

Technological Perspectives and Economic Aspects of Green Hydrogen in the Energetic Transition: Challenges for Chemistry

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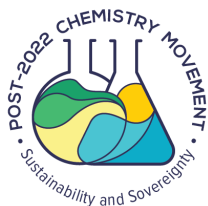
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Green hydrogen is a fuel capable of promoting sustainable energy development and is gaining attention in the current global energy transition framework. The global shift toward decarbonization has triggered a substantial boost in the hydrogen industry. This study presents an overview of the current status of hydrogen production, regulation of the green hydrogen segment, hydrogen storage, distribution, and transportation, and final use and application. We also critically discuss the viability of adopting green hydrogen in terms of possible economic and environmental impacts as well as the main challenges and opportunities it represents for the Chemical Sciences.

Keywords: green hydrogen, energy transition, sustainable development, decarbonization, defossilization, clean and affordable energy

1. Introduction

Since the Paris Climate Agreement in 2015, governments and businesses worldwide have stepped up, taking the actions needed to reach a global average temperature target well below 2 °C above the pre-industrial levels.¹ Several initiatives are related to reducing greenhouse gas (GHG) emissions (CO₂, CO, NO_x, among others) that can occur with the use of technologies aimed at decarbonizing various sectors. Many initiatives have been taken to solve this problem, including encouraging and using biofuels such as biodiesel^{2,3} and ethanol. However, green H₂ has been standing out in recent years due to its properties and application possibilities. The global shift toward decarbonization has triggered a substantial boost in the

hydrogen (H₂) industry. This industry, in turn, offers several alternatives for the use of hydrogen in the transition toward a low-carbon economy: as an energy carrier and storage medium for conversion back to electricity, as a fuel for all modes of transport and mobility, and as a potential substitute for fossil hydrocarbons in industries such as steel and petrochemicals.⁴ H₂ has gained importance because it is a carbon-free fuel with high heating value and a high energy carrier with less volume, which can significantly reduce carbon emissions.⁴

In the last ten years, there has been an apparent increase in interest in research on hydrogen. From 2010 to 2021, the number of published studies on hydrogen more than doubled (Figure 1). VOSviewer software⁶ was used to construct networks of scientific publications about “hydrogen” through a search on the Science Direct platform⁵ clusters which were built using the words used in the titles and abstracts of the works obtained on hydrogen

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(Figure 2a). The formed word clusters show the trends in hydrogen research: as a renewable energy source (signed in red; Figure S1, Supplementary Information (SI) section), as a reagent or product of chemical and physical reactions (green color; Figure S2, SI section), its use in photocatalytic production methods (dark blue; Figure S3, SI section), its use in engines and impact on pollutant emissions (yellow; Figure S4, SI section), its interaction with other materials (purple; Figure S5, SI section), its production through electrochemical reactions using electrocatalysts (light blue; Figure S6, SI section), and ways of storage (orange; Figure S7, SI section). It is interesting to observe in Figure 2b an organization of the clusters formed in relation to the years of publication. The most consolidated themes on hydrogen are closer to the yellow clusters, and the state-of-the-art research is the purple clusters. It means that the topics covered in this review are at the frontier of knowledge about hydrogen, which will be discussed in detail below.

2. The Hydrogen Atom and Molecule

After the Big Bang, the universe was populated by particles such as protons, neutrons, and electrons. In the Nucleosynthesis Era, a sequence of thermonuclear reactions rapidly combined protons and neutrons to give rise to deuterium nuclei and then helium.⁷ So, the hydrogen nucleus

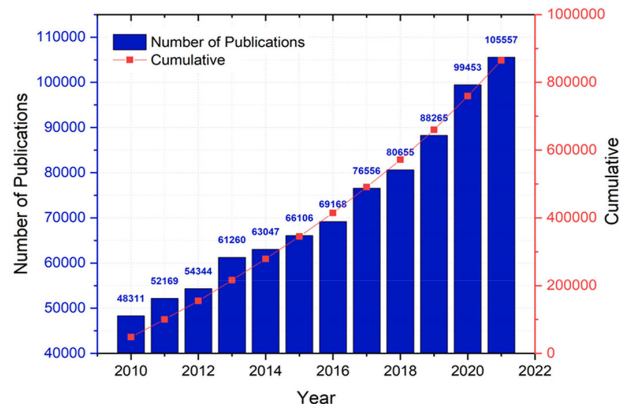


Figure 1. Number of publications on hydrogen *per* year from January 2010 to September 2021. Source: Science Direct Platform⁵ using “hydrogen” as keyword.

with a single proton was the precursor for all other nuclei. Hydrogen is, by far, the most abundant chemical element in the universe, accounting for around 90% of the matter. It is already well established that the stars’ radiant energy derives from internal sources caused by nuclear events in which lighter nuclei as protium are fused to create heavier nuclei releasing the energy stored in the nucleus. In nature, the most common type of explosion with nuclear fusion is the hydrogen-rich core-collapse supernovae, known as type II supernovae, observed in star-forming galaxies by the presence of prominent hydrogen lines in their spectra.^{8,9}

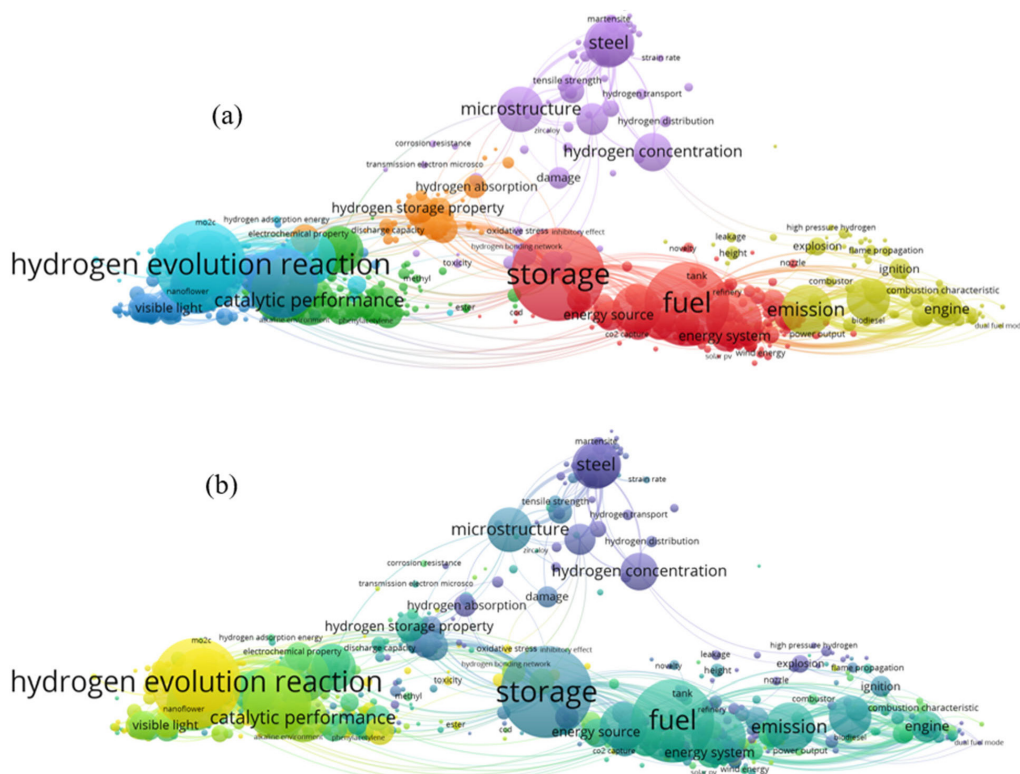


Figure 2. (a) Seven clusters of 725 items using “hydrogen” as the search term and (b) clusters of the evolution of terms over time, which the yellow represents the most consolidated topics.

On Earth, hydrogen is the third most abundant element on the surface when considering the number of atoms and the tenth most abundant by mass. Hydrogen is found in minerals, oceans, fossil fuels, and all living organisms. Hydrogen predominantly occurs as protium, an isotope with a single proton in the nucleus (${}^1\text{H}$ or P), accounting for 99.986%, followed by deuterium atoms (${}^2\text{H}$ or D), in which the nucleus also contains a neutron, accounting for 0.014%. The addition of a second neutron in the nucleus forms tritium (${}^3\text{H}$ or T), a very unstable isotope.

Hydrogen was first isolated and identified by Henry Cavendish¹⁰ in 1766 by reacting several acids with iron, zinc, and tin, showing that it was much lighter than air. Hydrogen was already part of Lavoisier's table of 33 elements, published in his book, *Traité Élémentaire de Chimie*, in 1789.¹¹ Currently, hydrogen occupies the first position in the periodic table of the elements with the simplest electronic configuration, $1s^1$, with a small radius allowing to form more compounds than any other element.

When hydrogen is combined as a diatomic molecule, it forms dihydrogen (H_2), a stable, colorless, odorless, tasteless, and nontoxic gas. As a homonuclear diatomic molecule, dihydrogen shows nuclear spin isomers, *ortho*- and *para*-hydrogen, with parallel and antiparallel spins, respectively. The different internal energies in *o*- H_2 and *p*- H_2 lead to significant differences in physical properties. At low temperatures, the lower energy *p*- H_2 state is favored, and the equilibrium concentration of *o*- H_2 gradually increases until it reaches room temperature, when it contains 75% *o*- H_2 and 25% *p*- H_2 .⁷ The main physical property affected by the nuclear-spin isomerism of hydrogen is thermal conductivity, which is more than 50% greater than for the *p*- H_2 . Dihydrogen is also a nonpolar and poorly polarizable molecule, implying virtually nonexistent intermolecular forces.

Thus, molecular hydrogen is a gas in the standard state with a very low boiling point. When compressed, the gas deviates from the ideal behavior, with a compressibility factor higher than 1 ($Z > 1$, where $Z = \frac{PV}{RT}$, P = pressure; V = volume; T = temperature; R = universal gas constant), indicating that the H_2 molecules repel each other when they are too close. In addition to the low density, these properties make it challenging to store hydrogen gas. Table S1 (SI section) summarizes some important physical properties of hydrogen gas.

