

Review Article

The hydrogen supply chain — A comprehensive literature review incorporating purity analysis

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ABSTRACT

Hydrogen is an important energy vector for the transformation of the energy system towards greenhouse gas neutrality. For accurate infrastructure planning, it is necessary to consider the entire hydrogen supply chain and the different states of hydrogen. A crucial dimension for hydrogen infrastructure planning is the purity of the hydrogen. This review paper aims to provide an overview of the different purity levels of hydrogen throughout the supply chain stages of production, purification, transport, storage, and application. The results show that purification is critical in the system when hydrogen is used as a feedstock material for the chemical industry and fuel cell vehicles (≥ 99.97 mol%). For thermal applications, lower purity levels are sufficient (≥ 98 mol%). Green hydrogen production methods based on electrolysis produce higher purity levels compared to fossil hydrogen production routes. For high purity applications, purification or treatment is required for all hydrogen production methods. Pressure swing adsorption can serve as a versatile purification technology, reaching high purity levels at investment costs of 143 EUR/kW. Different transport and storage options can either introduce new impurities, maintain the purity level, or remove impurities in the associated conversion processes.

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1. Introduction

Hydrogen is seen as a key cornerstone in the transition to greenhouse gas-neutral energy systems. The development of green hydrogen supply chains is gaining momentum. Newly developed hydrogen technologies are being deployed in the real world. However, there are still several unknowns that affect the design of future hydrogen supply chains. One of these is the level of hydrogen purity that will be provided, maintained and required at different stages of the supply chain. Several research projects and individual researchers have examined multiple, but often not all parts of the hydrogen supply chain. These include the *Hy4Heat* project (2019) [1], the *H₂-Rein* project (2022) [2] and research by Linde GmbH engineer Peschel (2020) [3]. There are also reviews and research articles dealing with individual stages of the supply chain. These include studies by Nikolaidis et al. (2017) [4] on hydrogen production processes, by Du et al. (2021) [5] on purification technologies, and by Usman (2022) [6] on hydrogen storage methods.

The purpose of this paper is to combine these sources and fill in missing data to provide a comprehensive overview of the major hydrogen technologies and their corresponding hydrogen purity levels throughout the supply chain. In detail, this includes the selection of the main hydrogen technologies, a systematic literature review of the hydrogen purity and the impurities, a categorization of the technologies into different purity levels, and a visualization of the research results.

The structure of the paper follows the steps of the hydrogen supply chain as described in Fig. 1. The hydrogen supply chain is divided into three parts that make up the three sections of the paper: Sources of impurities during production, transportation, and storage; Purity requirements at application and end-use; and Purification of hydrogen to achieve the desired purity levels. Within these sections, technology selection, literature review, and purity classification are discussed.

1.1. Technology selection

Fig. 1 shows which technologies have been considered in this paper for each step of the supply chain. The selection is based on the

assessment of their Technology Readiness Level (TRL), which is used to evaluate the applicability of technologies. The TRL rating system ranges from 1 (basic principles have been observed and reported) to 9 (actual system has been proven itself through successful operation) [7,8]. It can be expected that technologies that have not yet been tested beyond the laboratory scale will not make a significant contribution to the transformation. Therefore, the main criterion for technology selection in this study is that the technology in question must have a TRL value of at least five.

1.2. Structured literature review

The identification of purity data is based on the procedure for performing a systematic literature review by Kitchenham [9]. The search terms used and the number of research papers identified are presented in the supplementary material in Section 1. The purity analysis is performed for the entire hydrogen supply chain, including hydrogen production, purification, transportation, storage, and use. The hydrogen purity data presented in this paper are based on original research papers, review studies, standards and technical reports.

1.3. Purity grade classification

To reduce the complexity of the individual purity levels and contamination for each process, the technologies are clustered into purity grades. The clustering is based on the ISO 14687:2019(E) [10] standard for hydrogen fuel quality and the hydrogen gas groups defined by the DVGW e.V. [2,11], the Association of the German Gas and Water Industry, presented in Table 1.

The gas grades defined by the DVGW are based on the standard. Therefore, purity grade D is defined in the same way. For purity grade A, the DVGW specifies more specific values for use in practice. It should be noted that the maximum allowable impurity level of 300 ppm for grade D applies only to inert gases. Other impurities, such as catalyst poisons for fuel cells like carbon monoxide and sulfur-containing compounds, have much lower limits of less than 1 ppm.

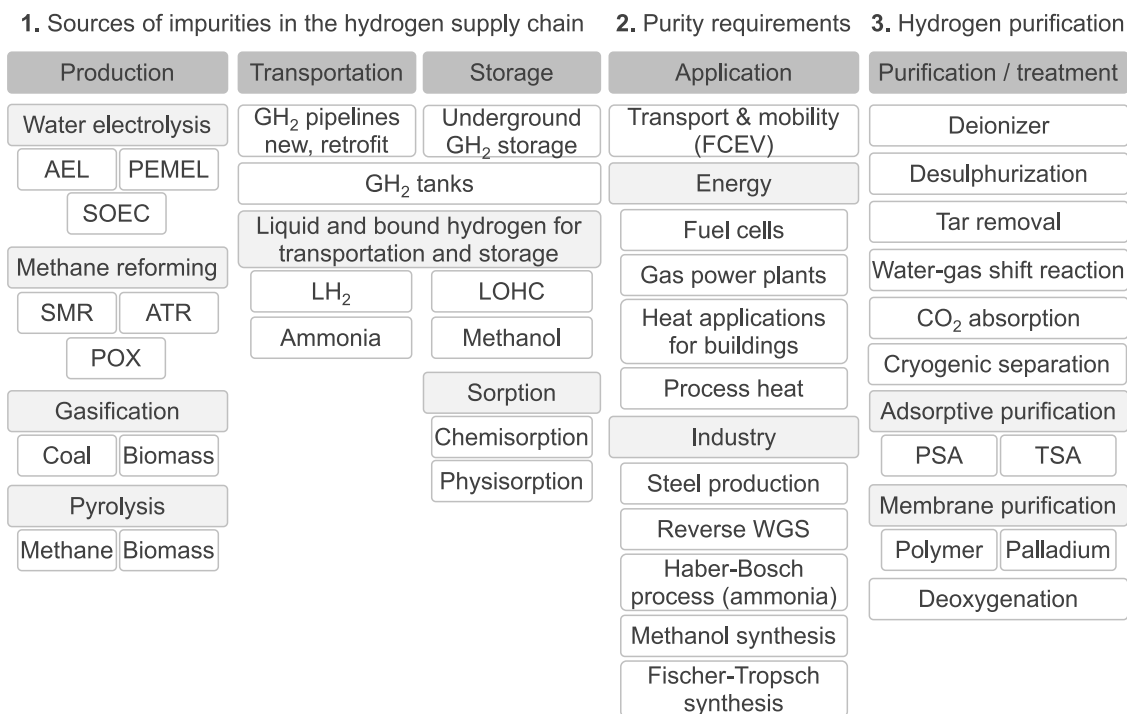


Fig. 1. Overview of the technologies and applications of hydrogen along the supply chain investigated in this paper. The structure of this paper follows these technology groups. AEL: alkaline electrolysis, PEMEL: PEM electrolysis, SOEC: solid oxide electrolysis, SMR: steam methane reforming, ATR: autothermal reforming, POX: partial oxidation, LOHC: liquid organic hydrogen carriers, FCEV: fuel cell electric vehicle, WGS: water-gas shift reaction, PSA: pressure swing adsorption, TSA: temperature swing adsorption.

Table 1

Classification of hydrogen purity grades according to ISO 14687:2019(E) [10] and DVGW e.V. [2,11].

	Grade A ISO 14687	Grade A DVGW	Grade D ISO 14687/DVGW
H ₂	98 mol%	98 mol%	99.97 mol%
H ₂ O	Non-condensing at all ambient conditions	200 mg/m ³ (MOP ≤ 10 bar) 50 mg/m ³ (MOP > 10 bar)	5 ppm
O ₂	Σ O ₂ , N ₂ , Ar ≥1.9 mol%	In L-gas net: 3 mol% without L-gas: 3 mol% further(*): 0.001 mol%	5 ppm
N ₂	–	–	300 ppm
Ar	–	–	300 ppm
He	–	–	300 ppm
CO	Σ CO, CO ₂ ≤1 ppm	0.1 mol%	0.2 ppm
CO ₂	–	4 mol% (MOP < 16) 2.5 mol% (MOP ≤ 16)	2 ppm
CH ₄	cf. C _n H _m	cf. C _n H _m	100 ppm
C _n H _m	100 ppm (including CH ₄)	Condensation point: –2 °C at 1 to 70 bar	2 ppm
S-total	2 ppm	10 mg/m ³ (with odorization) 6 mg/m ³ (without odorization)	0.004 ppm
H ₂ S, COS	cf. S-total	5 mg/m ³	cf. S-total
Formaldehyde	–	–	0.2 ppm
Formic acid	–	–	0.2 ppm
NH ₃	–	10 mg/m ³ (+ amines)	0.1 ppm
Halogenated compounds	–	–	0.05 ppm
Fog, dust, liquid	–	–	1 mg/kg

MOP: maximum operating pressure.

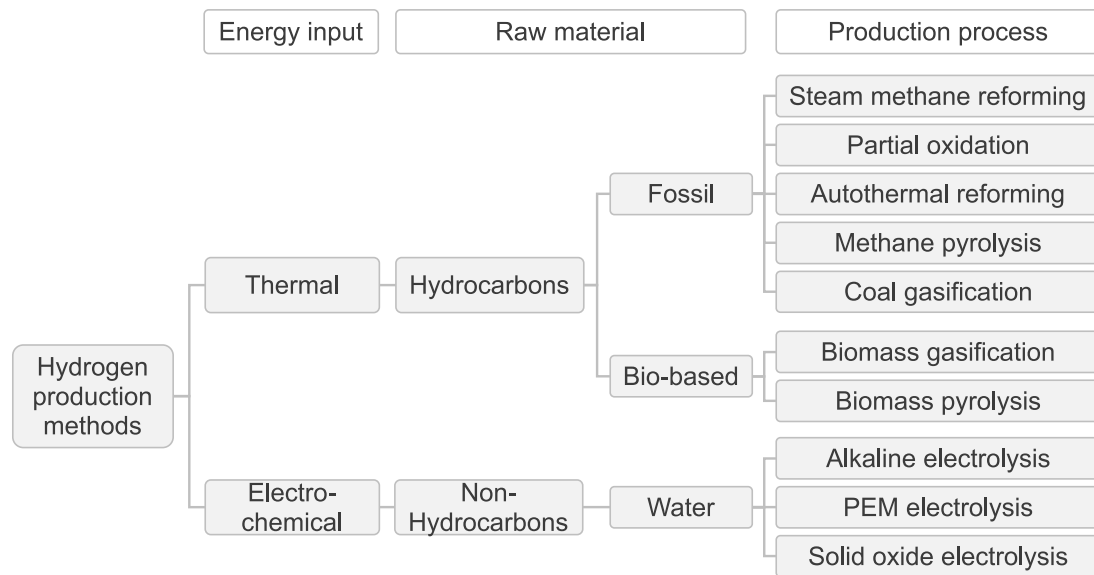


Fig. 2. Overview of the selected hydrogen production processes (based on [13]).

For ease of communication and possible implementation of the technologies in energy system models, the required hydrogen purity and the allowable impurity levels are grouped into three hydrogen grades:

1. Grade D: The highest purity grade with a hydrogen purity level of ≥ 99.97 mol% and impurity tolerances according to Table 1.
2. Grade A: The second-highest purity grade with a hydrogen purity level of < 99.97 mol% and ≥ 98 mol% and impurity tolerances according to the DVGW thresholds in Table 1.
3. Low Purity: Hydrogen with a purity level below 98 mol% is subsumed in the third category.

The purity levels are color-coded within this paper in green for grade D, blue for grade A, and orange for Low Purity hydrogen.

2. Sources of impurities throughout the hydrogen supply chain

This section of the paper looks at the impurities that occur at the beginning and middle of the hydrogen supply chain. It discusses the level of hydrogen purity achieved by different means of hydrogen production in the first part. The second part of this section looks in more detail at transportation and storage options. We discuss the purity requirements for the necessary conversion processes, the output purity of the reconversion processes, and the impurities introduced during the storage and transportation process itself.

2.1. Hydrogen production

The categorization of hydrogen production processes is based on two main factors, see Fig. 2: the type of energy input and the raw material [12]. The focus of this paper is on electrical and thermal forms of energy. The raw materials associated with these energy carriers are hydrocarbons and non-hydrocarbons. Fossil and bio-based/renewable raw materials fall into the category of hydrocarbons, while water falls into the category of non-hydrocarbons [13,14].

The following section provides an overview of the processes involved in the production of hydrogen. It outlines the basic operating principles, their key advantages and disadvantages, and the hydrogen purity level of these processes as derived from literature research.

The key findings of the literature review on hydrogen purity in production processes are shown in Fig. 3. The overview also contains

the purity levels achieved with the treatment and purification of the product. The purification technologies are discussed in depth in the section *Hydrogen purification and treatment*.

The findings indicate that electrolysis technologies exhibit the highest degree of purity. They reach purity levels of grade A without treatment and grade D with subsequent purification. The methane reforming processes on the other hand have significantly lower purity levels. With multiple steps of separation and purification, high purity levels can be achieved. The gasification and pyrolysis processes show significantly lower quantities of hydrogen in the product stream in some cases. An important influencing factor is the oxidation medium with pure hydrogen, leading to higher hydrogen purities.

2.1.1. Water electrolysis

Water electrolysis refers to the splitting of a water molecule into hydrogen and oxygen using electrical energy [13,15]. The gross reaction equation is



and takes place in an electrolyte cell [15,16]. This cell consists of two electrodes where the products are formed, a diaphragm that hinders the products to mix back together, and an electrolyte as the reaction medium [4,15]. Hydrogen is produced at the cathode and oxygen at the anode [16]. An abstract representation of the process diagram of water electrolysis is shown in Fig. 4.

The three most promising water electrolysis processes are: (1) alkaline electrolysis (AEL), (2) PEM electrolysis (PEMEL) and (3) solid oxide electrolysis (SOEC) [17]. Of the three water electrolysis processes, AEL is the most established and is used industrially on a large scale with a TRL 9 (2024) [18]. The technological development of PEMEL and SOEC leads to a TRL reaching 9 and 8 (2024) [18]. Due to the comparatively low technological maturity, TRL 6 (2024) [18], Anion exchange membrane (AEM) water electrolysis is not further investigated in this paper [19]. An overview of the respective advantages and disadvantages of the processes can be found in Table 2.

PEMEL is more expensive than AEL, primarily due to the higher cost of both the power electronics and the electrolysis stacks, which require titanium and critical platinum group metals (PGM) [27]. However, the benefits of better controllability and purity of the product stream are expected to provide an economic advantage by 2030 [22]. A key advantage of PEM electrolysis is the high hydrogen output pressure [24]. The subsequent compression required for the AEL significantly reduces

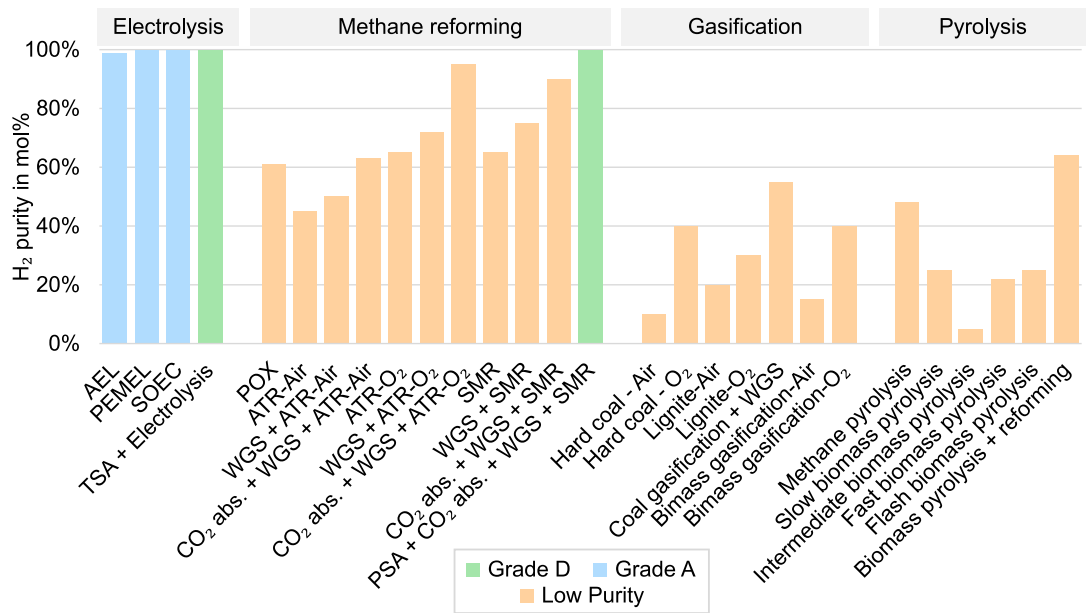


Fig. 3. Overview of the purity of hydrogen production processes according to the literature review. The figure also includes production in combination with selected purification and treatment technologies. AEL: alkaline electrolysis, PEMEL: PEM electrolysis, SOEC: solid oxide electrolysis, TSA: temperature swing adsorption, PSA: pressure swing adsorption, POX: partial oxidation, ATR: autothermal reforming, SMR: steam methane reforming, WGS: water–gas shift reaction.

