

# Hydrogen Energy: Production, Storage, Transportation and Safety

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Lecture - 53

Tutorial - 06

Hello everyone, I am Saurabh Tiwari I am PhD student at IIT Bombay. I am also TA of this coursework. In the last lecture we have studied about the various Design and Development of Metal Hydride Hydrogen Storage in which we studied about how we have developed the metal hydride reactor according to the applications that is being used for a particular metal hydride hydrogen storage.

In this lecture we have studied some example to so, that we are able to understand how we will able to develop these metal hydride hydrogen storage systems. In this tutorial we will initiate with the design of for the absorption case.

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Q1. Design a metal hydride reactor considering  $\text{LaNi}_5$  as metal hydride to store 50 g of hydrogen. Considering the shape of metal hydride as cylinder, calculate the length and diameter of cylinder if L/D ratio is 3. Based on this system calculate the mass of hydrogen absorbed ( $\text{kg}/\text{m}^3\text{-s}$ ) at time 't' at  $T = 303 \text{ K}$ , and at a supply pressure of 10 bar, 20 bar and 30 bar. Finally, comment on the effect of pressure on the system.


The density at saturation state is  $8534 \text{ kg}/\text{m}^3$ , density at particular time 't' is  $8467 \text{ kg}/\text{m}^3$  and density of metal hydride without hydrogen is  $8400 \text{ kg}/\text{m}^3$ .

The porosity of metal hydride is assume to be 0.5 and expansion volume as 20%. The reaction constant for this condition is  $59.187 \text{ s}^{-1}$  and activation energy is  $21179.6 \text{ J}/\text{mol}$ .

Solution : L/D = 3 ✓  
L = 3D ✓

- Amount of hydrogen to store = 50 g = 0.05kg
- Gravimetric capacity of  $\text{LaNi}_5$  = 1.6 wt%
- Amount of metal hydride required =  $\frac{100}{1.6} \times 0.05 = 3.125 \text{ kg}$
- Density of MH =  $8400 \text{ kg}/\text{m}^3$
- Volume of MH required =  $\frac{3.125}{8400} = 3.72 \times 10^{-4} \text{ m}^3$

$\frac{100}{g} \times m_{H_2}$

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In the question that we have seen on our slide we have to design a metal hydride reactor which contain  $\text{LaNi}_5$  as metal hydride reactor. So, from  $\text{LaNi}_5$  we are able to understand what is the density of metal hydride, what is the gravimetric capacity of metal hydride, in this we want to store 50 gram of hydrogen. Now, in the question it is also given that if we

consider the shape of metal hydride reactor as cylinder and then we will need to calculate the length and the diameter according to the L/D ratio which is given as 3.

Based on this system we also need to calculate the mass of hydrogen that is being stored at a certain time  $t$  at a temperature of 303 kelvin. So, there are three supply pressure that is being given in this question which is 10 bar, 20 bar and 30 bar and finally, we need to understand what is the effect of the supply pressure on the amount of mass absorbed.

There are some other properties which is the density of metal hydride at saturation state, this is when the hydrogen is absorbed inside the metal hydride and at a saturated state. That is the hydrogen is absorbed at the maximum level which will be accompanied by the metal hydride.

Density at a particular time  $t$  is also given 8467 kg per meter cube and the density of metal hydride without hydrogen is 8400 so, it is a pure density of metal hydride. The porosity of metal hydride is also given as 0.5 and the expansion volume is 20 percent. The reaction constant for this condition is given and activation energy is given. So, how will we proceed with this problem?

So, initially we have seen that the L/D ratio of 3 is given. So, from here we will find out that the length is equal to the 3 times of the diameter that of the cylinder. Now, the second is the amount of hydrogen that we need to store is 50 gram which is 0.05 kg, from the metal hydride which is LaNi<sub>5</sub> we have seen that the gravimetric capacity of LaNi<sub>5</sub> is 1.6 weight percent and that you have studied in the previous lectures.

