relationship in equation 1. So, you can put, putting I can, putting equation 3 in equation 1 we get what,  $F A_0$  minus  $F A_0 X_1$  plus  $k_1 C A_0$  times  $1$  minus of  $X_1$  minus of  $k_2$  by  $k_1$   $k_1 x$  one, this is clear, minus of  $x_1$ . Go through this now.

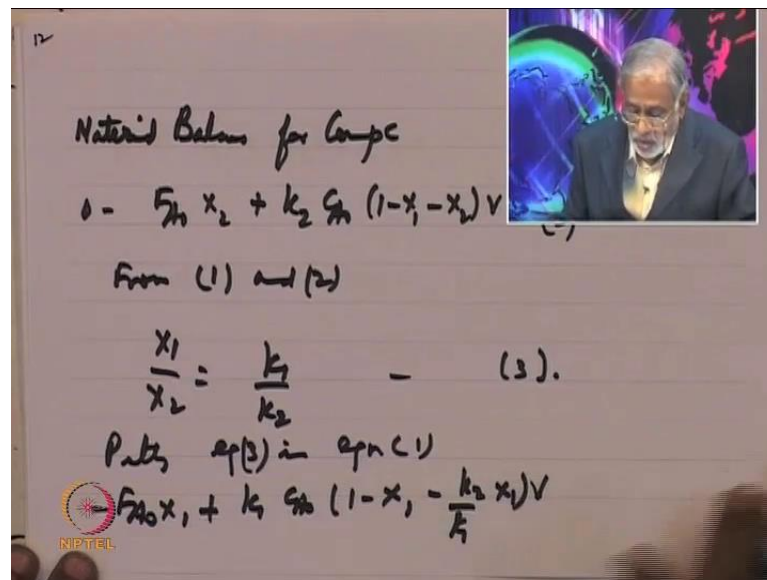
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A photograph of a hand-drawn equation on a piece of lined paper. The equation is  $x_1 (1 + k_1 \tau + k_2 \tau) = k_2 \tau$ . The paper has horizontal lines and a small circular logo in the bottom left corner with the word "MPTTEL" underneath it. The number "13" is written in the top left corner of the paper.

So, this gives us, simply rearranging,  $X_1$  multiplied by  $1$  plus  $k_1$  tow plus plus  $k_2$  tow equal to  $k_1$  tow.

(Refer Slide Time: 27:39)



Material Balance for Comp C

$$0 = F_{m1} x_2 + k_2 C_m (1 - x_1 - x_2) V$$

From (1) and (2)

$$\frac{x_1}{x_2} = \frac{k_1}{k_2} \quad (3)$$

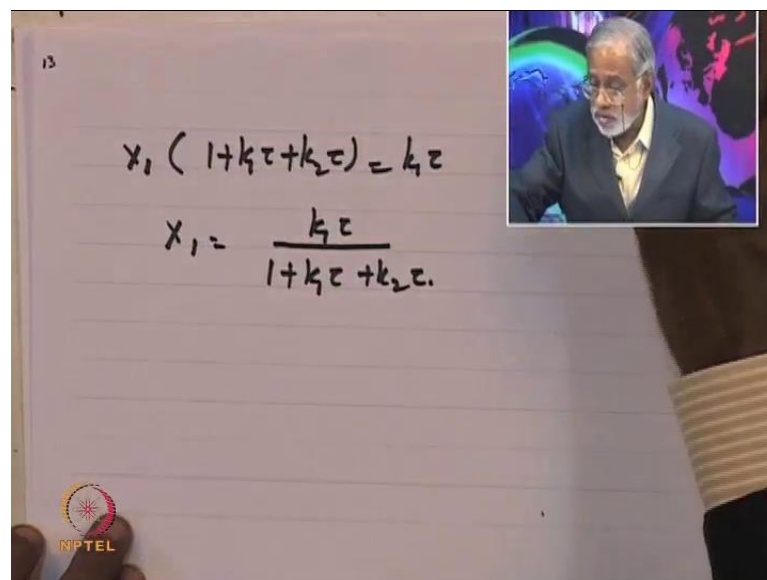
Put eq (3) in eqn (1)

$$-F_{m0} x_1 + k_1 C_m (1 - x_1 - \frac{k_2 x_1}{k_1}) V$$

The image shows a whiteboard with handwritten mathematical equations. The equations are:  $0 = F_{m1} x_2 + k_2 C_m (1 - x_1 - x_2) V$ ,  $\frac{x_1}{x_2} = \frac{k_1}{k_2} \quad (3)$ , and  $-F_{m0} x_1 + k_1 C_m (1 - x_1 - \frac{k_2 x_1}{k_1}) V$ . There is a small inset video of a man in the top right corner and an NPTEL logo in the bottom left corner.