The energy within the chemical bond between the hydrogen atoms (Table S1) can easily be transformed into either heat or electricity. In Lavoisier's table, hydrogen was already described as flammable gas, and in the early 19th century, François Isaac de Rivaz developed the first

internal combustion device powered by a mixture of hydrogen and oxygen. The combustion reaction produces water and releases -286 kJ mol^{-1} of energy, equivalent to the energy content of ca. 140 MJ kg^{-1} , which is greater than any other fuel.¹²

The cold electrochemical combustion of hydrogen, or any other gaseous fuel, is the principle of a fuel cell discovered by Sir Grove more than 180 years ago. However, commercial interest only started in the 1960s, when NASA used fuel cells to provide electrical power for spacecraft in the space program.¹³

A direct current is produced in a fuel cell when hydrogen is oxidized to protons in a gaseous diffusion electrode, releasing electrons to the opposite gaseous diffusion electrode, where oxygen is reduced, with water as the final product. The device converts the chemical energy of the hydrogen fuel into electricity. It will continue to generate electricity as long as external fuel and an oxidant are supplied and do not require recharging. In this way, the versatility of hydrogen in energy conversion with zero carbon emission makes it a perfect energy vector when extracted from a decarbonized source. Although it has a flame temperature similar to other fuels, under the presence of ambient oxygen, its propagation, buoyancy, and laminar burning speed are higher compared with other fuels.¹⁴

Among the main advantages of the use of hydrogen is its property of producing carbon-free emissions during combustion. In addition to its high calorific power, hydrogen is the lightest reactive gas, making it very economical to be produced from specific routes, becoming an attractive green energy alternative compared with fossil fuels.¹⁵

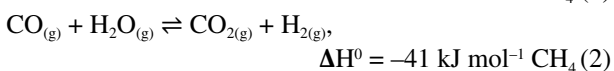
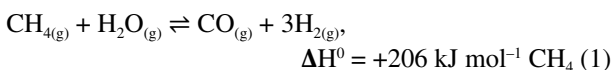
3. Possible Sources of Hydrogen

In nature, hydrogen is associated with other elements such as oxygen in water, carbon in hydrocarbons, and other elements in biomass. Nature has developed its own set of catalysts to produce hydrogen or use it as an energy source, such as hydrogenases. A hypothesis is that the genesis of hydrogenase enzymes probably occurred when the Earth had a hydrogen-rich atmosphere, during the first stages of life on our planet, and existing primitive organisms depended on this molecule as an energy source. This enzyme is found in many microorganisms, mainly archaea, and bacteria, but also in some eukaryotic organisms.¹⁶

Conventional H_2 production technologies include steam reforming of natural gas (methane) and petroleum, catalytic decomposition of natural gas, partial oxidation of heavy hydrocarbons, and coal or coke gasification. These technologies are energy-demanding since high temperatures are applied. In addition, 96% of these H_2

sources come from fossil fuels.^{14,17} Nowadays, the most used and affordable technology to produce H₂ is natural gas reforming, which will likely persist in the near future, although it is linked to various GHG emissions, including carbon dioxide and NO_x.¹⁴

For a long time, H₂ has been produced using fossil fuels as its primary raw material. A classic example is the steam reforming of natural gas (NG), which accounts for 48% of global production.^{16,18} In this process, the methane (CH₄) present in greater amount in NG reacts with water (steam) and produces, in addition to H₂, carbon monoxide (CO), in a second reaction (water-gas shift) reacts with steam producing carbon dioxide (CO₂) and hydrogen (equations 1 and 2).



On the other hand, other methods can be used to produce hydrogen with low carbon content, such as thermochemical biomass conversion, water by electrolysis, and biochemical methods involving bacteria and algae through anaerobic digestion and fermentation.¹⁷ Thus, the conventional methods used for the production of H₂ are (i) thermochemical, (ii) electrochemical, (iii) photobiological, and (iv) photoelectrochemical processes.¹³ Additionally, energy from sustainable resources and water must be used to produce green H₂, also known as H2G. Moreover, hydrogen allows using sustainable energy sources, namely biomass, hydro, geothermal, solar, and wind.^{14,19}

A carbon-free hydrogen society has been the goal of the hydrogen energy transition. Thus, the production of the so-called green H₂ has been approached preferentially based on hydrogen production through the electrolysis of water using renewable energy sources. These processes have been in progress for some time, and the production of hydrogen via alkaline water electrolysis is now a mature technology with commercially available megawatt (MW) scale installations.¹⁹

In this sense, there are two paths to produce “clean” H₂: (i) production from nonrenewable raw material sources (e.g., NG) together with carbon capture and sequestration, or (ii) H₂ production, avoiding and/or minimizing the formation of CO₂ and making use of renewable sources of raw materials (e.g., biomass, biogas, among others) and energy (e.g., solar, wind, among others). The latter include the so-called zero-carbon routes, without CO₂ generation and with low carbon (with CO₂ generation reduced to acceptable levels).²⁰

Using renewable raw material energy sources does not guarantee that CO₂ will not be formed. Examples

are biomass and biogas, which lead to CO₂ formation in gasification and biofuel reforming processes, among others. However, there are cleaner processes (e.g., electrolysis) that can use a renewable energy source and use it to separate the H₂ present in water without forming CO₂. Considering how clean a particular technology is in relation to the H₂ and CO₂ formed has motivated several discussions worldwide to establish international standards that indicate acceptable limits of CO₂ emissions in the production of H₂ by different technological routes.²⁰

The possibility of obtaining “clean” or renewable H₂ with zero or minimal GHG emissions led to the designation “green H₂”. The first reference on this subject is a 1995 publication²¹ that used the term “renewable hydrogen” (hydrogen produced from renewables). As early as 2006, California²² defined green H₂ as the one produced cleanly and sustainably, using renewable energy sources such as solar or wind. The first mention of green H₂ in the European Union (EU) was in a document establishing the green H₂ economy in Europe.²³ It is possible to find several definitions of green H₂ in the literature, according to the type of energy source and GHG emissions as any:²⁰ (i) renewable source; (ii) renewable energy source with an explicit mention of air pollution, safety, and global climate issues; (iii) renewable energy source with an explicit mention of low GHG intensity factors; (iv) renewable source or other zero carbon energy grid with carbon capture and sequestration and/or emissions offsets; (v) renewable and nuclear source; (vi) source (renewable or not) with low-intensity GHG emissions; (vii) low carbon energy source with low environmental impact.

There is a better agreement in recognizing that green H₂ requires using renewable sources, either with or without paying attention to GHG emissions. “Renewable sources” are well defined in the EU Directive 2018/2001/EC (or RED 2).²³ However, from a legal point of view, additional eligibility criteria such as carbon emission intensity limits may be interpreted differently by governments and standards or certification bodies.

Furthermore, there is still no consensus around the world regarding criteria, standards, norms, and legislation that define and certify how green or sustainable a particular route or process is for H₂ production.²⁰ The lack of a global green H₂ market has been driving several national and international standardization entities intending to facilitate a green H₂ market with a regional and global scope.

3.1. Color-coded hydrogen classification

Just as the term “green hydrogen” has been used, there is an expanded color-based hydrogen nomenclature according

to its energy source, production route, and GHG footprint (Figure 3).²⁴⁻²⁶ Green hydrogen, the main focus of the present study, is produced from water electrolysis powered by electric energy generated from renewable sources, such as wind, solar, hydro, geothermal, and tidal. It is considered to be zero or minimal carbon emissions.

By the Figure 3 we can identify a palette of at least eight different colors of hydrogen, and among them, green hydrogen. Keeping in mind there is no harmonized systematically defined color-classified hydrogen gas internationally, some definitions may be overlapping to each other or even ambiguous, depending on the interpretation of a given stakeholder^{20,27-30} or researcher. In this classification (Figure 3), the black/gray, brown, blue, and turquoise hydrogen are generated from fossil fuels while the green, yellow, and pink/purple/red hydrogen are generated from water electrolysis. In addition, white hydrogen is produced as a byproduct of industrial processes.

Accordingly, brown hydrogen is a product of coal gasification, and black/gray hydrogen is a product of natural gas reforming. Both of them are related to high GHG footprints.³⁰ In turn, although blue and turquoise hydrogen also are derived from fossil sources, they are considered low-carbon emission if about 90% of the generated GHG is sequestered by carbon capture, and storage (CCS).^{28,31} Indeed, if applying an efficient CCS step, blue hydrogen becomes sustainable, possibly achieving negative-carbon emissions.²⁹ Turquoise hydrogen is produced by natural gas pyrolysis, yielding solid carbon as byproduct, which can be repurposed in the industry sector.

Yellow hydrogen is produced by water electrolysis powered by grid electricity of a given country or region. Grid electricity may be variable (mixed-origin) energy, depending on the electric energy matrix considered. For instance, for a country which has a high share of

renewables (such as hydroelectric or solar power, among others) in their grid, in terms of carbon footprint, the yellow hydrogen generated may be considered “greener” than the yellow hydrogen generated from a grid electricity which is derived from other energy sources (i.e., thermoelectric). In turn, pink hydrogen is also produced by water electrolysis, but powered by nuclear energy. Since the current nuclear energy technology is based in nuclear fission of radioactive elements, it is not a carbon-related energy source. For this reason, even though there is a negative sense associated to nuclear power, mainly derived from the associated to long-lived radioactive waste and the Chernobyl (1986) and Fukushima (2006) accidents, nuclear power is considered a clean and sustainable way of producing hydrogen. Some advantages of using nuclear fuel are: (i) it is a kind of very dense energy, so it produces minimal waste;³² and (ii) its GHG emission is virtually inexistent.^{31,33,34} In terms of decarbonization and climate neutrality, nuclear-produced hydrogen is considered sustainable if the radioactive waste is disposed correctly (following the strictest international legislation). Indeed, in February 2022 the European Commission³⁵⁻³⁷ has agreed with this argument although some critics have declared it as “greenwashing”.³⁸

From the color classification for hydrogen (Figure 3), probably the most confuse denomination is the one from the white hydrogen due to multiple concepts found in the literature. According to NACFE,²⁴ OceanBased Perpetual Energy,²⁵ and GEI,²⁶ the definition of white hydrogen is the one formed as byproduct of industrial processes. For instance, startups are developing a closed loop plastic depolymerization industrial process. This process yields a syngas.³⁹ This syngas can be transformed into a variety of substances, and among them, methane, and white hydrogen. This innovative route is environmentally beneficial in different ways: (i) since it is a closed-loop process,

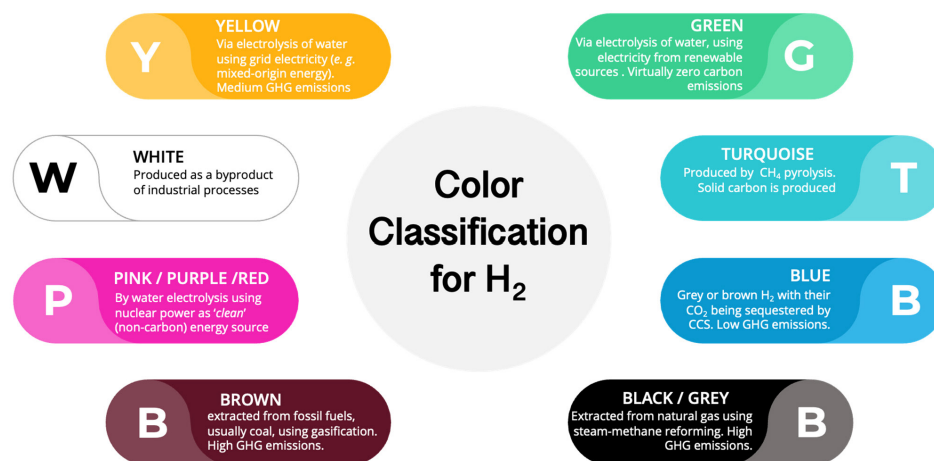


Figure 3. Color spectrum classification for hydrogen gas according to its energy source, production route, and GHG footprint (adapted from NACFE,²⁴ OceanBased Perpetual Energy,²⁵ and GEI).²⁶

virtually no emissions are released; (ii) it reutilizes end-of-life plastic residues accumulated in the environment; and (iii) it generates methane and hydrogen which can be repurposed to generate energy in different ways. The hydrogen produced by the mentioned route is classified as white since it is an industrial byproduct. On the other hand, white hydrogen is also defined as “a naturally-occurring geological hydrogen found in underground deposits and created through fracking” by some other entities and organizations.⁴⁰⁻⁴² The search for viable strategies for storage of H₂ in underground deposits is still a challenge. However, considering fracking is an industrial process to exploit unconventional fossil fuels from shale formations, the first definition of white hydrogen is correctly applied for both cases.