Now, to store 50 gram of hydrogen in LaNi<sub>5</sub> we have to understand what amount of metal hydride we required. So, amount of metal hydride is calculated by this formula that is being given in the last lecture which is  $100$  upon gravimetric capacity 'g' times the mass of hydrogen to be stored, which will give us the value of amount of metal hydride required. Now, from the metal hydride we also understand the density of metal hydride which is given as 8400, the density of LaNi<sub>5</sub> is 8400 which is given here.

Now, from here we know the mass of metal hydride, now we know the density of metal hydride, from here we are able to calculate volume of metal hydride required which is mass upon volume which will give us this volume of  $3.72 \times 10^{-4}$  meter cube.

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- Considering Porosity of 0.5, the volume of metal hydride =  $\frac{3.72 \times 10^{-4}}{0.5} = 7.44 \times 10^{-4} \text{ m}^3$  ✓
- Further considering expansion volume of 20 %, volume of metal hydride =  $1.2 \times 7.44 \times 10^{-4} = 8.93 \times 10^{-4} \text{ m}^3$  ✓
- Now, the shape of reactor is cylinder
  - $\frac{\pi}{4} \times D^2 \times L = 8.93 \times 10^{-4}$  (3D)
  - $D = 0.0723 \text{ m}$ ,  $L = 0.2169 \text{ m}$  ✓
  - $\Rightarrow L = 3D$   $L/D = 3$
- For any time 't',
  - $T = 303 \text{ K}$  ✓
  - $P_s = 10, 20, 30 \text{ bar}$  ✓
  - For  $\text{LaNi}_5$ ,  $\Delta S = 108 \text{ J/mol.K}$  ✓
  - $\Delta H = 30800 \text{ J/mol}$  ✓
- Mass of hydrogen absorbed
  - $P_{eq} = P_{ref} \exp\left(\frac{\Delta S}{R} - \left(\frac{\Delta H}{R T_s}\right)\right)$  ✓
  - $P_{eq} = 2.14 \text{ bar}$  ✓
  - $\dot{m} = C_a \exp\left(\frac{-E_a}{R T_s}\right) \ln\left(\frac{P_s}{P_{eq}}\right) (\rho_{sat} - \rho_s)$  ✓
  - $\dot{m} = 1.234 \text{ kg/m}^3\text{-s}$  (for 10 bar) ✓
  - $\dot{m} = 1.978 \text{ kg/m}^3\text{-s}$  (for 20 bar) ✓
  - $\dot{m} = 2.336 \text{ kg/m}^3\text{-s}$  (for 30 bar) ✓
  - Mass absorbed increases with increase in supply pressure

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After calculating this volume, we need to consider the porosity of metal hydride also. So, if you are assuming a porosity of 0.5, then the volume of metal hydride will increase by this content. So, like we have calculated the volume of metal hydride as  $3.72 \times 10^{-4}$  meter cube and when the porosity is 0.5. So, to accompany this porosity we have to divide this value by 0.5 and the volume required is  $7.44 \times 10^{-4}$  meter cube.

Now, in the last lecture we have studied that when the hydrogen is absorbed inside the metal hydride reactor there is expansion of metal hydride also to compensate that volume, we have to provide a expansion volume inside the metal hydride reactor which is 15 to 25 percent. So, in this example we are assuming this expansion volume as 20 percent.

So, if we assuming as 20 percent so the volume of metal hydride comes out to be  $8.93 \times 10^{-4}$  meter cube. This is the final volume of metal hydride reactor required to hold the metal hydride with the porosity of 0.5 and after providing an expansion volume of 20 percent also. Now, in the question that we have seen it is also given that the shape of the metal hydride reactor is cylindrical and L/D ratio is 3. So, from here we calculate that L is 3 time of diameter.

Now, from the shape of the cylinder we are able to calculate that the volume of cylinder is given by this formula and this volume need to be equal to this volume which is required for the metal hydride reactor. So, from here if you put  $L = 3D$  so, we have only one variable

diameter left in this equation. So, from here we are able to calculate the diameter of reactor and also the length of the reactor.

