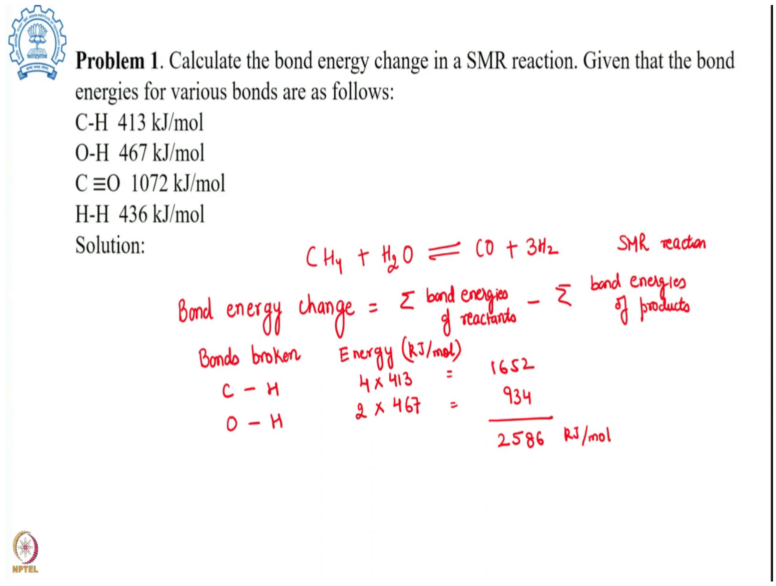
Hydrogen Energy: Production, Storage, Transportation and Safety
Prof. Pratibha Sharma
Department of Energy Science and Engineering
Indian Institute of Technology, Bombay

Lecture - 07
Tutorial - 1

Let us do certain problems on the steam reformation, we will start with very basic problems to just get a background and we will just brush up certain concepts which we have studied long back. And then later on we will move on to increase the complexity of the problem.

(Refer Slide Time: 00:42)



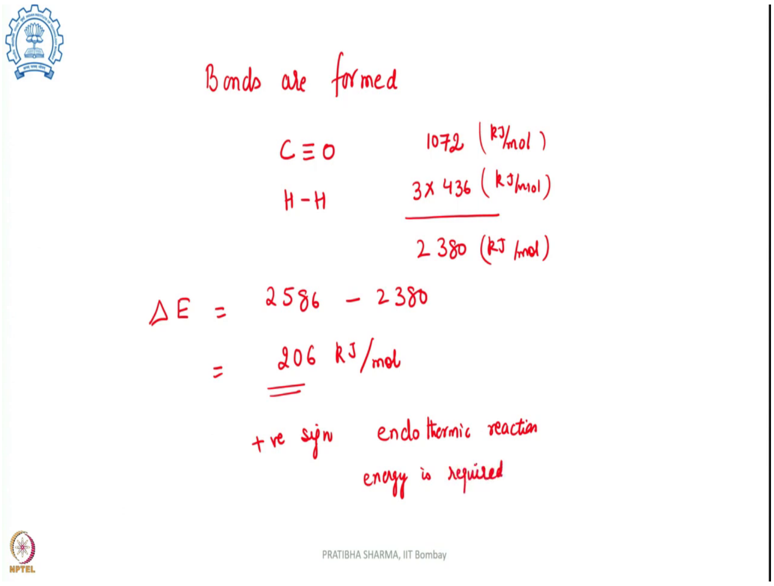
So, let us look at the first problem, this is a very simple problem wherein, it is asked to calculate the bond energy change in a steam methane reforming reaction. And the bond energy of various bonds is given in the problem.

So, how to solve that? Let us first look at the steam reformation reaction. So, we know that methane reacts with steam which is H_2O and then it forms syn gas which is nothing but carbon monoxide and hydrogen. Now, if you look at this reaction, which is the SMR reaction, how can we find the change in the bond energy? So, bond energy change can be obtained by finding the difference in the bond energy on the reactant side and that on the product side.