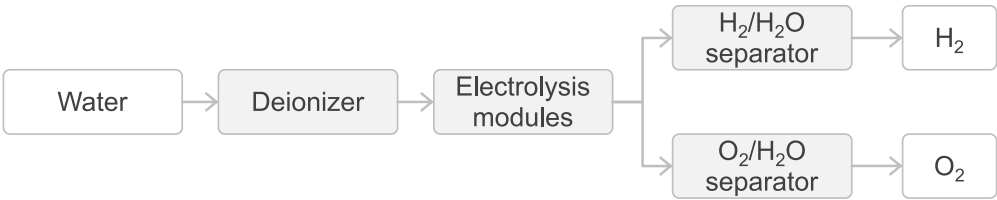


Fig. 4. Flow diagram of a water electrolysis process with integrated deionization of the water feed and water separation at the O₂ and H₂ product streams (based on [4]).

Electrolysis process:	AEL	PEMEL	SOEC
Advantages	<ul style="list-style-type: none">• Industrial experience• High durability• Low capital cost	<ul style="list-style-type: none">• High purity• Good dynamic operation• High operating pressure• High power density• High cell efficiency	<ul style="list-style-type: none">• High electrical efficiency• Fuel cell operation possible• Co-electrolysis possible
Disadvantages	<ul style="list-style-type: none">• Lower purity than PEMEL• Bad dynamic operation• Low operating pressure	<ul style="list-style-type: none">• Medium durability• High material costs• High complexity	<ul style="list-style-type: none">• Low maturity• Lower purity• Low durability• Bad dynamic operation

AEL: alkaline electrolysis, PEMEL: PEM electrolysis, SOEC: solid oxide electrolysis.

its cost advantage [27]. SOEC has several advantages over the other technologies: The high operating temperature creates favorable thermodynamics and reaction kinetics [17]. This leads to high conversion efficiencies, making SOEC the water electrolysis process with the highest electrical efficiency of about 80% [28]. It also enables co-electrolysis operation, in which hydrogen and carbon monoxide are produced from water vapor and carbon dioxide, and can be operated like a fuel cell. The cost of materials is also low [23,25,26].

Typical product compositions for hydrogen production using AEL, PEMEL, and SOEC are listed in Table 3. The data availability for the SOEC is comparatively sparse. The hydrogen purity value of 99.9 mol% listed in Table 3 is not based on empirical or theoretical studies, but on an estimate by electrolysis experts [22]. Therefore, no further impurities are listed. The process configuration corresponds to that shown in

Fig. 4 and includes water purification before and water separation after electrolysis.

As can be seen from Table 3, the water electrolysis processes under consideration are able to provide hydrogen with a purity exceeding 99 mol%. Due to the virtual absence of carbon and sulfur in the process, those compounds are only present in small proportions of under one ppm in the product [32]. The impurities are mainly water and oxygen [10].

Haug et al. [33,34] and Lubenau et al. [2] list some causes that can lead to impurities in electrolysis processes. These include: (1) dissolved vapors and gases in the electrolyte; (2) gas transfer across the separation membrane (cross-over); (3) pre- and post-treatment of the electrolyzer; (4) interfacial exchange with the water in the electrolyzer; (5) reaction of the oxygen with the hydrogen to form water and (6) deposits on the technical equipment [2,33,34].

Table 3

Crude gas composition of selected electrolysis processes after water separation.

Electrolysis process:	AEL	PEMEL	SOEC
H ₂	≈99 mol%	99.9 mol%	≈99.9 mol%
H ₂ O	0.2 mol%	≈100 ppm	
O ₂	0.2–0.6 mol%	18–500 ppm	
N ₂	100 ppm	1.2–4.5 ppm	
Ar	>300 ppm	<0.5 ppm	
He	>300 ppm	<9 ppm	
CO	<0.5 ppm	<0.02 ppm	
CO ₂	0.24 ppm	0.2–0.54 ppm	No literature data identified for contaminants
CH ₄	0.1 ppm	0.02–0.1 ppm	
H ₂ S	cf. S-total		
C _n H _m	0.5 ppm	0.08–0.2 ppm	
NH ₃	<0.1 ppm	<0.1 ppm	
S-total	<0.0012 ppm	<0.0036 ppm	
Formaldehyde	<0.1 ppm	<0.005 ppm	
Formic acid	<0.01 ppm	<0.1 ppm	
References	[1,29,30]	[31]	[22]

Sparse data availability for the SOEC; hydrogen purity value based on expert estimation.

AEL: alkaline electrolysis, PEMEL: PEM electrolysis, SOEC: solid oxide electrolysis.

<: Concentration is below the measurement limit, ≥: Concentration decreases or increases over time to the value.

Unlike AEL, PEM electrolysis does not use a liquid electrolyte, eliminating the first source of contamination. The *cross-over* activity is reduced compared to AEL due to the use of denser membranes [24]. In addition, the oxygen that diffuses to the other electrode is partially by at the catalysts, so that the total oxygen impurities are lower than in AEL (see Table 3).

Overall, it should be noted that water electrolysis processes can produce pure hydrogen (>99.0 mol%). PEMEL achieves the highest purity (99.9 mol%), while the purity of the AEL is lower. It should be noted in particular that the raw gas compositions listed here refer to stationary operation of the water electrolyzers. Load-flexible operating modes, such as those aimed for in demand side management (DSM), are not taken into account, but can lead to quality losses [33].

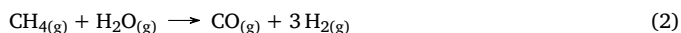
2.1.2. Methane reforming

In the following section, selected methane reforming processes are presented, followed by a comparison of their characteristics and their industrial application in the subsequent subsection.

This paper uses the term “methane”, even if the feedstock material is often natural gas. Conventional natural gas usually contains around 96 vol% methane (on a dry basis). The remaining components usually consist of higher hydrocarbons and CO₂ [35]. The higher hydrocarbons are broken down during the reforming process, while CO₂ is produced as a byproduct [36]. Since this paper does not focus on the raw feedstock of the production processes, no further distinction is made between natural gas and methane.

2.1.3. Steam reforming of methane (SMR)

Steam methane reforming (SMR) refers to the catalyzed reaction of methane with steam at high temperatures to produce a CO–H₂ mixture [37]. Nickel is used as the catalyst [38]. The reaction equation for the reforming reaction is [36]:



The product is a mixture of carbon monoxide, hydrogen, carbon dioxide and unreacted water vapor and methane [37]. Fig. 5 shows the flow diagram for a simple SMR process.

In accordance with industrial practice¹, methane is assumed to be desulfurized before entering a reformer in order to suppress the formation of hydrogen sulfide [36]. Subsequently, methane and water vapor

react in a tubular reactor at temperatures of 800–900 °C according to Eq. (2) [38,39]. These whole process includes secondary reformers and *Water–Gas–Shift* reactors. The *Water–Gas–Shift* process is separately discussed in the section *Hydrogen purification and treatment*. SMR is an industrially established process (TRL ≥ 9) and the most widely used process for producing hydrogen worldwide [20,40].

2.1.4. Partial oxidation of methane (CH₄-POX)

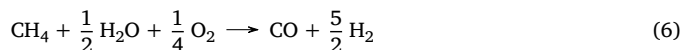
The partial oxidation of methane (CH₄-POX) is a sub-stoichiometric combustion of methane with oxygen [41]. It can be operated both catalyzed and non-catalyzed [4]. Since the reaction with methane is usually catalyzed, only this variant is discussed below [42]. The reaction equations of the exothermic, catalyzed CH₄-POX are [38,43]:



The goal of the process is to produce a CO–H₂ mixture. In addition to the target components, the product contains water, carbon dioxide, methane and, if air was used as the oxidant instead of pure oxygen, nitrogen [41]. Fig. 6 shows the flow diagram of the process. Catalytic partial oxidation of methane is an established industrial process (TRL ≥ 9) [13].

2.1.5. Autothermal reforming of methane (ATR)

Autothermal reforming (ATR) is a combination of steam reforming and partial oxidation (CH₄-POX) of methane [37]. The exothermic partial oxidation process provides the energy supply for the endothermic steam reforming process, resulting in a self-sustaining balanced process [44]. Combining all partial reactions in Eqs. (2), (3), (4), and (5) gives the gross reaction equation for the ATR [45]:



Similar to the SMR product, the product consists mainly of CO, H₂, CO₂, H₂O and CH₄ [37]. However, ATR processes are differentiated according to the oxidizing agent, which can either be concentrated oxygen (ATR-O₂, O₂: Oxygen) or ambient air (ATR-A, A: Air). The oxygen in the ambient air is predominantly diluted by nitrogen, so that the product stream of ATR-A is also diluted [38,46]. A simple ATR process is shown in Fig. 7.

ATR is an industrially established process (TRL ≥ 9) and is used in particular for synthesis gas production in the Haber–Bosch process [46]. An ATR process scheme, as it is common in industry, is shown in the supplementary material in Section 2.2.

¹ Section 2.1 in the supplementary material contains an example of an industrially operated methane reforming plant and its downstream process steps.

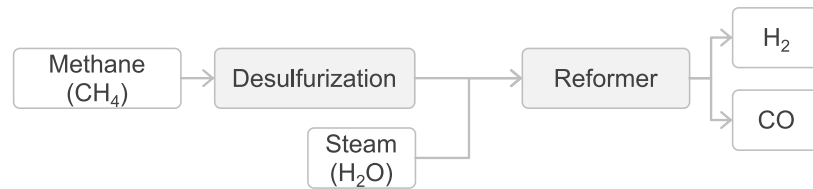


Fig. 5. Process flow diagram of steam methane reforming (SMR) including the integrated desulfurization processes (based on [4]).

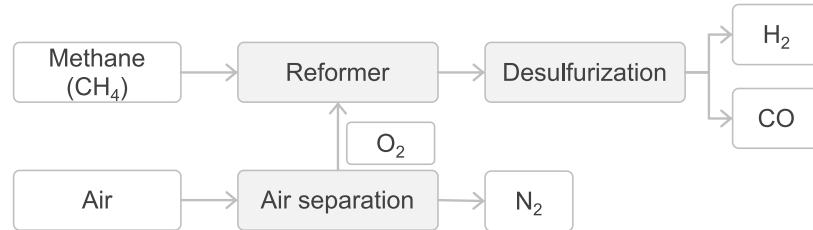


Fig. 6. Process flow diagram of catalytic partial oxidation of methane (CH₄-POX) including the integrated synthesis gas desulfurization processes (based on [4]).

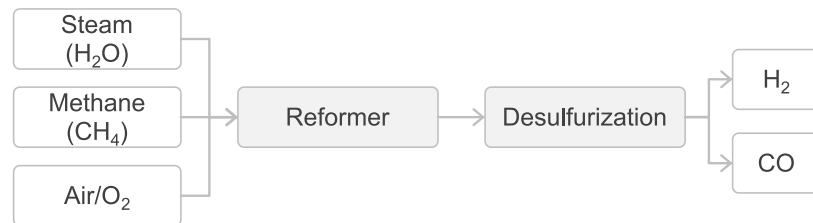


Fig. 7. Flow diagram of autothermal methane reforming (ATR) including the integrated desulfurization processes of the synthesis gas (based on [4]).

Table 4

Comparison of the advantages and disadvantages of selected methane reforming processes (based on [4,32,41,42,45,47]).

Reforming process:	SMR	CH ₄ -POX	ATR-O ₂	ATR-A
Advantages	<ul style="list-style-type: none"> Industrial experience No O₂ requirement Lowest temperature Best H₂/CO ratio for H₂ production 	<ul style="list-style-type: none"> Simple system No catalyst required Low methane slip Decreased desulfurization 	<ul style="list-style-type: none"> Barely N₂ dilution 	<ul style="list-style-type: none"> Lower temperature than CH₄-POX Low methane slip Requires less O₂ than CH₄-POX N₂ dilution beneficial for Haber–Bosch process
Disadvantages	<ul style="list-style-type: none"> Highest GHG emissions Complexity 	<ul style="list-style-type: none"> Deposits increase process complexity Very high temperature Low H₂/CO ratio O₂ required 	<ul style="list-style-type: none"> Requires O₂ 	<ul style="list-style-type: none"> Limited experience Very high temperature Air required N₂ dilution

SMR: steam methane reforming, CH₄-POX: partial oxidation of methane, ATR-O₂: autothermal reforming with oxygen, ATR-A autothermal reforming with air.

2.1.6. Comparison of methane reforming processes

Table 4 contains a comprehensive comparison of the advantages and disadvantages of the various methane reforming processes. Among these processes, the partial oxidation of methane is not common in industrial practice, while methane steam reforming (SMR) is the standard process for hydrogen synthesis [40].

Autothermal reforming (ATR) is mainly used to produce synthesis gas for the Haber–Bosch process [38]. In this two-stage process, methane steam reforming is used in the primary reformer. The product stream of the primary reformer is then fed into an air-driven ATR in the secondary reformer, resulting in an H₂-N₂ mixture in the final product stream. Since the mixture can be used as an inflow for the Haber–Bosch process, the disadvantage of the N₂ dilution becomes an advantage in the application case [46]. An exemplary process scheme is shown in the supplementary material in Section 2.2.

The raw gas compositions of steam reforming of methane (SMR), catalyzed partial oxidation of methane (CH₄-POX), and autothermal reforming of methane (ATR) are listed in Table 5. The ATR is further

differentiated according to the oxidants used during operation, air or oxygen.

With a hydrogen purity of 65 mol%, the SMR achieves the same value as an oxygen-driven ATR (ATR-O₂). In contrast, the air-driven ATR (ATR-A) shows a nitrogen dilution and therefore a lower hydrogen concentration. Partial oxidation achieves purity levels similar to SMR. However, enriched oxygen is required for CH₄-POX, as ambient air would dilute the product and thus reduce the product purity.

In summary, the reforming processes can achieve similar hydrogen purity ranges between 60 and 65 mol%. The need for enriched oxygen for operation puts CH₄-POX and ATR-O₂ at a disadvantage compared to SMR.

2.1.7. Coal gasification

Coal gasification refers to the sub-stoichiometric combustion of coal [36]. The oxidants used are either purified oxygen, ambient air or steam. While air is the least expensive option, it has the disadvantage of nitrogen dilution in the product stream. Using pure oxygen prevents

Table 5

Raw gas composition of selected reforming processes. The composition of the product gas can vary considerably depending on the composition of the natural gas input.

Reforming process:	SMR	CH ₄ -POX	ATR-O ₂	ATR-A
H ₂	65 mol%	61 mol%	65 mol%	45 mol%
CO	12 mol%	35 mol%	28 mol%	13 mol%
CO ₂	10 mol%	3 mol%	5 mol%	9 mol%
CH ₄	7 mol%	0.5 mol%	1 mol%	0.4 mol%
N ₂	1 mol%	0.5 mol%	0.7 mol%	32 mol%
Ar	N/A	0.1 mol%	0.6 mol%	0.4 mol%
References	[1,38,48]	[38,48]	[1]	[1]

SMR: steam methane reforming, CH₄-POX: partial oxidation of methane, ATR-O₂: autothermal reforming with oxygen, ATR-A autothermal reforming with air.

