Material and Energy Balance Computations
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Lecture –18
Introduction

Hello everyone, welcome back once again in the NPTEL online certification course on material and energy balance computations. Today we will start a new module that is on chemical reaction stoichiometry. So, until now whatever we have discussed in the material balance that was for non-reactive system. For those systems we have seen how the material balances are done for single unit processes as well as the multiple unit processes.

In multiple units we have emphasized on recycle as well as bypass cases. Now when the scenario is that it is not for the non-reactive species that means some feed in which we have couple of components which reacts with each other in an appropriate condition and it creates or forms some products. Now in such cases how do we apply this material balance be it a single unit process or multiple unit processes.

Now before going into the details we need to understand couple of terms and we are we need to revise couple of things that we are already aware. One of such thing is the stoichiometry.

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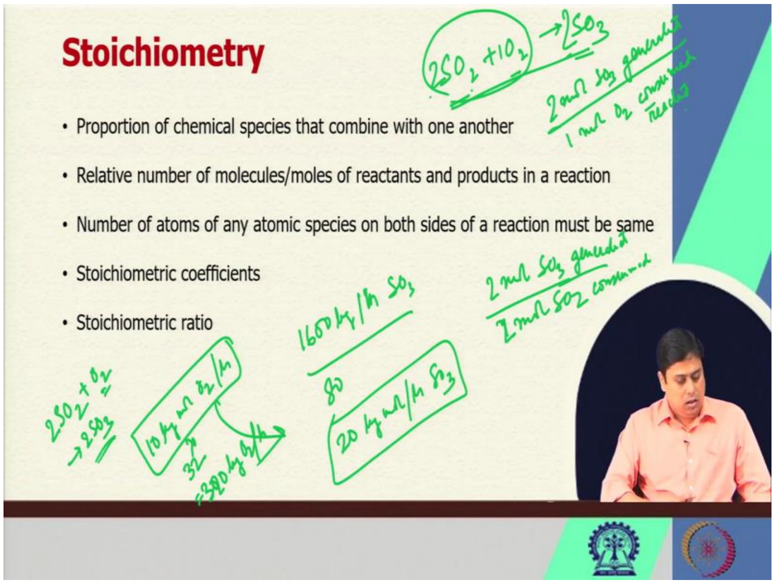

Stoichiometry

- Proportion of chemical species that combine with one another
- Relative number of molecules/moles of reactants and products in a reaction
- Number of atoms of any atomic species on both sides of a reaction must be same
- Stoichiometric coefficients
- Stoichiometric ratio

The stoichiometry is the study where we see or we estimate the proportion of chemical species that are needed for combining with each other in order to create some product. So, the stoichiometry when we say it is basically we calculate or we estimate or we know that the relative number of molecules or moles of reactants and products that are involved in a typical reaction. Now without the knowledge of stoichiometry we cannot proceed for the material balance on a reactive system.

This is because say we have a reaction that is $SO_2 + O_2 \rightarrow SO_3$. Now the point is that we understand that SO_2 is one reactant O_2 is another reactant if this reacts under appropriate condition temperature pressure and other desirable condition then it creates SO_3. But is this reaction that the way I have written here is fine it is not because the atomic species are not balanced in this reaction because atoms you cannot create not destroy at the atomic level.

So, here we can see we have 4 atomic oxygen's and on the right hand side we see only 3. So, which means it is not balanced. So, the number of atoms in any atomic species on both the sides of a reaction must be same or we must say the stoichiometry must be balanced. A stoichiometry reaction or reaction stoichiometry if we mention that is invariably that it is a balanced form of the reaction.

So, what we should do either we should write here $2SO_2 + O_2 \rightarrow 2SO_3$. Now this 2 and in for oxygen the one these are the stoichiometric coefficients. So what it tells this equation or this reaction it says that 2 molecules of SO_2 combines with one molecule of oxygen to produce 2 molecules of SO_3 or say 2 gram moles of SO_2 or 2 kilo moles of SO_2 reacts with 1 kilo mole or gram mole of O_2 in order to create 2 kilo mole or gram mole of SO_3, now depending on the units that we use.