4. Regulation of the Green Hydrogen Segment

The transition from a carbon-based energy matrix to matrix-supported hydrogen energy from a renewable source brings a discussion of a regulatory framework to guarantee the sustainable character of these primary energy sources. In addition, it involves the inclusive participation of all regions of a country.

The design of the developmental model of this new era, with a focus on energy and socio-environmental sustainability, is under construction. It will demand from all of us (academia, governments, industry, and society) the elaboration of a regulatory framework that gives direction, pace, and long-term vision compatible with environmental, social, and governance (ESG) criteria, in a circular economy with conscientious consumption. In addition to the criteria described above, this new regulatory framework must consider the technical and safety peculiarities of this vector (H₂) with its positive externalities and aspects to be mitigated, always with broad participation from organized society.

In global terms, this discussion demands each established form of government interacting with their regulatory agencies,⁴³ with the legislative houses, universities, research institutions, and representative associations of the industrial and commercial segments to give legitimacy to the new standards and ensure that they will be accepted. In Brazil, notably the regulatory agencies ANEEL (Brazilian Electric Energy Agency) and ANP (Brazilian Agency for Petroleum, Natural Gas and Biofuels) together with the other relevant actors (federal government, legislative representatives, private sector, and research institutions) are central for those discussions.

It is immediately necessary to identify regulatory gaps that inhibit investment and rules that make it challenging

to install plants that produce green hydrogen using the infrastructure available in the country (or even prevent their installation). The vision must be comprehensive regarding the green hydrogen production chain and its current and future uses to create an environment of greater legal security for investors in this new market.

Among the gaps that already exist, the lack of criteria for clean and renewable energy injected into the national interconnected system (SIN) can be removed from the same submarket, maintaining its original characteristics and giving the products derived from it all the attributes of sustainability, subsequently enabling the certification of a green product.⁴⁴

The fiscal and tax aspects should deserve special attention, compatible with the effort to carry out an energy transition without losing sight of the fact that eventual trade barriers can strongly affect the current Brazilian export agenda, which is still largely carbonized. Encouraging policies for the decarbonization of our production has become urgent, in line with the expansion of green hydrogen production in Brazil.

5. Hydrogen Preparation in the Bench and Industrial Scales

Hydrogen preparation methods including low- to zero-carbon energy sources is gaining the interests of the energy sector. Worldwide, it has been achieved when the hydrogen production plant is linked with renewable or nuclear energy.^{20,27-30} Yet, biological processes are proving to be promising alternatives for sustainable hydrogen production using renewable energy sources, especially concerning waste use and management.

Moreover, the so-called biohydrogen is produced from the conversion of water molecules and organic substrates into hydrogen, by the action of microorganisms, through the catalytic activity of two main enzymes, hydrogenase and nitrogenase.¹⁹ The possibility to use waste resources such as wastewater significantly contributes to sustainable H₂ production. In addition to the use of low-cost substrates and energy sources, this route can contribute to the major environmental issue of waste management.¹⁹ Although the most suitable energy sources for H₂ production are wind and solar energy, as they have been considered more suitable for this purpose, studies have been conducted regarding combining renewable energy sources (such as solar and geothermal).¹⁹ In general, green H₂ can be produced from different energy sources and renewable raw materials.

In general lines, Table 1 presents the main green H₂ production methods with their respective classifications.

Currently, more than 95% of H₂ is produced from fossil fuel thermochemical reformation, accounting for around 3% of global CO₂ emissions *per* year. But there are relatively unused technologies to produce clean hydrogen from water that show great promise in the near term.⁴⁵ These, so far, relatively small-scale hydrogen production technologies based on water splitting comprise different methods, such as electrolytic, thermochemical, photoelectrochemical, photocatalytic, and photobiological methods.⁴⁶ Water is the most abundant hydrogen decarbonized source. However, extracting hydrogen from a very stable molecule demands a great amount of energy, since hydrogen and oxygen are strongly bonded to each other (O–H bond, ΔH = 464 kJ mol⁻¹). Splitting water into H₂ and O₂ is an endergonic process (reaction 3), which means it is a thermodynamically non-spontaneous reaction where ΔH° (enthalpy) = 286 kJ mol⁻¹, ΔG° (Gibbs free energy) = 237 kJ mol⁻¹, E°_{overall} (overall standard potential) = -1.23 V, and hv (λ ≅ 1000 nm).



The primary energy source supplied to break the O–H bond will determine how clean the hydrogen produced by water splitting will be. Electrical, thermal, nuclear, or photonic energy can be used to generate hydrogen from water (equation 3).

5.1. Electrochemical method

Electrolysis was first performed in 1802 by Sir Humphrey Davy, who noted that a galvanic cell could produce hydrogen and oxygen.⁴⁷ Many different electrolyzer designs were developed in the 1920s and 1930s.⁴⁸ Nowadays, electrolysis is the most well-established technology for producing hydrogen from water. Water electrolysis involves the hydrogen (H₂) evolution reaction on a cathode and the oxygen (O₂) evolution reaction on an anode driven by electrical energy in an electrolytic cell.

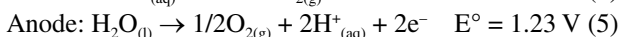
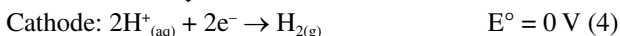
Table 1. Classification of green H₂ production methods

| Type of energy used | H ₂ production method | Raw material | |
|--|--|---|--|
| Electric | electrolysis | water | |
| | plasma arc decomposition | natural gas | |
| | thermochemical processes | – | |
| | with catalysis | H ₂ S splitting water splitting biomass conversion | H ₂ S water biomass |
| Thermal | without catalysis | water splitting gasification reform H ₂ S splitting | water biomass biofuels H ₂ S |
| | Photonics | photovoltaic electrolysis | water |
| | | photocatalysis | water |
| | | photoelectrochemical | water |
| biophotolysis | | water | |
| Biochemical | dark fermentation | biomass | |
| | enzyme | water | |
| Electric + thermal | high temperature electrolysis | water | |
| | hybrid thermochemical cycles | water | |
| | catalytic term cracking of fossil fuels (with CO ₂ capture and storage) | fossil fuel | |
| | coal gasification (with CO ₂ capture and storage) | water | |
| Electrical + photonics + biochemistry + thermal | fossil fuel reform | fossil fuel | |
| | photoelectrolysis | water | |
| | thermophilic digestion | biomass | |
| Photonics + biochemistry | biophotolysis | biomass, water | |
| | photofermentation | biomass | |
| | artificial photosynthesis | biomass, water | |

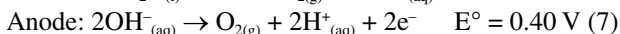
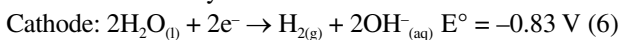
Source: adapted from Dincer³¹ and El-Emam and Özcan.³³

The half-reactions and respective standard potential (E°) at 25 °C and 1 atm in acid and alkaline electrolytes are written as follows (equations 4 to 7):

In acidic electrolyte



In alkaline electrolyte



In both acidic and alkaline electrolytes, the overall reaction, and the theoretical decomposition voltage (1.23 V) are the same (equation 3). However, in practice, when the theoretical decomposition voltage is applied to the electrolytic cell, water electrolysis is kinetically reversible, and additional overpotentials (η) are required to overcome the energy barrier for both cathode and anode reactions.^{49,50} The magnitude of the overpotential is highly dependent on the cathode material and thus can be divided into three classes: (i) metals with high overpotential, such as Cd, Tl, Hg, Pb, Zn, Sn, among others; (ii) metals with medium overpotential, Fe, Co, Ni, Cu, Au, Ag, and W; and (iii) metals with low overpotential, Pt, and Pd.⁵¹

The first technology available on the market for water electrolysis was the alkaline electrolysis cell (AEC) because alkaline electrolytes are less corrosive than acidic ones (Figure 4). Presently, the most widely used cathode material in AECs is nickel or its alloys with molybdenum.⁵⁰ AEC technology is the most commercially established. However, the limited current densities (below 400 mA cm⁻²), low operating pressure, and low energy efficiency led to a new approach with the development of an anion exchange membrane (AEM) built of polymers with anionic conductivity (Figure 4).⁵² With the same operating principles, proton exchange membrane (PEM) electrolysis was conceived by Grubb⁵³ in the 1950s

and developed by General Electric in 1966, using proton conductor membranes (Figure 4).⁵⁴ PEM water electrolysis has significant advantages over AEC, such as high current density (above 2 A cm⁻²), high efficiency, and fast response. Even though PEM overcomes the drawbacks of alkaline water electrolysis, it is more expensive, mainly due to the high cost of the electrode materials based on platinum for the cathode and iridium for the anode (Figure 4).⁵²

Besides AEC, AEM, and PEM technologies, solid oxide (SOC) electrolysis and microbial electrolysis (MEC) cells are also in development. The SOC cathode and anode are isolated by solid electrolyte and operate at high temperatures (600-1000 °C). In SOC, water is decomposed to H₂ and O²⁻ on the cathode, and oxide ions are transported through the solid electrolyte to the anode, where they are oxidized to O₂.⁵⁰ MEC can produce hydrogen gas from organic matter in wastewater using exoelectrogenic microorganisms on the anode.⁵⁵

Although water electrolysis has been known for more than 200 years and is the most popular among all water-splitting methods, it still contributes to only 4% of the total hydrogen production worldwide because the production cost is much higher than that for reforming fossil fuels. So, extracting hydrogen from water at a large scale in a sustainable way is still a challenge for chemistry. Sustainable electrolysis based on solar and wind energy can produce hydrogen with high purity and is a green and straightforward process (Figure 4). Undoubtedly, using renewable energy sources to produce clean H₂ with water electrolysis is the main path in the energy transition to the so-called hydrogen economy.