Please, you can divide, this v is here. So, if we divide throughout, this 0 becomes C A0, cancels off V 0, this becomes k 1 tow 1 plus k 1 tow and this is what I have done.

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$$x_1 (1 + k_1 \tau + k_2 \tau) = k_1 \tau$$
$$x_1 = \frac{k_1 \tau}{1 + k_1 \tau + k_2 \tau}$$

The image shows a whiteboard with handwritten mathematical equations. The equations are:  $x_1 (1 + k_1 \tau + k_2 \tau) = k_1 \tau$  and  $x_1 = \frac{k_1 \tau}{1 + k_1 \tau + k_2 \tau}$ . There is a small inset video of a man in the top right corner and an NPTEL logo in the bottom left corner.

So, this gives you X 1 equal to K 1 tow divided by 1 plus k 1 tow plus k 2 tow. Is this clear? The rest value is straight forward. Let us just, just go through what we have done once again because it is important, that we understand what we have done.



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Handwritten diagram of a CSTR reactor with an agitator. Below the diagram, the following reactions and rate expressions are written:

$$A \rightarrow B \quad r_1 = k_1 C_A \quad (\text{Desired})$$

$$A \rightarrow C \quad r_2 = k_2 C_A \quad (\text{Undesired})$$

The NPTEL logo is visible in the bottom left corner of the slide.

We have let me go through, one second. We have a stirred tank, we have a stirred tank, say, this is, this is CSTR and then this reaction, A goes to B, A goes to C, rate function  $r_1$  and  $r_2$ , two are given. Now, what we are saying is, that when we write the material balance, when you write the material balance, we have input minus of output plus generation equal to accumulation. So, what is the rate, which this gets generated? The rate functions are given here. So, you can see here,  $r_B$  is generated from reaction one, A goes to B, correct, A goes to B, therefore  $r_B$  is generated. It is positive, this is what we have written here.

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Handwritten material balance for component C in a CSTR:

$$0 = F_{A0} x_2 + k_2 C_A (1 - x_1 - x_2) V$$

From (1) and (2)

$$\frac{x_1}{x_2} = \frac{k_1}{k_2} \quad (3)$$

Subs eq (3) in eqn (1)

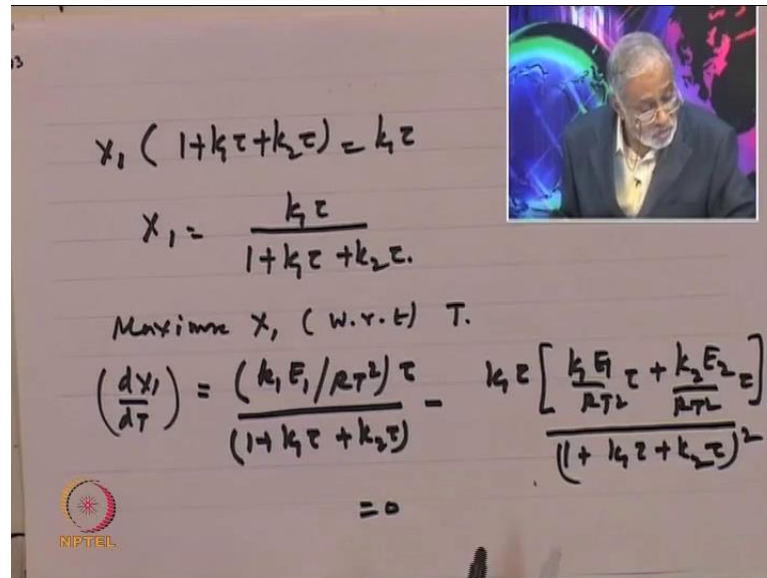
$$F_{A0} x_1 + k_1 C_{A0} (1 - x_1 - \frac{k_2 x_1}{k_1}) V$$

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Similarly,  $rC$ , you can see here,  $rC$ , it is generated,  $A$  goes to  $C$ , if  $A$  goes to  $C$  also. So, that is what we have plus sign here. Therefore, we have put it in the same form and dividing throughout by  $V_0$  and then cancelling off  $CAC_0$ , we get this relationship.