So, either in molecular numbers or in moles we can represent this or this has to be balanced one. Now this 2, 1 and 2 in the case of sulphur dioxide, oxygen and sulphur trioxide here we can understand that these are the stoichiometric coefficient and the ratio that means the ratio of the stoichiometric coefficients. So, which means that 2 mole SO_3 generated per one mole of O_2 either you can say it is consumed or reacted.

So, stoichiometry ratio of 2 molecular species that are involved in a reaction is there the ratio of the stoichiometric coefficient when it is in balanced form or in a balanced reaction equation. So, the stoichiometry ratio in this case 2 : 1 for SO_2 and O_2. So, similarly it is 1 : 1 for SO_3 and SO_2. Now here one typical writing convention that we should follow in order to avoid any confusion is that if we just write say 2 mole SO_3 per 2 moles of SO_2 that means one mole of SO_3 per one mole of SO_2 you may confuse with the form or there are chances of being confused

confusion is that say there will be one mole of SO_3 in one mole of SO_2 which is completely wrong. So, we should not end here while writing the stoichiometry ratios we should be ending with 2 moles of SO_3 generated per 2 moles of SO_2 consumed or reacted as I mentioned.

So, what it does this stoichiometric coefficient also helps us in estimating or calculating the other constituents or the species that are needed if we know the amount of one reactant beforehand. So, for example say we know in this case that say 1600 kg per hour of SO_3 we have to produce. So, how much O_2 is required this we can easily calculate based on our understanding on the stoichiometry and a balanced chemical reaction.

So, the equation is that $2SO_2 + O_2 \rightarrow 2SO_3$, we need 1600 kg/h of SO_3. So, we need to convert this amount to kg mole per hour of SO_3 that we need to produce. Now from this conversion you are already aware. So, what it it would be so, 1600 / 80 because 80 is the molecular weight of this sulfur trioxide SO_3 here. So, we have here 20 kg mole per hour of SO_3. Now we look at the balanced equation which says that for 2 moles of SO_3 or 2 kg mole of SO_3 production we need 1 kg mole of O_2.

So, we need 20 kg mole which means we require 10 kg mole of O_2 per hour in order to produce this 20 kg mole of SO_3 per hour and now we can easily convert this kg mole to kg of O_2 per hour if that is the question that we have that how much O_2 we need. So, kg mole to kg would be the measurable quantity that means we have to multiply this with 32 which is the molecular weight of oxygen and we get 320 kg of O_2 per hour.

So, that means if we know one species amount in a balanced chemical reaction with the help of stoichiometric coefficient and stoichiometric ratio we can easily estimate the other components.

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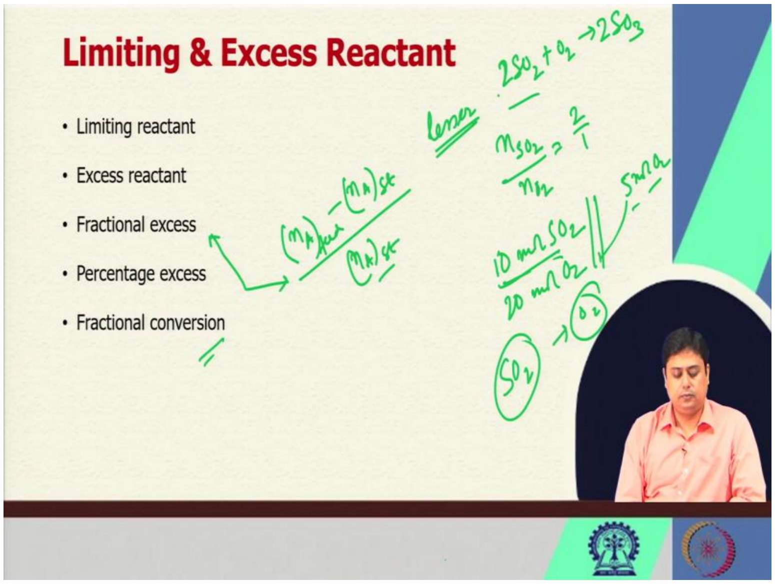

Limiting & Excess Reactant

- Limiting reactant
- Excess reactant
- Fractional excess
- Percentage excess
- Fractional conversion

Now, coming to the limiting and excess reactant concept so, the point is that when we have a reaction it is very unlikely that everything is provided in stoichiometric proportion that exactly the amount that is needed in order to react. In some cases some of the constituents or the species would be comparatively lesser. Now this term lesser is compared to their stoichiometric requirement.