So, let us look at the bonds which are broken in the process, these are C - H bonds, 4 C - H bonds are broken and 2 O - H bonds are broken. So, the associated average bond energy which is in kilojoule per mole can be written as, the bond energy for C - H bond is 413 kilojoule per mole. And for O - H bond, 2 such bonds are broken from the reactant side and the associated bond energy for O - H bond is 467 kilojoule per mole.

And which corresponds to 1652 kilojoule per mole and 934 kilojoule per mole, a total of 2586 kilojoule per mole for the reactants.

(Refer Slide Time: 03:28)

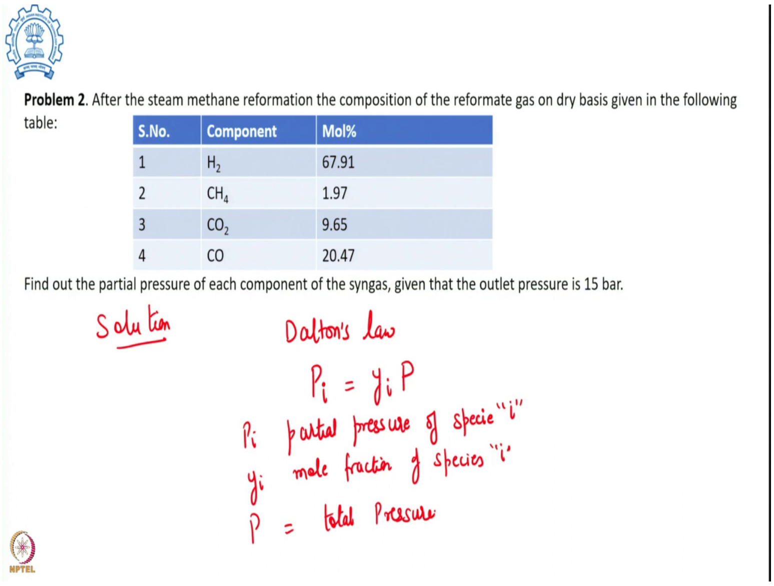


Now, let us look at the product side. On the product side bonds are formed. So, which bonds are formed? CO is formed carbon monoxide which is a triple bond. So, 1 mole of CO is being formed in the process.

So, the associated bond energy we have seen is 1072 kilojoule per mole and 3 moles of hydrogen is being formed. The associated bond energy for hydrogen is 436 kilojoule per mole, 3 such bonds are being formed which corresponds to total energy of 2380 kilojoule per mole for the product side. So, if you want to find the change in energy in the process, the energy associated with bonds being broken, the total we have found 2586 and the energy associated with the bonds being formed in the product side is 2380. And that is equal to 206 kilojoule per mole.

Now, if we remember this was the value we have seen in the SMR reaction and this is corresponding to the energy change. Since this is positive in sign; that means, SMR reaction is an endothermic reaction and energy is required in the process. So, this is a very simple problem which we have seen.

(Refer Slide Time: 05:36)



