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Review

Hydrogen Purity: Influence of Production Methods, Purification Techniques, and Analytical Approaches

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Abstract: Hydrogen purity plays a crucial role in the expanding hydrogen economy, particularly in applications such as fuel cells and industrial processes. This review investigates the relationship between hydrogen production methods and resulting purity levels, emphasizing the differences between reforming, electrolysis, and biomass-based techniques. Furthermore, it explores state-of-the-art purification technologies, including pressure swing adsorption (PSA), membrane separation, and cryogenic distillation, highlighting their effectiveness and limitations in achieving ultra-pure hydrogen. Analytical methods such as gas chromatography, mass spectrometry, and cavity ring-down spectroscopy are also discussed in terms of their accuracy and application scope for hydrogen quality assessment. By integrating findings from global and domestic studies, this paper aims to provide a comprehensive understanding of the challenges and advancements in hydrogen purity, offering insights into optimizing hydrogen for a sustainable energy future.

Keywords: hydrogen purity; hydrogen production; purification technology; energy transition; electrolysis

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1. Introduction

The increasing urgency to combat climate change and transition to sustainable energy sources has propelled hydrogen to the forefront of global energy strategies. Hydrogen, as a clean and versatile energy carrier, is uniquely positioned to decarbonize hard-to-abate sectors such as transportation, heavy industry, and power generation [1–4]. Its potential to act as a bridge between renewable energy sources and end-use applications highlights its importance in the global pursuit of net-zero carbon emissions [5–7]. However, the effectiveness and efficiency of hydrogen as an energy carrier depend critically on its purity, which directly impacts its performance in applications like fuel cells, chemical synthesis, and advanced manufacturing processes [8–15].

Hydrogen purity varies significantly depending on the production method. Fossil fuel-based processes, such as steam methane reforming (SMR) and coal gasification, remain the dominant methods for hydrogen production, contributing to the majority of the global hydrogen supply [16–21]. However, these processes often yield hydrogen with impurities such as carbon monoxide (CO), methane (CH_4), and other hydrocarbons, necessitating advanced purification technologies [22–25]. Conversely, water electrolysis—powered by renewable energy sources—can produce high-purity hydrogen, albeit at a higher energy cost [26–28]. Emerging methods such as biomass gasification and bio photolysis also contribute to the diversity of production pathways, each with unique challenges and implications for hydrogen purity [29–34].

Achieving the high purity levels required for applications, particularly in proton-exchange membrane (PEM) fuel cells, involves sophisticated purification processes. Technologies such as pressure swing adsorption (PSA), membrane separation, cryogenic distillation, and catalytic purification are widely employed to remove impurities [35–41]. Each technology offers distinct advantages and limitations, often influenced by the scale of production, feed gas composition, and desired purity levels. For instance, PSA is highly effective in removing impurities from reformate hydrogen, while membrane-based separation is advantageous for its energy efficiency and modular design [42–48]. Advanced hybrid purification systems are also gaining traction, combining multiple techniques to optimize performance and cost-effectiveness [49–52].

In addition to production and purification, the analysis of hydrogen purity is critical to ensure compliance with stringent quality standards. Analytical techniques such as gas chromatography (GC), mass spectrometry (MS), and Fourier-transform infrared spectroscopy (FT-IR) play vital roles in identifying and quantifying trace impurities [53–60]. These methods provide the precision and reliability required to meet the specifications outlined by international standards such as ISO 14687 [61], which governs the quality of hydrogen used in fuel cells and other critical applications [62–65]. Recent advancements in analytical technologies, including cavity ring-down spectroscopy (CRDS) and ion chromatography (IC), have further enhanced the ability to detect ultra-trace levels of contaminants [66–70].

Despite significant progress being made, challenges remain in achieving the cost-effective and scalable production of ultra-pure hydrogen. Economic barriers, particularly for renewable energy-driven electrolysis, must be addressed to ensure widespread adoption [71–76]. Additionally, the integration of purification systems with production facilities requires careful optimization to balance efficiency, cost, and environmental impact. Research and development efforts are focused on enhancing the durability and efficiency of purification technologies, as well as advancing analytical techniques for the real-time monitoring of hydrogen quality [77–88].

This review explores the interconnected aspects of hydrogen production, purification, and analysis, providing a comprehensive overview of current technologies and their implications for hydrogen purity. By examining the state-of-the-art advancements and identifying existing gaps, this paper aims to inform future research and development efforts, ultimately supporting the transition to a hydrogen-based economy [89–99]. The insights presented here are intended to guide stakeholders in academia, industry, and policy as they work towards optimizing hydrogen systems for a sustainable energy future [100–109]. This review explores the interconnected aspects of hydrogen production, purification, and analytical techniques, providing a comprehensive overview of current technologies and their implications for hydrogen purity. By examining traditional and state-of-the-art purification technologies, this review aims to contribute to the optimization of hydrogen systems for a sustainable energy future.

2. Hydrogen Production Based on Feedstock

Hydrogen production technologies are broadly classified by the type of feedstock used, energy sources applied, and the chemical reactions involved. Feedstocks include fossil fuels, water, biomass, and waste materials, while energy sources range from thermal and electrical to nuclear energy. From an environmental perspective, hydrogen production methods are further categorized into green, gray, and blue hydrogen. Green hydrogen is produced via water electrolysis powered by renewable energy, resulting in zero carbon emissions. Gray hydrogen relies on the conventional reforming of fossil fuels, and this process releases a significant amount of CO_2. Blue hydrogen, however, mitigates emissions through carbon capture, utilization, and storage (CCUS) technology [11–15].

Byproduct hydrogen is a notable method, derived as a secondary product from industrial processes like petroleum refining, chemical production, and steelmaking. After purification and dehydration, this hydrogen achieves high purity. Its primary advantage is economic efficiency, as it utilizes existing industrial waste gases without requiring major additional investment. However, its supply is inherently dependent on the scale and nature of the associated industries, limiting its scalability and availability. In 2018, approximately 48 million tons of byproduct hydrogen was produced globally, accounting for nearly one-third of the world's hydrogen demand [11,14].

Reforming hydrogen remains the dominant method, involving hydrocarbon-based feedstocks such as natural gas, coal, and petroleum. Common techniques include steam methane reforming (SMR), partial oxidation, and dry reforming. SMR is particularly popular due to its low cost and reduced CO_2 emissions compared to other processes. Global leaders in reforming hydrogen include France's Air Liquide, which operates 145 plants worldwide, and Germany's Linde, which provides scalable reforming solutions. In South Korea, the industry is in its early stages, with key players like SK Innovation and Korea Gas Corporation focusing on hydrogen reformers for fueling stations and integrated renewable energy systems [11–23].

Non-reforming hydrogen offers an eco-friendly alternative by utilizing CO_2-neutral feedstocks like biomass and biological fermentation. Biomass encompasses a diverse range of materials, such as agricultural residues, municipal waste, and algae, offering a sustainable and versatile pathway for hydrogen production. However, economic viability remains a challenge due to the complexities of feedstock collection and processing [12–20].

Water electrolysis hydrogen represents one of the cleanest production pathways, leveraging electrochemical reactions to split water into hydrogen and oxygen. Key technologies include alkaline electrolysis (AEC), proton-exchange membrane electrolysis (PEMEC), and solid oxide electrolysis (SOEC). When powered by renewable energy, water electrolysis generates zero carbon emissions. Despite its sustainability advantages, the high cost of renewable electricity and electrolyzer systems poses a challenge to its large-scale adoption. Globally, water electrolysis accounted for less than 0.1% of hydrogen production in 2018, but investments in technology are accelerating. Germany, for instance, is expanding its Power-to-Gas (PtG) projects, while South Korea is advancing domestic electrolysis systems through government-supported R&D [15–27,68,69].

Hydrogen production methods vary widely in terms of feedstock, scalability, and environmental impact. While reforming remains the dominant method, advancements in water electrolysis and non-reforming technologies are paving the way for a more sustainable hydrogen economy. The classification of hydrogen production technologies by feedstock is summarized in Table 1.