So, now, we have the diameter, we have the length of the reactor. Now, it is also given for any time 't' we have the temperature is 303 kelvin. Now, normally in the previous lecture we have told that there is an energy equation which is being used to calculate the temperature at a particular time and at a particular space that is at a particular distance or in the metal hydride reactor, but in this case it is given that at a particular time t. So, we do not require the differential equation it is directly given that the temperature is 303 kelvin and the supply pressure is these three.

So, from here we will calculate the equilibrium pressure. So, the equilibrium pressure is P reference exponential entropy of the reaction and the enthalpy of the reaction. Now, it is given that for LaNi<sub>5</sub> the entropy and the enthalpy is this 108 J/mol-K and 30800 joule per mole. If you put this value in this formula, we are able to calculate the equilibrium pressure which is 2.14 bar. Now, we have the equilibrium pressure.

In the last lecture, we have also studied that the rate of mass of hydrogen that is being absorbed inside the metal hydride reactor is given by this formula, where Ca is the reaction constant, Ea is the activation energy, R is a universal gas constant, this Ts is the temperature of the metal hydride reactor, Ps is the supply pressure, Pequilibrium we have already calculated from the above equation,  $\rho_{\text{saturation}}$  is the density of metal hydride at saturated level and  $\rho_s$  is the density of metal hydride at a particular time t.

Now, from this formula we have calculated the rate of mass absorbed inside the metal hydride reactor and this mass comes out to be this. So, we have all the values given in the question  $\rho_{\text{saturation}}$  is given,  $\rho_s$  is given. So, we have to change this value Ps from 10, 20 and 30, one by one and accordingly we will calculate rate of mass of hydrogen absorbed inside the metal hydride reactor. So, these are the three calculated rate of mass of hydrogen absorb.

From here we have seen that when a supply pressure is increasing from 10 to 30 bar or rate of mass of hydrogen is also increasing. So, why it is happening? In the last lecture I have told you that supply pressure minus equilibrium pressure of metal hydride is the main driving force. So, when we increase the supply pressure from 10 to 30 bar this difference between the supply pressure and the equilibrium pressure is continuously increasing which will allow us

to have a more hydrogen that is being rate of hydrogen that is being absorbed inside the metal hydride reactor.

So, this is how we will calculate. So, the effect of pressure is that is being asked in the question is when we increase the supply pressure the driving force will increase which will increase the amount of mass that is being absorbed inside the metal hydride reactor.

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Q1. Design a metal hydride reactor considering  $\text{LaNi}_5$  as metal hydride to store 50 g of hydrogen. Considering the shape of metal hydride as cylinder, calculate the length and diameter of cylinder if L/D ratio is 3. Based on this system calculate the mass of hydrogen desorbed ( $\text{kg}/\text{m}^3\cdot\text{s}$ ) at time 't' when temperature  $T = 303\text{ K}, 313\text{ K}, 323\text{ K}, 333\text{ K}$  and at an outlet pressure of 1 bar. Finally, comment on the effect of temperature on the system.

The density at saturation state is  $8534\text{ kg}/\text{m}^3$ , density at particular time 't' is  $8467\text{ kg}/\text{m}^3$  and density of metal hydride without hydrogen is  $8400\text{ kg}/\text{m}^3$ .

The porosity of metal hydride is assume to be 0.5 and expansion volume as 20%. The reaction constant for this condition is  $9.5\text{ s}^{-1}$  and activation energy is  $16473\text{ J}/\text{mol}$ .

Solution : L/D = 3 ✓  
L = 3D ✓

- Amount of hydrogen to store = 50 g = 0.05 kg ✓
- Gravimetric capacity of  $\text{LaNi}_5 = 1.6\text{ wt}\%$  ✓
- Amount of metal hydride required =  $\frac{100}{1.6} \times 0.05 = 3.125\text{ kg}$  ✓
- Density of MH =  $8400\text{ kg}/\text{m}^3$  ✓
- Volume of MH required =  $\frac{3.125}{8400} = 3.72 \times 10^{-4}\text{ m}^3$  ✓

description

Refrigeration

LaNi5

Secondary MH for HTMH → Thermal storage

Coming to the next question carry forward that the previous question we have seen that this is the amount of hydrogen that is being absorbed. So, the maximum hydrogen that is being absorbed according to 1.6 wt.% and the density at that portion is 8534 per meter cube, density at particular time t again is same and the density of metal hydride without hydrogen is also given now this is the case of desorption, in which the same 50 gram of hydrogen is already being stored, the shape of the metal cylinder the L/D ratio is 3.