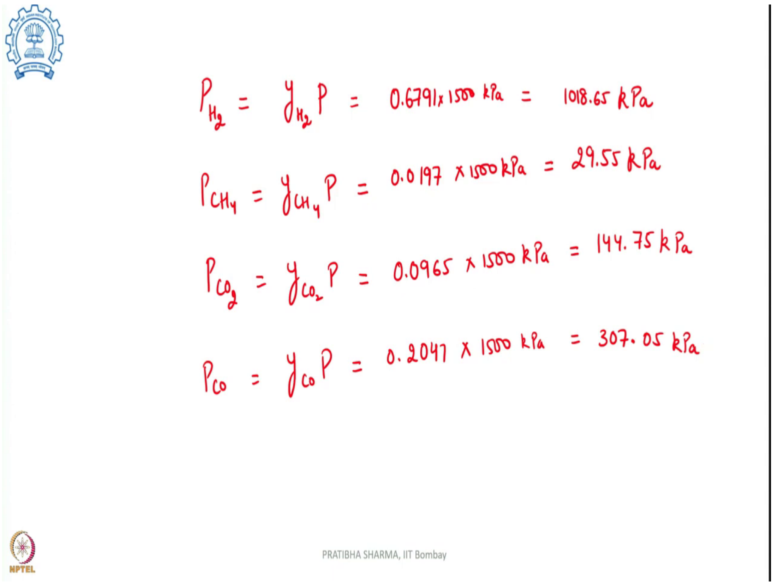
Let us look at another problem; this is again very simple problem which states that after the steam methane reforming the product gas which is obtained after reforming process called reformate gas has the composition which is shown in the table, this is on the dry basis.

So, removing the moisture content and this is given by the component wise in the mole percent and we need to find out the partial pressure of each component of the syn gas, provided that the outlet pressure, the total pressure is 15 bar in the process.

Now, let us solve this problem, this is again a simple problem, how to solve it let us see. Now, we know that Dalton's law which is actually for ideal gas, but can be applied for hydrogen, because the temperature of the reaction in SMR which we are considering is very high, 700 to 950 degree centigrade and under that conditions we can still apply the Dalton's law which says that, the partial pressure is equal to the mole fraction and the total pressure.

So, what is P i? P i is partial pressure of any species which is reacting say i and the corresponding mole fraction of that species is represented by yi. P is the total pressure, which is given in the problem.

(Refer Slide Time: 07:40)



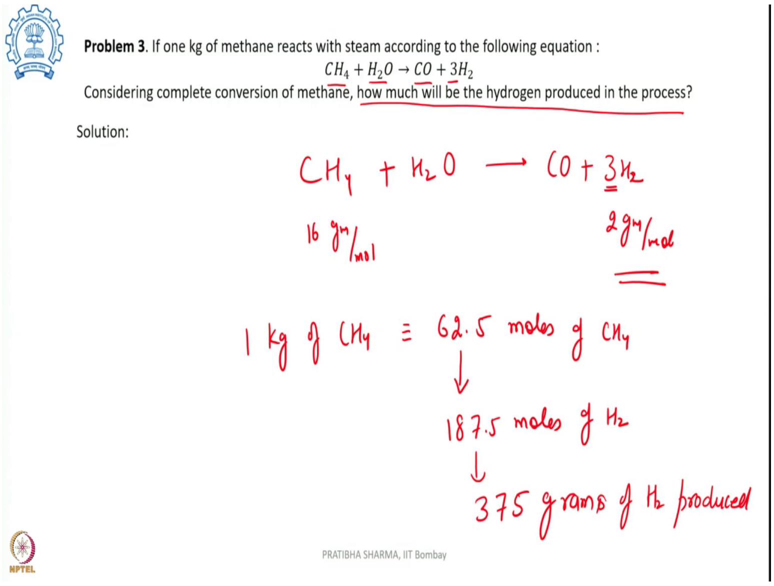
So, let us do that. Now, the partial pressure of hydrogen can be obtained as the mole fraction of hydrogen and the total pressure. So, given that the mole fraction of hydrogen in the problem is 0.6791, it was the mole percent. Now we have converted it into 15 bar which is nothing but 1500 kilopascal and that gives a value of 1018.65 kilopascal.

So, this is the partial pressure of hydrogen which we have got. Similarly, we can find for other species which is methane, again the mole fraction into the total pressure for methane given that the mole fraction is 0.0197, total pressure 1500 kilopascal and that gives a value of 29.55 kilopascal.

Partial pressure of carbon dioxide also we can get in the similar manner, its mole fraction time is the total pressure, given that the mole fraction is 0.0965 into 1500 kilopascal, which gives the value of 144.75 kilopascal.

