

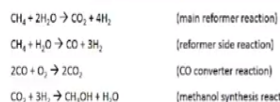
Material and Energy Balances
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Module No # 06
Lecture No # 28-2
Mechanical Balances: Part 2

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Example

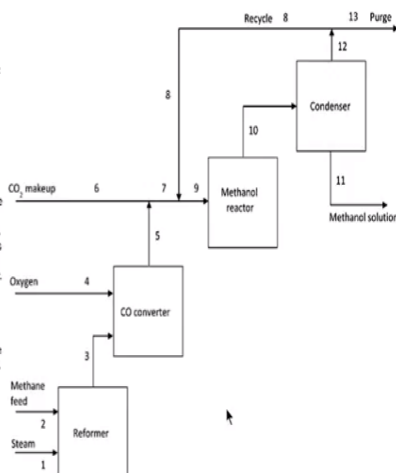
A process for methanol synthesis is shown here. The reactions involved are:



Ten percent excess steam, based on the main reformer reaction is fed to the reformer, and the conversion of methane is 100%, with a 90% yield of CO_2 . Conversion in the methanol reactor is 55% on one pass through the reactor. A stoichiometric quantity of oxygen is fed to the CO converter, and the CO is completely converted to CO_2 . Additional makeup CO_2 is then introduced to establish a 3:1 ratio of H_2 to CO_2 in the feed stream to the methanol reactor. The methanol reactor effluent is cooled to condense all the methanol and water, with the non-condensable gases are recycled to the methanol reactor feed. The H_2/CO_2 ratio in the recycle stream is also 3:1. Since the methane feed contains 1% nitrogen as impurity, a portion of the recycle stream is purged to prevent nitrogen accumulation in the system. The purge stream analyzes 5% nitrogen. For every 100 moles of impure methane feed, calculate:

- Moles of H_2 lost in the purge
- Moles of makeup CO_2 required
- Recycle to purge ratio in mol/mol
- Quantity (in kg) and composition of methanol solution produced

Problem adapted from Himmelblau and Riggs, Basic Principles and Calculations in Chemical Engineering, 7th Edition, Prentice Hall India



Here is the example problem a process for methanol process is shown here the reactions involved are methane + water forming carbon dioxide and hydrogen methane + water forming carbon dioxide and hydrogen methane + water forming carbon monoxide and hydrogen and carbon monoxide + oxygen forming carbon dioxide. And carbon dioxide reacting at hydrogen perform methanol and water.

So these reactions are labeled as main reformer reaction, reformer side reaction, carbon monoxide convertor reaction and methanol synthesis reaction 10% excess steam based on the main reformer reaction is fed to the reformer and the conversion of methane is 100% with the yield of 90% for CO_2 . Conversion of methanol reactor is 55% on one pass through the reactor the stoichiometric quantity of oxygen is fed in the CO converter.

And the CO is completely converted to CO_2 addition make up CO_2 is then introduced to established 3 is to 1 ratio of hydrogen to carbon dioxide in the feed stream to the methanol reactor. Methanol reactor effluent is cooled to condense all the methanol and water with the non-

condensable gases being recycled to the methanol reactor feed the hydrogen to carbon dioxide ratio in the recycle stream is also 3 is to 1.

Since the methane feed contains 1% nitrogen as impurity a portion of the recycle stream is purged to prevent nitrogen accumulation in the system. The purge stream analysis 5 % nitrogen. For every 100 moles of impure methane feed they are asked to calculate the moles of hydrogen lost in the purge moles of makeup carbon dioxide required recycled to purge ratio in moles per mole and quantity in kilograms composition of methanol solution is reduced.

So this problem covers all the aspects of chemical reactions with recycle and purge for a multiunit system.

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Example



CH₄ balance:
 $C_{ms} = 99 \text{ mol}$
 $\text{Output} = I - C$
 $= 0 \text{ mol}$

CO₂:

$I - O + G - X = \Delta$

$0 = G$

$99 \text{ mol CH}_4 \text{ consumed}$

$\left(\frac{90}{100} \times 99\right) \text{ mol CO}_2 \text{ gen}$

$\text{CO}_2 \text{ gen} = 89.1 \text{ mol}$

$\Rightarrow \text{Stream 3} = 89.1 \text{ mol CO}_2$

Let us try to solve this problem the problem statement gives us that 100 moles of impure methane is fed which means stream 2 would contain 100 moles which would be 99% methane and 1% nitrogen given as 99 moles of methane and 1 mole of nitrogen in stream 2. So our base is would be 100 moles in stream 2 so this contains 99 moles of methane and 1 mole of nitrogen so we have also been told that stream 1 is 10% excess water vapor which is being fed or steam which is being fed.