Table 1. Classification of hydrogen production energy source and chemical reaction by feedstock.

Feedstock	Energy Source	Chemical Reaction
Fuels (Natural Gas, LPG, Naphtha, Coal, etc.)	Reforming Reaction	Gas Fuel (LNG, LPG) Byproduct Gas Synthesis Fuel (Methanol, DME)
	Gasification Reaction	Coal/Petcoke Gasification
	Biological Conversion Reaction	Biological CO Conversion
Biomass, Waste Resources	Combustible Waste Gasification	
	Biomass Gasification	
	Biological Fermentation	

Table 1. *Cont.*

Feedstock	Energy Source	Chemical Reaction
Water	Electrolysis (Electrolysis)	Alkaline Electrolysis (AEC) Proton-Exchange Membrane Electrolysis (PEMEC) Solid Oxide Electrolysis (SOEC)
	Photo-chemical Decomposition	Photoelectrochemical (PEC) Photocatalytic Photobiological
	Thermal Decomposition	Thermochemical Cycles Redox Cycles
	Nuclear	High-Temperature Gas Reactors

3. Reactions and Purity in Hydrogen Production Processes

Hydrogen production from hydrocarbons involves various reforming methods, including steam methane reforming (SMR), partial oxidation (POX), and autothermal reforming (ATR). These processes typically produce hydrogen along with byproducts such as carbon monoxide (CO) and carbon dioxide (CO_2). SMR is the most widely used method due to its cost efficiency and scalability. By introducing high-temperature steam and a catalyst to hydrocarbons like natural gas, SMR achieves hydrogen yields of approximately 65–70% under industrial conditions.

In the petrochemical sector, hydrogen is also generated as a byproduct of processes like heavy straight-run naphtha reforming for BTX (benzene, toluene, xylene) production and naphtha cracking for olefin manufacturing. These processes yield relatively low hydrogen outputs, with BTX reforming achieving 3–4% efficiency and naphtha cracking achieving 1–2% [12]. Advanced reforming techniques, such as partial oxidation and autothermal reforming, integrate oxygen or steam into the reaction, enhancing hydrogen production under controlled thermal conditions [19–23].

Steam Reforming	$C_nH_m + nH_2O \leftrightarrow nCO + (n + 0.5m)H_2$	(1)
Partial Oxidation	$C_nH_m + 0.5nO_2 \leftrightarrow nCO + 0.5mH_2$	(2)
Auto-Reforming	$C_nH_m + 0.5nH_2O + 0.25nO_2 \leftrightarrow nCO + 0.5(n + m)H_2$	(3)

Biomass-derived hydrogen is produced through thermochemical and biological processes. In thermochemical methods, biomass undergoes gasification at high temperatures (500–1400 °C) to generate synthesis gas, a mixture of hydrogen, CO, and methane. Biological processes involve microbial activity, such as photobiological water splitting and anaerobic fermentation. These methods utilize light energy or organic substrates to produce hydrogen. While the purity of hydrogen from biomass varies widely (50–68%), innovations in processing technology have improved methane conversion rates to over 80% [30–33].

Thermochemical	Biomass + Air $\rightarrow H_2 + CO + N_2 + CH_4 + H_2O$ + Tar+ Charcoal Biomass + Steam $\rightarrow H_2 + CO + N_2 + CH_4$ + Tar+ Charcoal	(4)
Biological (Photodecomposition)	$H_2O + Light \rightarrow 2H_2 + O_2$	(5)
Biological (Fermentation)	$C_6H_{12}O_6 + 2H_2O \rightarrow 2CH_3COOH + 4H_2 + 2CO_2$	(6)

Water splitting technologies, such as electrolysis, thermochemical processes, and photo electrolysis, represent clean methods for hydrogen generation. Electrolysis, the most developed of these technologies, splits water into hydrogen and oxygen using electrical energy. Alkaline electrolysis is the most established and cost-effective but suffers from lower efficiency. Proton-exchange membrane (PEM) electrolysis offers higher efficiency but comes with higher costs, while solid oxide electrolysis (SOEC) achieves the

highest efficiencies, though it remains in the pre-commercial stage. Thermochemical water splitting involves heating water to extreme temperatures (>2500 °C) to decompose it into hydrogen and oxygen. Despite its simplicity, the process requires substantial energy input, limiting its practical application. Photo electrolysis, still in the research phase, utilizes sunlight and semiconductor materials to drive the reaction. Current conversion efficiencies for this method remain low, at approximately 10–30%. The purity of hydrogen varies significantly across production methods. Hydrocarbon-based processes typically achieve purities between 40 and 70%, depending on the methane conversion rate and downstream processing. Biomass-based hydrogen production achieves similar purities (50–68%), influenced by the type of feedstock and operational conditions. Electrolysis, on the other hand, can theoretically achieve purities exceeding 99.8%, although practical operations may reduce this slightly due to residual moisture or impurities [14–17].

Electrolysis	*PEM* Anode $2H_2O \rightarrow O_2 + 4H^+ + 4e^-$ /Cathode $4H^+ + 4e^- \rightarrow 2H_2$ *Alkaline* Anode $4OH^- \rightarrow O_2 + 2H_2O + 4e^-$ /Cathode $2H_2O + 2e^- \rightarrow 2OH^- + H_2$ *SOEC* Anode $2O^{2-} \rightarrow O_2 + 4e^-$ /Cathode $H_2O + 2e^- \rightarrow H_2 + O^{2-}$	(7)
Pyrolysis	$H_2O + \text{Heat} \rightarrow H_2 + 0.5O_2$	(8)
Photovoltaic	Anode $2p^+ + H_2O \rightarrow 0.5O_2 + 2H^+$ /Cathode $2H^+ + 2e^- \rightarrow H_2$	(9)

4. Hydrogen Purity Measurement Equipment

4.1. Gas Chromatography (GC)

Gas chromatography (GC) is one of the most commonly used techniques for analyzing hydrogen purity. The principle of GC relies on the separation of gases in a sample based on their interaction with a stationary phase within a column. In this technique, a gaseous sample is introduced into the system and carried through the column by a carrier gas, such as helium or hydrogen. Different components of the sample interact differently with the stationary phase of the column, causing them to separate as they pass through the column at varying rates. The time it takes for each component to elute from the column (known as retention time) is recorded and used for quantification and identification of the components. The main components of a GC system include the carrier gas supply, which ensures the flow of gas through the system; the sample injector, which vaporizes the sample for introduction into the column; the column, where separation occurs; and the detector, which detects the separated components. Common detectors used in GC include Flame Ionization Detectors (FIDs), Thermal Conductivity Detectors (TCDs), and Electron Capture Detectors (ECDs), each offering varying sensitivities for different types of compounds. After the sample is separated, the detector sends a signal to the data processing system, where the results are analyzed. The components of GC are shown in Figure 1.

GC is highly regarded for its speed, sensitivity, and precision. It offers a fast analysis time, with separation and quantification often occurring within minutes. Furthermore, GC can provide high separation efficiency, even for complex mixtures, and it is capable of detecting compounds at low concentrations, typically at the ppm (parts-per-million) level. One of the key advantages of GC is its ability to offer both qualitative and quantitative analysis simultaneously, providing detailed insights into the composition of the sample. However, GC also has limitations, such as its inability to analyze non-volatile compounds and the potential for sample matrix effects, which can interfere with the analysis [65].