5.2. Thermochemical method

The endothermic reaction of water splitting also can be driven by heat. However, for water splitting (equation 1) to become a spontaneous reaction, it is required to raise

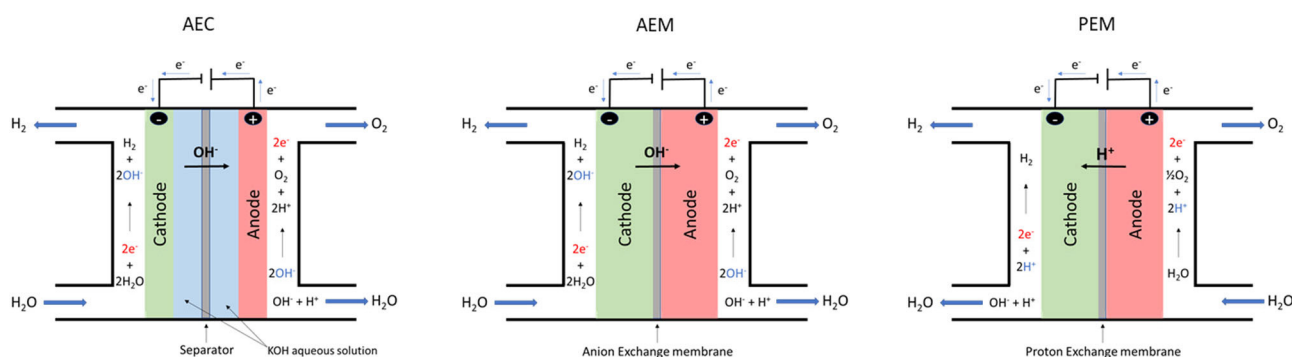


Figure 4. Schematics of electrolytic cells main types, alkaline electrolysis cell (AEC), alkaline electrolysis cell with anion exchange membrane (AEM), electrolysis cell with proton exchange membrane (PEM).

the temperature to at least 2000 K (1 atm), when free energy variation is negative and temperatures up to 4260 K are necessary to obtain a 50% hydrogen yield.⁴⁹ Moreover, at such temperatures, it is challenging to separate hydrogen and oxygen in time, which results in a mixed gas prone to explosion. The thermochemical cycle technology introduced by Funk and Reinstrom⁵⁶ in the 1960s is an alternative to the high temperatures required for water thermolysis.^{56,57} The reaction temperature in thermochemical cycles for hydrogen production, around 1100 K, matches the high-temperature thermal energy provided by nuclear power plants or solar energy.⁵⁸ The thermochemical cycle process is still in the research stage, in which hydrogen and oxygen are indirectly obtained through water splitting through cyclic chemical reactions that require heat. Except for water, all the other chemicals in a thermochemical cycle can be continuously recycled through repetitive series of chemical reactions using intermediate reactions and substances recycled during the process.⁵⁹ Among the thermochemical methods for water splitting, the most studied are two-step and three-step cycles.

In a two-step thermochemical cycle, a metal oxide (M_xO_y) acts as an intermediate medium for the decomposition of water. In the first step, the higher-valence metal oxide is initially thermally reduced to a lower-valence metal oxide in an endothermic process to produce oxygen, which requires temperatures higher than 1500 °C. In the second step, the lower-valence (or zero) metal oxide is oxidized in an exothermic process to produce hydrogen through water splitting, which generally requires temperatures lower than 1000 °C (Figure 5). The reduction and oxidation reactions are represented in equations 8 and 9, respectively.

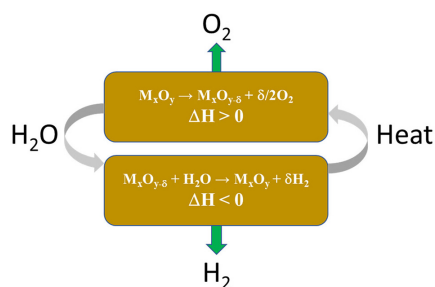
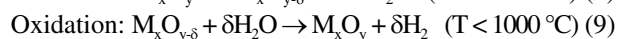
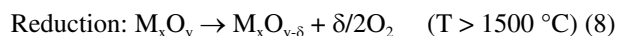
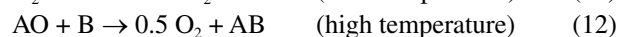
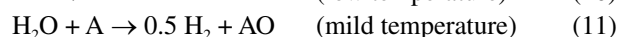
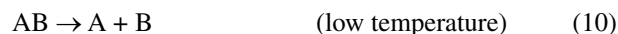


Figure 5. General scheme of a two-step thermochemical cycle.



Several candidates have been proposed for use as redox material in the two-step thermochemical cycle for water splitting metal oxide based redox pair reactions, including ZnO/Zn, Fe₃O₄/Fe, SnO₂/SnO, CeO₂/Ce₂O₃, Mn₂O₃/MnO, Co₃O₄/CoO, CdO/Cd, and GeO₂/GeO.⁵⁷⁻⁵⁹

A three-step thermochemical cycle can be derived from a two-step thermochemical cycle in which the highest temperature reaction is replaced by a two-step reaction process as follows:



Currently, many three-step thermochemical cycles are under research and development. Among them are the sulfur-iodine (S-I), copper-chlorine (Cu-Cl), and magnesium-chlorine (Mg-Cl) cycles.⁶⁰ In the most advanced stage is the iodine-sulfur cycle, initially proposed in the 1970s by General Atomic.⁶¹ Countries such as Japan, the USA, France, and China have conducted investigations of a scaled-up S-I thermochemical cycle. The results predict an efficiency of 52% when a high-temperature nuclear reactor is integrated with this cycle.⁵⁷ Figure 6 illustrates the main steps of the S-I thermochemical cycle, in which the maximum reaction temperature is 850 °C, compared with 530 °C in the Cu-Cl thermochemical cycle, but the latter involves an electrolysis step. The Mg-Cl thermochemical cycle is another low-temperature cycle that operates at maximum temperatures within 450-550 °C.⁴⁷ Cu-Cl, Mg-Cl, and S-I thermochemical cycles are considered more promising than others, but further research is needed to address the higher efficiency and lower cost to produce hydrogen on a large scale.

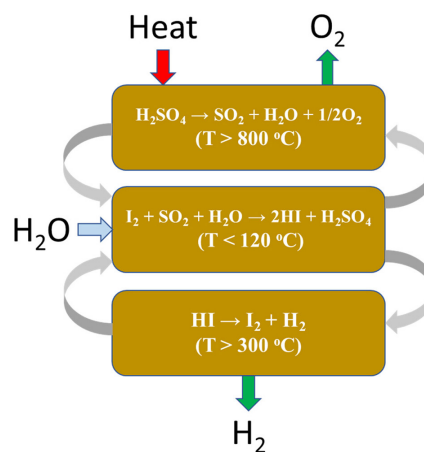


Figure 6. Scheme of a three-step S-I thermochemical cycle.

5.3. Photocatalytic method

Artificial photosynthesis is considered ideal since this process can capture solar energy and directly convert it into strategic fuels such as hydrogen and non-fossil hydrocarbons.⁶² Photocatalytic H₂ production is a form of artificial photosynthesis inspired by nature that is widely

exploited in the generation of H₂ based on water splitting assisted by a semiconductor particle, which acts as an artificial leaf. The photoelectrolysis of water was first reported by Fujishima and Honda⁶³ in 1972 using TiO₂ (semiconductor electrode) connected to a platinum counter-electrode exposed to ultraviolet radiation. A semiconductor particle with a small amount of a noble metal, such as platinum, deposited on the surface is essentially a miniature photoelectrochemical cell; water is oxidized directly on the semiconductor surface and reduced on the noble metal surface (Figure 7).

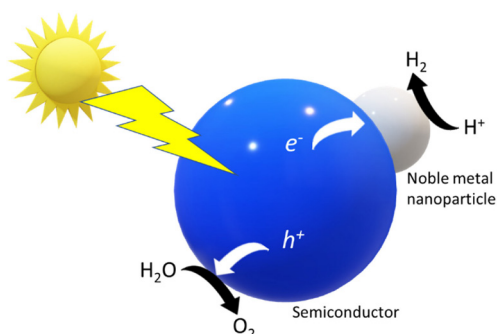
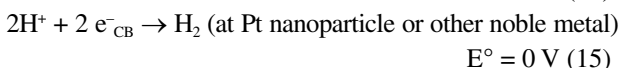
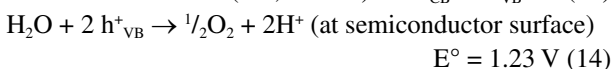
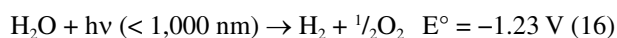


Figure 7. Schematic representation of photocatalytic water splitting on a semiconductor powder particle with co-catalyst (noble metal nanoparticle).

The decomposition of water molecules to produce hydrogen and oxygen is an uphill reaction ($\Delta G^\circ = +238 \text{ kJ mol}^{-1}$; $E^\circ_{\text{overall}} = -1.23 \text{ V}$; equation 3), a semiconductor can conduct it with suitable band potential and incident light with a wavelength shorter than 1000 nm (i.e., 1.23 eV ca. 1000 nm), the energy required to split water. In order to achieve the overall water splitting, the bottom of the semiconductor's conduction band must be located at a more negative potential than the reduction potential of H⁺ to H₂ ($E^\circ = 0 \text{ V vs. NHE}$ (normal hydrogen electrode) at pH 0). On the other hand, the top of the valence band must be more positively positioned than the oxidation potential of H₂O to O₂ ($E^\circ = 1.23 \text{ V vs. NHE}$).^{64,65} The energy required to split the water molecule matches the UV-visible-near-infrared (NIR) light found in sunlight, composed of 5% ultraviolet, 43% visible, and 52% infrared light.⁶⁶ The photocatalytic process allows water to be decomposed into oxygen and hydrogen at room temperature without the application of external voltage, according to the following equations:



The overall reaction is:



Thus, water splitting using particulate photocatalysts is a possible mean of achieving solar hydrogen production. On the other hand, the complete oxidation of an organic compound to CO₂ and H₂O in the presence of oxygen is a down-hill reaction ($\Delta G < 0$). However, the free energies of the reforming reaction can be positive, as is the case of reforming glycerol and ethanol (4 and 97 kJ mol⁻¹, respectively). Such reactions, and the reforming reaction of other biomass derivatives, can also be induced by photons using semiconductor particles irradiated with ultraviolet or visible light. The combination of water photolysis and photodecomposition reactions of organic compounds in a photocatalytic cell under anaerobic conditions leads to H₂ and CO₂ production.⁶⁵ Several studies demonstrate that it is possible to obtain H₂ from the photocatalytic reforming of an aqueous solution of biomass derivatives under ambient conditions.^{65,67,68} In addition to biomass derivatives, it is also possible to use wastewater with a high organic matter content and reduced sulfur compounds as sacrificial agents (hole scavengers).⁶⁸⁻⁷¹ Hole scavengers increase the half-life of electrons in the conduction band, increasing the efficiency of photocatalytic hydrogen production.

A wide variety of photocatalysts semiconductor has been investigated so far, such as chalcogenides (ZnS, CdS, CdSe, MoS₂),⁷²⁻⁷⁵ metal oxides (TiO₂, SnO₂, BiTaO₄, ZnO, LaFeO₃, ZrO₂),⁷⁶⁻⁷⁹ carbonaceous materials (g-C₃N₄),^{80,81} solid solutions (Cd_xZn_(1-x)S_ySe_(1-y))⁸¹ and metal-doped semiconductors (SrTiO₃:Al, Cd-SnO₂/CdO/CdS).^{68,69} The best choice to produce photocatalysts for water splitting is not to use toxic chemical methods or metals, so the hydrogen produced will, in fact, be green.

