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Assignment :03
SEE607:HYDROGEN ENERGY:PRODUCTION, STORAGE AND UTILIZATION

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Problem:01

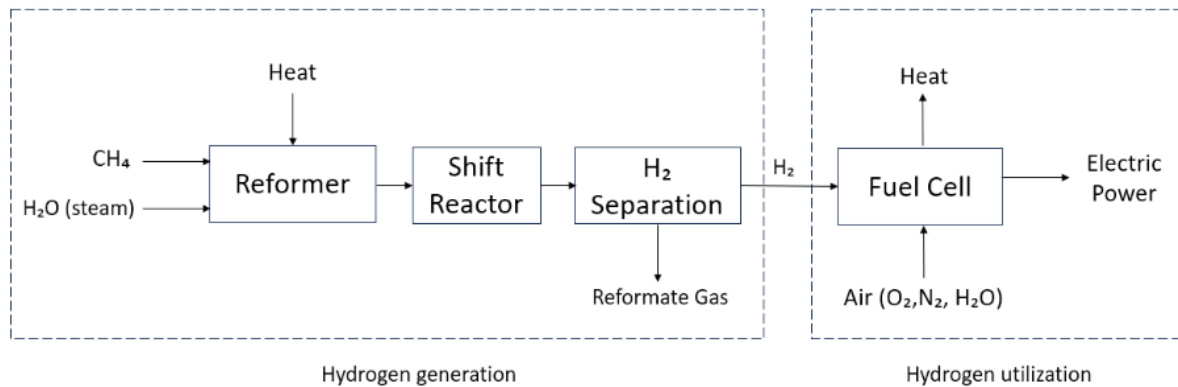


Fig:1 Schematic of Overall system

a) Fuel Cell: In this report I have used PEM Fuel cell as it is the most promising one for hydrogen utilization systems. PEM fuel cells provide equivalent efficiency at low temperatures as compared to other fuel cells, which is why it is selected for the hydrogen utilization system. Additionally, a lower operating temperature extends the life of the catalyst and the membrane, reducing the need for replacement. PEM fuel cells have high permeability and operating cost is less comparatively to other fuel cells.

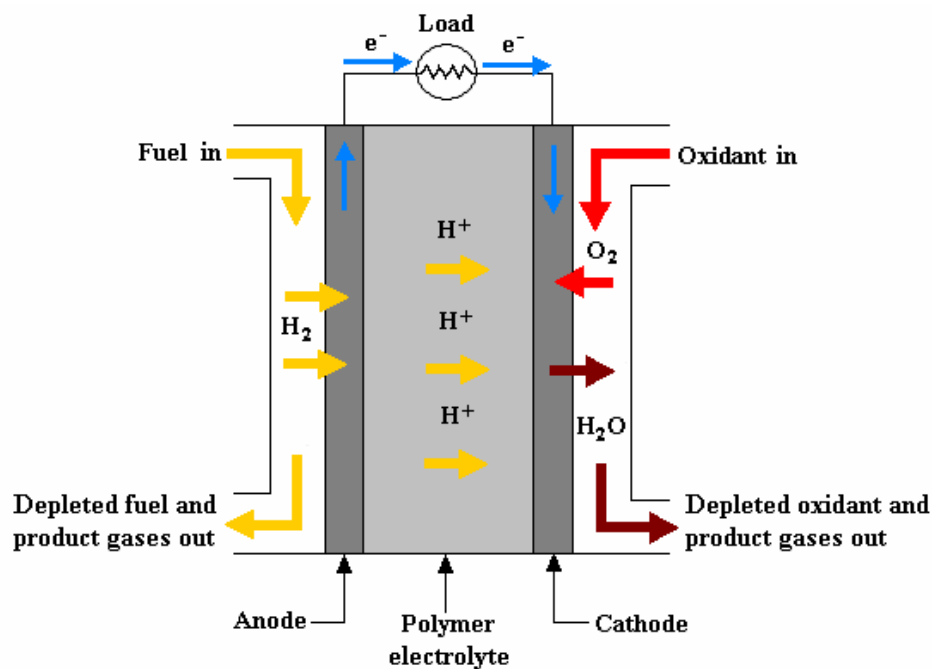


Fig:2 PEM Fuel cell Schematic

Anode side reaction: $\text{H}_2 \longrightarrow 2\text{H}^+ + 2\text{e}^-$

Cathode side reaction: $\frac{1}{2}\text{O}_2 + 2\text{H}^+ + 2\text{e}^- \longrightarrow \text{H}_2\text{O}$