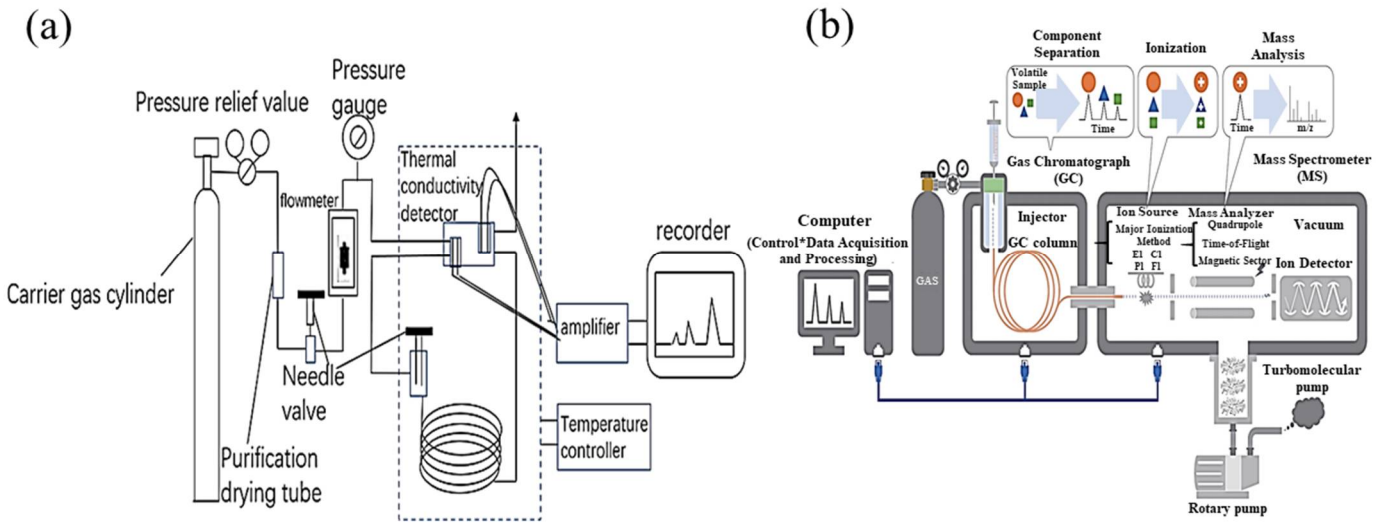


Figure 1. The components of (**a**) GC and (**b**) GC-MS [65].

4.2. Gas Chromatography–Mass Spectrometry (GC-MS)

Gas chromatography–mass spectrometry (GC-MS) combines the separation power of GC with the identification capabilities of mass spectrometry. In this method, the sample is first separated using GC, and the components are then introduced into a mass spectrometer. The mass spectrometer ionizes the separated components and analyzes them based on their mass-to-charge ratio (m/z), allowing for both qualitative and quantitative analysis. The components of GC-MS include the GC column and detector, similar to those used in GC, but with an additional mass spectrometer. The mass spectrometer contains an ionization source (e.g., Electron Ionization (EI) or Chemical Ionization (CI)), which ionizes the separated components. After ionization, the ions are sent to a mass analyzer, such as a quadrupole or time-of-flight (TOF) analyzer, where they are separated based on their m/z ratio. The resulting ion spectra are compared to a database to identify the compounds present, and the intensity of the signals is used to quantify the concentration of each compound. GC-MS provides several advantages, including extremely high sensitivity, with detection limits in the ppb (parts-per-billion) to ppt (parts per trillion) range. It allows for the simultaneous identification and quantification of compounds in complex mixtures, which is particularly useful for analyzing trace impurities in hydrogen. However, the technique is expensive, requires a high level of expertise, and can be prone to matrix effects, where the presence of interfering substances in the sample can affect the accuracy of the analysis [65].

4.3. Inductively Coupled Plasma Mass Spectrometry (ICP-MS)

Inductively coupled plasma mass spectrometry (ICP-MS) is a highly sensitive technique used for detecting trace elements and impurities in hydrogen. This method involves the use of an inductively coupled plasma (ICP) to ionize the sample, followed by mass spectrometric analysis of the resulting ions. In ICP-MS, the sample is introduced into the plasma, where it is atomized and ionized by the high-energy argon plasma. These ions are then transported to the mass spectrometer, where they are separated based on their mass-to-charge ratio (m/z) and detected. The key components of an ICP-MS system include the plasma torch, which generates the high-temperature plasma necessary for ionization; the sample introduction system, which introduces the sample into the plasma; the mass spectrometer, which separates the ions; and the detector, which measures the intensity of the ions. ICP-MS is particularly well suited for multi-element analysis, providing high sensitivity and accuracy for detecting trace elements at concentrations as low as parts per trillion (ppt). However, the method is costly and requires regular maintenance, as well as

a stable supply of argon gas. Additionally, matrix effects can interfere with the analysis, particularly in complex samples [66].

4.4. Fourier Transform Infrared Spectroscopy (FT-IR)

Fourier-transform infrared spectroscopy (FT-IR) is a non-destructive analytical technique that measures the absorption of infrared light by a sample. When the sample absorbs infrared radiation, its molecular bonds undergo vibrational transitions. These vibrations correspond to specific wavelengths of infrared light, and by measuring the absorption at different wavelengths, FT-IR can provide detailed information about the chemical composition of the sample. The components of an FT-IR system include an infrared light source, an interferometer that modulates the infrared light, a sample chamber where the sample interacts with the infrared light, and a detector that measures the transmitted light. FT-IR provides a spectrum that shows the amount of absorption at each wavelength, which is characteristic of the sample's molecular structure. FT-IR is advantageous for its non-destructive nature, as it can be used for real-time monitoring without altering the sample. The technique is also fast, with results obtained in a matter of minutes, and can be used to analyze a wide range of sample types, including gases, liquids, and solids. However, FT-IR has limitations, particularly in terms of its sensitivity for trace impurities in hydrogen. Water vapor and other contaminants can interfere with the measurements, and the interpretation of spectra for complex mixtures can be challenging [67,68].

4.5. Cavity Ring-Down Spectroscopy (CRDS)

Cavity ring-down spectroscopy (CRDS) is an advanced technique used for the ultrasensitive detection of gases, including hydrogen. In CRDS, a laser is directed into an optical cavity with highly reflective mirrors. As the laser light passes through the cavity, it interacts with the sample, and the presence of absorbing substances in the sample causes the light intensity to decay. The rate at which the light decays is proportional to the concentration of the absorbing substance, which can be used to quantify the substance. The key components of CRDS include a tunable laser source, which generates light at specific wavelengths, a high-reflectivity cavity, and a detector that measures the decay of the light signal. CRDS is highly sensitive, with the ability to detect gases at concentrations in the parts-per-billion (ppb) to parts-per-trillion (ppt) range. It offers real-time, continuous measurements without direct contact with the sample, which is particularly useful for monitoring hydrogen purity over time. However, CRDS requires precise control of environmental conditions, such as temperature and pressure, and the accuracy of the results can be affected by laser stability and other system factors [69].

4.6. Ion Chromatography (IC)

Ion chromatography (IC) is a technique used to separate and quantify ionic species in a sample. In IC, the sample is injected into a column packed with ion-exchange resin, and the ions in the sample are separated based on their affinity for the stationary phase. The elution of the ions from the column is monitored using a detector, typically a conductivity detector, which measures the ionic conductivity of the eluted solution. The main components of an IC system include the eluent (a solution that helps separate the ions), the column (which contains the ion-exchange resin), the detector (usually a conductivity detector), and the data processing system. IC is widely used for detecting inorganic ions, such as chloride, sulfate, and nitrate, and can also be used to analyze organic acids and bases. It is a highly sensitive technique, capable of detecting ions at concentrations as low as the parts-per-million (ppm) to parts-per-billion (ppb) range. However, IC has limitations, particularly with complex samples, where matrix effects can interfere with the separation and detection of target ions [70].

4.7. Electrochemical Sensors

Electrochemical sensors are widely used for detecting gases, including hydrogen. These sensors work based on the principle that the oxidation or reduction of a target substance on an electrode surface generates a measurable electrical signal. The signal, which can be in the form of current, voltage, or impedance, is proportional to the concentration of the target substance. The types of electrochemical sensors include amperometric, potentiometric, impedimetric, and conductometric sensors. Amperometric sensors measure the current generated by the electrochemical reaction, while potentiometric sensors measure the voltage difference between electrodes. Impedimetric sensors measure changes in impedance, and conductometric sensors detect changes in conductivity. Electrochemical sensors offer several advantages, including real-time monitoring, high sensitivity, and relatively low cost. They are commonly used in portable and online monitoring devices for hydrogen purity. However, the lifespan of these sensors is limited by the degradation of the electrode material, and environmental factors such as temperature, humidity, and gas matrix effects can impact the accuracy of the measurements [80].