Several methods have been proposed and applied for hydrogen production, as mentioned. Recently, studies^{82,83} have highlighted the possibility of H₂ production via the photocatalytic route from glycerol, a byproduct of biodiesel production.

5.4. Gray, blue, and green hydrogen

As presented in Figure 8, according to CertifHy, one possible certification for hydrogen production,¹⁸ blue H₂, is produced by non-renewable raw materials and energy (e.g., NG) and whose CO₂ emissions are below 36.4 g CO₂ eq MJ⁻¹ H₂. Interestingly, in Figure 8 it is presented that by replacing gray hydrogen by blue hydrogen, there is an estimative of 60% reduction in the GHG emissions, with a low-carbon threshold value of 36.4 g CO₂ eq MJ⁻¹ H₂ has been proposed by some experts

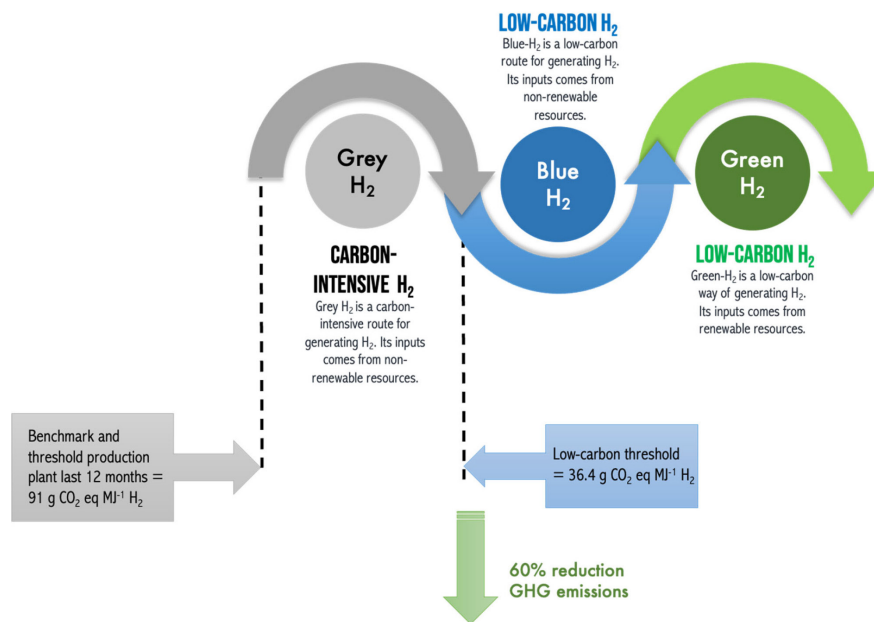


Figure 8. Categorization of hydrogen according to its source of energy and emission intensity (adapted from Velazquez and Dodds).²⁰

as a “quantitative criteria” to a given hydrogen production route to be classified as a “low-carbon” technology.^{20,34}

The production of green hydrogen in the short and medium-term has been debated, and many companies favor its use for several reasons. Initially, it was argued that the high cost and lack of standardization and definitions regarding the demand price limited the end-use sectors where H₂ can be more impactful. Without the necessary demand, investments in new or upgraded production lines and distribution networks, and new storage infrastructure, become unjustified.²⁰

International consortia such as the Hydrogen Council⁸⁴ and industries, and intergovernmental strategies such as the European Union Hydrogen Backbone Project, have already started investment actions to transform the hydrogen economy. Each believes that this transformation should occur gradually in the order: gray → blue → green (Figure 8). This strategy has three limitations that can be overcome with continued use of blue H₂: (i) the availability of resources varies geographically; (ii) there are energy inefficiencies in the electrolysis process; (iii) the H₂ supply is intermittent due to the constant demand for use of the product.

Furthermore, the production of H₂ requires an abundant amount of low-cost water or simple hydrocarbons (preferably methane). Green H₂ consumes at least 9 kg of water *per* kg of H₂, while gray and blue H₂ require half this amount (when produced by steam reforming methane with a gas-water exchange reaction). As already discussed, water is a limited resource in many regions, with uses in several sectors, such as energy, agriculture, and sanitation.

In many regions, the scarcity of this resource does not allow for the production necessary to meet local demand. In addition to the higher water consumption, green H₂ requires approximately 11 times more energy *per* unit of H₂ produced when compared with non-renewable routes (before carbon capture), which need to be cheap.⁸⁵⁻⁸⁷

Greening the global H₂ supply would require approximately 3.90 TWh of electricity annually, representing 60% more than the combined energy generated globally by wind and solar photovoltaics in 2020 (2.44 TWh).⁸⁶

Currently, electrolyzers can only reach the competitive limit of USD 2 kg⁻¹ when operating on “free” electricity 30% of the time or more, dramatically limiting the supply of H₂. In 2020, without the necessary demand, 1.6 TWh of renewable energy had to be wasted by the California Independent System Operator (CAISO), an amount corresponding to 28.9 kt H₂. However, CAISO data show that only 50 MW electrolyzers could achieve a capacity factor of 30% of the wasted energy, enough to produce only 451 t of H₂.⁸⁶

While H₂ is seen as an alternative to reduce the waste of excess renewable energy (for more information, read about renewable curtailment), converting the excess energy into H₂ may subsequently reflect losses of up to 70% in turbines or fuel cells (energy → gas → energy).

The simplest solution to avoid wasting energy would be to increase demand. The problem lies in a business model that focuses on the worldwide use of electrolyzers, whose production cost is not yet appealing for industries to start buying energy to produce green H₂ continuously, thus causing intermittent production. On the other hand, blue H₂

is not associated with the electricity supply network, has a low cost, and can be continuously produced, as NG is also continuously produced in several locations.⁸⁸

In summary, the main purpose of using H₂ is to decarbonize the economy, and it makes sense to use the H₂ that offers the most significant environmental benefit. However, there are cases where the use of blue H₂ is more appropriate. For instance, if a natural gas plant has access to the entire transport infrastructure, it makes sense to use this H₂, contributing to emission reductions with a carbon capture process. Regardless of whether H₂ is green or blue, caution must be exercised when embarking on projects aimed at building new transport networks or H₂ plants based on non-renewable sources, due to the high construction cost of new infrastructure and the long-time horizon of these projects. It is necessary to include in the equation whether the option for blue H₂ with carbon capture will justify the investment in the long term.⁸⁸

5.5. Biohydrogen

The use of a wide variety of biologically available raw materials contributes to improvements in the energy and socioeconomic sphere of developing countries, such as Brazil.

The H₂ production can take place with virtually any raw biomaterial. In Brazil, due to its wide availability, ease of production, operation, and high conversion to H₂, ethanol has been the most promising raw biomaterial. Table 2 presents the top ten ethanol producers in the world.

The production of pure H₂ (99.99 vol%) has been shown to be an interesting alternative through the introduction of ethanol pre-treatment and pre-reformation to the reforming methane steam process. This route can be intensified by including palladium (Pd) membranes, which are selective to H₂, as already reported in the literature.⁸⁹ It has also proved to be a competitive route as the carbon market consolidates and membrane costs decrease.

Table 2. Ten largest bioethanol producers in the world

| Country | Production in 2016 / (× 10 ⁹ L) |
|-------------------|--|
| USA | 57730 |
| Brazil | 27616 |
| Europe | 5213 |
| China | 3199 |
| Canada | 1651 |
| Thailand | 1219 |
| Argentina | 1113 |
| India | 852 |
| Rest of the world | 1855 |

Source: adapted from Mosca.⁸⁹

A very promising route is hydrogen production by anaerobic digestion (AD).⁹⁰⁻⁹² Among the many other biotechnological processes for H₂ production, also known as dark fermentation, it is the most robust process, as it can convert all types of biomass, including food and agricultural waste, sewage sludge, and distillery waste, among others, into biogas that contains CH₄ and H₂.⁹³

The AD process does not require sunlight, requires moderate process conditions, and has lower energy demands. Furthermore, this process' hydrogen yield and hydrogen production rate are more attractive than other processes.⁹⁴ A complete review of AD applied to biogas production covered all aspects, such as factors affecting efficiency (temperature, pH, C/N ratio, organic loading rate (OLR), and retention time), accelerators (green biomass, pure biological culture, and inorganic additives), reactors (conventional anaerobic reactors, sludge retention reactors, and anaerobic membrane reactors), and biogas processes.⁹⁵

6. Hydrogen Storage

Storage of chemical energy (including H₂) represents the only technically feasible and scalable approach to interseason storage of renewable energy, but this only makes sense if the renewable energy supply exceeds 70% of demand. Thus, it is unlikely that the excess supply of renewable energy will somehow accelerate the use of green H₂ in the short term.⁹⁶

There are different ways of storing H₂: compressed hydrogen gas reservoirs, liquid hydrogen reservoirs, metal hydrides, carbon adsorption, and microspheres. Compressed hydrogen gas reservoirs are the most commonly used for high-pressure gas storage. Most vehicles powered by fuel cells use this form of hydrogen storage in cylinders, similar to those used with compressed natural gas.^{97,98}

High-pressure cylinders typically store hydrogen at a pressure of 3600 psi (250 bar), but some cylinders can handle 5000 psi (350 bar). However, there has been the development of new materials in order to increase the storage capacity, and consequently the pressure, so that explosions do not occur.⁹⁹ Currently, cylinders are made with thin plates using highly resistant materials with excellent durability. In general, these are classified into four types, according to the material used: type 1, made entirely of aluminum or steel; type 2, made with a thin layer of aluminum or steel surrounded by another composite, usually carbon fibers, in a circular shape; type 3, made with a thin layer of steel or aluminum fully enveloped by other compounds such as carbon fibers; and type 4, made with a layer of tough plastic-wrapped in another tough compound.

Table 3 presents some examples of applications of the different types of storage that can be used for hydrogen. The use of cylinders is indicated for hydrogen storage at small and medium scale. At larger scales, hydrogen can be stored cryogenically as a liquid and in pipes or porous storage underground, as an underground geological method (most economical),¹⁰³ or in interactions between hydrogen and hydrocarbons dissolved in reservoir rocks through microbial metabolism, for example.¹⁰⁴

Underground storage is possible in different types of reservoirs, but what is more viable are salt caves, which are also used for storing fossil gases. This type of storage is best suited for large volumes and long periods (weeks or seasons), and it has low operating pressure (50-250 bar). Caves of this type are found worldwide with different levels of storage ability. Although they are found in the Asia Pacific, South America, Southern Europe, and the west coast of North America, only the US and UK use this type of cave to store H₂.¹⁰⁰

In terms of technology, some research aims to develop new materials that can be used in the H₂ storage process, such as H₂ adsorption using carbon nanostructures.¹⁰⁵ One nanostructure that has been heavily investigated is graphene-based.^{106,107} The use of this material can significantly increase storage efficiency, offering high stability.