Table 6

Raw gas composition after coal gasification.

Process:	Coal gasification			
Coal type:	Hard coal		Lignite	
Oxidant:	Oxygen	Air	Oxygen	Air
H ₂	40 mol%	10 mol%	30 mol%	20 mol%
CO	40 mol%	20 mol%	60 mol%	20 mol%
CO ₂	20 mol%	6 mol%	5 mol%	15 mol%
CH ₄	0.1 mol%	0.2 mol%	N/A	5 mol%
N ₂	0.4 mol%	60 mol%	1 mol%	40 mol%
C _n H _m	N/A	0.0 mol%	N/A	0.01 mol%
References	[38]			

The data is summarized for the burner types and differentiated by oxidant and coal type. The composition of the product gas can vary considerably depending on the coal quality.

the nitrogen dilution, but the air separation required increases the costs. Steam represents a cost compromise of these methods [20]. The reaction equations of coal gasification are [49]:



The product of coal gasification consists mainly of carbon monoxide and hydrogen. Analogous to partial oxidation, desulfurization is assumed to take place after raw gas production in the coal gasification process (see Fig. 6) [4]. Coal gasification is an industrially established process (TRL ≥ 9) and is used especially in China for hydrogen production [40,45,50]. Table 6 shows the raw gas composition after the gasification of coal. The data is broken down by coal type, hard coal or lignite, and by oxidant, oxygen or air.

Similar to autothermal reforming, the choice of oxidant has a major impact on the product purity achieved. The use of air results in a dilution of the product with nitrogen. With oxygen, a purity of about 40 mol% is achieved, while air leads to a purity of 20%. In addition to the oxidant, the composition of the raw gas from coal gasification is highly dependent on the coal feedstock used, the burner design and case-specific parameters [51]. With a subsequent water–gas shift reaction, described in the section *Hydrogen purification and treatment*, the hydrogen content in the gasification product stream can be further increased [18].

2.1.8. Biomass gasification

Biomass gasification is similar to coal gasification and can also be performed with different oxidants (air, oxygen, steam) with the corresponding advantages and disadvantages [51,52]. To assess the hydrogen purity in the product stream, we assume that desulfurization and a tar removal step take place after the biomass gasification as shown in Fig. 8. The air separation unit is optional.

Table 7

Raw gas composition after biomass gasification.

Process:	Biomass (lignocellulosic) gasification	
Oxidant:	Oxygen (O ₂)	Air (A)
H ₂	40 mol%	15 mol%
CO	45 mol%	20 mol%
CO ₂	15 mol%	15 mol%
CH ₄	1 mol%	4 mol%
N ₂	0 mol%	44 mol%
C _n H _m	N/A	2 mol%
References	[51,53,54]	[38,51,53–59]

The data is summarized for the different burner and biomass types. Further differentiations by burner type and biomass source are included in Table 11 and 12 in the supplementary material.

Biomass gasification is less common than coal gasification, but still reaches a TRL of 7 [20]. Table 7 lists typical raw gas compositions after the biomass gasification. Additionally, Table 11 and 12 in the supplementary material list the compositions differentiated by biomass type and burner type. The values in Table 7 summarize the different biomass and burner types with rounded numbers.

Similar to autothermal reforming and coal gasification, the raw gas composition of biomass gasification depends on the choice of oxidizing agent, whereby the use of air leads to a nitrogen dilution of the raw gas. While the hydrogen content in operation with pure oxygen is around 40 mol%, the nitrogen dilution when using air leads to a reduction in the hydrogen content to 15 mol%. Overall, biomass gasification achieves similar raw gas compositions to the gasification of coal.

2.1.9. Methane pyrolysis

Low emission hydrogen can be produced via methane pyrolysis [60]. In this process, methane reacts under high heat to hydrogen and solid carbon (carbon black) according to the gross reaction equation [61]:



Methane pyrolysis is the only fossil-based production process considered in this work that theoretically has no process-related emissions, provided that the energy supply is greenhouse gas-neutral reaching a TRL of 8 (2024) [18]. Greenhouse gas emissions and environmental damage resulting from extraction, transportation, and slippage limit sustainability [60,62]. Most methane pyrolysis process variants have a low TRL of around 5 [61]. The literature on the purity of individual processes is very limited [2]. Based on theoretical considerations, methane pyrolysis should produce pure hydrogen and pure, solid carbon when the conversion is complete [61]. In the case of incomplete conversion, unreacted methane from the reactant stream should still be found in the product [44]. Lubenau et al. [2] point out that the idealized assumption that the reactant stream consists only of methane is usually not correct. Instead, they point out that in addition to unconverted methane, other components of natural gas can be expected in the product. In accordance with Muradov et al. [44] and the considerations of Lubenau et al. [2], the product composition from Table 8 is assumed for methane pyrolysis. It should be emphasized that the information given results from theoretical considerations and does not correspond to measured values. Furthermore, methane pyrolysis refers to a number of different processes that differ in terms of their raw gas composition. Due to the low level of technological maturity, no further differentiation is made.

2.1.10. Biomass pyrolysis

Biomass pyrolysis refers to two different processes. One is the conventional biomass pyrolysis, whose product consists of a solid, a liquid and a gaseous component; the other is the steam reforming of pyrolysis oil, which is obtained by fast biomass pyrolysis (*Fast Pyrolysis Steam Reforming* - FP-SR).

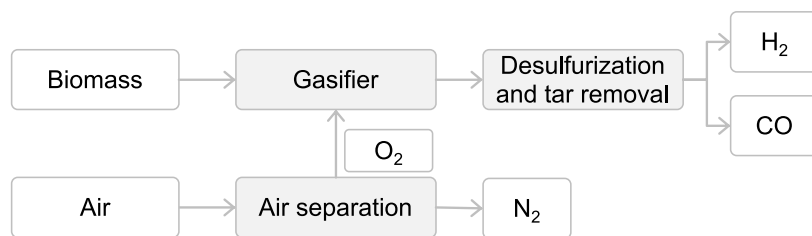


Fig. 8. Process scheme of biomass gasification including integrated desulfurization and tar removal from synthesis gas. The air separation unit is optional.

Table 8

Crude gas composition after pyrolysis of natural gas. The data is not based on measurements but on theoretical considerations.

Process:	Methane pyrolysis
H ₂	48 mol% ^a
CO	0 mol%
CO ₂	4 mol%
CH ₄	48 mol%
C _n H _m	0 mol%
References	[2,44]

^a Lower boundary. Higher values may be achieved by repeating the process.

Biomass pyrolysis is based on the pyrolytic decomposition of biomass [63]. The process can be divided into slow, medium, fast and flash pyrolysis according to the temperature level, heating rate, and residence time [64]. The product of biomass pyrolysis consists of a solid (char), a liquid (oil), and a gaseous (syngas) component. Hydrogen is obtained from the syngas component of the pyrolysis product [63].

The steam reforming of pyrolysis oil is a subsequent process step [65]. The liquid phase of the pyrolysis product is first separated into an oil and an aqueous phase. The oily phase is then reformed with steam so that hydrogen is present in the product gas. The oil from rapid biomass pyrolysis is usually used for this purpose [13,20]. In the further course of the paper, FP-SR therefore refers to the steam reforming of the oil from fast pyrolysis. Overall, the TRL of both pyrolysis processes is around 5–6 (2024) [18,63].

The hydrogen content in the raw gas of biomass pyrolysis is dependent on the speed of the process. According to Vuppaladiyam et al. [63], the ranges of hydrogen content are 9–44 mol% for slow, 1–8 mol% for intermediate, 1–45 mol% for fast, and 9–44 mol% for flash pyrolysis. Except for intermediate pyrolysis, which reaches 8 mol%, the different processes can reach hydrogen contents of up to around 45 mol%. A second driver for the hydrogen purity beside the speed is the temperature at which the pyrolysis is conducted. Table 9 shows a clear dependence of the raw gas composition on the process temperature, with higher temperatures favoring higher hydrogen contents.

With a downstream steam reforming process of the fast pyrolysis oil (FP-SR), the hydrogen purity can be increased to 64 mol% as shown in Table 10. In addition, the carbon monoxide content in the raw gas of the FP-SR is lower than in the gas phase of the biomass pyrolysis product.

Taken together, the raw gas compositions of biomass pyrolysis are strongly dependent on the pyrolysis duration and temperature. Although steam reforming of the pyrolysis oil from a fast biomass pyrolysis process can increase the hydrogen content in the raw gas up to 64 mol%, further process steps are also required for this.

2.2. Transport and storage of hydrogen

As the technologies for hydrogen transport and hydrogen storage overlap, they are discussed together within this section. Hydrogen can be transported in a gaseous, liquid or bounded state, as shown in Fig. 9 [66]. In this context, bound hydrogen refers to hydrogen transported

in the form of liquid organic hydrogen carriers (LOHC), hydrogen adsorbed on solids, or hydrogen that has been converted to ammonia or methanol for transport. After the corresponding conversion process, hydrogen is transported via pipelines or gas and liquid containers [67].

Hydrogen storage can be based on both physical and chemical conversion processes, analogous to the transport options shown in Fig. 9 [67]. Depending on the state of the hydrogen, physical storage can be divided into compressed, liquefied and cryocompressed hydrogen storage [6,67,68]. Material-based storage systems that follow a chemical conversion process are divided into solid-state storage and liquid-organic hydrogen carriers according to the state of the H₂ carrier. Hydrogen binds to H₂ solid-state storage systems, either by physisorption or chemisorption. A further distinction is made by the adsorbent, which in the case of physisorption includes carbon-based materials, zeolites and metal-organic frameworks. Based on the compound formed, chemisorption can be divided into the storage of chemical hydrides, intermetallic hydrides, and multicomponent systems [6,67–70].

Ammonia and methanol synthesis are typical examples of hydrogen applications in the industrial sector. For a detailed explanation of the synthesis processes, please refer to the section *Purity requirements for hydrogen applications and end-use*. Table 11 shows a comparison of the examined transport options.

When selecting a suitable transport option, a compromise is usually sought between the technical complexity and the energy storage density of the transport mode. For example, the conversion of gaseous hydrogen into liquid hydrogen, ammonia, or methanol requires a lot of energy, but allows higher storage densities than the transport of gaseous hydrogen. An important advantage of GH₂ pipeline transport in the context of techno-economic optimization is the existence of natural gas pipelines, that can be converted to hydrogen pipelines at comparatively low cost. Fig. 10 shows the results of the hydrogen purity review in transport. As the technologies for hydrogen transport and hydrogen storage overlap, both are shown in Fig. 10.

With gaseous hydrogen, the quality can be sustained during transport and storage when new vessels and pipelines are built. On the other hand, infrastructures with lower investment costs like retrofitted natural gas pipelines and salt caverns lead to a contamination of hydrogen.

Converting hydrogen to LH₂, LOHC, Ammonia, and Methanol and reconverting it can have different effects on the hydrogen purity. Liquefaction requires a high purity level to begin with. This purity is sustained during storage or transport, resulting in high purity output. LOHC has low purity requirements and a high purity output. For Ammonia, the input requirements are high, but the output is lower. Depending on the reconversion process, the hydrogen reaches above or below 98 mol%. Similarly, for the Methanol reconversion, the hydrogen purity depends on the chosen process, leading to hydrogen of over 99.97 mol% or hydrogen well below 98 mol%.

2.2.1. Transport and small-scale storage of compressed gaseous hydrogen

Gaseous hydrogen (GH₂) is transported either in vessels by truck, train, and ship or in pipelines [76]. GH₂ transport vessels are considered mature with a TRL ≥ 9 according to Müller et al. [77] and Peschel [3]. They assign GH₂ pipeline transport a TRL of 8 to 9.

Table 9

Composition of the gas phase of the biomass pyrolysis product. The processes are differentiated by their process temperature and speed.

Process:	Biomass pyrolysis (here: sugarcane bagasse)					
Temperature:	480 °C		580 °C		680 °C	
Speed:	Slow	Fast	Slow	Fast	Slow	Fast
H ₂	9.6 mol%	8.7 mol%	21.3 mol%	15.2 mol%	28.8 mol%	45.3 mol%
CO	60.1 mol%	13.9 mol%	25.1 mol%	18.7 mol%	37.7 mol%	20.5 mol%
CO ₂	11.7 mol%	52.4 mol%	20.7 mol%	58.1 mol%	23.9 mol%	14.4 mol%
CH ₄	17.6 mol%	21.5 mol%	31.1 mol%	6.9 mol%	7.2 mol%	17.0 mol%
C _n H _m	1.0 mol%	3.6 mol%	1.8 mol%	1.1 mol%	2.5 mol%	2.8 mol%
References	[64]					

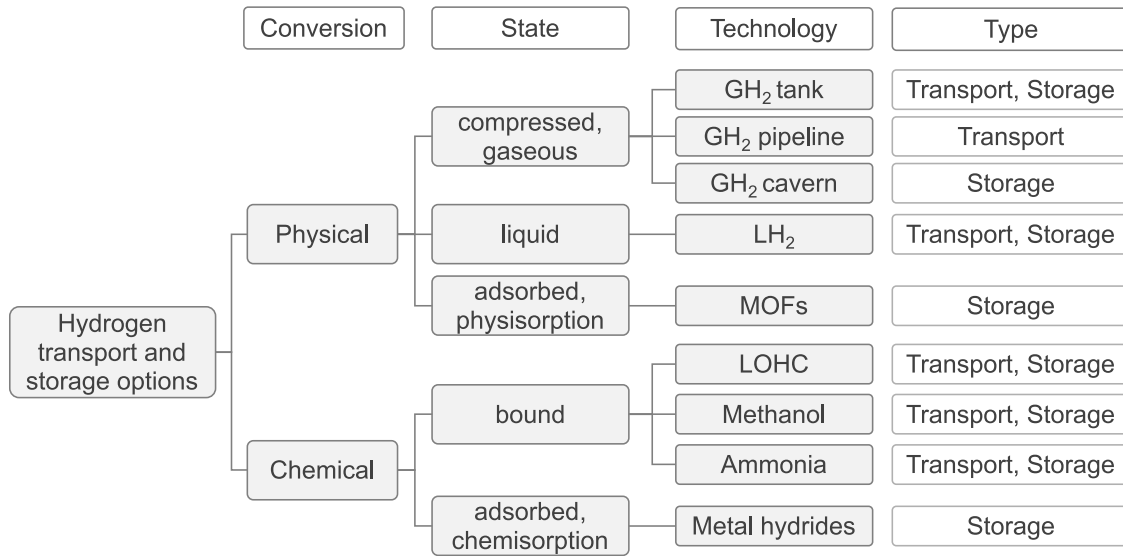


Fig. 9. Overview of selected hydrogen transport and storage options (based on [3,67]). MOFs: metal–organic frameworks, LOHC: liquid organic hydrogen carriers.

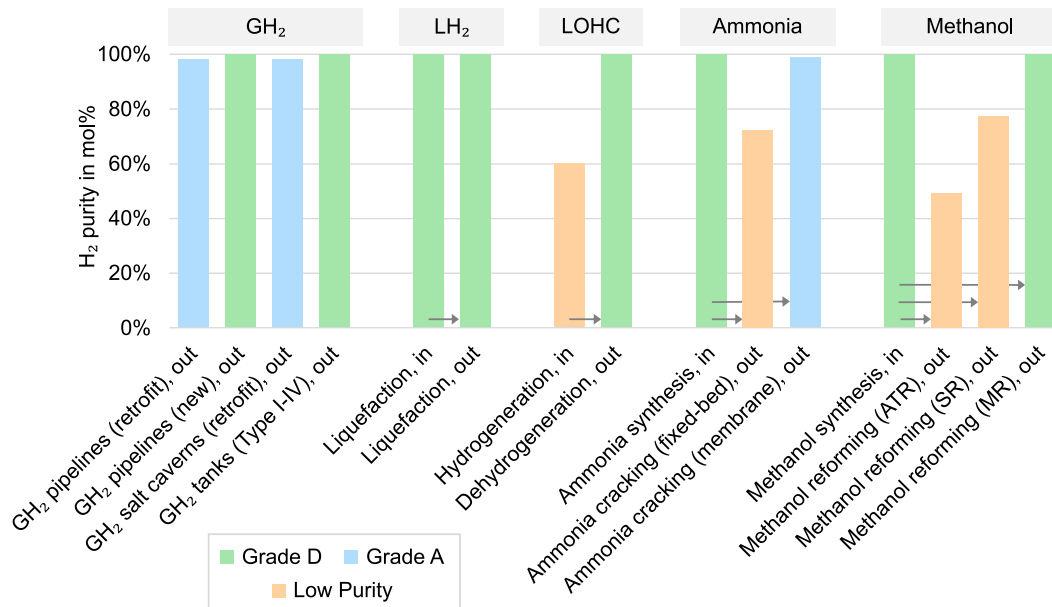


Fig. 10. Overview of hydrogen purity levels in transport and storage according to the literature review. In: value refers to the required input purity; out: value refers to the obtained output purity. LOHC: liquid organic hydrogen carriers, ATR: autothermal reforming, SR: steam reforming, MR: membrane reactor.

