Technologies for Clean and Renewable Energy Production

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Lecture - 25
Tutorial 5

Hi friends, now we will have a tutorial session which is based on the last 4 classes. In this class, we will solve some numerical problems.

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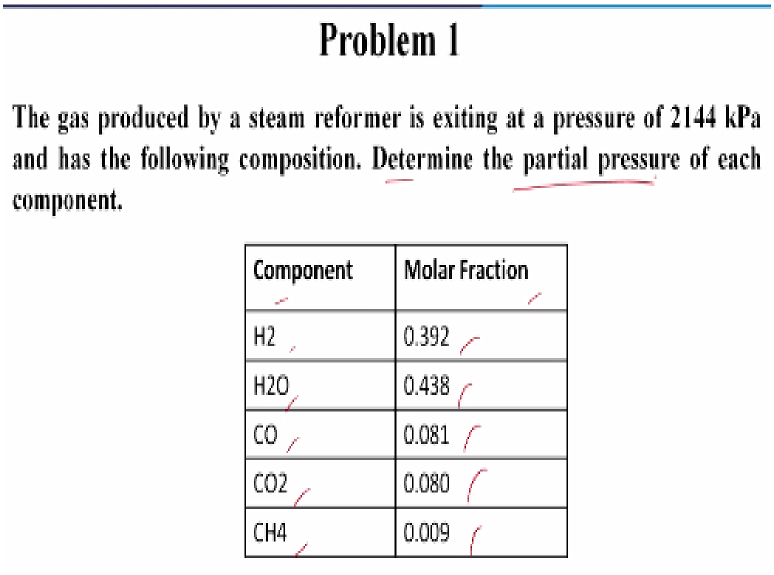

Component	Molar Fraction
H2	0.392
H2O	0.438
CO	0.081
CO2	0.080
CH4	0.009

Our first problem statement says the gas produced by steam reformer is exiting at a pressure of 2144 kilopascal and has the following composition. Determine the partial pressure of each component. So here a table is given component and molar fraction that is hydrogen, H_2O, CO, CO_2, CH_4. Hydrogen is 0.392, H_2O 0.438, CO 0.081, CO_2 0.080, and CH_4 0.009. So this is the problem statement and we have to determine the partial pressure of each component, mole fraction is given and total pressure is also given, so we can measure it. Now let us see.

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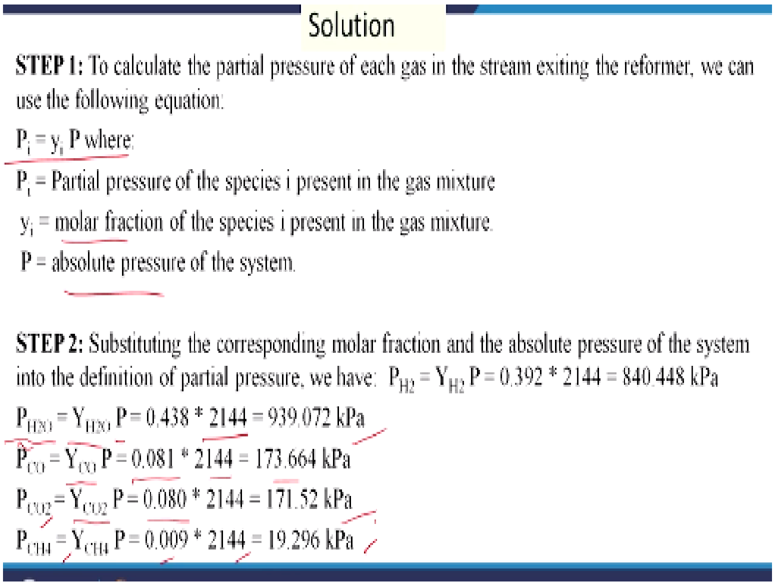

So what is our step one, we have to calculate the partial pressure of each gas in the steam exiting the reformer. So we can use which formula, that is $P_i = Y_i \times P$ where P_i is the partial pressure, Y is the mole fraction and then P is the absolute pressure, the total pressure of the system. So in our case what is our P_{H2O}, partial pressure of steam, then that is equal to mole fraction into the absolute pressure. So absolute pressure is given, that is the total pressure, that is 2144 kilopascal, this into the mole fraction of H_2O.