Table 3. Overview of hydrogen storage types and their peculiarities

| Reference | Scale | Type of storage | Type of tank | Requirements | Note |
|-----------|--------|---|--------------------------|--|--|
| 97,98 | small | board vehicles | 2, 3 or 4 | 5-10 kg compressed gas at 350-950 bar | high pressures require tanks to be reinforced with carbon fibers or pre-stressed concrete |
| 100 | small | buffer hydrogen | 2 or 4 | 100 kg | – |
| 91,101 | small | tube trailers for hydrogen delivery to refueling stations | 4 | 1000 kg at 540 bar | – |
| 100 | medium | spherical vessels or underground pipe facilities | – | ca. 20 bar | protection from adverse weather conditions and no requirement for shaft structures |
| 93,102 | large | cryogenically as a liquid | spherical tanks | LH2 at 20 K two 3200-m ³ spheres, 21.3 m in diameter, each capable of storing 230 t of LH2 | hydrogen liquefaction process requires very high energy and is costly largest LH2 storage facility at NASA's Kennedy Space Center |
| 100 | large | underground pipes | type-1, API 5L X52 pipes | < 20 t H ₂ | more economical than geological caverns but estimated capital cost is high |
| 100 | large | underground lined rock caverns | – | > 750 t useable H ₂ requires multiple caverns | installed capital cost of lined rock caverns decreases with increased H ₂ storage |
| 100 | large | underground salt caverns | – | 50-250 bar | installed capital cost of salt caverns decreases with increased H ₂ storage salt caverns are more economical than lined rock caverns |

LH2: liquid hydrogen.

Hydrogen storage in vehicles can be done in two forms: liquid and gaseous hydrogen fuels. Figure 9 presents hydrogen-based systems in vehicles.

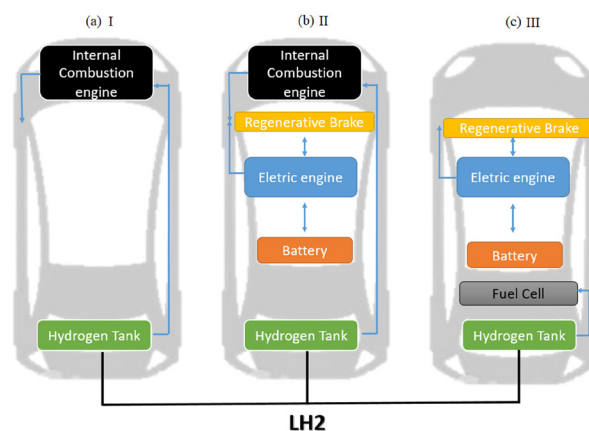


Figure 9. Systems of (a) internal combustion engine vehicle; (b) hybrid electric vehicle; (c) fuel cell vehicle. LH2: liquid hydrogen (adapted from Ugurlu and Oztuna).¹⁰⁸

7. Hydrogen Transport

The energy sector has extensive experience with transporting gases over long distances. However, H₂ has additional challenges due to its physical properties. Despite

having a high energy density by mass of 33.3 kWh kg⁻¹ (the value for CH₄ is 13.9 kWh kg⁻¹), it has a low energy density by volume of 3 kWh m⁻³ (the value for CH₄ is 10 kWh m⁻³ under standard conditions).¹⁰⁹ Thus, to transport the same amount of energy, larger volumes of H₂ must be considered. For this reason, H₂ is treated to reduce its volume for transport. Currently, the solutions for H₂ transport are compression, liquefaction, use of liquid organic hydrogen carriers (LOHCs), or conversion to ammonia. Each of these solutions increases the energy density by volume.

Compressed H₂ can be transported by truck or gas cylinders with 200 to 700 bar pressures. However, this modality is only viable for short distances (a few hundred kilometers) and reduced volumes. For long distances, H₂ is usually transported in its liquid form, and the liquefaction process requires cooling it to a temperature of -253 °C or lower. Up to 3500 kg of H₂ can be transported by truck.¹⁰⁹ However, as the distance increases, the trucks become a less viable option.

For longer distances, where it is unfeasible to use trucks for transport, compressed H₂ pipes are used, thus increasing the volume transported to thousands of tons *per* day. The H₂ distribution network is still short (approximately 5000 km) compared with natural gas (3 million km) in Asia, Europe, and North America. An alternative is to inject green H₂ into natural gas lines, but it requires replacing valves, regulators, compressors, and measuring devices. In some cases, complete replacement of piping is necessary. Pipes can also transport ammonia, and some are already in operation. An example is the Togliatti-Odesa pipeline in Russia, with

2700 km.¹¹⁰ Another modality is to transport H₂ via ships. This option favors the transport of liquid H₂, ammonia, LOHC, methanol, and synthetic liquids. The Japanese government has started feasibility studies for these options.

8. Uses of Hydrogen

In terms of renewable H₂ applications, its energy conversion can be highlighted in different types of energy such as power-to-X (P2X), power-to-power (P2P), power-to-chemical, and power-to-mining. The process of converting energy generated from solar (photovoltaic) and wind sources into different types of energy for use in various sectors of the economy, or even to be reconverted into energy, has the potential to increase the flexibility of the electricity grid significantly. Optional locations can be built to place temporary surplus energy by displacing fossil fuel energy sources, contributing to net-zero carbon emissions.¹¹¹ Green H₂, produced by electrolysis from renewable energy sources, appears to be a relevant alternative to obtain much-needed carbon neutrality in various sectors of the economy, such as the transport, chemical, and general industries. A representation of the possible applications of H₂ produced by electrolysis from renewable energy sources is presented in Figure 10.

In the P2P application, producing H₂ by electrolysis from renewable energy sources and storing and reconverting hydrogen into electricity by fuel cells or gas turbines are promising processes for applications outside of the grid, in remote locations or rural communities, or as a power

FLOW OF APPLICATIONS

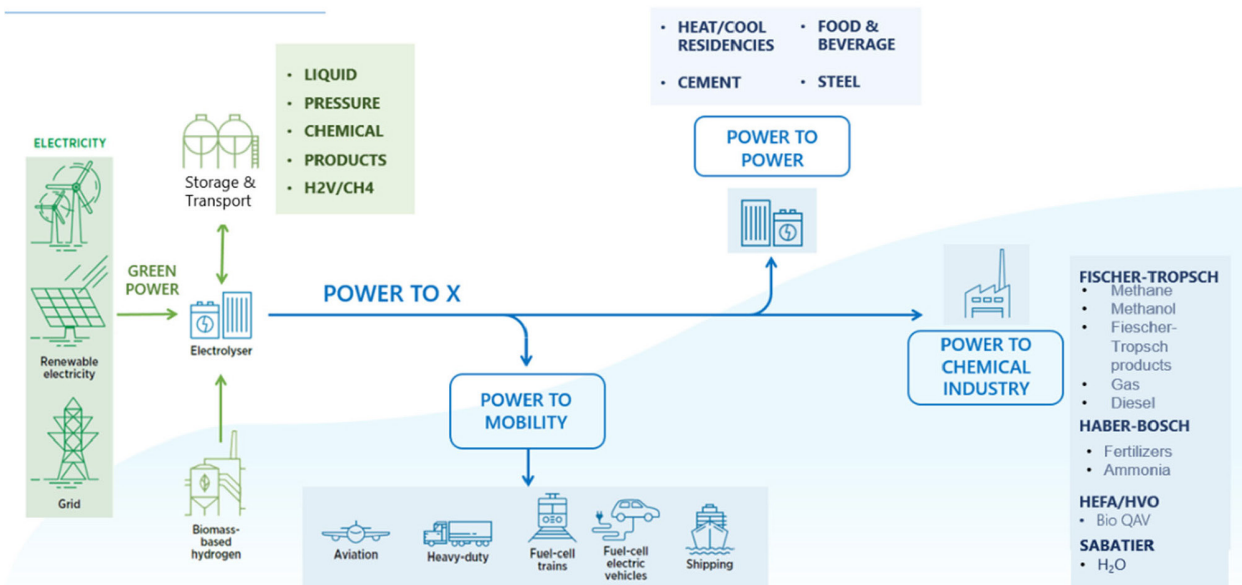


Figure 10. Possible applications of green hydrogen (adapted from IRENA).¹¹²

reserve. It is not yet a competitive process for connection to the grid.¹¹³ This is due to the low efficiency of the entire system, as it currently varies in the range of 30 to 40%.¹¹⁴ In this case, underground storage in salt caves, aquifers, or depleted oil and gas fields is mentioned as the most economical way to store large volumes of hydrogen.¹¹⁵ Another possibility is the use of combined H₂ storage to compensate for the variations in electrical energy produced by wind and photovoltaic generators, minimizing the use of thermal generating plants, which use fossil fuels. It could also be an alternative to reduce the adverse effects caused by the uncertainty of climate forecasts regarding hydroelectric plants.

Globally, the industry already produces and uses H₂ in a variety of catalysts and catalytic processes, ranging from the synthesis of ammonia to asymmetric hydrogenation processes for pharmaceuticals.¹⁶

The largest share of H₂ demand is from the chemical and refining sectors, and steam methane reforming is the principal option, although coal gasification is also used for metal and petrochemical production. Other industrial sectors also use H₂, but their cumulative share of global demand is small, just 1%,¹¹⁶ and include the manufacturing of glass, food products (hydrogenation of fats), bulk and specialty chemicals, and semiconductors, the cooling of large stationary electrical generators, the production of propellant fuel for aerospace vehicles, and others. Hydrogen produced by electrolysis can be mainly used as a raw material in industrial processes such as the following: (i) chemical: ammonia (Haber-Bosch process), methanol, and urea (with carbon capture, use and/or storage (CCUS)); Fischer-Tropsch products such as light/heavy naphtha, kerosene, gas, diesel, and others (with CCUS); polymers, and resins are relevant markets for industrial hydrogen;¹¹⁷ (ii) refining: hydrogen is used for hydrocracking and hydrotreating processes (removal of sulfur from fuels). Refineries represent very important consumers of industrial hydrogen; (iii) HEFA/HVO process: hydrogen is used in hydrotreating vegetable oil (HVO), commonly referred to as renewable diesel, and in hydroprocessed esters and fatty acids (HEFAs). Hydroprocessing of oils and fats is an alternative to esterification to produce diesel from biomass. The HVO/HEFA process produces straight chain paraffinic hydrocarbons free of aromatics, oxygen, and sulfur and has high cetane numbers. HEFAs can typically be used in all diesel engines as aviation bio-jet fuel.^{118,119}

As a permanent material that can be continuously recycled, steel is a fundamental material for industry and society in general. Its production has been growing substantially, reaching 1.9 billion tons in 2020 (Figure 11).¹¹¹

