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**ANALYSIS OF PERFORMANCE AND FEATURES OF HYDROGEN  
AS AN ENERGY CARRIER**

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# INTRODUCTION

Energy has become an essential component of all activities and plays a significant role in any country's economic development. Energy demand in all sectors continues to rise because of increased consumption, population growth, lifestyle changes, and technological advancement. Almost every industry is reliant on energy, the majority of which comes from fossil fuels. Renewable energies are playing an important role in addressing all the issues. For these reasons, the world and governments are developing new policies, particularly in the major industrialized countries, which are attempting to reduce their dependence on fossil fuels. Aiming to increase the proportion of its energy produced from renewable sources in search of solutions, researchers and scientists suggest "hydrogen" due to its properties. The density of hydrogen is smaller than that of air. The gravimetric density of hydrogen is approximately twice that of fossil fuels. Hydrogen is a fuel that can be used instead of traditional fossil fuels such as natural gas. Hydrogen is a promising energy carrier because it can store and deliver energy in usable form. The energy density of hydrogen ranges between 120 MJ/kg (LHV) and 142 MJ/kg (HHV). Depending on the production pathways, it has a relatively high-power density and low carbon emissions when consumed over its life cycle. It can also be combined with natural gas to meet the fuel requirements of various energy systems. However, hydrogen production must be both environmentally and economically competitive, which has sparked significant research and development efforts. As an essential part of the energy system, fossil fuel not only meets human demand but also causes ecological damage and pollution. Adjusting and optimizing energy structure is an effective way to address this issue. According to the US Energy Information Administration, global energy consumption will rise by 56% between 2010 and 2040. According to this forecast, conventional fossil fuels will account for approximately 78% of the total, with the remainder coming from renewable and nuclear sources. The widespread use of fossil fuels is to blame for climate change, greenhouse gas emissions, and pollution (e.g. CO, CO<sub>2</sub>, SO<sub>x</sub>, NO<sub>x</sub>, ashes etc.). All these gases and air pollutants deplete the stratospheric ozone layer and contribute to smog formation. As a result, people will consequently have health issues like blood disease, eye discomfort, and lung and respiratory illnesses. After electricity generation, the transportation sector is the second largest consumer of energy, with high consumption of petroleum and other liquid fuels (industrial). Annual energy consumption in

the transportation sector rises by 1.1 percent, with fossil fuels meeting most of the energy demand. These negative results encourage researchers to look for fossil fuel alternatives and much work has been done in this context. Paris Agreement On climate change in 2015, many countries set the goal of limiting global warming to 2°C or less by the end of the century. In the subsequent global collaboration projects and national roadmaps, it is clear that hydrogen completes the toolset required for nations to reduce domestic greenhouse gas emissions and achieve deep decarbonization on a scale of 80% or more. As researcher and scientists suggests, hydrogen is abundant on earth, along with other chemical elements such as water and natural gas. It has no color, odor, or toxicity. It produces no acid rain or harmful emissions and provides 2-3 times the energy of other common fuels. In fact, hydrogen can be produced using a variety of methods from readily available abundant sources. Again, most of the hydrogen is produced from fossil fuels via a process known as steam reforming of natural gas, which emits massive amounts of greenhouse gases. About 48% of hydrogen demand is met by natural gas, 30% by the petroleum industry, 18% by coal gasification, 3.9% by electrolysis, and the remaining 0.1% by other processes. Scientists are still looking for large-scale renewable hydrogen production sources. Currently, 96% of hydrogen is produced through the steam methane reforming (SMR) process, which uses fossil natural gas (primarily methane [CH<sub>4</sub>]) as a feedstock. This process is energy-intensive, necessitating high temperatures for the reforming process, and it emits a significant amount of CO<sub>2</sub> (CO<sub>2</sub>). Both CH<sub>4</sub> and CO<sub>2</sub> are greenhouse gases (GHGs) that must be tracked to perform an environmental assessment of the hydrogen life cycle. As a result of high GHG emissions, this process is far from sustainable. It has a global warming potential of approximately 13.7 kgCO<sub>2</sub>equivalent per kilogram net hydrogen (Muradov NZ, 2005;).CO<sub>2</sub>is a by-product of the main reactions involved, so some of these emissions are unavoidable. Other thermo-chemical conversion technologies allow hydrogen production through different pathways starting from coal, oil, biomass-derived fuels, biomass and wastes Nicolas-LyMBERopoulos. However, all these approaches are not GHG-free. The Power-to-Gas concept, based on water electrolysis utilizing electricity derived from renewable energies (wind, solar, geothermal, hydro) is the most environmentally friendly approach. This attractive method for hydrogen generation, based on a mature technology, currently accounts for only 4% of the hydrogen production but its large expansion is expected in the next few years: a share of 22% is predicted for 2050. An uncompressed state of gas the

energy content and density of hydrogen are quite low. In other words, there are some technical issues with the widespread usage of this substance as fuel. The most common method of storing hydrogen is as a compressed gas in tanks, though there are other methods as well. In this case, high pressure levels are preferable. However, construction constraints, cost of production and maintenance and operational safety of the tanks and compressors limit the extent to which the gas can be pressurized. The energy content of hydrogen in liquid form is much higher than in compressed gas form. The true advantage of storing liquefied hydrogen is its high density at low pressure. These characteristics enable compact and light-weight storage as well as efficient delivery options Carpetis, 1982. Hydrogen liquefies at temperatures below  $-250\text{ }^{\circ}\text{C}$  and that is why the liquefying process of hydrogen adds an excess 30% to the production power demand. Furthermore, using gas liquefiers adds sophistication to the production system. As a result, liquid hydrogen is 4-5 times more expensive than compressed gas hydrogen. Storing hydrogen in high pressure vessels is currently the method of choice for most of the vehicle manufacturers due to the efficiency, design, cost, and environmental advantages. Gas compression is recognized as the most time and energy efficient method for providing a convenient source for consumers. The main disadvantage of this method is its low storage density. As a result, many experts believe that hydrogen storage in high-pressure cylinders is unlikely towards becoming popular in the future Zhou, 2005.

# STATE OF ART REVIEWS

The authors Ramin Moradi, Katrina M. Groth. report on their paper (Hydrogen storage and delivery: Review of the state-of-the-art technologies and risk and reliability analysis). Hydrogen is becoming an increasingly viable clean and green option for transportation and energy storage among all introduced green alternatives. In this literature review states the current state of the art in risk and reliability analysis for hydrogen technologies, and identify research needs and gaps relevant to ensuring continued safe and reliable operation The emphasis is on two critical aspects of the hydrogen economy: hydrogen delivery and hydrogen storage. Hydrogen storage in a variety of capacities and operating conditions is required to meet consumer demand, and hydrogen delivery is critical to making this green energy carrier widely available. In comparison to fossil fuels, hydrogen has a low energy density by volume (9.9MJ/m<sup>3</sup>) LHV (Lower Heating Value) As a result, extremely large storage vessels may be required. To avoid this, at least one of the three following features must be present to store an adequate amount of hydrogen: high storage pressure, low storage temperature, or the use of a material that attracts many hydrogen molecules. In physical based hydrogen storing as compressed gas, cold/cryo compressed, and liquid storage. Material based has chemical & physical sorption. Especially in chemical sorption, metal hydrides play a promising role in storing large-scale hydrogen productions with low cost and weight, and operating temperature and it is necessary to discuss safety aspects of hydrogen storage and delivery. In addition, they review the main existing safety and reliability challenges in hydrogen systems. List of factors that can negatively impact reliability of hydrogen systems.

Authors Joakim Andersson, Stefan Gronkvist describes in their report that the storage of hydrogen is challenging, even though it is the lightest material with very low density for example 1kg of hydrogen gas occupies over 11m<sup>3</sup> at room temperature and atmospheric pressure, thus hydrogen storage is economically viable, and it needs more density storage. Hence the large-scale storage of hydrogen plays a crucial role in the potential future hydrogen economy. Although salt caverns are already used to preserve the gaseous hydrogen as storage it is not flexible for every geographical condition therefore, we need more methods to store it. The other physical storage liquid hydrogen, its primary concern

for the storage of liquid hydrogen is the energy-intensive liquefaction process. After that hydrogen has been liquified it is essential that it can be stored so that evaporation is minimized heat transfer through the tank's walls. Generally, liquid hydrogen has another aspect that must consider in hydrogen from metal hydrides, can be achieved in two ways heating (thermolysis) or reaction with water(hydrolysis) these approaches are radically different. although a vast array of metal hydrides has been developed and investigated for thermolysis based storage, few have been applied for hydrolysis with any significant success. The most notable and promising metal hydrides for hydrolysis is sodium borohydride. Most of the metallic elements can form binary compounds with hydrogen i.e., elemental hydrides most of them are not suitable for storing hydrogen storage vessels are double walled with a high vacuum applied between the walls.in this literature review paper states. various options for storing the hydrogen on a large scale and reviewed and compared the various aspects according to thermodynamics and engineering. the liquid hydrogen, methanol, ammonia and dibenzyl toluene had certain storage technologies for different application in these we can observe great benefits in terms of storage density, cost of storage and safety. High densities storage technologies are associated with high electricity for the hydrogen release process. If hydrogen produced via electrolysis and stored during a time of low electricity prices in an industrial setting, these are variable costs that may be tolerable.

In every system has its own characteristics to attain its properties, in the same way this hydrogen energy-based system has its properties to get a promising result. Authors Furat Dawood, Martin Anda, G.M. Shafiullah describes a production model so their report (an overview of hydrogen production) they stated that the hydrogen system comprises 4 different stages production, storage, safety, and utilization. In this literature authors discussed about the hydrogen production pathways and associated technology. These production pathways have been characterized by 4 main categories which are electrolysis, photolysis, biolysis and thermolysis each one has prominent characteristics and efficiency. Researchers are considered in the hydrogen production some of the energy additives to the process as catalytic energy to increase the process efficiency. Moreover, few second energy types like radiation, plasma, and biological energy amongst the main energy categories for hydrogen production. many pieces of works of literature are considered different

production pathways. Hence the authors are introduced an innovative model to define the category of production pathways. Another aspect that we need to consider is hydrogen cleanness they decried with, 3 main colour code: green, blue, and grey, the green hydrogen refers to a 100% renewable energy source for hydrogen production. Grey hydrogen is a polluting type of hydrogen. Blue hydrogen defines the Carbon Capture and Storage (CCS) inclusive in the grey hydrogen. But this current colour model fails to determine how clean is that hydrogen because it fails to determine how much greenhouse gas emitted during the production process subsystems or from the life cycle of equipment used. The authors of this paper have identified the uncertainty and inaccurate colour coding precisely describing the cleanness of any produced hydrogen. Moreover, the current superficial colour coding model fails to describe how deep is that cleanness assessment. Therefore, an innovative colour spectrum concept in a colour coding model has been introduced to resolve this imprecise issue in the current colour coding model.

From the report (Hybrid Hydrogen Home Storage for Decentralized Energy Autonomy) the authors Kevin Knosala, Leander Kotzur, Fritz T.C. Röben, Peter Stenzel, Ludger Blum, Martin Robinius, Detlef Stolten stated the around 40% of global energy consumption is considered for the building sectors for heating, cooling, ventilation, hot water, and lighting. In further year years charging stations for the battery electric vehicles placed on buildings will significantly add to building energy demand. Therefore, measures for sustainable development and the reduction of greenhouse gases are highly relevant to the sector. It has been admitted that increased self-consumption is beneficial in the context of large shares of distributed renewable generation and falling feed-in tariffs and therefore public and academic interest in – at least partly – “leaving the grid” or “living off-grid” is growing. In this paper, the authors present a building level techno-economic study of an energy self-sufficient single building for a family along with that authors are shows how a heat-integrated hydrogen storage unit equipped with a liquid organic hydrogen carrier (LOHC) storage system and reversible solid oxide cells (RSOCS) enables cost-effective, self-sufficient residential buildings with only rooftop PV installed. For residential building, hydrogen application is Fuel cell– combined heat and power systems for residential buildings based on PEM fuel cells and solid oxide (SO) fuel cells are state-of-the- art and commercially available from different suppliers. They process natural gas (from the gas grid) into hydrogen in fuel

processor units based on steam or auto-thermal reforming, operating at temperatures above 800 °C. hydrogen storage with pressure vessels and metal hydrides storage systems are already commercially available for residential applications. However recent technological developments are improving its efficiency handling and space requirements of hydrogen storage units. Hydrogen absorbing compounds such as metal hydrides allow for the compression and storage of hydrogen without the use of moving components another storage technology uses LOHCs as a carrier fluid that can be enriched with hydrogen in a catalytic, exothermic, hydrogenation reaction. Although both technologies allow for the efficient integration of residential heating and cooling with the storage process, this study focuses on LOHCs as an alternative storage solution. Most applications of LOHC storage stores solutions utilize dibenzyltholuene(DBT) as anon flammable carrier fluid DBT can be enriched in the hydrogenation process to a capacity of 6.4 wt.% hydrogens (1.75k WhH<sub>2</sub>/kg DPT) and easily recovered after dehydrogenation.

Authors (N.A.A. Rusman, M. Dahari) describes in their report( A Review on the Current Progress of Metal Hydrides Material for Solid-State Hydrogen Storage Applications) that Hydrogen fuels can be preserved in various forms like liquid gasses or solid these are the key priorities to develop hydrogen storage systems that are safe and cost-effective and eco-friendly, and hydrogen has high energy densities current technology are used for hydrogen storage includes high-pressure compression of about 70mpa, liquefaction at cryogenic temperatures and adsorption into solid-state compounds. Among the three hydrogen storage technologies, solid state compounds appear to best the most flexible solution since it a safer and more convenient method compared to high-pressure compression and liquefaction technologies. In this review, paper authors are stated that the latest technological developments are in metal hydrides because of their potential chemical compounds for solid hydrological storage and in fact, many studies are carried out that to synthesize low-cost metal hydrides with low adsorption/desorption temperatures high gravimeter, volumetric hydrogen stores good resistance to oxidation and good reversibility and cyclic ability fast kinetics and reactivity and moderate thermodynamic stability in general, these studies describes that the adsorption/desorption properties of hydrogen might be improved by the addition of catalysts into the metal hydrides, alloying and Nano structuring. metal-nitride-based systems (simply known as metal-N-H systems) composed of

amide and binary hydrides have gained significance as candidate materials for on-board hydrogen storage applications owing to their capability in releasing hydrogen in appropriate conditions. It shall be noted that the binary hydrides used in these systems are compounds formed between hydrogen and an active metal from the Periodic Table of Elements, which is typically an alkali metal or alkaline earth metal. Chemical hydrides can exist in either solid or liquid state, and can be heated directly, passed through a catalyst containing reactor, or combined with water (i.e. hydrolysis) or other reactants to produce hydrogen. Unlike reversible complex hydrides, chemical hydrides are irreversible and generally intended as “one-way” single-use fuels. Besides, the left-over by-product must be removed from the vehicle for offboard regeneration. Among chemical hydrides, ammonia borane (AB) is reported as a potential material for hydrogen storage due to its high hydrogen capacity. Mg based alloys have high hydrogen storage capacities up to 7.6 wt.% as well as good kinetics. More importantly, Mg is inexpensive, and it is available in abundance within the Earth's crust. Mg based alloys also have excellent heat resistivity, good recyclability, and they can form solid solutions and compounds with other elements in their equilibrium states.

Authors Riccardo Amirante, Egidio Cassone, Elia Distaso, Paolo Tamburrano stated in their report (overview on recent developments in energy storage: Mechanical, electrochemical and hydrogen technologies) about 95% of the worldwide hydrogen production involves non-renewable resources. Hydrogen is extracted from natural gas utilizing an endothermic process at high temperatures (800–1000 °C) in presence of a catalyst. In such a technique, called Steam Reforming, natural gas acts both as raw material for hydrogen production and as fuel since it is burned to increase the temperature of the process. A natural gas amount comprised of between 3 and 20% is used to keep alive the reaction. For each ton of hydrogen produced, 2.5 tons of CO<sub>2</sub> are released. Hydrogen extraction from coal has been widely investigated. Such a process has a heavier environmental impact in comparison to the extraction from NG (5 Tons of CO<sub>2</sub> are released for each ton of H<sub>2</sub> produced). To contain the environmental impact, either the Pressure Swing Adsorption (PSA) or the Carbon Capture System (CCS) techniques have been developed. CCS enabled plants to have higher (22%) Hydrogen costs. To reduce overall H<sub>2</sub> cost, electricity co-production (by gasified coal) has been considered. In relatively new technique hydrogen is produced starting from gasoline and diesel fuels. This process, called Partial Dehydrogenation (PDH),

leads to high purity hydrogen (up to 99%) and allows the recovery of the original fuels. The reaction acts in presence of a catalyst, like Platinum, at 400 °C and 0.1 MPa. About 1800 NI/h and 3500 NI/h of Hydrogen for a kilogram of catalyst mass are produced respectively from gasoline and diesel. The catalyst life is about 300 h for gasoline and 29 h for diesel. Hydrogen productions by using water electrolysis and biomass amount to, respectively, 4% and 1% of the total production. In water electrolysis electricity is employed to break the water molecule bonds, generating oxygen and hydrogen atoms. The production rate is higher in presence of an electrolyte, commonly KOH (which is reusable). The efficiency of this kind of process is high (up to 75%), and the purity of the produced hydrogen can reach 99.9%. However, its costs are high because of the electricity consumption (about 4.49 kW h/m<sup>3</sup> are required) and the expensive coated electrodes (Platinum) required in the process. The introduction of a Cobalt phosphate catalyst allowed to decrease the costs.