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$$X_1 (1+k_1\tau+k_2\tau) = k_1\tau$$

$$X_1 = \frac{k_1\tau}{1+k_1\tau+k_2\tau}$$

Maximize  $X_1$  (w.r.t)  $T$ .

$$\left(\frac{dX_1}{dT}\right) = \frac{(k_1 E_1 / R T^2) \tau}{(1+k_1\tau+k_2\tau)} - k_1\tau \left[ \frac{\frac{k_1 E_1 \tau}{R T^2} + \frac{k_2 E_2 \tau}{R T^2}}{(1+k_1\tau+k_2\tau)^2} \right]$$

$$= 0$$

What is it that we would like to maximize? We would like to maximize, see, we would like to maximize, maximize  $X_1$  with respect to, with respect to  $T$ , which means, that we have to differentiate  $dX_1$  by  $dT$ . So, we have  $dX_1$  by  $dT$ . We have to find out what is it equal to, we can differentiate this. Now, I am just writing down differentiation, differentiation of  $k_1$ . See, we know this, this is not new to you, derivative of  $d$  by  $dk$ ,  $d$  by  $dT$  of  $k$  is  $k_1 E_1$  by  $R T^2$ . So, I write here  $k_1 E_1$  by  $r T^2$ ,  $r T^2$  square times  $\tau$  divided by  $1$  plus  $k_1 \tau$  plus  $k_2 \tau$ .

Second term is,  $k_1 \tau$  and then we have to differentiate the denominator. So,  $k_1 E_1$  by  $r T^2$  square  $\tau$  and then  $k_2 E_2$  by  $r T^2$  square  $\tau$  divided by  $1$  plus  $k_1 \tau$  plus  $k_2 \tau$  whole square. So, this is what we have to set equal to  $0$ . Now, it is, we can do some algebraic manipulations and so on, so we will not spend too much time on that.

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$$E_1(1+k_2\tau) = k_2E_2\tau$$
$$k_2\tau = \frac{E_1}{E_1 - E_2}$$

$\infty$  |  $A \rightarrow B$   
 $A \rightarrow C$

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When you do that and go through algebra you will find, that the result you will get is  $E_1$  by  $1 + k_2\tau$  equal to  $k_2E_2\tau$  or  $k_2\tau$  equal to  $E_1$  divided by  $E_1$  minus of  $E_2$ . This is what we will get. So, the result, that we have wanted to prove, we have been able to show.

Now, it is important to understand what we have done. So, what is being said is the following, is, that we have a stirred tank and then this reaction,  $A$  goes to  $B$ ,  $A$  goes to  $C$  and these rate constants are given as it is given. So, then the best choice to get the maximum production of  $B$  is simply to choose your  $k_2$  such that this equality is satisfied.

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15

$$E_1 = 15000 \text{ Cal/mole}$$
$$E_2 = 25000 \text{ Cal/mole}$$
$$(k_2 \tau) \text{ for Max B} = \frac{15000}{25000 - 15000} = 1.5$$
$$\tau = \frac{V_R}{v_0} = \frac{(1.0)}{0.066} = 15.1 \text{ s}$$
$$(k_2) \tau = 1.5$$
$$k_2 = 1.5 / \tau = 1.5 / 15.1 = 0.1 \text{ s}^{-1}$$