And same way we can find out for the last species that is a CO in the problem, its mole fraction and the total pressure given that the mole fraction is 2047 into 1500 kilopascal and that makes it 307.05 kilopascal, so it is very simple. So, we are trying to build up the foundation to do the problems on the reforming reaction.

(Refer Slide Time: 09:54)

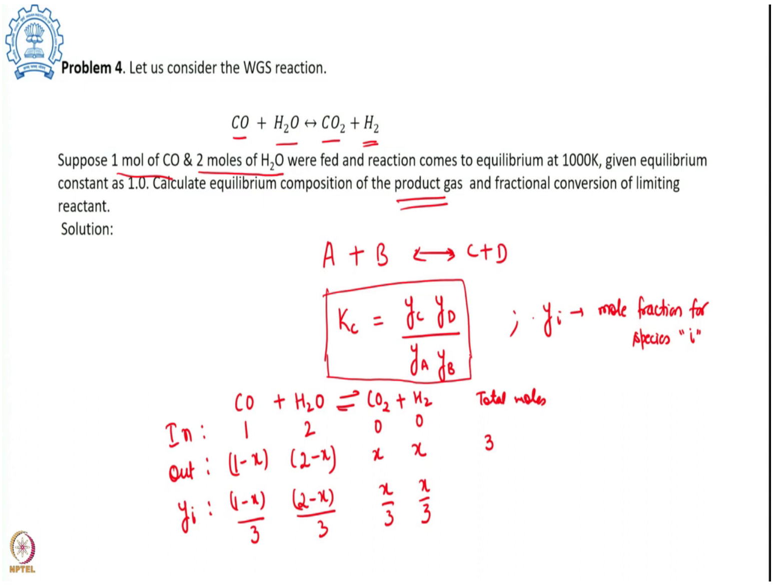


Let us look at another problem which states that, if 1 kg of methane reacts with steam producing syn gas, carbon monoxide and hydrogen and that undergoes the reaction. Let us assume that there is a complete conversion of methane which occurs.

So, the problem is how much amount of hydrogen will be produced in the process. So, this can be done, considering we know that if we look at this process. So, if you look at the molar mass so 16 gram per mole for CH 4 and that is producing 1 mole of methane and 3 moles of hydrogen. So, 2 gram per mole for hydrogen.

So, if we look at 1 kg of methane being used in the process, that is equivalent to say 62.5 moles of methane; now these 62.5 moles of methane produces, in fact, three times hydrogen which is equivalent to 1870.5 moles of hydrogen. There can be several ways of doing this and that if converted using the molar mass will give us the amount of hydrogen which is being produced is 375 grams.

(Refer Slide Time: 12:05)



So, this way we can do very simple small calculation. Now, let us consider problem number 4 here, this is the next step of the SMR that is after reforming which is water gas shift, wherein carbon monoxide again reacts with one mole of steam to produce carbon dioxide and more amount of hydrogen is produce. So, this process we remember is water gas shift reaction, also known as carbon monoxide shift reaction.

Now, let us assume the problem states that, if 1 mole of CO reacts with 2 moles of steam and these are fed in the reaction such that the reaction comes to equilibrium at 1000 K and it is given that under these reaction condition the equilibrium constant is 1. So, what we need to do is, we have to calculate the equilibrium composition which is obtained for the product gas and what is the fractional conversion of the limiting reactant in the process.

Now, let us consider any general equation. Let us say two reactants which are reacting to produce two products, which are say A B are the reactants and they are reacting to produce products C and D. Let us say this is a sort of reversible reaction, like the reforming or the water gas shift reaction. Now, the equilibrium constant we know, this is given by their mole fraction ratio of the product to that of the reactants.