Authors Cevahir Tarhan, Mehmet Ali Çil, describes in their study about on hydrogen, a clean hydrogen for the future & hydrogen storage methods. Hydrogen can be pressurized in suitable structures up to 700 bar and stored in the form of gas in cylinders, containers, underground cavities. Zheng et al. In their study stated that more than 80% of hydrogen refuelling stations in the world used the compressed gas storage method for 2010. Compressed gas storage containers are made of steel, aluminium and carbon fibre reinforced plastic composite materials The low-pressure liquid hydrogen storage system has a low cost. While liquid hydrogen can be stored at -253°C, pressurized gas hydrogen can be stored at ambient temperature. In the liquid hydrogen storage method, the boiling point of hydrogen is low. Therefore, special containers with insulation systems are required to protect the hydrogen efficiency. Borohydrides have high hydrogen storage capacity and can dissolve in water. LiBH<sub>4</sub> (lithium borohydride), Mg (BH<sub>4</sub>)<sub>2</sub> (magnesium borohydride), NaBH<sub>4</sub> (sodium borohydride) and Ca (BH<sub>4</sub>)<sub>2</sub> (calcium borohydride) are hydrides with high hydrogen storage densities among metal borohydrides. LiBH<sub>4</sub> has a high hydrogen storage capacity of 18.5 wt.%. LiBH<sub>4</sub> does not react reversibly under high decomposition temperature and practical conditions, it is not suitable for the hydrogen storage process as such. However, with the addition of silicon oxide (SiO<sub>2</sub>) catalyst, its thermodynamic properties have improved. Hydrogen storage efficiency has increased by adding Ti and Mg (Magnesium) as catalysts. Zinc borohydrides (Zn (BH<sub>4</sub>)<sub>2</sub>) have a hydrogen storage capacity of 8.4 wt.%.

NaBH<sub>4</sub> has a high hydrogen storage capacity of 10.8 wt.%. It requires a high degree of decomposition temperature, so it is not preferred for hydrogen storage.

In their paper (Hydrogen and ethanol: Production, storage, and transportation) authors describes ethanol as a promising and sustainable feedstock to hydrogen production should be based on a premise the ethanol itself is renewable and sustainable; and thus bioethanol, the ethanol derived from biomass, is the 'ethanol' in the future. The production of bioethanol comes from the conversion of glucose from renewable biomass materials. From the perspective of GHG emissions, most emissions come from the agricultural stage in which the types of machinery on growing and transporting crops released amounts of emissions for the combustion of fossil fuels in the industrial stage, sugar beet and corn still rely on fossil fuels as an energy source, but sugarcane could burn the residues to obtain energy for converting sugarcane into ethanol. From the perspective of energy transmission, the higher productivity makes sugarcane could be continuously harvested more times in the same cultivated area, 11 which ensures sugarcane requires less energy in the agricultural stage; meanwhile, in the industrial stage, compared to corn that requires more energy to convert starch and sucrose into glucose, the energy demand during the bioethanol production from sugarcane is further reduced. Therefore, sugarcane could be more sustainable for the first-generation bioethanol due to the reduced GHG emissions which far exceeded the net savings in emissions released by straw burning and the lower energy demand. A bulk application of them to bioethanol production is little sustainable in the current; however, using the lignocellulosic materials from the residues and non-grain crops (even municipal wastes) are taken as the feedstock to (second-generation) bioethanol could alleviate the problem. Albeit the chemical properties of bioethanol are different from ethanol for the existence of impurities (like heavy alcohols, organic acids, aldehydes, and esters), it does not make distinct differences in the storage. Under standard conditions (the environment for the most storage), (bio-)ethanol is an odorous liquid with slight toxicity. Due to the hydroxyl groups and short carbon chains, (bio-) ethanol is easier to combine with hydrogen bonds than other similar organic compounds, which leads to higher viscosity and weaker polarity. Ethanol is high volatile to easily form the azeotrope with slight exothermic phenomena into the water and most organic solvents, and it can easily be burned into the air within an invisible blue flame. Aluminium, a promising material satisfied by the trend about

lightweight, is commonly used for (bio-)ethanol storage, but the problem of corrosive pitting due to the electrical coupling of two different metals for the change in electrical conductivity, occurs and rapidly spreads across the surface when the Ni-surface coating of the storage container has fallen off makes it has hidden risk of leakage. the solid-state storage of hydrogen can be divided into alloy hydrogen storage, coordination hydride storage and carbonaceous adsorption storage. Such storage manner mainly relies on electrochemistry, different electrical potentials combined with different materials capture H atoms at the interface of an electrode, and the diffusion of H atoms on the surface of lattice realizes the storage of hydrogen in solid form.

Authors Ahmed M. Elberry, Jagruti Thakur, Annukka Santasalo-Aarnio, Martti Larmi reported (Large-scale compressed hydrogen storage as part of renewable electricity storage systems) that there are two key components for the compressed hydrogen gas storage system: the storage means and also the compressor used for reaching the storage pressure, because of properties of materials, investment costs, and issues of safety, storing large quantities of compressed hydrogen gas at pressures exceeding 200 bar have many hindrances, which may be tackled with research and technology. Pressure vessels are commonly employed in industrial, automotive, commercial, and aerospace applications, ranging from tiny bottles to massive storage tanks. Their design, manufacture, use, and maintenance are regulated by different standards, with well-defined safety guidelines. Some metals are subject to embrittlement caused by hydrogen adsorption and dissociation at surfaces of these materials, which reduce the strength and sturdiness of the fabric. Suitable materials that are mostly used for the pressure cylinders are austenitic stainless steel, aluminium, and copper alloys, which are known for his or her resistance and opposition to the effects of hydrogen at ambient temperatures. Hydrogen gas is sometimes compressed to pressure values ranging from 100 and up to 825 bars for large-scale storage. Hence, materials choices are crucial, considering such high-pressure requirements. Typically, hydrogen storage systems comprise different components like valves, sensors, storage containers, etc. These components are manufactured from different materials which will be categorized into metallic, polymer, and composites parts. hydrogen embrittlement (HE) is that the main issue for metal components. The industry and academia have put plenty of effort into tackling the (HE) issues by examining the HE mechanisms well, manufacturing development of the alloys,

component assembling, and assessing the materials' mechanical testing. Gas permeation may be a common phenomenon for gasses in direct contact with polymers. It results from the absorption, diffusion, and desorption<sup>4</sup> of gas molecules through complex physical and chemical processes. This is predicated on the unification of two different materials with a range of various compositions, of which fibre reinforced composites are the foremost common for hydrogen storage tanks. Seamless hydrogen storage vessels are made up of high strength seamless 7 tubes, and that they are commonly utilized in hydrogen fuel stations. The inner diameter of this type of vessel is proscribed to 6.1 m and their maximum overall length rely on the most important pipe length (usually  $\leq 12\text{m}$ ) or the available pipe weight. Thus, seamless hydrogen storage vessels have a limited volume. Nevertheless, for storing large quantities of hydrogen, seamless vessels are often employed in multivessel assemblies, which are denoted as cascade storage, where the seamless vessels are assembled through valves and interconnection piping manifolds, resulting in more hydrogen leak points. The multifunctional steel layered hydrogen storage vessel (MSLV) was developed.

In their report (Hydrogen: A brief overview on its sources, production, and environmental impact) authors Sema, Z. Baykara describes, hydrogen plays a vital role in industrial processes mostly as feedstocks. Currently, fossil fuels account for the main sources for hydrogen production, chemical grade hydrogen is possible by water electrolysis. Approximately 95% of the hydrogen produced is used captive. The utilization of hydrogen as a fuel grows and as the global temperature has risen, it will be necessary to produce a large scale using diminishing amounts of fossil resources. Several studies are available for this hydrogen production, methods are available from fossil fuels especially from methane, natural gas, coal from biomass water: compounds like metal hydrides and  $\text{H}_2\text{S}$  and biological sources. Fossil based hydrogen production method is commercialized mature technologies established at higher efficiency and low-cost products. Natural gas is mostly methane and SMR (steam reforming of methane) process widely used at an efficiency range 65-75%. Another process is partial oxidation of natural gas which has low efficiency of 56%. For coal gasification, the Koppers-totzek process is the leading technology producing capacity is 97% pure hydrogen might be possible with fossil-based system through an application of carbon sequestration and solar thermal processes. From biomass & coal hydrogen can be produced

via pyrolysis/gasification processes, even though its calorific value is low compared to coal. Thermal chemical hydrogen production from water is possible through single or multi step processes above 2000K direct thermal decomposition of water is possible. The extent of single extent water dissociation varies directly with temperature. Lowering pressure has a suitable effect in the process. Hydrogen can be produced at lower temperatures through thermochemical cycles where dissociation of water into hydrogen and oxygen is possible through two or more successive reaction steps involving redox materials such as sulfur and some metal oxides. Sulfur-based cycles can be operated at lower temperatures ( $T < 1200\text{ K}$ ) relative to metal oxide cycles. Nearly 2000-3000 thermochemical cycles were studied but 20-30 are suitable for large scale hydrogen production. Hydrogen production is possible through pyrolysis and hydrolysis of metal hydrides. Lithium and magnesium hydride ( $\text{LiH}$ ,  $\text{MgH}_2$ ), lithium and sodium borohydride ( $\text{LiBH}_4$ ,  $\text{NaBH}_4$ ), lithium and sodium aluminium hydride ( $\text{LiAlH}_4$ ,  $\text{NaAlH}_4$ ) are often considered. Most known potential source in hydrogen production, hydrogen sulfide technology which involves thermal, thermochemical, electrochemical, photochemical and plasma chemical methods are at different levels of maturity. Fossil based centralized hydrogen production methods have commercial, mature technology and established feedstock infrastructure. Although carbon sequestration helps extend the utilization of fossil-based technology, large scale land damage caused due to extraction of fossil fuels and risk of oil spills in oceans during transportation of petroleum by tankers remain to be dealt with. Water electrolysis has well-developed technology and uses electricity from the grid and therefore the existing infrastructure.

Authors Meiling Yue, Hugo Lambert, Elodie Pahon, Robin Roche, Samir Jemei, Daniel Hissel in their report (Hydrogen energy systems: A critical review of technologies, applications, trends, and challenges) describes the prospects of hydrogen penetration and decarbonization are stated, however, key hydrogen technologies and the current progress of developing hydrogen technologies have not been fully addressed. In some review papers detailing about the challenges in terms of social aspect & technologies evolution are not discussed. Authors are devoting to treating the hydrogen powered energy systems as a whole and analysing the attention of hydrogen in the energy systems. Hydrogen has four principles hydrogen integrated applications including energy storage, power to gas

applications, co and tri generation and transportation are introduced and interpreted by remarkable projects. Current status on hydrogen applications is analysed statistically in terms of cost, consumption, efficiency, and durability, which justifies the need of further progress in the related technologies. Some Hydrogen technologies are typically used in hydrogen power systems introduced along with electrolytic hydrogen production, hydrogen re-electrification using fuel cell, hydrogen production methods like steam reforming, coal gasification and electrolysis of water are majorly used today for industrial hydrogen production. Today, with the declining cost for renewable electricity, there is a growing interest in water electrolytic hydrogen production, which consumes electricity to extract hydrogen from water while causing no carbon by-products like CO<sub>2</sub>. In water electrolysis cell, two electrodes are come up with the electrolyte solution and are connected to the power supply to conduct current. When a sufficiently high voltage is applied between the electrodes, water is decomposed to produce hydrogen on the cathode and oxygen on the anode. The addition of an electrolyte raises the conductivity of the water, which facilitates the continuous flow of electricity. Acids and solid polymer electrolytes are commonly used in water electrolysis and use different ions as charge carriers the reactions of water electrolysis at the electrodes with different charge carriers may be different, but the overall reaction is always the same. Hydrogen can first be re- electrified through combustion. Similar to internal combustion engines running on gasoline, some combustion engines or 15 turbines can also run directly on hydrogen. However, hydrogen combustion engines are less efficient than gasoline combustion engines, with a thermodynamic efficiency of around 20%- 25%. This is because hydrogen has relatively a low volumetric energy density. Besides, when combusting hydrogen, nitrogen oxides are emitted while no CO<sub>2</sub> is released.

In their report (Magnesium based materials for hydrogen-based energy storage: Past, present, and future) authors M. Baricco, N. Bourgeois, C.E. Buckley, J.M. Bellosta von Colbe, J.- C. Crivello, F. Cuevas, R.V. Denys, M. Dornhei stated that the Magnesium started an investigated as a means to store the hydrogen around 50 year ago, since it has the advantages of fulfilling the natural targets of (1) high abundance (2% of earth surface composition and virtually unlimited in sea water), (2) non toxicity and (3) relative safety of operation as compared to other light elements and their hydrides that quickly and exothermically oxidize in air. Moreover, magnesium is produced by a well- established

technology and its raw materials cost is relatively low. This, as well as its high volumetric (0.11 kg H/l) and gravimetric (7.6 mass% H) capacities, places magnesium as a feasible material to store hydrogen and it has attracted huge attention during recent year. international magnesium group experts contribute to IEA recently they published a task about hydrogen based energy storage in those 2 papers presenting activities of the group focused on Mg based compound's for the hydrogen and energy storage hydrogen storage materials for the future.  $\alpha$ magnesium dihydride ( $MgH_2$ ) can be synthesized directly from magnesium metal and hydrogen gas as a product of reversible interaction and by chemical methods, starting from magnesium organic compounds. In contrast to the chemically synthesized  $MgH_2$  being a very active material which self-ignites when exposed to air and intensively reacts with water, magnesium hydride obtained by interaction of metallic Mg with  $H_2$  gas is relatively inert and safe during handling.  $MgH_2$  is a stoichiometric hydride having a mixed ionic-covalent type of chemical. hydrogen sorption kinetics in bulk coarse-grain Mg are extremely slow. This results from kinetic limitations on both dissociation of hydrogen molecules at the Mg surface and diffusion of hydrogen atoms in bulk Mg. Surface limitations can be overcome by decoration of the metal surface with catalysts. The use of  $Nb_2O_5$  as additive is a paradigmatic example of this approach. Bulk limitations are attributed to the formation of a blocking hydride shell over the Mg metal. Indeed, the diffusion coefficient of hydrogen in magnesium hydride is very low. The dehydrogenation of Mg-based hydrides requires rather a high temperature, even above  $300^\circ C$ , 16 which must be overcome for practical applications. To enhance the hydrogen absorption/desorption rate and reduce the reaction temperature of Mg based hydrogen storage alloys, different improving strategies, such as alloying, nanosizing, nanoconfinement, catalysing and compositing, have been applied to tune the dehydriding/hydridding thermodynamics and kinetics. It should, however, be noted that the beneficial effect of tuning a certain other service characteristic. Thus, tailoring is usually aimed at improving one specific property without destroying other features relevant for hydrogen storage.

The report from authors Mengjiao Wang, Guizhou Wang, Zhenxin Sun, Yukui Zhang, Dong xu. describes a review on renewable energy-based hydrogen production process sustainable energy innovation. A photovoltaic (PV) water electrolysis system comprises PV panels, DC bus bar, AC grid, accumulator battery set, electrolyzer, and hydrogen storage canisters. This

system can compensate for low reliability caused by intermittent instability of solar power generation and can provide stable and reliable power within a certain range. water thermolysis based on solar energy involves using solar concentrators to directly collect solar energy to heat water to 2500 K, at which temperature it decomposes into H<sub>2</sub> and O<sub>2</sub>. However, there are problems associated with this approach; the primary ones include achieving high temperature using a solar concentrator and effective separation of H<sub>2</sub> and O<sub>2</sub> at high temperature. To address these problems, Kogan proposed the use of a catalyst in water, which could allow for the decomposition of water in multiple steps, while considerably reducing the required heating temperature. In the nuclear-assisted hydrogen production process, the high heat provided by the reactor is used for thermolysis of water; to achieve this with a fourth-generation reactor, processes like I-S cycle, Cu-Cl cycle, Ca-Br cycle, or U-C cycle are used.