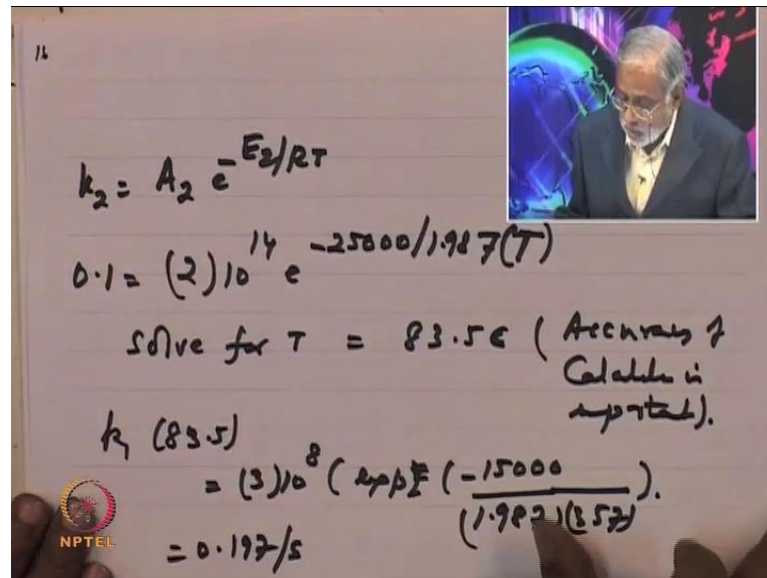
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Now, now that we know what is the best way to do this reaction, now we have put some numbers to see what it has to say. In the data, E 1 is given as, E 1 is given as 15000 units of calories per mole, E 2 is given as 25000, the units of calories per mole. Therefore, if you put these conditions into this one, therefore you should have k 2 tow for max production of B, max B equal to 15000 divided by 25000 minus of 15000, correct. That is equal to what? 1.5.

So, we should have and what is tow? Tow, by definition, is reactor volume V naught, that is, reactor volume is given and then, V naught is given as 0.066. So, that is equal to 15.1 second. So, tow is known, 15.1 seconds. Therefore, k 2 tow, which is equal to 1.5, therefore k 2 equal to 1.5 divided by tow, that is, 1.5 divided by 15.1 that is equal to 0.1 second.

So, what have we found out here? What we have found is, that the temperature, the value of k 2 that we should choose should be such, that k 2 should be 0.1 per second. So, that comes out of all.

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Handwritten mathematical derivation on a whiteboard:

$$k_2 = A_2 e^{-E_2/RT}$$
$$0.1 = (2)10^{14} e^{-25000/1.987(T)}$$

Solve for T = 83.5°C (Accuracy of calculation is important).

$$k_2 (83.5) = (3)10^8 \left( \exp\left(\frac{-15000}{(1.987)(83.5)}\right) \right)$$
$$= 0.197/s$$

The whiteboard also features an NPTEL logo in the bottom left corner and a small video inset in the top right corner showing a man in a suit speaking.

We know, we know that from our  $k_2$ , so we know that  $k_2$  equal to  $A_2 E$  to the power of minus of  $E_2$  by  $RT$ . This we know. This  $A_2$  is given as  $2 \times 10^{14}$   $e$  to the power of, this is given as 25000,  $R$  is 1.987 and  $T$ . So, essentially, this equation defines temperature at which we must operate the reaction. So, we can solve, solve for  $T$  and that turns out to be about 83.5 C. Please note, that accuracy of calculation is important, of calculation is important in this particular case.

Now, if we know the temperature to be 83.5, so notice, here you get this temperature  $T$  in Kelvin and it is converted to centigrade. So, what is  $k_1$  at 84, 83.5? To find this out we can say, that is equal to  $3 \times 10^8$   $e$  to the power of 8. It is all given exponential of, exponential of minus 15000 divided by 1.987 and then, temperature is 357, which is 83. This is what is given, that turns out to be 0.197 per second.

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$$X_1 = \frac{k_1 T}{1 + k_1 T + k_2 T}$$
$$= \frac{(0.197)(15.1)}{1 + (0.197)(15.1) + (0.1)(15.1)}$$
$$X_1 = 0.542$$
$$X_2 = \frac{k_2}{k_1} X_1 = \frac{(0.542)(0.1)}{0.197} = 0.273$$

So, we have got  $k_2$  from there, we have got temperature from there,  $k_1$  we have got, 0.197, therefore what is the value of... Now, we, we want to know what is the composition. What is the  $X_1$ ? We want to find out what is  $X_1$ , which is  $k_1 T$  plus  $k_2 T$  to  $T$ . So,  $k_1 T$  is 0.197,  $T$  is 15.1 second divided by 1 plus  $k_1 T$  is 0.197 multiplied by 15.1. And then,  $k_2 T$  is 0.1 multiplied by 15.1. So, that gives you  $X_1$  as 0.542. And then,  $X_2$  by definition you already got, that it is  $k_2$  by  $k_1$  times  $X_1$ , that is, 0.542 multiplied by 0.1 divided by 0.197. So, that comes out to 0.273.