For both options, the hydrogen is first compressed using dry-running piston or diaphragm compressors that minimize the introduction of impurities [3,78]. A comparison of the two compressor technologies is given in Table 12.

Compressed hydrogen is stored in pressure vessels during transportation by truck, train, or ship. These tanks usually correspond to one of four designs, the characteristics of which are summarized in Table 13. In addition to the four types, a type V tank is being developed [79].

Table 10

Gas composition of the crude gas after steam reforming of pyrolysis oil from fast biomass pyrolysis.

Process:	Biopyrolysis reforming
H ₂	64 mol%
CO	8.7 mol%
CO ₂	25 mol%
CH ₄	1.7 mol%
C _n H _m	0.7 mol%
References	[65]

As type V tanks are currently not widely used commercially and are mainly used in space travel, they will not be discussed further [72,80].

Metals, polymers, and composites are used as materials for the pressure tanks [83]. These include stainless steel or chromium–molybdenum steel (usually 34CrMo4) and aluminum 6061 or 7060 [76,81] for the metallic components. Tank types I and II are made of both steel and aluminum, while tank type III is usually made of aluminum [83]. Polyethylene or polyamides are used for the polymer components [81]. Type I and II containers are used for stationary storage, with type II being advantageous at higher pressures [82]. Hydrogen is usually transported in type III or IV tanks [82].

Pipeline transportation of GH₂ takes place either in newly built hydrogen pipelines or retrofitted natural gas pipelines [84]. The pipeline network can be divided into a distribution network and a transmission network [85]. Transmission pipelines are used for large-scale transportation from the production site to the distribution network, where the gas is then distributed to the final consumer. Transmission pipelines operate at higher pressures, have larger diameters, and are made of steel. In contrast, the pressure and diameter of distribution pipelines are lower and most of today's distribution pipelines are made of polyethylene (PE). For the new construction of dedicated hydrogen pipelines, the use of low-carbon steel is recommended for both the transmission and distribution networks [76,86].

The results of the gaseous hydrogen transport are summarized in Table 14. The literature review shows that the transport via pressure tanks of type I, II and III takes place without contamination. Type IV tanks can also be used to transport pure hydrogen if the polymer components are made of either polyethylene (PE) or pre-dried polyamide (PA). When using a type IV tank made of polyamide that has not previously been degassed, water degassing occurs. The water contaminates the hydrogen to at least 5 ppm, so that some quality requirements are no longer met. One example would be the use of hydrogen in mobile PEM fuel cells.

For the pipeline transport of gaseous hydrogen, Moradi et al. [72], Omoniyi et al. [29], and the National Hydrogen Council of the German Federal Government in a statement on hydrogen transport [89] point out that quantitative measurements on the behavior of individual impurities are still missing. The results presented in Table 14 are mainly based on work commissioned by the German Technical and Scientific Association for Gas and Water (DVGW e.V.). The assessment of contamination during pipeline transport is one of the subjects of the *GetH₂ TransHyDE* research project (running from 2021 to 2025) [90].

According to the research of Lubenau et al. [2], gaseous hydrogen of quality grade A can be transported in both retrofitted transmission and distribution networks regardless of the previous use and the conversion status of the pipeline network. The results of Lubenau et al. [2] are presented in the supplementary material in sections 3.4.2 and 3.4.3. For higher quality requirements, a distinction has to be made whether the pipeline was previously used by pure natural gas or a mixture of natural gas and biogas or a gas enriched with odorants. A distinction is also made between a time before and after the conversion phase. The conversion phase, summarized in Table 14 in the supplementary material, essentially consists of cleaning a pipeline until constant concentrations are achieved. The duration of the conversion phase can range from

months to years. The contamination of GH₂ in retrofitted natural gas pipelines is largely unknown, according to Lubenau et al. In newly constructed pipelines, it is known that the transportation of grade D hydrogen is possible. An exception is contamination with water, about which no statement can be made. Table 14 shows the summarized results on pipeline transport.

2.2.2. Transport and storage of liquefied hydrogen

Liquefied hydrogen (LH₂) is stored in containers and transported by train, truck, and ship [85,91–93]. LH₂ storage and transport is considered a mature process (TRL ≥ 9) [3,77]. The tanks consist of an inner pressure vessel, a separating layer and an outer protective jacket. The materials used are stabilized austenitic stainless steels and aluminum alloys [81,82]. Gaseous hydrogen is liquefied to provide LH₂ [94]. This requires hydrogen that is as pure as possible in order to avoid damage to the equipment caused by condensed and frozen impurities. The first step of liquefaction involves optional compression to 2 to 8 MPa followed by pre-cooling to 80 K and adsorptive purification to remove further impurities. This is followed by cryogenic cooling to 30 K. The final step of liquefaction is an adiabatic expansion to 20 to 23 K and 0.1 to 0.2 MPa [95,96]. The reconversion of LH₂ into GH₂ is considered a simple process and usually takes place via heat exchange with the environment, mostly through indirect contact with ambient air or seawater [85].

To transport hydrogen in liquid form, gaseous hydrogen is compressed, liquefied, stored and then transported in a container before arriving at its final destination. There it can be used in liquid form or converted back to gaseous hydrogen. The gas composition for liquefied hydrogen is summarized in Table 15. The liquefaction process itself has high purity requirements. During liquefaction, hydrogen is cooled to temperatures so low that many other gases become liquid or solid first. To prevent damage to the liquefaction plant, the sum of all impurities must first be reduced to 1 ppm, so that the purity requirement is about 99.999 mol% [82,95,97–99]. In reality, the hydrogen purity requirement is slightly lower, as the helium content in the gas mixture is not relevant for the 1 ppm limit.

Liquefaction itself can be seen as an integrated purification process [87]. The component proportions listed in Table 15 are measured in an LH₂ container. The gas phase that was in contact with the liquid phase in the container was investigated. No data could be identified for the gas composition after complete regasification and transfer to a GH₂ container.

2.2.3. Transport and storage of LOHC-bound hydrogen

The storage of hydrogen in liquid organic hydrogen carriers (LOHC) is “based on a reversible hydrogenation and dehydrogenation of carbon double bonds” [100]. Teichmann et al. [101] define LOHC systems as liquid organic, energy bearing compounds that switch between a high and a low energy state. The LOHC concept is thus based on a reversible, heat-releasing hydrogenation of a liquid, organic compound and a subsequent dehydrogenation by heat [85,100].

For storage and transport of LOHC, existing infrastructure can be used, making these steps of the supply chain highly mature with a TRL ≥ 9 [3,18,77]. LOHC can be stored in mineral oil tanks [100] and transported in specially coded chemical tankers [18]. While LOHC-bound H₂ is usually transported in containers, pipeline transport is also conceivable [85,102].

An overview of possible LOHC systems is given in Table 16. A comparison of the properties and the advantages and disadvantages of some LOHC systems can be found in the work of Usman [6]. They come to the conclusion that two LOHC systems are particularly recommendable: first, the MTH (methylcyclohexane/toluene) system, since large-scale production already exists, the substances are not harmful to health and toluene is liquid at ambient conditions; second, the Hx-DBT (perhydro dibenzyl toluene/dibenzyl toluene) system. Dibenzyltoluene is an industrially used heat transfer oil, fulfills the requirements for

Table 11

Comparison of the advantages and disadvantages of selected hydrogen transport methods (based on [3,71,72]).

Process	Advantages	Disadvantages
GH ₂ pipelines	<ul style="list-style-type: none"> • Mature • Large-scale transport 	<ul style="list-style-type: none"> • Low volumetric capacity
GH ₂ vessels	<ul style="list-style-type: none"> • Mature • Low infrastructure requirement 	<ul style="list-style-type: none"> • Low volumetric capacity • No large-scale transport
LH ₂	<ul style="list-style-type: none"> • Mature • High volumetric capacity 	<ul style="list-style-type: none"> • Boil-off • High purity & energy requirement
LOHC	<ul style="list-style-type: none"> • First experiences • Relatively cheap 	<ul style="list-style-type: none"> • High pressure and temperature • Low maturity
Ammonia transport	<ul style="list-style-type: none"> • Mature • High storage capacity 	<ul style="list-style-type: none"> • Boil-off^a • Toxicity • High energy requirement
Methanol transport	<ul style="list-style-type: none"> • Mature • High storage capacity 	<ul style="list-style-type: none"> • Low purity • Toxicity • High energy requirement

^a Due to its higher boiling temperature and latent heat of vaporization, the boil-off rate of liquefied ammonia is much less critical at ~0.025 vol%/day [73] compared to up to 5 vol%/day [74] for LH₂. Through immediate reliquefaction, net boil-off losses can be largely eliminated for ammonia [75].

Table 12

Comparison of commercially available hydrogen compressors (based on [3]).

Compressor technology:	Membrane	Dry-running piston
Scale	Small-middle	Small-large
Throughput	1–4000 m ³ /h	10–115,000 m ³ /h
Maximum release pressure	300 MPa	130 MPa
Advantages	Good availability Δp independent of molar weight No contamination	Good availability Δp independent of molar weight

Table 13

Comparison of the four common types of pressure vessels for the storage and transport of gaseous hydrogen (based on [81,82]).

Storage/transport option:	Pressure tank			
Tank type:	Type I	Type II	Type III	Type IV
Operating pressure	≤50 MPa	Unlimited	≤45 MPa	≤100 MPa
Maturity	Mature (TRL ≥ 9)	Mature (TRL ≥ 9)	Mature (TRL ≥ 9)	First commercial series
Material and construction	Metal	Metallic liner	Metallic liner	Polymeric liner
		Fiber-resin composite	Carbon fibers in a polymer matrix	Carbon fibers in a polymer matrix
Cost-performance	++	+	–	–
Weight-performance	–	0	+	++

Table 14

Achievable output purity levels of transport options of gaseous hydrogen.

Transport option:	Pressure tank		Pipeline	
Type:	I–III, IV (PE), IV (PA) dry	IV (PA) wet	Retrofit	New
H ₂	≈100 mol%	<99.9995 mol%	98.0 mol%	99.97 mol%
H ₂ O		>5 ppm		
O ₂				
N ₂				
Ar				
He				
CO				
CO ₂	No contamination	Only water contamination	Contamination according to purity grade A	Contamination according to purity grade D
CH ₄				
H ₂ S				
C ₂ H ₄				
NH ₃				
S				
Formaldehyde				
Formic acid				
References	[72,78,81,87]	[72,81]	[2,88]	[2,88]

The gas groups correspond to the gas groups from Table 1. Further details on impurities of transmission and distribution grids listed in Table 15 and 16 in the supplementary material. The tank types correspond to those listed in Table 13.

PA: polyamide, PE: polyethylene, dry: water degassing takes place before the H₂ filling.

Table 15

Purity requirements and impurity tolerances for hydrogen liquefaction and the resulting composition after liquefaction. The composition measured after liquefaction refers to the composition of the vapor phase in equilibrium with the liquid phase in the liquid tank container.

Process:	Hydrogen liquefaction	
State:	Requirement	Liquefied
H ₂	≈99.999 mol%	>99.9995 mol%
H ₂ O		<0.5 ppm
O ₂		<0.2 ppm
N ₂		<0.5 ppm
Ar		<0.1 ppm
He		<4.0 ppm
CO		<0.02 ppm
CO ₂		<0.01–0.018 ppm
CH ₄	Sum of all impurities except for helium: 1 ppm	<0.005 ppm
H ₂ S		N/A
C ₂ H ₄		N/A
NMHC		<0.02 ppm
NH ₃		<0.03 ppm
Total-S		<0.001 ppm
Formaldehyde		<0.005 ppm
Formic acid		<0.005 ppm
Halogenates		<0.038 ppm
Reference	[82,95,97–99]	[87]

NMHC: non-methane hydrocarbons.

Table 16

Selected dehydrogenated LOHCs and their corresponding hydrogenated organic hydrides.

Dehydrogenated product	Organic hydride	References
Benzene	cyclohexanes	[6,70]
Toluene	methylcyclohexane (MCH)	[6,70,104–106]
Benzyltoluene	perhydro-benzyl toluene	[6,105]
Dibenzyltoluene	perhydro dibenzyl toluene (H ₁₈ -DBT)	[6,105,106]
Indoles	indolines	[6]
1,3-Dimethylbenzenes	1,3-Dimethylcyclohexanes	[70]
1,2,4-Trimethylbenzenes	1,2,4-Trimethylcyclohexanes	[70]
1,2,3,4-tetramethylbenzenes	1,2,3,4-tetramethylcyclohexanes	[70]
N-ethylcarbazole	perhydro-N-ethylcarbazole	[105]

Table 17

Purity requirements and product compositions for LOHC hydrogenation and dehydrogenation using a Hx-DBT complex (perhydro dibenzyl toluene).

Process:	LOHC-bounding		
State:	Input requirement hydrogenation	Output dehydrogenation	Output advanced ^a dehydrogenation
H ₂	≥60.0 mol%	99.96 mol%	99.999 mol%
CO	≤7.0 mol%	2 ppm	0.2 ppm
CO ₂	≤50.0 mol%	7 ppm	N/A
CH ₄	N/A	120 ppm	N/A
C _n H _m	N/A	95 ppm	N/A
Reference	[107]	[107–110]	[108]

^a Advanced dehydrogenation: use of pre-purified and recycled LOHC as described by Bulgarin et al. [108].

an LOHC system and is already produced on a large scale [103]. In summary, Usman [6] recommends the use of the MTH system for mobile applications and the Hx-DBT system for stationary applications.

Table 17 summarizes the results of the literature research on hydrogen purities in LOHC transport. LOHC transport includes the hydrogenation of a LOHC complex, storage and transportation, mainly in containers, and final dehydrogenation. Following dehydrogenation, the product is purified by distillation as standard.

The results from Table 17 apply to the LOHC complex perhydro dibenzyl toluene (Hx-DBT complex). A distinction is made between the standard purification and an advanced purification, which is explained below.

For the standard process, investigations have shown that hydrogenation is possible with hydrogen contents of at least 60 mol% and CO and CO₂ contents of a maximum of 7 and 50 mol% respectively [107]. The prerequisite for this is the use of palladium as a catalyst. This means that the extraction of hydrogen from a synthesis gas mixture can be regarded as an integrated purification step in LOHC hydrogenation [107].

After dehydrogenation and simple distillation, the hydrogen purity averages 99.96 mol%. The proportion of CO and CO₂ is in the single-digit ppm range, while the proportions of methane and other hydrocarbons are significantly higher. In particular, the product also contains residues of the organic carrier material [107–110].

In addition to the standard process, additional purification of the H₁₈-DBT complex prior to dehydration is also possible, which reduces the impurities. Bulgarin et al. [108] recommend the use of LOHC material that has already been hydrogenated and dehydrogenated several times. This removes production-related impurities. Alternatively, the complex can be further purified.

Taken together, hydrogen purities of 99.96 mol% can be achieved in the standard process. Further upstream purification and recycling steps make it possible to increase the hydrogen product purity to up to 99.999 mol%.

2.2.4. Transport and storage of ammonia

The ammonia pathway consists of the ammonia synthesis using the Haber–Bosch process, explained in the section *Purity requirements for hydrogen applications and end-use*, its storage and transport, and finally cracking, to obtain hydrogen. Under normal conditions (0 °C, 1 atm), ammonia is gaseous, but can be liquefied either by cooling to –33 °C or by pressurizing to 8.6 bar [111]. For large-scale storage (up to 50,000 t), double-wall double integrity tanks storing refrigerated ammonia at atmospheric pressure are preferred over pressurized tanks, as they offer more economical storage solutions [18].

