Hydrogen as fuel

Introduction

Hydrogen is a clean fuel. It is an energy carrier that can be used for a broad range of applications. Also it could serve as a possible substitute to liquid and fossil fuels. Its physical properties could be stated as following. At standard temperature and pressure, hydrogen is a nontoxic, nonmetallic, odorless, tasteless, colorless, and highly combustible diatomic gas with the molecular formula H_2.

Occurrence and storage

Speaking of its natural occurrence, it is the most abundant element in the universe. The sun and other stars are composed largely of hydrogen. Astronomers estimate that 90% of the atoms in the universe are hydrogen atoms. Hydrogen is a component of more compounds than any other element. Water is the most abundant compound of hydrogen found on earth.

Molecular hydrogen is not available on Earth in convenient natural reservoirs. Most hydrogen on Earth is bonded to oxygen in water and to carbon in live or dead and/or fossilized biomass. It can be created by splitting water into hydrogen and oxygen. Water is again formed, when hydrogen is used.

On the other hand, its preparation could be done by breaking the chemical bonds from compounds. A few common methods include electrolysis, from steam and hydro carbon or carbon, reaction of metals with acids, ionic metal hydrides with water, etc. Currently, global hydrogen production is 48% from natural gas, 30% from oil, and 18% from coal; water electrolysis accounts for only 4%.

Its storage is important because it has wide range of applications. They range from stationary power, portable power to transportation, etc. Also it has the highest energy per mass of any fuel. However, its low ambient temperature density results in a low energy per unit volume, therefore requiring the development of advanced storage methods that have potential for higher energy density.

Hydrogen can be stored physically as either a gas or a liquid. Storage of hydrogen as a gas typically requires high-pressure tanks (350–700 bar [5,000–10,000 psi] tank pressure). Storage of hydrogen as a liquid requires cryogenic temperatures because the boiling point of hydrogen at one atmosphere pressure is −252.8°C. Hydrogen can also be stored on the surfaces of solids (by adsorption) or within solids (by absorption).

Hydrogen as a fuel

Hydrogen is considered an alternative fuel. It is due to its ability to power fuel cells in zero emission electric vehicles, its potential for domestic production, and the fuel cell's potential for high efficiency. In fact, a fuel cell coupled with an electric motor is two to three times more efficient than an internal combustion engine running on gasoline. Hydrogen can also serve as fuel for internal combustion engines. The energy in 2.2 pounds (1 kilogram) of hydrogen gas contains about the same as the energy in 1 gallon (6.2 pounds, 2.8 kilograms) of gasoline.

Potential Applications

· Production of electricity, heat and water for various end uses · Industrial

applications
· Vehicular transportation
· Residential applications
· Commercial applications, including in telecom towers for providing back-up power

Advantages and disadvantages of Hydrogen fuel cells

Advantages

- **It is readily available**. It is a basic earth element and is very abundant. However, it time consuming to separate hydrogen gas from its companion substances. While that may be the case, the results produce a powerful clean energy source.
- **It doesn't produce harmful emissions.** When it is burned, it doesn't emit harmful substances. Basically, it reacts with oxygen without burning and the energy it releases can be used to generate electricity used to drive an electric motor. Also, it doesn't generate carbon dioxide when burnt, not unlike other power sources.
- **It is environmentally friendly**. It is a non-toxic substance which is rare for a fuel source. Others such as nuclear energy, coal and gasoline are either toxic or found in places that have hazardous environments. Because hydrogen is friendly towards the environment, it can be used in ways that other fuels can't even possibly match.
- **It can be used as fuel in rockets.** It is both powerful and efficient. It is enough to provide power for powerful machines such as spaceships. Also, given that it is environmentally friendly, it is a much safer choice compared to other fuel sources. A fun fact: hydrogen is three times as powerful as gasoline and other fossil fuels. This means that it can accomplish more with less.
- **It is fuel efficient.** Compared to diesel or gas, it is much more fuel efficient as it can produce more energy per pound of fuel. This means that if a car is fueled by hydrogen, it can go farther than a vehicle loaded with the same amount of fuel but using a more traditional source of energy. Hydrogen-powered fuel cells have two or three times the efficiency of traditional combustion technologies. For example, a conventional combustion-based power plant usually generates electricity between 33 to 35 percent efficiency. Hydrogen fuel cells are capable of generating electricity of up to 65 percent efficiency.
- **It is renewable**. It can be produced again and again, unlike other non-renewable sources of energy. This means that with hydrogen, you get a fuel source that is limited. Basically, hydrogen energy can be produced on demand.