4.8. Gravimetric Analysis (GA)

Gravimetric analysis is a classical technique used to determine the concentration of a substance by measuring the mass of a precipitate or residue formed during a chemical reaction. In this method, the substance of interest is precipitated, filtered, dried, and weighed. The mass of the precipitate is then used to calculate the concentration of the target substance. Gravimetric analysis is highly accurate and precise, capable of detecting trace amounts of substances with minimal interference. However, the process is time-consuming as it requires multiple steps, including filtration, drying, and weighing, which limits its applicability for high-throughput analysis. Despite this, gravimetric analysis remains valuable for confirming the purity of hydrogen in applications where high accuracy is required.

Each of the components of the equipment and an example of the analysis result are shown in Figures 1–6. Table 2 shows the capabilities of each analytical device for hydrogen gas quality testing.

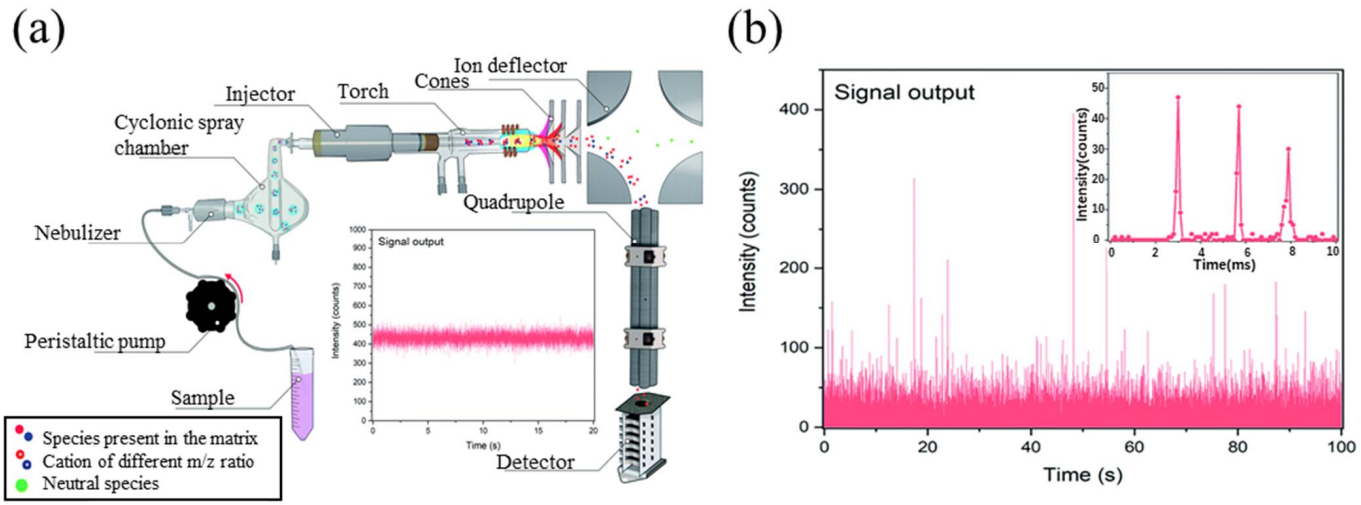


Figure 2. (**a**) The components of ICP-MS; (**b**) example of analysis result [66].

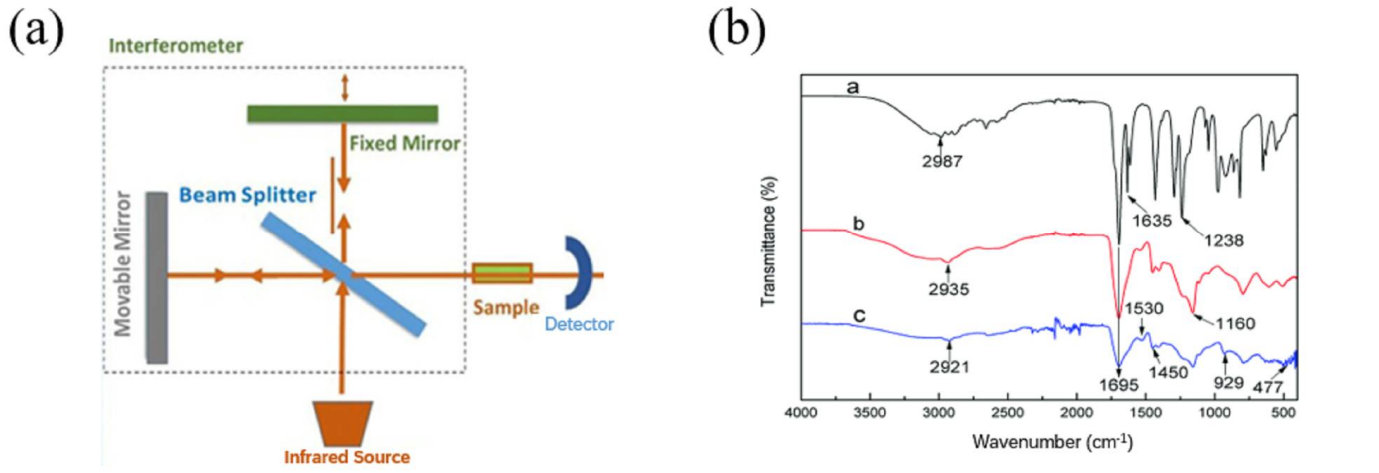


Figure 3. (**a**) The components of FT-IR; (**b**) example of analysis result [61,67,68].

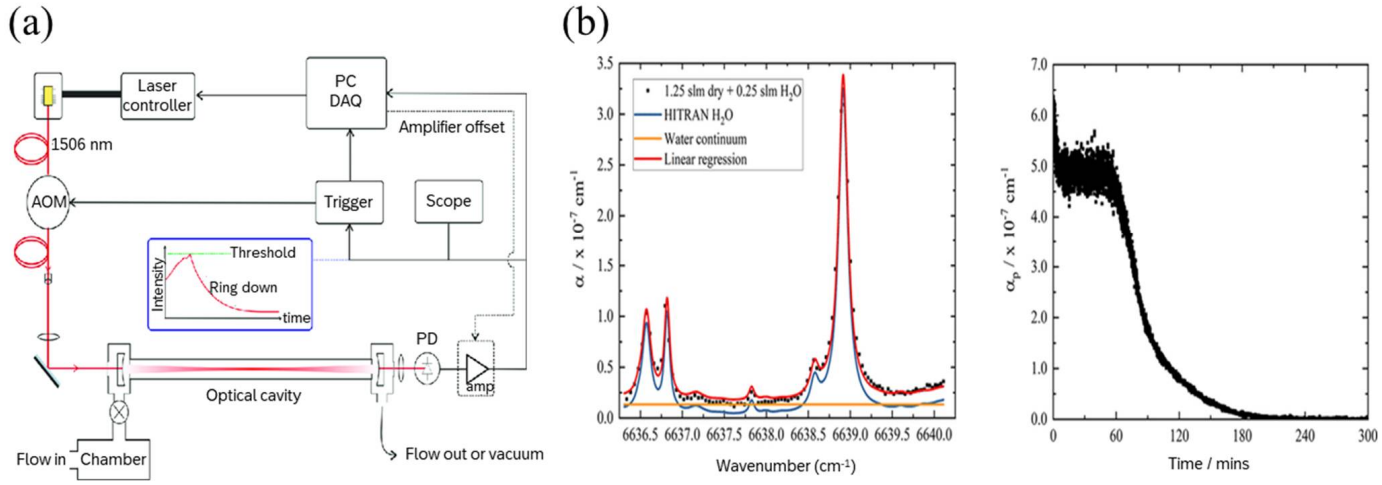


Figure 4. (**a**) The components of CRDS; (**b**) example of analysis result [69].

