H_2-Rein

H_2 short study: Hydrogen quality in an all-German hydrogen network

Study

Legal notice

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Client

Implementation

Project management

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Abbreviations

WGV	Working gas volume
API	American Petroleum Institute
BMWK:	Bundesministerium für Wirtschaft und Klimaschutz [Federal Ministry of Economics and Technology]
dena	German Energy Agency
DGMK:	Deutsche Wissenschaftliche Gesellschaft für nachhaltige Energieträger, Mobilität und Kohlenstoffkreisläufe e.V. [German Society for Sustainable Energy Carriers, Mobility and Carbon Cycles]
R&D	research and development
GEB	Gaserstbefüllung [first gas filling]
GGV	Gesamtgasvolumen [total gas volume]
Group A	Hydrogen quality ≥ 98 mol %
Group D	Hydrogen quality ≥ 99.97 mol %
i.N.	in standard condition (0°C, 1.01325 bar)
KGV	Kissengasvolumen [cushion gas volume]
Max.	maximum, maximal
Min.	minimum, minimal
NMHC	Non-methane hydrocarbons
NWR	National Hydrogen Council [German National Hydrogen Council]
OTA	Obertageanlage [surface plant]
Pd	palladium
PSA	pressure swing adsorption
PtG	power to gas
PtL	power to liquid
PtX	Power to X, definition at dena (synthetic fuels) different from other cases
s.	see
SMR	steam methane reforming
TEG	triethylene glycol
TN	Treibhausgasneutralität [greenhouse gas neutrality]
UGS	underground gas storage facility
USAV	Untertagesicherheitsabsperrventil [underground safety shut-off valve]
Vol.	volume
WGS	water gas shift reaction

Formula symbol	Explanation	Unit
p	Pressure	[bar]
T	Temperature	[°C, K]

1 Introduction

1.1 Background and aim of the study

Against the background of the energy transformation, hydrogen (H_2) is a key source energy. Its areas of application range from industry and mobility to catalytic processes (e.g. (petro-)chemistry, PtX processes (power-to-X)) to energetic areas of application (e.g. heat market, reverse power generation). Depending on the respective application, different qualities are required at the place of use; these are regulated in ISO 14687: 2019 [1] and DIN EN 17124:2019 [2]. Based on this, hydrogen was included as a fifth new gas family in two qualities (Group A: ≥ 98 mol % and Group D: ≥ 99.97 mol %) in the worksheet of the DVGW G 260 (2021) [3].

In order to meet the demand for hydrogen throughout Germany, various production processes are being discussed. For this purpose, both temporal and spatial variants of hydrogen production are being considered.

The gas industry is both willing and able to make the existing natural gas infrastructure available for the transport and storage of hydrogen. Fluctuations in renewable energy and green hydrogen production can be compensated for by using underground gas storage facilities (UGS), and site-specific peaks and valleys can be evened out by transporting them via a hydrogen network. Seasonal changes in demand require the large-scale storage of energy. For hydrogen, this is possible through underground gas storage.

The requirements for hydrogen quality present the gas industry with completely new challenges. On one hand, highly pure hydrogen is necessary for sensitive applications such as mobility or the PEM fuel cells used for it; on the other hand, burners such as those in lime or cement works can be readily supplied with an H_2/natural gas mixture. This balancing act with regard to the necessary gas quality requires an assessment of the individual components of the entire value chain with regard to their influence on the hydrogen quality as well as any necessary processing steps.

The use of the existing gas infrastructure is seen as a cost-efficient and favourable option for making the hydrogen demand for the whole of Germany available on a decentralised basis. In order to ensure that the quality required by each customer is available, an overview of the hydrogen qualities required by the relevant customer groups is necessary. The state of the art for measures to increase H_2 quality are to be described. In this context, the assessment of the economic aspects is just as important as the efficient use of renewable energy resources.

Within the framework of the short study, an initial general overview of the system of generation, the transport, the storage, and the application of hydrogen is to be given with regard to the requirements of the different hydrogen qualities in order to be able to derive a scope of investigation for the detailed main study to follow.

1.2 Boundary conditions

In preparation for the short study, boundary conditions for the considerations were agreed upon with the client. The background to this is the considerable breadth of the range of H_2 gas quality to be considered – from H_2 generation and transport to storage and application. The following was determined:

- The consideration of the H_2 demand is based on an established scenario (dena pilot study Towards Climate Neutrality [4])
- The converted state of the infrastructure is considered. This applies in particular to pipelines and storage facilities. The conversion phase is not the subject of this study.
- A regionalised presentation of the H_2 demand is not provided.
- With regard to underground storage, the focus is on cavern storage facilities.
- Transport and distribution networks are considered; these are referred to as “hydrogen networks” according to the EnWG.

The focus of the study is the statements on gas processing of hydrogen of quality ≥ 98 mol %. Mixtures of natural gas and hydrogen are not considered.

2 WP 1: Estimation of the H_2 requirement

The first step towards an overall view of a future hydrogen system consisting of production, transport, storage, and application is estimating the quantities of hydrogen that will be needed. These will give an initial impression of the rough dimensioning of the overall system. In particular, the design of networks and storage facilities is driven not only by the total quantity but also by the distribution of demand among different sectors and industrial processes as well as the location and number of entry and exit points.

This chapter, for which Frontier Economics is responsible, therefore provides a literature-based estimate of hydrogen use in a climate-neutral Germany in 2045 (Section 2.1). In addition, the distribution of use among (sub-)sectors is considered (Section 2.2), and an outlook on a possible regional distribution of hydrogen demand and the market ramp-up to the target scenario 2045 is made (Section 2.3). The following text box summarises the main findings of the chapter.

Results at a glance

- The evaluation of various studies reveals a wide range of expected hydrogen demand in Germany. With an expected hydrogen demand of 515 TWh in 2045, the dena pilot study II is in the median of the more recent estimates considered (as of January 2022). For comparison: The current natural gas consumption is about 1000 TWh per year.
- Hydrogen consumption will be distributed among the industrial, energy, building, transport, and PtX sectors. However, it can be assumed that there will be a considerable shift in the use of natural gas compared to its current use – almost 95% of which is used for energy (for electricity and heat generation) and only 5% for materials (chemical processes, refineries).
- In accordance with the dena pilot study II [4], less than **60% of hydrogen will be used for energy in 2045** (in the energy and building sector), a **considerable part will** be used in **catalytic processes** (in the chemical industry and for the production of hydrogen derivatives, PtX) or directly in **mobility** (in fuel cells).[1] This implies that the **requirements for hydrogen quality** will be **higher** than if a usage structure analogous to current natural gas consumption were assumed (see Chapter 3).
- The exact customer structure is not yet clearly predictable. While a **considerable role of hydrogen in industry and power generation** is **largely undisputed**, there are **still greater uncertainties** regarding the extent of **hydrogen use in the transport and building sectors**. However, because of the change in use compared with natural gas and the presumably more decentralised feeding-in of hydrogen (compared with natural gas), it is foreseeable that the structure of an efficient hydrogen network will differ from that of the current natural gas network.

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[1] In the steel industry, hydrogen will be used proportionately for energy and materials (as part of direct reduction). However, unlike in the chemical sector, the material use in iron and steel production does not result in high requirements for the purity of the hydrogen.

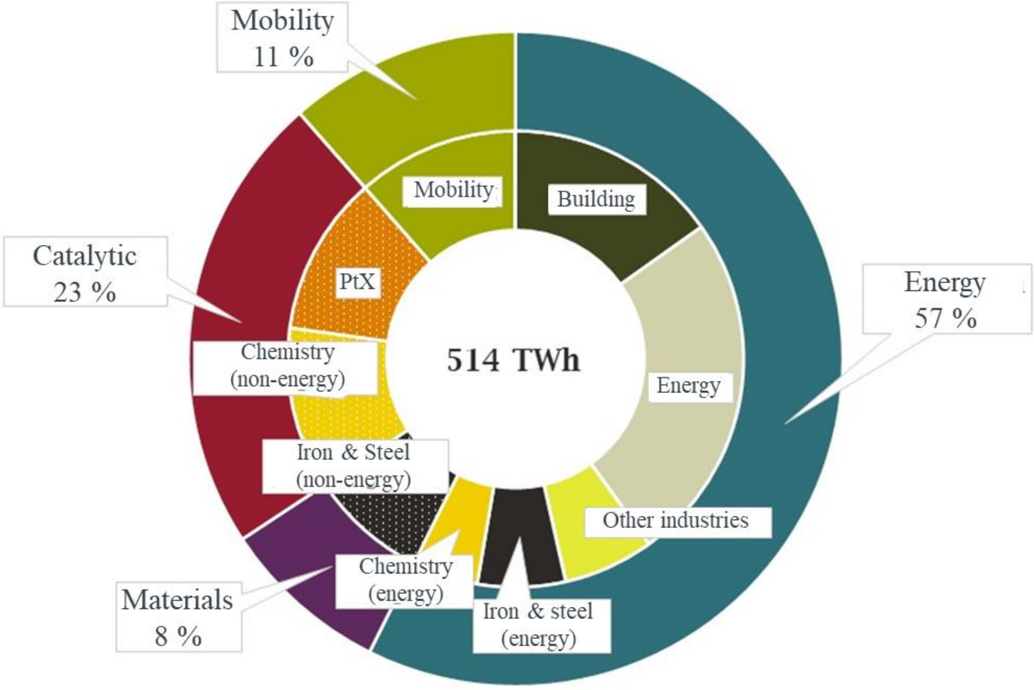


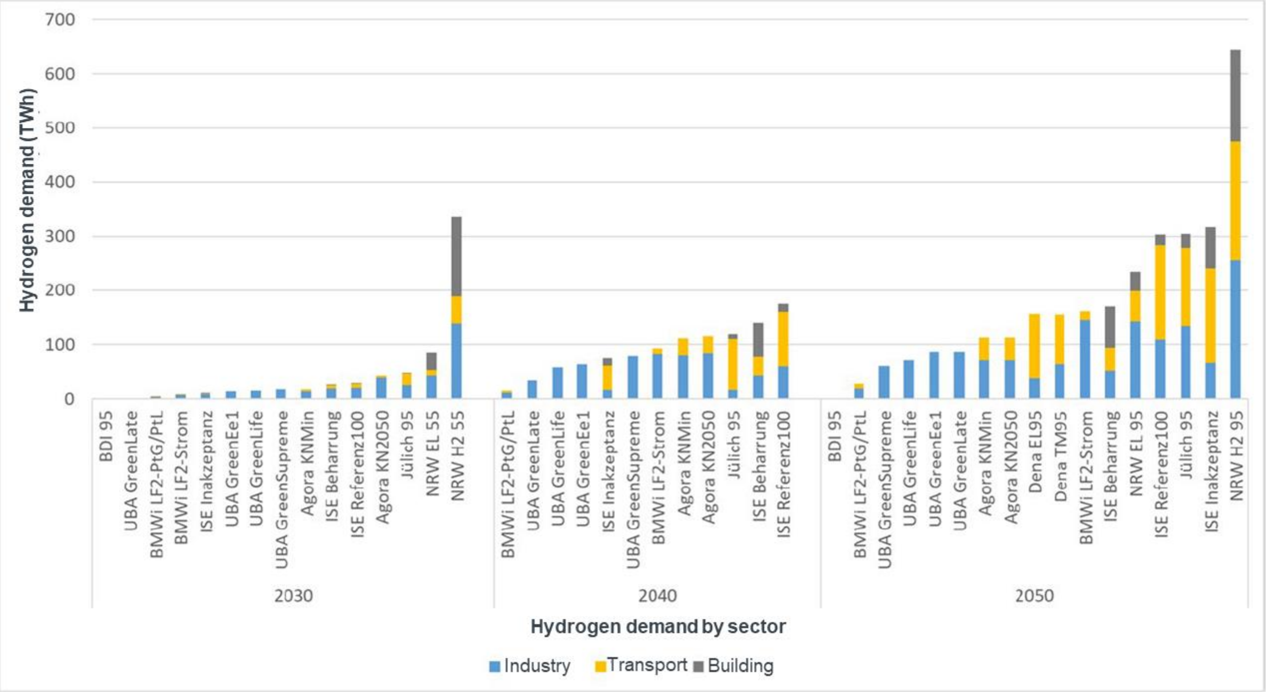
Figure 1: Distribution of H_2 quantities among (sub-)sectors in 2045 in accordance with the *dena pilot study Towards Climate Neutrality*

In Chapter 3, the requirements of the various consumption sectors with regard to hydrogen quality will then be analysed so that a target scenario of the consumption quantities per hydrogen quality can be estimated for 2045.

2.1 Evaluation of the meta-analysis

At the current time, there are still considerable uncertainties about the hydrogen demand in a climate-neutral German economy. Various studies have forecast the future demand and cover a wide field. For this study, only those estimates that achieve climate neutrality in 2045 and cover all relevant sectors (industry, transport, buildings, and energy) are evaluated. *Disclaimer: All the studies analysed here as well as the hydrogen demand estimates derived from them do not take into account possible implications of recent developments in Russia and Ukraine.*

In order to make as reliable and well-founded a forecast as possible with regard to future quantities, various existing meta-studies, in particular the “Meta-study Hydrogen – Evaluation of Energy System Studies” commissioned by the National Hydrogen Council (NWR), were used for this purpose. Many studies were evaluated and processed for this purpose (Figure 2). It therefore seems particularly suitable as a starting point for a forecast of hydrogen demand.



Source: (Wietschel, et al., 2021)

Figure 2: H_2 demand in the demand sectors in Germany in 2030, 2040, and 2050

A closer look at the evaluation of the NWR reveals two crucial limitations. Although the study was published in June 2021, the policy objective has changed decisively since then. Instead of 2050, climate neutrality is to be achieved as early as 2045.[2] This aspect can be neglected if the target state of the studies under consideration describes a “steady state” (i.e. the end point of the transformation); for this, it is irrelevant whether it is reached in 2045 or 2050. This affects only the start-up of the hydrogen system, which is not the subject of this study.

In addition, updates have been made to some of the core studies in the median evaluation of the NWR since publication (also because of changes in the political framework). This applies to the dena pilot study, the evaluation by Agora Energiewende, and the Fraunhofer ISE.

In order to take these factors into account, the evaluation of the NWR was supplemented with the results of the updates of the above studies. As Figure 3 shows, the future hydrogen demand has once again been revised upwards in all recently published studies. This is also the case in the “*dena pilot study towards Climate Neutrality*”; here, instead of approx. 170 TWh/a, almost 500 TWh/a of hydrogen (without hydrogen for PtX products) are now expected. This increase is due both to an increase in the expected quantities of hydrogen of the individual sectors (such as industry) and the addition of previously unconsidered sectors (especially the energy sector). The *dena pilot study* thus lies in the median of the volume forecasts of the supplemented current studies and is thus a suitable starting point for the further analyses of this study.

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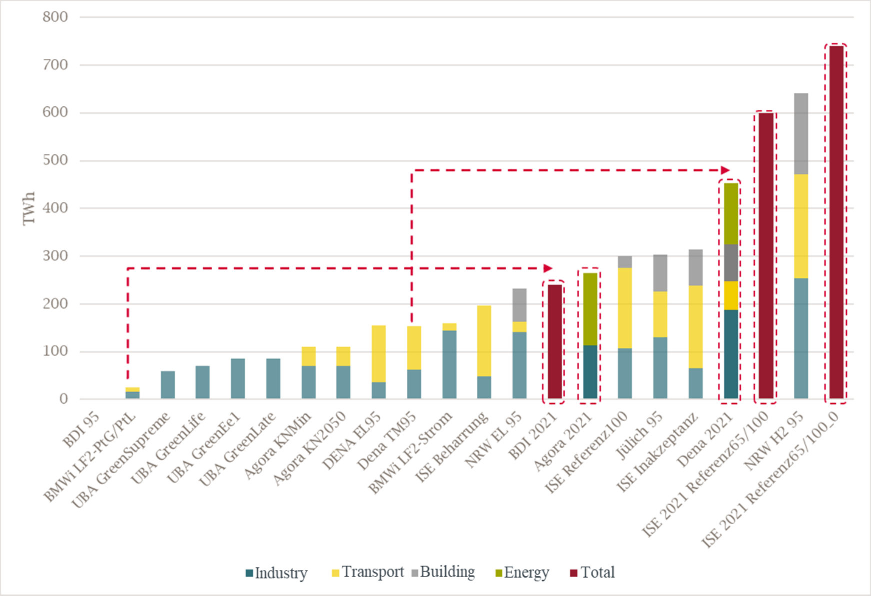
[2] Federal Government, 2022

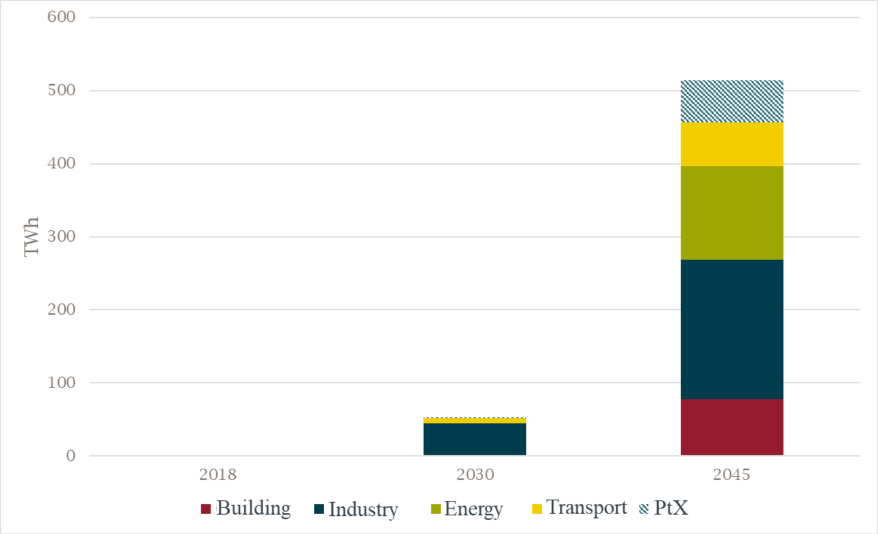


Source: Frontier Economics based on (Wietschel, et al., 2021), (BCG, 2021), (Brandes, et al., 2021), (dena, 2021), (Prognos, Öko- Institut, Wuppertal-Institut, 2021). The five scenarios of the three studies, which were published after the NWR meta-study was prepared in December 2020, are outlined in red.