The transport of ammonia in liquid form is carried out by various modes including truck, rail, ship, and pipeline [18,111]. In particular, existing liquefied petroleum gas (LPG) infrastructure can be used to transport ammonia. Fully refrigerated, non-pressurized vessels designed for LPG are suitable for ammonia transport, as LPG has a lower boiling point (–42 °C) compared to ammonia (–33 °C) [18,111]. However, when using LPG carriers for ammonia, it is critical to ensure that it does not come into contact with non-ferrous metals such as copper or zinc and its alloys due to corrosion [18,112]. Both, storage and transport of ammonia are mature technologies, with TRL ≥ 9 [18].

Following transportation, the ammonia is converted back into hydrogen as required, usually called ammonia cracking [113]. The gross reaction equation of the ammonia decomposition is [114]:



An operating temperature of around 800 °C is favorable for shifting the equilibrium of this endothermic reaction towards the hydrogen product [104]. Using highly active ruthenium-, nickel-, iron-, or cobalt-based catalysts allows for operating temperatures of 350–650 °C [115]. However, these temperatures and the associated energy requirements continue to challenge the economics of the process [104]. Currently, ammonia cracking processes are commercially available in metallurgy [116]. The TRL of ammonia reconversion for hydrogen is at least 4–5 (2024) [18,116,117]. Table 18 shows the product compositions after the reconversion of ammonia into hydrogen by means of ammonia cracking. The first column refers to the raw gas composition resulting from ammonia cracking in a *Fixed-Bed* reactor. The last column represents the composition after reconversion in a membrane reactor.

As can be seen, the raw gas composition in the *Fixed-Bed* reactor of 72 mol% is in a similar range to the methanol reconversion processes. The majority of the impurity consists of nitrogen [104,118]. Membrane reactors achieve significantly higher purities of around 99 mol% [119].

Table 18

Composition of the product gas after the reconversion of ammonia to hydrogen by ammonia cracking.

Process:	Ammonia cracking	
Type:	Fixed-Bed reactor	Membrane reactor
H ₂	72 mol%	99 mol%
N ₂	24 mol%	N/A
NH ₃	4 mol%	1 mol%
References	[104,118]	[119]

2.2.5. Transport and storage of methanol (MeOH)

The methanol pathway for hydrogen transport and storage consists of the methanol synthesis, which will be later discussed in the section *Purity requirements for hydrogen applications and end-use*, transport and storage itself and the reconversion to retain the hydrogen.

Under normal conditions (0 °C, 1 atm), methanol is a liquid, which makes it safer to handle than gaseous hydrogen [120]. Methanol is already a common cargo, routinely transported by ship, rail, truck, and pipeline [18,121,122]. The transport and storage itself consists of mature TRL ≥ 9 technologies [18] that can potentially be scaled up with the growth of the hydrogen and methanol economy.

When it reaches the end user, methanol is either used as is or reconverted to hydrogen, depending on the application [104]. According to Dalena et al. [123], the reconversion can take place in several ways. These include in particular:

1. Direct decomposition of methanol
2. Steam reforming of methanol (MeOH-SR, MeOH-MR)
3. Partial oxidation of methanol
4. Autothermal reforming of methanol (MeOH-ATR)

In direct decomposition, methanol is decomposed into hydrogen and carbon monoxide with the addition of heat [123]:



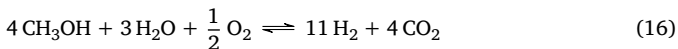
The steam reforming of methanol is carried out according to the gross reaction equation



However, two important side reactions occur in addition to this main reaction: Methanol decomposition (Eq. (13)) and a *Water–Gas–Shift* reaction (Eq. (26)) [124]. Steam reforming of methanol is the most commonly used back-conversion route [104]. The partial oxidation of methanol is described by the equation



while autothermal reforming proceeds according to Eq. (16) [123, 124]:



For methanol reconversion, the discussed technologies are limited to steam reforming and autothermal reforming. The direct decomposition and partial oxidation of methanol are not discussed further.

This section deals with the product gas composition after the reconversion of methanol into hydrogen. The raw gas compositions after reconversion using the upstream processes autothermal reforming (MeOH-ATR) as well as steam reforming with a conventional reactor (MeOH-SR) and with a membrane reactor (MeOH-MR) are listed in Table 19. Autothermal reforming is carried out with air as the oxidizing agent.

It can be seen that simple back-conversion processes such as steam reforming and autothermal reforming with a resulting H₂ purity of 75 to 80 mol% for SR and 46 to 51 mol% for ATR cannot provide pure hydrogen (>99.9 mol%). The air-driven MeOH-ATR leads to a dilution

Table 19

Composition of the product gas after the reconversion of methanol to hydrogen, differentiated by type of conversion process.

Process:	Methanol reconversion		
Type:	MeOH-ATR	MeOH-SR	MeOH-MR
H ₂	49 mol%	77.5 mol%	≈100 mol%
N ₂	21–27 mol%	N/A	N/A
CO	4 mol%	1.5 mol%	<10 ppm
CO ₂	20 mol%	23 mol%	N/A
CH ₄	5 mol%	N/A	N/A
References	[125,126]	[5,104]	[127–129]

MeOH-ATR: autothermal reforming of methanol (with air as the oxidizing agent); MeOH-SR: steam reforming of methanol in a conventional reactor; MeOH-MR: steam reforming in a membrane reactor (use of a dense Pd-based membrane with a CuO/Al₂O₃/ZnO/MgO catalyst).

of the product with nitrogen [5,104,125,126]. Alternatively, the reconversion can take place in an intensified process in conjunction with a membrane (MeOH-MR). The membrane reactor shown here is based on a palladium membrane with a catalyst of CuO/Al₂O₃/ZnO/MgO. The H₂ product purity is over 99.999 mol% and is thus in the range of some purification processes presented in the section *Hydrogen purification and treatment* [127–129]. Taken together, the product compositions of the methanol conversion processes are in a similar range to the compositions of the methane reforming processes (see section *Hydrogen production*).

2.2.6. Large-scale underground storage of compressed gaseous hydrogen

Underground storage facilities in geological formations offer a promising option for the large-scale storage of gaseous hydrogen [69, 130,131]. Both salt caverns and porous rock reservoirs, such as depleted oil and gas reservoirs and saline aquifers, can be considered for storage [131,132]. While the overall experience with storage in porous rock is limited and no relevant data is available for depleted oil fields, underground storage in salt caverns is rated with a TRL of 7 to 8 (2020) [132,133] and up to 9 (2024) [18]. In contrast, storage in porous structures only has a TRL of 3 to 4 (2024) [18,132].

Salt caverns. Salt caverns are created by a process known as leaching, in which water is injected into a salt dome. This dissolves the salt in the water, creating a brine, which is then pumped out, leaving behind an artificial cavity, the salt cavern [130,134].

During salt extraction, a protective medium consisting of hydrocarbons called blanket can be used. The application of hydrocarbons as a film around the edge of the borehole prevents the uncontrolled spread of salt water [135].

The storage of gaseous hydrogen in salt caverns always leads to contamination of the hydrogen. Table 20 lists possible impurities, their origin and conditions for their occurrence.

Saturation with water vapor occurs in new hydrogen salt caverns as well as in retrofitted natural gas salt caverns [2]. Water separation is therefore necessary after hydrogen storage. Further contamination results from possible previous use and the geological and microbiological conditions of the underground storage site. In the case of retrofitted salt caverns, natural gas and crude oil residues may lead to direct contamination. Oil residues may also be present in former natural gas storage facilities, as oil blankets are often used to protect salt caverns.

Bacterial activity can also occur in both newly constructed and retrofitted salt caverns [138]. Microorganisms consume hydrogen and carbon or sulfur sources and produce some contaminants listed in Table 20. The extent of bacterial activity varies greatly depending on the geological site, so that individual monitoring of each salt cavern is recommended in the literature [139].

A summary of the gas compositions after GH₂ storage in newly constructed and retrofitted salt caverns and in salt caverns in which there is no bacterial activity is shown in Table 21. According to research

Table 20
Contamination, contamination sources and conditions for the occurrence of contamination in new and retrofitted salt caverns (based on [2,136–138]).

Contaminant	Source of contamination	Condition for occurrence
H ₂ S	S-/SO ₄ ²⁻ -reduction	Halophilic bacteria Sulfate or sulfur deposits
CO ₂	Acetate decomposition Dissolved in brine	Acetogenic bacteria Mostly: Previous use with hydrocarbons Rarely: Natural occurrence
Acetate		Hydrogenotrophic bacteria
CH ₄	Methanogenesis	CO ₂ contaminant CO ₂ reducing bacteria Guess: Salinity ≤150 g/L Pre-use with natural gas
Acetic acid	CO ₂ reduction	CO ₂ contaminant CO ₂ reducing bacteria
Metals	H ₂ -metal-reaction	Non-suitable steels
Biofilm	Subterranean bacterial reaction	Bacterial activity
Hydrocarbons	Diesel blanket Natural gas/oil residues	Use of blanket Pre-use with natural gas/oil
Saline solution	Swamp	<i>none</i>
H ₂ O	Water vapor from cavern and swamp	<i>none</i>
N ₂	Blanket residual	<i>none</i>

Table 21
Gas composition after storage of gaseous hydrogen in salt caverns.

Storage option:	Salt caverns		
Cavern state:	After conversion	No pre-use	No pre-use no carbon and sulfur sources
H ₂	≥98.0 mol% <i>saturated</i>	≥98.0 mol% <i>saturated</i>	≥99.97 mol% <i>saturated</i>
H ₂ O			
O ₂			
N ₂			
Ar			
He			
CO			
CO ₂			
CH ₄			
H ₂ S			
C _n H _m			
NH ₃			
S-total			
Formaldehyde			
Formic acid			
References	[2]	[2]	[2,140]

The gas groups correspond to the gas groups from Table 1. For a precise statement about the gas composition, the impurities in salt caverns must be determined on a case-by-case basis (see [139]).

by Lubenau et al. [2] in the H₂Rein project, the storage of hydrogen of quality grade A should be possible for new and retrofitted salt caverns.

A more precise classification of impurities is not possible with the current state of the literature. However, the purity requirements and sources of contamination for GH₂ storage in salt caverns are the subject of current research activities. H₂-ReNoWe and HyCavMobil are two of these projects led by the German Aerospace Center (DLR), which are investigating the storage of hydrogen in salt caverns and its use in electricity generation and fuel cell vehicles [141–144]. Comprehensive results of these projects on GH₂ storage in salt caverns have not yet been published at the time of writing.

Porous underground storage. Studies on impurities in the storage of gaseous hydrogen in porous underground storage facilities are limited and mostly consist of numerical investigations. According to studies by Okoroafor et al. [145], based on preliminary studies by Pfeiffer et al. [146], the achievable hydrogen purity correlates with the gas

withdrawal rate: the higher the gas withdrawal rate, the lower the achieved hydrogen purity. The authors use a productivity index to determine an advantageous operating point for the storage tank. According to the authors of the study, the highest productivity index is achieved at a low extraction rate of about 750,000 m³/d. The hydrogen purity achieved at this point is 90 mol% [145]. According to the current state of the literature, porous underground storage facilities are therefore not capable of storing hydrogen of DVGW gas group qualities A and D.

2.2.7. Storage by means of chemisorption and physisorption

In the process of chemisorption, the hydrogen forms a chemical bond with the surface atoms of the adsorbent material [147]. Metal hydride storage is a prominent representative of this group [67]. For this storage type, dissociated monatomic hydrogen binds to the lattice of metals or metal alloys. The hydrogen is then released again by increasing the temperature or reducing the pressure [6,67,68]. Due to the small-scale fields of application, it is not expected that storage using metal hydrides will play a significant role in the subsequent infrastructure design. For this reason, storage using metal hydrides is not discussed further in this study. Metal hydrides are considered to have a low TRL of 3 to 5 (2024) [3,18,77]. Due to the small-scale fields of application, it is not expected that storage using metal hydrides will play a significant role in the subsequent infrastructure design. For this reason, storage using metal hydrides is not discussed further in this study.

Physisorption involves the reversible and adsorptive binding of hydrogen to a porous material [148]. According to Usman [6], the material can consist of carbon, zeolites or metal–organic frameworks (MOFs). Adsorptive storage processes generally have a low level of maturity (TRL < 5) [3,77]. This is true for all physisorption processes mentioned [77]. Therefore, physisorption storage will not be discussed further.

3. Purity requirements for hydrogen applications and end-use

This section of the paper looks at the end use and application of hydrogen, giving us a clear picture of the maximum hydrogen purity levels required at the end of the supply chain.

The hydrogen applications fall into the sectors energy supply, transport & mobility, and industry. In the industrial sector, hydrogen is

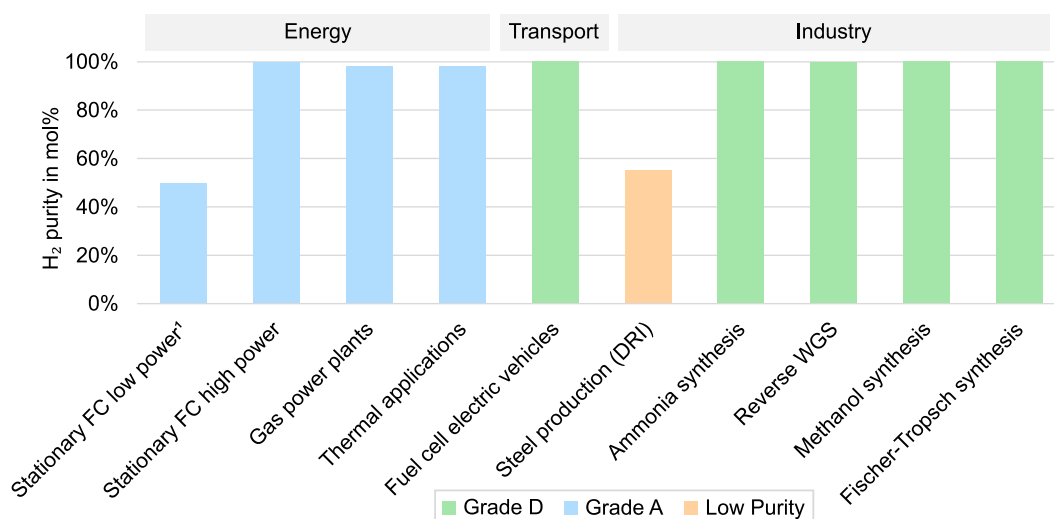


Fig. 11. Overview of hydrogen purity requirements for hydrogen applications according to the literature review.

FC: fuel cell, DRI: direct reduced iron, WGS: water–gas shift reaction.

¹ Classified conservative, higher inert gas tolerance possible.

used both as an energy carrier and as a chemical feedstock [149]. The hydrogen technologies used in the individual sectors are explained in the following section. Fig. 11 shows the results of the purity review for different hydrogen applications.

The results show that the lowest purity requirements are in applications where hydrogen is used solely for thermal applications, such as process heat and smelting in the steel industry. Stationary fuel cells with low power output requirements also tolerate hydrogen purity levels as low as 50 mol% [10]. Fuel cells with higher efficiency and power output, as well as gas turbines, require higher purity levels of grade A, ≥ 98 mol%. The highest purity requirements come from fuel cell vehicles and the chemical industry, where the hydrogen content is at least 99.97 mol%. The definition of purity grade D is derived from the requirements of fuel cell vehicles.

3.1. Energy supply

The use of hydrogen in stationary fuel cells, gas-fired power plants and thermal applications is part of the hydrogen-based energy supply.

3.1.1. Stationary fuel cells

Fuel cells convert the chemical energy of hydrogen and oxygen into electrical energy following the exothermic gross reaction



under the formation of water, representing the reverse reaction of the electrolysis [150].

Stationary fuel cells in the building sector. In the building sector, hydrogen can be used in small-scale stationary polymer electrolyte fuel cells (PEMFC) to generate electricity [10]. PEMFC in the building sector have a TRL of 9 (2024) and can also be used as small scale combined heat and power plants by utilizing the waste heat [18]. For the consideration of purity requirements, stationary PEMFCs are divided into three different classes depending on the required power and efficiency, which result from the application: Firstly, applications that require low power and high efficiency; applications that require high power; and applications that require high power and high efficiency [10].

It is to be expected that PEM fuel cells that have very high efficiencies and can handle very high load cases will not be used in the building sector. Therefore, the purity requirement for stationary PEMFC applications in the building sector is in most cases 50 mol% [10]. The

Table 22

Purity requirements and tolerances for impurities for stationary PEM fuel cells.