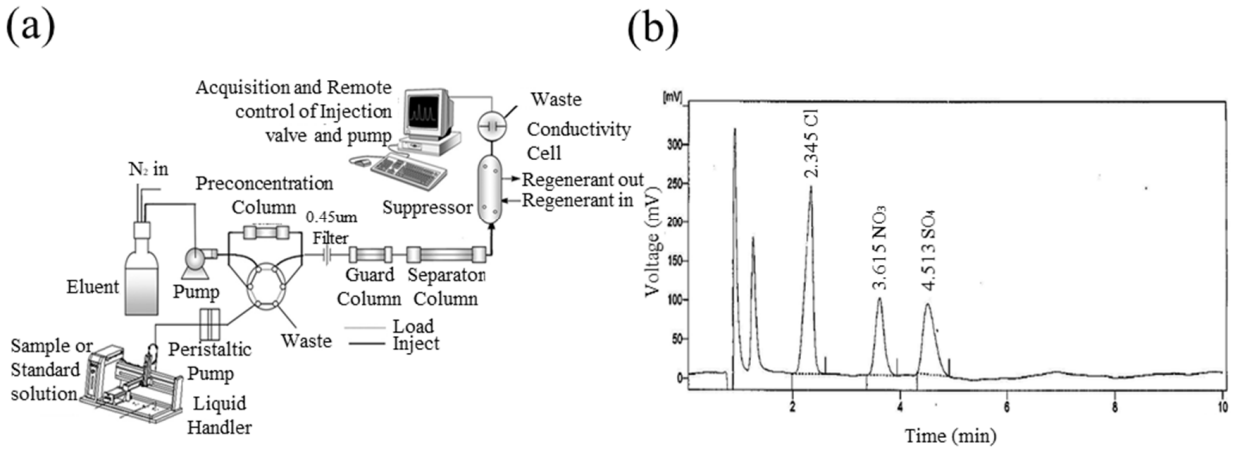


Figure 5. (**a**) The components of IC; (**b**) example of analysis result [70].

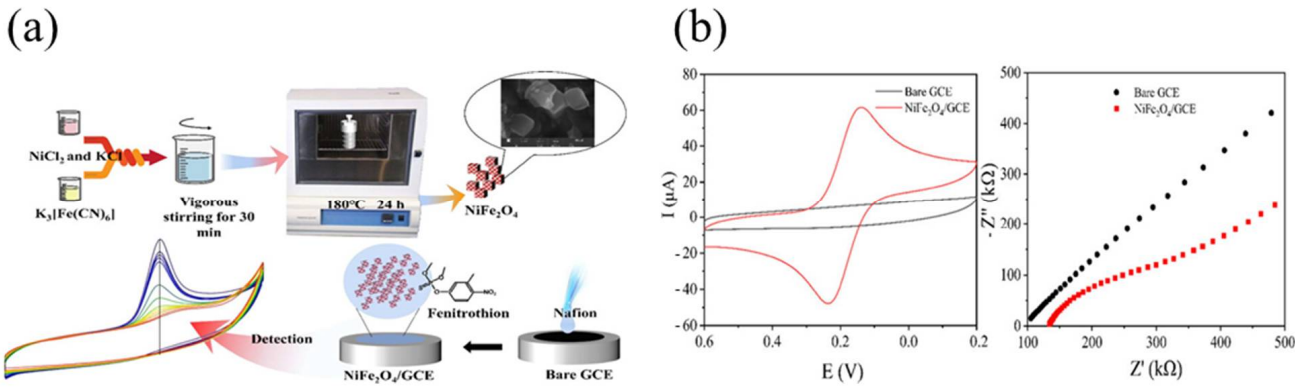


Figure 6. (**a**) The components of electric sensor; (**b**) example of analysis result [80].

Table 2. Comparison of hydrogen gas quality testing suitability for different analytical devices (O: possible to analyze the test item, X: not possible to analyze the test item).

Test Item	GC/GC-MS (ppb~ppm)	FT-IR (ppm~%)	ICP-MS (ppt~ppb)	IC (ppb~ppm)
Purity	O	X	X	X
Moisture (H_2O)	X	O	X	O
Total Hydrocarbons (THC)	O(FID)	X	X	X
Oxygen (O_2)	O(TCD)	X	X	X
Helium (He)	O(TCD)	X	X	X
Nitrogen/Argon (N_2/Ar)	O(TCD)	X	X	X
Carbon Dioxide (CO_2)	O(TCD)	O	X	O
Carbon Monoxide (CO)	O(TCD)	O	X	X
Total Sulfur (Total S)	X	X	O	O
Organic Acids	O	O	X	O
Formaldehyde (CH_2O)	O	O	X	X
Ammonia (NH_3)	O	O	X	O
Halogen Compounds (HX)	O	O	X	O
Particle Concentration	X	X	O	X

5. Purification Technologies

Hydrogen purification methods can be broadly categorized into mechanical methods (such as adsorption, membrane separation, and cryogenic techniques), chemical methods (including metal hydride separation and catalytic purification), and physical methods. The choice of purification method is determined by factors such as the quantity of hydrogen and the nature of the impurities present during production. Pressure swing adsorption (PSA) and gas membrane separation are among the most commonly used methods for hydrogen purification. PSA, in particular, tends to be more energy-intensive and costly when the hydrogen purity is low, prompting recent developments in membrane separation technologies. There are commercially available inorganic and organic membrane products for such processes [28,103–108]. One notable study involved the integration of membrane and cryogenic separation technologies into a hybrid membrane-cryogenic process, which achieved hydrogen purity of 99.99% with a recovery rate of 95.9%, while reducing energy consumption to 2.37 kWh/kg. This study also evaluated the total operational cost of equipment, including compressors and coolers, providing a comprehensive economic analysis [103]. The proposed process overcomes the limitations of single-technology methods, offering potential for applications requiring high-purity hydrogen, such as fuel cells and liquid hy-

drogen production. Another experimental study focused on improving hydrogen recovery rates in PSA processes under variable hydrogen conditions (65–98% hydrogen content, 25–60 bar pressure). By dividing the gas recovery process into four stages, the researchers successfully produced high-purity hydrogen (99.95%) and identified effective operational strategies, flexible process control mechanisms, and the need for advanced components to ensure stability under dynamic conditions [104]. Simulation-based analyses have also provided valuable insights, as demonstrated by a study using the CHEMCAD program to simulate the production of nitrogen, oxygen, and argon with purities ranging from 99.49% to 99.99%. By optimizing the process parameters, this study evaluated efficiency, practicality, and specific gas production rates, offering critical data for future designs [106].

In another case, a VSA (vacuum swing adsorption) process was designed to economically produce high-purity hydrogen from low-concentration hydrogen mixtures. Experimental setups involving a 10% hydrogen and 90% methane mixture demonstrated a two-stage process, achieving 99% hydrogen purity. This study also validated performance using Aspen simulations, confirming the superior recovery rates and lower energy consumption of the two-stage VSA process compared to single-stage alternatives [107].

5.1. Adsorption Method

The adsorption method involves separating hydrogen from a gas mixture by selectively adsorbing impurities onto a solid surface. The process relies on solid adsorbents (typically porous materials) to selectively capture specific gases. The adsorption method can achieve hydrogen purification when the feed purity is higher than 40% by volume [29,71,104].

5.1.1. Principle of PSA (Pressure Swing Adsorption)

In this process, a gas mixture is passed through an adsorbent at high pressure, where impurities are trapped by the adsorbent. The pressure is then reduced to release the adsorbed impurities, while the hydrogen continues to pass through. PSA is commonly used in large-scale industrial applications, such as hydrogen purification from steam methane reforming (SMR) processes, where impurities like CO_2, methane, and CO are removed. The key advantage of PSA is its high hydrogen recovery rate (over 99%), making it suitable for large-scale applications where maintaining high purity is critical [29]. The flow scheme of PSA is shown in Figure 7.