# HYDROGEN

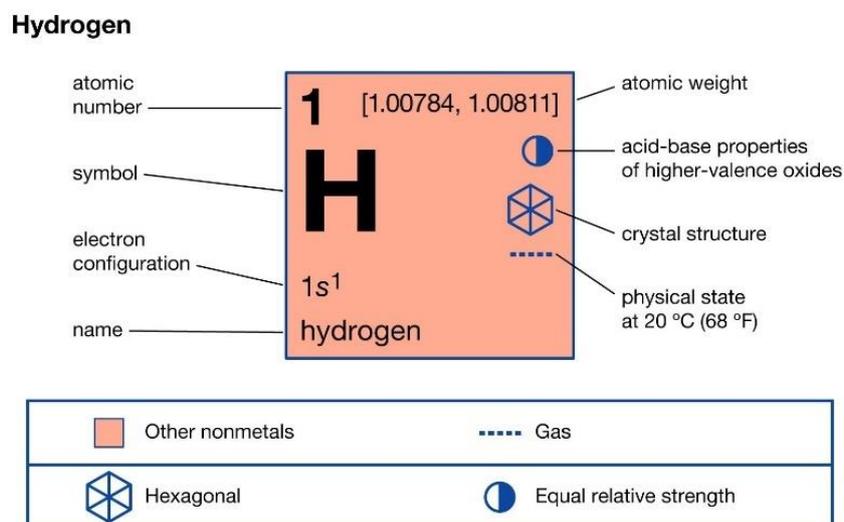


Figure 1 chemical properties of hydrogen

Source: <https://www.britannica.com/science/hydrogen>

Hydrogen (H), the simplest member of the chemical element family, is a colourless, odourless, tasteless, flammable gaseous substance. The hydrogen atom has a nucleus that consists of a proton with one unit of positive electrical charge and an electron with one unit of negative electrical charge. Under normal circumstances, hydrogen gas is a loose aggregation of hydrogen molecules, each of which contains a pair of atoms, a diatomic molecule, H<sub>2</sub>. The earliest known significant chemical property of hydrogen is that it burns with oxygen to form water, H<sub>2</sub>O; in fact, the name hydrogen is derived from greek words that mean "maker of water." Although hydrogen is the most abundant element in the universe (three times more abundant than helium, the next most abundant element), it accounts for only about 0.14 percent of Earth's crust by weight. It does, however, occur in massive amounts as part of the water in oceans, ice caps, rivers, lakes, and the atmosphere. Hydrogen is found in all animal and vegetable tissue, as well as in petroleum, as a component of numerous carbon compounds. Even though it is commonly stated that there are more known carbon compounds than any other element, the truth is that because hydrogen is present in almost all carbon compounds and forms a plethora of compounds with all other elements (except some of the noble gases). There are three known isotopes of

hydrogen. The mass numbers of hydrogen isotopes are 1, 2, and 3, with the mass 1 isotope being the most abundant (symbol H, or  $^1\text{H}$ ) but also known as protium. The mass 2 isotope, with a nucleus of one proton and one neutron and dubbed deuterium, or heavy hydrogen  $^2\text{H}$  (symbol D, or  $^2\text{H}$ ), accounts for 0.0156 percent of the ordinary hydrogen mixture. Tritium (symbol T, or  $^3\text{H}$ ), the mass 3 isotope, has one proton and two neutrons in each nucleus and accounts for about  $10^{-15}$  to  $10^{-16}$  percent of hydrogen.

**Table 1: properties of hydrogen (R.B.C. Rivkin, 2015) (Blumenthal, 2013)**

<b>Properties</b>	<b>SI Units</b>
Discovery date/by/Chemical formula	1766/Henry Cavendish/ $\text{H}_2$
Isotopes	$^1\text{H}$ (99.98%), $^2\text{H}$ , $^3\text{H}$ ,
	( $^4\text{H}$ – $^7\text{H}$ Unstable)
Equivalences; Hydrogen solid, liquid and Gas at Pressure = 981 mbar and Temperature = 20 °C	1 kg = 14,104 l = 12,126 m <sup>3</sup>
Molecular weight	1.00794
Vapor pressure at (–252.8 °C)	101.283 kPa
Density of the gas at boiling point and 1 atm	1.331 kg/m <sup>3</sup>
Specific gravity of the gas at 0 °C and 1 atm (air = 1)	0.0696
Specific volume of the gas at 21.1 °C and 1 atm	11.99 m <sup>3</sup> /kg
Specific gravity of the liquid at boiling point and 1 atm	0.0710
Density of the liquid at boiling point and 1 atm	67.76 kg/m <sup>3</sup>
Boiling point at (101.283 kPa)	–252.8 °C

<b>Properties</b>	<b>SI Units</b>
Freezing/Melting point at (101.283 kPa)	-259.2 °C
Critical temperature	-239.9 °C
Critical pressure	1296.212 kPa, abs
Critical density	30.12 kg/m <sup>3</sup>
Triple point	-259.3 °C at 7.042 kPa, abs
Latent heat of fusion at the triple point	58.09 kJ/kg
Latent heat of vaporization at boiling point	445.6 kJ/kg
Solubility in water vol/vol at 15.6 °C	0.019
Dilute gas viscosity at 26 °C (299 K)	$9 \times 10^{-6}$ Pa s
Molecular diffusivity in air	$6.1 \times 10^{-5}$ m <sup>2</sup> /s
C <sub>p</sub>	14.34 kJ/(kg) (°C)
C <sub>v</sub>	10.12 kJ/(kg) (°C)
Ratio of specific heats (C <sub>p</sub> /C <sub>v</sub> )	1.42
Lower heating value, weight basis	120 MJ/kg
Higher heating value, weight basis	141.8 MJ/kg
Lower heating value, volume basis at 1 atm	11 MJ/m <sup>3</sup>
Higher heating value, volume basis at 1 atm	13 MJ/m <sup>3</sup>
Stoichiometric air-to-fuel ratio at 27 °C and 1 atm	34.2 kg/kg

# HYDROGEN SAFETY

The safe use of any fuel focuses on avoiding situations in which the three combustion factors are present: ignition source (spark or heat), oxidant (air), and fuel. We can design fuel systems with appropriate engineering controls and establish guidelines to enable the safe handling and use of a fuel if we have a thorough understanding of its properties. Hydrogen's combustion properties, such as its wide range of flammability, low minimum ignition energy, and high burning velocity, make it an excellent alternative fuel, there are a number of safety concerns associated with its use and storage. As shown in Table 2, hydrogen has a very low boiling point, density, and ignition temperature of 585 °C, but a high diffusion coefficient in air. Hydrogen also has a low ignition energy of 0.017 MJ but a high latent heat of combustion of 141.6 MJ/kg. Hydrogen detonation can occur at volumetric concentration ratios of hydrogen to air ranging from 4% to 75%. Hydrogen is a substance that is extremely sensitive to explosion.

Although its combustion efficiency is truly exceptional and is welcomed as a future fuel of choice, it inevitably poses several safety challenges in production, storage, and transportation. When hydrogen reacts with oxygen, it produces water as its only by-product, either explosively in combustion engines or quietly in fuel cells. Hydrogen is not found on the planet. It is, however, available in the form of oxygen and carbon chemical compounds. Water, for example, contains hydrogen; fossil hydrocarbons such as coal, petroleum, and natural gas; and biomass such as carbohydrates, protein, and cellulose. When compared to conventional fuels such as methane (natural gas), liquefied petroleum gases (LPG), and liquid fuels such as gasoline, hydrogen has both similarities and differences. See below table 2. The technical and economic challenges of implementing a "hydrogen economy" require a solution to the fundamental problem of renewable energy production, which is not always available, expensive, and fraught with problems of capture and conversion issues. Many issues must be addressed before hydrogen can be used as a universal energy medium, including difficulties with hydrogen production, transportation, storage, distribution, and end use. As previously stated, its large oxygen mixture range of ignition and detonation demonstrates how vulnerable its storage is. The auto-ignition temperature of a fuel is one of the most essential safety concerns while handling it. This

phrase refers to the temperature at which a substance will ignite in the absence of any external ignition sources.

The auto-ignition temperature is known to be negatively related to the pressure or oxygen content of the surrounding environment. However, due to hydrogen's flammability range, its auto ignition temperature is expected to stay constant at greater pressures or oxygen concentrations. On the other hand, hydrogen has the greatest auto-ignition temperature of any fuel.

Furthermore, when exposed to hydrogen, some metals can become brittle, so selecting appropriate materials is critical in the design of safe hydrogen systems. Training in safe hydrogen handling practices, in addition to designing safety features into hydrogen systems, is a critical component for ensuring the safe use of hydrogen. As additional hydrogen demonstrations take place, the safety record of hydrogen will improve, raising confidence that hydrogen can be as safe as conventional fuels. Moreover, some metals can become brittle when exposed to hydrogen, therefore selecting appropriate materials is crucial in the design of safe hydrogen systems. In addition to designing safety aspects into hydrogen systems, training in safe hydrogen handling procedures is a vital component for guaranteeing the safe use of hydrogen. Tank leak testing, garage leak simulations, and hydrogen tank drop tests further demonstrate that hydrogen can be safely generated, stored, and supplied.

**Table 2 properties of hydrogen related to safety (guptha, 2008)**

	<b>H<sub>2</sub></b>	<b>CH<sub>4</sub></b>	<b>Gasoline</b>
Diffusion	The rapid dispersion rate of H <sub>2</sub> in air is its greatest safety asset		
Buoyancy	H <sub>2</sub> rises more rapidly (14 times lighter than air → moves fast upward → drop in ignition hazards)		$P_{\text{gas}} = 5.82 \text{ kg/m}^3$
Flammability range	4–75%	4.3–15 vol%	1.4–7.6 vol%
Ignition energy (@ $\Phi = 1$ )	0.02 mJ	0.28 mJ	0.24 mJ
Detonation level	H <sub>2</sub> is detonable over wide range of concentration when confined		
Flame velocity		0.38 m/s	0.42 m/s
	It is difficult to arrest H <sub>2</sub> flames. Explosion confinement is more difficult. In detonations velocity is 30 times faster		
Flame temperature @ $\Phi = 1$		1917 °C	2307 °C
Limiting O <sub>2</sub> index	No flame propagation if mixture contains <5% by volume O <sub>2</sub>		
Liquefied H <sub>2</sub>	<ol style="list-style-type: none"> <li>1. Frostbite burns or hypothermia</li> <li>2. Vents and valves (accumulation of ice formed from moisture in the air).</li> <li>3. Storage vessels must be kept under +ve pressure to prevent air from entering and producing flammable mixtures.</li> <li>4. Electric current carrying capacity is small → charge buildup is not a concern in flowing liquefied H<sub>2</sub></li> </ol>		

**Table 3 Comparison of combustion properties of hydrogen with other fuel.**

Fuel	LHV (MJ/kg)	HHV (MJ/kg)	Stoichiometric air/fuel ratio (kg)	Combustible range (%)	Flame temperature °C	Min. ignition energy (MJ)	Autoignition temperature °C
Methane	50.0	55.5	17.2	5–15	1914	0.30	54–630
Propane	45.6	50.3	15.6	2.1–9.5	1925	0.30	450
Octane	47.9	50.1	15.1	0.95–6.0	1980	0.26	415
Methanol	18.0	22.7	6.5	6.7–36.0	1870	0.14	460
Hydrogen	119.9	141.6	34.3	6.7–36.0	2207	0.017	585
Gasoline	44.5	47.3	14.6	1.3–7.1	2307	0.29	260–460
Diesel	42.5	44.8	14.5	0.6–5.5	2327		180–320

### **Safety in Transmission**

To be transported, hydrogen must be in the safest possible condition, while also being cost-effective and energy efficient. There are three main ways to transport hydrogen:

1. Pipelines and tube trailers for transporting gaseous hydrogen or a mixture of hydrogen and natural gas
2. Trucks, rails, barges, and ships outfitted with cryogenic tanks for delivering liquefied hydrogen
3. High energy-density carriers, such as ethanol, methanol, and other liquids derived from renewable biomass, that can be transported and converted to hydrogen at the point of use.

Transportation is still developing, and methods are dependent on a variety of factors; however, safe, cost-effective, and energy-efficient delivery technologies are required. Economic strategies and safety are the primary delivery barriers.

## **Safety in Pipelines**

A pipeline network infrastructure is mostly used to transport large amounts of hydrogen over long distances, owing to its safety in operation, particularly with small diameters and operating at low and constant pressures.

As a result, hydrogen transmission requires significantly more power and energy for compressors. Furthermore, lubricants used in normal compression applications can cause unacceptable contamination problems in fuel cells. More dependable, low-cost, and efficient pipeline compression technologies are required. Alternatively, compressor-less hydrogen transmission pipelines based on current high-pressure-output electrolyzer technology are being explored.

## **Sensors: Leak Detection**

All liquid and gas fuels have the possibilities to leak, particularly during transportation. Human senses cannot detect hydrogen. Because people can smell hydrogen, adding odorants to it is one option for leak detection. These odorants, however, are not suitable for hydrogen because they are too heavy to "travel with" hydrogen and disperse at the same rate. Fuel cells, a popular hydrogen application, are also contaminated by odorants. As a result, odorants may pose a problem when used to odorize hydrogen gas.

Sensors for detecting hydrogen leaks are required for hydrogen delivery infrastructure. Hydrogen sensors that are both affordable and dependable, such as optical fiber leak detection technologies, are being developed.

The sensor must be sensitive and fast enough to detect leaks early enough to act before the explosive limit in the air is reached. Using a fiber-optic sensor configuration may provide the best chance of meeting the goals of fast response and low cost and reliability.

It can be concluded that hydrogen is primarily transmitted through pipes, with the challenge of safety being in the manufacture of materials capable of handling hydrogen. Hydrogen can

either permeate or embrittle a material over time. The use of sensors to detect leaks is an important application for safe use.

## HYDROGEN COSTS

As was previously said, hydrogen can be manufactured using a variety of basic energy sources, production methods, and levels of maturity. However, now there are most discussed colours for hydrogen are green, blue, and Gray, but in our case, we consider black hydrogen and green hydrogen prices which are listed below sections. Although most hydrogen is used in industrial processes (such as the production of ammonia, steel, methanol, and refining), demand for hydrogen is rising quickly. However, most of this hydrogen is produced using fossil fuels, which releases CO<sub>2</sub> into the atmosphere. The final cost of hydrogen may vary greatly depending on the energy source and technique of generation. The prices for grey hydrogen are the most affordable, often ranging between 0.8 and 2.1 € per kilogram of hydrogen. Due to greater expenses for carbon capture and storage, blue hydrogen may be much more expensive than grey hydrogen. However, the scenario where hydrogen is produced in an electrolyzer using electricity from RES currently has the greatest hydrogen costs (see below fig 2). In the literature, the price range for green hydrogen is typically between 2.2 and 8.2 € per kilogram of hydrogen.

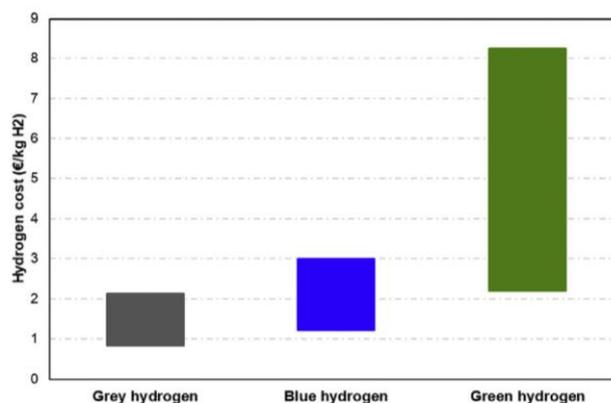


Figure 2 Reported cost of hydrogen production for different production pathways in the literature Midilli A, 2021, Longden T, 2022, Ji M, 2021, Noussan M, 2021

The wide range of projected hydrogen production costs in the literature is due to a variety of factors, mainly coming from different assumptions regarding possible operating hours and the cost of fossil fuels or electricity. Both rely on the area in which they are used. It's

important to keep in mind that grey hydrogen is currently the primary production method when comparing the costs of various hydrogen colours. Different assumptions about the number of feasible operating hours and the cost of fossil fuels or electricity. Both rely on the area in which they are used. It's important to keep in mind that grey hydrogen is currently the primary production method when comparing the costs of various hydrogen colours. with plants in the GW range, whereas, for example, green hydrogen is still deployed with much smaller capacity, both on the side of the electrolyzer technologies as well as the respective renewable electricity generation. In regions with low natural gas prices, grey hydrogen can be produced at 0.8 € per kg of hydrogen. The IEA recorded the lowest prices for SMR in the middle east, the US and Russia, all below 1 € per kg of hydrogen. The highest prices were in Europe and China. The same applies to blue hydrogen. The investment costs for coal gasification are higher than SMR, but fuel input is cheaper than natural gas with a production cost range of 1.2-2 € per kg of hydrogen. The production costs of biomass gasification are slightly higher, ranging from 1.6 to 3 € per kg of hydrogen.

Although producing hydrogen from fossil fuels is now the most cost-effective method, green hydrogen production has the potential to become an attractive alternative in the future as technology advances and RES-generated power production rises. According to IRENA, a combination of cost reductions in power generation and electrolysis due to increased efficiency, as well as an increase in the quantity of full-load hours, might result in a drop of up to 80% in the price of hydrogen. From 2030 onwards, green hydrogen is anticipated to be more affordable than blue hydrogen.

In the case of green hydrogen, the two most significant components of the cost are the investment cost of the electrolyzer and electricity price. Currently, electricity price represents about 90% of the total operating costs. Current capital costs for alkaline electrolyzers are in the range of 500-1000 USD/kW and 700-1700 USD/kW for PEM electrolyzers. However, these costs are expected to decrease significantly. In 2050 capital costs for electrolyzers could be below 200 USD/kW.

**Table 4 Key parameters for AEM & PEM (IRENA, 2020)**

	2020- Alkaline	2020- PEM	2050- Alkaline	2050-PEM
System efficiency(kWh/kg)	50-78	50-83	<45	<45
Lifetime(1000h)	60	50-80	100	100-120
Capital costs (USD/kWe), system size >10MW	500-1000	700-1400	<200	<200

The cost of producing hydrogen is heavily influenced by the investment costs of the hydrogen production facility, the cost of raw materials or electricity used, and the operating hours of the hydrogen production technology. Depending on the manner of production, the price of electricity will only go down if excess renewable energy is utilised. But because of this, there are fewer full-load hours per year, which raises the overall cost.