Figure 3: NWR meta-study supplemented by new publications

In addition, the *dena pilot study Towards Climate Neutrality* also fulfils the previously mentioned criteria that climate neutrality will be achieved in 2045 and that all relevant sectors (transport, buildings, industry, energy) will be taken into account. Therefore, the quantities determined in the pilot study are used as a starting point for the further analyses of this study.

Figure 4 shows the forecast quantities of hydrogen per sector according to dena in detail.



Source: Frontier Economics based on the data appendix (results) of the dena pilot study expert report (Institute of Energy Economics at the University of Cologne (EWI), 2021).

Figure 4: Total hydrogen demand in accordance with the dena pilot study Towards Climate Neutrality

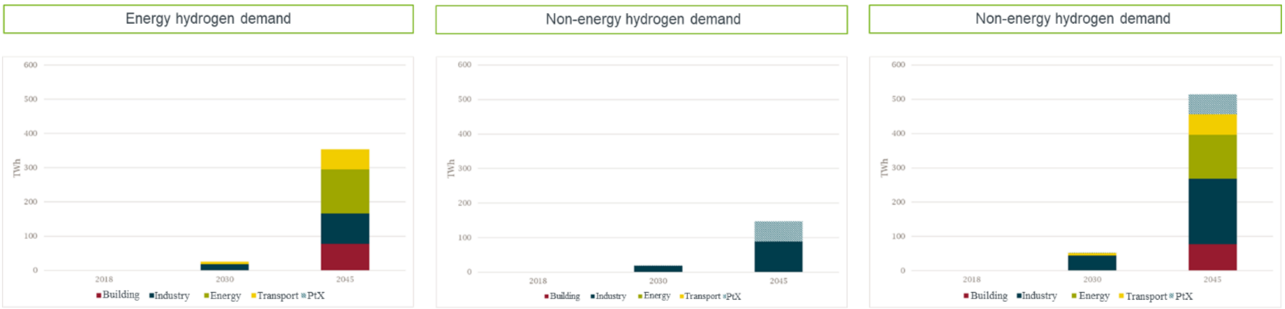
2.2 Sector comparison

The requirements for the purity of hydrogen vary greatly depending on the sector and the intended use. Therefore, not only the total amount of hydrogen expected to be needed in 2045 but also how this is distributed among various sectors and what the hydrogen is used for in the respective sectors is relevant.

The dena pilot study not only provides the breakdown into the four sectors of industry, transport, buildings, and energy that can already be seen in Figure 4 but also differentiates between energetic and non-energetic use. Furthermore, forecasts are provided for the demand for Power-To-Liquid (PtL) products, which are also based on hydrogen.[3]

In the area of PtL products, the dena pilot study sees production mainly abroad so that only the end product (i.e. as synthetic naphtha) is imported. This can make use of location advantages abroad (e.g. more hours of sunshine) as well as the easier transport of the derived products compared with hydrogen itself.

Because various projects for the domestic production of PtX products are already being planned, this study deviates from dena in assuming that 20% of PtX production will take place in Germany and that the required hydrogen must be available locally and flow through networks in Germany. The aim here is not to make an exact forecast of the expected hydrogen demand but rather to also take into account the interdependencies and quality requirements for the overall system that result from domestic production of hydrogen derivatives.



Source: Frontier Economics based on the data appendix (results) of the dena pilot study expert report (Institute of Energy Economics at the University of Cologne (EWI), 2021)

Figure 5: Allocation of hydrogen demand to energy and material demand in accordance with the *dena pilot study Towards Climate Neutrality*

The demand and use of hydrogen and, as a result, the quality requirements differ considerably depending on the sector:

- In the transport sector, hydrogen is expected to be used in particular for heavy-duty transport as well as for bridging long distances in road transport in fuel cells. In addition, synthetic fuels, especially hydrogen-based synthetic paraffin, will be used in particular in air transport[4]. However, other synthetic fuels will also be used in road, rail, and inland waterway transport.[5]

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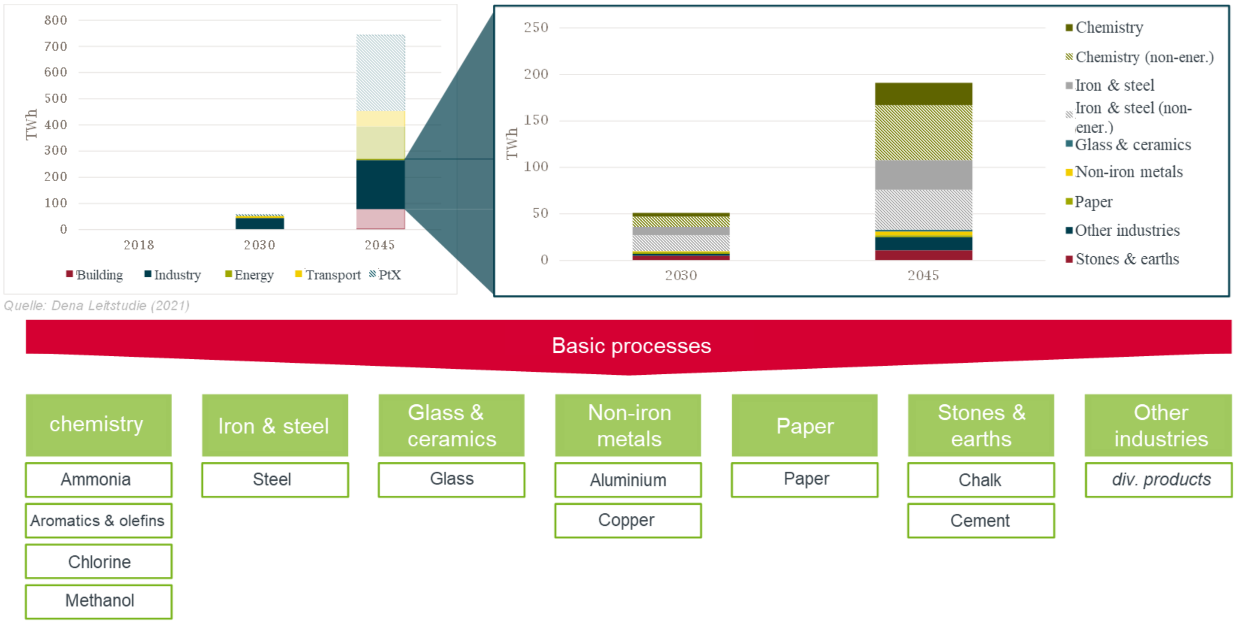
[4] (dena, 2021) pg. 260

[5] (dena, 2021)pg. 273

- In the building sector, hydrogen will be used to generate heat. Thus, by 2045, 65% of the demand for gaseous energy carriers is to be covered by hydrogen; this corresponds to a consumption of 79 TWh.[6] In addition, synthetic hydrogen-based heating oil is used sporadically for oil heating.[7]
- Hydrogen will also be of central importance for the energy sector in order to replace fossil fuels. Especially with regard to controllable power, coal and (fossil) gas-fired power plants are to be almost completely replaced by hydrogen-based CCGT power plants by 2045.[8]

For the industrial sector, hydrogen will play a major role both energetically and non-energetically. Various processes (Figure 6) will be converted to the use of hydrogen by 2045. Within the industrial sector, the chemical and steel sectors in particular are key drivers of hydrogen demand – in terms of both energy and materials. Overall, the industrial sector will need 191 TWh of hydrogen in 2045 according to the forecast of the dena pilot study. In addition, there is “green” naphtha, which is produced synthetically based on hydrogen.[9]



Source: Frontier Economics based on the data appendix (results) of the dena pilot study expert report (Institute of Energy Economics at the University of Cologne (EWI), 2021)

Figure 6: Hydrogen demand from the industrial sector in accordance with the *dena pilot study Towards Climate Neutrality*

Because the energy quantities for hydrogen derivatives are shown only with regard to the end products, the efficiency of the fuel synthesis must also be taken into account in order to determine the respective quantities of hydrogen required. An average efficiency of 68% is assumed for a Fischer–Tropsch synthesis.[10]

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[6] (dena, 2021) pg. 270

[7] (dena, 2021) pg. 273

[8] (dena, 2021(pg. 271

[9] (Energiewirtschaftliches Institut an der Universität zu Köln (EWI), 2021) pg. 265.

[10] (FVV, 2021), pg. 50.

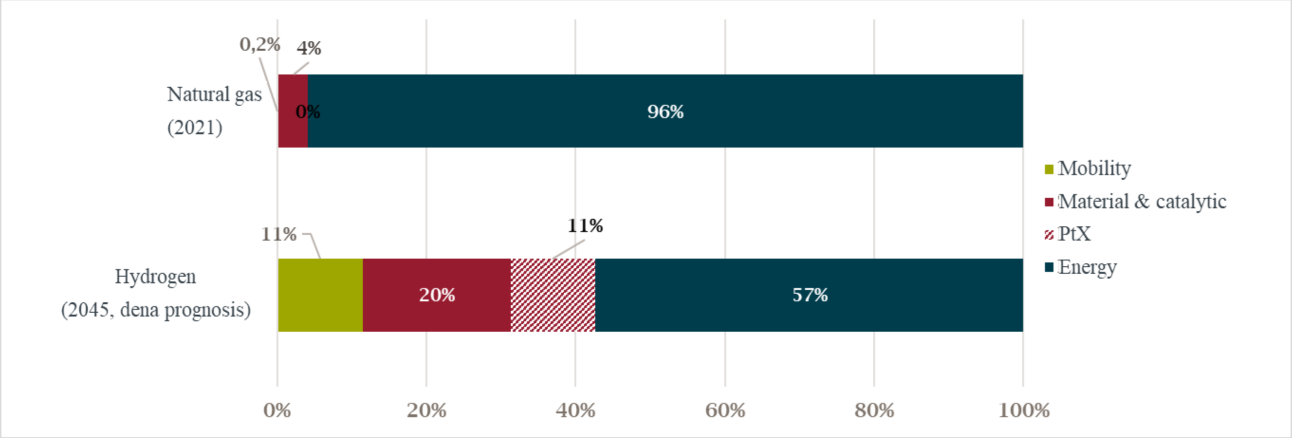
Overall, this results in the following distribution of total demand among the various (sub)sectors:

Table 1: Hydrogen demand by sector

Sector		Unit	H_2 demand	Use
Building		*TWh*	78	*Energetic*
Energy		*TWh*	128	*Energetic*
Traffic		*TWh*	59	*Mobility*
PtX		*TWh*	58	*Catalytic*
Industry, of which		*TWh*	191	
	Stones and soils	*TWh*	11	*Energetic*
	Other industry	*TWh*	14	*Energetic*
	Paper	*TWh*	2	*Energetic*
	Non-ferrous metals	*TWh*	4	*Energetic*
	Glass and ceramic	*TWh*	2	*Energetic*
	Iron and steel (non-energetic)	*TWh*	43	*Material*
	Iron and Steel (energetic)	*TWh*	32	*Energetic*
	Chemistry (non-energetic)	*TWh*	59	*Catalytic*
	Chemistry (energetic)	*TWh*	24	*Energetic*

Source: Frontier Economics based on the data appendix (results) of the dena pilot study expert report (Institute of Energy Economics at the University of Cologne (EWI), 2021).

The distribution of the future use of hydrogen among the areas of mobility, energetic, material, and catalytic processes and the resulting quality requirements thus differ considerably from the current use of natural gas. Most natural gas is currently used for energy purposes; only 4% of the total volume is used as a material in industry, and only 0.2% is used for mobility applications (Fig. 6). In contrast, a considerable proportion of the expected quantity of hydrogen will be used for catalytic processes. In particular, just under 8% of the total amount will be spent on power-to-X processes based on the assumption that 20% of the required PtX products will be produced in Germany and 80% imported from abroad. If the establishment of the required supply chains is not achieved or is delayed, the proportion of total demand is expected to increase. Use in the transport sector will also play a much more important role. This shift in use also affects the requirements for the overall hydrogen system.



Source: Frontier Economics based on Statista (2022), Zukunft Gas (2022), and the data appendix (results) of the dena pilot study expert report

Figure 7: Current use of natural gas compared with the expected future use of hydrogen

2.3 Outlook

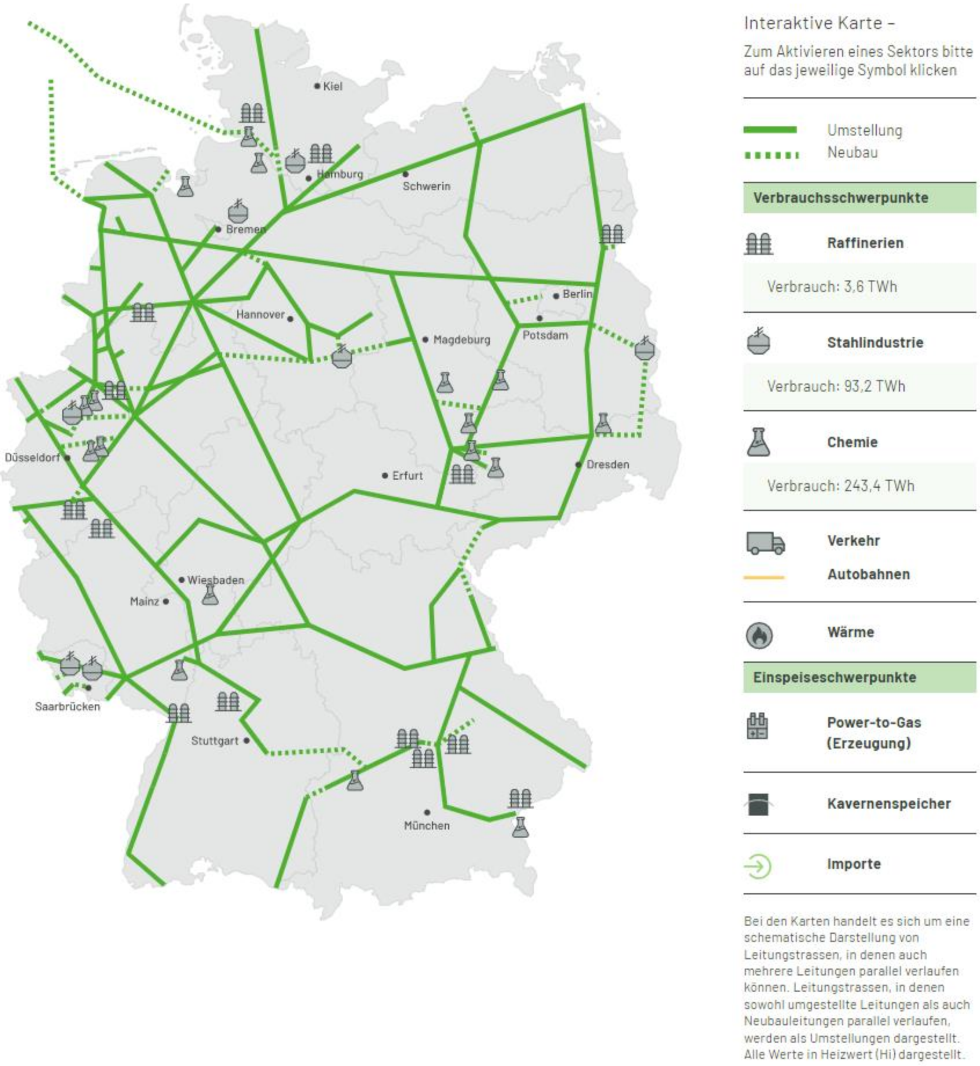
This short study is limited to a consideration of Germany-wide hydrogen use in the target scenario 2045 (climate neutrality) in order to obtain an initial estimate of the target scenario of the hydrogen economy. For the planning of the hydrogen system, further analyses of hydrogen use (and production) are needed – in terms of both regional distribution and the time axis.

2.3.1 Regionalisation

For the design of the overall hydrogen system of the future, the regional distribution of consumption (as well as generation and storage) plays a considerable role in addition to the consumption volumes. In the transport and building sector, demand is expected to be distributed over the entire federal territory in terms of area – essentially in proportion to population density. In the industrial sector in particular, however, demand will probably be distributed differently from region to region because of industrial centres. The connection to a hydrogen supply would thus have to be explicitly taken into account.

An estimation of the regional distribution of hydrogen consumption is not part of this short study. However, Figure 7 shows an example of the 2050 hydrogen network drawn up by the association of long-distance gas network operators FNB Gas as well as the current locations of likely future large hydrogen consumers in the chemical and steel industries and in refineries. It becomes clear that there are some regional clusters (e.g. in the Rhine-Ruhr area or in the east of Germany), where the demand for hydrogen is expected to be particularly high.