Overall cell reaction: $\text{H}_2 + \frac{1}{2}\text{O}_2 \longrightarrow \text{H}_2\text{O}$

Theoretical fuel cell efficiency:

For a fuel cell, the energy input is equivalent to the enthalpy of reaction (combustion), and the useful energy output is electrical energy produced. If all the Gibbs free energy produced is converted to electricity, then the thermodynamic fuel cell efficiency at 25°C (77°F) temperature and 1 atmosphere pressure is the ratio of the change in Gibbs free energy (ΔG°) to the change in enthalpy (ΔH°) of the fuel cell reaction (using the HHV of hydrogen)

$$\eta = \Delta G / \Delta H = (237.1 \text{ kJ/mol}) / (286.0 \text{ kJ/mol})$$

$$\eta = 83\%$$

Thermodynamic energy conversion efficiency for fuel cells:

$$\eta = V_{\text{cell}} / 1.48$$

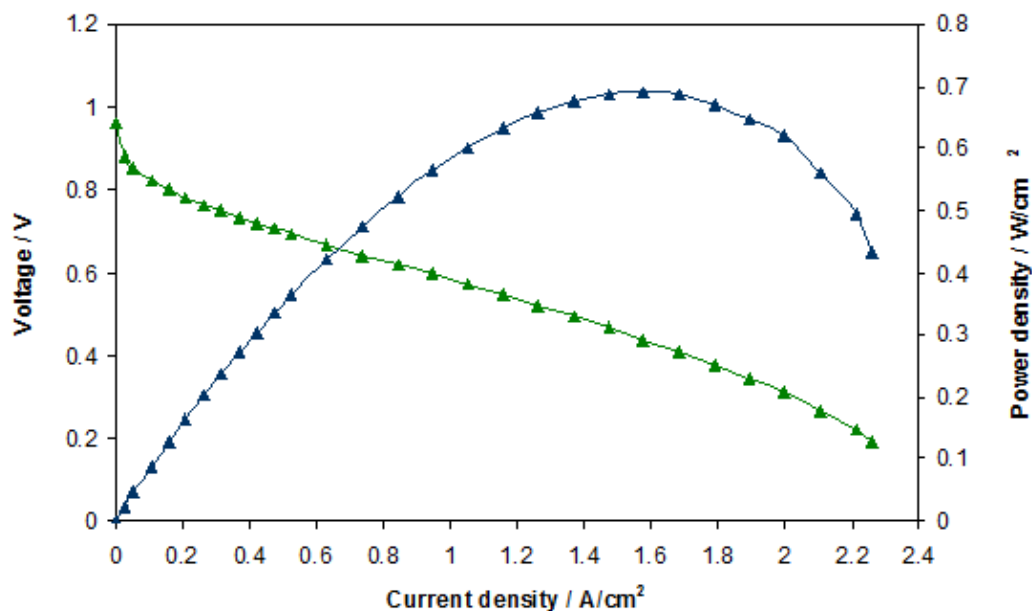


Fig:3 Polarization curve for PEM Fuel Cell (from literature)

In order to use the least number of cells to get the required 500KW power. Each cell must operate at maximum power density. Based on the above polarization curve we can see that the maximum power density is around 0.7 W/cm^2 , which is at a current density around 1.6 A/cm^2 and the cell voltage at 1.6 A/cm^2 current density is around 0.45V .

Therefore each cell is operating at ($i = 1.6\text{A/cm}^2$ $V_{\text{cell}}=0.45\text{V}$).