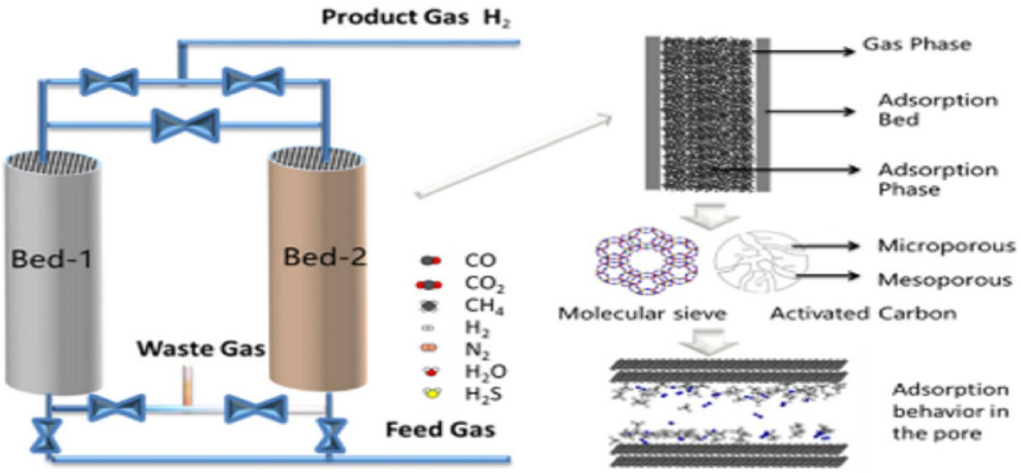


Figure 7. Flow scheme of the classical pressure swing adsorption (PSA) system [30].

5.1.2. Temperature Swing Adsorption (TSA)

TSA relies on the temperature variation to adsorb and desorb impurities. It is mainly used for removing water or light impurities from hydrogen. Since the process operates at atmospheric pressure, it consumes less energy and is typically applied for hydrogen that needs to be dried or purified for specific uses [31,108]. The process is shown in Figure 8.

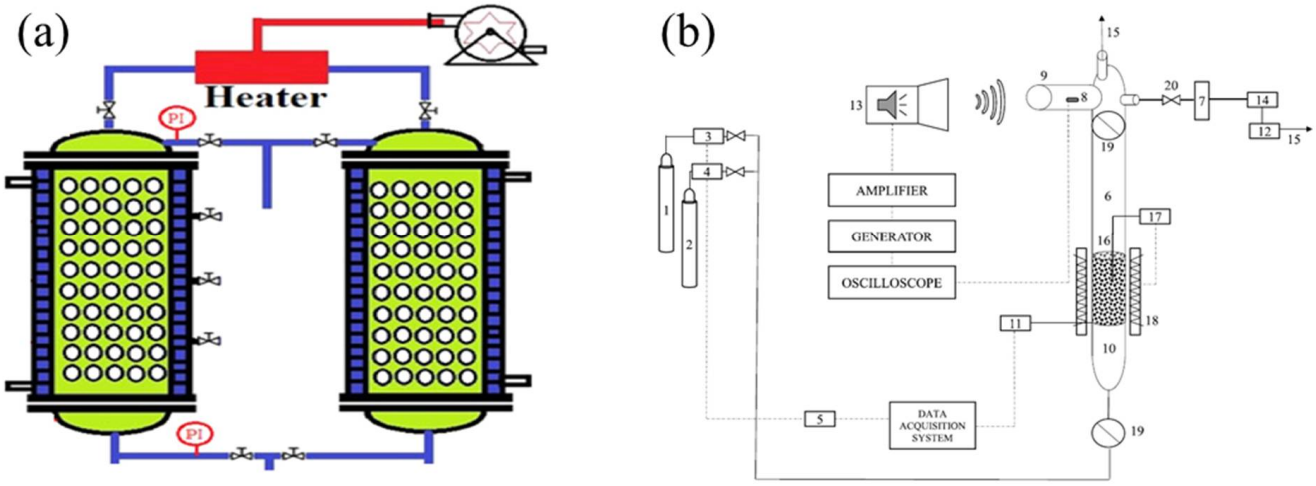


Figure 8. (**a**) TSA system adsorption for H_2 purification; (**b**) experimental apparatus [31,32].

5.1.3. Vacuum Swing Adsorption (VSA)

VSA is similar to PSA, but it uses a vacuum instead of a pressure swing to remove impurities. This method is especially useful for hydrogen purification processes that operate at lower pressures, offering advantages such as lower energy consumption and higher efficiency in small-scale applications [33,34,106].

5.2. Membrane Separation Method

In membrane separation, hydrogen is purified by selectively passing through a membrane that separates it from other gases based on molecular size or chemical characteristics. Since hydrogen has the smallest molecular size, it can be selectively separated from larger impurities, such as CO_2, CO, and methane, using different types of membranes. Figures 9 and 10 show the penetration mechanism of penetrants through membrane and other membrane separation processes, respectively [45–51].

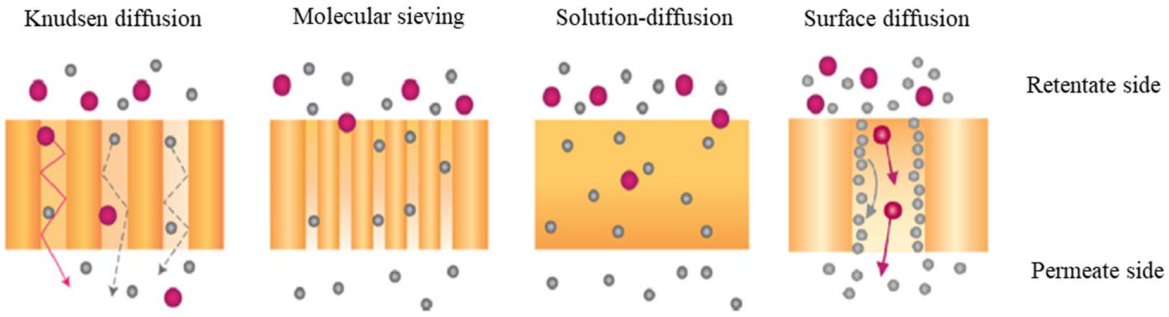


Figure 9. The penetration mechanism of penetrants through membrane [46].

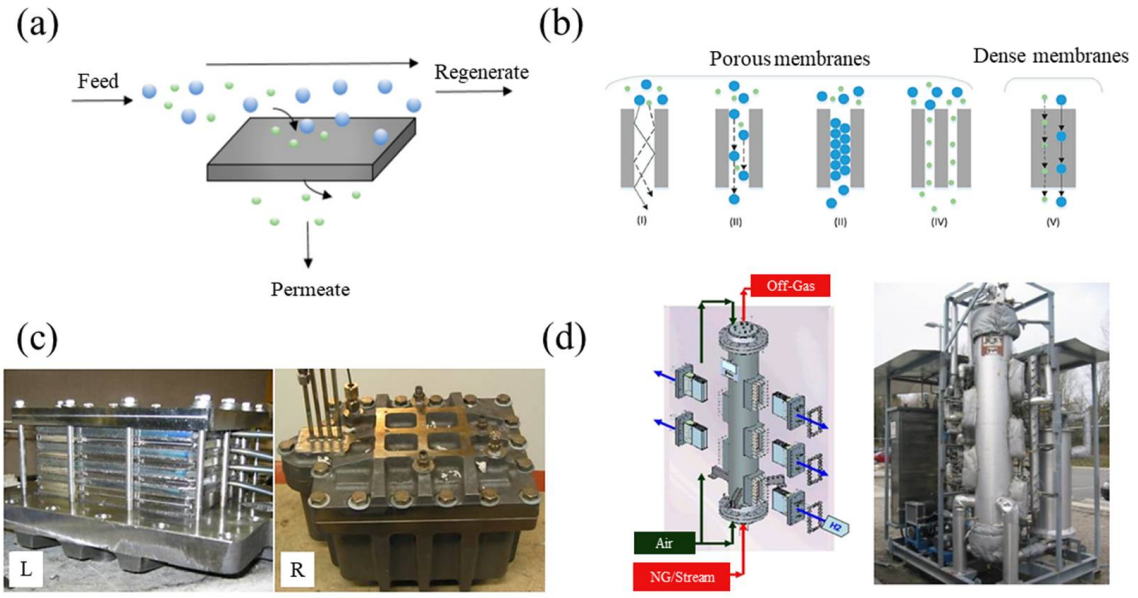


Figure 10. (**a**) Schematic of membrane separation, (**b**) transport mechanism for membranes, (**c**) L: purifier for town gas, R: membrane stack and purifier prototype, and (**d**) unit for pure hydrogen production [50,51].