How much it is, mole fraction is 0.438. So we will write here 0.438 x 2144, it is coming 939.072 kilopascal. Similarly for carbon monoxide, the mole fraction of carbon monoxide into total pressure, so we are having 0.081 x 2144, so 173.664 kilopascal. Similarly for carbon dioxide, partial pressure = Y_{CO2} x P, so that is = 0.080 x 2144, so 171.52 and similarly for methane that is equal to 0.009 x 2144 = 19.296 kilopascal.

(Refer Slide Time: 03:23)

Problem 2

In the steam reforming process for producing hydrogen, part of the reformer exit gas is being burned with 10 % excess oxygen from air in order to supply heat for the reforming reaction to occur. The fuel being burned has the following composition:

The combustion reactions occurring inside the firebox are shown below; The combustion of methane is only 87 % complete.

1) $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

2) $CO + 1/2O_2 \rightarrow CO_2$

3) $H_2 + 1/2O_2 \rightarrow H_2O$

Component	Mol %
H_2	41.9
H_2O	5.1
CO	1.7
CO_2	41.9
CH_4	9.4

Determine the composition of the gas produced by the combustion reaction assuming an air composition of 21 mol % oxygen and 79 mol % nitrogen.

So now we will come to problem number 2. So problem number 2 states that in the steam reforming process for producing hydrogen, part of the reformer exit gas is being burned with 10% percent excess oxygen from air in order to supply heat for the reforming reaction to occur. The fuel being burned has the following composition, that is component and mole percent. So H_2 41.9%, H_2O 5.1%, CO 1.7%, CO_2 41.9%, CH_4 9.4%. The combustion reactions occurring inside the firebox are shown below.

These are the reaction that is $CH_4+2O_2 \rightarrow CO_2 + 2H_2O$, $CO+1/2O_2 \rightarrow CO_2$, and $H_2+1/2O_2 \rightarrow H_2O$. The combustion of methane is only 87%, another condition is methane conversion is 87% complete. So determine the composition of the gas produced by the combustion reaction assuming an air composition of 21 mol % oxygen and 79 mol % nitrogen. So in this problem, what we have to do? We have to determine the composition of the gas produced by the combustion reaction in the outside of the reforming tube.

So if we have one reformer here, so these are the tubes. When the reforming is taking place, then under reforming the gas is going out and here we are putting this gas that is your some part of this gas is recycled back and then it is fed here and this is burnt in this chamber, this is burnt, and then the burnt gas is getting out. So we have to calculate the composition at this position, here, what is the gas composition and this is the gas composition which is given it is coming here.

We are also providing oxygen or basically here oxygen plus nitrogen. So oxygen plus nitrogen is provided here at the outside of the tubes and some gas with this composition is burnt here and is getting out, basically it is a combustion problem, although it is related with reformer, but it is basically a combustion problem. So mass balance will do and we will be able to determine the composition of the gas which is going out from this.

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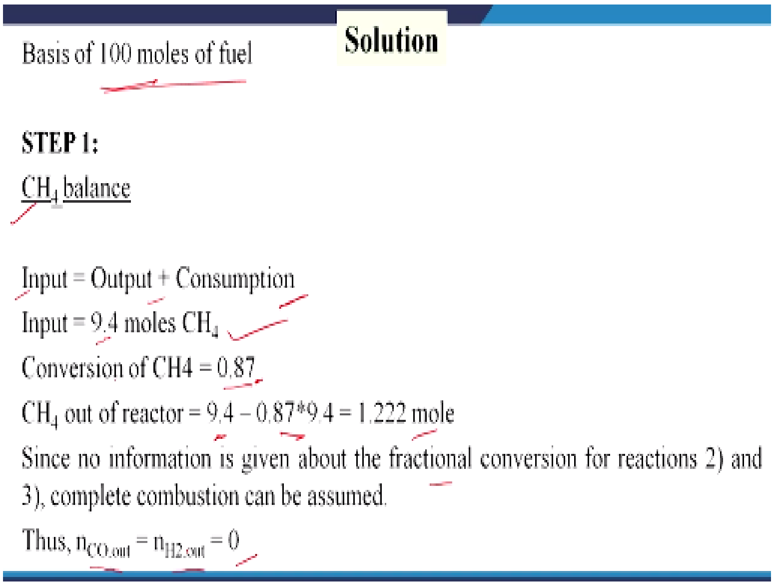

See for this problem, we will take one basis. So our basis is 100 moles of fuel gas which we are using for the combustion in the outer side of the reformer and then we will go for mass balance. So for CH_4 balance, methane balance, we have input = output + consumption. Obviously input = output + consumption because the CH_4 is consumed, so how much input we had minus consumption is our output. In this case input is equal to how much 9.4%. So we have 100 moles, so 9.4 moles of CH_4 we are getting.