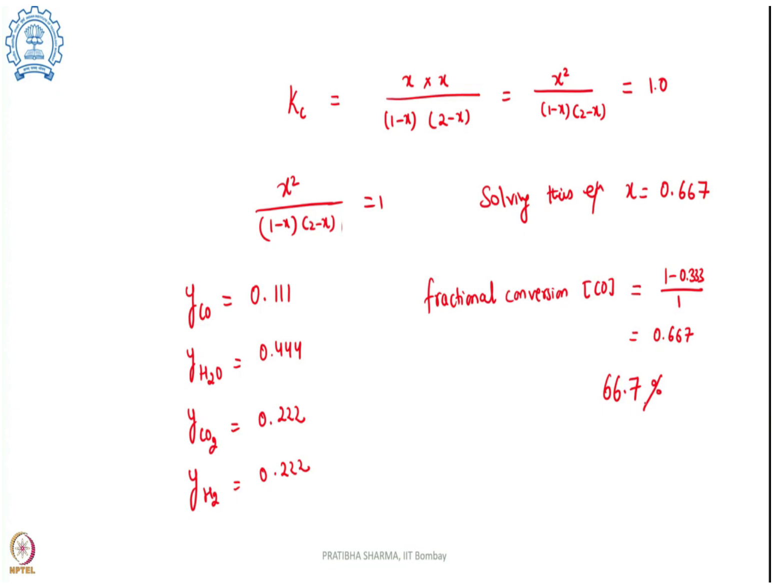
So, y is nothing but the mole fraction for species let us say i. Now, let us look at the reaction wherein CO reacting with H_2O giving us CO_2 plus H_2. Now, if we look at the input side, given that 1 mole of CO reacts with 2 moles of H_2O, so at the input side it is 2 and 0 however, at the out output side.

Since, it will depend upon the equilibrium certain amount of unreacted CO could be there, that can be represented by 1 minus x. Similarly, certain amount of steam could be left out. So, 2 minus x and the amount of CO_2 formed on the product side, let us say it is x and H_2 is also x.

Now, these are 3 moles. So, if we look at the total number of moles then this can add up to give us 3. So, we can also find out the mole fraction from here. So, mole fraction is the moles which we have found in the output side, divided by the total number of moles. So, 1 minus x by 3, 2 minus x by 3, x by 3 and x by 3.

Now, let us use these mole fractions in the equilibrium constant equation to find out the product gas composition.

(Refer Slide Time: 16:01)



Now, using that we can substitute the equation for Kc and we find that x into x in the numerator and 1 minus x into 2 minus x in the denominator. So, that is x square over 1 minus x and 2 minus x. It is already given in the problem that this value is equal to 1.

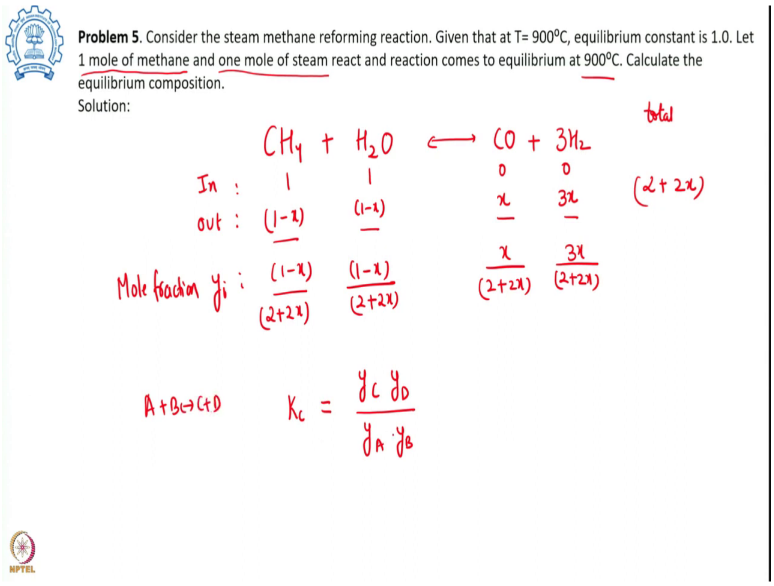
So, what we will do is, now we will solve this quadratic equation x square upon 1 minus x into 2 minus x equal to 1. And if we solve this equation, solving this equation we get the value of x and that comes out to be 0.667. Now, if we use this value of 0.667 into the table that we have made. So, here in we can get the values of the CO, H_2O, CO_2 and H_2 in the output side.