Disadvantages

- **It is expensive.** While widely available, it is expensive. A good reason for this is that it takes a lot of time to separate the element from others. If the process were really simple, then a lot would have been doing it with relative ease, but it's not. Although, hydrogen cells are now being used to power hybrid cars, it's still not a feasible source of fuel for everyone. Until technology is developed that can make the whole process a lot more simpler, then hydrogen energy will continue to be an expensive option.
- **It is difficult to store.** Hydrogen is very hard to move around. When speaking about oil, that element can be sent through pipelines. When discussing coal, that can be easily carried off on the back of trucks. When talking about hydrogen, just moving even small amounts is a very expensive matter. For that reason alone, the transport and storage of such a substance is deemed impractical.
- It is not easy to replace existing infrastructure. Gasoline is still being widely used to this day. And as of the moment, there just isn't any infrastructure that can support hydrogen as fuel. This is why it becomes highly expensive to just think about replacing gasoline. Also, cars need to be refitted in order to accommodate hydrogen as fuel.
- **It is highly flammable.** Since it is a very powerful source of fuel, hydrogen can be very flammable.

In fact, it is on the news frequently for its many number of risks. Hydrogen gas burns in air at very wide concentrations – between 4 and 75 percent.

- It is dependent on fossil fuels. Although hydrogen energy is renewable and has minimal environmental impact, other non-renewable sources such as coal, oil and natural gas are needed to separate it from oxygen. While the point of switching to hydrogen is to get rid of using fossil fuels, they are still needed to produce hydrogen fuel.

The main hydrogen production processes can be classified into

- electrolysis,
- photolysis,
- thermolysis.

Electrolytic hydrogen production processes involve the use of electric or thermal energy to trigger a chemical reaction for splitting water molecules into hydrogen and oxygen. The main examples of electrolytic processes are water electrolysis (conventional process) and thermolysis (steam electrolysis). Photolytic processes involve technologies that use the energy of light, and its main examples are the photobiological and photoelectrochemical systems. Hydrogen production through thermochemical processes essentially comprise the raw material, being either from fossil or renewable sources, heat and catalysts so as to trigger chemical reactions for transforming the raw material (for example, ethanol, natural gas, methanol, gasoline) into hydrogen. The main thermochemical hydrogen production processes are: biomass gasification and pyrolysis, steam reforming, partial oxidation, autothermal and oxidative reforming.

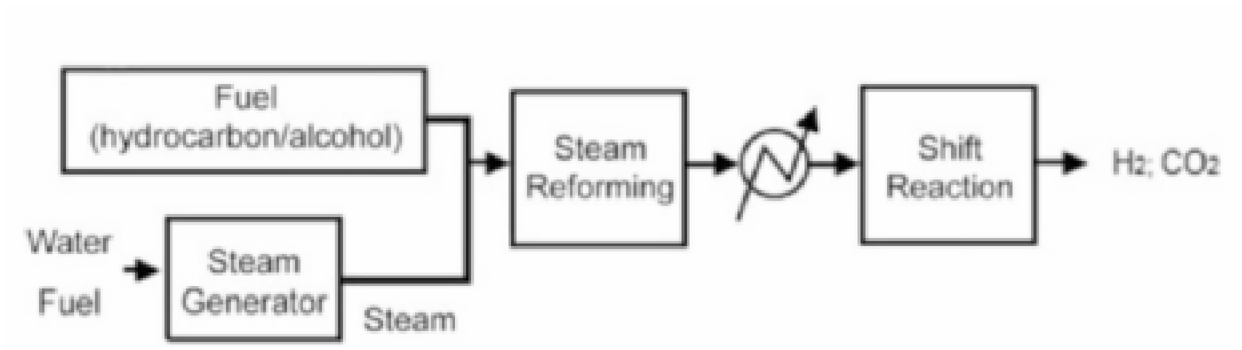
Thermolysis

Steam Reforming for Hydrogen Production

Steam reforming has been used as the main process for hydrogen production, which accounts for 50% of the world's total production. The popularity of this process derives from its high conversion efficiency and cost-effectiveness in comparison with other processes.