So we can calculate the requirement for water vapor based on the reformer reaction the main reformer reaction given as methane + 2 H₂O gives CO₂ + 4H₂. So this means for every mole of

methane fed you require two moles of water vapor or steam. So here 99 moles of methane is fed which means 198 moles of steam is required we know that 10% excess is actually fed this implies 198 times 1.1 will be the actual number of moles fed in steam 1.

So this is 217.8 moles of water vapor being fed so stream 1 is 217.8 moles. Now we need to calculate the information about steam 3 for this reason we will choose the reformer as the system and perform material balance calculation. So we can write methane balance we know that 100% methane is consumed so which means methane consumed would be 99 moles so output methane in steam 3 which would be equal to input – consumption would be 0 mole.

So similarly we can write component balances for carbon dioxide so carbon dioxide balance would be input – output + generation – consumption = accumulation at steady state there would not any accumulation carbon dioxide is a product so it is only generated there is no input of carbon dioxide so your output is actually equal to generation we have been told that 90% of methane consumed produces carbon dioxide so we know 99 moles of methane was consumed.

So 90% of this converted to carbon dioxide so number of moles of carbon oxide produced would be 90 divided by 100 times 99 so CO₂ generated would be equal to 89.1 moles so this implies steam 3 contains 89.1 mole of CO₂.

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Example



$$CO: O = G$$

$$\Rightarrow 9.9 \text{ mol } CH_4 \equiv 9.9 \text{ mol } CO$$

$$Out = 9.9 \text{ mol } CO$$

$$H_2: O = G_1 + G_2$$

$$= 89.1 \times 4 + 9.9 \times 3$$

$$Out = 386.1 \text{ mol}$$

$$H_2O: I - O - C = 0$$

$$0 = I - C$$

$$= 217.8 - (89.1 \times 2)$$

$$- (9.9 \times 1)$$

$$Out = 29.7 \text{ mol}$$

$$N_2 = 1 \text{ mol}$$

$$\text{Stream 1:}$$

$$CO_2 = 89.1 \text{ mol}$$

$$CO = 9.9 \text{ mol}$$

$$H_2 = 386.1 \text{ mol}$$

$$H_2O = 29.7 \text{ mol}$$

$$N_2 = 1 \text{ mol}$$

Similar to carbon dioxide we can also perform carbon monoxide balance which would again be output = generation so we knew that 90% of methane which was consumed went into main reformer and the rest 10% went into side reformer reaction this implies 9.9 moles of methane went into formation of carbon monoxide based on stoichiometric this would have produced 9.9 moles of carbon monoxide.

So output would be equal to 9.9 moles of carbon monoxide we can also write a balance equation for hydrogen. So hydrogen is not coming in it is only being generated so your output would again be equal to generation but here you would have two generation terms from reaction 1 and reaction 2 based on stoichiometric we know that for every mole of carbon dioxide produced 4 moles of hydrogen is being produced.

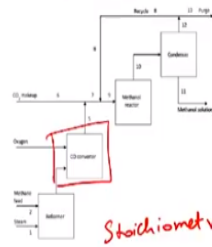
So 89.1×4 would be the generation of hydrogen by the main reformer reaction from the side reaction you would have every mole of carbon monoxide produced 3 moles of hydrogen being produced this means 9.9×3 moles of hydrogen is being produced. So the total output of hydrogen would be 386.1 moles.

If you were to write a balance for water we know that input – output – consumption would be equal to 0, because water is not generated as a reactant and accumulation would be 0 or steady state thereby output is actually equal to input – consumption so input is 217.8 based on the stoichiometric we know that every mole of carbon dioxide produce 2 moles of water was consumed. So for 89.1 moles you have 89.1×2 moles of water consumed.

Similarly for the side reaction for every mole of carbon monoxide produced 1 mole of was consumed. So 9.9×1 mole of water was consumed so output for water was 229.7 moles as nitrogen does not take part in the reaction output for nitrogen would be 1 mole. So based in this steam 3 composition would be as follows stream 3 contains carbon dioxide 89.1 moles carbon monoxide 9.9 moles hydrogen 386.1 mole water 29.7 moles and nitrogen 1 mole.