In order to specify the conception of hydrogen networks, further analyses of the regional distribution of hydrogen consumption and production will be required in the follow-up to this short study. It is already foreseeable that the supply task of the hydrogen network will differ from the supply task known today from the natural gas network. As a result, a sensible hydrogen network will not resemble the current natural gas network 1:1. This is due in particular to the fact that hydrogen production is likely to be much more decentralised than natural gas production. As with natural gas, it can be assumed that hydrogen will also be imported to a considerable extent because of limited domestic renewable energy potential. However, domestic hydrogen production is expected to be characterised by a larger number of smaller production units than current or historical domestic natural gas production. This must also be taken into account when designing hydrogen quality. On the consumption side, there may also be shifts in the regional structure compared to natural gas consumption (e.g. through comparatively higher use of hydrogen in large-scale industrial applications yet the possibly lower use of hydrogen in decentralised heat supply).



Source: FNB Gas (https://fnb-gas.de/wasserstoffnetz/h2-netz-2050/)

Figure 8: H_2“Network” 2050 of FNB Gas, including regional distribution of large industrial consumers

2.3.2 Market ramp-up

In this short study, the focus is on hydrogen use in 2045. This is because Germany has set itself the goal of becoming climate neutral by 2045. In this respect, the hydrogen use expected for 2045 corresponds to the “target scenario” from today’s perspective. The future hydrogen infrastructure should be oriented towards this.

In order to prepare decisions on the prioritisation and chronology of the development of a hydrogen network, a more detailed understanding of the hydrogen demand (and generation) in the transformation phase up to 2045 is needed beyond the 2045 target scenario. Regarding the quality design of hydrogen networks, the focus of this short study, an understanding of the expected market ramp-up, is particularly relevant if different ramp-up rates are expected between sectors with different hydrogen quality requirements. Many studies on the development of hydrogen use – including the dena pilot study II (Figure 5) – assume, for example, that hydrogen will be used primarily in large industrial applications such as for direct reduction in steel production in the coming decade. Meanwhile, the share of direct hydrogen use in transport (e.g. example in 2030) is still considered quite low; more precise estimates of the market ramp-up of this application area with high demands on hydrogen quality are lacking yet necessary.

3 WP 2: Generation and tolerance of the applications

The starting point for the evaluation of hydrogen qualities is a consideration of the production sources as well as the recording of the technical requirements of the various hydrogen users. In summary, the following statements can be made:

Results at a glance

- Depending on the manufacturing process, there are different impurity profiles of the hydrogen. Each of the processes generates one or more added components.
- All processes require gas treatment to achieve a feed-in quality into a hydrogen network. The expense of this gas treatment depends on the accompanying components and differs considerably in terms of technical and financial outlay.
- There are normative requirements regarding hydrogen purity. These are based on the process-related requirements for the use of hydrogen. As knowledge evolves regarding the tolerance of individual applications, there will be further development of this set of rules.
- Several application areas can be defined; these lead to different quality areas. These are the **energetic** quality range (H_2 quality of Group A), the **catalytic** range, and the requirement range for **fuel cells** (Group D).
- The catalytic application range is below the fuel cells in terms of requirements; for individual components such as nitrogen, higher limit values than in Group D are technically permissible. Accordingly, the quality range lies between those of Group A and Group D of the DVGW Code of Practice G 260 and is not yet part of a defined set of rules. The quality range of catalytic processes includes applications in the chemical industry, refineries, and PtX processes.
- Theoretically, considerably lower hydrogen contents can also be provided for combustion processes – but then with a low fluctuation. In general, the fluctuation of H_2 quality or concentration is also limited in energy use.

3.1 Overview of H_2 production qualities.

In nature, hydrogen exists almost exclusively in bound form (e.g. in the form of water, hydrocarbons such as methane, and various other chemical compounds). The technical application of hydrogen accordingly always requires the production of the hydrogen. Depending on the starting material and the selected process, added gases that may require appropriate processing can arise.

Within the scope of the short study, the three most important processes for the production of green (electrolysis), blue (reforming with CCS), and turquoise (methane pyrolysis) hydrogen were considered with regard to purity and required processing.

3.1.1 Hydrogen from electrolysis (green hydrogen)

In electrolysis, water is split electrochemically into hydrogen and oxygen. The two gases are produced in separate fluid spaces separated by membranes.

$$H_2O \rightleftarrows H_2 + 0{,}5O_2 \qquad \Delta_r H^0 = 286\ kJ/mol \qquad \text{Gleichung 1}$$

There are several approaches for technical implementation. These include alkaline electrolysis (AEL), polymer electrolyte membrane electrolysis (PEMEL), solid oxide electrolysis (SOEL), and anion exchange membrane electrolysis (AEMEL). Of these, AEL and PEMEL have reached the highest technical maturity. Both differ with regard to the function of the membrane and the structure; these differences can also influence the hydrogen purity that can be achieved.

In alkaline electrolysis, the electrodes and fluid spaces are separated by a membrane that is permeable to hydroxide ions (OH^-). Both sides are filled with electrolyte solution (potassium hydroxide solution). The hydrogen produced can thus contain electrolyte vapours and gases that are introduced in dissolved form with the electrolyte. In addition, minor gas transfers between the fluid chambers via the membrane (cross-over) cannot be ruled out, especially in part-load operation. Small amounts of oxygen can thus also be present in the hydrogen.

In PEM electrolysers, on the other hand, the electrodes and fluid spaces are separated by a proton-conducting membrane, and the water required for the reaction is supplied without the addition of electrolytes. The hydrogen produced in PEM electrolysis also contains water vapour and, in the case of gas transfer across the membrane (cross-over, especially in partial load), small amounts of oxygen. The latter may be partially converted on the precious metal catalysts used on the cathode side so that low oxygen contents are to be expected.

With both technologies, however, the achievable purity depends on the system design and the mode of operation. Differences in purity are therefore to be expected between modules from different manufacturers. Exemplary manufacturer specifications are shown in Table 2. Both electrolysis concepts already enable > 99% purity after drying the hydrogen. As a rule, the oxygen content is also separated with the aid of a deoxo unit so that purities ≥ 99.99% are achieved.

Corresponding processing modules are available from the manufacturers and enable the provision of hydrogen – even in high purity (> 99.97 mol %). An additional possible source of contamination is the flushing/inertisation of the electrolyser; this can lead to the brief introduction of nitrogen after maintenance work, for example.

Table 2: Hydrogen purities achieved for different electrolysis systems

Type	Manufacturer	Purity before preparation	Purity after preparation
PEMEL	Siemens Energy [5]	Not specified	99.999 vol. %
	ITM POWER [6]	Not specified	99.999 vol. %
	H-TEC SYSTEMS [7]	99.9 vol. %	99.999 vol. %
	iGas energy GmbH [8]	Not specified	99.999 vol. %
	Nel ASA [9]	99.95 vol. %	99.9995 vol. %
	Elogen [10]	Not specified	99.999 vol. %
	AVX/Kunatec [10]	Not specified	99.999 vol. %
AEL	Green Hydrogen Systems [11]	Not specified	99.998 vol. %
	Sunfire [12]	99.6 vol. %	99.999 vol. %
	thyssenkrupp [13]	99.95 vol. %	99.999 vol. %
	Enapter [10]	99.9 vol. %	99.999 vol. %

3.1.2 Hydrogen from reforming with CCS (blue hydrogen)

Both steam reforming and autothermal reforming are suitable for producing hydrogen by reforming natural gas.

Steam reformation is a technically established, marketable process for the production of hydrogen in which hydrocarbons or fluids containing hydrocarbons (e.g. natural gas) are converted to hydrogen and CO_2 in a multi-stage process.

The hydrocarbons are first desulphurised and mixed with steam and fed into the reformer. There, the catalytic conversion of hydrocarbons (e.g. methane) with water vapour to hydrogen, carbon monoxide, and CO_2 takes place at high temperatures (Equation 2 and Equation 3). Because both reactions are endothermic, heating of the reformer is required. This is usually done by a natural gas-fired burner.

$$CH_4 + H_2O \rightleftarrows CO + 3H_2 \qquad \Delta_r H^0 = 206\ kJ/mol \qquad \text{Gleichung 2}$$

$$CH_4 + 2H_2O \rightleftarrows CO_2 + 4H_2 \qquad \Delta_r H^0 = 165\ kJ/mol \qquad \text{Gleichung 3}$$

The reformate produced is cooled and fed into a second reaction stage in which further hydrogen is formed according to the water gas shift reaction with water vapour.

$$CO + H_2O \rightleftarrows CO_2 + H_2 \qquad \Delta_r H^0 = -41\ kJ/mol \qquad \text{Gleichung 4}$$

After the condensation of unreacted water, the reformate stream is further processed to separate the by-products, some of which also contain combustible components and can thus be used to heat the reformer. A schematic representation is given in Figure 9.

Because the reactions that take place and the heating of the reformer produce CO_2 as a result of the process, the emission of which must be avoided in the interest of climate protection, various options for CO_2 separation have also been developed for steam reforming; these differ not only in terms of technical implementation but also primarily in terms of their integration into the process. It is thus possible to separate CO_2 from the reformate (cfFigure 9, Positions 1), the by-product stream after processing (Positions 2), or the exhaust gas stream of the reformer heating. Items 1 and 2 are preferable in terms of technical effort because they have lower volume flows with higher CO_2 contents.

However, the disadvantage is that the emissions caused by heating the reformer are not recorded there. On the other hand, separation in the flue gas stream (Position 3), allows the CO_2 to be separated to a large extent; however, this is technically more complex.

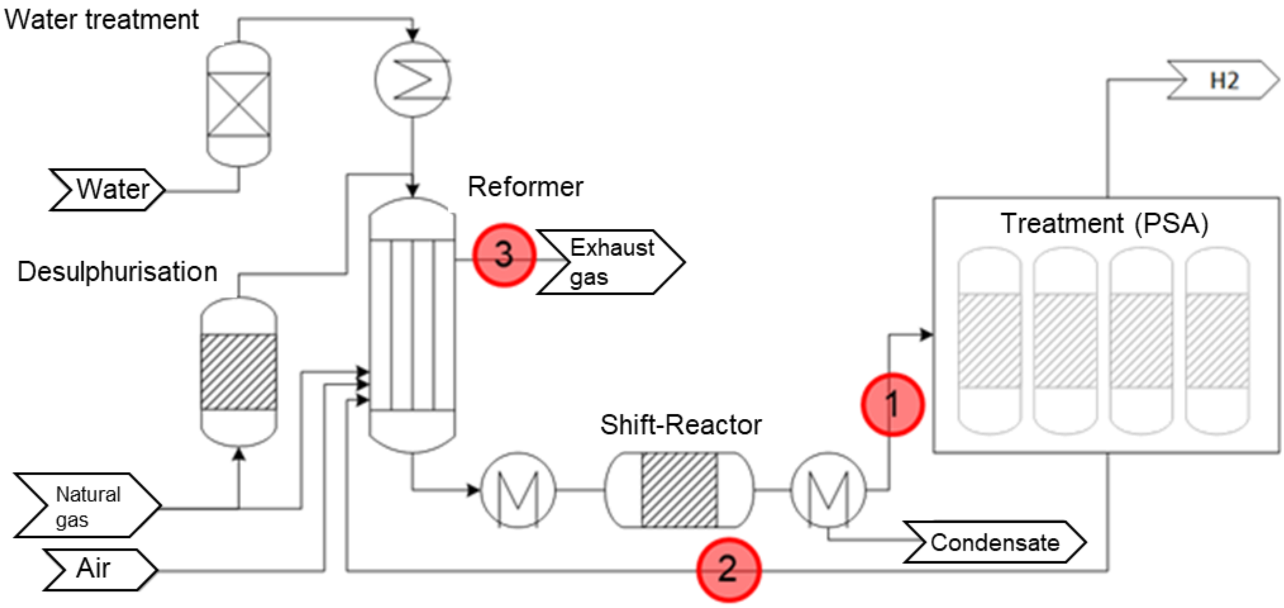


Figure 9: Schematic process of steam reforming with options for CO_2 separation

In addition to the possible CO_2 separation rate, the position of the CO_2 separation also directly influences the achievable hydrogen purity before further processing. Thus, in addition to the input materials and the process conditions, there is another influencing parameter; this is considered below.

In principle, hydrogen of sufficient purity cannot be provided by steam reforming without further treatment. According to Equation 2, hydrogen and CO_2 are formed in a ratio of 4:1 so that stoichiometrically a hydrogen content of maximum 80 vol. % is achieved. However, under real conditions, this hydrogen content is not achieved because of various influencing factors. Thus, both the reforming reactions and the water gas shift reaction are subject to thermodynamic equilibrium. The achievable conversions are limited depending on the operating conditions; in addition to hydrogen and CO_2, the product gas also contains unreacted methane and carbon monoxide. In addition, the input material natural gas also contains inert gases (nitrogen, noble gases), CO_2, and higher hydrocarbons. The latter are also converted during reforming but allow lower H_2 contents stoichiometrically.

Exemplary compositions of the reformate stream before treatment are shown in Table 3 based on “North Sea” natural gas according to DVGW worksheet G 260. The product gas contains approx. 75 vol. % hydrogen. At approx. 17 vol. %, CO_2 is the main minor constituent; methane, carbon monoxide, and nitrogen also occur in considerable proportions. Even if CO_2 is separated directly from the reformate stream (Position 1) to reduce emissions, sufficient hydrogen quality is not yet achieved (cf Table 3). With hydrogen contents of approx. 91 vol. %, the requirements for distribution in hydrogen networks are not met. Further treatment of the reformate stream is absolutely necessary and is currently also carried out in industrial applications. For this purpose, pressure swing adsorption is state of the art, and purities of up to 99.9999 vol. % are possible.

Table 3: Exemplary reformate composition of steam reforming for natural gas “North Sea” according to DVGW G 260, calculated for reforming at 20 bar, 850°C, S/C = 3 and WGS at 400°C with and without CO_2 separation in the reformate stream

Product gas before H_2 treatment		**Without CO_2 separation**	**With CO_2 separation**
Methane	Vol. %	4.0	4.9
Nitrogen	Vol. %	0.2	0.2
Carbon dioxide	Vol. %	17.5	0.0
Carbon monoxide	Vol. %	3.1	3.8
Hydrogen	Vol. %	75.2	91.1

Analogous to steam reforming, autothermal reforming also converts hydrocarbons with steam to hydrogen, carbon monoxide, and carbon dioxide (Equations 2 and 3). However, oxygen is additionally supplied to the reformer in order to compensate for the endothermy of the reforming through the exothermic partial oxidation of the hydrocarbons and to balance the heat balance without external heating.

$$CH_4 + 0{,}5O_2 \rightleftarrows CO + 2H_2 \qquad \Delta_r H^0 = 36\,kJ/mol \qquad \text{Gleichung 5}$$

On one hand, this reduces the design requirements for the reactor, enables higher operating temperatures, and achieves advantages with regard to CO_2 emission reduction because no separate burners are required for heating. On the other hand, compared with steam reforming, the hydrogen yield and the hydrogen content in the reformate also decrease. Exemplary compositions of the reformate before processing are given for natural gas “North Sea” in Table 4. In addition to the lower hydrogen content, a lower residual methane content or a higher methane conversion can also be achieved because of the modified operating conditions. On the other hand, the CO_2 content is considerably higher than in reformate gases from steam reforming. Nevertheless, especially in view of the high CO content, the separation of CO_2 from the reformate (emission reduction) is not sufficient to meet the hydrogen purity requirements (cf Table 4). Downstream reprocessing is mandatory. If this is done by pressure swing adsorption as in industrial practice, purities of up to 99.9999 vol. % are possible.

Table 4: Exemplary reformate composition of autothermal reformation for natural gas “North Sea” according to DVGW G 260, calculated for reforming at 20 bar, 1,000°C, S/C = 2, λ = 0,3, and WGS at 400°C with and without CO_2 separation in the reformate stream

Product gas before H_2 treatment		**Without CO_2 separation**	**With CO_2 separation**
Methane	Vol. %	0.2	0.2
Nitrogen	Vol. %	0.2	0.3
Carbon dioxide	Vol. %	24.3	0.0
Carbon monoxide	Vol. %	3.9	5.2
Hydrogen	Vol. %	71.4	94.3

3.1.3 Hydrogen from methane pyrolysis (Turquoise hydrogen)

The pyrolysis of methane is increasingly coming into focus in connection with low-emission hydrogen production. Because the methane is thermally split into hydrogen and solid carbon, practically no CO_2 is produced. The carbon formed can be used as a material or stored.

$$CH_4 \rightleftarrows C + 2H_2 \qquad \Delta_r H^0 = 75\,kJ/mol \qquad \text{Gleichung 6}$$

However, the technical implementation of methane pyrolysis is demanding, especially because of the necessary energy supply at a high temperature level combined with the formation of solids. Various solutions have been and are being developed. However, so far, they have not reached market maturity comparable to the reform. However, in some cases, an advanced development level (TRL) has already been reached.

The achievable hydrogen purity also depends on the solution approach and the specific technical design. Values between 45 and 99.7 vol. % are known from the literature; however, the early stage of development and the breadth of solution approaches must be taken into account. However, irrespective of this, it can be assumed that other components in addition to hydrogen are present in the product gas. On one hand, because inert gases and CO_2 are also supplied with the natural gas and transferred into the product gas. On the other hand, because complete methane conversion is not achieved for thermodynamic and kinetic reasons. By-/intermediates such as alkanes, alkenes, alkynes, aromatics, polycyclic aromatic hydrocarbons, and ammonia can be formed. Treatment at the production site is accordingly necessary and can be carried out (e.g. by pressure swing adsorption).