In that case the constituent or the reactant that is lesser than its stoichiometric requirement is called the limiting reactant with respect to that the other components or the other reactants are in excess. So, for example again in this case if we go back to that same example that $2SO_2 + O_2 \rightarrow 2SO_3$. So, the stoichiometric coefficient says that, that is the moles of SO_2 that would be required in the feed composition with respect to O_2 would be 2 : 1.

Now if that is provided in a lesser quantity that means say in a feed we are feeding with 10 moles of SO_2 and 20 mole of O_2. So, what will happen here in this reaction if it is in a reactor with appropriate operating condition in a reactive condition? Then what will happen that we know from here that 2 moles of SO_2 will consume 1 mole of O_2 in order to complete the reaction. So, 10 moles of SO_2 okay would eventually require five mole of O_2 because that is the stoichiometry ratio 2 : 1.

If it is 2 mole we require one mole of O_2 if it is 10 mole SO_2 we will require 5 mole of O_2 but it is provided with 20 moles of O_2. So, what will happen after a certain time the reactor will be out of SO_2 the all SO_2 will be consumed at that point the reactant that disappears first is called the limiting reactant with respect to that O_2 here is the excess reactant. Now in order to quantify this that how much is the excess there are certain terminology either it is called the fractional excess or percentage excess when it is multiplied by 100.

And the fractional conversion the fractional conversion is also similar to what I just explained but the point is that it hardly happens that one of the quantity is completely or the component is completely reacting for the product. So, what happens that some of the reactant comes out of the reactor along with the product which is separated and again sent back as recycle. So, the point is that even though it is a limiting reactant but it has not been consumed to its 100% or it has not reacted completely.

So, means there is certain amount left even after the limiting reactant and that is the fractional amount that is left and with respect to that how much it has converted that is the fractional conversion. And again fractional conversion if we multiply that with 100% we get percentage conversion of the reactant. Now this is not only for the limiting reactant it can be with respect to any of the reactant that are involved in the reaction.

So, percentage conversion of a certain reactant this is how we typically call that or fractional conversion of a certain reactant. The point that I try to make is that this fractional conversion of limiting reactant can also happen. Because hardly any reaction goes for 100% conversions in a single pass. The reactants are typically separated and recycled even the limiting reactants. So the point is that, that means the fractional excess the way we should define it is that say the amount that is there in the product if we say that say certain component we have in A.

n_A that we have the amount in the feed – number of moles of A that is stoichiometrically that we require this is the excess with respect to the stoichiometric requirement. This is we call as fractional excess once we multiplied that with 100% we get the percentage excess.

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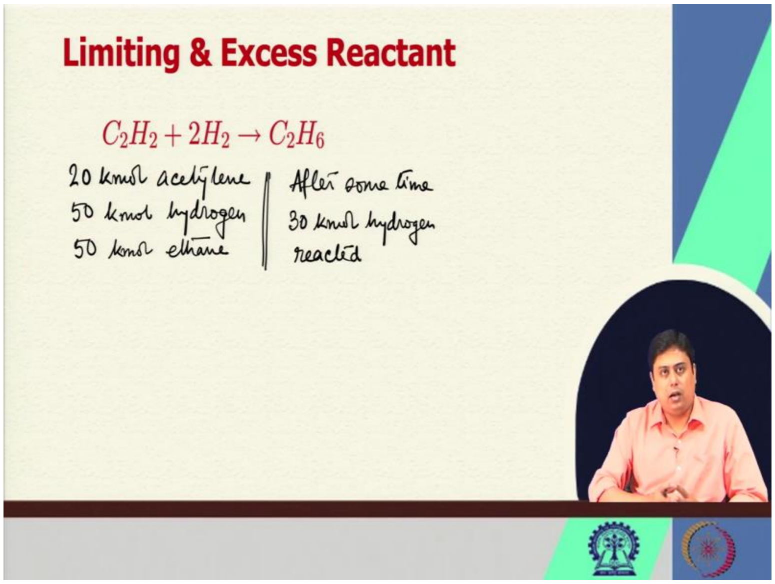