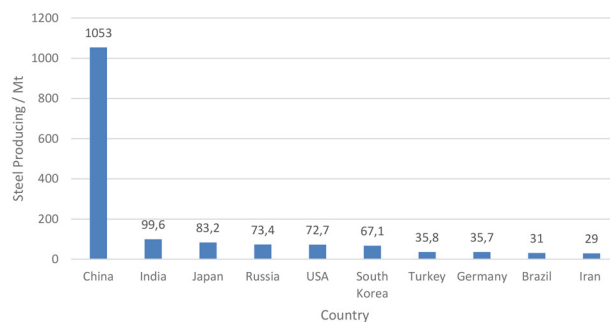


Figure 11. Steel-producing countries in 2020.¹¹⁰

The steel industry is heavily dependent on coal and accounts for approximately 8% of global CO₂ emissions.^{120,121} With increasing pressure on the carbon-intensive mining industry to reduce emissions, the world's leading players are working hard to decarbonize the sector. Several options are being considered for the decarbonization process: increasing the efficiency of current production processes, recycling steel, using carbon capture and storage, and using hydrogen. Regarding the last option, H₂ can reduce emissions in the steel production process to participate in the decarbonization process in two ways: using it as an auxiliary reducing agent in the production process called the basic oxygen furnace route in a blast furnace (BF-BOF) or as an agent for reducing iron in the process known as direct iron reduction (DRI or H₂-DRI).¹²²

Ito *et al.*¹²⁰ evaluated the situation in the steel industry and examined the possible technologies that could be used to achieve carbon neutrality. Most steel production is carried out by the primary route, in which the iron ore is processed to obtain a sintered material or iron pellets, which are subsequently melted in a blast furnace with coke to make pig iron and then processed in a basic oxygen furnace to produce steel. The remaining steel production comes from the secondary route by heating scrap metal in an electric arc furnace. Processes in the primary route emit mainly direct greenhouse gases, and those in the secondary route emit mainly indirect greenhouse gases, which vary depending on the electricity mix used in the electric arc furnace.

Carbon capture, use, and storage (CCUS) is a method to capture CO₂ emissions and either process them for further utilization as fuel or store them in geological formations such as exhausted undersea gas reservoirs. CCUS alone cannot achieve carbon neutrality, but it could mitigate emissions into the atmosphere.

The second kind of potential technology involves replacing coke or natural gas with alternative reductants of iron ore, including hydrogen and direct electric current. The advantage is that this can probably make steel production fully green. However, developing these technologies will

require much more time and money than what is required for CCUS.

The method of direct hydrogen reduction of iron uses the element to reduce iron ore in a shaft furnace or a fluidized bed reactor. The shaft furnace still has an inconvenience: it requires iron ore pellets, and the process to produce them can cause significant emissions depending on the heat source of the pellet plant. A great amount of hydrogen is also required for both reactors, requiring a large amount of electrolyzers. In the case of the fluidized bed reactor, the use of iron fines removes the need to pelletize, cutting down the CO₂ emitted during this process. Additionally, it can reach higher levels of metallization. On the other hand, fluidized bed reactors in steelmaking are less developed than shaft furnaces and require a larger investment.

Some other processes are already in development, producing carbon-neutral steel, such as biomass-based ironmaking with CCUS, suspension ironmaking, plasma direct steel production, and electrolytic processes. These last three technologies are at the early stages of development. Their technical and economic viability in large-scale production must be proved, and there is a high degree of uncertainty over their industrial utilization.

Hydrogen-based reduction technologies are more developed and have lower technological risks, but there is no sufficiently large-scale hydrogen electrolyzer available, a prerequisite to produce sufficient green H₂ for the reduction process. Furthermore, these energy sources are still costly, and the whole process is not competitive compared with the coking process. Much time and great effort in research and development are still needed to reach competitiveness for these new direct reduction processes.

One of the mechanisms still underway for energy conversion systems for thermal use for heating or its generation comes from combustion. Fossil fuels are still used in liquid, solid or gaseous form, including hydrogen via unsustainable routes (gray H₂).

By looking ahead to the following decades, combustion will still be used in energy conversion, and given the decarbonization in progress, the use of green H₂ should be considered, especially as an energy source in the chemical industry. Recently, research has been carried out (2018-2021) regarding using hydrogen in combustion, considering its importance for the H₂ economy that is expected to develop. The possibility of its use in thermoelectric plants, chemical processes (such as ammonia and green cement production), and the production of fuels (e-fuels) for vehicles and heavy transport opens up an important field of research.

The combustion of green H₂ follows some of the main routes as the origin of its formation: mixed with CO and fractions of biomass gasification (syngas), as a result of

water together with oxygen electrolysis, from the reform or biotechnological processes of biogas, and from the combustion of products formed from green H₂, such as green ammonia.

Along these lines, work was carried out to evaluate the energy and environmental impacts, flame structure and stability, and association with modern techniques used in combustion. Studies^{110,123-133} have analyzed the influence of parameters on the characteristics of hydrogen flames or mixtures of hydrogen with other fuels, evaluating their stability and efficiency. The flame flow aspects of CH₄/H₂ mixtures with the rotational flow were evaluated, verifying the velocity stability characteristics in the studied mixtures.¹²⁶ The curvature in the flow for flame development and its propagation were investigated to understand better joint combustion between H₂ and NH₃.¹¹⁰ Flame velocity and mass diffusion aspects as well as propagation stability were studied in the combustion of a mixture of CH₄, H₂, and air, allowing a better understanding under the evaluated conditions.¹³⁰

A modern technique called low-oxygen dilution (moderate or intense low oxygen dilution, MILD) combustion was analyzed with several mixtures of CH₄ and H₂, evaluating aspects of NO_x emissions and their routes, supporting the environmental analysis of associations of modern techniques for the combustion of H₂.¹²⁵

Combustion propagation studies evaluating the velocity uncertainty of hydrogen flame were developed, allowing a better understanding of the operation under specific conditions of feeding gases to the burning.¹³¹

Stabilization of rotational flows, very common in industrial combustion equipment, was analyzed in synthetic natural gas flames mixed with H₂, evaluating aspects of flame velocity, NO_x formation, and combustion stability.¹¹⁰

Studies with ammonia and dimethyl ether (DME) as e-fuels for energy applications have been an important research area. Experimental and numerical studies were better carried out to understand combustion and its energetic and emission aspects.^{131,133-139}

The use of polyoxymethylene dimethyl ether (OMEn), a promising e-fuel, was studied for possible applications in engines.¹³⁵ The flame structure and CO and NO_x emissions were evaluated for its use as a possible fuel for the green H₂ chain.

The combustion of ammonia, CH₄, and H₂ mixture was investigated through experimental and numerical studies. The stability of flames with swirling flow with the addition of ammonia under different conditions and the emissions of NO_x and CO were evaluated.¹³⁷

The combustion of e-fuel oxymethylene ether 1 (OME1) and its blends with *n*-dodecane was also studied,¹³⁸

evaluating the performance in engines. The process of ignition and soot formation was analyzed, verifying the fundamental characteristics for possible expansion of its use with the decarbonization process.

Turbulent ammonia flames were evaluated using the oxygen-enriched combustion technique at high pressures. Turbulence effects on flame stability and propagation velocity and the comparative influence of turbulence and reaction effects were evaluated.¹³⁹ This line of study supports the possibility of developing combustion equipment for the industrial use of ammonia coming from the green H₂ chain.

With the same objective, studies of syngas and biogas combustion, either enriched with H₂ or not, are being carried out to understand better combustion and possible applications in energy production and industrial thermal applications.^{110,138,140-142}

A review¹⁴⁰ of the fundamental characteristics of syngas combustion was conducted, identifying important points of stability and efficiency of syngas combustion and indicating gaps in the development of combustion devices for better industrial use of this fuel, which will play an essential role in the green H₂ chain.

Comparative studies of gas turbines between natural gas and biogas were carried out. The influence of swirling flow, combustion efficiency, and CO and NO_x emissions were analyzed.¹⁴¹

Syngas flames were analyzed under the conditions of the modern oxy-fuel combustion technique, evaluating combustion stability and emissions and verifying the environmental behavior of the syngas burner operation.¹³⁸

Turbulent syngas flames were also studied.¹¹⁰ The influence of the equivalent ratio and turbulence intensity on the flame stability and velocity were analyzed, supporting the research on turbulent syngas combustion and its operating conditions for further industrial applications.

By presenting these recent studies, a vital interest of the academic community in the role of combustion in the green H₂ chain is identified. Therefore, important possibilities open up for a better understanding of the benefits and impacts of this chain with the technological route of combustion.

Due to the properties highlighted above, H₂ was chosen as one of the alternatives for the main automotive industry sources in relation to the transition from electric vehicles to fuel cells. Although many power systems have been implemented in electrical system vehicles, the hydrogen-based energy system is favored by consumers. This is because it offers many advantages, as saving excellent efficiency and being environmentally friendly.

Although H₂ does not emit any dangerous by-products during combustion, some points still need to be considered in its production and storage, as it is highly reactive in the presence of oxygen, which can lead to explosive action. Therefore, H₂ sensors must be attached to vehicles to detect any hydrogen leakage that might happen.^{143,144} Internal combustion engines accompanied by hydrogen can also be seen in the automotive market.¹⁴

In-vehicle systems that use H₂ (Figure 9), the pressure produced by the combustion of the H₂ pushes down the pistons in the cylinders of the internal combustion engine (system I, Figure 9a). In hybrid vehicles (system II, Figure 9b), hydrogen is the combustion engine fuel responsible for rotating the wheels, which works as an energy source to charge the vehicle's battery. Unlike previous vehicles, fuel cell vehicles (system III, Figure 9c) do not have internal combustion engines. They are powered by hydrogen through fuel cells that create electricity for the battery. Based on the three types of vehicles with a hydrogen engine, system III has the lowest emissions of volatile organic compounds, followed by II and I.¹⁴⁵

9. Economic and Environmental Impacts

Cost reduction and improvements in novel technologies encourage companies and governments to invest time and financial resources in new regulations, policies, and alternatives to decarbonize industries, especially the transport and heating sectors and most society's activities.

One possible solution to reach this goal is to use H₂ as one of the leading energy vectors, especially green and clean H₂, when it comes from clean energy sources such as solar, wind, and hydroelectric power. Although currently there are many established ways to produce hydrogen, none of them can help to achieve the goals of the Paris Agreement to 2030 and 2050. In addition, it is estimated that up to 2020, the industry sector demand for hydrogen was 51 Mt, with chemical production consuming ca. 46 Mt, attesting to the importance of the hydrogen market and this activity worldwide.¹³² To understand the importance, 90% of all hydrogen produced is directed to industrial use, especially ammonia, methanol, and steel plants.¹²⁴

For this reason, the implementation of a production chain based on green H₂ has brought about relevant discussions among governments to define strategic plans for the sector. In this context, both the economic aspects of the benefits and the bottlenecks in the chain and the environmental aspects associated with decarbonization have been discussed in the literature. Recent works^{88,146-159} have discussed green H₂ in several countries and the value chain. On the other hand, the implementation of green hydrogen

production has been researched based on the potential of generating renewable energy, verifying the application of this new energy source for the decarbonization of the transport and industrial sectors.^{88,146-149,153,155,157,159}

The use of hydroelectric energy and its expansion for the production of green hydrogen and the replacement of fossil fuels, and its impact on decarbonization, was studied in Nepal.¹⁴⁹ In Pakistan, a study¹⁴⁸ was carried out on implementing the green hydrogen economy using solar energy, biomass, and municipal solid waste as sources, supporting the country's decarbonization and enabling it to be a global supplier. The formation of an e-fuel production chain between countries was also studied,⁸⁸ with the connection of renewable generation in Iceland (via geothermal energy and hydropower) and the surplus of renewable energy production in Germany.