For our calculations, black hydrogen and green (AEL & PEM Electrolysis). By including above mentioned parameters, hydrogen costs are calculated as

**Equation 1**

*Cost of hydrogen*

$$= \frac{\text{investment cost} * \text{capital recovery factor} + \text{cost of operating and maintainance costs}}{\text{time}} + \left( \text{cost of fuel} \frac{\text{price}}{\text{efficiency}} \right)$$

**Table 5 input data for the hydrogen production costs (A. Ajanovic M. Sayer, 2022)**

	SMR	SMR WITH CCUS	AEL	PEM
INVESTMENT COST (\$/Kw)	910	1778	2600	2900
OPERATION AND MAINTENNACE COST(\$/Kw)	42.77	53	39	43.5
EFFICIENCY(LHV)	76	69	65	74
OPERATING HOURS	60	8322	40	40
ENERGY PRICE(\$/kWh)	0.03	0.03	0.04	0.04

It can be clearly seen that SMR is, to date, the most economic hydrogen production method due to its low investment costs of the reformer technology. However, in the future, due to technological learning, substantial cost reductions of electrolyzer technology are expected. Furthermore, the electricity costs will further decrease with a high number of renewables in the electricity system, whereas fossil fuel costs will increase due to higher CO<sub>2</sub> costs. Since SMR is already a fully mature technology, no further learning effects are to be expected. In the future, it will be essential to increase the full load hours of the electrolyzers, especially for green hydrogen production and to utilize low electricity prices.

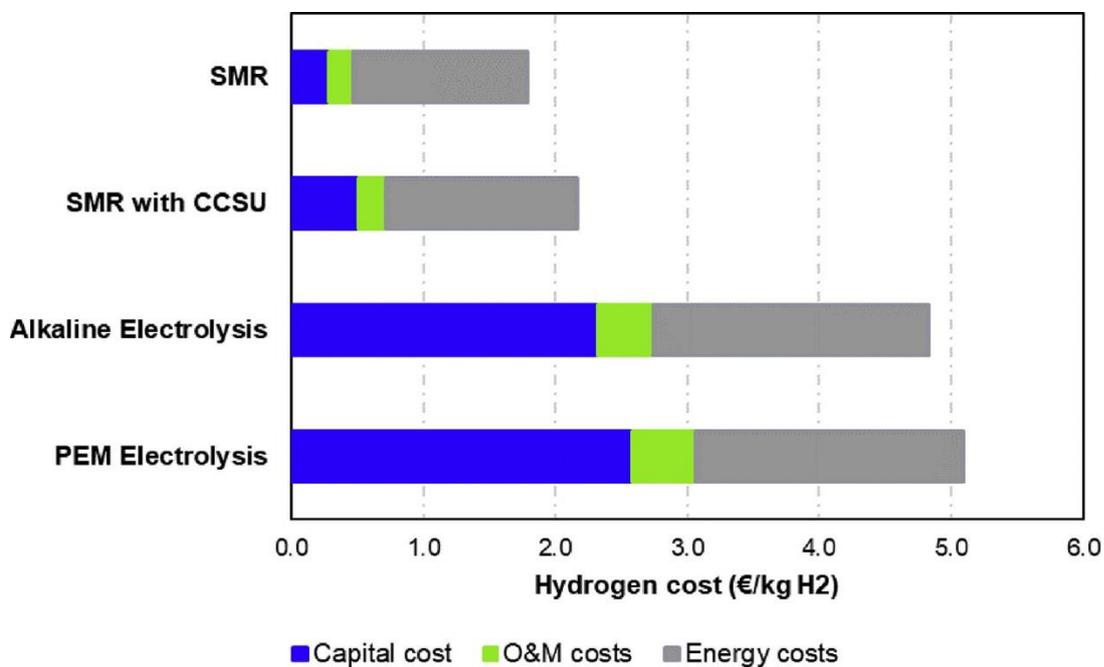


Figure 3 Hydrogen production costs of grey (SMR), blue (SMR with CCUS) and green hydrogen (PEM and Alkaline Electrolysis) (A.Ajanovic, 2022)

# HYDROGEN STORAGE TECHNOLOGIES

Due to the vast multitude of possible hydrogen storage options, it makes sense to organize these into categories. However, finding an optimal categorization system is not trivial, and most authors appear to use slightly different systems. The categorization that will be applied here is based on the nature of the interaction between the stored hydrogen and the storage vessel or material and is graphically represented in below Fig 4.

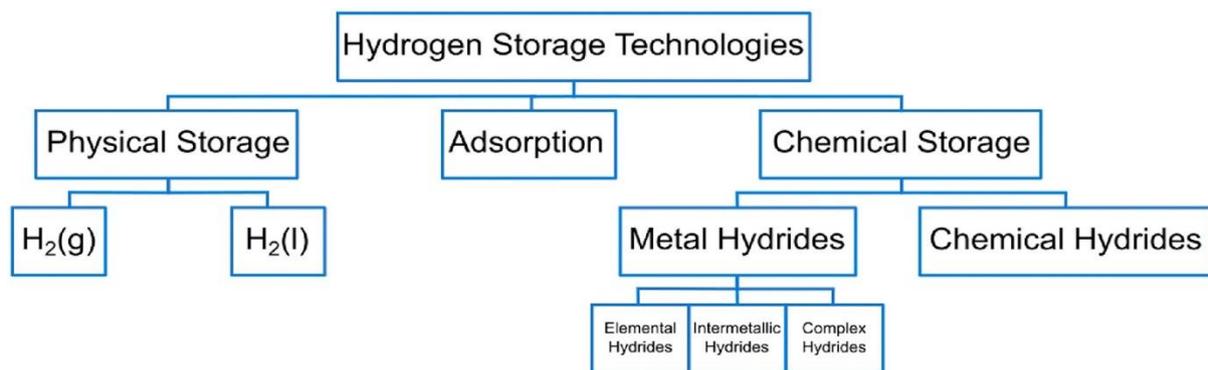


Figure 4 categorization of hydrogen storage technologies (Andersson and Grönkvist 2019)

There are three types of hydrogen storage technologies:

- hydrogen can be stored as a gas or a liquid in pure, molecular form with no significant physical or chemical bonding to other materials
- molecular hydrogen can be adsorbed onto or into a material with relatively weak physical van der Waals bonds
- atomic hydrogen can be chemically bonded (absorbed).

Furthermore, the storage technologies based on chemical bonding can be divided into two subcategories: metal hydrides and chemical hydrides. Because these materials have fundamentally different hydrogen storage properties, this division makes sense. Metal hydrides, as the name implies, contain metal atoms. Hydrogen can be bonded to a metal atom directly (elemental metal hydrides and intermetallic hydrides) or as part of a complex ion that is bonded to a metal atom (complex metal hydrides). Chemical hydrides, on the

other hand, are made up entirely of non-metallic elements, typically some combination of carbon, nitrogen, boron, oxygen, and hydrogen.

## COMPRESSED HYDROGEN STORAGE

The most common method of hydrogen storage is high-pressure compressed hydrogen. Hydrogen compression is not only a mature technology, but it also provides high rates of hydrogen filling and release. Furthermore, no energy is used in the hydrogen release. However, compressing hydrogen to high pressure consumes approximately 13-18% of its lower heating value, affecting the overall economics of the process. The good news is that increasing the pressure only slightly increases the amount of power required for compression. Because spherical vessels are difficult to fit onboard, hydrogen is stored in cylindrical vessels. It is necessary to use a lightweight, low-cost vessel material that can withstand high pressure. The chosen material must be resistant to hydrogen diffusion and embrittlement caused by the stored hydrogen.

For the storage of compressed hydrogen gas, four different types of vessels are used based on the criteria listed above.

Type 1: Fully metallic pressure vessels. This type is the most conventional, least expensive, and heaviest with approximately 3.0 lb/L. They are normally made from aluminium or steel and can contain pressures up to 50 MPa.

Type 2: Steel pressure vessel with a glass fibre composite overwrap. The steel and composite material share about the same amount of structural load. Manufacturing Type 2 vessels costs about 50% more than Type 1, but they offer 30–40% less weight. This type of pressure vessel has the highest-pressure tolerance.

Type 3: Full composite wrap with metal liner. The structural load is mainly carried by the composite structure (carbon fibre composite) and the liner (aluminium) is for sealing purposes. In this type of pressure vessel, the metal liner shares about 5% of mechanical load. This type of pressure vessel has proven to be reliable for 45 MPa working pressure but still has problems with passing the aging tests at 70 MPa. Type 3 provides 0.75–1 lb/L weight, which is about half of the type 2 but their cost would be twice the cost of Type 2.

Type 4: Fully composite. Commonly a polymer like high density polyethylene, HDPE, is used as liner and carbon fibre or carbon-glass composites are used for carrying the structural load. This type of pressure vessel is the lightest yet again the price is still relatively very high. These pressure vessels can withstand pressures up to 100 MPa.

There is also a full composite, liner less pressure vessel (so-called Type 5) which is pre-commercial. This type was first developed in 2010 by Composites Technology Development Inc. Its first built vessel was 20% lighter than similar type IV and had an operational pressure of 1.37 MPa which at this stage is far less than pressures required to store enough hydrogen outside of laboratory use.

With a refueling time of less than 3 minutes and a driving range of 500 kilometers, hydrogen stored at 700 bar in a Type 3 or Type 4 vessel may provide a practical solution. Hydrogen has an energy density of 5.7 MJ/L at 700 bar in a Type 4 vessel (E. Rivard, 2019). Onboard pressurized vessels, on the other hand, have less public acceptance and are more likely to explode due to sudden possible shocks. To reduce the pressure from 700 bar to engine inlet pressure, sophisticated valve technology is required. Energy can ideally be recovered during the expansion process, but this necessitates a complex design and additional weight of the turbine on the vehicle. There are also practical issues with refueling at 700 bar and associated safety issues at the filling stations. Furthermore, hydrogen fuel infrastructure, including transportation and storage, is being developed.

## LIQUID HYDROGEN

In addition to compression, pure hydrogen's density can be increased by liquefaction (condensation). Liquefaction has the advantage of achieving very high hydrogen storage densities at atmospheric pressure: saturated liquid hydrogen has a density of 70 kg/m<sup>3</sup> at 1 bar. Liquid hydrogen has been evaluated as a medium for hydrogen distribution, where its high density is a significant advantage.

The energy-intensive liquefaction process is the primary source of concern for liquid hydrogen storage. The extremely low boiling point of hydrogen (253 °C at 1 bar) and the fact that hydrogen gas does not cool down during throttling processes (adiabatic, isenthalpic expansion) for temperatures above around -73 °C. The latter problem necessitates

precooling in the liquefaction process, most often by the evaporation of liquid nitrogen. Nonetheless, hydrogen liquefaction is relatively well-established: the total installed capacity of hydrogen liquefaction is around 355 tonnes per day (tpd); the largest plant currently in operation has a capacity of 34 tpd. The world's largest hydrogen liquefaction plants were built for NASA between the 1950s and 1970s; most recently built plants are small in comparison (1–10 tpd). The most modern hydrogen liquefaction plants have a specific energy demand of about 10 kWhel/kg, but it is believed that values closer to, or even below, 6 kWhel/kg can be achieved in larger plants with various process improvements (minimum theoretical work for 25 bar feed is 2.7 kWh/kg). Nonetheless, even if liquefaction's specific energy demand can be significantly reduced, the capital costs of a liquefaction plant are still a significant part of the overall costs of liquefaction, even for larger plants. For instance, it has been estimated that the capital investment constitutes around 40–50% of the specific liquefaction costs for a new 100 tpd liquefaction plant.

After the hydrogen has been liquefied, it must be stored to minimize evaporation. Evaporation of liquid hydrogen results in a loss of not only the energy spent liquefying the hydrogen, but also, eventually, a loss of hydrogen as the evaporated gas must be vented due to pressure build-up inside the storage vessel. This gradual loss of stored hydrogen is known as boil-off, and it is frequently expressed as a percentage of stored hydrogen lost per day: the boil-off rate. Heat transfer from the environment to the stored liquid hydrogen, and thus the boil-off rate, is reduced by reducing the surface-to-volume ratio of tanks by making them spherical and by using advanced insulation to reduce heat transfer through the tank walls. Most liquid hydrogen storage vessels are double walled with a high vacuum between the walls. The vacuum reduces heat transfer through conduction and convection. Additional materials in the space between the vessel walls include alumina-coated polyester sheets, alternating layers of aluminium foil and glass fiber, and aluminium, silica, or perlite particles. These materials' purpose is to protect against heat transfer via radiation. Boil-off rates for larger spherical tanks are typically less than 0.1% per day due to the high degree of insulation and low surface-to-volume ratio. NASA operates the largest current storage vessels for liquid hydrogen at Cape Canaveral, Florida, with 230-270 t of hydrogen stored in these vessels. With current technology, even larger spherical liquid hydrogen storage vessels with storage capacities exceeding 900 t should be possible. Despite their relative

complexity, liquid hydrogen storage tanks appear to be less expensive per weight of hydrogen stored than larger-scale vessels for pressurized gaseous hydrogen.

It should be noted that boil-off is less of an issue in applications where the liquefaction plant and liquid hydrogen storage are close together. In such cases, cold boil-off gas from the storage vessel(s) may be injected back into the liquefaction process at a later stage using an ejector. Because the storage's boil-off gas is already close to boiling, reliquefaction is accomplished at a low additional cost. In addition, if reliquefaction is not a viable option, boil-off gas may be utilized in downstream applications.

## ADSORPTION

Adsorption-based hydrogen storage takes advantage of physical van der Waals bonding between molecular hydrogen and a material with a large specific surface area. Because of the weakness of the van der Waals bonding, low temperatures and high pressures are usually required to achieve significant hydrogen storage densities through adsorption. Liquid nitrogen (boiling point:  $-196\text{ }^{\circ}\text{C}$ ) is by far the most common refrigerant used for hydrogen adsorption. The hydrogen pressure applied is typically 10-100 bar, but it varies depending on the adsorbent and the intended application. Higher pressures are not advantageous beyond a certain threshold because the presence of the adsorbent may no longer improve the hydrogen storage capacity compared to storing pressurized gas in the same vessel, the reason being the space occupied by the adsorbent.

Many adsorbents for hydrogen storage have been proposed, including porous carbon-based materials, metal-organic frameworks (MOFs), porous polymeric materials, and zeolites. Certain activated carbons and MOFs have achieved excess hydrogen adsorption of 8-10% (wt) hydrogen at  $196\text{ }^{\circ}\text{C}$ , making them the most successful adsorbents. However, due to the low density of most applied adsorbents and the need for additives to improve effective heat conductivity, the volumetric hydrogen storage density suffers, and achieving a vessel-level deliverable hydrogen storage capacity of much greater than  $40\text{-}50\text{ kg/m}^3$  at  $196\text{ }^{\circ}\text{C}$  is likely difficult using currently available adsorbents.

## MATERIAL BASED STORAGE

In this storage both physical and chemical storages sorption's, some of the base materials are initially in powder form some are liquid form such as liquid organic hydrogen. during discharge and charge process of hydrogen heat is being adsorbed and powder shape material are not an efficient form of material when it comes to heat transfer. Thus, the base materials are pre-process are followed by different methods which are casting, templating, foaming coating, and uniaxial pressing. Then processed material will be fitted into a containment. In most cases a heat exchanger for thermal management purposes is embedded in the design of the containment, and connections for controlling hydrogen flow and filtration of the input and output hydrogen gas

## METAL HYDRIDES

Metal hydrides are formed when hydrogen chemically interacts with metals and metal alloys. When a hydrogen molecule is dissociated into atomic hydrogen at the surface, it diffuses into the bulk and becomes chemisorbed in the metal or alloy structure. The lattice may expand to 20-30% of its original volume because of this chemisorption. The formation of hydrides occurs either through the direct reaction of hydrogen with the metal or through the electrochemical dissociation of water molecules. The following are the two reaction mechanisms:

Mechanism 1: Direct hydrogen reaction:  $M + x/2H_2 \leftrightarrow MH_x$

Mechanism 2: Electrochemical dissociation of water:  $M + x/2H_2O + x/2 e^- \leftrightarrow MH_x + x/2 OH^-$

In metal hydrides, hydrogen is chemically bonded. These bonds are much stronger than the physical bonds involved in hydrogen adsorption. As a result, more energy is required to liberate the chemically bonded hydrogen. The stronger bonding, on the other hand, allows hydrogen to be stored at high density even at ambient temperatures. The hydrogen can be obtained in two ways: through heating (thermolysis) or through a reaction with water (hydrolysis). These approaches are fundamentally different: thermolysis is endothermic, whereas hydrolysis is exothermic; thermolysis is reversible in some cases, whereas hydrolysis is generally in solution; and thermolysis requires elevated temperatures, whereas

hydrolysis may be spontaneous at room temperature. Although a vast array of metal hydrides has been developed and investigated for thermolysis-based storage, relatively few have been applied for hydrolysis with any significant success. The most notable and promising metal hydride for hydrolysis is sodium borohydride ( $\text{NaBH}_4$ ).