5.2.1. Polymer Membranes

Polymer membranes are lightweight, low-cost, and porous structures that allow for hydrogen to permeate while blocking larger molecules. They are primarily used in industries like petrochemicals and are suited for low-pressure applications [45–47].

5.2.2. Metal Membranes

Made from palladium or palladium alloys, these membranes are highly selective for hydrogen and can achieve ultra-high purity (99.999%). These are used in applications requiring extremely pure hydrogen, such as fuel cell production or high-purity hydrogen processes [48].

5.2.3. Ceramic Membranes

These membranes have excellent thermal stability and chemical resistance, allowing them to operate in high-temperature and corrosive environments. They are often used in processes involving the separation of hydrogen from CO_2 or SO_2, such as in gasification and power plants [49].

5.2.4. Composite Membranes

These combine polymer, metal, or ceramic materials to create membranes with high selectivity, durability, and mechanical strength, allowing them to perform effectively across various conditions. They are used in large industrial plants and fuel cell applications [49].

5.3. Cryogenic Distillation Method

Cryogenic distillation is a physical separation technique where hydrogen is separated from other gases based on their boiling points. In this process, hydrogen is cooled to extremely low temperatures, causing it to liquefy, while the other gases remain in the vapor phase. This method produces very-high-purity hydrogen (99.999%) but requires significant energy and complex cooling systems [64]. The process is shown in Figure 11.

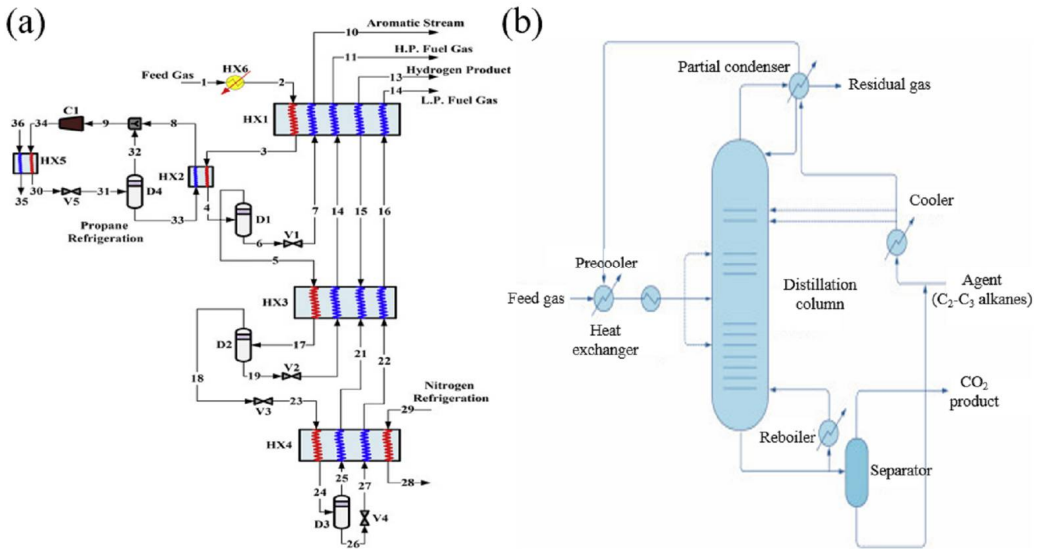


Figure 11. (**a**) Process of the cryogenic method; (**b**) schematic of a cryogenic distillation unit consisted of a packed distillation column and an equilibrator [52,63,109].

5.3.1. Metal Hydride Separation

Metal hydride separation is a chemical method where hydrogen is absorbed by metals or alloys to form metal hydrides. These hydrides can absorb and release hydrogen under specific temperature and pressure conditions. This method is useful for separating hydrogen from other gases, as metal hydrides can selectively absorb hydrogen and reject other impurities. The advantages include high selectivity, low-temperature operation, and the ability to store and purify hydrogen simultaneously [24]. The metal hydride separation method is shown in Figure 12 [64,73,77,80,107].

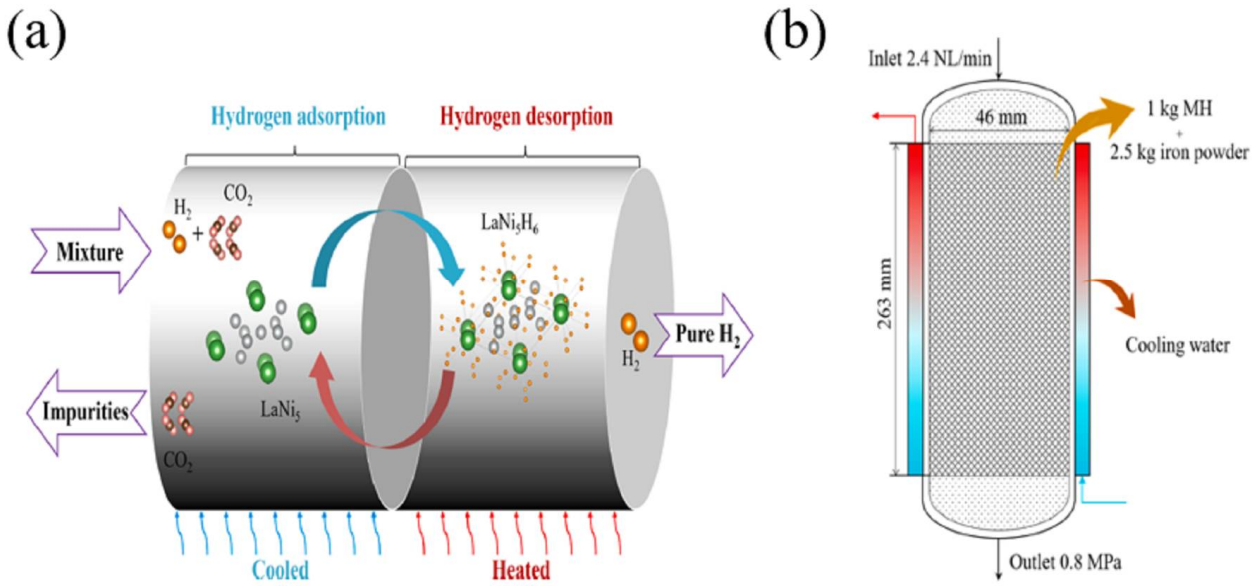


Figure 12. (**a**) The diagram of MH method for hydrogen recovery and purification; (**b**) the reactor of MH method [64].

5.3.2. Catalytic Purification

Catalytic purification removes impurities from hydrogen by promoting chemical reactions that convert unwanted gases into harmless byproducts. For instance, carbon monoxide (CO) is removed from hydrogen by reacting it with water to form CO_2 and hydrogen via the water–gas shift reaction (WGS) using catalysts like iron, copper, or palladium.

Other impurities, like methane and nitrogen oxides, are also removed through catalytic reactions at high temperatures. This method is widely used in producing high-purity hydrogen for fuel cells and ammonia production processes [28]. Table 3 summarizes the advantages and disadvantages of hydrogen purification technologies [19,20,27,28,30,36,91].

Table 3. Comparison of hydrogen refining technologies [19,20,27,28,30,91].