Process:	Stationary PEM fuel cells		
Power requirement:	Low	High	High
Efficiency requirement:	High	–	High
H ₂	50 mol%	50 mol%	99.9 mol%
H ₂ O	non-condensing		
O ₂	200 ppm	200 ppm	50 ppm
N ₂ , Ar, He	$\Sigma \leq 50$ mol%	$\Sigma \leq 50$ mol%	$\Sigma \leq 0.1$ mol%
CO	10 ppm	10 ppm	0.2 ppm
CO ₂	N/A	N/A	2 ppm
CH ₄	5 mol%	1 mol%	100 ppm
C _n H _m	10 ppm	2 ppm	2 ppm
NH ₃	0.1 ppm	0.1 ppm	0.1 ppm
S	0.004 ppm	0.004 ppm	0.004 ppm
Halogenated compounds	0.05 ppm	0.05 ppm	0.05 ppm
Formaldehyde	3 ppm	0.2 ppm	0.2 ppm
Formic acid	10 ppm	0.2 ppm	0.2 ppm
References	[10]		

research results on the use of hydrogen in stationary fuel cells are summarized in Table 22.

The carbon monoxide limit value of 0.2 ppm is particularly critical when using hydrogen in stationary PEMFCs with high load and efficiency requirements. The sulfur limit value of 0.004 ppm is also very low for all stationary PEMFC applications.

Stationary fuel cells in the power sector. For large-scale fuel cells in the power sector, high-temperature solid oxide fuel cells (SOFC) with a TRL of 8–9 (2024) [18] are preferred over low-temperature PEM fuel cells [151,152]: Due to higher operating temperatures, they have greater tolerance to carbon monoxide contamination [151]. Fuel flexibility is another advantage of SOFC as they can be operated on hydrocarbon fuels, syngas, biogas, ammonia and pure hydrogen [151–154]. Third, SOFC can perform reversible operation, producing hydrogen when there is a surplus of electricity and reconverting hydrogen when there is a demand for electricity [151].

Data on purity requirements for SOFCs are scarce and are not included in ISO 14687:2019. Exports say that the purity requirements for stationary PEMFC in ISO 14687:2019 can serve as a baseline, but SOFC tend to be more resistant to impurities [1].

Table 23

Purity requirements and tolerances for impurities for gas power plants.

Process:	Gas power plants
H ₂	98.0 mol%
H ₂ O, O ₂ , N ₂ , Ar	$\Sigma \leq 1.9 \text{ mol\%}$
CO	1 ppm
C _n H _m	100 ppm
S	2 ppm
References	[10]

Table 24

Purity requirements and tolerances for impurities for small scale domestic heat applications like boilers and cookers.

Process:	Domestic heating appliances
H ₂	98.0 mol%
CO	20 ppm
H ₂ S	3.5 ppm
O ₂	0.2 mol%
Ar, N ₂ , He	$\Sigma \leq 2 \text{ mol\%}$
CO ₂ , CH ₄ , C _n H _m	$\Sigma \leq 1 \text{ mol\%}$
S-total	$\leq 35 \text{ ppm}$
References	[1]

3.1.2. Gas power plants

Hydrogen can be used in gas-fired power plants to generate electricity and heat, acting as a low emission alternative to natural gas fired power plants [155]. Gas-fired power plants are characterized by high flexibility and efficiency, which makes them particularly interesting for use in a fluctuating power grid [156]. Lubenau et al. [2] assume hydrogen for gas turbines to be of quality grade A. According to ISO 14687:2019 this results in the purity requirements presented in Table 23.

There is a significantly reduced purity requirement of 98.0 mol% compared to some stationary and especially compared to mobile PEM fuel cell applications. Stationary PEMFCs with high efficiency and high load require 99.9 mol% purity, while mobile PEMFC applications are operated with a hydrogen purity of 99.97 mol%.

Lubenau et al. [2] point out that in heat applications, the exact quality of the hydrogen is less important than a constant quality supply. Nevertheless, in terms of infrastructure-wide technology integration, a minimum hydrogen content of 98.0 mol% is prescribed [2,11].

3.1.3. Thermal applications

In addition to electricity, hydrogen can also be used for heating. This includes small-scale applications for buildings as well as large-scale applications such as industrial process heat.

Small-scale heating applications. The small-scale heat applications of hydrogen in the context of this work primarily include the use of H₂ in heating systems and stoves [10,156]. A comprehensive study of hydrogen purity for these applications was carried out as part of the Hy4Heat project commissioned by the UK Department for Business, Energy & Industrial Strategy, which published its results in 2019 [1]. The results of their study are presented in Table 24.

As in ISO 14687:2019(E), the total hydrogen purity level is recommended to be at least 98.0 mol%. Compared to the standard, the tolerances recommended in the Hy4Heat project are higher for the impurities studied.

Process heat and large scale heating applications. The temperature level of the heat required in the industrial sector is generally much higher than in the building sector. Temperatures above 400 °C are often required [157]. To provide process heat at high temperature levels, hydrogen is burned in burners [156,158]. For heating applications, DVGW e.V. and ISO 14687:2019(E) suggest purity grade A with a hydrogen content of 98.0 mol% [10,11]. The contamination levels are similar to those of natural gas, and the variation of the Wobbe index,

Table 25

Purity requirements and tolerances for impurities for mobile PEM fuel cells.

Process:	Mobile PEM fuel cells
H ₂	99.97 mol%
H ₂ O	5 ppm
O ₂	5 ppm
N ₂	300 ppm
Ar	300 ppm
He	300 ppm
CO	0.2 ppm
CO ₂	2 ppm
CH ₄	100 ppm
C _n H _m	2 ppm
NH ₃	0.1 ppm
Total sulfur	0.004 ppm
Halogenated compounds	0.05 ppm
Formaldehyde	0.2 ppm
Formic acid	0.2 ppm
References	[10]

the ratio of the higher heating value to the specific gravity of hydrogen, should be of less than 2% [2].

3.2. Transport & mobility

PEMFC are a promising and widely used technology in hydrogen powered vehicles, especially in the passenger car sector [159]. The basic mode of operation corresponds to that of stationary PEMFCs. The hydrogen purity requirements for mobile PEMFC are well-defined in ISO 14687:2019(E) and listed in Table 25. They constitute the purity grade D in the norm.

Similar to stationary PEM fuel cells, the limit values for carbon monoxide and sulfur compounds in particular are very low. In the literature, the purity requirement for mobile PEM fuel cells of 99.97 mol% is often used as a guide value for high purity [5].

3.3. Industry sector

In the industrial sector, green hydrogen is used to decarbonize process heat and as a carbon-free feedstock [157,158,160–162].

3.3.1. Steel production

Hydrogen can be used to produce steel, offering an alternative to coke-fired blast furnaces. [163]. In a first step, hematite (Fe₂O₃) is reduced to iron (Fe) in order to be enriched with carbon in the second step, whereby small amounts of cementite (Fe₃C) are formed. Alternatively, the reduction of the hematite and the reaction to cementite can be integrated in one step [164]. The product of the first step is called direct reduced iron (DRI). The gross reaction equation of the DRI formation is [165]:



Purity requirements and impurity tolerances in steelmaking are listed in Table 26. The processes can be distinguished in carbon-free DRI and cementite (Fe₃C) enriched DRI. The permissible proportions of H₂, CO, CO₂ and H₂O are described by a value range referred to as the low and high hydrogen content pathway.

Hydrogen with a purity of 97 mol% is sufficient for the synthesis of carbon-free DRI from [165]. Steel enriched with cementite is not synthesized using pure hydrogen, but with a mixture of carbonaceous substances and hydrogen [164].

3.3.2. Ammonia synthesis/Haber–Bosch process

Ammonia can be produced by various synthesis routes. In addition to the conventional Haber–Bosch process (HBP), electrochemical, thermochemical and integrated processes are also conceivable [166]. Since

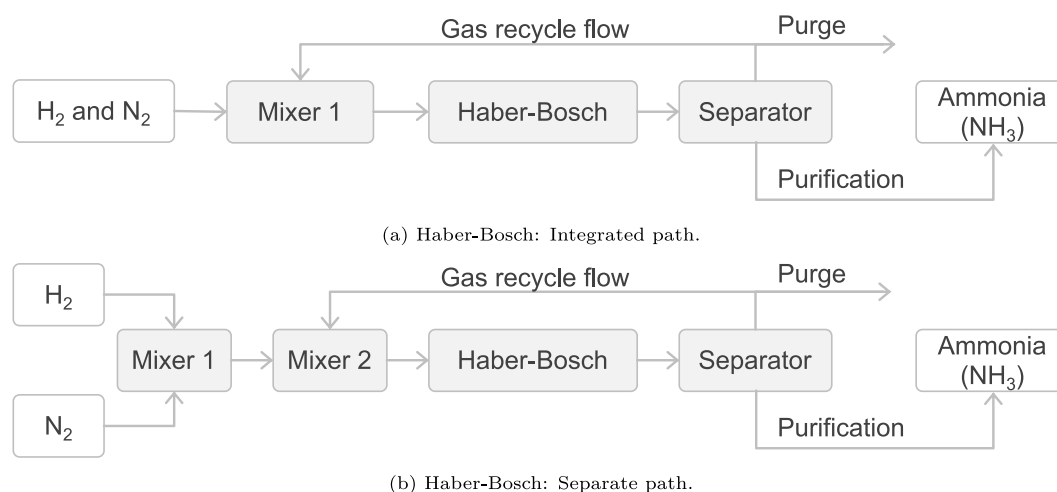


Fig. 12. Process scheme of two possible ways to feed the reactants to the Haber-Bosch process:

(a) Integrated supply of N_2 and H_2 , e.g., by air-driven autothermal reforming of methane (see also Section 2.2 in the supplementary material).

(b) Separate supply of N_2 and H_2 , for example via an air separation and an electrolysis unit.

Table 26

Purity requirements and tolerances for impurities in the production of direct reduced iron (DRI) using hydrogen. DRI can be carbon-free or carbon-containing. Carbonaceous DRI can be synthesized with either a high or low hydrogen content.

Process:	Direct reduced iron (DRI)		
Carbon content:	Carbon-free	Carbon-containing	
H_2 content:	–	Low	High
H_2	97 mol%	55 mol%	90 mol%
H_2O	3 mol%	15 mol%	5 mol%
CO_2	N/A	5 mol%	0 mol%
CO	N/A	30 mol%	5 mol%
CH_4	N/A	≈1 mol%	
References	[164,165]	[164]	

Table 27

Purity requirements and impurity tolerances for the Haber-Bosch process.

Process:	Haber-Bosch process
H_2	99.99 mol%
H_2O	10 ppm
O_2	10 ppm
N_2	educt
Ar	As low as possible
He	N/A
CO, CO_2	$\Sigma \leq 10$ ppm
CH_4	As low as possible
NH_3	product
References	[46,168–172]

the International Renewable Energy Agency and the Ammonia Energy Association expect the Haber-Bosch process to remain the standard process in the coming decades, especially for large-scale production plants, only the HBP is discussed here [116]. The gross reaction equation for the exothermic ammonia synthesis of HBP is [46]:



The process is usually operated at 460 °C and 200 bar catalyzed by iron [46,167]. The reactants of the HBP, N_2 and H_2 , can be introduced into the process in two different ways as shown in Fig. 12 [116]: Either together in an integrated pathway as shown in Fig. 12(a) or in a separate pathway as shown in Fig. 12(b).

The integrated pathway in which nitrogen and hydrogen are synthesized together represents the classic process implemented, for example, via an SMR coupled with an air-driven ATR (see also Section 2.2 in the supplementary material). It makes use of the fact that the product stream of methane reforming contains the reaction product hydrogen as well as the inert nitrogen introduced to the process via the air supply.

In the separate pathway, hydrogen and nitrogen are sources individually. The hydrogen can stem from an SMR or an oxygen driven ATR, as demonstrated in the Linde Ammonia Conversion concept [46]. It can also be provided by water electrolysis, providing means for green ammonia production. Nitrogen is provided with the use of air separation.

After the H_2 - N_2 mixture is provided to the process, both pathways are the same. Recirculated gas is added to the mixture, the resulting mixture enters the reactor and reacts incompletely according to Eq. (19) to form a NH_3 - N_2 - H_2 mixture. The reactants are separated from the product, and a portion of the gas mixture is purged to prevent a concentration of impurities and inert gases. The remaining portion of

the unreacted reactants is returned to the feed via the recycle stream and re-enters the reactor chamber [46]. Purity requirements for the separate pathway are collected from multiple literature sources are presented in Table 27.

Appl [46] states as a criterion that all oxygen-containing compounds should be reduced to a very low concentration level in the ppm range. De Klerk et al. [173] further specify that the cumulative fraction of CO and CO_2 should be below 10 ppm. Moghaddam et al. [172] state a limit value of 5 ppm for water and oxygen, while Lee et al. [171] recommend 3 ppm for oxygen. The compounds listed so far, CO, CO_2 , O_2 , and H_2O , are considered catalyst poisons [172].

In contrast, argon and methane are considered inert gases. The inert gas content in the Haber-Bosch process can vary between 0 and 15 vol% due to recirculation [46]. With integrated reactant feed, it is typically 1 vol%.

For hydrogen purity in the separated path, 99.99 mol% is recommended [168,169]. According to Linde, 98.0 mol% is also possible [169]. However, the reduced purity is probably only permissible if the additional impurity consists of the inerts CH_4 and Ar.

3.3.3. Reverse water-gas shift reaction

The reverse water-gas shift reaction (RWGS) is used to produce carbon monoxide from carbon dioxide and hydrogen [174]. The gross reaction equation is [175]:



The RWGS is usually integrated as a process sub-step, for example, in the Fischer-Tropsch synthesis, in order to synthesize a reaction mixture of hydrogen and carbon monoxide [176]. The input requirement for

Table 28

Purity requirements and impurity tolerances for methanol synthesis.

Process:	Methanol synthesis
H ₂	99.99 mol%
H ₂ O	5 ppm
O ₂	145 ppm
N ₂ , Ar, He	As low as possible
CO	<i>educt</i>
CO ₂	<i>educt</i>
CH ₄	As low as possible
Sulfur	100 ppb
C ₂ H ₄	5 ppm
NH ₃	100 ppb
Halides	10 ppb
References	[173,177,181]

the RWGS is a low water content according to Kaiser et al. [176]. This is due to the shift of the reaction equilibrium towards the reactants when additional water is added. Since the RWGS is carried out today in many variants using different catalysts, it is hardly possible to specify concrete purity requirements [174]. A minimum hydrogen purity of 99.9 mol% is derived from the water content recommendation. It should be noted that the purity requirement results from an efficiency requirement and not from catalyst deactivation.

3.3.4. Methanol synthesis

Methanol can be synthesized on the basis of carbon dioxide and carbon monoxide [177]. The gross reaction equation of the CO₂-based synthesis is



In contrast, the CO-based reaction takes place according to:



The synthesis according to Eq. (21) is called the CO₂ pathway, the synthesis according to Eq. (22) CO pathway. While the CO₂ pathway uses as pure hydrogen and CO₂ streams as possible [177], the carbon reactant stream of the CO pathway usually consists of a CO–CO₂ mixture [178]. It is recommended that the composition of the synthesis gas be chosen so that the stoichiometric number, *S*, is slightly above 2 [178–180]. The stoichiometric number is defined as

$$S := \frac{v_{\text{H}_2} - v_{\text{CO}_2}}{v_{\text{CO}} + v_{\text{CO}_2}}, \quad (23)$$

where *v_i* stands for the volume fraction of the component *i* [178]. Derived from the stoichiometric number of 2, a volume fraction of 66–75 vol% can be calculated for H₂, 0–34 vol% for CO, and 0–25 vol% for CO₂. Since, strictly speaking, a stoichiometric number slightly greater than 2 is required, the permissible proportions may vary slightly. A common composition in the CO path consists of about 74 vol% H₂, 15 vol% CO₂, and 8 vol% CO [178].

Analogous to the Haber–Bosch process, a distinction can be made between the reactant feed in methanol synthesis. A separate feed is referred to as a separate CO or CO₂ pathway, while an integrated feed is referred to as an integrated CO or CO₂ pathway.