Area of each fuel cell = 600 cm^2

Power required to produces by each cell

$P_{\text{cell}} = p_{\text{cell}} \times \text{Area}$

$P_{\text{cell}} = 0.7 \times 600 = 420\text{W}$

No of cells required to produce 500 KW

$n_{\text{cell}} = P_{\text{stack}} / P_{\text{cell}}$

$n_{\text{cell}} = 500000\text{W} / 420\text{W}$

$n_{\text{cell}} = 1191$

Total power generation

Total power = $n_{\text{cell}} \times P_{\text{cell}}$

Total power = 500.220 KW

Each cell's total current

$I_{\text{cell}} = i_{\text{cell}} \times \text{Area}$

$I_{\text{cell}} = 1.6 \times 600$

$I_{\text{cell}} = 960\text{A}$

Total current produced

$I_{\text{stack}} = n_{\text{cell}} \times I_{\text{cell}}$

$I_{\text{stack}} = 1143360\text{A}$

Rate of hydrogen need to produced (mol/sec)

$R_{\text{H}_2} = I_{\text{stack}} / (n \times F)$

$R_{\text{H}_2} = 5.9250 \text{ mol/sec}$

The thermoneutral voltage of fuel cell

$E_{\text{th}} = \Delta H / nF$

$E_{\text{th}} = 1.48\text{V}$

Thermodynamic efficiency (η)

$\eta = V_{\text{cell}} / E_{\text{th}}$

$\eta = 0.45 / 1.48$

$\eta = 0.3040$ (low efficiency due to low voltage)

The cell is operating at thermodynamic efficiency = 0.3040

The fraction of heat been loss = $(1 - 0.3040) = 0.6959$

The electric power 500 KW is 0.3040 fraction of total heat produced

Total heat (Et) = $500000 / 0.3040$

Et = 1644.736 KW

Heat loss = 0.6959×1644.736

Heat loss = 1144.572 KW

Heat Generation: $(1 - \eta) * 500000$

Heat Generation = 348000W

Cooling requirement: $N_{coolent} = 348000 / (4186 * 10)$ where $c_p = 4186 \text{ J/kg}$ $\Delta T = 10^\circ\text{C}$

$N_{coolent} = 8.3134 \text{ kg/sec}$

b) Natural gas steam reforming, or SRM, is the most popular way to produce hydrogen today.

The endothermic steam reforming (SR) reaction produce carbon monoxide (CO) and (H₂) by using steam and methane(CH₄).The CO can be further transformed by the exothermic water-gas shift (WGS) reaction, producing more hydrogen and carbon dioxide (CO₂). Methane is efficiently converted into carbon dioxide and hydrogen when these processes come together to produce a larger reaction.

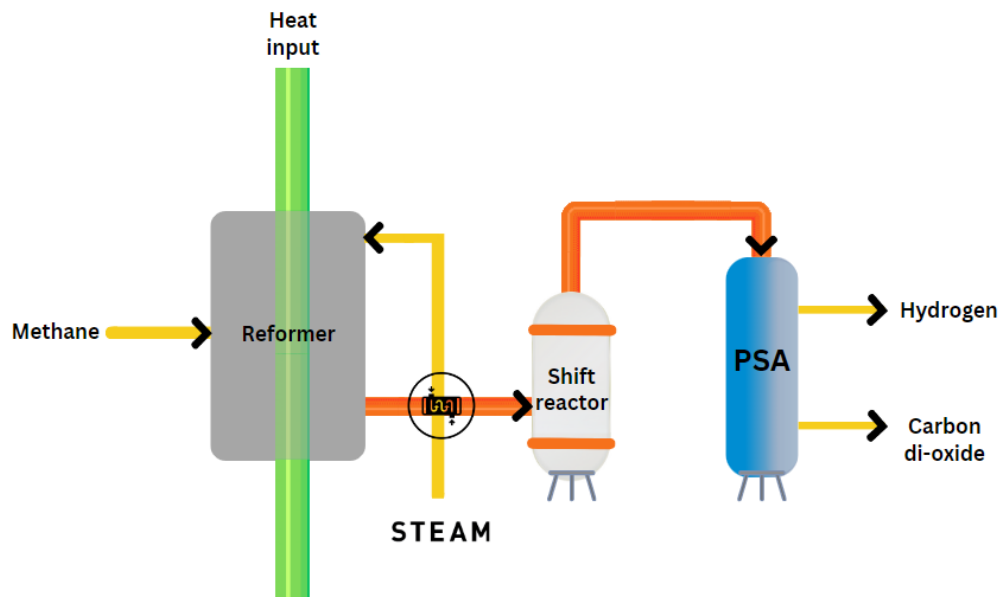


Fig:4 Schematic of Steam Methane Reformer

$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$, $H = +206.2 \text{ kJ/mol}$ (Endothermic)