## ELEMENTAL METAL HYDRIDES

Most metallic elements can form binary compounds with hydrogen, i.e., elemental hydrides. However, most of these are not suitable for hydrogen storage due to thermodynamics, hydrogen storage capacity, or both. The elemental metal hydrides considered most promising for the large-scale storage of hydrogen are magnesium hydride ( $\text{MgH}_2$ ) and aluminium hydride ( $\text{AlH}_3$ ). Magnesium and its alloys are the subject of extensive research for on-board hydrogen storage because of their high hydrogen-storage capacity by weight and low price. Furthermore, Mg-based hydrides have high-quality functional properties such as heat resistance, vibration absorption, reversibility, and recyclability. In recent years, therefore, much attention has been paid to investigations on specific material properties of Mg alloys for the development of new functional materials.

Magnesium hydride ( $\text{MgH}_2$ ) has the highest energy density (9 MJ/kg Mg) of all reversible hydrides suitable for hydrogen storage.  $\text{MgH}_2$  combines a high  $\text{H}_2$  capacity of 7.7 wt% with the low cost of abundantly available magnesium and good reversibility.

The main disadvantages of  $\text{MgH}_2$  as a hydrogen store are its high discharge temperature, slow desorption kinetics, and high reactivity to air and oxygen. The magnesium hydride system's thermodynamic properties have been investigated. The results revealed a high operating temperature that is unsuitable for practical on-board applications. Due to its high thermodynamic stability, it has a relatively high desorption enthalpy, which corresponds to an unfavourable desorption temperature at 1 bar  $\text{H}_2$ .

## INTERMETALLIC HYDRIDES

Intermetallic compound research for hydrogen storage began more than 20 years ago. The discovery of hydrogen absorption and FeTi opened new avenues for industrial advancement. However, due to the weight penalty and poor hydrogen-storage capacity, they remained at the prototype stage for on-board storage.

Intermetallic compounds (AB<sub>5</sub>, AB<sub>2</sub>, AB, and A<sub>2</sub>B) are currently the most common alloying materials for metal hydrides, with hydrogen storage capacities of 1.5, 2.0, 1.8, and 3.0 wt. percent, respectively. There are also solid solution alloys available, such as vanadium-based solid solution alloys with body-centered cubic structures and Mg-based alloys with hydrogen storage capacities of about 2 and 5 wt percent, respectively. To date, most hydrogen storage alloys can effectively store about 2–3 wt percent of hydrogen, but this is insufficient for on-board vehicular applications based on the US Department of Energy's targets. Metal hydrides made of lightweight elements such as lithium (Li), boron (B), nitrogen (N), magnesium (Mg), and aluminium (Al) have shown great promise for use as hydrogen storage materials. Complex hydrides are the only group of metal hydrides having high volumetric and gravimetric hydrogen storage densities.

Table 6 Properties of some of the most common intermetallic metal hydrides A. Szajek, 2007

Intermetallic compound	Intermetallic hydride	Hydrogen storage capacity (wt%)	Temperature at 1 bar (K)
LaNi <sub>5</sub>	LaNi <sub>5</sub> H <sub>6</sub>	1.37	295
FeTi	FeTiH <sub>2</sub>	1.89	185
Mg <sub>2</sub> Ni	Mg <sub>2</sub> NiH <sub>4</sub>	3.59	255
ZrMn <sub>2</sub>	ZrMn <sub>2</sub> H <sub>2</sub>	1.77	440

## COMPLEX HYDRIDES

Because conventional metal hydrides are mostly composed of heavy elements in the Periodic Table of Elements, complex hydrides composed of light elements such as lithium (Li) and sodium (Na) have gained importance as hydrogen materials. Because of their high hydrogen storage capacities, high hydrogen storage densities, and mild pressures and temperatures, lightweight complex hydrides emerge as potential candidates for hydrogen storage applications. Alanates and borohydrides are examples of Group III complex hydrides that can bond four H<sub>2</sub> atoms with an alkali metal, ionic compound, or partially covalent compound. Despite their high energy densities, complex hydrides are difficult to handle safely and may decompose into highly stable elements that are difficult to refuel with hydrogen on board a motor vehicle.

## SODIUM BOROHYDRIDES

Sodium borohydrides (NaBH<sub>4</sub>) are complex metal borohydrides that have high reversible hydrogen storage capabilities of up to 10.8 wt%. Hydrolysis (reaction with water) is the only way to release hydrogen from NaBH<sub>4</sub>, and it is an irreversible process. The thermodynamic parameters of NaBH<sub>4</sub> are judged undesirable for hydrogen storage applications in the absence of a catalyst or additive because the decomposition temperature is exceedingly high, with a value of 673 K. Furthermore, the traces of BH compounds generated during the heat decomposition process are not only harmful to the fuel cell membranes, but they are also poisonous to the fuel cell catalysts.

Even though NaBH<sub>4</sub> is stable in alkaline aqueous solutions, it can decompose catalytically. NaBH<sub>4</sub> solutions can be stabilized by adding sodium hydroxide (NaOH). However, it should be noted that the addition of this stabilizing compound (1–10% by weight) reduces the amount of stored hydrogen and creates undesirable conditions that make hydrogen recovery difficult. The catalytic hydrolysis of NaBH<sub>4</sub> has piqued the interest of researchers working on hydrogen production systems for on-board vehicular applications. Catalytically active materials for catalytic hydrolysis of NaBH<sub>4</sub> include ruthenium (Ru), platinum (Pt), platinum-palladium (Pt–Pd) and platinum-ruthenium (Pt–Ru) alloys, Raney cobalt and nickel, cobalt, and nickel borides, and fluorinated Mg<sub>2</sub>Ni alloys.

Table 7 Various methods of hydrogen storage P. Preuster, 2017, E. Rivard, 2019, H. Barthelemy, 2017, L. Zhou, 2004.

Storage method	Hydrogen content (wt% H <sub>2</sub> )	Volumetric density (g/L)	Volumetric energy density (MJ/L)
Compression			
1 bar, RT	100	0.0814	0.01
350 bar, RT	100	24.5	2.94
700 bar, RT	100	41.4	4.97
700 bar, RT, (incl. Type IV tank)	5.7	40.8	4.9
Liquid hydrogen			
1 bar, -253 °C	100	70.8	8.5
1 bar, -253 °C (incl. tank)	14	51	6.12
Cryo-compression			
350 bar, -253 °C	100	80	9.6
Metal hydrides			
MgH <sub>2</sub>	7.6	110	13.2
FeTiH <sub>2</sub>	1.89	114	13.7
Complex hydrides			
NaAlH <sub>4</sub>	7.5	80	9.6
Physical adsorbents			
Activated carbon @77 K and 30–60 bar	5.0	38.5	2.4
Zeolite (NaX) @77 K and 40 bar <sup>€</sup>	2.55	20	2.4
MoF (MOF-210) @77 K and 80 bar	7.9	25.8	3.1
Liquid hydrogen organic carriers			
Methylcyclohexane/toluene	6.2	47.3	5.68
perhydro-benzyltoluene/benzyltoluene	6.2	56.0	6.72

## HYDROGEN PRODUCTION

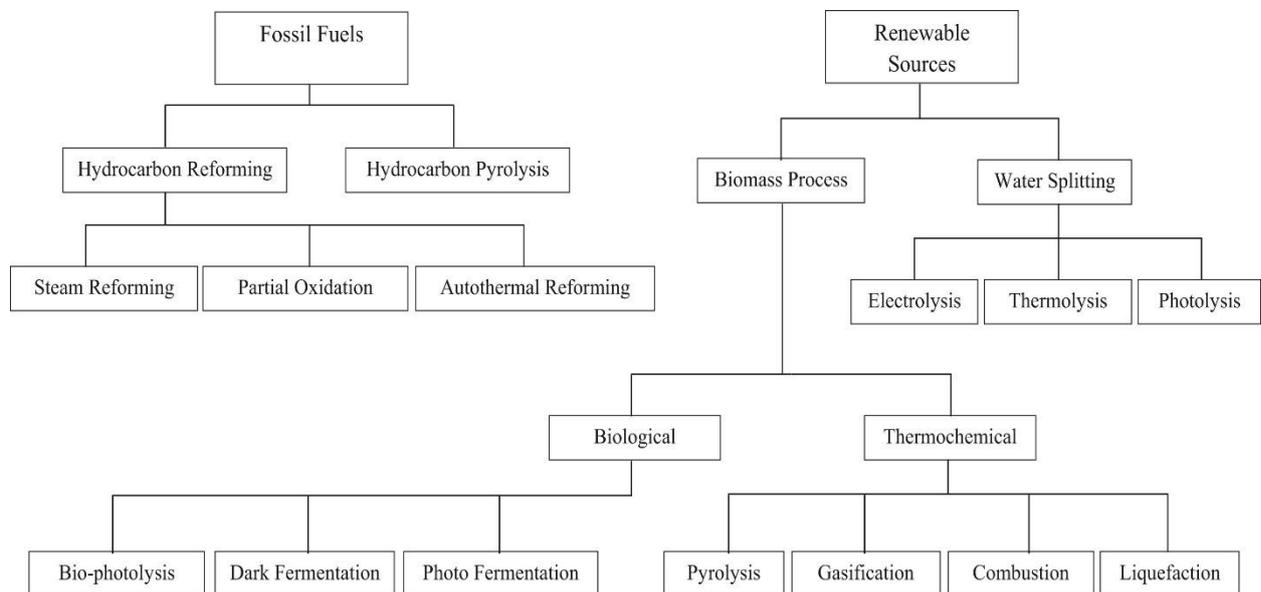


Figure 5 hydrogen production methods sourced from ( Poullikkas, 2017)

## MODES OF HYDROGEN PRODUCTION

Nowadays, over 90% of hydrogen recovered from fossil fuels is recovered, and annually, approximately 830 million tonnes of carbon dioxide are released. From 1975 to 2018, hydrogen production increased to 115 million tonnes per year. Hydrogen production pathways have been divided into two categories: non-renewable energy resources such as steam methane reforming, gasification, and pyrolysis, and renewable energy resources such as electrolysis, biohydrogen, photocatalysis, thermochemical cycles, and plasmolysis. In a different light, few literatures reveal that hydrogen cleanness was described and labelled using three primary colour codes: grey, blue, and green Mulder, 2019, Mulder P. , 2019, T. Bridges, 2019. Regardless of deep cleanness assessment, the colour of hydrogen is determined solely by the type of energy or additional technology used to produce that hydrogen. As a result, grey hydrogen is regarded as a polluting type of hydrogen. Blue hydrogen, on the other hand, defines Carbon Capture and Storage (CCS), which includes grey hydrogen. A 100% renewable energy source for hydrogen production is referred to as

green hydrogen. As a result, green hydrogen is regarded as a clean (low-carbon-emissions) form of hydrogen energy. This raises the question of whether all renewable energy resources emit less pollution than the blue method of hydrogen production. The current colour coding model fails to determine how clean (low-carbon-emission) hydrogen is because it does not account for the amount of GHG emitted during the manufacturing process, subsystems, or the lifecycle of the equipment used. Furthermore, the colour coding identifies the use of RE or CCS (energy type/origin) rather than how clean the hydrogen produced.

Color	<b>GREY</b> HYDROGEN	<b>BLUE</b> HYDROGEN	<b>TURQUOISE</b> HYDROGEN*	<b>GREEN</b> HYDROGEN
Process	SMR or gasification	SMR or gasification with carbon capture (85-95%)	Pyrolysis	Electrolysis
Source	Methane or coal 	Methane or coal 	Methane 	Renewable electricity 

Note: SMR = steam methane reforming.  
\* Turquoise hydrogen is an emerging decarbonisation option.

Figure 6 colours of hydrogen, source: <https://www.weforum.org/>

Thermal processes include natural gas reforming or biofuels/biogas gasification, coal and biomass gasification, and thermochemical processes. The most widely used technology today is reforming, which uses high-temperature steam (700°C-1000°C) to produce hydrogen from a carbon source such as methane. Natural gas, biogas produced from various biogenic renewable sources, and biomass can all be used as sources. Biomass gasification is an exciting near-term technology that has yet to be commercialized on a large scale. Thermal reforming can be used at both the central and distributed scales. Heat (500°C-2000°C) is used in other emerging thermochemical processes to drive a series of chemical reactions that produce hydrogen from water. Water-splitting processes based on thermochemistry will be best suited for large-scale central production.

Electrolytic processes use electricity in an electrolyzer to produce hydrogen and oxygen from water. Electrolyzers can range in size from small, appliance-sized units suitable for small-scale distributed hydrogen production to large-scale, central production facilities. When low-carbon or zero-carbon electricity is used to produce hydrogen, greenhouse gas

emissions are reduced. Low temperature electrolyzers are commercially available and used in some hydrogen fuelling stations. High-temperature electrolysis systems, which typically operate at temperatures above 750°C and have higher electrical efficiency than lower temperature electrolyzers, are suitable for use in nuclear reactors and solar thermal facilities, utilizing the high-grade heat generated by these technologies.

**Photolytic Processes:** Photolytic processes use sunlight's energy to separate water into hydrogen and oxygen. They are further classified into two broad categories: photoelectrochemical (PEC) and photobiological. Specialized semiconductor devices use sunlight to split water in PEC hydrogen production. Specialized microorganisms, such as green algae and cyanobacteria, use sunlight energy to produce hydrogen in photobiological production. These pathways have long-term potential for sustainable hydrogen production with low environmental impact in the future, but they are still in the early stages of research and development.

## RENEWABLE HYDROGEN PRODUCTION

Water is considered as the most abundant source of hydrogen, which is composed of hydrogen and oxygen. As a result, if enough energy is applied to it, its molecules will split into hydrogen and oxygen. To split the water, several technologies can be used. Some of these technologies are discussed in greater detail in the sections that follow.

Water electrolysis can be accomplished using a variety of electrolyte systems, including anion exchange membranes (AEMs) electrolysis, alkaline water electrolysis (AWE), solid oxide water electrolysis (SOE), and proton exchange membranes (PEMs) electrolysis. They operate on the same principle, but under different conditions and with different materials.

### ALKALINE ELECTROLYZER

Alkaline electrolyzers perform by transporting hydroxide ions (OH<sup>-</sup>) from the cathode to the anode via the electrolyte, with hydrogen generated on the cathode side. For many years, commercially available electrolyzers used a liquid alkaline solution of sodium or potassium hydroxide as the electrolyte. On the lab scale, newer approaches that use solid alkaline exchange membranes (AEM) as the electrolyte are showing promise.

When the electrodes relate to a direct current, hydrogen is produced at the cathode and oxygen is produced at the anode. Maximize ionic conductivity, this assembly is immersed in a liquid electrolyte, which is typically a highly concentrated aqueous solution of KOH (25-30 wt.%).

Other electrolyte solutions, such as NaOH or NaCl, are less commonly used. The main disadvantage of alkaline electrolytes is their corrosive nature.

In an alkaline electrolysis cell, the following reactions occur:

1. Anode  $4\text{OH} \rightarrow \text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^-$
2. Cathode:  $4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2$
3. Sum:  $2\text{H}_2\text{O} \rightarrow \text{O}_2 + 2\text{H}_2$

A diaphragm separates the reaction zones and prevents the produced gases from mixing. As a result, the diaphragm is permeable to water ions but not to gases. Asbestos diaphragm material with a thickness of 3 mm is used in conventional electrolyzers. The operating temperature of a conventional alkaline electrolyzer is limited to 80 °C due to the material properties of asbestos.

The reduction in energy required to compress hydrogen to storage pressure levels is a significant advantage of high-pressure electrolysis. Its disadvantage is that it reduces the purity of the product gases because high pressures and temperatures increase the permeability of the membrane to gases. The energy demand of an alkaline electrolyzer is determined by the electrode characteristics and operational conditions.

Atmospheric electrolyzers require approximately 4.1-4.5 kWh/Nm<sup>3</sup> H<sub>2</sub>, whereas pressurized electrolyzers require approximately 4.5-5 kWh/Nm<sup>3</sup> H<sub>2</sub>. Furthermore, the atmospheric electrolyzers require energy for hydrogen compression, resulting in a total plant energy demand of approximately 4.5-7 kWh/Nm<sup>3</sup> H<sub>2</sub>.

The efficiency of atmospheric electrolyzers can reach 85% (HHV), while high-pressure electrolyzers can reach 78%. (HHV). An alkaline electrolyzer has a reported lifetime of up to 30 years, though a general overhaul is required every 7-15 years to replace/reactivate the electrodes and diaphragms.

Alkaline water electrolysis is a well-established technology. These electrolyzers are dependable and secure. As a result, they are the most extensive electrolysis technology at the commercial level in the world. The investment costs range from \$1,000 to \$5,000 per kW, depending on the production capacity.

## ELECTROLYSIS

Electrolysis is a non-spontaneous chemical decomposition technique in which an electric current is applied to an ion-containing solution in an electrolyzer (electrolyte, anode-cathode electrodes, and separator). The various electrolysis methods that could be used for hydrogen production include alkaline water electrolysis, solid oxide electrolysis (SOES), PEM electrolysis, and high-temperature water electrolysis. The alkaline water and PEM electrolyzers work at low temperatures (373 K), whereas the SOSE electrolyzer works at high temperatures (800–1273 K). The high temperature electrochemical breakdown of steam has two advantages over the low temperature electrolysis technique. For first, a high temperature electrolysis method is more efficient than standard room-temperature electrolysis because heat is less expensive than electrical power.