Then what is the conversion of CH_4, 87% of it is converted, so 0.87 x 9.4, so that is equal to will be the conversion of it. So how much methane is remaining in the outlet, so that is equal to input - consumption. So input is our 9.4 and consumption is 0.87 x 9.4, so this one, so = 1.222 mole. So this mole of methane is getting out of the reactor, that is for methane, and since no information is given about the fractional conversion of reaction 2 and 3, so what are the reactions 2 and 3, CO to CO_2 and H_2+1/2O_2 it is giving us H_2O.

So these reactions either the CO is converted completely or not hydrogen is completely or not, so we are assuming that the CO is completely converted to CO_2 and H_2 is completely converted to H_2O. So under this condition, how do you get, $nCO_{out} = nH_{2out} = 0$, that means these are completely converted, so no CO, no H_2 is available in the output of this.

(Refer Slide Time: 08:39)

STEP 2:

CO_2 balance

Input + Generation = Output

By looking at the chemical reactions, it can be seen that both reactions 1) and 2) are generating carbon dioxide. From the stoichiometric coefficients of these reactions, and considering CO_2 balance

$n_{CO2,generated} = n_{CH4,reacted} + n_{CO,reacted}$

$= 9.4*0.87 + 1.7 = 9.88$ moles CO_2

Thus, by the material balance equation for CO_2:

$n_{CO2,out} = 41.9 + 9.88$ moles $= 51.78$ moles

Then we go for carbon dioxide balance. So carbon dioxide balance will again use input + generation = output. In this case, carbon dioxide is generated unlike methane, methane was being consumed, but here carbon dioxide is generated, so this expression will be used. So we have to find out that generation. So how we can determine the generation? We have to see the reactions first. So what are the reactions? We have these reactions. So these reactions also give carbon dioxide, this reaction also give carbon dioxide, so reaction 1 and reaction 2.

So how many moles of methane is used that many moles of carbon dioxide is also produced and how many moles of CO is used that much of carbon dioxide is also produced, so that part we will discuss. So what is this, consumed equal to number of moles of CH_4 reacted and number of CO reacted and what is this number of nCH_4 reacted, that is 9.4 x 0.87, this part, and what is nCO, the percentage of CO is 1.7, so out of 100, 1.7 moles was present, so this is this plus this, that is equal to 9.88 moles of CO_2 is generated.

So this is the generation of CO_2. Then what would be the output of this, input + generation. So what was the input, that carbon dioxide was available in it as 41.9%, so 41.9 moles are originally available in the inlet of the gas and now 9.88 moles is generated during the process, so this plus this will be 51.78 moles of carbon dioxide will be available at the output.

(Refer Slide Time: 10:38)

STEP 3:

H_2O balance

Input + Generation = Output

Input = 5.1 moles

The amount of water generated by the chemical reactions will be given by:

$$n_{H2O,generated} = n_{H2,reacted} + 2n_{CH4,reacted}$$

Substituting numeric values into this equation, we have:

$$n_{H2O,generated} = 41.9 + 2*0.87*9.4 = 58.256 \text{ moles}$$

By substituting this result into the material balance equation for H_2O:

$$n_{H2O,out} = 5.1 + 58.256 = 63.356 \text{ moles}$$

Next we see the H_2O balance, mass balance for H_2O. Then what we will get, again input + generation = output, the same formula we will use. In this case, what is the input, input is given as 5.1%, so we are having say 5.1 moles, so it is given here in this table 5.1, so that 5.1% we are considering, 5.1 moles. The amount of water generated by the chemical reactions will be given by this, $nH_2O_{generated} = nH_{2reacted} + 2nCH_{4reacted}$ because this was the formula, here the reactions, so $H_2 + 1/2O_2 \rightarrow H_2O$.