3.1.4 More options

In addition to the options presented for hydrogen production through electrolysis, reformation, and methane pyrolysis, there are other options for supply that were not considered in detail within the scope of the short study. Examples include the use of the by-product hydrogen from industrial processes (e.g. chlor-alkali electrolysis) and production from biomass, especially residual and waste materials. In addition to the question of generation qualities, the technical implementation of the expected import also influences the hydrogen quality. If hydrogen is transported in liquid form (LH_2), a high degree of purity can be assumed in principle. However, if hydrogen-containing compounds such as ammonia or liquid organic compounds (LOHC; liquid organic hydrogen carrier) are used in view of their better transport properties, the hydrogen must be released from these compounds. Impurities, incomplete conversion, and possible by-products can also influence the hydrogen purity and may require appropriate treatment.

3.2 Requirements for H_2 quality – normative requirements

With regard to the use of hydrogen as a fuel and for PEM fuel cells, there are quality requirements that clearly exceed the requirements for natural gas with regard to individual limit values. Depending on the intended application (e.g. burner, fuel, power generation), the requirements from ISO 14687-2 (Hydrogen fuel quality – Product specification) or DIN EN 17124 (Hydrogen as a fuel – Proton exchange membrane (PEM) fuel cell applications for road vehicles) vary but are still considerably higher than natural gas for track components.

As the recognised regulator of the gas industry, the DVGW e.V., has reacted to the challenge of hydrogen and revised the DVGW G 260 (A) Code of Practice and presented it in September 2021. Hydrogen was introduced as a fifth new gas family “hydrogen” in addition to the already possible feeding-in as an additional gas in gas networks of the second gas family.

In this worksheet, this fifth gas family has been newly included in two qualities. The nomenclature is based on ISO 14687:2019. Group A quality is hydrogen of purity ≥ 98 mol%; Group D quality requires a purity of 99.97 mol %.

The areas of application of the various standards are listed below:

ISO/DIS 14687 (2018)	Hydrogen fuel quality — Product specification This international standard specifies the minimum requirements for hydrogen distributed for use in mobile and stationary applications.
DIN EN 17124 (2019)	Hydrogen as a fuel – Product specification and quality assurance Proton exchange membrane (PEM) fuel cell applications for on-road vehicles

DIN EN 17124 thus sets the narrower framework for the application of hydrogen only as a fuel. In addition to the quality requirements listed in Table 5 for the use of hydrogen as a fuel with PEM fuel cells, ISO/DIS 14687 describes other uses of hydrogen for which the quality requirements are less stringent. These include use for combustion plants, for power and heat generation, and in aerospace applications. These H_2 qualities still below Group A have not found their way into the G 260. However, hydrogen of Group A quality (≥ 98 mol%) can be used for these processes in any case.

In February 2022, a recommendation (Common Business Practice CBP) was also issued by EASEE-Gas [14]; this describes in detail how a future “industrial hydrogen” could be structured.

In addition to the normative requirements, the following table lists the requirements of Linde for H_2 feeders as defined by Linde as part of a research project for distribution network operators as an example of an industry quality requirement.

Table 5 Compilation of various quality requirements for hydrogen, maximum values for impurities, supplemented by Linde requirements for gas suppliers in research projects

Parameter	DVGW G 260 H_2, Group A	DVGW G 260 H_2, Group D	DIN EN 17124 (PEM FC for road vehicles)	Linde (e.g. feeding-in requirements)
Hydrogen	≥ 98 mol %	≥ 99.97 mol %	≥ 99.97 mol %	≥ 99.96 vol. %
Non H_2 gases		300 µmol/mol	300 µmol/mol	
Water	200 or 50 mg/m³	5 µmol/mol	5 µmol/mol	Dew point (30 bar) ≤ −40°C
Non-methane hydrocarbons	-	2 µmol/mol	2 µmol/mol	≤ 3 µmol/mol
Methane		100 µmol/mol	100 µmol/mol	≤ 3 µmol/mol
Hydrocarbon condensation point	−2°C at 1 to 70 bar	-	--	
Oxygen	0.001 mol % / 1 mol %	5 µmol/mol	5 µmol/mol	≤ 1 µmol/mol
Helium		300 µmol/mol	300 µmol/mol	
Nitrogen		300 µmol/mol	300 µmol/mol	≤ 400 µmol/mol
Argon		300 µmol/mol	300 µmol/mol	
Carbon dioxide	2.5 / 4 mol %	2 µmol/mol	2 µmol/mol	≤ 2 µmol/mol
Carbon monoxide	0.1 mol %	0.2 µmol/mol	0.2 µmol/mol	≤ 2 µmol/mol
Total sulphur	10 mg/m³ (with odourisation)	0.004 µmol/mol[11]	0.004 µmol/mol[12]	
H_2S, COS as S	5 mg/m³	see total sulphur	see total sulphur	
HCHO		0.2 µmol/mol	0.2 µmol/mol	
HCOOH		0.2 µmol/mol	0.2 µmol/mol	
Ammonia	10 mg/m³ (NH_3 + amines)	0.1 µmol/mol	0.1 µmol/mol	
Halogenated compounds		0.05 µmol/mol	0.05 µmol/mol	
Mist, dust, liquid		1 mg/kg	1 mg/kg	
Total volatile silicon	0.3 or 1.0 mg Si/m³	-	-	

In general, the various standards, including G 260, list completely different units, some of which make it difficult to get a quick overview. Additional footnotes exist; these are not reproduced here for reasons of clarity.

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[11] Total sulphur and sulphur compounds

[12] Total sulphur compounds (basis H_2S)

Some special features can be identified based on Table 5 :

- The requirements for hydrogen quality of Group A are based on the second gas family (methane-rich gases) in the added gases. The required limit values are thus known from the transport and distribution of natural gas.
- The hydrogen quality of Group A is not sufficient to supply hydrogen filling stations (for the supply of PEM FC vehicles) according to DIN EN 17124. For the distribution of hydrogen quality of Group D, a supply of hydrogen filling stations is possible.
- For the distribution of Group D quality, parameters that have not played an analytical role in the gas compartment up to now (e.g. HCOOH (formic acid) or HCHO (formaldehyde)) must be observed.

3.3 Requirements for H_2 quality – technical requirements

3.3.1 Catalytic use of hydrogen

The catalytic use of hydrogen (e.g. in the chemical industry) has considerably higher demands on hydrogen purity compared with thermal use. For catalytic processes, a quality that is clearly above the requirements of Quality A but partly (depending on the catalytic process) below the requirements of Quality D is required. Special attention is paid not only to the hydrogen concentration but also to the added gases. The following describes the H_2 qualities required for various industries.

3.3.2 Ammonia

There are precise requirements for ammonia synthesis. In Table 6, these requirements are compiled with regard to various impurities. Sulphur, fluorine, chlorine, and phosphorus in particular are catalyst poisons and should be avoided accordingly.

Table 6: Maximum permissible impurities for ammonia synthesis [15]

Components	Maximum concentration
Sulphur	1 ppb
Halogens (F, Cl, Br, I, At)	1 ppb
O_2, CO, CO_2	5 ppm
Water vapour	30 ppm
Inert (CH_4,Ar, He)	As low as possible

3.3.3 Methanol

Table 7 shows the maximum permissible impurities for methanol synthesis. Again, the limiting factors are the catalysts (copper/zinc) because these show a tendency to catalyst poisoning.

Table 7: Maximum permissible impurities for methanol synthesis [15]

Components	Maximum concentration
Sulphur	50 ppb
Halogens (F, Cl, Br, I, At)	1 ppb
Iron	5 ppb
Nickel	5 ppb
Hydrogen chloride	2 ppb
Total nitrogen	0.5 vol. %
Methane	3 vol. %

3.3.4 Fischer–Tropsch synthesis

The maximum permissible impurities are due to the iron catalysts used. The sulphur content in particular must be kept low. Table 8 shows the currently known requirements for impurities.

Table 8: Maximum permissible impurities in hydrogen for Fischer–Tropsch synthesis [16]

Components	Fluctuation range	Unit
Sulphur	5–100	ppb
Halogens	10	ppb
Ammonia	10	ppmv
Hydrogen cyanide	0.2	ppmv
Nitrogen oxide	10	ppb
Total nitrogen	50	ppb

3.3.5 Power-to-X processes (PtX)

Power-to-X processes refers to various technologies using renewable energies and serve to network electricity with the heat, chemical, and mobility sectors. In the context of this report, the generation of gases such as hydrogen and methane (power-to-gas = PtG) and the production of liquids such as methanol and synthetic fuels (power-to-liquid = PtL) are relevant. These processes can also be classified as part of a chemical industry. The requirements of these processes are addressed separately here because these PtX processes[13] are often presented separately in the various studies on H_2 demand (see 2.2).

PtX processes are catalytic processes. The catalyst is the decisive component that defines the requirements for the quality of the hydrogen feedstock.

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13 dena has made a different definition to determine the quantities (see Chapter 1)

The effect of the various impurities on catalysts varies and depends strongly on the material of the catalyst (precious metal, other metals, or mixtures). Strong catalyst poisons that permanently reduce the effect of a catalyst are:

- Carbon monoxide
- formaldehyde
- formic acid
- sulphur compounds
- halogen compounds

Ammonia, water, non-methane hydrocarbons, and suspended particles can also damage catalysts. On the other hand, inert gases and methane, lead to a drop in performance mainly because of the dilution of the hydrogen.

The H_2 quality of Group D ensures a gas quality that should be suitable for all PtX processes. With the lower quality of 98% mol % (Group A), this is only partially the case. The catalyst poisons must be removed.

One example is the production of methane (methanation). This process can be carried out in a mixture of natural gas and hydrogen and was evaluated under the aspect of plant protection in DVGW Report G 201611 of 2018 . The presence of methane and the various saturated hydrocarbons does not interfere with the process. However, desulphurisation is provided to protect the catalytic converters. If CO and ammonia are present in the output gas, these would also have to be removed.

In summary, it can be said that an H_2 quality of Group A of 98% or even lower may well be sufficient for a PtX process but that individual compounds with properties harmful to catalysts must be removed in any case.

3.4 Energetic use

3.4.1 Crude iron production

No uniform hydrogen quality requirements are yet known from crude iron production. The current blast furnace route produces coke oven and converter gases as well as blast furnace gases along the production chain; these have different hydrogen contents ranging from 1–5% (blast furnace gas) to 65% (coke oven gas). Hydrogen can be used directly in the blast furnace to reduce iron ore. However, it is currently not possible to completely eliminate carbon from the blast furnace route. Alternatively, crude iron can be produced via hydrogen direct reduction on electric furnaces. However, the product here differs greatly from the product from the blast furnace route so that additional carburisation is necessary later. Because of the combined use as fuel and reducing agent, crude iron production with hydrogen is not a purely energetic use but rather also uses the hydrogen as a material.

It is therefore currently assumed that it will be possible to work with different hydrogen contents on both routes. Various research projects on this topic are currently under way.

3.4.2 Industrial firing plants

Detailed studies on the exact quality requirements of industrial furnaces are still lacking. In principle, the requirements from the DVGW projects on gas quality also apply to hydrogen. These suggest a maximum fluctuation range of 2% of the Wobbe index. Otherwise, the requirements of a furnace are less specific than in the chemical industry: Currently, it can be assumed that Group A according to G 260 is a sufficient quality requirement. It should be noted that components such as CO_2 or N_2 in particular are harmless to the processes; water vapour is also not critical. Sulphur components should be present in the same proportion as natural gas or less because the experience levels here are sufficiently high in terms of how to deal with them.

In general, combustion processes do not react to a certain hydrogen content in natural gas to a particularly specific extent. More important than high purity requirements is a stable gas composition. Industrial furnaces and heating processes can also be converted to 75% hydrogen content. However, they react sensitively to strong fluctuations. However, because a basis for a uniform hydrogen supply should be found, Group A is specified as the possible hydrogen quality in each case. This also corresponds to the EASEE gas CBP. The purity requirements for additional components are much more specific depending on the product but should be in line with the current purity requirements for natural gas.

Table 9 shows examples of some industrial sectors and their respective gas qualities for combustion processes.

Table 9: Hydrogen quality in industrial combustion processes

Plant type	Quality	Impurities	Special features
Glass/ceramics	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Sensitive to fluctuations; if possible, fluctuations in the Wobbe index of less than 2%
Non-ferrous metals	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Sensitive to fluctuations; if possible, fluctuations in the Wobbe index of less than 2%
Steel	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Sensitive to fluctuations; if possible, fluctuations in the Wobbe index of less than 2%
Paper	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Limit fluctuations; if possible, fluctuations in the Wobbe index of less than 2%
Boiler plants	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Limit fluctuations; if possible, fluctuations in the Wobbe index of less than 2%
Other industry (e.g. drying plants, crematoriums)	ISO Grade A or worse/DVGW G260 Group A	Comparable to natural gas	Limit fluctuations; if possible, fluctuations in the Wobbe index of less than 2%

3.4.3 Domestic and commercial heaters

Domestic and commercial heaters generally show a robust behaviour towards fluctuations in the gas composition and are insensitive to the composition of the fuel gas because of their pure heating function without contact with products or the like. Based on the development in projects such as Hy4Heat [17] in the UK, where hydrogen applications are used in larger numbers, the Hy4Heat composition specifications in Table 10 provide a good guide to the requirements of the heaters.

Table 10: Recommended fuel gas composition in the Hy4Heat project in the UK [18; 19; 15]

Components	Value	Explanations
Hydrogen (at least)	98 mol %	Compromise between cost and performance
CO	20 (µmol/mol)	Based on production limit from reforming
H_2S	≤ 5 mg/m^3 3.5 ppm (µmol/ mol)	Component protection from GSMR:1996
Total sulphur	≤ 50 mg/m^3 35 ppm (µmol/mol)	
Oxygen	≤ 0.2 mol %	
Dew point of hydrocarbons	−2°C	GSMR:1996 and EASEE gas
Dew point of water	−10°C	
Methane, carbon dioxide, CO_2, hydrocarbons	≤ 1% mol %	
Total argon, nitrogen, helium	≤ 2% mol %	Avoidance of transport costs through higher inert proportions (ISO 14687-2019) and the limitation of fluctuations in the Wobbe index
Wobbe band	42–46 MJ/m^3	
Impurities	The gas should not contain any solid, liquid, or gaseous components that endanger the safe operation of pipes and end use.	

Fuel cell systems are an exception for hydrogen purity in domestic and commercial heating. Fuel cell systems require hydrogen quality according to DVGW Code of Practice G 260 Group D because the fuel cell stacks are highly sensitive and react to impurities in the hydrogen with loss of performance and reduction of the lifetime of the stacks.

3.4.4 Gas turbines

Gas turbine burners react sensitively to fluctuations in the gas composition. Accordingly, it is more important to define the maximum range of variation than the exact nature. Currently, a permissible fluctuation range of ± 5% of the Wobbe index is assumed. Group A again provides the basis for the hydrogen content. The same conditions apply to impurities as to natural gas.

3.4.5 Gas engines

Stationary gas engines are relatively robust in the face of fluctuations in the Wobbe index and heating value. In principle, as with all combustion processes, the composition of the gas is less important than a consistent nature. Accordingly, the quality of Group A also provides a good orientation here. Table 11 summarises the requirements for stationary engines. The same conditions apply to impurities as to natural gas.

Table 11: Hydrogen quality for gas engines [17, 14]

Parameter	Window min–max	Remarks
Heating value and fluctuation in the Wobbe index	± 5%	If necessary, the rate of change must be defined
CO, CH_4, CO_2, N_2, hydrocarbons		No effects to be feared as long as Wobbe index and heating value are complied with
Sulphur	Comparable to natural gas	
Dew point of water/hydrocarbons	Comparable to natural gas	
Dust/particles	Comparable to natural gas	
Other	Comparable to natural gas	

3.5 Overview of the sectors and their requirements

A statement on the quality requirements of the individual (sub-)sectors is not possible in a generally valid manner in every case. The following Table 12 should make this clear.

In the building, energy, and transport sectors, hydrogen can be used by means of combustion processes as well as in fuel cells. While combustion processes accept H_2 of the “lower” quality of Group A, this does not apply to fuel cell systems.

From a technical point of view, however, there is also the ability for sensitive (e.g. catalytic) systems to accept “impurities” in the hydrogen. This by no means concerns catalyst poisons but rather nitrogen or increased water concentrations. From a technical point of view, this makes it possible to use a “catalytic”, medium H_2 quality. In the table, a quality of 99 mol % is assumed as an example.

From a technical point of view, this possibility concerns PtX processes, processes in the chemical industry, and fuel cells.

Table 12: Comparison of estimated H_2 demand and different H_2 qualities

		H_2 demand (dena 2021) in TWh	Group A ≥ 98 mol % H_2 “low” quality requirement	≥ 99 mol % H_2 “medium” quality requirement	Group D ≥ 99.97 mol % H_2 “high” quality requirement
Building		78	(✓)	(✓)	✓
Energy		128	(✓)	(✓)	✓
Traffic		59	(✓)	(✓)	✓
PtX		58	-	(✓)	✓
Industry (Examples)		191			
	Stones and soils		✓	✓	✓
	Paper		✓	✓	✓
	Glass and ceramic		(✓)	✓	✓
	Iron and steel		✓	✓	✓
	(Petro-)chemistry[14]		-	(✓)	✓

The possible suitability of this H_2 quality marked by parentheses makes it clear that, in this case, there is a dependence on the type of component in the hydrogen and the type of use.