The results of the purity requirements and impurity tolerances for methanol synthesis are summarized in Table 28. A distinction of the different pathways is not necessary when considering the purity requirements for hydrogen.

The catalyst for methanol synthesis (Cu/ZnO/Al₂O₃) must be protected from sulfur and halogen compounds, in particular. The limits are therefore in the ppb range. In addition, oxygen is also a catalyst poison [181]. Cordero-Lanzac et al. [177] point out that the required purity of the hydrogen feed stream in the separate CO₂ pathway is determined by two factors:

Table 29

Purity requirements and impurity tolerances for Fischer–Tropsch synthesis using iron (Fe-FTS) or cobalt (Co-FTS) as catalyst.

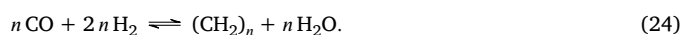
Process:	Fischer–Tropsch synthesis	
Catalyst:	Iron (Fe-FTS)	Cobalt (Co-FTS)
H ₂	99.99 mol%	99.9 mol%
H ₂ O	As low as possible	Low
O ₂	N/A	
N ₂	As low as possible	
CO	<i>educt</i>	
CO ₂	5 mol%	
CH ₄	2 mol%	
NH ₃	1 ppm	
S	1 ppm	4 ppb
Halides	10 ppb	
References	[173,176,181,184]	

1. The purity of the other reactant streams. In the following, it is assumed that the other reactant streams are completely pure material streams.
2. The recirculation rate of the unreacted gases. With a gas recirculation rate of 99% and a resulting purge fraction of 1%, the allowable oxygen contamination limit in the hydrogen feed is reduced from 300 ppm to 145 ppm [177].

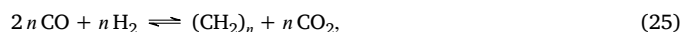
The work of Cordero-Lanzac et al. [177] makes it clear that rigorous studies of the accumulation of impurities in the reactor chamber are necessary to accurately determine the allowable limits with separate reactant feed.

3.3.5. Fischer–Tropsch synthesis/synfuel synthesis

Fischer–Tropsch synthesis (FTS) is based on the hydrogenation of CO to synthesize a mixture of liquid hydrocarbons [182]. FTS processes are usually divided into high-temperature (HTFT) and low-temperature (LTFT) processes. HTFT processes are catalyzed by iron, while cobalt is usually used in LTFT [183]. The gross reaction equation of the cobalt-catalyzed FTS is [182]:



The iron-catalyzed reaction, on the other hand, takes place after



since a WGS occurs in parallel in the reactor [182].

In accordance with the previous sections, the reactant feed in the FTS is divided into a separate and an integrated path.

The purity requirements and impurity tolerances in Table 29 apply to the Fischer–Tropsch synthesis. The results are divided into an iron-catalyzed process (Fe-FTS) and a process that is operated with a cobalt-based catalyst (Co-FTS).

The two processes differ primarily in the limits for sulfur compounds and water. The cobalt catalyst has a very low tolerance to sulfur and requires a much lower proportion at 4 ppb than the iron catalyst at 1 ppm [185].

The literature information on water contamination is less clear. The lowest possible water content is required because water can lead to reduced kinetics with the iron catalyst and to reoxidation with the cobalt catalyst [176]. Therefore, water should be reduced as much as possible in the Fe-FTS, while it is considered less critical in the Co-FTS.

In summary, the process requirements for hydrogen purity in Fischer–Tropsch synthesis are not clearly defined. It is assumed that a hydrogen purity of 99.99 mol% is required for the Fe-FTS, while the Co-FTS can be operated at 99.9 mol% due to its higher tolerance to water impurities.

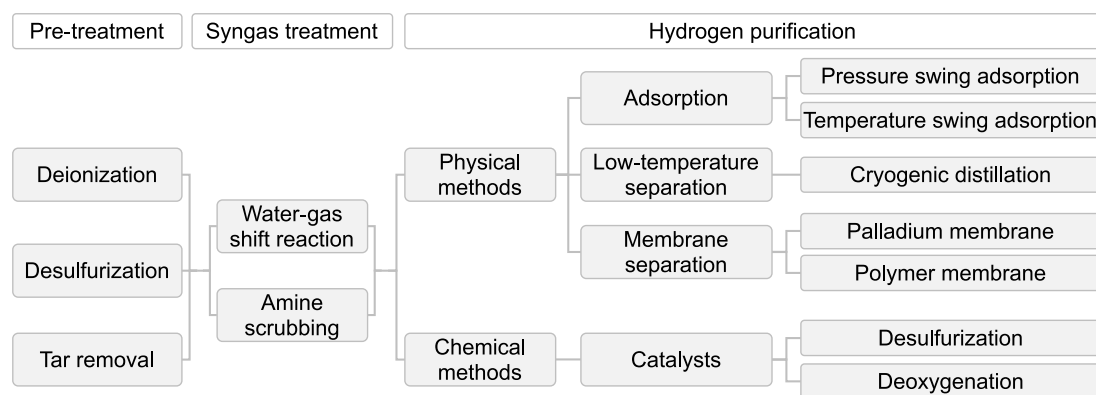


Fig. 13. Overview of the selected hydrogen purification and treatment processes (based on [5]).

4. Hydrogen purification and treatment

The third section of the literature review deals with the part that bringing together the different elements of the supply chain, the purification and treatment of hydrogen. Different processes are used to purify hydrogen in different stages of the process: First, there are processes to purify the feedstock material [5]. These include the deionization of water in electrolysis processes, the desulfurization of hydrocarbons, and the tar removal in the biomass gasification process. Second, there are a number of processes used to remove impurities and increase the hydrogen content of the resulting syngas. These include the water–gas shift (WGS) reaction and carbon dioxide removal. Third, there is the class of processes for the purification of pure (>90 mol%) hydrogen, as shown in Fig. 13.

According to Du et al. [5], the hydrogen purification processes are divided into physical and chemical methods. The physical methods include adsorptive, low-temperature, and membrane methods. The chemical methods include catalytic processes such as deoxygenation and purification processes using metal hydrides.

Fig. 14 shows the results of the literature review of hydrogen purification technologies. The highest levels of purity can only be achieved with TSA/PSA, and palladium membrane systems. Deoxygenation is highly efficient at removing oxygen and achieving high purity levels, when oxygen is the only contaminant, but is not a general purpose purification system. WGS and amine scrubbing are efficient in converting and removing carbon monoxide and carbon dioxide. Because they are only intermediate steps in a purification chain, they do not achieve high purity by themselves. Cryogenic distillation and polymeric membranes represent general purpose purification systems, but do not achieve the high purity levels of grades A and D.

The following technologies are primarily used on an industrial scale. A comprehensive assessment of the technology maturity level is provided in each section.

4.1. Deionizer

According to ISO 22734:2019(E) [186], all electrolyzer manufacturers must define the requirements for the water used. Typically, deionized water is required that meets at least water quality type II of the *American Society for Testing and Materials* standard [187,188]. The standard specifies that water must have a minimum resistivity of 1 MΩ cm, a maximum conductivity of 1 μS/cm, and a maximum TOC (total organic carbon) of 50 ppb [187–189]. To meet these requirements, water is usually deionized before it is fed into the electrolyzer [190].

4.2. Desulfurization

Desulfurization is a common process step, especially in natural gas reforming [4,36]. Sulfur is a catalyst poison in methane reforming and can therefore affect the process [38,191]. Zinc oxide is used to absorb hydrogen sulfide and sulfur compounds [38].

4.3. Tar removal

Gasification of biomass leads to tar formation [192]. Two approaches are recommended to counteract this [193]:

1. Primary methods, where removal occurs during gasification
2. Secondary methods where tar removal occurs after gasification

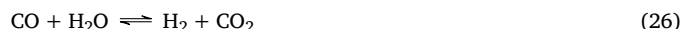
In industrial practice, a combination of secondary methods based on physical, thermal and catalytic technologies is usually used in addition to primary removal [193].

4.4. Water–gas shift reaction (WGS)

In the synthesis of hydrogen from hydrocarbons, carbon dioxide and carbon monoxide are usually present in the product stream in addition to hydrogen [194]. The water–gas shift (WGS) reaction can be used to both reduce the CO content and increase the hydrogen content [1]. Boll et al. [195] list three use cases for WGS:

1. adjustment of the carbon monoxide content in carbon monoxide-rich gases,
2. conversion of toxic carbon monoxide to carbon dioxide,
3. increase in the hydrogen content.

The gross reaction equation of the WGS is [47]:



Carbon monoxide and water react to form hydrogen and carbon dioxide. Because the reaction is exothermic, the reaction equilibrium is favorable at low temperatures [1]. On the other hand, the reaction kinetics are more favorable at high temperatures [195]. In order to combine the advantages of both temperature levels, a multi-stage reactor is used, combining a high-temperature WGS at 315 to 450 °C and a low-temperature WGS at 190 to 250 °C [1,196,197]. The product compositions resulting from the purification of common raw gases with a multi-stage WGS reactor are presented in Table 30.

The WGS significantly reduces the carbon monoxide content down to 2 mol% (SMR, 12 mol% before WGS) to 0.5 mol% (ATR-A, 13 mol% before WGS). For the most common industrial hydrogen production process, SMR, the WGS simultaneously increases the hydrogen purity from 65 mol% (see Table 5) to 75 mol% (see Table 30), which is still below the purity level of the electrolysis processes (see Table 3).

4.5. CO₂-absorption

Carbon dioxide removal is part of most hydrocarbon-based hydrogen production processes [39]. It can be accomplished by means of absorption, adsorption, distillation, membrane separation and hydrates [198]. This section deals only with absorptive CO₂ separation.

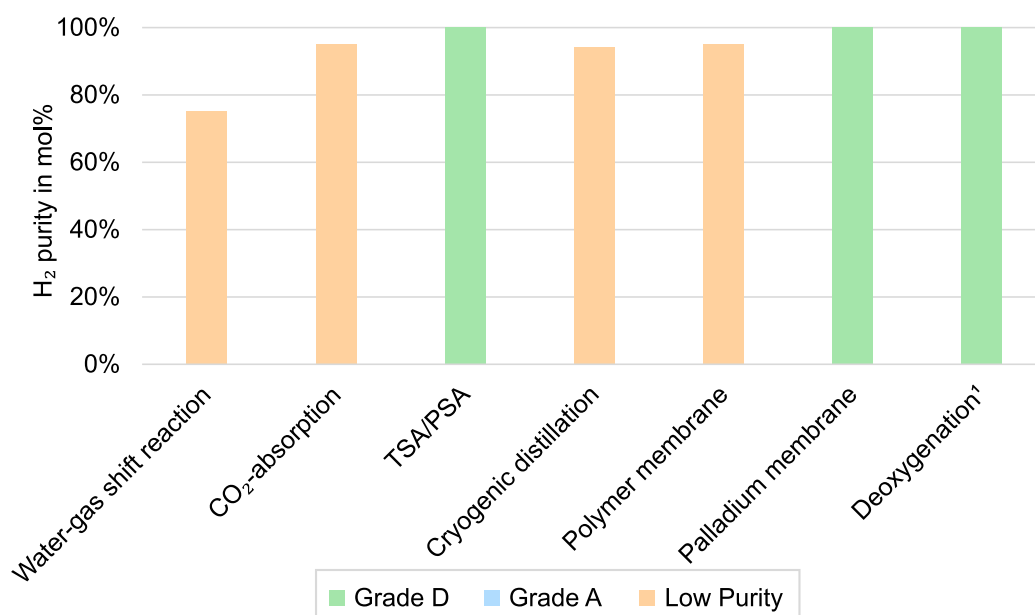


Fig. 14. Overview of achievable hydrogen purity levels through purification and hydrogen treatment according to the literature review.

TSA: temperature swing adsorption, PSA: pressure swing adsorption.

¹Grade D achievable when O₂ is the only contamination.

Table 30

Gas composition after purification of common synthesis gases in a high-temperature-low-temperature water-gas shift reactor.

Process:	Water-Gas shift reaction			
Upstream process:	SMR	ATR-O ₂	ATR-A	CG-O ₂
H ₂	75 mol% (65 mol%) ^a	72 mol% (65 mol%) ^a	50 mol% (45 mol%) ^a	55 mol% (40 mol%) ^a
H ₂ O	0.15 mol%	0.1 mol%	0.1 mol%	0 mol%
O ₂	0 mol%	0 mol%	0 mol%	0 mol%
N ₂	0.1 mol%	0.08 mol%	30 mol%	3 mol%
Ar	0 mol%	0 mol%	0.4 mol%	0.7 mol%
CO	2 mol% (12 mol%) ^a	0.7 mol% (28 mol%) ^a	0.5 mol% (13 mol%) ^a	1.2 mol% (40 mol%) ^a
CO ₂	20 mol%	27 mol%	18 mol%	41 mol%
CH ₄	4.5 mol%	1.3 mol%	0.15 mol%	≤1.33 mol%
H ₂ S	20 ppm	10 ppm	10 ppm	≤0.06 mol%
References	[1,49]	[1]	[1,49]	[49]

SMR: steam methane reforming, ATR-O₂: autothermal reforming with oxygen, ATR-A: autothermal reforming with air, CG-O₂: coal gasification with oxygen.

^a The value in brackets indicates the component proportion before the water-gas shift reaction.

The other processes also apply to the separation of other contaminants and are described in separate sections.

Absorption describes a process in which gaseous components pass into a liquid solvent [199]. Depending on whether the gas components remain chemically unchanged or not, the processes are divided into physical and chemical absorption [195,199]. Chemical CO₂-absorption processes include the industrially common absorption in amine solutions (amine scrubbing) [1,198]. Physical absorption processes include the *Selexol*[®] process licensed by Honeywell UOP [200] and the *Rectisol*[®] process licensed by Linde and Lurgi [201]. A comprehensive list of possible absorption processes can be found in the reviews by Rufford et al. [198] and Boll et al. [195].

Table 31 shows the product compositions after amine scrubbing of gas mixtures from common methane reforming processes. The gas composition refers to a process where the CO₂-absorption follows a WGS process, as is common in the industry.

Amine scrubbing allows for a significant reduction of the carbon dioxide content from 18–27 mol% down to 1–0.5 mol% in the different

Table 31

Gas composition after purification of common synthesis gases with amine scrubbing.

Purification process:	Amine scrubbing (CO ₂ -absorption)		
Upstream process:	SMR	ATR-O ₂	ATR-A
H ₂	90 mol% (75 mol%) ^a	95 mol% (72 mol%) ^a	63 mol% (50 mol%) ^a
H ₂ O	0.2 mol%	0.2 mol%	0.2 mol%
O ₂	0 mol%	0 mol%	0 mol%
N ₂	0.15 mol%	0.7 mol%	34.5 mol%
Ar	0 mol%	0 mol%	0 mol%
CO	2 mol%	1 mol%	0.5 mol%
CO ₂	0.5 mol% (20 mol%) ^a	1 mol% (27 mol%) ^a	0.5 mol% (18 mol%) ^a
CH ₄	4 mol%	1.5 mol%	0.15 mol%
H ₂ S	25 ppm	25 ppm	25 ppm
References	[1]	[1]	[1]

SMR: steam methane reforming, ATR-O₂: autothermal reforming with oxygen, ATR-A: autothermal reforming with air.

^a The value in brackets indicates the component proportion before purification.

methane reforming processes. Even after the purification of common raw gases with a combination of WGS reactor and amine scrubbing, the purities achieved are not yet at the level of the electrolysis processes (see Table 3).

4.6. Low-temperature separation

Du et al. [5] divide the low-temperature processes into (1) cryogenic distillation and (2) low-temperature adsorption. Cryogenic distillation takes advantage of the fact that hydrogen has a lower dew point than some common impurities. By lowering the temperature, distillative separation can be achieved [5,202]. The process is used in particular to separate hydrocarbons, carbon monoxide and nitrogen from a hydrogen mixture [5]. The disadvantage is that CO₂, H₂S and water impurities must be removed beforehand, as they solidify at cryogenic temperatures and can damage the apparatus [203,204].

Cryogenic distillation is a low-temperature separation process that can achieve hydrogen purity of about 94 mol% [1,2,5]. Cryogenic distillation is mainly used to remove hydrocarbons from the gas mixture [5,205]. In addition, the scope of application of this process

Table 32

Hydrogen content in the product gas after membrane purification of common synthesis gases.