But in this case we want to calculate the mass of hydrogen desorbs at a particular time t when temperature of metal hydride reactor is these. So, in this we want to calculate the effect of temperature on the amount of mass desorbs from the metal hydride reactor.

Now, two important things which is need to be seen is the reaction constant is much more lesser as compared to what is in the absorption case and the activation energy is also less in this case. So these values are lower as compared to what you guys in the absorption case.

So, this desorption is generally used for the refrigeration case in which when the hydrogen is desorbed the temperature of the metal hydride reactor will decrease and this will provide us the cooling effect. In the LaNi5 cases these type of desorption cases are also being seen in the as a secondary metal hydride reactor for high temperature metal hydride.

This is in case of thermal energy storage systems which means when the hydrogen is dissolved from the high temperature metal hydride it is being absorbed in the low temperature metal hydride and accordingly the desorption will be as fast as possible. So, that more and more hydrogen is present at the high temperature metal hydride reactor. So, that it will generate more heat and that will be available for the utilization for particular cases.

Now, this problem is again start with we have the L/D ratio of 3 from here we were able to calculate the L=3D is, amount of hydrogen store is again 50 gram, 0.05 kg, gravimetric capacity is 1.6 weight percent and accordingly the amount of metal hydride required is 3.125 kg, the density of metal hydride is 8400 from where the we have calculated the volume of metal hydride.

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- Considering Porosity of 0.5, the volume of metal hydride =  $\frac{3.72 \times 10^{-4}}{0.5} = 7.44 \times 10^{-4} \text{ m}^3$
- Further considering expansion volume of 20 %, volume of metal hydride =  $1.2 \times 7.44 \times 10^{-4} = 8.93 \times 10^{-4} \text{ m}^3$
- Now, the shape of reactor is cylinder

$$\frac{\pi}{4} \times D^2 \times L = 8.93 \times 10^{-4}$$

- D = 0.0723 m, L = 0.2169 m

- For any time 't',

$$T = 303\text{K}, 313\text{K}, 323\text{K} \text{ and } 333\text{K}$$

$$P_0 = 1 \text{ bar}$$

For LaNi<sub>5</sub>,  
 $\Delta S = 108 \text{ J/mol.K}$   
 $\Delta H = 30800 \text{ J/mol}$

$$P_{eq} = P_{ref} \exp\left[\left(\frac{\Delta S}{R}\right) - \left(\frac{\Delta H}{R T_s}\right)\right]$$

- Mass of hydrogen desorbed

$$\dot{m} = C_d \exp\left(\frac{-E_d}{R T_s}\right) \left(\frac{P_d - P_{eq}}{P_{eq}}\right) (\rho_s - \rho_{emp})$$

$P_d > P_0$

Now, considering the again considering the porosity of 0.5 when and the volume of metal hydride is coming out to be  $7.44 \times 10^{-4}$ -meter cube. Again we have considered the expansion volume, the volume of metal hydride comes out to be  $8.93 \times 10^{-4}$ -meter cube and as we have not seen in the last question also.