$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$, $H = -41.1 \text{ kJ/mol}$ (Exothermic)

$\text{CH}_4 + 2\text{H}_2\text{O} \rightarrow \text{CO}_2 + 4\text{H}_2$, $H = +164.9 \text{ kJ/mol}$

Operating parameter:

Inlet fuel(CH_4)	Inlet Steam	Reformer	Shift reactor
$T = 298 \text{ K}$	$T = 483.15 \text{ K}$	$T = 973 \text{ K}$	$T = 573 \text{ K}$
$P = 10 \text{ atm}$	$P = 10 \text{ atm}$	$P = 10 \text{ atm}$	$P = 10 \text{ atm}$

Effectiveness of membrane=0.90

Effectiveness of heat exchanger= 0.81

Design: I) For Reformer

$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$ (In this process we are assuming that methane is fully consumed)

Compounds	N_{in}	$H_{\text{in}}(\text{kJ/mol})$	N_{out}	$H_{\text{out}}(\text{kJ/mol})$
CH_4	x	-110.52	0	0
H_2O	$3x$	-219.142	$2x$	-214.84
CO	0	0	x	-88.39
H_2	0	0	$3x$	20.24

The enthalpy of compounds are calculated as per NIST JANAF Table.

II) For Water Gas-Shift Reaction(WGS):

$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$

Compounds	Nin	Nout
CO	x	0
H ₂ O	x	0
CO ₂	0	xz
H ₂	3x	4x

Total hydrogen production is 4x

As we have assuming 0.9 effectiveness of Pressure Swing Adsorption (PSA) the net output of H₂ will be 0.9*4x

Flow Rate calculation: The required H₂ (mol/sec) of fuel cell to produce 500 KW power is 5.9250 mol/sec.

$$0.9 \cdot 4x = 5.9250$$

$$x = 1.64583 \text{ mol/sec}$$

Compound	Nin	Nout
CH ₄	1.64583	0
H ₂ O	4.93749	0
H ₂	0	5.9250

Methane Conversion: (No of moles of methane reacted)/(Total no of mol of methane fed in feed stream of reactor)

Conversion : 100%

Hydrogen Conversion: $(N_{in} - N_{out})_{H_2} / N_{inH_2} = 100\%$

Hydrogen Yield: $N_{outH_2} / (2 \cdot N_{inCH_4} + N_{inH_2O})$

Hydrogen Yield: 72%

c) Hydrogen Fuel Cell Storage:

The Fuel Cell operates 6 hours per day

$$RH_2 = (H_2(\text{kg}) \cdot 500(\text{mol/kg})) / (6(\text{hr}) \cdot 3600(\text{sec/hr}))$$

H₂(kg) = 255.96 kg of hydrogen (gas)

34 Type III cylinders are used for the storage of 255.96 kg of gaseous hydrogen, connected in parallel to enhance thermal safety and extend service life.