Purification process:	Polymer membrane	Palladium membrane
H ₂	95 mol%	99.9999 mol%
References	[1,2,5]	

is limited because only pre-purified gas mixtures can be used. In particular, carbon dioxide and water must be separated before the purification step [5]. Overall, the cryogenic distillation product has a lower hydrogen purity of 94 mol% than the adsorptive purification processes.

4.7. Membrane purification

Membranes for H₂ purification are made of organic or inorganic materials. The class of organic membranes is called polymeric membranes. Inorganic membranes include metal and carbon molecular sieve membranes [5]. Contaminants are separated from the product stream at the membrane by driving forces resulting from either pressure, concentration or potential differences. The membrane is not permeable to all components in the stream, so that some components are retained and concentrate in the retentate, while permeating components accumulate in the permeate [206,207].

Metal membranes are classified as dense inorganic membranes [208]. Palladium-based metal membranes are commonly used [5,208]. The material is either pure palladium or a palladium alloy [209].

Carbon-based membranes are classified as porous inorganic membranes [208]. They include carbon molecular sieve membranes (CMSM) and graphene-based membranes [5].

Polymer membranes are usually classified as dense organic membranes [209,210]. Common polymers are polysulfones (PSF), polyimides (PI) and polyamides (PA) [5]. In addition to pure polymers, polymer blends and mixed matrix membranes are also used. In the latter case, zeolites, silica, carbon molecular sieves or other inorganic materials are added to the polymer [5].

Membrane processes are generally highly mature (TRL ≥ 9), with polymer membranes in use since the 1980s [211]. Metal membranes made of palladium, which are still under development, are an exception [1]. The hydrogen content obtained after purification of a gas mixture using polymer or palladium membranes is listed in Table 32.

Polymer membranes typically achieve a hydrogen purity of 92 to 98 mol%, while palladium membranes can achieve up to 99.9999 mol% hydrogen purity. Table 32 shows that no information about other impurity components could be determined. Overall, the hydrogen purity achievable with polymer membranes is in the range of the hydrogen purity of cryogenic distillation processes, while palladium membranes can achieve even higher hydrogen purities than adsorptive processes.

4.8. Deoxygenation

Deoxygenation is often used in electrolytic hydrogen production to catalytically remove oxygen impurities [5,29]. The process reduces the oxygen content by recombining the oxygen with the hydrogen according to the gross reaction equation [212]:



As the oxygen and hydrogen content decreases, the water content increases according to Eq. (27). Accordingly, water removal is usually required after catalytic oxygen removal [2,30]. Deoxygenation is mainly used in electrolytic processes where oxygen is the main impurity here [29]. The gas composition obtained after purification with deoxygenation is shown in Table 33.

Table 33

Gas composition after deoxygenation of the product gas of an alkaline electrolysis (AEL).

Purification process:	Deoxygenation
H ₂	99.999 mol%
H ₂ O	3 ppm
O ₂	<0.015 ppm
N ₂	6 ppm
Ar	<0.07 ppm
CO	<0.029 ppm
CO ₂	0.24 ppm
CH ₄	<0.01 ppm
S-total	<0.0012 ppm
Formaldehyde	<0.1 ppm
Formic acid	<0.01 ppm
Ammonia	<0.01 ppm
Total halogenated compounds	<0.032 ppm
References	[29]

<: The concentration is below the measuring limit.

Deoxygenation achieves hydrogen purities of 99.999 mol% when used after alkaline electrolysis. Table 33 shows that most of the impurities are below the measuring limits of the instruments. Exceptions are water, nitrogen and carbon dioxide. For these components, too, the content is only in the single-digit ppm range.

4.9. Adsorptive purification

In adsorption purification, gaseous or liquid contaminants are removed from the product stream by reversibly binding to the surface of another component, called the adsorbent [148]. To subsequently remove the adsorbed contaminants from the adsorbent, a change in temperature or pressure is applied. This changes the chemical equilibrium that separates the contaminants from the adsorbent and the process can start again [196,213]. According to Boll et al. [195], three types of adsorbents are particularly suitable for adsorptive gas purification on an industrial scale: (1) activated alumina oxide or silica gels; (2) molecular sieves; (3) activated carbon.

A further distinction is made between adsorptive purification processes is based on the regeneration method. Temperature swing adsorption (TSA) is used in the case of a temperature change, while pressure swing adsorption (PSA) is used in the case of a pressure change [148]. Both are industrially established processes (TRL ≥ 9).

Since PSA is usually used downstream of an SMR or ATR, Table 34 shows the product purity after purification of an industrial SMR gas by PSA. For TSA, common upstream processes are PEMEL and AEL.

All ISO 14687:2019(E) impurities are measured in the cited study and are based on measurements in real industrial plants [29]. A further differentiation according to different types and adsorbents is given in Table 13 in the supplementary material, but the studies cited there do not meet all quality criteria.

Adsorptive purification processes achieve very high levels of hydrogen purity. Most impurities are below the measurement limit of the instrumentation used (indicated by <). Except for water, nitrogen, argon and possibly helium, all impurities are below 1 ppm. Because some impurities are below the measurement limit, the hydrogen purities listed are lower limits (indicated by >).

The high level of achievable purity level and the industrial experience make adsorptive purification processes and especially PSA plants versatile options for purifying hydrogen. For this reason, we also include a review of PSA investment cost data. Techno-economic data of PSA plants are strongly dependent on the intended use of the plant (based on interview with a PSA plant manufacturer [214]). In particular, the components of the feed gas and the product purity to be achieved have an influence, with not only the desired molar hydrogen purity but also the desired limits for individual impurity components playing a decisive role. As an example, it is stated that a required

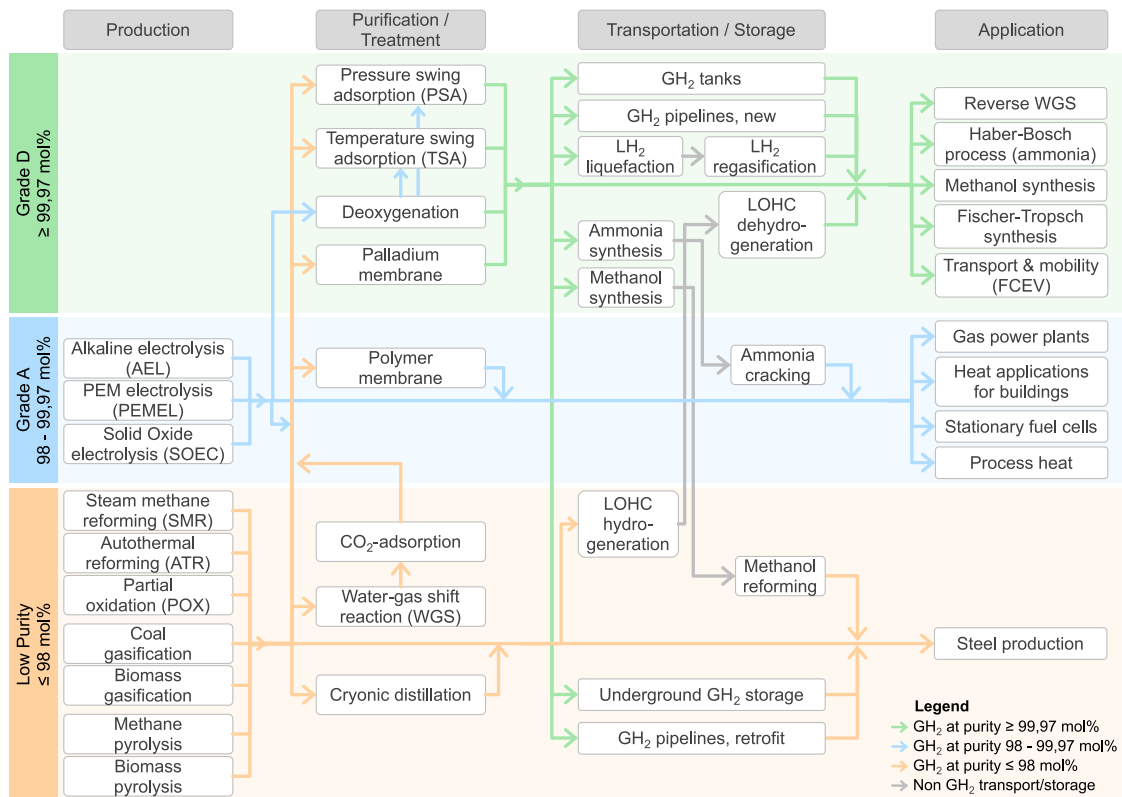


Fig. 15. Purity levels across the hydrogen supply chain.

Table 34

Gas composition after purification by common adsorptive purification methods. Hydrogen purity data for various PSA types are given in the supplementary material in Table 13.

Purification process:	PSA	TSA
Upstream process:	SMR	PEMEL, AEL
H ₂	>99.997 mol%	>99.996 mol%
H ₂ O	1.46 ppm	≈5.87 ppm
O ₂	<0.24 ppm	<0.24 ppm
N ₂	<0.09 ppm	6.89 ppm
Ar	1.74 ppm	<0.07 ppm
He	<28 ppm	<28 ppm
CO	<0.029 ppm	<0.029 ppm
CO ₂	<0.29 ppm	0.61 ppm
CH ₄	<0.01 ppm	<0.01 ppm
H ₂ S	cf. S-total	
C ₂ H ₆	<0.015 ppm	<0.015 ppm
NH ₃	<0.01 ppm	<0.01 ppm
S-total	<0.0012 ppm	<0.0012 ppm
Formaldehyde	<0.1 ppm	<0.1 ppm
Formic acid	<0.01 ppm	<0.01 ppm
References	[29]	[29]

PSA: pressure swing adsorption, TSA: temperature swing adsorption, SMR: steam methane reforming, PEMEL: PEM electrolysis, AEL: alkaline electrolysis.

<: The proportion of the component is below the measurement limit, >: The proportion of the component is at least at this level.

oxygen limit of 0 ppm compared to a limit of 10 ppm can result in a 50% higher adsorber height with corresponding additional costs. The literature review provided data on the techno-economic parameters of five different PSA systems. The data is shown in Table 35.

The data shows that the specific investment costs for the different PSA plants vary widely. The figure from Wickham et al. [216] is based on additional assumptions that may explain the high value of

720 EUR/kW. The investment costs quoted by DVGW e.V. [2] are considered to be too high, as they include the costs of desulfurization, oxygen removal and drying in addition to the PSA. The data presented in the Hy4Heat report [1] seem to be the most reliable, as they come from a survey of plant manufacturers. However, in this case, the input purity is unknown. The data presented in Hy4Heat –1 of 143 EUR/kW is considered to be the most accurate.

4.10. Comparison of the purification processes

A useful parameter to characterize the performance of hydrogen purification processes is the recovery rate r . It describes the ratio of the amount of hydrogen purified $n_{H_2,p}$ to the total amount of hydrogen feed $n_{H_2,f}$ [218]:

$$r = \frac{n_{H_2,p}}{n_{H_2,f}} \quad (28)$$

Table 36 contains a comparative analysis of the advantages and disadvantages of the purification methods according to Du et al. [5]. The adsorptive processes are characterized by their wide industrial application [1,214,217].

Although comparable degrees of purity can be achieved with palladium membranes, such membranes are not yet fully developed and are prohibitively expensive [2]. In contrast, polymer membranes are much more mature, even if they do not achieve high degrees of purity [5]. The main disadvantages of adsorptive processes are the relatively high hydrogen loss and the fact that they are carried out as batch processes, which makes them difficult to implement in stationary plants [217].

Deoxygenation and cryogenic processes are hampered by the fact that they are only suitable for certain impurities [5,30]. Deoxygenation

Table 35

Techno-economic data for PSA systems from the literature review.

Ref.	H ₂ purity input	H ₂ purity output	Recovery rate	Invest EUR/kW	Annotation
Hy4Heat-1 [1]	<i>impure</i>	<i>pure</i>	90%	143	Based on stakeholders, Large-scale
Hy4Heat-2 [1]	N/A	99.99 mol%	90%	152	Based on stakeholders, Medium-scale
Yao [215]	95.7 mol%	99.99 mol%	85%	284	Based on simulation, Small-scale
DVGW [2]	98.0 mol%	99.97 mol%	90%	238	Further purification steps
Wickham [216]	95.0 mol%	99.99 mol%	N/A	720	Based on assumptions

Hy4Heat-1 and -2 are the result of a stakeholder survey, while Yao refers to a study dealing with an integrated PSA system. The DVGW parameters refer to a combination of PSA, desulfurization and drying. Wickham is based on data for a natural gas–hydrogen mixture. Yao, DVGW and Hy4Heat-2 refer to small to medium scale plants (3.5 MW, 30 MW and 37 MW input power respectively), Hy4Heat-1 and Wickham refer to large scale plants (939 MW input power for Hy4Heat-1). For comparison, 1 GBP is assumed to be 1.1 EUR.

Table 36

Comparison of the advantages and disadvantages of selected hydrogen purification processes (based on [1,2,5,13,217]).

Process	Advantages	Disadvantages
PSA and TSA	<ul style="list-style-type: none"> Industrial experience High purity 	<ul style="list-style-type: none"> Low recovery Batch process
Cryogenic distillation	<ul style="list-style-type: none"> High recovery 	<ul style="list-style-type: none"> Only suitable for certain impurities Low purity
Deoxygenation	<ul style="list-style-type: none"> High recovery High purity 	<ul style="list-style-type: none"> Only suitable for oxygen impurities Water contamination
Palladium membrane	<ul style="list-style-type: none"> High recovery High purity 	<ul style="list-style-type: none"> Expensive Low maturity
Polymer membrane	<ul style="list-style-type: none"> Mature Medium recovery Cheap 	<ul style="list-style-type: none"> Low purity

only reduces oxygen impurities while enriching water impurities. Cryogenic processes can be hampered by certain impurities, making pre-cleaning necessary [203]. However, both cryogenic and deoxygenation processes are well established [5].

5. Summary and conclusion

The goal of matching hydrogen purity levels between production and application, while maintaining desired purity levels throughout the supply chain, is a complex challenge as shown in Fig. 15. Green hydrogen production methods, particularly water electrolysis, demonstrate high purity levels, compared to conventional fossil-based processes. At the other end of the supply chain, end-users in the chemical industry and fuel cell vehicles require high purity hydrogen. In the intermediate steps, transport and storage may introduce new impurities.

The impurities occurring throughout the hydrogen supply chain can be attributed to the following aspects:

- Externally introduced contamination. This contamination occurs, for example, when using retrofitted infrastructure such as pipelines and underground storage systems.
- Not or not fully converted reactants. This is the case when hydrogen is produced from methane pyrolysis. Only a fraction of the methane can be converted into hydrogen. This type of impurity can be reduced by repeating the process and concentrating the desired product.
- By-products passing through. An example of this is reforming processes where air is used instead of pure oxygen. The nitrogen from the air does not react but reduces the purity of the hydrogen in the product stream.
- Unwanted reaction products. The reforming process produces unwanted intermediates, such as CO and CO₂, which must be separated from the hydrogen.

Especially the end-users in the chemical industry and fuel cell vehicles impose high purity requirements in the hydrogen supply chain.

If hydrogen was only used for thermal applications, lower purity grades would be acceptable. High purity requirements lead to additional costs for purification. Furthermore, new key questions emerges regarding the optimal design of the hydrogen supply chain. Multiple potential pathways present themselves of how to configure hydrogen infrastructure to cater a high purity hydrogen demand:

- The development of specialized, high-purity transport and storage infrastructure to maintain the high quality of green hydrogen throughout the supply chain. This could mean purification at the point of production and building a network of new high-purity hydrogen pipelines.
- The utilization of more economical retrofitted infrastructure, coupled with an additional purification step at the point of end-use.
- The import, storage, and transport of high purity liquid or bound hydrogen and the reconversion into elemental hydrogen at the location of the final consumer.

To determine the most efficient and cost-effective approach to managing hydrogen purity throughout the supply chain, comprehensive optimization models can provide valuable insights. This model should take into account production methods, infrastructure costs, purification technologies, and end-use requirements.

CRediT authorship contribution statement

Toni Busch: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Jonas Derichs:** Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Data curation. **Theresa Klütz:** Writing – review & editing, Supervision, Conceptualization. **Jochen Linßen:** Writing – review & editing, Conceptualization. **Detlef Stolten:** Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.ijhydene.2025.04.532>.

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