Second, the energy expended in high temperature electrolysis is minimal due to the low theoretical breakdown voltage at high steam temperatures. The main disadvantage of electrolysis for hydrogen generation is its high cost in comparison to the SMR technique. A high-cost metal oxide electrolyte is required to deal with the high SOSE operating temperature and massive thermal energy. The process's electrical power consumption decreases as the SOSE working temperature rises, while the required thermal energy rises. SOSEs do not require expensive catalysts because they operate at high temperatures; however, certain chemical, thermal, and structural conditions must be met. The cost of hydrogen generation is determined by the cost of energy consumption. Water electrolysis meets 4% of global hydrogen demand.

Hydrogen can be produced by electrolysis of aqueous methanol. It has been reported that hydrogen can be produced at low voltage and low cost by electrolyzing aqueous methanol, but carbon dioxide, a greenhouse gas, is released. The feedstock has a large impact on the efficiency of hydrogen production in electrolysis. However, methanol is made from biomass, this method is time-consuming and energy intensive. Water electrolysis is regarded as a

viable method of hydrogen production. Because hydrogen and oxygen evolve at different electrodes, one of the primary benefits of electrolysis is that no external separation sources are required, and pure hydrogen can be obtained. The disadvantage of this method is that it consumes a lot of energy when compared to other electrolysis methods. It has been reported that commercial water electrolyzers consume approximately 4.5-5 kWh/Nm<sup>3</sup>, which is significantly higher than other methods. However, if energy is supplied by renewable sources such as wind and light, its energy efficiency could be increased (PV electrolysis) (R. Kothari, 2008).

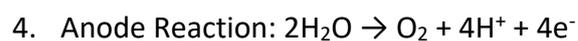
## POLYMER ELECTROLYTE MEMBRANE (PEM)

In a polymer electrolyte membrane (PEM) electrolyzer is a solid specialty plastic material.

At the anode, water reacts to produce oxygen and positively charged hydrogen ions (protons).

The electrons are routed through an external circuit, while the hydrogen ions move selectively across the PEM to the cathode.

Hydrogen ions combine with electrons from the external circuit at the cathode to form hydrogen gas.



PEM electrolyzers are commercially available for small-scale production. Without the use of auxiliary purification equipment, the hydrogen purity is typically greater than 99.99 vol.% (in some cases up to 99.999 vol.%). Furthermore, the polymeric membranes' low gaseous permeability reduces the risk of flammable mixture formation. PEM electrolyzers operate at temperatures around 80 degrees Celsius and pressures of up to 15 bar.

PEM electrolyzers typically have capacities ranging from 0.06 to 30 Nm<sup>3</sup>H<sub>2</sub>/hr. Specific energy demand is typically in the 6-8 kWh/Nm<sup>3</sup> H<sub>2</sub> range, but it can be as low as 6 kWh/Nm<sup>3</sup>H<sub>2</sub> in large-scale systems producing more than 10 Nm<sup>3</sup>H<sub>2</sub>/hr. Their efficiencies range from 67-82%. PEM electrolyzers have some drawbacks as well. The main problem is

the high investment cost associated with the membranes and noble metal-based electrodes. The production capacity needs to be increased for their wider commercialization.

## SOLID OXIDE ELECTROLYZER

Solid oxide electrolyzers, which use a solid ceramic material as the electrolyte and selectively conduct negatively charged oxygen ions ( $O_2$ ) at elevated temperatures, produce hydrogen in a slightly different way.

Steam combines with electrons from the external circuit at the cathode to form hydrogen gas and negatively charged oxygen ions.

The oxygen ions pass through the solid ceramic membrane and react with oxygen gas at the anode, generating electrons for the external circuit.

Solid oxide electrolyzers must operate at temperatures high enough for the solid oxide membranes to function properly (around 700°-800°C, as opposed to PEM electrolyzers, which typically operate at 70°-90°C and commercial alkaline electrolyzers, which typically operate at less than 100°C). Advanced lab-scale solid oxide electrolyzers based on proton-conducting ceramic electrolytes are promising for lowering operating temperatures to 500°-600°C. The solid oxide electrolyzers can use the heat available at these high temperatures (from a variety of sources, including nuclear energy) to reduce the amount of electrical energy required to produce hydrogen from water.

Table 8 Typical specification of alkaline, polymer electrolyte and solid oxide electrolyzers, Smolinka, 2014

Specification	Unit	Alkaline	PEM	SOEs
Technology maturity		State of the art	Demonstration	R & D
Cell temperature	°C	60–80	50–80	900–1000
Cell pressure	Bar	<30	<30	<30
Current density	A/cm <sup>2</sup>	0.2–0.4	0.6–2.0	0.3–1.0
Cell voltage	V	1.8–2.4	1.8–2.2	0.95–1.3
Power density	W/cm <sup>2</sup>	Up to 1.0	Up to 4.4	–
Voltage efficiency	%	62–82	67–82	81–86
Specific energy consumption, system	kWh/Nm <sup>3</sup>	4.5–7.0	4.5–7.5	2.5–3.5
Partial load range	%	20–40	0–10	–
Cell area	m <sup>2</sup>	<4	<300	–
Hydrogen production, system	Nm <sup>3</sup> /hr	<760	<30	–
Lifetime, stack	hr	<90000	<20000	<40000
System lifetime	yr	20–30	10–20	–
Purity of hydrogen produced	%	>99.8	99.999	–
Cold start up time	min.	15	<15	>60

Table 9 Comparison of different types of electrolyzers in their operation temperature, stack voltage efficiency and pros and cons, Schmidt O., 2017.

Type	Operating temperature	Stack voltage efficiency	Pros and cons
Alkaline electrolyser (AEL)	<80 °C	62%–82%	Pros: good durability and maturity. Cons: low partial load range, low current density.
Proton exchange membrane electrolyser (PEMEL)	<80 °C	67%–82%	Pros: good compactness and efficiency, fast response. Cons: more expensive and lower durability.
Solid oxide electrolyser (SOEL)	>700 °C	Around 100%	Pros: high efficiency and operation pressure, reusable heat. Cons: low maturity, not widely commercialised

# NON-RENEWABLE HYDROGEN PRODUCTION

## STEAM METHANE REFORMING

Steam methane reforming is a well-established and widely used method for producing hydrogen (SMR). SMR generates more than 80% of hydrogen, which is higher than electrolysis. As a first step, natural gas and other hydrocarbons containing methane are sent to the steam system to be heated and sulfur removed, which can contaminate and slow hydrogen production and catalyst activity. Sulfur could be removed using hydrodesulfurization and adsorption techniques with activated carbon. By using an endothermic reaction, steam and purified methane are passed through a catalyst and converted into hydrogen.

A reforming reactor, water shift reactors (WGS, High Temperature, and Low Temperature), syngas purification, CO<sub>2</sub> compression, transportation, sequestration, and hydrogen storage are depicted in the process flow diagram (Fig 6). First, we'll look at the case for carbon capture and storage. Natural gas reacts with steam at high pressure in the reforming reactor to produce syngas (a mixture of hydrogen and carbon monoxide). In the presence of nickel-based catalysts, the reaction produces carbon monoxide and hydrogen-rich syngas. The syngas is cooled and fed into water-gas shift (WGS) reactors, where it is converted to carbon dioxide and hydrogen by the addition of steam. The HT and LT WGS reactors are linked together by Fe<sub>2</sub>O<sub>3</sub>-Cr<sub>2</sub>O<sub>3</sub> and CuO/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts. The hydrogen produced is purified in the syngas purification unit (amine unit). It is then pressurized and stored in the storage tanks. CO<sub>2</sub> emissions from the syngas purification unit are compressed and transported through a pipeline to an underground cavern. For the case without CCS, the syngas from the WGS reactors is directly sent to the syngas purification/pressure swing adsorption (PSA) unit after cooling. CO<sub>2</sub> produced is released directly into the atmosphere.

Steam-Methane Reforming Reaction  $\text{CH}_4 + \text{H}_2\text{O} (+\text{heat}) \rightarrow \text{CO} + 3\text{H}_2$

Water-Gas Shift Reaction  $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2 (+\text{small amount of heat})$

In partial oxidation, the methane and other hydrocarbons in natural gas react with a limited amount of oxygen (typically from air) that is not enough to completely oxidize the hydrocarbons to carbon dioxide and water. With less than the stoichiometric amount of

oxygen available, the reaction products contain primarily hydrogen and carbon monoxide (and nitrogen, if the reaction is conducted with air rather than pure oxygen), and a relatively small amount of carbon dioxide and other compounds. Subsequently, in a water-gas shift reaction, the carbon monoxide reacts with water to form carbon dioxide and more hydrogen. Partial oxidation is an exothermic process—it gives off heat. The process is, typically, much faster than steam reforming and requires a smaller reactor vessel. As can be seen in chemical reactions of partial oxidation, this process initially produces less hydrogen per unit of the input fuel than is obtained by steam reforming of the same fuel.

Partial oxidation of methane reaction  $\text{CH}_4 + \frac{1}{2}\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2$  (+ heat)

Water-gas shift reaction  $\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$  (+ small amount of heat).

Table 10 steam reforming of methane, process conditions and performance data were taken from SRI Consulting report. Naqvi, 2007

<b>Pre-reformer section</b>	
Temp (°C)	474–550
Pressure (psia)	365
<b>Reformer section</b>	
Temp (°C)	700–875
Pressure (psia)	325
<b>Reformer outlet composition (mol %, dry basis)</b>	
H <sub>2</sub>	73.44
CH <sub>4</sub>	4.59
CO	13.05
CO <sub>2</sub>	8.92
Methane conversion (%)	81.27
<b>Water–gas shift reactor</b>	
Temp (°C)	370–438
Pressure (psia)	300

Water-gas shift reactor outlet composition (mol %, dry basis)	
H <sub>2</sub>	75.57
CH <sub>4</sub>	4.22
CO	3.98
CO <sub>2</sub>	16.87
CO conversion (%)	66.87

## AUTO - THERMAL REFORMING (ATR)

ATR is a commercial technology commonly used in the production of ammonia and methanol. ATR is now being proposed as a preferred technology to produce pure hydrogen from natural gas because it allows capture of carbon at higher rates than conventional SMR, at lower cost. Compared to SMR, ATR has a simpler production stream, with a high concentration of carbon dioxide. This makes it easier to capture a higher percentage of carbon emissions in the conversion process.

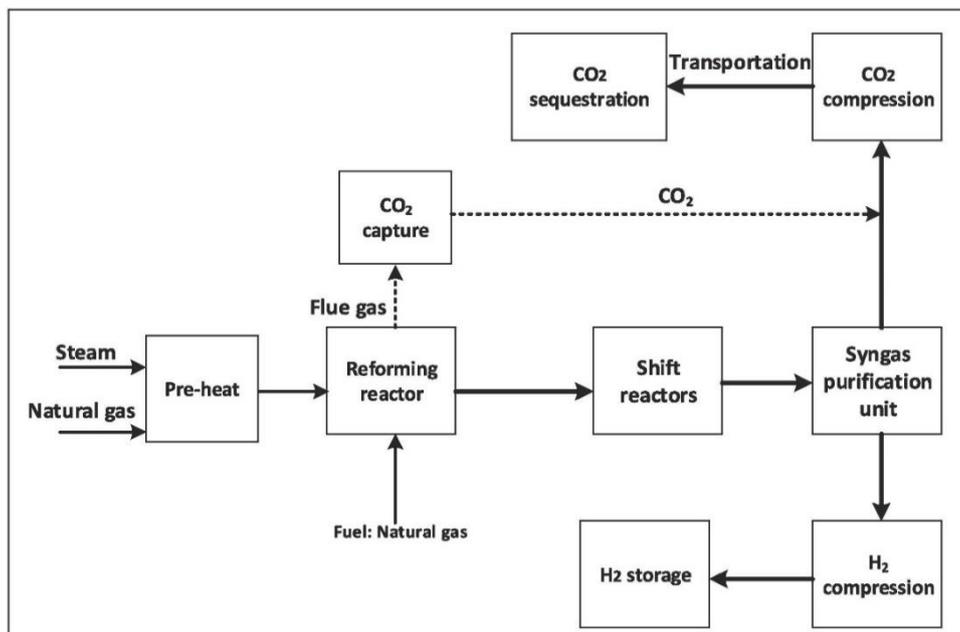


Figure 7 Simplified process flow diagram of steam methane reforming with carbon capture storage (SMR-CCS) source from: (Abayomi Olufemi Oni, 2022)

## GASIFICATION

Coal is a viable option for producing hydrogen in large plants due to global reserves and commercially available technologies. Gasification is more suitable for converting coal to hydrogen than existing methods (such as electrolysis). Coal is partially oxidized with steam and oxygen in a high-temperature, high-pressure reactor during the coal gasification process. The main products are CO and H<sub>2</sub>, which are mixed with steam and CO<sub>2</sub> (syngas). A shift reaction occurs in the syngas to increase the hydrogen yield. The gas can be cleaned conventionally to recover elemental sulphur (or to produce sulphuric acid). Electricity can be generated by using some of the syngas in a gas turbine.

The main concern with coal gasification is the high carbon content of coal, which results in higher CO<sub>2</sub> emissions than other feedstock options. CCS (Carbon Capture and Storage) technologies are being developed to address this issue. The cost of producing hydrogen in a large coal gasification plant is currently slightly higher than the cost of producing hydrogen from natural gas. However, coal gasification techniques are less well-defined than those used in natural gas steam reforming. In terms of economics, hydrogen production from coal differs from other fossil fuels in that the unit raw material costs are lower while the unit capital costs for coal gasification plants are higher.

## THERMOCHEMICAL WATER SPLITTING

Hydrogen can be produced using nuclear reactors and thermochemical water-splitting cycles operating at temperatures of 500 °C or higher. Higher temperatures allow for faster reaction rates and higher efficiencies. Over 100 different high temperature water-splitting thermochemical reactions have been proposed thus far. The thermochemical Cu-Cl and S-I cycles are investigated in this study. The thermochemical Cu-Cl cycle was proposed for the first time in the 1970s. Some commercially available Cu-Cl cycles are currently being tested. Cu-Cl cycles are expected to have efficiencies of around 40% at operating temperatures around 550 °C (cogeneration of electricity is ignored). A key challenge of thermochemical Cu-Cl cycles is lowering the required temperatures for high efficiencies. With thermochemical S-I cycles, it is possible to reach higher efficiencies (around 60%, with cogeneration of electricity). However, these cycles require higher temperatures, around 825–900 °C. These thermochemical cycles need special reactors that are constructed

using special chemically inert materials capable of resisting high temperatures. Developing these special materials in an economically feasible way is another significant challenge of thermochemical cycles. However, thermochemical cycles show promising results to be considered as potential methods to produce hydrogen.

## BIOMASS GASIFICATION

As biomass resources for hydrogen production, wood processing, forestry and agricultural residues, municipal and animal waste, and/or crops can be used. The biomass gasification process is currently incapable of producing hydrogen on a large scale at a competitive price. However, energy from household and agricultural waste can be recovered in a clean manner using this method. Because CO<sub>2</sub> released when biomass is oxidized can be absorbed from the atmosphere and fixed by photosynthesis in the biomass growing process, this option has the potential to reduce net CO<sub>2</sub> emissions more than fossil fuels. One major concern with this method is the possibility of natural resource and land requirement issues because of growing large amounts of biomass as energy crops.

Table 11 steam reforming of methane, process conditions and performance data were taken from SRI Consulting report. Naqvi, 2007.

Natural gas steam reforming	Coal and biomass gasification	Thermo-chemical	Water electrolysis
<b>Key benefits</b>			
Most viable approach in the near term	Low-cost synthetic fuel in addition to H <sub>2</sub>	Clean and sustainable	No pollution with renewable sources
Lowest current cost	Abundant and affordable		
Existing infrastructure			
<b>Critical challenges</b>			
Capital, operation, and maintenance costs	Reactor costs		Low efficiency
	System efficiency	Effective and durable materials of construction	Capital costs
	Feedstock impurities Carbon capture storage		Integration with renewable energy sources

# LIFE CYCLE ASSESSMENT OF HYDROGEN

## BASIC PRINCIPLES

LCA quantifies the environmental impacts of a product or service over its entire life cycle, beginning with resource extraction and continuing through intermediate processing stages, use, and final disposal. It includes consumption of fossil and mineral resources, land use, and emissions to air, water, and soil. The International Organization for Standardisation (ISO) has established international standards for life cycle assessment (LCA) (ISO, 2006). There are four major steps: goal and scope definition, inventory assessment, impact assessment, and interpretation. Conducting an LCA is typically an iterative process due to the comprehensive approach and interdependent assessment steps.