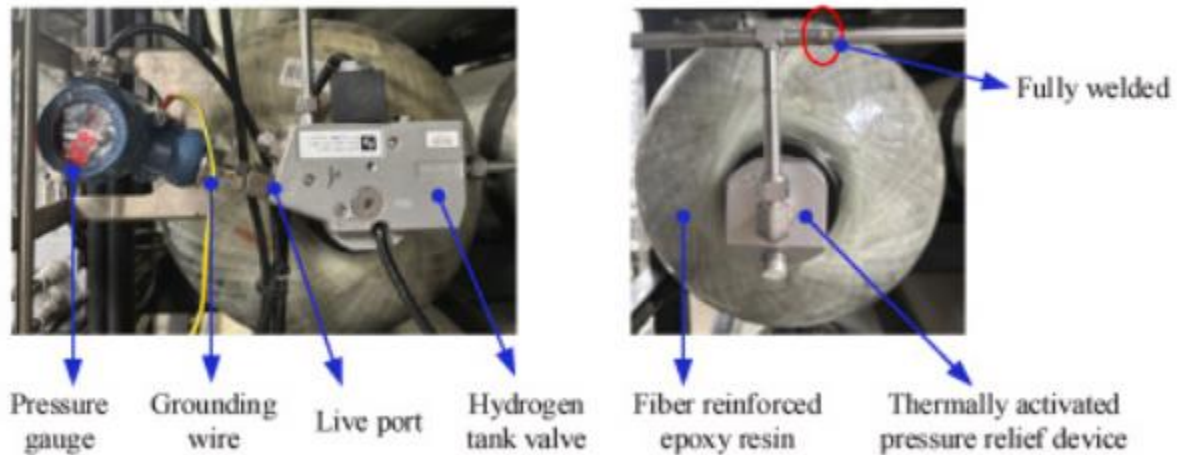


Fig:5 Head and Tail view of Type III compressed cylinder

Cylinders are made up of aluminium, reinforced by fully-wrapped carbon fiber.

Two TPRDs are installed at both ends of each cylinder to safely vent hydrogen to open air if temperature reach 110 °C

Design parameters:

The outer diameter of the cylinder is 408mm.

The length of the cylinder is 3400 mm.

Remote monitoring of pressure and local display via explosion-proof indicators (Ex IIC T6, measuring range from zero to 50 MPa) is facilitated for each cylinder.

Problem:02 Cryogenic Storage: Cryogenic storage involves storing hydrogen in its liquid form at extremely low temperature around (-253°C).

Advantages: i) Higher energy density per volume compared to compressed gas.
ii) Suitable for applications where space is limited and weight savings are critical.

Disadvantages: i) Requires significant energy to liquefy hydrogen.
ii) Boil-off losses due to heat ingress are common.
iii) Expensive and complex insulation and handling systems.

Compressed hydrogen system: Compressed Storage involves storing hydrogen gas under high pressure, typically at 350–700 bar.

Advantages: i) Simpler and more mature technology.
ii) Lower energy input compared to liquefaction.
iii) Easier to refill and handle at fueling stations.
Disadvantages: i) Lower energy density per volume than cryogenic.
ii) Heavy and bulky storage tanks are needed to withstand high pressures.

Problem:03 Liquid organic hydrogen carriers (LOHCs) is an attractive and promising technology for hydrogen storage. This method involves two stages: the first stage is the charging of hydrogen into LOHCs through a catalytic hydrogenation reaction and the second stage in the discharging of hydrogen through a catalytic dehydrogenation reaction. LOHCs are materials that might experience the reversible hydrogenation/dehydrogenation process that take place in the liquid state in the hydrogenation/dehydrogenation process.



Fig:6 LOHC

- use the existing infrastructure (low cost).
- Storage viability
- 1 year (long term).

In this method, the hydrogenation and the dehydrogenation could be performed at the same temperature. **The main advantages of the LOHC are the high gravimetric and volumetric density, easiness of storage and transportation of generated hydrogen at ambient temperature, and low level of operation and investment risk since the existing infrastructure for fuel could be used to store and transport hydrogen in the form of LOHC.** In addition, LOHC charging conducts and catalytic hydrogenation occurs under high hydrogen pressure while the release of hydrogen from the LOHC occurs under low hydrogen pressure (under 5 bar). **Moreover, explosion risk could be reduced in this case due to the low amount of hydrogen in a LOHC system.**

References

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- PROTON EXCHANGE MEMBRANE or POLYMER ELECTROLYTE MEMBRANE (PEM) FUEL CELLS *Ryan Baker and JiuJun Zhang* , Institute for Fuel Cell Innovation , National Research Council of Canada, 4250 Wesbrook Mall, Vancouver, British Columbia V6T 1W5, Canada