So, if we substitute that and find out the mole fraction. So, mole fraction will be again 1 minus let us say for CO, it is 1 minus 0.667 upon 3. If you just look back for CO mole fraction is 1 minus x upon 3. Let us substitute that and on substituting we get a value of 0.111. Same way we can find out the mole fraction for the rest of the species, like for H_2O, this is 0.444.

For CO_2, it is 0.222, for hydrogen this is again 0.222. One more thing is asked in the problem and that is fractional conversion of limiting reactant. Now, if we looked at the values, we can easily identify here that the limiting reactant is CO. So, the fractional conversion of limiting reactant can simply be written as, which is CO in this case; we know that the fractional axis could be the number of moles fed, minus the number of moles corresponding to the stoichiometric amount divided by the number of moles corresponding to the stoichiometric amount.

So, if we try to find out that, at equilibrium we know that the number of moles for CO is 1 minus x. So, fractional it could be given by 1 minus 0.333 divided by 1 and that is again 0.667. The same value as x and we can find out the percentage also by multiplying it by 100; so that comes out to be 66.7 percent.

(Refer Slide Time: 19:43)



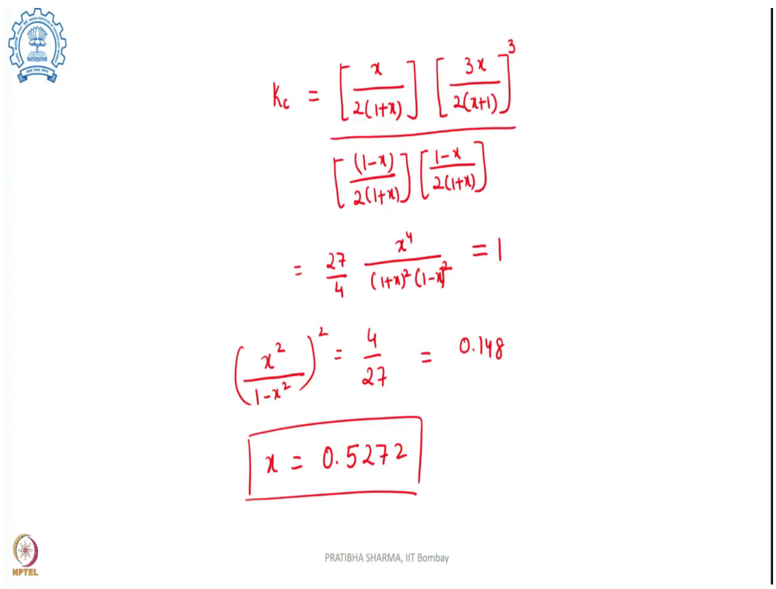
Now, let us look at one more problem which is on steam methane reforming. And it is stated that for steam methane reforming reaction, the temperature is given as 900 degree centigrade, equilibrium constant as 1 and it is mentioned that 1 mole of methane and 1 mole of steam, they react together and the reaction it comes at equilibrium to equilibrium at 900 degree centigrade. So, we have to again calculate the equilibrium composition.

Now, we know what the steam methane reforming is. So, if we again write down the in and out species one mole given methane reacting with one mole of steam. So, at input side, these two were 0. Now, what is remaining at the output is 1 minus x and 1 minus x, such that x moles of CO and 3 x of hydrogen is being found. Now, if we sum total this, then the total of this comes out to be of 1 minus x, 1 minus x, x and 3x that comes out to be 2 plus 2x, this will be used for finding out the mole fraction.