So how much hydrogen is used that much H_2O is produced and this is how much methane is used two of that will be the H_2O production. So that is why we will be getting this balance number of moles of hydrogen reacted = number of moles of hydrogen reacted + 2 x number of moles of methane reacted. So number of moles of hydrogen reacted as we are considering that hydrogen is 100% converted, so 41.9 it is available as the hydrogen concentration in the inlet gas is 41.9%.

So out of 100 moles that is 41.9 moles of hydrogen is available + 2 x methane converted. So methane how much was available 9.4 x 0.87 that was the conversion and 2 moles will be generated, 2 moles of H_2O will be generated from 1 mole of methane, so 2 x this x this will be our H_2O generated due to methane. So this overall we are getting moles of H_2O generated = 58.256 moles. So what would be the output, input + generation, so input how much we have 5.1% and so 5.1 moles we had out of 100 moles and now we are getting 58.256, so we are getting 63.356 moles of H_2O.

(Refer Slide Time: 12:49)

STEP 4:

To determine the oxygen exiting in the product stream, we will perform a material balance for molecular oxygen:

This value can be calculated by multiplying the amount of fuel in the feed (carbon monoxide, methane or hydrogen) by the stoichiometric ratio of fuel to oxygen. Thus,

$n_{O2,r1}$ = 9.4 moles CH_4(2 moles O_2/mol CH_4) = 18.8 moles O_2

$n_{O2,r2}$ = 1.7 moles CO(1/2 moles O_2/mol CH_4) = 0.85 moles O_2

$n_{O2,r3}$ = 41.9 moles H_2(1/2 moles O_2/mol CH_4) = 20.95 moles O_2

Next we will see our oxygen balance because we have to determine the composition of the outlet gas which will be containing nitrogen also, so where from the nitrogen is coming, from the oxygen it is coming. So oxygen we have used 10% excess, that means I have to determine stoichiometrically how much oxygen is required, so 10% of that as excess is provided. So here we need not to consider how much methane is converted in the reactor in real case, we have to consider stoichiometrically how much oxygen is required for the conversion of all the methane available in it, so that we will consider here.

So what is this nO_2 number of moles of oxygen required for methane conversion is your 2 moles of O_2 per mole of methane, that is why for complete conversion stoichiometrically, we need 2 x 9.4 moles as 9.4 moles of methane is available originally in the inlet gas. So 2 x 9.4 = 18.8 moles of oxygen is required for the conversion of CH_4 to H_2O and CO_2 and then similarly for CO, carbon monoxide to CO_2 conversion, we need 1 / 2 mole of oxygen for 1 mole of CO, this is not CH_4 this is CO, so what we are getting 1.7 x mole of CO, we have 1.7 x half of it, so that is equal to 0.85 moles O_2 is required.

Then for the hydrogen to H_2O production, we need oxygen and that 1/2 mole of O_2 is required for 1/2 mole of hydrogen, therefore hydrogen is present 41.9 and all hydrogen is converted, so 1/2 of 41.9 that is 20.95 moles oxygen is required for this reaction.

(Refer Slide Time: 15:03)

Knowing the values of oxygen consumed by each reaction, we can calculate the total amount of oxygen required by this process:

Consumption $= n_{O2,r1} + n_{O2,r2} + n_{O2,r3}$

$= 40.6$ moles O_2

Since there is 10 % excess oxygen, the number of moles of oxygen entering the reactor will be given by:

Input = 1.10 * 40.6 = 44.66 moles

O_2 actually react through all the reactions = 2*0.87*9.4 + 1.7*1/2 + 41.9*1/2

= 38.156 moles O_2

O_2 out of reactor = 44.66 -38.156 = 6.504 moles O_2

So what will be our total oxygen consumption? The oxygen consumed for the methane reaction for the CO and for the hydrogen, so that is 40.6 moles we have got, that is equal to 20.95+18.8+0.85, so this is equal to 40.6, so that moles we are getting. So now this is the stoichiometric requirement, now 10% excess has been provided. So what was the oxygen provided, so there is 1.10 x 40.6 moles that is equal to 44.66 moles, so that much of oxygen is provided.

So oxygen actually consumed equal to how much, that is equal to 87% of methane conversion. So 2 x 0.87 x 9.4 + 100% of carbon monoxide and hydrogen. So 1.7 x 1 / 2 + 41.9 x 1 / 2 = 38.156 moles of O_2, so this 44.66 we are giving and 38.156 moles of O_2 is being used for the conversion process, so remaining will be available in the exit gas so 44.66-38.156 = 6.504 moles of oxygen will be available.