Limiting & Excess Reactant

$C_2H_2 + 2H_2 \rightarrow C_2H_6$

20 kmol acetylene
50 kmol hydrogen
50 kmol ethane

After some time
30 kmol hydrogen
reacted

So, let us see one example and then we will realize that how to estimate or how to identify which one is the limiting reactant and how much is the excess that is the other reactant in the which amount those are excess. So, for example here we have C_2H_2 reacting with hydrogen to produce ethane. So, acetylene + hydrogen giving us ethane. So, say initially we had in the feed 20 kilo mole of acetylene, 50 kilo mole of hydrogen and 50 kilo mole of ethane this is charged into a reactor.

And then after a certain time we estimate that 30 kilo mole of hydrogen has reacted. So, the question is what would be our final composition. Now before we come to that we have to understand another point that is the extent of reaction. Now before we go to this extent of reaction.

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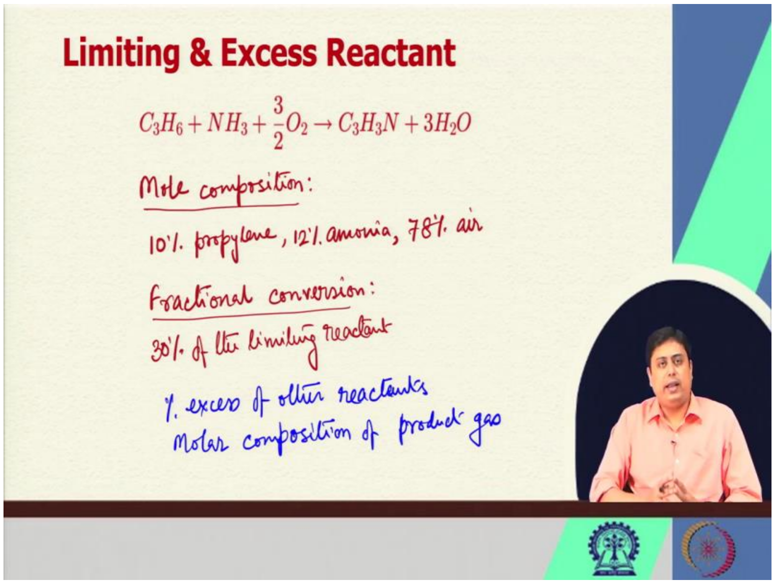

Limiting & Excess Reactant

$$C_3H_6 + NH_3 + \frac{3}{2}O_2 \rightarrow C_3H_3N + 3H_2O$$

Mole composition:

10% propylene, 12% amonia, 78% air

Fractional conversion:

30% of the limiting reactant

% excess of other reactants

Molar composition of product gas

Let me show you another example where we will see that what is the limiting and the excess reactant that before identifying what is extent of reaction and how do we calculate let us at first have an understanding that how to identify the limiting and excess reactant. So, say this reaction is happening. So, in this reaction we see that ammonia and oxygen where the mole composition is mentioned as air because this is the primary source of oxygen.

So, here what we have is that C_3H_6 reacting with ammonia and oxygen in order to give us C_3H_3N + $3H_2O$. So, in this reaction first of all when we write we have to ensure that this is balanced this is a balanced chemical reaction which we can clearly see that here it is balanced we have 3 C's, H we have 9 which is here on the right hand side and O we have 3 which is 3 here the atomic species balances we can see that it is balanced we cross check it.

Because based on this stoichiometric coefficient as well as stoichiometry ratio we will initially identify that which one is the limiting reactant and what is the percentage of other reactants that are in excess and the molar composition of product gas. So here what we have the mole composition initially it is 10% propylene 12% ammonia and rest air that is there in the feed and it is said that 30% fractional conversion has happened of the limiting reactant.

So, which means we have to at first identify what is the limiting reactant here which one is the limiting reactant. With respect to that we have 2 questions that is the percentage excess of other reactant and molar composition of product gas.