So, what have we said? What we have said is, that if we have chosen the temperature, which maximizes the production of B and that temperature is given by this equation, which you have already derived, the temperature comes from this  $T$ , is specified in the problem. Therefore, we can find  $k_2$ . Once we can find  $k_2$ , we can solve for  $k_2$  from here where  $T$  is the temperature in Kelvin, which is converted to centigrade here. Once we know value of temperature, we can find  $k_1$  also, Arrhenius dependence is given. Therefore,  $k_1$  value is known. Once  $k_1$  value is known, we have already derived this,  $X_1$  is given by  $k_1 T$  by 1 plus  $k_1 T$  plus  $k_2 T$ . Therefore,  $X_1$  is 0.5 and  $X_2$  is  $k_2$  by  $k_1$ , we found 0.273.

So, what we are saying is, that in this multiple reaction where A goes to B, A goes to C,  $X_1$  about 54 percent is  $X_1$  and about half of it is component  $X_2$ , which is component

C. Notice here, that in the rate functions are such, that a significant part of the, of the, of the reactions go towards undesired product, which is not very desirable.

This problem itself is chosen to illustrate you that a huge quantity of the reaction material is often going towards products, which are wasteful and this is where choice of good catalyst, so that the specificity towards our desired product is required. Therefore, required development of suitable catalyst to target towards your required product is very, very important in reaction, which ((Refer Time: 37:31)).

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18

$$\sum N_i \frac{dH_i}{dT} = \sum F_{i0} (H_{i0} - H_i) + \sum_{r=1}^{p+r} r_i (-\Delta H_r^*) V + Q - W_s$$

$$H_i = H_i^*(T_R) + \int_{T_R}^T C_{p,i} dT$$

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Next question is, how much energy, see we have already said now, that we have, we have how much heat or heat is to be added or removed, to be able to achieve what we want. So, for that we, we look at our energy balance, which says,  $\sum N_i \frac{dH_i}{dT}$  equal to  $\sum F_{i0} (H_{i0} - H_i)$  plus  $\sum_{i=1}^p r_i (-\Delta H_i^*) V$  plus  $Q - W_s$ .

What we are saying is, to be able to achieve what we have achieved here, what we have achieved here we need to be able to ensure, that the heat, that is required for the process is appropriately added or removed. So, that we have to find out. How do you find out? Now,  $\frac{dH_i}{dT}$  is, let us go through this calculations. So, what is  $H_i$ ?

$H_i$  is equal to  $H_i$  at 0 at some reference temperature plus  $C_p$  times  $T$  minus of  $T_R$ , correct. Now, these, these effects are not important, then it is, you know, we can simplify, the whole thing simplifies. Let us put all the numbers to see how it works out.

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$$0 = \nu_0 C_p (T_0 - T) + \nu_1 v (-\Delta H_1^\circ) + \nu_2 v (-\Delta H_2^\circ) + Q$$