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[14] non-energetic

4 WP 3: Gas treatment

The processing of hydrogen poses considerably greater challenges for the future operators of a hydrogen infrastructure than the processing of natural gas does. These result from the hydrogen quality requirements of the catalytic processes and the fuel cells. As a result of the study, the following key statements can be made:

Results at a glance

- The type of impurities (substance groups) to be expected is known. Potential sources of unwanted components in hydrogen are hydrogen production itself, storage in UGS, and the transport of hydrogen in former natural gas pipelines.
- Various gas treatment processes with a TRL of 9 are available. These processes can produce a Group D grade with a hydrogen concentration of ≥ 99.97 mol %.
- This gas treatment incurs additional costs, the amount of which depends on the process, the location of the treatment plant, its size, and the type of components to be removed. While some processes manage without hydrogen losses and thus lower OPEX, processes with hydrogen losses (e.g. PSA) are to be classified as cost-intensive.

4.1 Sources of H_2 impurities

There are three potential sources of hydrogen impurities:

- the production of hydrogen
- the storage of the hydrogen
- the transport of the hydrogen

These sources also exist after the conversion and “stabilisation” of the integrated infrastructure. Accordingly, these three potential sources of contamination must be taken into account in the long term when evaluating any necessary treatment steps.

In all three cases, special operating procedures such as flushing, cleaning, and inertisation can lead to the entry of components into the hydrogen. This potential component input is not system- or process-related and can be prevented or minimised (e.g. by technical measures).

The following summarises some basic statements on the introduction of secondary components into hydrogen; this is explained in detail in the chapters on the production, storage, and transport of hydrogen.

4.1.1 Production

Depending on the production process, different substance groups can occur as gas-accompanying substances or impurities. A risk assessment regarding the possibilities of contamination (type and source) can be found in Appendix C of DIN EN 17124.

Table 13: Type and source of possible secondary components from the production process

Method	potential secondary components
Steam-methane reforming with pressure swing adsorption	N_2, CH_4, CO, HCOH, CO_2
Alkaline and PEM electrolysis with temperature swing adsorption	O_2, H_2O
Methane pyrolysis	N_2, O_2, H_2O, CO_2, hydrocarbons, halogens, sulphur compounds,
Ammonia (transport medium)	NH_3, N_2, NO_x

Other production processes for hydrogen are gasification processes (e.g. biological waste, refuse), which are not considered in detail here.

When supplying or accepting an H_2 quality of ≥ 98 mol %, there is a possibility that other substance groups in addition to the “possible impurities” of Table 13 fill the open 2% gap. Regardless of the manufacturing process, the G 260 with Grade A quality gives the possibility that:

- methane up to 2 mol %
- other hydrocarbons (ethane, propane, butane) also up to 2 mol % if the CHP condensation point is maintained
- Gases such as nitrogen (N_2), argon (Ar), and carbon dioxide (CO_2)

can fill this gap. Possible but limited are carbon monoxide CO (0.1 mol %), water, and sulphur compounds in hydrogen.

It should be explicitly pointed out here that even when complying with G 260, Grade A, there is leeway with regard to the H_2 composition under the responsibility of the H_2 producer. The use of the leeway by the producer (e.g. the targeted admixture of N_2 or CO_2) can lead to effects (e.g. in the form of a necessary gas treatment at the gas distribution or the H_2 user) or to a restriction of the H2 user group.

DIN EN 17124 lists further “highly unlikely” secondary components that could occur in individual cases. These are not to be regarded as the current state of the art in every case. At the moment, investigations are being carried out to

- verify such compounds and their presence or concentration in the hydrogen in the first place
- better process the starting product of the electrolysis (water) because every impurity also influences the lifetimes of the various electrolysers. The manufacturers of the electrolysers thus have their own interest in using highly pure starting products (water).

4.1.2 Underground storage of H_2 in caverns

Sufficient experience is available from the storage of natural gas with regard to the possible introduction of components into the gas to be stored; this can be incorporated into the evaluation of the storage of hydrogen [20] [21].

The following components can be additionally introduced into the hydrogen via the storage process:

Table 14: Type and source of possible impurities, storage in caverns

Cause	Components	Probability
Cavern (brine)	Water	Fluent
Cavern (brine)	Sulphur compounds	possible
Cavern, compressor	higher hydrocarbons	possible (blanket[15], compressor oils)
Cavern (brine)	CO_2, methane	possible (residual gases in cavern wall and dissolved in brine)

In any case, the stored gas absorbs water until saturation. Depending on the retention time of the hydrogen and the flowing gas volumes, saturation with water vapour may be delayed, but gas drying cannot be dispensed with in any case.

The use of hydrocarbons as compressor oil in the compressors and as blanket (see Chapter 5.) can lead to traces of these components in hydrogen. The occurrence of an increased concentration of hydrocarbons in the hydrogen is to be classified as reservoir-specific, analogous to the microbiological activity (see below).

It is assumed that hydrogen of high purity is stored in a UGS. If hydrogen of Group A quality (98 mol %) should be stored even for a short time, the delivery of Group D quality is not possible without additional gas treatment.

If a cavern is converted from natural gas to pure hydrogen (Group D) by using brine (i.e. the natural gas is displaced by brine), the hydrogen subsequently contains fewer residues of the natural gas or blanket. However, there may be “pockets” in the cavern walls where natural gas or blanket is “trapped” and cannot be removed by brine. Remnants of the blanket or gas residues could also remain in the roof area. When converting oil-filled caverns to H_2, oil residues on the cavern walls must also be assumed; this requires removal of these in the aboveground plant in order to achieve Group D quality.

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[15] Covering medium on the brine, separation of the brine from the gas space

4.1.3 Transport

The cause of the introduction of various compounds into a gas to be transported are compounds adsorbed on the wall of the pipeline and deposits/condensates. In addition to hydrocarbons and sulphur compounds from natural gas and odourisation, components from biogas and the processing of this are also to be expected in some places.

Figure 10: Deposits from a transport pipeline, second cleaning pigging

A risk assessment with regard to the possibilities of contamination was again carried out in Appendix C of DIN EN 17124, which lists the type and sources of “possible” and “unlikely” components from pipelines. However, the listing of N_2 and O_2 as possible secondary components from a pipeline indicates that the statements of this standard are not to be accepted without comment.

The chemical and refinery industry has experience with the transport of hydrogen using high-pressure pipelines. The transport of a pure hydrogen of high quality is, in principle, no problem. The following facts are known:

- Hydrogen is transported exclusively via networks in which no other gas was previously transported. These are therefore **not** converted networks. At no time did hydrocarbons or sulphur compounds enter these pipelines
- In Germany (Linde network Leuna), the hydrogen network is operated with an H_2 quality greater than or equal to 99.96 mol %. The reason for the somewhat lower value compared with Group D is greater caution towards the customer because minimal quality changes could occur during construction work, switching operations, or the like.

- Qualities of 99.99 vol. % H_2 can be transported; the input qualities are controlled accordingly (e.g. hydrogen network Texas/US).
- In the H_2 network in Texas (US), **no** oil-free compressors are used; nevertheless, the limits for hydrocarbons are complied with.

With regard to converted natural gas pipelines, it is therefore permissible to conclude that a high hydrogen quality can be maintained, transported, and distributed after setting a high H_2 quality (i.e. after removing all relevant impurities). However, the period of discharge of these impurities is uncertain.

4.2 Substance groups and preparation methods

4.2.1 Assignment to substance groups

The aforementioned compounds can be grouped together in different substance groups regardless of their origin; this makes it easier to assign them to the gas treatment processes.

Table 15: Substance groups or substances in hydrogen

Group/substance	Common components	Rarely
Sulphur compounds	H_2S, Mercaptane, THT, COS	CS_2; sulphides (DMS)[20]
Gases/permanent gases	N_2, O_2, Ar, He, CO_2, CO, CH_4	
Hydrocarbons	From ethane to > C30 (e.g. compressor oils, natural gas condensates)	Naphthalene, terpenes[16]
Other		Glycols; ammonia, halogen compounds, formaldehyde, formic acid
Water	x	
Dust	Rust, metals, sand, bound sulphides (FeS)	

The sulphur compounds represent a thoroughly inhomogeneous group with regard to polarity, adsorption behaviour, and vapour pressure. Nevertheless, they are considered as a group with regard to a necessary removal (desulphurisation). Natural gas fuel cells (manufacturer e.g. Panasonic) have a desulphurisation unit upstream of the reformer; this can retain all compounds of this group. A combination of different adsorbents is used.

In the group of sulphur compounds, COS (carbon oxide sulphide) and CS_2 (carbon disulphide) are to be regarded as highly critical because according to the experience of Panasonic in FC development, these two compounds are poorly adsorbed and thus cause problems for FC manufacturers. CS_2 has already been detected in distribution networks where biogas was transported.

The group of gases includes components (e.g. nitrogen and helium), the presence of which has no harmful effects on chemical processes or catalysts. CO is an exception.

The group of hydrocarbons is remarkably homogeneous in terms of polarity; this makes the removal of these from the hydrogen much easier.

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[16] Source biogas

4.2.2 Processing method

There are treatment processes for substances or groups to be removed at a TRL of 9. This means that these methods can be used immediately. There is therefore no fundamental problem with regard to the processing of hydrogen to the desired quality.

The following table lists substance groups and the relevant treatment processes.

Table 16: Substance groups and suitable preparation processes for H_2 preparation

Method	Components	Gas volume ≤ 1000 m³/h TRL	Gas volume ≥ 1000 m³/h TRL	Comments
Adsorption (physisorption)	CO_2, CO, HC (including CH_4), H_2O, N_2, NH_3	9	9	Purification possible up to the ppb level[17] Temperature change adsorption in the case of drying COS, CS_2 are critical
Chemisorption/catalytic conversion	O_2, sulphur compounds	9	9	
Liquefaction (cryogenic process)	N_2	9	9	Also offered for small outputs in the semiconductor industry
Absorption	H_2O	(9)	9	Low-capacity plants possible but not relevant for drying small volumes
Membrane process	H_2	9 / 6	9 / 6	See below for explanation.
Filter	Dust	9	9	

These methods can be used regardless of the installation site.

4.2.2.1 Adsorption

Adsorptive processes involve the attachment of molecules from the gas or liquid phase to a solid surface (adsorbent). This surface is provided in the form of macro-, meso-, and micro-pores. The separation effect of an adsorptive process is usually based on the different strength of interaction of the components with the adsorbent (equilibrium) and, in some cases, on adsorption at different rates (kinetics) as well as through size exclusion (steric). All three effects must be taken into account when designing adsorption processes. Heat is released during adsorption (adsorption heat).

Physisorption (physical adsorption) can be reversed by desorption without changing the adsorbed compound and the adsorbent.

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[17] There are various statements regarding the cost and feasibility of individual components from the point of view of gas manufacturers and users of clean gases.

In temperature swing adsorption (TSA), desorption is based on the reduction of the equilibrium load as a result of an increase in temperature. For this purpose, energy is supplied either indirectly via heating elements or directly via warm inert gas. Depending on the thermal stability of the adsorbate (adsorpt and adsorbent), even strongly bound components can be desorbed at high temperatures. The main disadvantage of this method is the high time requirement for heating and cooling processes. An example of this process is gas drying using a molecular sieve or silica gel (Figure 12).

In pressure swing adsorption (PSA), the loaded adsorber is depressurised and flushed; this also reduces the partial pressures of the individual gas components. The pressure reduction thus leads to an equilibrium shift in the direction of the gas phase with the release of adsorbed molecules (desorption). The main process advantage lies in the short desorption times, which allow a high cycle frequency for the overall process (and thus smaller apparatus). A disadvantage is the need for electrical energy for compression during the loading phase if the feed gas is not already under pressure. Figure 11 shows the principle of both desorption processes in the equilibrium diagram.

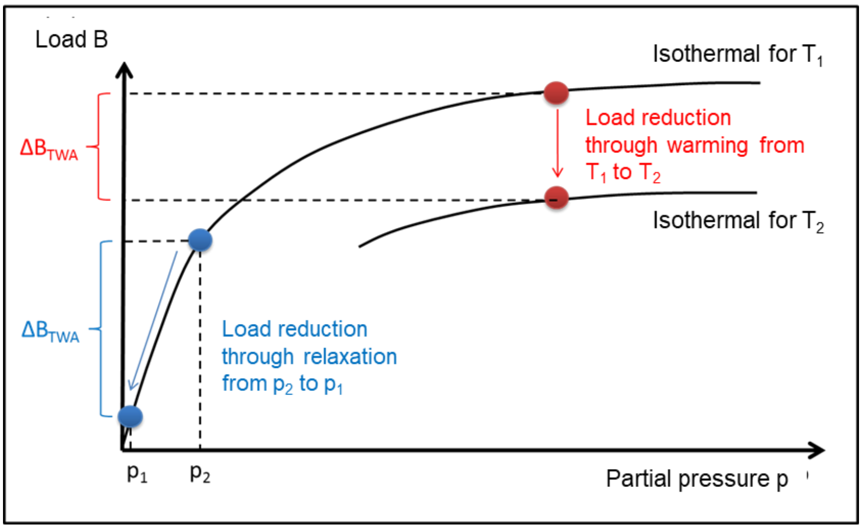

Figure 11: Operating modes of adsorption: desorption through temperature or pressure change (source DVGW report G1-04-16)

Hydrogen and helium are not adsorbed under normal conditions. Hydrogen is purified by adsorbing the impurities and allowing hydrogen to pass through the adsorber with little interaction with the adsorbent. Nitrogen also exhibits low adsorption forces or interactions. The removal of nitrogen is based on its adsorption (e.g. on molecular sieve/zeolites)

A prerequisite for the regeneration of an adsorbent is that the compounds can be desorbed without expending too much energy. In the present case, this is not the case with long-chain hydrocarbons such as compressor oils; the adsorbent must therefore be changed. The adsorption capacity depends on the adsorbent, the input concentration of the substance to be removed, and the presence of competing components.

Figure 12: Siloxa adsorption dryers type 400 and 700 (Siloxa product sheet).

Adsorption processes with and without regeneration are state of the art. High-purity hydrogen is produced from synthesis gas by means of a PSA stage. Desorption is operated close to ambient pressure, and the combustible waste gas is used to heat the reformer.

The following framework parameters are given by Air Liquide regarding pressure swing adsorption for hydrogen purification [22]:

- Recovery of hydrogen with a purity of up to 99.9999%
- Availability factor usually above 99.9%
- Input gases in a wide range
- patented exchange cycles and state-of-the-art adsorbents
- designed for unmanned outdoor operation
- compact and pre-assembled on frames
- Capacity: 5,000 to 200,000 standard cubic metres per hour
- H_2 recovery rate: 60 to 90%
- Partial load operation: up to 25%

In comparison, Linde quotes capacities of up to 400,000 Nm^3/h, recovery rates of 93–98% (two-stage), and a greater margin for part-load operation (up to virtually 0%).

The indication of the H_2 recovery rate suggests a disadvantage of this process (i.e. the losses of hydrogen as a result of the regeneration of the adsorbers). For fine purification from 98 mol % to 99.97 mol %, these losses can usually be estimated at 2–10% of the gas used. A similar situation is known from biogas upgrading; the biomethane losses are indicated at the PSAs of biogas upgrading plants at approx. 3% and make catalytic post-combustion of the captured CO_2 necessary, for example.

Separators without regeneration (Figure 13 and Figure 14) are less complex in terms of circuitry. These are used when small quantities of strongly adsorbing components must be separated. Losses of hydrogen are practically non-existent; the tanks need only to be depressurised to change the adsorbent. The design takes into account the adsorption capacity so that relatively few adsorbent changes (e.g. once per year or less) are necessary. In the example, the adsorbers are connected in such a way that they can be operated both in series and in parallel. The example shown below is from a deodourisation project. Deodourisation will also become relevant for the processing of hydrogen.

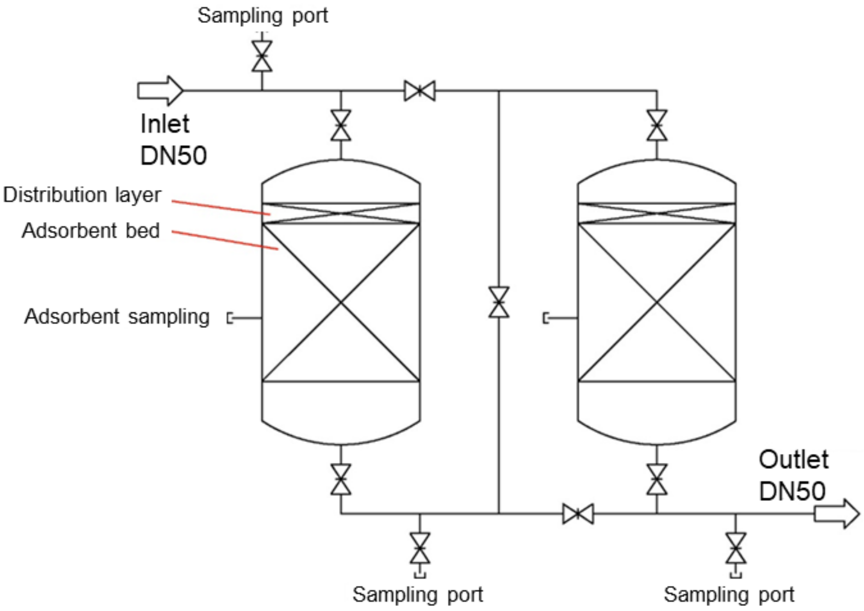

Figure 13: Schematic diagram of a separator with two adsorbers

Figure 14: Example Fangmann Industrie – separator skid with two adsorbers (DN 250; DP64)

Zeolite-based adsorbents are also used for the desulphurisation of gaseous material flows. Because of the pore size, zeolites 13X are particularly suitable for the separation of sulphur compounds. The water content and the proportion of higher hydrocarbons influence the absorption capacity of the adsorbent. Regeneration of the loaded adsorbent by means of hot gas is theoretically possible but is not carried out (e.g. in the case of odourants) because of the odour pollution, especially in smaller plants. Activated carbons can also be used for fine desulphurisation. This is implemented, for example, in the natural gas fuel cells from Panasonic. There, an (unknown) combination of different adsorbents is used to protect the catalysts.