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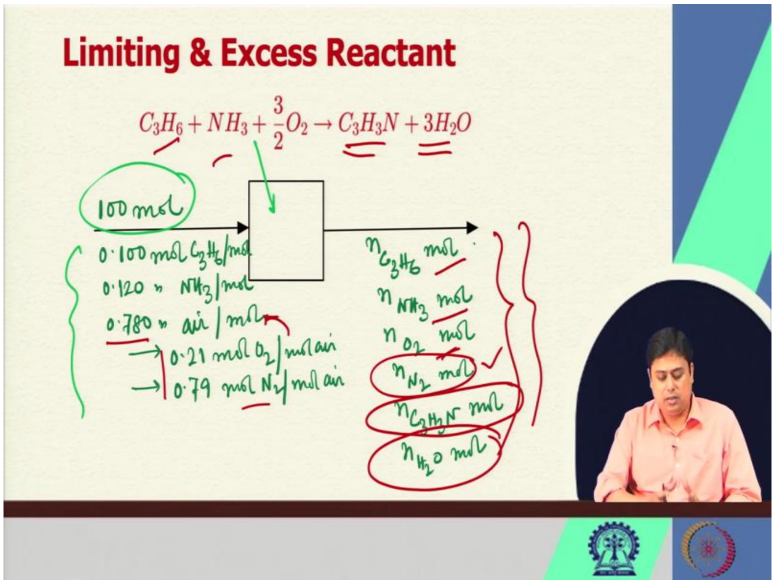

Limiting & Excess Reactant

$$C_3H_6 + NH_3 + \frac{3}{2}O_2 \rightarrow C_3H_3N + 3H_2O$$

So, the first thing that we have learnt till now is to draw a flowchart quickly. This is a simple system we assume the basis of calculation as 100 mole which is again a logical deduction because the mole composition is given. This percentages are by mole this is the feed composition. So, if we consider that 100 moles of feed that is coming in to the reactor where this reaction is happening we know the molar composition of the inlet which are 0.100 mole of C_3H_6 per mole of this feed, 0.12 mole of ammonia per mole of this feed and 0.78 mol of air per mole of this feed.

So, then what happens the point if you remember I mentioned earlier as well that when the air composition is typically not mentioned which will not be in future as well. If it is explicitly not mentioned in any problem statement you need to consider you need to remember this composition that it contains 79 mole percent nitrogen and 21 mole percent oxygen. If the inert composition or the other constituents or the species are not explicitly mentioned because air will also contain some other inert gases carbon dioxide, carbon monoxide etc., those are in trace amount.

Now if those are explicitly not mentioned if only air is mentioned which is a source of oxygen as well as nitrogen in several places we consider. Then you have to write on the flowchart that we have 0.21 mole of oxygen in this much mole of per mole of this much air. So, 0.79 mole of nitrogen per mole of this air and on the right hand side on the flow chart we clearly see or we have to write what are the product gas constituents.

Now we can see that these are the products that are fine. So, which means C_3H_3N its number of moles that is unknown and H_2O these 2 are unknown clearly these are through the product stream. But the problem statement says that we have 30% conversion of the limiting reactant. So, which means in the product stream not only the limiting reactants would be it would be the other constituents as well because limiting reactant itself has not converted to its 100% extent.

So, which means the other components would definitely be there in the product stream. Now other component means here since we have not identified yet which one is the limiting reactant. So, all the constituents or the all the reactants would be there in the product stream as well. So, the reactants the components were C_3H_6, ammonia, oxygen and you must not forget that the air content nitrogen which is inert in this case will also be there in the product stream.

So, these 6 components constitute our product stream. We need to identify or we need to estimate these n values but before that we have to identify which one is the limiting reactant that means which one is fed lesser compared to its stoichiometric requirement. So the take home message where I will stop here today and will start our discussion from this problem. So, that we can solve it with ample discussion is that the limiting reactant is the reactant which would run out first in a reactor compared to the other reactants.

And this based on the limiting reactant its stoichiometric ratio the other components would be calculated for its percentage excess. So, with this I will stop today and will resume our discussion on solving this problem in the next class, thank you for your attention.