$$0 = (0.066)(720)(0.8)(54.5 - 83.5) + (0.066)(15)(0.54)(9060) + (0.066)(15)(0.27)(-13880) + Q$$

$$Q = +13 \text{ kcal/s}$$

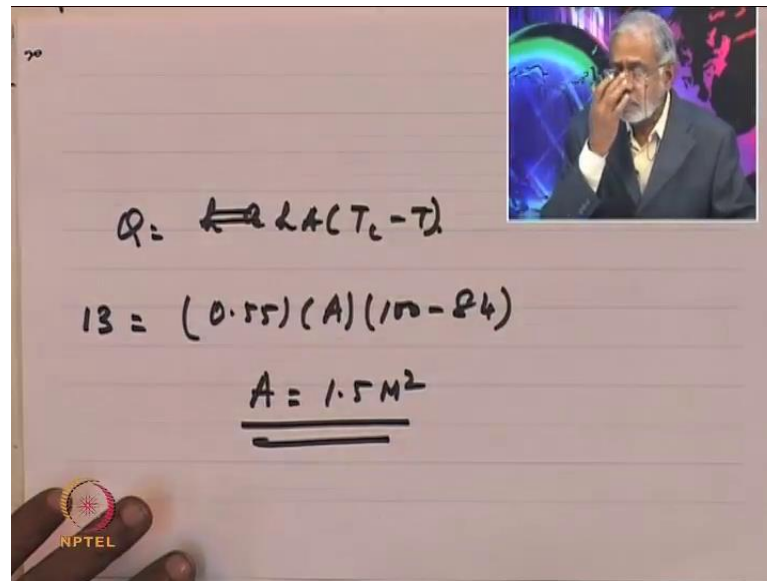
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So, we have here, putting all the numbers here we get  $v$  naught. So, so the energy balance simplifies like this for our case, plus  $r_1 v$  minus of  $\Delta H_1^\circ$  plus  $r_2 v$  minus of  $\Delta H_2^\circ$  plus  $Q$ . So, I will put all the numbers here, which is 0.066 into 720 into 0.8 into 54.5 minus of 83.5. So, this is the ((Refer Time: 39:36)) temperature to reacted temperature plus, next is  $r_1 v$ , we notice here, that this is equal to  $F_{A0} X_1$  is very elementary. This is equal to  $F_{A0} X_2$ , this, this  $r_1 v$  equal to  $F_{A0} X_1$ . I am putting, that  $F_{A0} X_1$  is  $F_{A0}$  is 0.066 multiplied by 15 multiplied by 0.454 into 9060, this is the, and then the next one is 0.066 15 into 0.27 to minus of 13880.

Notice here, please notice here, our heat of reaction, the data that is given, we can see here,  $\Delta H_1$  is exothermic,  $\Delta H_2$  is endothermic. So, this is a factor taken into account, minus  $\Delta H$  positive minus  $\Delta H$  negative. Here, we can see plus  $Q$ . We put all the numbers, we will find, that  $Q$  equal to 13 is positive, 13 kilocal per second,  $Q$  equal to, if you put all the numbers here, you get  $Q$  equal to 13 cal per second.



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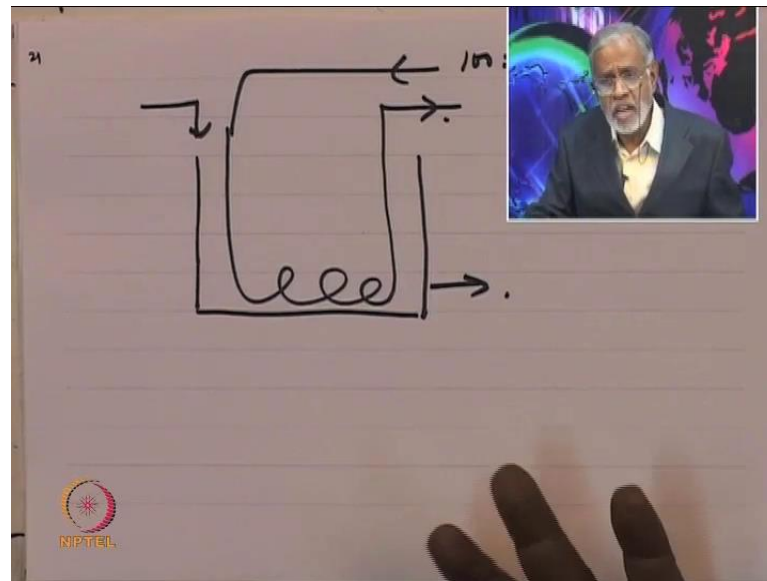
The image shows a whiteboard with handwritten mathematical equations. The first equation is  $Q = h A (T_c - T_h)$ . The second equation is  $13 = (0.55)(A)(100 - 84)$ . The third equation is  $A = 1.5 M^2$ , which is underlined. In the top right corner, there is a small inset video of a man with a beard and glasses, wearing a suit, speaking. In the bottom left corner, there is a small logo for NPTEL.

$$Q = h A (T_c - T_h)$$
$$13 = (0.55)(A)(100 - 84)$$
$$\underline{\underline{A = 1.5 M^2}}$$

Now, how do you ensure the 13 kilocal per second is actually achieved, that is, by looking at the heat transfer surface? We know, that  $Q$  equal to  $h$  times  $A$  heat transfer area, I will, I will put it like this,  $h A$  times  $T_c$  minus of  $T_h$  is given as, how much is  $h$ , heat transfer medium is given as 0.55 kilocal per second. So, it is 0.55 in the units of seconds.  $A$ , we do not know; coolant temperature is, is given as 100; and then, reactor temperature is given as 84 and  $Q$  is 13. So,  $A$  equal to ((Refer Time: 41:38)), it is about 1.5 meter square.