The processing of Group A quality hydrogen to Group D quality requires adsorptive processes. The removal of nitrogen, carbon dioxide, methane, and carbon monoxide requires a PSA; for hydrocarbons and sulphur compounds, adsorbers with alternating fillings are to be provided. Water can be dried by means of temperature swing adsorption (TSA).

4.2.2.2 Chemisorption/catalytic conversion

The coupling of an adsorption process (chemisorption) with a subsequent chemical change of the adsorbed components is relevant in the context of hydrogen processing with regard to the removal of oxygen and sulphur compounds.

For the removal of oxygen, a reaction in which the oxygen is catalytically converted with hydrogen to water is used. In electrolysis, this reaction serves to remove the oxygen residues from the hydrogen and is state of the art. The hydrogen content of the gas stream must be at least twice as high as that of oxygen for reasons of stoichiometry. The oxygen content can be reduced to concentrations < 1 ppmv with this method. Precious metal catalysts (containing platinum or palladium) are used; these work at ambient temperatures or slightly elevated temperatures (< 50°C). Other catalysts are conceivable; however, these require considerably higher temperatures. The water produced during the reaction must then be removed adsorptively.

Desulphurisation processes can also be used in combination of adsorption and subsequent conversion of the adsorbed components into sulphur to increase the adsorption capacity. Impregnated or doped materials achieve high absorption capacities, especially with regard to hydrogen sulphide. These materials are used in industrial applications for the separation of sulphur compounds in the trace range. However, it must be checked in advance whether oxygen is required for the conversion of the sulphur compound, which is not present in the hydrogen. This eliminates the need to use iodine-impregnated activated carbon. On the other hand, hydrogenation desulphurisation can be used to remove sulphur compounds from hydrogen:

$$\text{R-SH} + H_2 + \text{ZnO} \longrightarrow H_2S + \text{R–H} + H_2O \qquad \text{Equation 7}$$

The cobalt/molybdenum catalyst operates at 200–400°C; the uptake capacity of the ZnO bed is up to 30 mass %. Hydrogen as a required reaction component is present in excess in the hydrogen stream.

4.2.2.3 Liquefaction

Liquefaction is state of the art in terms of large and small-scale technology. In addition to the separation of components (air liquefaction), it serves to reduce the volume and pressure when transporting liquids (LNG, H_2).

At −253°C, the boiling point of hydrogen is considerably lower than that of other gases. It follows that in the case of an H_2 mixture present, the hydrogen can be separated as a separate phase only by liquefying all the other components. Another disadvantage is that the expansion process used for LNG (utilisation of the cooling Joule-Thomson effect) is not possible; this increases the energy requirement.

For LNG, the total energy requirement in terms of heating value needed to liquefy natural gas is given as 10–25%. Because the adsorptive processes offer energetically more favourable alternatives for the purpose of H_2 gas purification, the liquefaction of H_2 will not be discussed further below.

4.2.2.4 Absorption

In **absorptive processes**, the component to be removed is bound in a washing liquid. This process is reversible. Note that the scrubbing liquid (e.g. amines, glycols, water) can be introduced into the gas.

With regard to hydrogen, the relevant absorption process is gas drying. Drying by means of triethylene glycol (TEG) is standard on underground gas storage tanks, highly flexible in partial load behaviour, and is characterised by low operating costs compared with molecular sieve drying. The requirements of hydrogen quality of Group A are achieved with TEG drying on a UGS; a combination with molecular sieve drying as a second stage for drying hydrogen to achieve the quality of Group D is conceivable.

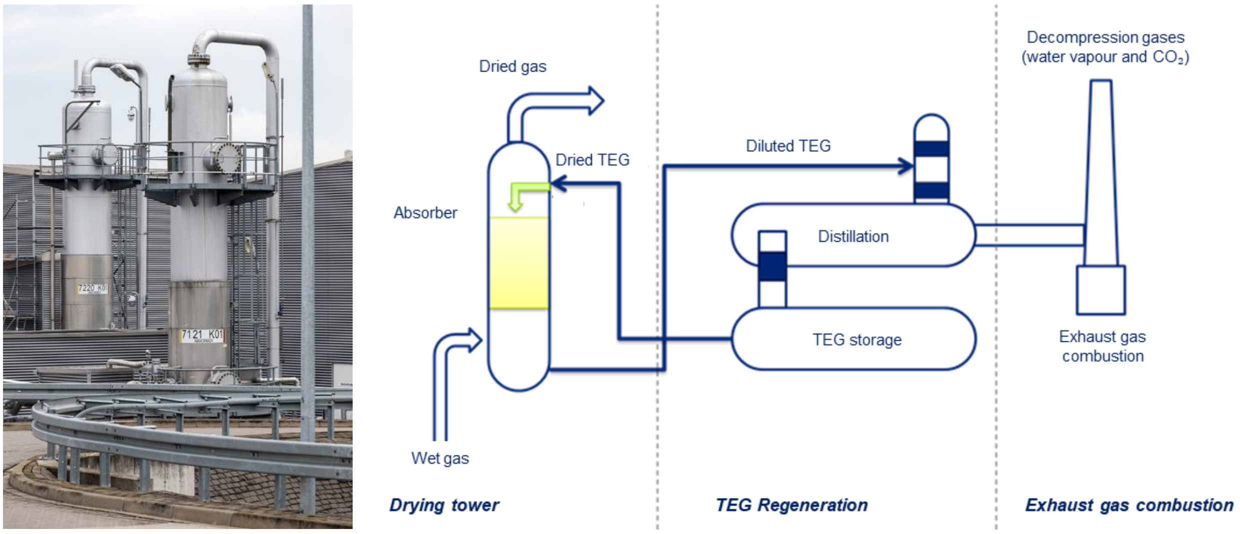

Figure 15: TEG drying at the UGS and principle diagram of gas drying by means of absorption

4.2.2.5 Membrane process

Another, theoretically possible treatment process for gases at a TRL of 9 are membrane processes.

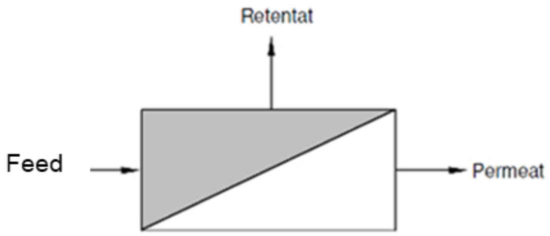

Figure 16: Schematic representation of the material flow separation at a membrane

Membrane processes have the following advantages over other separation processes:

- Low energy demand
- High flexibility with regard to changing material flows
- Modular design and thus easily expandable
- Fast start-up and shut-down of the plants possible
- No need for chemical additives, free of waste materials

With technological advancements in membrane technology, new membranes can be easily incorporated into existing equipment. These advantages are also countered by disadvantages. Membranes are not normally a method of fine gas purification. This is typically done by a downstream pressure swing adsorption unit.

Polymer membranes are relevant for the extraction of hydrogen from a natural gas-hydrogen mixture. However, these cannot undertake the purification from 98 mol% to 99.97 mol% considered within this study.

In the case of hydrogen, there are special features that nevertheless allow the use of membranes for fine purification. Whilst different membrane types (e.g. polymer membranes) allow the production of a 98 mol% quality of hydrogen, two membrane types allow the production of Group D quality. The reasons for this are the small size of the molecule as well as a highly specific interaction with palladium.

Palladium membranes are used in order to obtain high hydrogen purities of up to 99.9999%. A comprehensive overview of the status and problems of palladium membranes can be found in [23]. Pd membranes usually operate in the temperature range of 300–700°C.

A distinction is made between pure palladium membranes and Pd alloys. Palladium is highly sensitive. For pure Pd membranes, problems in dealing with CO, sulphur compounds, or water are described; these are partly temperature-dependent. With “palladium-based” membranes (i.e. palladium alloys), some of the problems can be circumvented.

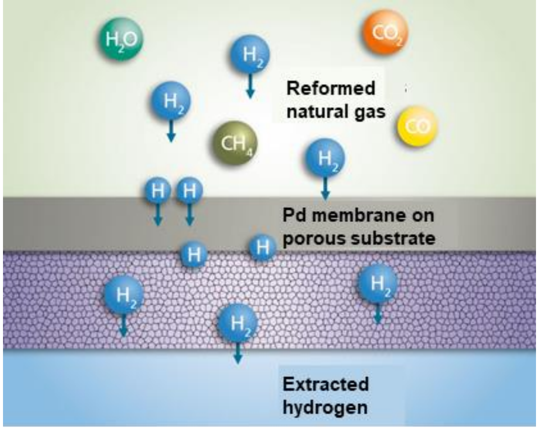

Figure 17: Diffusion through a palladium membrane (source Fraunhofer IST)

The disadvantage is that all the hydrogen must pass through the membrane; this requires a high permeability of the membrane and/or large membrane areas. The development is moving in the direction of reducing the Pd content in order to lower the costs of the membranes. But with this type of membrane, an alternative to PSA is available for the separation of N_2 from H_2 (e.g. for smaller applications). Palladium membranes can be formally classified as TRL 9. However, for cost reasons, they are currently used more for small-volume applications.

Recent research results show that carbon membranes can also produce a Group D hydrogen from a Group A hydrogen. The development status of this membrane type is classified as TRL 6. In general, it should be noted that although membrane technology has TRL 9, the individual membrane types can have a lower TRL.

5 WP 4: Underground gas storage

In a future system of production, transport, storage, and use of hydrogen, the underground gas storage facilities will play an important role for security of supply and for balancing fluctuations in production and consumption. The previous chapter describes the storage potential in Germany and the differences between the storage types. With a focus on cavern storage, quality-changing processes are explained.

The main findings of the chapter are summarised below.

Results at a glance

- The storage of gases in geological formations leads to quality changes depending on the type of UGS and the previous use.
- There are ways of converting caverns that minimise the subsequent introduction of accompanying components from residual natural gas into the hydrogen.
- The introduction of water into hydrogen in a cavern cannot be prevented. Microbiological processes can take place in caverns; the extent of these depends on parameters such as the microbiological activity in the brine.
- All components mixed in the hydrogen can be removed; the effort varies depending on the condition of the UGS. Caverns and pore storage facilities are to be evaluated differently in terms of conversion and their effects on hydrogen storage.

5.1 Storage structure in Germany

Underground gas storage facilities are the backbone of a stable energy supply and are necessary in the long term because they

- provide for an individual and flexible connection of energy suppliers and consumers
- balance fluctuations between energy production and demand, both seasonally and diurnally
- ensure security of supply because stored hydrogen volumes represent a reserve that can be drawn on in the event of the failure of other system components (e.g. accident of an import pipeline or failure of an energy producer).

In the case of hydrogen storage, underground gas storage facilities are once again becoming more important because

- volatile hydrogen produced from renewable sources means greater fluctuations in daily production; a more fluctuating demand can also be expected
- Underground gas storage facilities will be needed in greater numbers because the switch to renewable energies will also mean that greater quantities of energy will be generated domestically and consequently less will be imported.

In the case of large-volume energy storage, only underground gas storage facilities offer the necessary storage capacities. These are several magnitudes higher than other storage variants such as battery storage or pumped storage. This feature represents the decisive unique selling point of underground gas storage facilities. It is therefore necessary to deal with them specifically in connection with hydrogen.

The starting point for determining the H_2 storage potential in Germany was the current storage overview of the LBEG[18]. There are currently 47 UGS in operation in Germany (Figure 18); of these, 16 are pore storage facilities and 31 are cavern storage facilities.

Pore storage facilities are primarily characterised by their size (i.e. the storage volume). The disadvantage is that pore storage facilities contain residues of the gas that was contained in this geological structure before the planned use over a long period of time.

Cavern storage systems are characterised by a free cavity volume, great flexibility in switching between injection and withdrawal operation, higher feeding-in and out rates, relatively low cushion gas content, and a lower risk of contamination of the hydrogen by added gases or lower microbial activity in the cavern. The quality of the stored gas is determined mainly by the added gases that are also introduced into the cavern.

From a technical point of view, different conversion processes are to be expected in the two UGS types. In principle, caverns are suitable for hydrogen storage. This does not exclude case-by-case tests depending on the previous use and geometry of the cavern.

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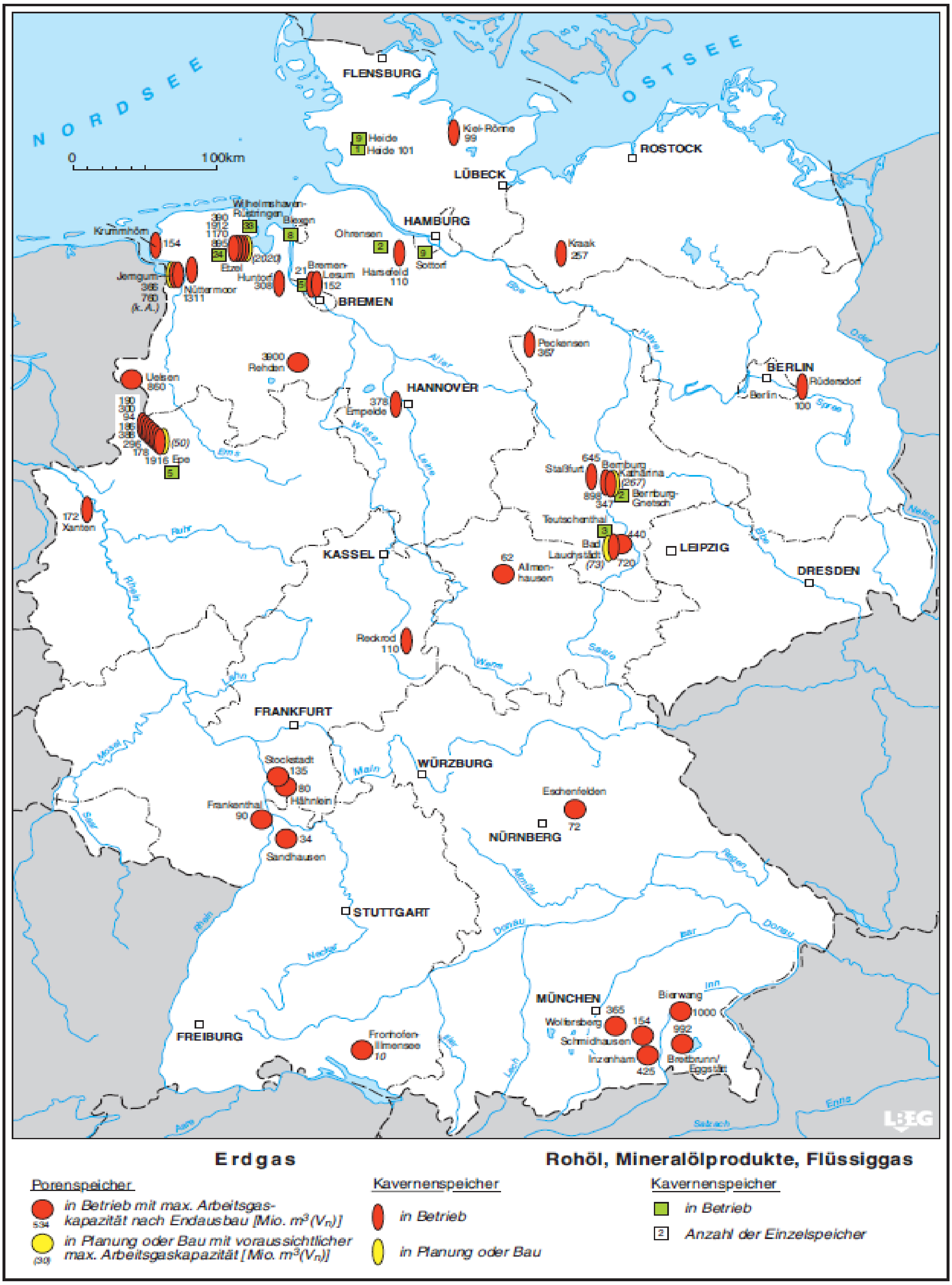
[18] LBEG – Status 2020, available at: https://www.lbeg.niedersachsen.de/erdoel-erdgas-jahresbericht/jahresbericht-erdoel-und-erdgas-in-der-bundesrepublik-deutschland-936.html



LBEG Hannover - L3.6 - Anl_14 Untertagespeicher_2020.fh11 Stand: 31.12.2020

Figure 18: Overview of gas storage facilities in Germany (LBEG – as of 2020)[19]

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[19] LBEG – Status 2020, available at: https://www.lbeg.niedersachsen.de/erdoel-erdgas-jahresbericht/jahresbericht-erdoel-und-erdgas-in-der-bundesrepublik-deutschland-936.html

5.2 Specific differences

Basically, two different types of underground gas storage facilities are distinguished:

- Pore storage facilities, which, in turn, can be divided into aquifers and depleted oil and gas reservoirs
- Cavity storage facilities, which can be divided into salt cavern reservoirs (the most common type in Germany) and special types such as old mines and rock caverns.