As illustrated in Fig. 2.1, this process occurs in two main steps, one that occurs at high temperatures (steam reforming), in which the fuel (hydrocarbon or alcohol) reacts with steam and is converted into a gaseous mixture of H2, CO, CO2, hydrocarbon or alcohol, and unreacted steam, and another one which occurs at lower temperatures in a shift reactor (water-gas shift reaction), where the CO present in the synthesis gas reacts with H2O to produce additional CO2 and H2.

1. Overall Reforming Reaction



The overall reaction of fuel conversion into hydrogen by steam reforming is shown in Eq. (1) Overall Reaction: Fuel + H_2O (gas) $\rightarrow$ CO_2+ H_2 (1)

Steam Reforming Reaction

Equation (2) shows the steam reforming reaction which consists of an endothermic catalytic reaction of the fuel with steam, mainly producing carbon monoxide and hydrogen:

Reforming Reaction:
Fuel + H_2O (gas) $\rightarrow$ CO + H_2 (2)

Water-Gas Shift Reaction

Equation (3) shows the catalytic water-gas shift reaction that produces additional hydrogen and eliminates part of the carbon monoxide, which is conducted through a catalytic reactor called as the shift reactor, i.e., the carbon monoxide reacts with steam so as to form carbon dioxide and hydrogen. This reaction is

$CO+H_2O \rightarrow CO_2+H_2$ (3)

Methane Formation Reaction

Equation (2.4) shows one of the reactions that can occur during the reforming process. The methane formation reaction is unwanted, since part of the produced hydrogen reacts with carbon monoxide, thus decreasing its composition in the final synthesis gas.

$CO + 3H_2 \rightarrow CH_4 + H_2O$

Steam Reforming of Alcohols

According to Silva (2005), a fairly feasible alternative is the production of hydrogen via the steam reforming of alcohols.

Overall Reaction: $C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 6H_2$

Reforming Reaction: $C_2H_5OH + H_2O \rightarrow 2CO + 4H_2$

Shift Reaction: $2CO + 2H_2O \rightarrow 2CO_2 + 2H_2$

The steam reforming reaction of ethanol occurs at temperatures between 400 and 700 C (Saebea et al. 2011), and the shift reaction occurs at temperatures between 200 and 300 C,

$$\text{Steam Reforming Reaction: } C_2H_5OH_{(g)} + H_2O_{(g)} \underset{773-923\ K}{\overset{NiCu\text{-}Al_2O_3}{\rightleftarrows}} 2CO_{(g)} + 4H_{2(g)}$$

$$\text{Water-Gas Shift Reaction: } CO_{(g)} + H_2O_{(g)} \underset{473-523\ K}{\overset{\frac{Cu}{ZnO}\text{-}\gamma Al_2O_3}{\rightleftarrows}} CO_{2(g)} + H_{2(g)}$$

Partial oxidation

With the growing interest in hydrogen fuel cells for energy generation, the need for a decentralized supply of hydrogen is also increasing. Partial oxidation is one of the processes currently in use for hydrogen production. The following article explains how this works and what types of partial oxidation are available.

What is partial oxidation?

Partial oxidation is one of the so-called reforming processes for hydrogen production. Even before electrolysis, reforming is one of the most important processes for producing hydrogen. More than 500 billion cubic meters of hydrogen are produced worldwide each year by reforming and around 15 billion cubic meters by electrolysis.[1]

Reforming requires extremely high temperatures and a catalyst. An oxidizing agent is also required, for example steam, oxygen or a mixture of both starting materials. If oxygen is used, this is called partial oxidation.[1]

What happens during partial oxidation?

The partial oxidation process for hydrogen is technically very mature. In this process, oxygen is added to the available raw material, i.e. natural gas or heavy hydrocarbons such as fuel oil or residual oils from petroleum processing.[4] This process is exothermic, i.e. heat is released. The starting materials are the residues produced in the refinery process, i.e. liquid hydrocarbons. Although these are liquid, they have a high viscosity, i.e. they are very viscous or viscous.[2]

In partial oxidation, the mixture of fuel and air is partially burned in a process furnace. [3] Via a dedicated burner, it enters the reactor, which is operated at 40 to 100 bar pressure. This process produces a synthesis gas rich in hydrogen (H2), carbon monoxide (CO) and carbon dioxide (CO2), making it suitable for further use in [fuel cell technology.](). The synthesis gas obtained is then cooled and the carbon dioxide is separated by amine scrubbing.[5]

What are the types of partial oxidation?