Studies have also evaluated the prospects of, and obstacles to, green H₂ chain deployment. For example, in Russia, studies^{146,153} identified the potential for generating renewable energy and producing green hydrogen and the bottlenecks and analyzed the costs and production payback. A similar study¹⁵⁶ was carried out in the Philippines, verifying the possibility of hydrogen production and how the country can participate in the decarbonization of the economy. The implementation of green H₂ production sites and production capacity in different regions of Uzbekistan was analyzed, using a hierarchical methodology multi-criteria decision-making (MCDM) method in addition to financial feasibility analysis.¹⁵⁵

In Brazil, the pros and cons and economic feasibility of producing green H₂ were studied based on the surplus production of hydroelectric and wind energy, identifying the possibility of production at costs comparable with the current production of gray hydrogen.^{147,157}

Studies on the implementation of green H₂ production and its value chain have begun to be intensely discussed in the literature. However, there is a need for further studies, including analyses of more consolidated data on production prices, coupling of production chains and uses, and regulation of the sector.

Projects related to green H₂ production are still expensive compared with those using fossil fuels. According to the International Energy Agency (IEA),¹⁶⁰ green H₂ from wind energy costs between USD 4-10 kg⁻¹ and USD 7-17 kg⁻¹ when solar energy is used, while gray H₂ produced from fossil fuels costs USD 1-2.50 kg⁻¹. However, the production of gray H₂ generates close to 9.5 kg CO₂ kg⁻¹ H₂. For this reason, the carbon market becomes an ally for projects involving green H₂ to become economically viable.¹⁶¹

The current domestic market demand for green H₂ is focused on industrial use, especially when safety issues

are considered. The industry currently has better resources to deal with this type of gas. Furthermore, it can reduce GHG emissions by replacing gray H₂ with the green one. For this reason, in the short term, most projects should be aimed at the needs of industry and foreign markets. Sectors such as heavy road transport, naval, aviation, chemical, cement, and steel, when combined, account for 30% of global GHG emissions and involve a complicated electrical transition. Despite the emissions, each sector has or will have a continuous demand for H₂. This would reduce the associated renewable energy waste due to prolonged storage based on a possible imbalance in supply/demand.

The realization of the green H₂ economy also depends on advances in technology such as electrolyzers. The installed capacity of electrolyzers is currently around 200 MW, still, far from the capacity required for the desired consumption of green H₂.¹⁰⁹ However, this capacity is expected to increase considerably as new electrolyzer projects are launched. For example, according to a 2021 report released by the International Renewable Energy Agency (IRENA),¹⁰⁹ over a 5 month period (November 2019 to March 2020), the expected capacity for 2030 increased from 3.2 to 8.2 GW. In addition, an electrolyzer with a capacity of 22 GW was announced in Australia. Further, new investments are being directed to the Arabian Peninsula. Three industries have announced a USD 5 billion project for a 4 GW green ammonia plant expected to start operating in Saudi Arabia in 2025.¹⁶² At the same time, a company at Al Duqm signed an understanding agreement with one group to invest USD 2.5 billion to start a green H₂ and green ammonia plant. China, in turn, expects to start operating electrolyzers of 70-80 GW by 2030.¹⁶³ In 2020 alone, 28 projects were announced across China. It is believed that by around 2030, the production of green H₂ will become competitive, reaching a level of USD 2.60 kg⁻¹ and less than USD 1.50 in 2050.⁸⁶ Until then, the blue H₂, with carbon capture, along with the production of green H₂ is the way to cleaner hydrogen production. This summarizes the main expansion projects in electrolyzer capacity by companies worldwide.

10. Green Hydrogen and Challenges for Chemistry

In the current global scenario, humankind is confronted with an oncoming scarcity of fossil fuel resources together with the ever-increasing need for energy. Energy is essential for human development and prosperity and a critical factor in achieving sustainable development.¹⁵²⁻¹⁵⁵ Hydrogen is considered by several experts, the energy carrier for revolutionizing the energy system since it is

a carbon-free fuel. Green hydrogen is a clean alternative for generating energy for the electricity, industry, heating, and transportation sectors and to meet the 2030 and 2050 agendas and, consequently, sustainable development.¹⁶⁴⁻¹⁶⁹

Considering hydrogen is a clean fuel capable of promoting sustainable energy development, a hydrogen economy is rising worldwide. Hydrogen fuel is crucial for decarbonisation and meeting climate neutrality (net zero) up to 2050. In regard to the UN Sustainable Development Goals (SDGs),¹⁶⁹ those goals are, by conception, indivisible and interlinked to each other. Or in other terms, when considering one specific SDG we should also consider many synergisms and some trade-offs among them, which are fully described by a matrix of 17 goals by 169 targets. At the Table S2 (SI section) we point out six SDGs and their associated targets closely related to the sustainable nature of adopting green hydrogen as energy resource in the future. Among the SDGs, at first, the most closely related is the Goal 7 (affordable and clean energy) and all its targets (Table S2), such as “ensure universal access to affordable and modern energy services”, including a “substantial increase of the share of renewable energy in the global energy mix” by “promoting investments in clean energy research technology”, and “ensuring modern and sustainable energy services for developing countries”. Accordingly, Goal 13 (climate action) is also met since transitioning from a carbon-based to a green hydrogen-based economy would considerably decrease GHG emissions, which are responsible for global warming. Synergistically, by meeting Goal 13, major improvements are also likely to be reached in regard to the Goals 14 (life below water) and 15 (life on land), not presented in Table S2.

Additionally, green hydrogen is also transversally related to some other SDGs, such as Goal 3 (good health and well-being, principally in relation to “the reduction of deaths and illnesses from hazardous chemicals and pollutants from air, water, and soil” and “global health risk reduction and management”) and Goal 9 (industry, innovation, and infrastructure by “developing sustainable and inclusive infrastructures and industrialization to significantly raise the industry share of employment and gross domestic product globally, but with special attention to the least developed countries”).

Green hydrogen economy is also associated to Goal 11 (sustainable cities and communities, in the way it corroborates to “affordable and sustainable transport systems”, and “to support positive economic, social, and environmental links to development planning, and also promoting inclusions, mitigation and adaptation to climate change”) as well as the Goal 12 (responsible consumption and production, by “achieving the sustainable management and efficient use of natural resources” and “responsible

management of chemicals and waste”), among others (Table S2).

By transitioning from a carbon-based economy to a hydrogen economy, there will be a drastic reduction in greenhouse compounds (GHGs) and the elevated-toxicity chemicals either exhausted from fossil fuel burning or during petroleum exploitation to all environmental compartments. Therefore, pollution-related diseases will also decrease proportionally. Goals 14 and 15 will also be met in a few decades by ceasing or drastically reducing onshore and offshore fossil fuel exploitation. Considering that 2021-2030 is the decade of the Ocean designed by the UN, the transitioning to a hydrogen economy could also synergistically go along with this movement and its actions. In fact, by decreasing the global dependency on fossil fuels for energy generation, it would alleviate considerably geopolitical tensions which historically occur among different countries. Ultimately, it would also corroborates with the Goal 16 (peace, justice, and strong institutions) and Goal 17 (partnership for the goals), which are critical to enable all the other SDGs.

Launching a hydrogen-based economy will demand from Chemistry, Engineering, and associated fields fast and solid actions to fill the gaps needed to become practical.¹³⁴ The bottlenecks in hydrogen-based energy open several opportunities for those fields. Furthermore, enabling conditions to adopt green hydrogen as an energy carrier for humankind will synergistically match Industry 4.0 and the Circular Chemistry/Circular Economy frameworks. However, there are some challenges ahead of us to be solved in the near future: (I) although the obvious benefits of employing green hydrogen as an energy source, it remains prohibitively expensive. New approaches for obtaining efficient and low-cost energy are required. Hydrogen as fuel needs to be equally affordable and readily available for every country around the world, regardless of its current degree of development; (II) hydrogen fuel plans are currently being implemented to address energy needs in some countries. On the other hand, those countries have varying maturity levels in using hydrogen in various contexts, using green hydrogen, fossil-based hydrogen (with or without carbon sequestration), or a combination of both at various scales. Widespread discussion and policy development are critical in order to determine how much green hydrogen will be genuinely adopted by society, hence determining how much infrastructure, research, development, and innovation will be done in the coming decades; (III) since green hydrogen relies on electrolysis, new electrolyzers and cost-effective and more efficient electrolyzer technologies (including the development of new materials) are critical to making green hydrogen competitive when compared with blue and brown

hydrogen; (IV) hydrogen storage and distribution is a key enabling factor to promote the hydrogen economy, and it is a real issue nowadays; (V) there is an urgency to transform the current infrastructure and materials for the (i) transportation (automotive, train, maritime, and aviation) system, (ii) industrial plants and processes; (iii) electricity grid (jointly to renewables, such as wind, biomass, solar PV, and tidal), and (iv) domestic sector by research and development and innovation (R&D&I); (VI) with the adoption of green hydrogen, some regions that are already facing freshwater scarcity will have to surpass this obstacle. It provides a new avenue for study into new methods for creating green hydrogen from seawater or wastewater.

11. Concluding Remarks

Humanity is assuming a significant change of direction towards conscient energy production and consumption, enabling the hydrogen economy and sustainable development. Although green hydrogen is still cost-effective and has important drawbacks, the development of new processes for guaranteeing the hydrogen chain seems feasible within the following decades. A large array of opportunities and challenges for the Chemical Sciences is ahead of us right now. We need to plan the energy matrix transition up to 2050, and the real clean hydrogen economy fully applied in all continents up to 2070.

Enabling sustainability necessitates ongoing efforts from various stakeholders in the political, industrial, economic, and social realms. Despite the numerous obstacles in (i) production, (ii) storage and distribution, and (iii) use and applications, the role of green hydrogen in the new world energy grid is conceivable and viable.

On a regional basis, South America plays a critical role in the green hydrogen chain. As a result, Brazil has a high chance of becoming a market leader in green H₂. The diversity of Brazil's renewable energy matrix (wind, solar, hydropower, and biofuels) creates opportunities for several projects in the short- and medium-terms, including production via mature technologies such as water electrolysis and use of renewable electricity via the existing grid, as well as storage and distribution of green H₂ in the context of a new grid.

Supplementary Information

Supplementary information is available free of charge at <http://jbcs.s bq.org.br> as PDF file.

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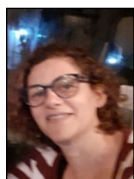


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