In the following sections, the essential characteristics of pore and cavern storage facilities are outlined. Depending on their geological conditions, different impurities of the storage gas are to be expected. Because of this, the processes that influence the gas quality must be dealt with in detail. This is done in Section 5.5.

The main differences between cavern storage and pore storage are storage capacity and storage flexibility.

- Pore storage facilities have much larger storage volumes; however, their geological conditions make them less flexible than caverns.
- Cavern storage facilities are characterised by a lower proportion of cushion gas (KGV) than pore storage facilities.

The main differences are summarised in Appendix 3. With regard to the gas quality in underground hydrogen storage, the following specific differences between pore and cavern storage facilities should be highlighted in particular:

- Injection and withdrawal rates: Cavern UGS are flexible and, because they are not bound to a pore structure, could technically be filled and emptied several times a year.

- Pore UGS have a heterogeneous environment; this leads to various possible added gases. Whilst gas drying is always necessary, gas treatment can be more complex for pore UGS than for cavern UGS because of the large number of added gases.

In summary, cavern storage facilities are much more flexible and thus easier to plan because of the lower technical requirements than for pore storage facilities.

In this study, the focus is on cavern UGS. Knowledge about possible contamination of hydrogen by processes in pore storage facilities is nevertheless necessary and should be the subject of further investigations because this affects not only German pore UGS but also pore UGS abroad. These will be used for hydrogen storage, after which the temporarily stored hydrogen will be exported to Germany with any additional accompanying gas substances.

Total and working gas volumes for natural gas are publicly available for both cavern and pore storage. Furthermore, data on the depth and the maximum injection and withdrawal rate are available.

The storable hydrogen volume (total and working gas volume) can be calculated individually based on the minimum and maximum pressures as well as the temperatures in the storage tank. In the context of this study, the work carried out in the reference project “HyReady”, WP 3 [24], was used: in this project, data on 725 UGS in Europe, the US and Canada were researched for the storage types cavern, aquifer, and depleted reservoir. The starting point was the Gas Infrastructure Europe database [25], which was supplemented with data from a wide range of sources of non-European UGS. Using this data, the working gas volumes of natural gas were converted to those of hydrogen by means of the gas equations for natural gas and hydrogen:

$$p \cdot V = m \cdot R_i \cdot T \cdot Z(p,T) \qquad \text{Equation 8}$$

$$V_N = V_{(p,T)} \cdot \frac{p_{res}}{p_N} \cdot \frac{T_N}{T_{res}} \cdot \frac{1}{Z(p,T)} \qquad \text{Equation 9}$$

Equation 9 can be set up for hydrogen as well as for natural gas. Because the value for the gas volume is the same under the pressure and temperature conditions in the storage tank ($V_{(p,T)}$), the following overall equation can be established.

$$WGV_{H_2} \cdot \frac{p_N}{p_{res}} \cdot \frac{T_{res}}{T_N} \cdot Z(p,T)_{H_2} = WGV_{Natural\ gas} \cdot \frac{p_N}{p_{res}} \cdot \frac{T_{res}}{T_N} \cdot Z(p,T)_{Natural\ gas} \qquad \text{Equation 10}$$

Equation (10) can be rearranged according to the working gas volume of hydrogen so that the quantities p_N, p_{res}, T_N, and T_{res} are truncated. The following equation results for the determination of the hydrogen working gas volume:

$$WGV_{H_2} = WGV_{Natural\ gas} \cdot \frac{Z(p,T)_{Natural\ gas}}{Z(p,T)_{H_2}} \qquad \text{Equation 11}$$

The results of the “HyReady” project were evaluated to determine whether average conversion factors between natural gas and hydrogen WGV – subdivided into the different UGS types – can be determined. For this purpose, the mean values of the WGV for hydrogen were compared with those of natural gas, and the conversion factors summarised in Table 17 were established:

Table 17: Conversion factors determined from comparative project

	Conversion factors natural gas volume: H_2 (mixed gas) volume
UGS types	100 vol. % H_2
Cavern storage	0.679
Pore storage facility	0.691

The reduced hydrogen working gas volume compared with natural gas (under the same pressure and temperature conditions and the same geometric storage volume) is due to the lower density and compressibility of hydrogen compared with natural gas.

The energetic storage capacity for hydrogen (blends) is additionally reduced by the approx. 3.5-fold lower heating value of hydrogen compared with natural gas. Furthermore, the publicly available data was used to determine how homogeneous or heterogeneous the cavern and pore storage facilities are. For this purpose, a comparison of the ratio of the working gas volume to the total gas volume was set up.

The cavern UGS are considerably more homogeneous in terms of the working to total gas volume compared with the pore storage facilities (Figure 19).

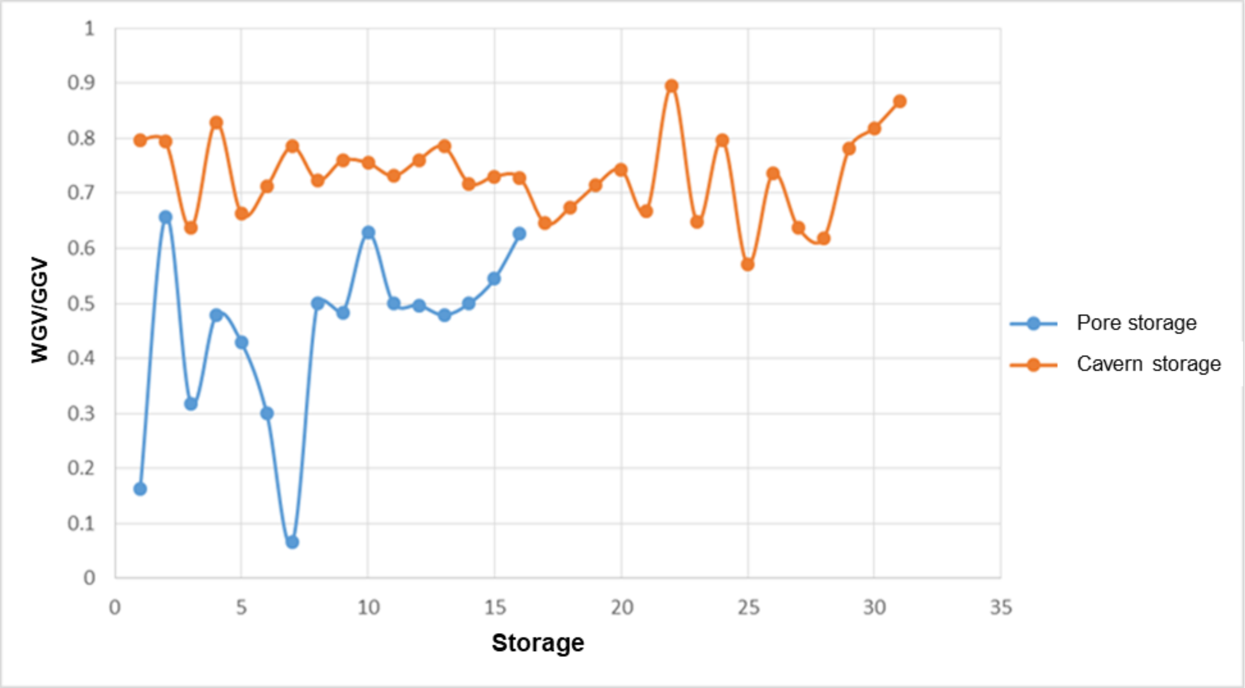

Figure 19: Relationship between WGV and KGV ratio for the German UGSs

Compared with natural gas operation, hydrogen operation requires about 3.5 times the volume flow in order to provide the same energy-equivalent injection and withdrawal capacity. However, this is not possible without further adaptation measures because of the limitations of

- pipe diameters and the limitation of flow velocities (avoidance of abrasion)
- in the case of cavern storage, the maximum permissible pressure change of 10 bar/d (guaranteeing geomechanical stability)
- in the case of pore storage tanks, by properties of the pore space (porosity and permeability)
- compressors because of their outlet pressure and
- in gas processing because of the efficiency of the processes (necessary residence time of the gas in the processing unit).

Accordingly, it is assumed that in operation with hydrogen (blends), the volumetric injection and withdrawal capacity remains unchanged compared with natural gas operation. Accordingly, the energetic injection and withdrawal capacity is reduced by a factor of 3.5 because of the lower heating value of hydrogen compared with natural gas. However, this energy supply can be increased by modifying the storage facility; this would simultaneously require an expansion of the surface facility and possibly additional caverns with larger tubing diameters as part of the new plant construction.

5.3 Comparison of hydrogen storage demand and theoretically available storage potential

In 2021, the BMWK developed various long-term scenarios for the decarbonisation of Germany by 2045 – including for the electricity and gas network. The central question was to clarify the techno-economic effects of different paths or scenarios. Here, the three scenarios listed below were modelled for the electricity and gas network under various assumptions; these differ in terms of their demand for hydrogen in the various sectors (transport, buildings, industry, and tertiary sector/appliances). Accordingly, different hydrogen storage needs were also identified at the network level.

- A scenario with heavy hydrogen use (TN-H2-G),
- An electrification scenario with heavy use of electricity (TN electricity)
- A scenario with the heavy use of synthetic hydrocarbons (TN-PtG/PtL)

The hydrogen storage requirements of the TN-H2-G and TN Electricity scenarios are summarised in Table 19 (because they contain the minimum and maximum expected H_2 storage requirements) and compared with the theoretically available hydrogen storage capacities when all existing UGS in Germany are converted (detailed gas volumes of the UGS in Germany can be seen in Appendix 2):

Table 18: Storage capacities UGS Germany and comparison with long-term scenarios BMWK

UGS types	**Cumulative storage capacity of existing UGS in Germany**					**Scenario 1: TN electricity**	**Scenario 2: TN-H_2-G**
	Natural gas WGV	H_2 WGV	H_2 WGV	Injection capacity	Withdrawal capacity	H_2 storage requirements 2045	H_2 storage requirements 2045
	million m^3 i.N.	million m^3 i.N.	TWh	1000 m^3/h	1000 m^3/h	TWh	TWh
Pore storage facility	8,615	5,952	18	3,273	6,075	73	47
Cavern storage facility	15,087	10,244	31	6,465	22,085		
Total	**23,702**	**16,196**	**49**	**9,738**	**28,160**		

To provide the H_2 storage capacities envisaged in the long-term scenarios, both the pore and cavern UGS are necessary. In the TN electricity scenario, the construction of additional storage facilities is to be expected. The expected hydrogen demand was already explained in WP1, which also includes imports.

Because of the complexity of pore storage systems, it is assumed that not all of them are suitable for hydrogen storage. Accordingly, additional caverns are necessary to cover the future hydrogen demand.

5.4 Quality changing processes in cavern storage facilities

5.4.1 General effects and processes

Caverns are usually homogeneous and dense and consist of a salt formation that does not interact with the gas during the storage process itself. Nevertheless, components are also introduced into the gas to be stored depending on the age and use of the cavern.

- Water and moisture in the cavern and sump
- Residual components of previous storage media
- Operating resources, solids

In the case of hydrogen storage, two further quality-relevant factors must be taken into account:

- Possibility of storing different hydrogen qualities (Group A or Group D) with different accompanying components
- Possibility of microbial processes in the cavern sump and transfer of gases formed here into the gas space and thus contamination of the storage gas. In particular, the formation of sulphur components, especially H_2S, must be taken into account.

The gas quality on the withdrawal side depends on the quality of the injected gas and the microbial processes that may occur in the cavern. The gas quality on the injection side can be controlled by prior treatment. However, the initial microbiology be influenced only by adding external media (e.g. pumping sterile water or bactericides). It must then be checked according to the utilisation path and the required gas quality whether it makes more sense to treat the gas before injection or after withdrawal.

In Germany, cavern storage facilities are characterised by temperatures of 15 to 60°C and the absence of oxygen. There is also a high salt content up to saturated brine and a high hydrostatic pressure.

In caverns, the micro-organisms can be introduced from outside (allochthonous) (e.g. by rinsing water during the brine process) or be present in the subsurface (autochthonous). Microbial activity is highly individual and site-specific. Initially, however, no micro-organisms occur in salt formations.

In numerous cavern UGS, the presence of thermophilic, barophilic (-tolerant), and halophilic (-tolerant) microorganisms was detected under anaerobic conditions. Figure 20 represents the diversity of micro-organisms that can be considered in a cavern storage facility based on experience.

The stimulation of microbial growth is achieved by partial hydrogen feed-in. Hydrogen serves as a universal electron donor for prokaryotes and, if suitable electron acceptors are available, is degraded with high affinity down to extremely small residual concentrations [26]. Suitable electron acceptors are nitrate (or nitrite), sulphate, metal ions (e.g. trivalent iron), elemental sulphur, and CO_2. The products are N_2 or NH_3 from nitrate reduction, H_2S from sulphate reduction and sulphur reduction, reduced Fe(II) salts from iron reduction, and methane or acetic acid from CO_2 reduction.

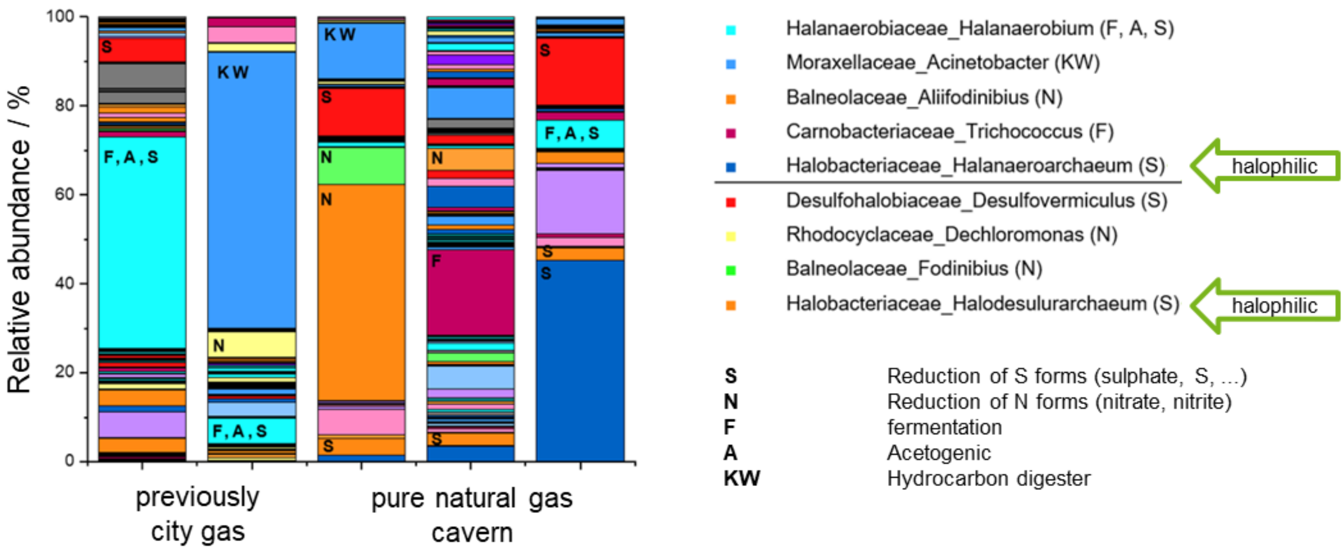

Figure 20: Microbial diversity of the barracks swamps (MicroPro)[20]

The Halobacteriaceae (halophilic) are highly important because they can cause sulphate reduction and thus the formation of H_2S (see Figure 21:).