There are two types of partial oxidation: Thermal Partial Oxidation (TPOX) and Catalytic Partial Oxidation (CPOX). While TPOX requires temperatures of at least 1200 degrees Celsius for the reactions, CPOX uses a catalytic medium. Therefore, the temperature required for the latter is only 800 to 900 degrees.[3]

Which technique is used in the reforming process depends on the amount of sulfur present in the fuel. If the sulfur content is less than 50 ppm, catalytic partial oxidation can be used. Since a higher sulfur content would lead to poisoning of the catalyst, Thermal Partial Oxidation is used for such fuels.[3]

Partial oxidation with coal is also possible. The chemical process is similar to the reaction of the oil, but before that a coal treatment takes place. In this step, the coal is ground and mixed into a suspension with the addition of water.[4]

What is released during partial oxidation?

The product of partial oxidation as a gasification reaction is a gas mixture that is used as a synthesis gas, as a heating gas or as a feedstock for hydrogen production. In addition to hydrogen, partial oxidation also produces carbon monoxide (CO), carbon dioxide (CO_2) and water.[5]

What are the advantages and disadvantages of partial oxidation?

Partial oxidation is an efficient and recognized process for the recovery of synthesis gas. The advantage is that the ratio between hydrogen and carbon in the synthesis gas can be individually adjusted by various process steps – for example, the use of a membrane. The ratios can thus be adapted to the customer’s requirements without any problems.[5] Another advantage of partial oxidation is that it allows the refinery residues used to be recycled particularly cleanly and economically.[6]

Case studies: partial oxidation of methane to produce hydrogen gas in a mixture of synthesis gas (CO, H2).

The low-temperature conversion of methane into value-added products is an appealing goal due to the abundance of methane in the form of natural gas.

Methane partial oxidation (MPO, $CH_4 + \frac{1}{2}O_2 \rightarrow CO + 2H_2$) is an appealing alternative to Methane steam reforming for the formation of synthesis gas. This reaction has the energetic benefit of being mildly exothermic ($\Delta H = -36$ kJ mol-1), as well as producing a H_2/CO ratio of ~2, which is more favorable for the synthesis of hydrocarbon fuels

Electrolysis method:

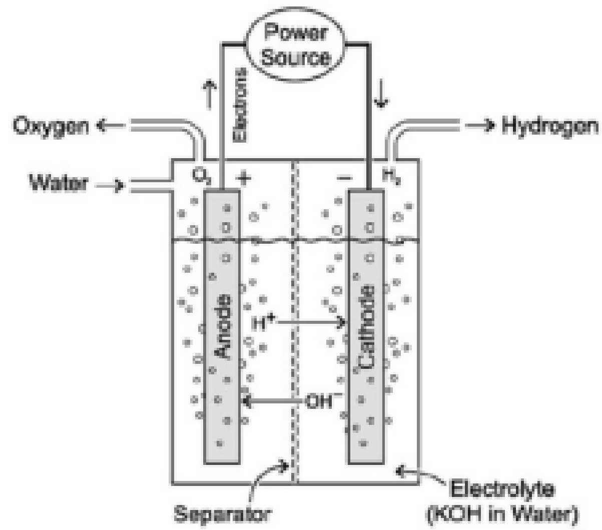
2.4 Alkaline Electrolysis (AEL)

From a technological point of view, alkaline electrolyzers are sufficiently well developed and ready to produce renewable hydrogen at significant rates. The equipment is reliable and secure, with total lifetime of up to 30 years, electrode and membrane exchange at every 8 years, operation efficiency ranging between 62 and 82 %, and production capacity from 1 to 760 Nm^3/h (Smolinka et al. 2011). It consists mainly of two electrodes immersed in an aqueous solution of KOH or NaOH (25–30 %). Hydrogen is produced at the cathode and oxygen at the anode. The reactions involved in the process are as follows:

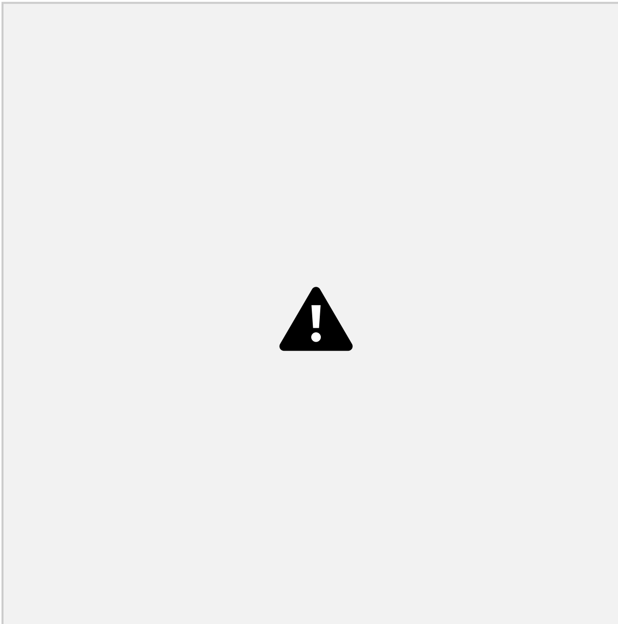
$$\text{Anode:}\ 4OH^- \rightarrow O_2 + 2H_2O + 4e^- \tag{2.29}$$

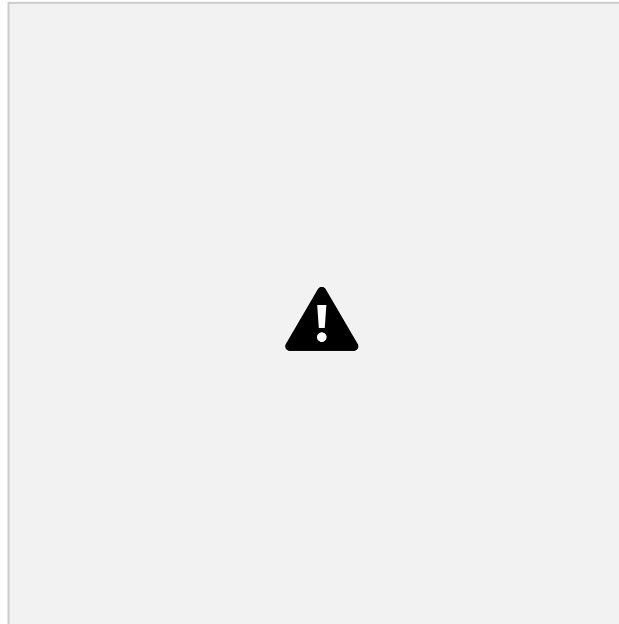
$$\text{Cathode:}\ 4H^+ + 4e^- \rightarrow 2H_2$$

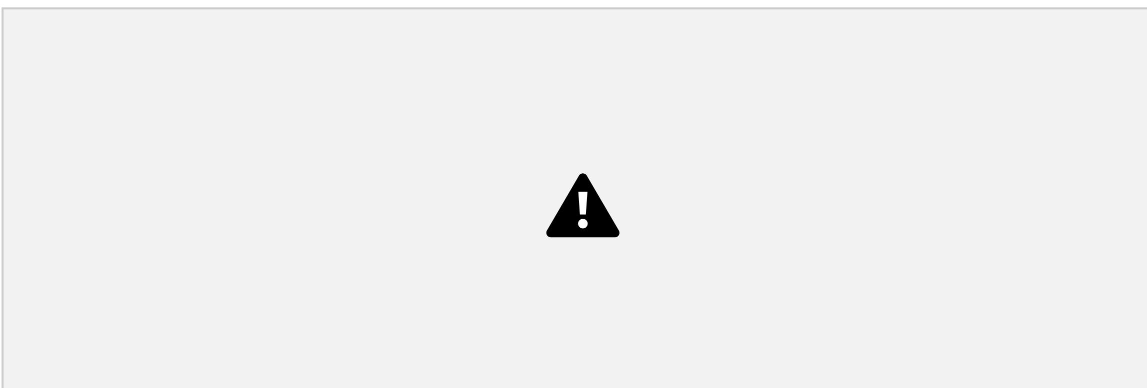
$$\text{Sum:}\ 2H_2O \rightarrow O_2 + 2H_2$$