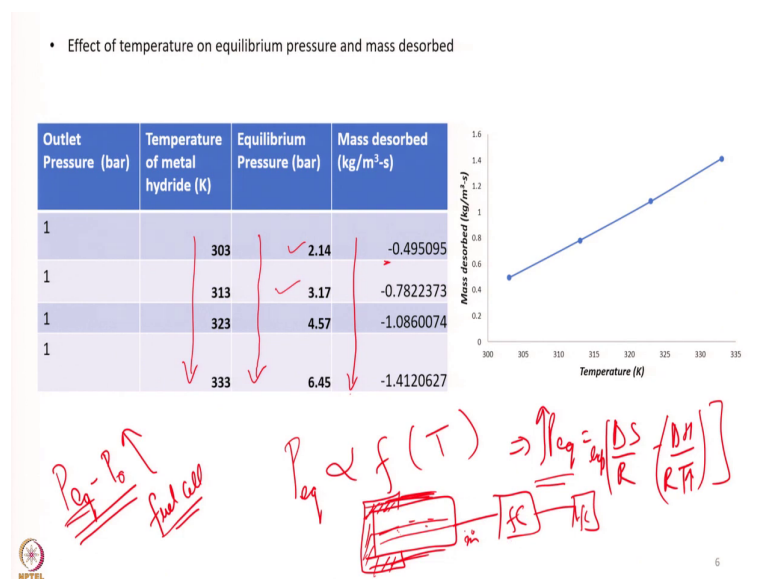
Now, again we have the shape of reactor cylinders. So, that we are able to calculate the diameter and the length of the reactor by having the volume of the metal hydride reactor required. Now, for any time  $t$  in this case we have given the temperature of 303, 313, 323 and 333 kelvin. And the outlet pressure is given as 1 bar.

So, if we have a metal hydride reactor and metal hydride is here and the hydrogen is already present inside this metal hydride reactor. So, when the desorption case is started so, the pressure at outlet need to be lower than the equilibrium pressure of metal hydride. So, when this pressure is when the equilibrium pressure is higher than the outlet pressure only then the hydrogen will transfer from inside to the outlet.

So, for the first case is  $P$  equilibrium pressure is greater than the  $P$  outlet pressure. So, here it is given that the  $P$  outlet pressure is 1 bar, similarly we will calculate as we see in the last question similarly we will calculate the equilibrium pressure also by this formula.

The mass desorbed is calculated by this formula it is important that this term in the mass desorbed is different as the formula that we have seen for the amount of mass absorbed. This is also a bit different as compared to the last, the reaction constant is lesser for the desorption case as we compared in the absorption case.

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So, from this formula we have calculated the value of equilibrium pressure. So, at 303 kelvin it is 2.14 bar, for 313 is 3.17 bar. So, what we have seen from here as we increase the

temperature, our equilibrium pressure is also continuously goes on increasing. If our equilibrium pressure goes on increasing the mass desorbed from the metal hydride reactor is also increasing. This negative sign indicates the desorption of hydrogen from the metal hydride reactor.

Now, when we increase the temperature equilibrium pressure increases and the mass amount of mass dissolved is also increasing. So, why it is happening is the equilibrium pressure we have seen that the equilibrium pressure is a function of temperature that is  $P_{\text{equilibrium}}$  is as I shown you in the last slide is the function of exponential  $\Delta S/R$  minus  $\Delta H/RT$ . So, when the temperature is increasing this equilibrium pressure is also going on increasing, if this equilibrium pressure is increasing the main driving force which is  $P_{\text{equilibrium}}$  minus  $P_0$  is continuously goes on increasing.

With this increase in the driving force the amount of mass desorbs is also continuously goes on increasing. This is very important when we want to design a particular metal hydride reactor for a particular cases so initially we have to see what we have to go what we have to consider suppose if we want to.

So, designer metal hydride reactor for fuel cell integration so, there is a hydrogen metal hydride reactor that is being connected with the fuel cell. So, this hydrogen need to be removed at a particular rate that is being that has gone into the fuel cell and that is being further used for the generation of electricity.

So, the control of this mass flow rate is done by the by increasing or decreasing the temperature. So, this to maintain this temperature there are different type of methods that is being used, some of them uses the flow of fluid at the outer boundary, some of them uses the cooling tube inside the metal hydride reactor to supply heat to the metal hydride reactor at a particular temperature. So, that this equilibrium pressure will increase and there will be an increase in the mass desorbed.

Thank you.