Refining Technologies	Advantages	Disadvantages	Purity (%)
PSA	High hydrogen recovery rates Widely used commercially	High energy consumption Expensive for low-purity	99.999
Membrane Separation	High hydrogen recovery rates Widely used commercially	High operating costs Membrane lifespan issues	95.8–99.9
Cryogenic Distillation	High hydrogen recovery rates Widely used commercially	High energy consumption Complex cooling systems Expensive to operate	99.999
TSA	High hydrogen recovery rates Widely used commercially	Limited application fields Restricted to the removal of certain lightweight impurities	95–98
VSA	High efficiency at low pressures Low energy consumption Suitable for small-scale applications	Unsuitable for large-scale applications	95–98
Metal Hydride Separation	High selectivity Operable at low temperatures Capable of storage and purification	Unsuitable for large-scale applications	99.95

6. Purification Based on Production Method

The type and concentration of impurities in hydrogen are largely determined by the production method used, and the corresponding purification methods are chosen accordingly [28–34,62].

6.1. Steam Methane Reforming (SMR)

This process typically produces hydrogen with impurities such as CO_2, CO, and methane. PSA is commonly employed for purification, often in conjunction with membrane separation technologies [28].

6.2. Electrolysis

Hydrogen produced through electrolysis has high purity, but trace impurities like water vapor or oxygen may still be present. Dehydration or drying technologies, such as TSA or specific water-removal devices, are used to further purify hydrogen [15].

6.3. Coal Gasification

Coal Gasification: In this process, coal is converted into hydrogen at high temperatures, producing large amounts of CO_2, CO, and other impurities. PSA is commonly used to purify hydrogen, and in some cases, chemical absorption is applied to remove CO_2. For large-scale CO_2 removal, carbon capture and storage (CCS) technology is often integrated [12].

6.4. Biomass Gasification

Similar to coal gasification, hydrogen is produced from biomass at high temperatures, yielding methane, CO_2, and CO. PSA is frequently used for purification, with membrane separation technology also being employed for improved efficiency [13].

6.5. Water–Gas Shift Reaction (WGS)

After SMR, CO is further converted to CO_2 and hydrogen through a reaction with water. This process generates large amounts of CO_2, which is typically removed through chemical absorption or PSA [28].

7. Hydrogen Purification Based on Purity Levels

The purification method employed depends on the hydrogen purity required and the composition of the feed gas. Each purification method is chosen based on the specific requirements of the hydrogen production process and the desired purity level, balancing energy efficiency, cost, and the effectiveness of impurity removal. High-purity hydrogen plays a crucial role in applications such as fuel cells, where impurities can contaminate electrodes and catalysts, leading to performance degradation and reduced lifespan. As hydrogen energy industries rapidly expand, the reliable supply of ultra-high-purity hydrogen ($\geq$99.99%) is becoming increasingly vital. Impurities not only lower system efficiency but also increase maintenance costs and risk equipment damage. Therefore, advancing and optimizing hydrogen purification technologies is essential for supporting the hydrogen economy and achieving sustainability goals [82–87].

7.1. Low Purity Feed Gas (40–70% Hydrogen)

Produced in processes like coal or biomass gasification, this feed gas contains impurities like CO_2, CO, methane, and nitrogen. Purification methods include PSA, chemical absorption (especially for CO_2), and membrane separation [29].

7.2. Intermediate Purity Feed Gas (70–90% Hydrogen)

Typically produced by SMR or the water–gas shift reaction, this feed gas is purified using PSA, membrane separation, and sometimes cryogenic methods for high-purity hydrogen [29].

7.3. High-Purity Feed Gas (90–99% Hydrogen)

Produced via processes like electrolysis or advanced reforming, the main impurities are water and oxygen. TSA and membrane separation are often used to remove these trace impurities [15].

7.4. Ultra-High-Purity Feed Gas (99% + Hydrogen)

Used in industries like aerospace, semiconductor manufacturing, and precision chemistry, ultra-high-purity hydrogen is purified using cryogenic distillation and advanced filtering systems. These methods remove the last traces of water and oxygen to achieve the highest purity levels [64].

8. Conclusions

Key hydrogen purification methods include pressure swing adsorption (PSA), membrane separation, and metal hydride-based separation. While PSA is widely adopted for its simplicity and cost-effectiveness, membrane technologies offer efficient separation based on molecular size and diffusion rates. Metal hydride-based separation enables theoretical ultra-high-purity hydrogen production with low operational complexity. However, these technologies face challenges such as high energy consumption, operational costs, and limited scalability. Real-time monitoring and analysis remain critical gaps, with current technologies lacking the capability to rapidly detect trace impurities in hydrogen. Furthermore, the intermittent and variable nature of renewable energy sources poses challenges

for consistent hydrogen production, requiring enhanced efficiency and stability in water electrolysis processes.

The future of hydrogen purification technologies is aligned with the global decarbonization and sustainability goals. Key directions include the following:

- Development of High-Efficiency, Low-Cost Technologies: Innovations in membrane materials, catalysts, and hybrid processes aim to enhance efficiency and reduce operational costs.
- Integration with Renewable Energy: Clean hydrogen production technologies, such as biomass gasification and advanced water electrolysis, are expected to leverage renewable energy sources like solar, wind, and hydro.
- Advances in Ultra-High-Purity Hydrogen Production: Hybrid processes combining PSA, membrane technologies, and metal hydride separation will enable production tailored to specific applications.
- Scalable Production Technologies: Large-scale hydrogen production technologies will address growing global demand and expand industrial applications.
- Digitalization and Real-Time Monitoring: Advanced digital tools and monitoring systems will improve the precision and safety of hydrogen purification processes.
- International Collaboration and Standardization: Global cooperation and standardization will ensure the seamless integration of hydrogen technologies across markets and regions.

By overcoming the current limitations and embracing innovation, hydrogen purification technologies will play a pivotal role in achieving a sustainable energy future, advancing the hydrogen economy, and supporting global decarbonization efforts.

Hydrogen's role as a clean energy carrier is central to achieving global sustainability and decarbonization goals. However, its effectiveness across various applications depends significantly on its purity, which is influenced by the production methods, purification techniques, and analytical processes employed. Fossil fuel-based methods, while currently dominant, introduce impurities that necessitate advanced purification strategies. Conversely, renewable-based production methods such as electrolysis offer pathways to ultra-pure hydrogen but require further cost reductions and technological advancements to achieve large-scale adoption. Purification technologies such as pressure swing adsorption, membrane separation, and cryogenic distillation have proven to be essential for delivering high-purity hydrogen. These techniques, combined with hybrid systems, can optimize both performance and cost, catering to the diverse purity requirements of industries ranging from fuel cells to chemical synthesis. Simultaneously, the growing sophistication of analytical tools, including gas chromatography, mass spectrometry, and cavity ring-down spectroscopy, ensures the precise monitoring of hydrogen quality, fostering confidence in its use across critical applications. Despite the progress made, challenges remain in scaling up renewable hydrogen production, integrating advanced purification systems, and meeting the stringent standards required for ultra-pure hydrogen. Addressing these challenges will require coordinated efforts across research, industry, and policy domains. Investments in R&D to enhance production efficiency, reduce costs, and develop real-time analytical techniques will be pivotal in overcoming these barriers.

In conclusion, the pathway to a hydrogen-based economy hinges on the ability to produce, purify, and analyze hydrogen effectively and efficiently. By addressing the current limitations and leveraging advancements in technology, hydrogen can fulfill its promise as a cornerstone of a sustainable and decarbonized energy future. This review underscores the importance of continued innovation and collaboration in realizing this vision (Figure 13).

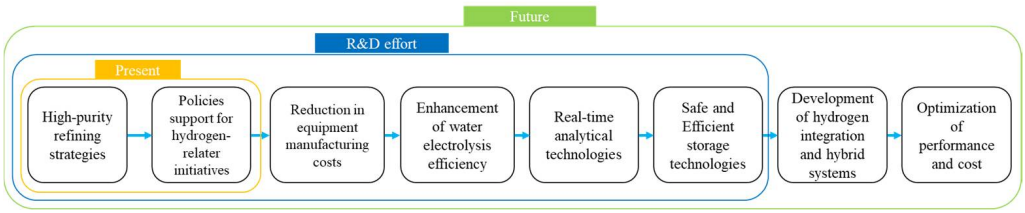


Figure 13. Challenges and future directions for hydrogen purity technologies.

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