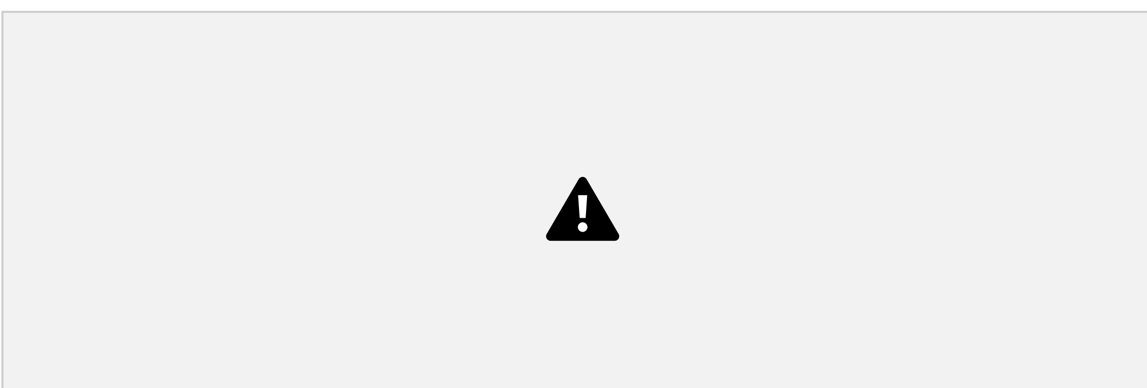


The electrodes are separated by a microporous membrane which is permeable to OH^- ions, but impermeable to gases. The anode is usually made of Nickel or Nickel-coated steel, while the cathode is made of steel coated with different catalysts. The distance between the electrodes is up to 5 mm and the operating temperature is usually limited to 80 °C (Bhandari et al. 2014). Figure 2.24 shows a scheme of the working principle of an alkaline electrolyzer.

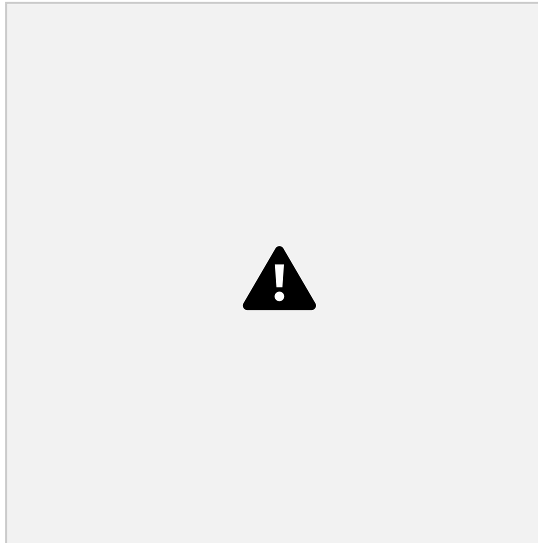




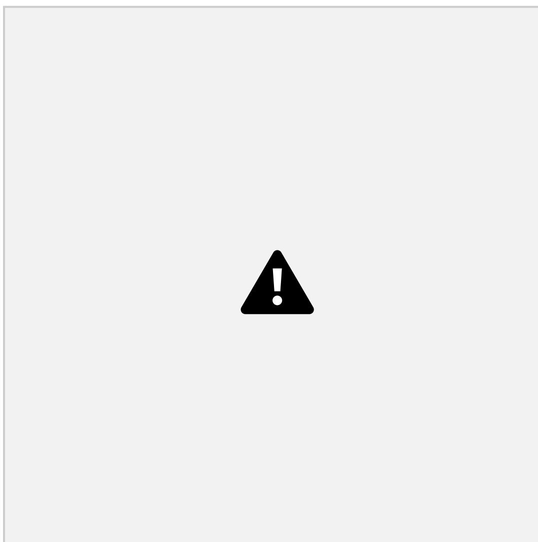




$H_2O \longrightarrow$



½ O2 + 2H+ + 2e



$2\ H^+ + 2e^- \rightarrow H_2$

2.6 High temperature steam electrolysis (SOEC)

$2O^{2-} \rightarrow O_2 + 4e^-$

$2H_2O + 4e^- \longrightarrow H_2 + 2O^{2-}$