(Refer Slide Time: 16:37)

STEP 5: However, all the nitrogen will exit in the product stream since it is not being consumed nor generated by the chemical reactions. Thus

N_2 balance

$$n_{N2,in} = n_{N2,out}$$

The amount of nitrogen fed into the system can be determined by multiplying the molar fraction of nitrogen in the air by the amount of air fed:

$$n_{N2,in} = n_{N2,out} = (0.79/0.21)*44.66 = 168.01 \text{ moles } N_2$$

Now that we know the amount of moles of all the species, we can calculate the total number of moles exiting the combustion chamber.

$$nout = n_{CH4} + n_{CO2,out} + n_{H2O,out} + n_{N2,out} + n_{O2,out}$$
$$= 1.222 + 51.78 + 63.356 + 168.01 + 6.504$$
$$= 290.87 \text{ moles}$$

Then what about the nitrogen, so as you know that nitrogen will not react, so how much nitrogen is getting in that will go out. So in this case, how much is in, that is how much oxygen is used if we know, then you can determine how much nitrogen is being used. So that 0.79 / 0.21 x the moles of oxygen used. So moles of oxygen used = 44.66 which is supplied to the inlet gas, so that is equal to 44.66, so it is coming is equal to 168.01 moles nitrogen.

So this nitrogen we are giving here. Now what will be the compositions of the outlet gas then? It will be having number of methane which is unconverted and the number of moles of carbon dioxide and the moles of steam and moles of nitrogen and moles of oxygen which is not used. So already we have got 1.222 for methane, for nCO_2 we have got 51.78, H_2O we have got 63.356, nitrogen we have got 168.01, and for oxygen we have got 6.504 which is going out. So total is 290.87 moles.

(Refer Slide Time: 18:07)

STEP 6:

The molar fraction of each component of the exhaust gases can be obtained by dividing the number of moles of each component by the total number of moles.

Thus, $Y_{CH4} = n_{CH4,out}/n_{out} = 1.222/290.87 = 0.0042$

$Y_{H2O} = n_{H2O,out}/n_{out} = 63.356/290.87 = 0.2178$

$Y_{O2} = n_{O2,out}/n_{out} = 6.504/290.87 = 0.0224$

$Y_{CO2} = n_{CO2,out}/n_{out} = 0.178 = \frac{51.78}{290.87}$

$Y_{N2} = n_{N2,out}/n_{out} = 168.01/290.87 = 0.5776$

So now we can determine the percentage, so what will be the percentage of methane equal to mole of methane/total mole x 100, so that way we will get it hence for mole of methane 1.222 / 290.87, so this is the fraction. For H_2O we are getting 63.356 / 290.87 that is 0.2178, this is 63.356 okay. Then we are getting for Y_{O2} that is equal to 6504 / 280.87 = 0.024 and for Y_{CO2} so 0.178 because this is equal to how much, we have carbon dioxide, so this is 51.78, so 51.78 / 290.87 = 0.17.

Then we are getting say Y_{N2}, Y_{N2} = moles of nitrogen / moles of total outlet stream, so that is equal 168.01 / 290.87 = 0.5776. So now we are able to get the composition of the outlet gas.

(Refer Slide Time: 19:31)

Problem 3

Dry methane is burned with dry air. Both are 25 °C initially. The flame temperature is 1300 °C. If the complete combustion is assumed how much excess air is being used? The reaction is

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Standard heat of reaction is -8.028*10^5 J/g mole of CH_4 reacted. Mean molar specific heat of gases between 25°C and 1300°C are in J/g (mole) K

CO_2	51.88
O_2	34.01
H_2O	40.45
N_2	32.21

So next problem statement says dry methane is burned with dry air. Both are 25 degree centigrade initially. The flame temperature is 1300 degree centigrade. If the complete combustion is assumed, how much excess air is being used. The reaction is $CH_4+2O_2 \rightarrow CO_2+2H_2O$. The standard heat of reaction is -8.028 x 10^5 joule per gram mole of CH_4.