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Example



Stoichiometric O_2 is fed
 $\Rightarrow 9.9 \text{ mol CO} = 9.9 \text{ mol CO}_2$
 $CO_2: I + G = O$
 $Out = 89.1 + 9.9$
 $= 99 \text{ mol}$

Stream 5:
 $CO_2 = 99 \text{ mol}$
 $H_2 = 386.1 \text{ mol}$
 $H_2O = 29.7 \text{ mol}$
 $N_2 = 1 \text{ mol}$

Stream 7:
 $H_2:CO_2 = 3:1$
 $\Rightarrow \text{Stream 7 } H_2 = 386.1 \text{ mol}$
 $\Rightarrow \text{Total } CO_2 \text{ in stream 7}$
 $= \frac{386.1}{3} = 128.7 \text{ mol}$

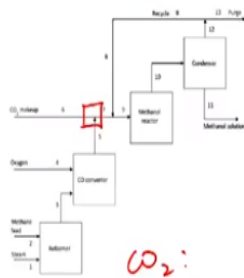
So now we have performed the calculations for the first system the next system of interest would be the CO convertor for the CO convertor we have been told that stoichiometric requirement of oxygen is fed and there is carbon monoxide to carbon dioxide. This implies the 9.9 moles of carbon monoxide gets converted to form 9.9 moles of carbon dioxide. So if you were to write a carbon dioxide balance you would have input + generation = output.

So the output would be $89.1 + 9.9$ giving you 99 moles of CO_2 leaving. So stream 5 would have the same component as in stream 3 except for carbon dioxide being 99 moles instead of 89.1 so this would be carbon dioxide being 99 moles and you do not have any carbon monoxide here this all been converted hydrogen would be 386.1 moles water would be 29.7 moles and nitrogen is stil not taking part of reactions so you have one mole of nitrogen leaving.

The problem statement gives us that steam 7 contains hydrogen to carbon dioxide ratio of 3 is to 1 the steam which is being mixed with steam 5 that is steam 6 is only CO_2 maker which means all the hydrogen present in steam 7 as to come from steam 5. This implies steam 7 contains hydrogen as 386.1 moles knowing this we can calculate total CO_2 in steam 7 as 386.1 divided by 3 which is 128.7 moles.

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Example



Stream 7:

$$\text{CO}_2 = 128.7 \text{ mol}$$

$$\text{H}_2 = 386.1 \text{ mol}$$

$$\text{H}_2\text{O} = 29.7 \text{ mol}$$

$$\text{N}_2 = 1 \text{ mol}$$

CO_2 :

$$I = 0$$

$$99 + I_6 = 128.7$$

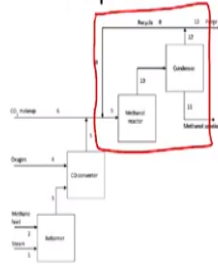
$$\Rightarrow \text{CO}_2 \text{ makeup} = 29.7 \text{ mol}$$

Now that we know 128.7 moles of CO₂ is present we can write a balance for a mixing point for CO₂. If the CO₂ balance for mixing point would be input = output so you have 2 inputs here one input comes from steam 5 which contains 99 moles of carbon dioxide and you have another input from the CO₂ make up steam will just call that I₆ would be equal to the output which know is 128.7 moles.

So this implies CO₂ make which is given = 29.7 moles so this is one of the values which is given to calculate. So steam 6 you have calculated to the CO₂ make up of 29.7 moles based on this we can also get the information on steam 7 the only component changing from steam 5 would be carbon dioxide which is being added so we now have carbon dioxide of 128.7 moles and hydrogen would be 386.1 moles and we have water as 29.7 moles and nitrogen is still being present as 1 mole.

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Example

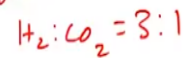


$$\text{Total purge} = \frac{1}{0.05} = 20 \text{ mol}$$

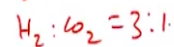
Stream 12:



Recycle:



⇒ Purge:



$$N_2: I = 0$$

⇒ Purge contains 1 mol N_2

⇒ 5% N_2

⇒ 1 mol = 5%

We have also been asked to calculate the amount of hydrogen which is lost through the purge steam taking the overall system into account the nitrogen which is entering through the methane feed would have to leave only through the purge steam. So if you were to write the nitrogen balance you would have input = output thereby our purge steam contains one mole of nitrogen. We also have one information about the purge steam which is purge steam contains 5% nitrogen this implies 1 mole accounts for 5%.

so total purge steam would be $1 / 0.05$ which is 20 moles. So we have 20 moles of purge being sent out of the system now that we have the total purge steam we still need to calculate the composition of the purge steam and we also need to identify how much methanol is produced. For this reason you will choose a different system let us choose this particular system which has the mixing point for recycle steam the methanol reactor and the condenser.