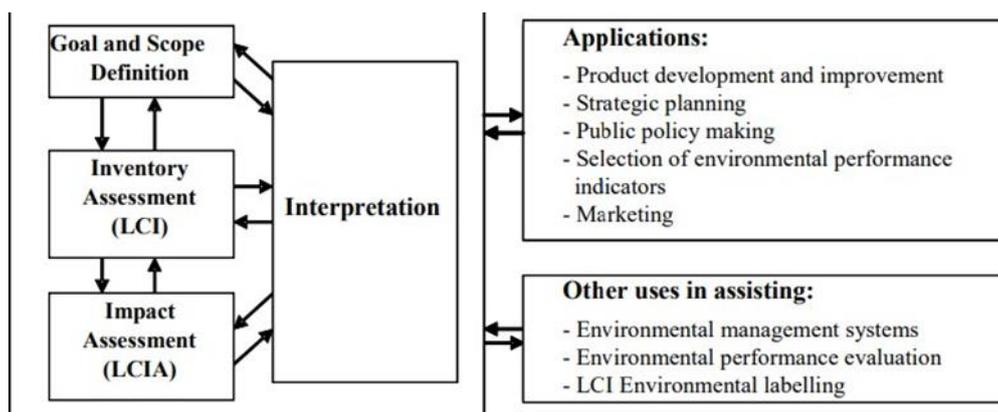


Figure 8 schematic of LCA, source from (ISO, 2006)

## GOAL AND SCOPE DEFINITION

The goal and scope define the fundamental characteristics and constraints of the LCA being conducted. Although the definitions of these aspects can also be iterated upon throughout the duration of a study, they provide a framework and guidelines for the collection of the inventory data. The inventory data are either then elementary (mass) flows of resources and emissions, the use and occupation of land, or the provision of services in the form of unit processes. Some of the main aspects for consideration when setting out the objectives and scope of the study include (ISO, 2006): Functional unit: the quantifiable unit of a product or service and according to which the inventory data are then related. System boundaries: the definition of the processes included, ideally considering all elementary flows into and out of the processes under focus. The level of detail considered in the study depends on the capabilities of the tools employed as well as the resources available. At the data level, system boundaries are defined according to temporal, geographical and technological constraints and should reflect the goals of the study. Cut-off criteria: the criteria for selecting the inputs and outputs according to the system boundary definition is an iterative process throughout an LCA, determined as various aspects are tested for their sensitivity to the final results. Data quality requirements: the description of requirements concerning temporal, geographical and technological aspects to enable the goal and scope to be met and to be able to properly interpret the results of the analysis. Definition of the type of critical review: Depends on the framework of the study and the audience addressed.

## LIFE CYCLE INVENTORY (LCI) ANALYSIS

The Life Cycle Inventory (LCI) analysis quantifies all elementary flows associated with single processes, i.e. mass (materials and resources) and energy flows, land use, emissions to air, water and soil and products of the processes as outputs. By linking the single processes, the elementary flows per desired functional unit are quantified. Eco invent LCA database contains more than 4'000 individual processes covering the whole economic system with focus on European production chains. For important globally traded goods (e.g., energy carriers like oil, gas, coal and uranium) regions outside of Europe are also considered. The inventories include more than 1000 individual elementary flows, i.e., emission species to air, water and soil, consumption of renewable and non-renewable energy, mineral resources as

well as various types of land use. These LCI data mainly refer to conditions existing around the years 2000-2005. For projection to the year 2035 the same background data is applied, with modifications made to significant datasets such as the European electricity mix and Russian natural gas production, according to expected developments.

## LIFE CYCLE IMPACT ASSESSMENT (LCIA)

Life Cycle Impact Assessment (LCIA) is the third step within an LCA and focuses on the aggregation of specific or total environmental burdens for the comparison of competing technologies. LCIA can also be used to analyse the contributions from system parts or for use in product optimization. Figure 2 shows the main aspects or steps of the LCIA: it contains several mandatory elements and certain additional options for a higher level of aggregation and a more comprehensive assessment. Implementation of all optional elements allows aggregation of all environmental burdens to a single indicator. The concept of category indicators for environmental impacts is the basis for LCIA. Each category has its own environmental mechanism, such as infrared radiative forcing for climate change or proton release for acidifying emissions. All mass flows considered in the LCI are classified and multiplied with specific characterization factors concerning the specific environmental impact for a specific impact category. Implementation of the optional elements depends on the intended assessment. Normalization allows the comparison of different category indicators by dividing the values with a selected reference value such as given emissions or resource uses for a certain area, e.g., the whole Europe. Grouping of impact categories allows a specific comparison depending on the interests defined in the goal and scope description. Certain characteristics can be grouped, such as emissions or resource consumptions, or impact categories can be ranked depending on value-based priorities. Weighting indicators allows for a differentiated rating of impacts, such as for an aggregation of the categories to a total environmental indicator. As the choice of weighting factors depends on personal value judgement and is not only based on scientific criteria but weighting also involves a strong element of subjectivity. Therefore, different weighting schemes as well as sensitivity analysis may be helpful for consolidation of results and conclusions.

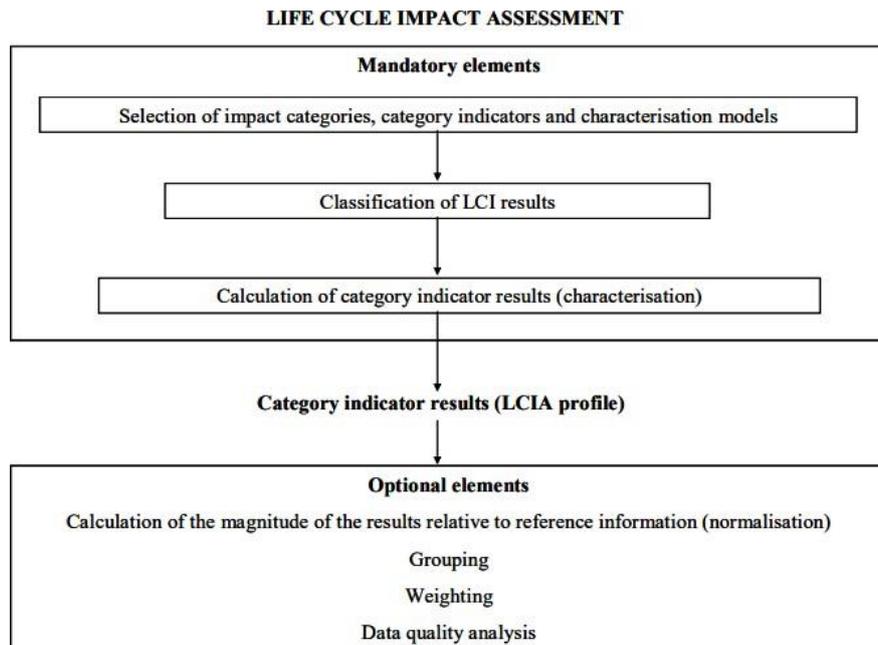


Figure 9 life cycle impact assessment, source from (ISO, 2006)

## GLOBAL WARMING POTENTIAL

Greenhouse gases (GHGs) warm the earth by absorbing energy and slowing the rate at which the energy escapes to space; they act like a blanket insulating the Earth. Different GHGs can have different effects on the earth's warming. Two keyways in which these gases differ from each other are their ability to absorb energy (their "radiative efficiency"), and how long they stay in the atmosphere (also known as their "lifetime"). The Global Warming Potential (GWP) was developed to allow comparisons of the global warming impacts of different gases. Specifically, it is a measure of how much energy the emissions of 1 ton of a gas will absorb over a given period of time, relative to the emissions of 1 ton of carbon dioxide (CO<sub>2</sub>). The larger the GWP, the more that a given gas warms the Earth compared to CO<sub>2</sub> over that time period. The time period usually used for GWPs is 100 years. GWPs provide a common unit of measure, which allows analysts to add up emissions estimates of different gases (e.g., to compile a national GHG inventory), and allows policymakers to compare emissions reduction opportunities across sectors and gases.

- CO<sub>2</sub>, by definition, has a GWP of 1 regardless of the time period used, because it is the gas being used as the reference. CO<sub>2</sub> remains in the climate system for a very long time: CO<sub>2</sub> emissions cause increases in atmospheric concentrations of CO<sub>2</sub> that will last thousands of years.
- Methane (CH<sub>4</sub>) is estimated to have a GWP of 27-30 over 100 years. CH<sub>4</sub> emitted today lasts about a decade on average, which is much less time than CO<sub>2</sub>. But CH<sub>4</sub> also absorbs much more energy than CO<sub>2</sub>. The net effect of the shorter lifetime and higher energy absorption is reflected in the GWP. The CH<sub>4</sub> GWP also accounts for some indirect effects, such as the fact that CH<sub>4</sub> is a precursor to ozone, and ozone is itself a GHG.
- Nitrous Oxide (N<sub>2</sub>O) has a GWP 273 times that of CO<sub>2</sub> for a 100-year timescale. N<sub>2</sub>O emitted today remains in the atmosphere for more than 100 years, on average.
- Chlorofluorocarbons (CFCs), hydrofluorocarbons (HFCs), hydrochlorofluorocarbons (HCFCs), perfluorocarbons (PFCs), and sulfur hexafluoride (SF<sub>6</sub>) are sometimes called high-GWP gases because, for a given amount of mass, they trap substantially more heat than CO<sub>2</sub>. (The GWPs for these gases can be in the thousands or tens of thousands.)

# METHODOLOGY

LCA is the technique used to evaluate the energy and material use which are associated with an energy production pathway or a product. Moreover, the results of LCA can help to change the environmental impact. Overall, the LCA methodology helps to evaluate the life cycle GHG emissions associated with energy an energy there are four steps in the LCA which are mentioned above section. The main purpose to carrying out the LCA is to describe our goal of the study. The description of functional unit is to measure performance of process or product to ensure fair results.

The hydrogen production systems considered in this study include more than one stage. For SCG-H2, the system boundary involves three stages

1. Coal mining and washing (S1)
2. Coal transportation (S2)
3. Hydrogen production (S3)

For, UCG-H2, the system boundary involves two stages

1. Wells and channels construction(S1)
2. Hydrogen production (S2)

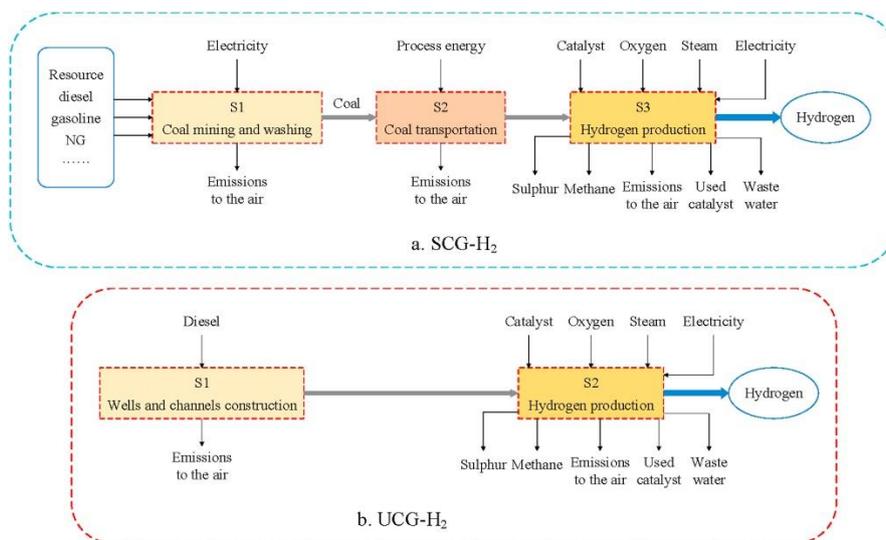


Figure 10 Life cycle boundaries of hydrogen production systems (Liu, 2021)

### Life cycle energy consumption (LCEC)

The amount of primary energy consumed during the life cycle of hydrogen production is referred to as energy consumption. As a result, the concept of primary fossil consumption factor (PFCF) is introduced into this study, and the PFCFs considered in this study are listed in Table 13. The LCEC calculation is based on the amount of process energy consumed and its PFCF, which can be noticed below.

Equation 2

$$LCEC = \sum_{s=1}^3 \sum_{i=1}^3 \sum_{j=1}^7 EC_{s,j} \times PFCF_{j,i}$$

where:

s represents the stages of hydrogen production systems

i is type of primary fossil energy, including coal, oil, and natural gas (NG)

j represents the type of process energy involved in this study

ECs, j represents the consumed process energy during the stages of hydrogen production systems.

### The life cycle of GHG emissions

The life cycle GHG emissions of hydrogen production systems include CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O emissions, which can be classified as direct or indirect emissions. Direct emissions are those produced and emitted into the atmosphere during the hydrogen production stage, whereas indirect emissions are those produced during the upstream stages, as well as the production of process energy used in hydrogen production systems. The following equation can be used to calculate CO<sub>2</sub>, CH<sub>4</sub>, and N<sub>2</sub>O emissions:

Equation 3

$$EM_{CO_2} = EM_{CO_2,direct} + EM_{CO_2,indirect} = \sum_{s=1}^3 \sum_{j=1}^7 EC_{s,j} \times (D_{CO_2,j} + I_{CO_2,j})$$

$$EM_{CH_4} = EM_{CH_4,direct} + EM_{CH_4,indirect} = \sum_{s=1}^3 \sum_{j=1}^7 EC_{s,j} \times (D_{CH_4,j} + I_{CH_4,j})$$

$$EM_{N_2O} = EM_{N_2O,direct} + EM_{N_2O,indirect} = \sum_{s=1}^3 \sum_{j=1}^7 EC_{s,j} \times (D_{N_2O,j} + I_{N_2O,j})$$

## Coal transportation (UCG AND SSG)

The calculation of energy consumption in the coal transportation stage requires data on the proportion of each transport mode and the average transportation distance obtained from the literature Feng, 2017 as well as the data on energy consumption intensity and process energy structure for each transport mode.

Table 12 Coal transportation stage related data

Transportation mode	Energy consumption intensity	Transportation distance	Proportion
Railway	240 kJ/(t·km), diesel (55%) and electricity (45%)	659 km	70%
Road	1200 kJ/(t·km), diesel (68%) and gasoline (32%)	310 km	10%
Waterway	148 kJ/(t·km), furnace oil (100%)	1410 km	20%

The GHG emissions in this stage consist of direct and indirect emissions. Direct emissions refer to the emissions during the usage of process energy in transportation devices, while indirect emissions come from the production of process energy. Based on the consumption amount of process energy (Table 12) and its corresponding direct and indirect emission factor, the direct and indirect emissions can be calculated respectively.

Table 13 Process energy consumption in each stage of hydrogen production systems

Hydrogen production system	Process energy consumption in each stage
<b>1. SCG-H<sub>2</sub></b>	
Coal mining and washing/(MJ coal)	Coal 0.066 MJ, NG 0.001 MJ, diesel 0.001 MJ, electricity 0.004 MJ
Coal transportation/(13,393 kg hydrogen)	Gasoline 9801 MJ, diesel 25,845 MJ, electricity 13,127 MJ, furnace oil 10,997 MJ
Hydrogen production/(13,393 kg hydrogen)	Coal 5,309,122 MJ, electricity 194,281 MJ, steam 676,650 MJ

Hydrogen production system	Process energy consumption in each stage
<b>2. UCG-H<sub>2</sub></b>	
Wells and channels construction/(13,393 kg hydrogen)	Diesel 5816 MJ
Hydrogen production/(13,393 kg hydrogen)	Coal 7,689,240 MJ, electricity 295,387 MJ, steam 256,521 MJ

### Wells and channels construction

The establishment of injection wells for injecting a gasifying agent into the coal seam, production wells for obtaining output syngas, and gasification reaction channels connecting injection and production wells is necessary for the implementation of UCG. The drilling equipment is driven by diesel, and the amount of consumption is estimated according to the existing works of literature A. Verma, 2015

### Hydrogen production

The hydrogen production stage data in this study is derived from Aspen Plus simulation results, and the hydrogen production capacity is 13,393 kg/h. The coal demand for SCG-H<sub>2</sub> and UCG-H<sub>2</sub> is determined to be 263.48 t/h and 381.6 t/h, respectively, based on site-specific composition data of gasifying agent and production goal, while unit operation specification data are generic. As for GHG emissions, this stage, like others, involves both direct and indirect emissions. The direct emissions in the hydrogen production stage are mostly from tail gas, which contains a lot of CO<sub>2</sub> but almost no CH<sub>4</sub> or N<sub>2</sub>O. The direct emissions in the hydrogen production stage mainly come from tail gas, which contains a large amount of CO<sub>2</sub>, and almost no CH<sub>4</sub> and N<sub>2</sub>O. The amount of CO<sub>2</sub> emitted to the air is 100,160 kg/h and 62,613 kg/h for UCG-H<sub>2</sub> and SCG-H<sub>2</sub> respectively under the circumstance of capturing 80% of the CO<sub>2</sub> in the tail gas. The captured CO<sub>2</sub> is compressed to 15 MPa and transported as a fluid in its supercritical state.