Mean molar specific heat of gases between 25 degree centigrade and 1300 degree centigrade are in joule per gram mole K that is equal to CO_2 51.88, O_2 34.01, H_2O 40.45, and N_2 32.21. So this is the problem statement and then what we have to do, how much excess air is required so that we have to calculate. So how we can do it, let us see.

(Refer Slide Time: 20:39)

SOLUTION:

- The reaction is given below:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

- Let y = number of moles of O_2 in the feed
- Reference temperature = 25 °C
- Therefore, enthalpy of both CH_4 and $O_2 + N_2$ is zero at 25 °C

So what is the reaction given, $CH_4+2O_2 \rightarrow CO_2+2H_2O$. Then let us assume that number of moles of O_2 in the feed is equal to y and the reference temperature is 25 degree centigrade and the enthalpy of both CH_4, O_2 and N_2 is 0 at 25 degree centigrade, this way base case it is given.

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- For Complete conversion of CH_4

	Inlet			Outlet		
Species	T(°C)	Moles	Enthalpy (J/mol)	T(°C)	Moles	Enthalpy (J/mol)
CH_4	25	1	0	1300	0	
O_2	25	y	0	1300	y-2	34.01(1300-25)
N_2	25	3.76y	0	1300	3.76y	32.21(1300-25)
CO_2				1300	1	51.88(1300-25)
H_2O				1300	2	40.45(1300-25)

Then for complete conversion of methane, what is our condition, say we have, this is our inlet, all are CH_4, oxygen and nitrogen it is there here we are providing. So nitrogen will be there, oxygen will be there, methane will be there. See we have 1 mole of methane, we are having y mole of O_2 and then 3.76 mole of nitrogen because 21% is oxygen and 79% is nitrogen, that is why this mole ratio will be 3.76. So if y is oxygen, then 3.76 will be nitrogen, enthalpy for all it is 0.

Then outlet temperature is 1300 degree centigrade and in this case methane will not be available, but oxygen will be available because excess oxygen is used, so how much y is given, so rest will be y - 2 because 1 mole methane consumes 2 mole of oxygen, so y - 2 is the remaining oxygen and then nitrogen how much was available that will be available, there is no reaction with it, so 3.76y. Then CO_2, 1 mole of methane will give 1 mole of carbon dioxide and 1 mole of methane will give 2 moles of H_2O.

So we are getting 2 mole of H_2O and then enthalpy of these already we can calculate that = 34.01 x 1300 - 25, why because these value are given here for CO_2 this one, oxygen 34.01, H_2O 40.45, and N_2 of 32.21. So at the outlet, all those gas will be available and their enthalpy values are also provided here okay, so this we have to multiply by the moles x this x this one, mCpdT, so mCpdT, m with respect to mole, so Cp is given here, so this is our dT 1300-25, so this is our enthalpy value.

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- **Rates of enthalpy:**

Accumulation = Input- Output + Generation (heat due to reaction)

$$= 0 - [(y-2)*34.01 + 3.76y * 32.21 + 51.88 + 40.45 *2](1300-25) + (-8.028 * 10^5)$$

$$= 155.12y + 64.76](1300-25) = 8.028*10^5$$

$$y = 3.6416 \text{ mole}$$

- % excess = [(3.64-2)/2]*100

= 82%

Therefore, 3.6416 mole O_2 was fed for each mole of CH_4

Then we will get the sheet balance. Then we will calculate the value of y and that will be the excess oxygen required for this combustion. So here accumulation = input - output + generation. So this is the heat balance we are consuming. So input equal to zero, ΔH is not there because all are at 25 degree centigrade so that is our base case, so minus output, y-2 oxygen is there, so x 32.01+3.76y for nitrogen and then 32.31+51.88+40.45x 2 that is the composition which we are getting, that is H_2O and CO_2 and then ΔT.

So this is your mC_P and this is your ΔT, mCpΔT that is the output which we are getting with the gas stream. Generation we are getting, what is that, during this heat generated that is equal to -8.028 x 10^5. So by this accumulation is equal to 0, so by rearranging we are getting this formula and y = 3.6416 moles, so this is our y we are getting. So then what is the excess air, why this much oxygen was required, 2 moles were stoichiometrically, so (3.64–2)/ 2 x 100 = 82% excess air was used.

Therefore 3.6416 moles oxygen was fed for each mole of CH4 and excess air was 82%. So now we are able to solve the problems, so up to this in this class. Thank you very much for your patience.