So, the mole fraction represented by yi for the species i, we can find out from here by dividing the individual composition by the total. Same way 1 minus x over 2 upon 2 plus 2x and x upon 2 plus 2x.

Similarly, 3x upon 2 plus 2x. Now, we will be using that in the equilibrium constant to find out the value of x for this equation. So, if we quickly write down these equation in the formula for equilibrium constant, the product side is CO and H_2. So, we know that the product if it is y_C y_D over the reactant, if the reaction is of the form A B, A plus B giving C plus D, then this is the equilibrium constant.

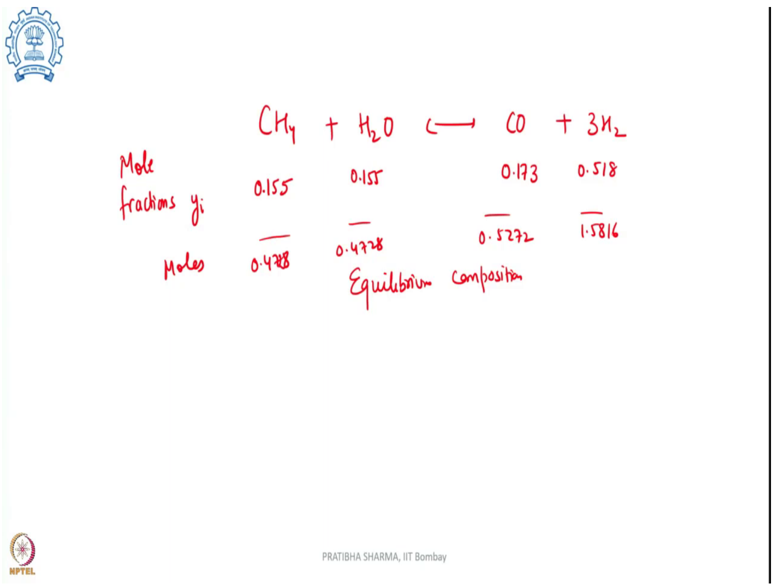
(Refer Slide Time: 22:41)



So, let us write down this kc for the problem. So, it comes out to be x upon 2 1 plus x, this is for CO. Similarly , for hydrogen, we can write as 3 x upon 2 times x plus 1, and this goes to stoichiometric coefficient because 3 moles of hydrogen are being considered. For methane it is 1 minus x, upon 2 1 plus x and same way for steam, 1 minus x upon 2 1 plus x. So, we will be solving this problem and that gives us a value of 27 by 4, solving this x to the power 4 upon 1 plus x square 1 minus x square.

And that is given in the problem is equal to 1. And this can be made further simplified by writing x square upon 1 minus x square whole square and that is equal to 4 by 27. That comes out to be somewhere 0.148. We can further solve this to get the value of x and the x on solving comes out to be 0.527. Now, this can be further used to find out the product gas composition for the individual species involved.

(Refer Slide Time: 24:30)



So, again writing back in terms of the mole fraction and we will be finding out the mole fractions now by substituting in the table. So, in the table if we see, mole fraction is given by for methane it is 1 minus x upon 2 plus 2x, for hydrogen it is 1 minus x upon 2 plus 2x, similarly, for CO and for hydrogen. So, substituting the value of x we can find out the mole fraction and that comes out to be for methane it is 0.155, these the higher digits are being rounded off 0.173 and 0.518.

So, these are the corresponding equilibrium compositions which we can get. We can find out the number of moles also by substituting in the same equation. So, if we want to write in terms of moles, it comes out to be number of moles 0.4728, same for this 0.5272 and 1.5816. So, this is how we can calculate and find out the equilibrium composition for either a water gas shift reaction or for a steam methane reforming reaction. So, these are some of the problems, simple problems that we have solved related to the steam methane reforming.

Thank you.