For this particular system of interest we know that all the information about steam 7 has been calculated and purge steam we know the total purge and we have some information about its composition also let us try to perform the material balances for this system. Based on what is been given to us in the problem steam level contains methanol and water only and steam 12 contains all the non-condensable components.

This means that steam 12 would contain all the non-condensable components which are entering into the system those non condensable component would be unreacted hydrogen carbon dioxide

and nitrogen which does not take part in the reaction the problem statement also gives us that the recycle steam contains hydrogen and carbon dioxide in the ratio of 3 is to 1. This means purge steam would also contain hydrogen and carbon dioxide at the ratio of 3 is to 1 using this we can calculate the amount of hydrogen which is leaving through the purge steam.

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Example

$3x + x + 1 = 20$
 $\Rightarrow x = 4.75 \text{ mol}$
 $4.75 \text{ mol } \text{CO}_2$
 $1 \text{ mol } \text{N}_2$
 $14.25 \text{ mol } \text{H}_2$

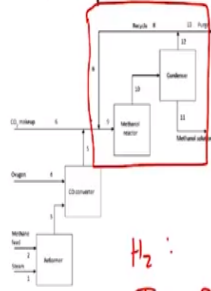
$\text{H}_2 : \text{CO}_2 = 3:1$
 $\Rightarrow 1 \text{ mol } \text{N}_2$
 $3x \text{ mol } \text{H}_2$
 $x \text{ mol } \text{CO}_2$ } Purge
 Total purge = 20 mol

So what we have here is hydrogen is to carbon dioxide in purge steam is 3 is to 1 this implies you have 1 mole of nitrogen 3X moles of hydrogen and X moles of carbon dioxide in the purge steam. The total purge is calculated already as 20 moles so what we can do is $3X + X + 1$ which is the total number of purge steam = 20 giving you X as 4.75 moles.

So the purge steam contains 4.75 moles of carbon dioxide 1 mole of nitrogen and 14.25 moles of hydrogen. So based in this we have calculated 14.25 moles of hydrogen is being purged in this process. For the system chosen we have methanol reactor where hydrogen is being consumed we can calculate hydrogen consumption based on information we have about input and output terms for hydrogen.

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Example



H_2 :

$$I - O = Cons$$

$$Cons = 386.1 - 14.25 \\ = 371.85 \text{ mol}$$

CO_2 :

$$I - O = Cons$$

$$Cons = 128.7 - 4.75 = 123.95 \text{ mol}$$

$$1 \text{ mol } CO_2 \equiv 1 \text{ mol } CH_3OH$$

$$\Rightarrow 123.95 \text{ mol } CH_3OH$$

CH_3OH :

$$O = Gen = 123.95 \text{ mol}$$

$$123.95 \text{ mol} \equiv 3966.4 \text{ kg } CH_3OH$$

Using this we will be able calculate how much methanol has been produced let us try and do this so if you were to write the balance equation for hydrogen for the system chosen we basically this what you would have is input – output = consumption we already know that input is 386.1 which is coming in through steam 7 and we calculated that the output was 14.25 from the purge steam so consumption is basically = distance between the 2 which is 371.85 moles.

So that is the total consumption of hydrogen in this system similarly we can calculate for carbon dioxide if you write the carbon dioxide balance which would be input – output = consumption again and consumption would be 128.7 - 4.75 giving you a value of 123.95 moles based in this stoichiometry we know that for every mole of carbon dioxide consumed we have 1 mole of methanol produced.

This implies 123.95 moles of methanol would have been generated in this system so if you were to write a methanol balance for the system chosen output would be equal to generation which is 123.95 moles. So from this equation we know that 123.95 moles of methanol was actually produced in the system. We have been asked to calculate the mass of methanol and the mass of fraction of methanol in the steam 11.

So 123.95 moles of methanol is actually equal to 3966.4 kilograms of methanol we also need to calculate the amount of water which is present in this steam. So that we can calculate the composition of steam level how much water would be present.