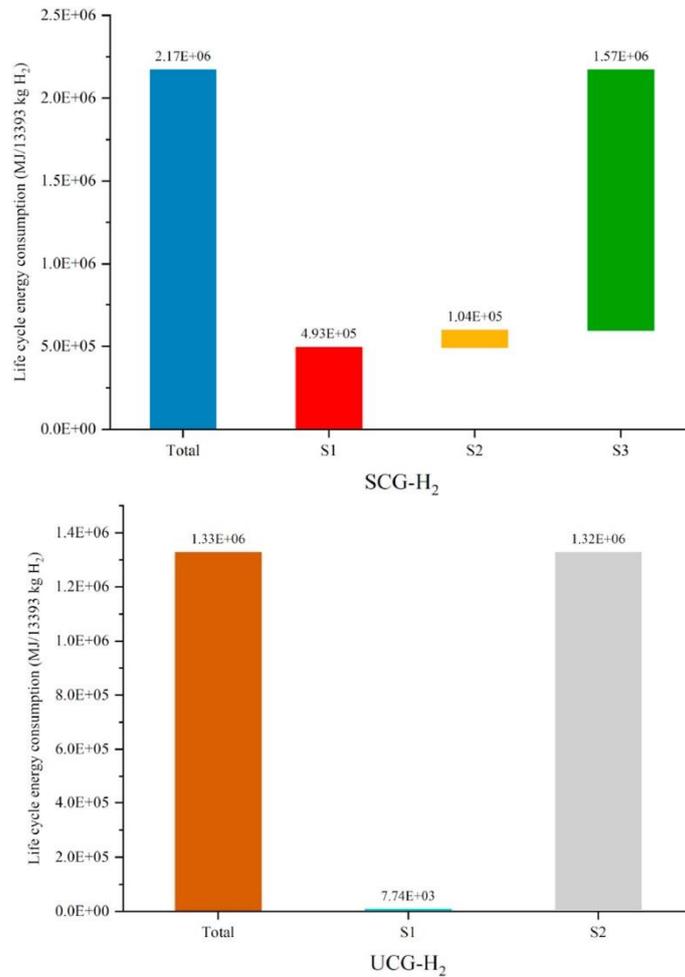


Figure 11 life cycle energy consumption of SCG -H<sub>2</sub> and UCG-H<sub>2</sub> (Liu, 2021)

The GHG emissions of hydrogen production systems are calculated according to Equations above based on the data . According to the calculation results, the GHG emissions of SCG-H<sub>2</sub> and UCG-H<sub>2</sub> are 197,419 and 207,582 kg CO<sub>2</sub>-eq when producing 13,393 kg hydrogen respectively, and the distribution of GHG emissions in each stage is presented in below Fig 11.

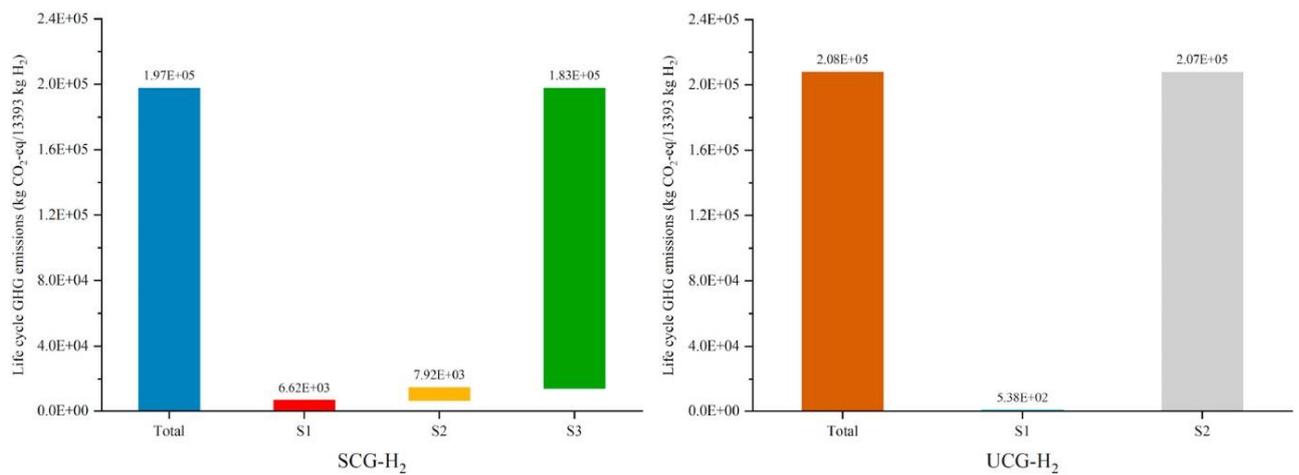


Figure 12 Life cycle GHG emissions of hydrogen production systems (Liu, 2021)

## RESULTS

### COST COMPARISON FOR DIFFERENT HYDROGEN TECHNOLOGIES

Depending on different hydrogen production methods and kind of energy used, final hydrogen costs could be very different. Currently the usage of fossil-based hydrogen production is the cheapest options, but in future the usage of electrolysis increase, its efficiency and as well as increasing number of full last hours could deliver up to 80% hydrogen cost reduction. According to IEA reports that green hydrogen will be cheaper than blue hydrogen from 2030 onwards. By keeping this statement, the calculation is fall in place in this section and compare the different technologies by adopting IEA and IRENA data (see table 4) which shows the significant components of costs for current & future electrolyzer.

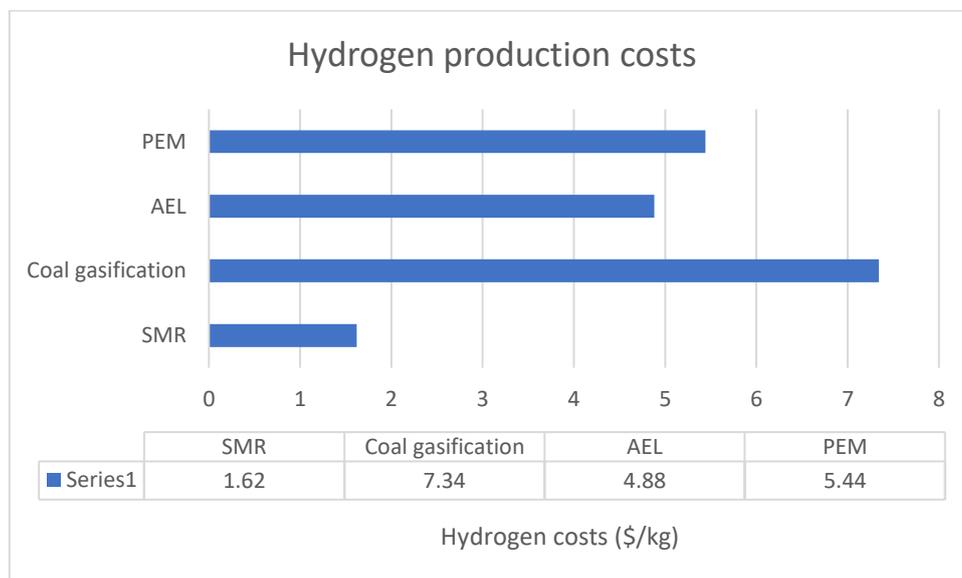
	2020- Alkaline	2020-PEM	2050- Alkaline	2050-PEM
System efficiency(kWh/kg)	50-78	50-83	<45	<45
Lifetime(1000h)	60	50-80	100	100-120
Capital costs (USD/kWe), system size >10MW	500-1000	700-1400	<200	<200

Costs of hydrogen production are very dependent on investment costs of hydrogen production, the cost of electricity used and operating hours of hydrogen production technology. The cost of electricity is dependent on production method, and it will decrease

only if surplus electricity from renewable energy is used. However, the calculation results that are included in this study are black and green and grey hydrogen by using above equation 1.

**Table 14** assumptions taken from (IEA, 2021) (IRENA, 2020)

	SMR	Coal gasification	AEL	PEM
INVESTMENT COST (\$/Kw)	910	2670	2600	2900
OPERATION AND MAINTENNACE COST(€/Kw)	42.77	133.5	39	43.5
EFFICIENCY(LHV)	76	60	65	74
OPERATING HOURS	60	40	40	40
ENERGY PRICE(\$/kWh)	0.03	0.03	0.04	0.04
CAPITAL RECOVERY FACTOR	0.06	0.06	0.06	0.06
HYDROGEN COSTS (\$/kg H2)	1.6232	7.343	4.88	5.44



**Figure 13** graphical representation of calculated hydrogen costs

## LIFE CYCLE ENERGY CONSUMPTION

In this study, the hydrogen production capacity were assumed as 35500 kg/h by consider the above tables in methodology in order to calculate the LCEC of SCG-H2 and UCG-H2. For calculation the adoption values are taken from Liu, 2021. The results shown in below indicates that the LCEC of SCG-H2 and UCG-H2 which are 7889301.92MJ/35500 kg hydrogen and 10323671.9 MJ/35500 kg hydrogen respectively, and the distribution of energy consumption in each stage is shown in below fig 13. As it can see from the results that comparing with SCG-H2, the LCEC of UCG-H2 is much lower, only 59.47%. The reason for this that LCEC represents the external energy demand to satisfy the production goal and for SCG-H2 the required coal for production needs mining and transported before it can be used therefore each stage contributes certain accounts which is 20.92% and 2.92%.

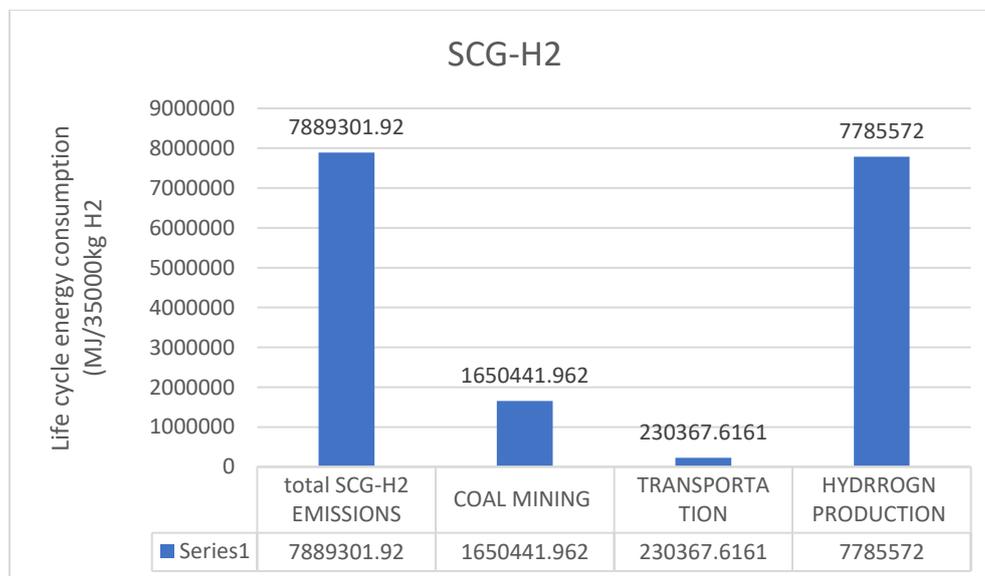


Figure 14 graphical representation of SCG- H2 calculated values

While for UCG-H2 the production required coal can accessed by constructing necessary injection and production wells and channels construction stage plays a similar role with coal mining and washing stage as well as coal transportation stage, but the energy consumption is only 7735.28 MJ/35500 kg of hydrogen accounting for only 0.23% of LCEC OF UCG-H2 which can be ignored.

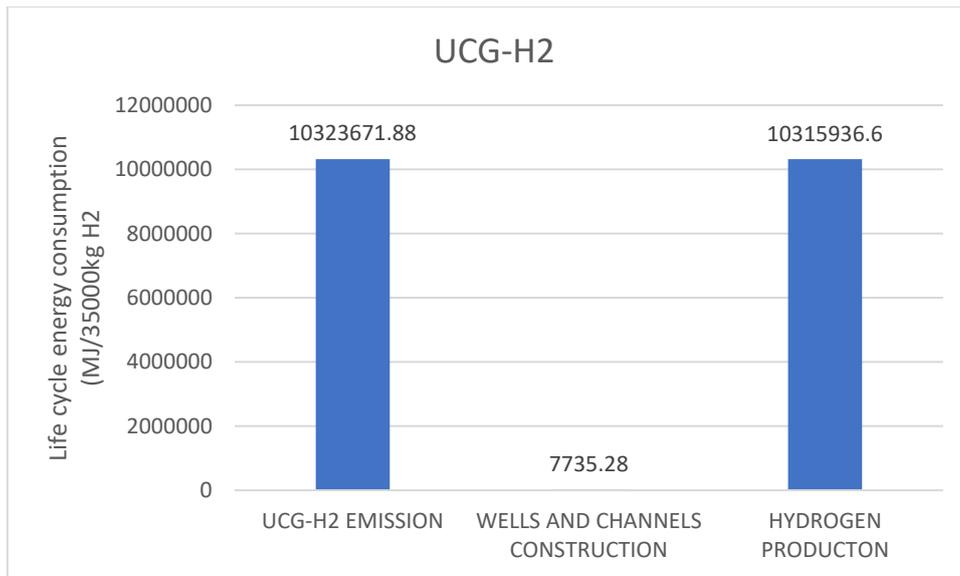


Figure 15 graphical representation of UCG-H2 calculated values

In hydrogen production stage the energy consumption of UCG-H2 is close to that of SCG-H2 which is 10315936.6 and 7785572 MJ/35000 hydrogen respectively, but main contributors are different.

The GHG emissions of hydrogen production are calculated by using above tables. According to the calculation results the GHG emissions of SCG-H2 and UCG-H2 are 495971.4 & 166081.9 kg CO<sub>2</sub>-eq when producing 35500 hydrogen respectively, and the distribution of GHG are presented in below fig 15.

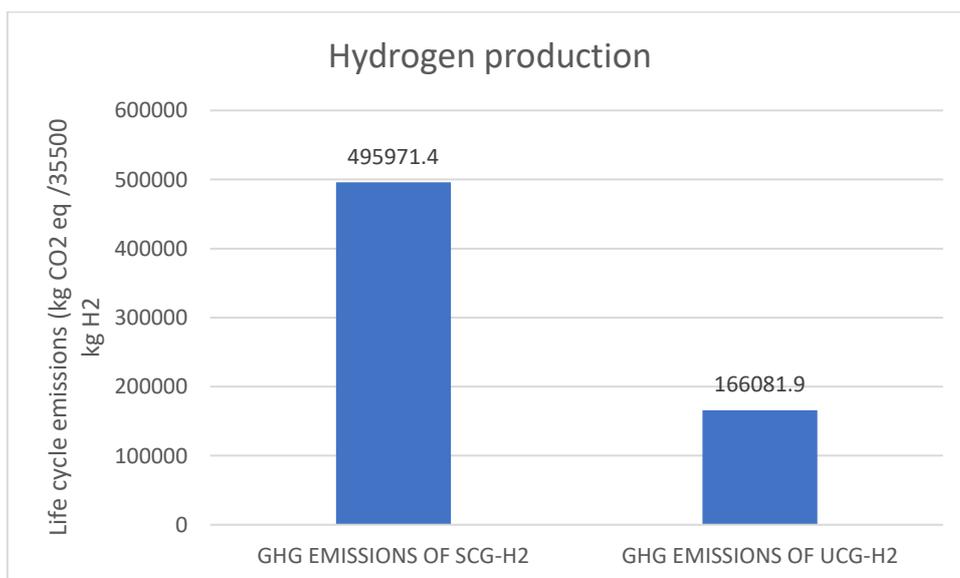


Figure 16 graphical representation of calculated hydrogen production life cycle emissions

As can be seen that the GHG emissions of SCG-H2 and UCG-H2 are close enough to compare and the distributions of GHG emissions are also similar. The observation that can be seen in hydrogen production stage the emissions are occupy a dominant position which accounting nearly 86% and 95% of total emissions respectively.

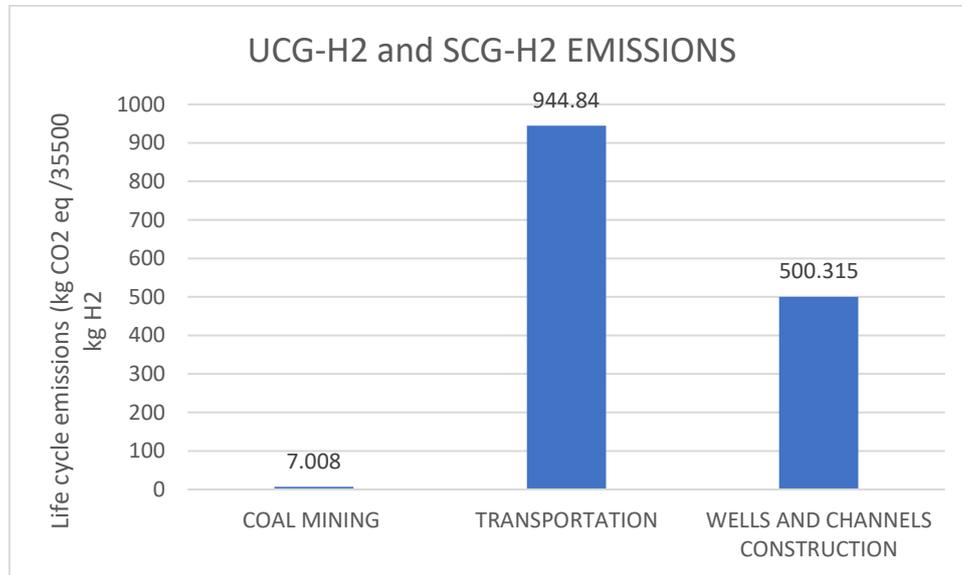


Figure 16 graphical representation of UCG-H2 and SCG-H2 life cycle emissions

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