So, what we said, that this problem  $A$  going to  $B$ ,  $A$  going to  $C$ , we need heat transfer surface about 1.5 square meter to be able to achieve the maximum production rate of component, component  $B$ . Is that clear? Alright.

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Let me just summarize what we have said without losing the thought. So, we have this multiple reaction in which you have found out the best conditions for achieving the desired, alright. Now, there is related question, that might, that might be of importance to us is, the related question is, let me just run through this once again.

So, we have this reactor here. We have this heating medium or cooling medium, whatever. In this case, it is the heating medium equal to  $T_c$ . Feed is coming in, feed is going out. Now, what we would like to know is, whether this reaction operation, that we have chosen, whether it is stable or unstable. Now, to questions like this are best answered by looking at our stability criteria, which we have already done and as per that stability criteria if we look at the values of  $L$ ,  $M$  and  $N$ , we will be able to tell whether the process is stable or unstable.

So, what we have tried to do in this, in this particular problem is, that we have taken two exercises. Case one, in which it is semi batch operation where we have tried to understand how we can deal with very explosive reactions, so that in and then ensure, that the temperature at which that reaction takes place is kept under the control. And also, related with that heat is also released because the reaction is also taken in account and we operate the process, so that there is no explosions, at the same time new products are formed at the rate, which you can handle. That was the first exercise we have done.

The second exercise we have done is an exercise in which there are two reactions, A goes to B, A goes to C in a stirred tank and then, try to see how best we can maximize production of the desired product, which is component B. What we have done, that we set up the equations for production of component B and then we said, alright, if this is the rate at which component B is produced what is the conditions, which we, maximum rate of production be obtained, which we did by differentiating the expression for  $X_1$  with respect to temperature. And we found out, that the best temperature at which we can operate this process is defined by this relationship, which is  $k_2$  to equal to  $E_1$  divided by  $E_1$  minus of  $E_2$ ; that is something that we did, correct. It is very,  $k_2$  divided by  $E_2$  minus  $E_1$ .

Now, once we did that what we said is, that then, clearly temperature at which we are going to operate the process can come by looking at the value of  $k_2$  and hence, finding out the value of temperature corresponding to the given value of  $k_2$  because all the ((Refer Time: 44:56)), you know, of parameters are given. So once  $k_2$  is known, we know, find out the  $k_1$  because temperature is known. Therefore, find  $X_1$ , which is the, which is the extent of reaction. And therefore, what is the composition outlet stream and also, what is the amount of product C, which is undesired product formed? You know desired product, we know undesired product.

The conditions under which this problem has been, problem statement has been given, we find, that desired product is 0.54 and undesired product is 0.27 showing, that the undesired product is not small at all. It is very significant indicating, that our design must look at this problem of wasteful production of undesired product, which means, that you know, we do not have the catalyst, which is good enough to specifically target your reactants towards the desired product. In fact, it is one of the most important decisions in developmental work, that we must do always to see, that our catalyst always ensures, that the reactants substantially goes towards the desired product and the production of undesired product is kept as low as possible.

Now, it is not just that the undesired. It may be, I mean, may be reactants may not be very, very, very expensive and therefore, we might be able to afford it through our way significant part of our reaction as an undesired product. But the question is, that whatever is the undesired product that is produced, this must, will go into our environment and create problems of pollution. So, since the cost of polluting the environment has become

quite serious as you all well understand, we cannot afford to have a product, which is producing a lot of undesired product. A process cannot afford to produce an undesired product. So, that is something that you and I must recognize and remember in our design making sure so that our, not only we have economically good process, we also have a process, which is environmentally surround, environmentally safe apart from the economically attractive.

Thank you.