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Example



$$\begin{aligned}
 \text{H}_2\text{O}: \\
 O &= G + I \\
 G &= 123.95 \text{ mol} \\
 I &= 29.7 \text{ mol} \\
 \text{Out} &= 123.95 + 29.7 \\
 &= 153.65 \text{ mol}
 \end{aligned}$$

$$153.6 \text{ mol H}_2\text{O} \approx 2765.7 \text{ g H}_2\text{O}$$

$$\begin{aligned}
 \text{Total stream 11} \\
 &= 6.7321 \text{ kg}
 \end{aligned}$$

$$\frac{3966.4}{6732.1} \times 100 = 58.9\%$$

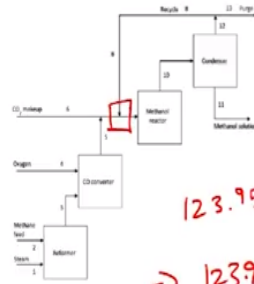
$$\begin{aligned}
 \text{Stream 11} \\
 6.7321 \text{ kg of } 58.9\% \text{ CH}_3\text{OH} \\
 \text{Soln.}
 \end{aligned}$$

For that we need to perform the water balance equation so the balance equation would again be output = generation + input so using stoichiometric generation would be equal to 123.95 moles of water being produced we already know input is 29.7 moles coming in through steam 7 this means our output for water in steam level would be 123.95 + 29.7 giving you a value of 153.65 moles.

So 153.65 moles of water is equivalent to 2765.7 grams of water so the total steam level mass would be 6.7321 kilograms mass percentage of methanol would be 3966.4 divided by 6732.1 times 100 giving you a value of 58.9% so steam 11 is basically 6.7321 kilograms of 58.9% methanol solution.

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Example



$$123.95 \text{ mol CH}_3\text{OH}$$

$$\Rightarrow 123.95 \text{ mol CO}_2$$

$$\Rightarrow \text{Gross CO}_2 = \frac{123.95}{0.55} = 225.36 \text{ mol}$$

$$\text{Gross H}_2 = 3 \times 225.36 = 676.09 \text{ mol}$$

For calculating the recycle steam we would like to write a balance equation for either the mixing point or for the splitting point the problem with the splitting would be we would have only one independent balance equation so it is better to write the balance for the mixing point so for writing the balance for the mixing point we would have to have information about steam line. How do we get information about steam line?

We have been told that the single pass conversion for methanol production was 55% of carbon dioxide coming in. So this means the amount of methanol which was being produced and removed from the system was based on 55% of carbon dioxide entering into the methanol reactor as the gross feed. So what we have is 123.95 moles of methanol being produced this implies 123.95 moles of carbon dioxide was consumed in this methanol reactor through a single pass.

So gross CO₂ entering would be 123.95 divided by 0.55 giving you a value of 225.36 moles as we know as we know that ratio of carbon dioxide to hydrogen is 1 is to 3 gross hydrogen entering would be 3 times 225.36 giving a value of 676.09 moles. Now that we have information about the carbon dioxide and hydrogen which is present in the total feed.

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Example



Total mol. recycle:

$$289.99 + 96.66 + 0.05x = x$$

$$x = 407 \text{ mol}$$

$$\Rightarrow \frac{R}{P} = \frac{407}{20} = 20.35$$

$$\text{CO}_2: I = 0$$

$$128.7 \left(\frac{I}{8} \right) = 225.36$$

$$\Rightarrow \text{CO}_2 \text{ in Stream 8} = 96.66 \text{ mol}$$

$$\text{H}_2: \text{H}_2 \text{ in stream 8} = 289.99 \text{ mol}$$

Let us write the balance equation for the mixing point the carbon dioxide balance would be input = output so input is 2 steam 1 is steam 7 and other is 8 and output is steam 9 we know that the output is 225.36 and input in steam 7 is 128.7 and the rest would be the input in the steam 8. So this would be the CO₂ input in steam 8 so this would be CO₂ steam 8 can be calculated as 96.66 moles.

Similarly writing a balance equation for hydrogen we would be able to calculate hydrogen in steam 8 as 289.99 moles this is not sufficient because we still need to calculate the amount of nitrogen which is coming in through the recycle steam we have 1 information about the nitrogen concentration which is 5%. So we know that the total moles of recycle would contains hydrogen at 289.99 moles carbon dioxide which is 96.66 moles + whatever would be the moles of nitrogen which is basically 5% of total moles which is 0.05 times X and is the total number of moles.

Using this we calculate the total number of moles which is recycled as 407 moles so the ratio of recycle to purge would be 407 to 20 which is 20.35 with this we have performed all the required calculations and we come to the conclusion of today's lecture. In the next class we will perform one more example where we consider a biochemical system with recycle until then thank you and good bye.