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[20] *MicroPro, Isodetect shown in consortium meeting H_2 UGS 20 April 2020*

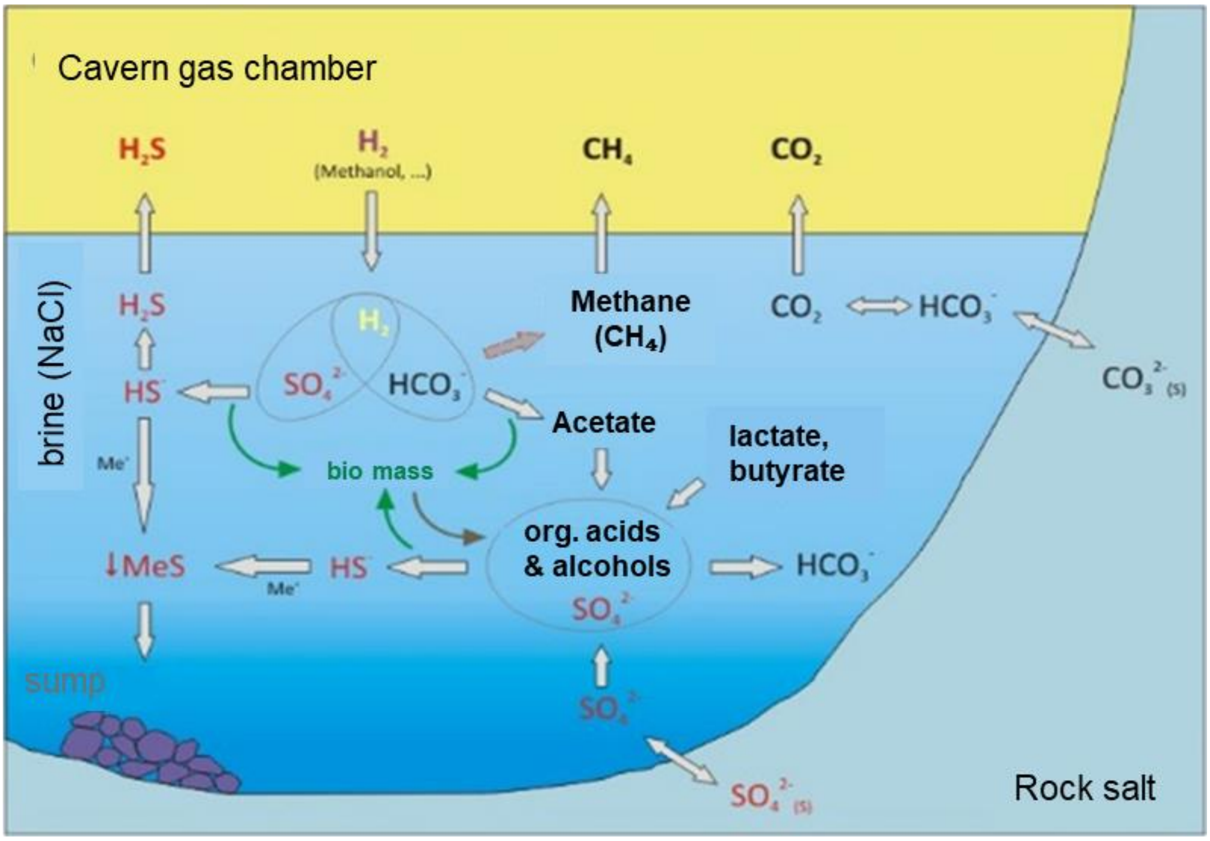

Figure 21:possible reactions in barracks swamp (MicroPro)[21]

In order for these metabolic processes and reactions to take place, a carbon and/or sulphate or sulphide source is necessary in addition to the energy source hydrogen. This is important in converted oil and gas caverns if a certain amount of residual natural gas or oil remains in the cavern or settles in the sump during the conversion process. Another carbon source is in the brine process if diesel was used as a blanket. Sulphur compounds are also introduced with the diesel.

On the other hand, whether methane or acetic acid is produced from CO_2 reduction is not readily predictable and depends on specific environmental parameters. Laboratory tests showed that methanogenesis ($CO_2 + 4H_2 \rightarrow CH_4 + H_2O$) does not take place at a salinity of more than 150 g/l.

If these reactions take place in the cavern, additional technical effort is required for gas treatment, and the well completion is subject to faster wear (e.g. because of the corrosion of the safety equipment (e.g. tubing, USAV, packers)).

The use of hydrocarbons as a blanket in the cavern serves to physically separate the brine from the gas phase above or to protect the cavern roof during solution mining. Mixtures of high-boiling hydrocarbons are used as blanks. From these mixtures, individual components – in this case hydrogen – can diffuse into the gas phase. The concentration in H_2 depends on the vapour pressure and thus on the chain length of the hydrocarbons. In this way, the concentration of high-boiling hydrocarbons could remain below the permissible value of 2 ppm in hydrogen – also depending on the gas temperature. Thus, the occurrence of an increased concentration of hydrocarbons in the hydrogen is to be classified as storage-specific. This did not play a role in natural gas; knowledge of the phase transition liquid (blanket)/gas phase (hydrogen) must therefore be classified as incomplete.

For the long-term protection of plant inventory and equipment and to ensure consistent gas quality or high

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[21] MicroPro, Isodetect shown in consortium meeting H_2 UGS 20 April 2020

hydrogen purity, avoiding contamination before the injection process is key. Practical examples show that this can be achieved for newly constructed caverns.

5.4.2 Microbial activity of newly constructed caverns

A prediction regarding the formation of sulphur compounds in caverns that have not yet been used for the storage of natural gas is hardly possible; the formation must therefore be classified as storage-specific. The basic prerequisites, the presence of the two necessary components hydrogen and sulphate in the brine, are assumed. The introduction of suitable bacterial strains for H_2S formation could take place via the brine process, for example.

The introduction of bacteria into UGS is not an exceptional case and has been documented more frequently for natural gas. With regard to hydrogen, the H2UGS project is conducting [27] a targeted sampling of the brine for the microbiological investigation. Microbiological activity was detected; H_2S formation is thus expected for this cavern of the Bad Lauchstädt UGS when converted to hydrogen. The concentration of the H_2S cannot be calculated in advance because, in addition to the uncertain formation rate, the mass transfer between the brine and the gas phase (i.e. the transition of the H_2S from the brine to the hydrogen) must also be taken into account.

In another case, an H_2 cavern in the US (Moss Bluff Dome, Texas, 70–135 bar) within a hydrogen network, no microbiological activity was detected. The operator, Linde, has so far not detected any hydrogen sulphide [28]. This cavern was never used for natural gas; hydrocarbons and CO_2 were thus never available as a “food source” for micro-organisms. Linde continuously measures the CO_2 concentration in the hydrogen after it has been withdrawn from the cavern. The background is the possibility of the presence of CO_2 in the brine, which could cause microbiological activity.

5.4.3 Overview of quality changing processes

Depending on the production processes and treatment methods as well as the transport route of the hydrogen, different impurities or added gases can occur. These added gases can cause various reactions in the subsurface (Figure 21:), thereby also reducing the gas quality in the withdrawal side. A listing of the possible contamination in the injection and withdrawal side can be seen in Table 19.

Table 19: Possible added gases in the injection and withdrawal side

Injection side					Withdrawal side			
Substance	Source	new cavern	relocated cavern	influenceable (yes/no)	Source	new cavern	relocated cavern	influenceable (yes/no)
N_2	Blanket, pipeline, filling stations, transport	X	X	yes	Blanket residue	X	X	no
H_2S					SO_4^{2-} reduction by sulphate-reducing bacteria	X[19]	X	no
CO_2	H_2 process (spec. SMR)				formed by the decomposition of acetate produced by hydrogenotrophic bacteria; dissolved in brine	X[19]	X	no
H_2O	H_2 process, transport	X	X	yes	Water vapour	X	X	no
CH_4	H_2 process (spec. SMR) steam methane reforming	X	X	yes	Methanogenesis and for converted caverns, the natural gas residues also count; Remains dissolved in brine	X[19]	X	no
O_2	H_2 process (spec. electrolysis), transport	X	X	yes				
CO	H_2 process (spec. SMR) steam methane reforming	X	X	yes				
Solids (e.g. metals, dust)	Long-distance pipeline contamination				H_2 metal reaction when using unsuitable steels	X	X	no
Saline solution					Sump	X	X	no
Biofilm					underground bacterial reaction	X[22]	X	no
HC (e.g. ethane, propane, butane)	Filling stations/dirt bin trailers	X	X	yes	Diesel blanket, residual natural gas, petroleum components	(X)[23]	X	no

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[22] Depends on location. Here, proof of the micro-organisms in the subsoil is required

[23] If a hydrocarbon blanket was used for solution mining

The gas quality is strongly determined by the amount of added gases (i.e. their concentration in the hydrogen). On the injection side, water from the generation process (electrolysis, pyrolysis, ammonia cracking, steam reforming) as well as various impurities found in the transport pipelines can contaminate the hydrogen. If possible, water should always be separated at the storage tank so that condensation in the pipeline and thus further technical problems can be avoided. The impurities on the withdrawal side are essentially determined by the conditions of the geological subsurface and, in particular, by the existing remnants of earlier storage media.

In newly constructed caverns, no or only minimal contamination is to be expected on the withdrawal side. The impurities listed in Table 19 can occur only if a source of carbon and/or sulphate is present in addition to micro-organisms. These substances always originate from externally introduced media but not from the salt formation itself.

Depending on the application, it may make more sense to install the preparation on the injection or withdrawal side or alternatively directly at the user. The decision in favour of one of the three processing variants depends on the integration of the storage facility into the network (island networks, transport networks, distribution networks) as well as the quality requirements of the consumers and the storage facility itself.

However, gas drying on the withdrawal side of a UGS must be provided in any case because water is always present and this is harmful to further equipment in the process chain.

In sum, it should be clear from the outset what quality the stored gas should have. Operating a cavern storage facility with withdrawal quality of Group D while feeding-in of Group A would be possible only with a great deal of effort because

- the gas treatment would have to be adapted
- Storage tanks have a “memory”, and traces of previously stored components always remain in the cavern; this, in turn, can mix with the stored gas.

Grade A (98 mol %) hydrogen can be provided by the cavern storage. The common processing variants are capable of separating the corresponding accompanying components.

6 WP 5: Networks

A future hydrogen network will be based on the existing transport and distribution network for natural gas. This is necessary and sensible from an economic point of view but requires technical adaptations to the network depending on the condition of the pipeline section from the point of view of the quality requirements for hydrogen.

Results of the work package at a glance

- Previous use of the pipelines and their operation can lead to the introduction of substances and thus to changes in H_2 quality. Hydrogen can be transported in high quality via newly built pipelines.
- For an assessment with regard to a possible gas quality to be transported, existing pipelines and new construction as well as distribution and transmission network must be differentiated. The piggability of a pipeline facilitates its conversion to hydrogen and subsequent use for high quality hydrogen. If mains gas or, more recently, biogas was still transported in pipeline sections, additional components from the pipelines can be introduced into the hydrogen. Odorant deposits in pipeline networks can also lead to the contamination of hydrogen with these substances.
- These impurities concern components that are subordinate in terms of quantity (e.g. hydrocarbons or sulphur compounds for which very low limit values are defined, especially for Group D).
- The substances introduced via the pipelines can be removed easily and relatively inexpensively by adsorptive cleaning of the gas. It may be possible to clean the pipes at the time of conversion; however, there is a lack of practical experience.
- Thus, in principle, it is possible to feed H_2 with a high degree of purity into the network and, if necessary, to separate the individual components that are introduced by deposits in the pipelines and the operation of the network according to need

6.1 Converting pipelines/networks to hydrogen

The gas industry has the following experience regarding the conversion of gas pipelines:

- From mains gas/coke oven gas to natural gas
- From L-gas to H-gas
- the conversions of odorants

These conversions cannot be compared with the conversion of a network to hydrogen. Nevertheless, some of the experiences from these conversions help to draw conclusions for the upcoming conversion of lines to H_2. Experience is available on the group of hydrocarbons and sulphur compounds.

The aforementioned conversions did not require any separate cleaning measures. Cleaning measures such as pigging take place primarily at regular intervals in order to remove deposits and condensates and to check the condition of the pipeline section. On the other hand, in the course of converting pipelines to hydrogen, the use of cleaning pigs will be part of the standard procedure.

> Experience with hydrocarbons
>
> Long-chain or high-boiling hydrocarbons can be detected in the pipeline network even after decades. This clearly concerns naphthalene and long-chain hydrocarbons, the introduction of which ended in 1992/93. For more than 20 years, some of these compounds were detectable in the gas phase in high-pressure pipes. In deposits from distribution networks of corresponding age, naphthalene can still be detected along with other PAHs (polycyclic aromatic hydrocarbons). There is also experience with glycols. These are transported long distances (>> 100 km) when entering from the TEG gas dryers and are also detectable for a long time.
>
> The concentration of these high-boiling compounds in the gas stream is not particularly high because of the low vapour pressure; specifically, an order of magnitude of 2–10 mg/m³ is to be expected. Fluctuations are to be expected depending on the residence time of the hydrogen (flow velocity). These substances fall into the group of non-methane hydrocarbons with a limit value of 2 ppm for the quality of Group D, which would be exceeded.
>
> Experience with sulphur compounds
>
> Various sulphur compounds are quite common in pipelines. In the high-pressure system without odorisation, H_2S was continuously introduced with the natural gas – meanwhile partly bound (e.g. as FeS or as elemental sulphur in the system). From odorant conversions, it is known that sulphur compounds can still be measured in the local network months after the conversion to sulphur-free odorants. The specified limit value of 0.004 ppm in H_2 is problematic. Currently, concentrations in the range of 0.5 ppm are recorded. There is thus a lack of knowledge about the required lower concentrations (e.g. after a conversion from sulphur-containing odorants to S-free). It should be noted that the quality of this substance group will not fall below that of Group A because of desorption from the network. A general assessment regarding Group D is not (yet) possible.

The examination of deposits as well as condensates from the past decades shows that the condition of the transport pipelines varies greatly. While in some pipelines, only dry solids are obtained from pigging, in other cases, a liquid mixture of hydrocarbons, glycol, and water is obtained. The reasons for these differences are:

- the age of the lines
- quality of the transported gas (L-gas, mains gas, storage gas from reservoir, H-gas)
- possible admixtures (biogas, LPG)
- the geometry of the pipeline (e.g. the number and age of the culverts)

For the transport network, Table 20 summarises which connections could occur during and after the changeover phase. Changeover phase means that

- the cleaning measures (pigging, rinsing processes) are completed
- the gas quality has stabilised with regard to the concentration of HC and sulphur compounds
- short-chain hydrocarbons (e.g. butanes and hexanes) are discharged with the H_2
- the system has dried out or has assumed the new constant water content.

The conversion phase itself requires separate measures and is not the subject of this assessment.

The potential impurities and the development of these are shown. In any case, there will be transport pipelines that have less impurities because of their history and thus possibly reach Group D quality in the transported H_2. There is currently no experience from such conversions in order to be able to make further statements.

The following is a summary of some of the other experiences of the gas industry that have been incorporated into the statements made in Table 20 and Table 21.

- Measurements at UGS and border transfer points show that low O_2 concentrations of << 10 ppm O_2 are the rule and stable in the long term. A continuous introduction of oxygen via the network itself cannot be discerned. Currently higher oxygen concentrations in places are due to the feeding-in of biogas
- Formaldehyde (HCHO), ammonia (NH_3), and formic acid (HCOOH) are occasionally mentioned as impurities from operational processes (DIN EN 17124) but are not relevant in the long term. On the other hand, components from a long-term biogas input, could have accumulated in the downstream network and must be assessed (example: terpenes).
- CO and CO_2 from pipelines are not to be expected because as their low adsorption capacity (e.g. on pipe walls) means that these compounds will no longer be relevant after the conversion phase.
- The concentration of water will decrease rapidly when an extremely dry gas is fed into the pipe. Experience from the conversion from mains gas to natural gas showed that the pipe networks dried out quickly with the dry natural gas.

The colour representation has the following backgrounds:

- Red: relatively certain statement; impurities are to be expected and can prevent the achievement of Group A or D quality
- Yellow: uncertain; lack of corroborative knowledge, especially about the temporal development of the concentration of the component concerned
- Green: no problems are expected

Table 20: Potential contamination in the transport network before (or during) and after conversion phase

		Gas network until 1980/90; operation with mains gas/metallurgical gas		Gas network (existing); operation with natural gas only		Gas network (existing); natural gas + other components (odorization, biogas)		New building	
		Limit value Group A	Limit value Group D	Limit value Group A	Limit value Group D	Limit value Group A	Limit value Group D	Limit value Group A	Limit value Group D
Material		Steel		Steel		Steel		Steel	
Cleaning/pigging necessary			yes		yes		yes		?
relevant substance groups/components	Hydrocarbons	🟩	🟥	🟩	🟥	🟩	🟥	🟩	🟩
	Water	🟩	🟨	🟩	🟨	🟩	🟨	🟩	🟨
	Sulphur compounds	🟩	🟨	🟩	🟨	🟩	🟥	🟩	🟩
	Inert gases + O_2	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩
	CO, CO_2, methane	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩
	Other	🟩	🟩	🟩	🟩	🟩	🟥	🟩	🟩
relevant substance groups after conversion	Hydrocarbons	🟩	🟨	🟩	🟨	🟩	🟨	🟩	🟩
	Water	🟩	🟨	🟩	🟨	🟩	🟨	🟩	🟨
	Sulphur compounds	🟩	🟨	🟩	🟨	🟩	🟨	🟩	🟩
	Inert gases + O_2	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩
	CO, CO_2, methane	🟩	🟩	🟩	🟩	🟩	🟩	🟩	🟩
	Other	🟩	🟩	🟩	🟩	🟩	🟨	🟩	🟩
		🟩	🟩	🟩	🟩	🟩	🟨	🟩	🟩

This representation reflects the expectation that the H_2 quality of Group A can be handed over to the buyers without major problems from the pipeline system. However, long-chain hydrocarbons, similar to sulphur compounds, are expected to remain an uncertainty for years, and their occurrence is possible even after the conversion period.

In contrast to the transport network, the **distribution** network (with a few exceptions) cannot be cleaned by pigging. Flushing with water analogous to sections of transport pipelines is also not possible because the water would not be easy to remove.

Thus, over longer periods of time and thus also beyond a changeover phase, connections that make it difficult to distribute H_2 quality of Group D are to be expected. Newer nets can make this possible if they have seen only gases with little added gases. The group “Other” contains rather gas-atypical compounds primarily from biogas plants. On average, these have a high technical standard with activated carbon filtration. Nevertheless, it is always noticeable that individual connections (e.g. CS_2) break through these and are detected in the downstream network.

Table 21: Potential contamination in the distribution network during and after the conversion phase

		Gas network until 1970/80; operation with mains gas		Gas network (existing); natural gas + other components (odorization, biogas)		New building	
		Limit value Grade A	Limit value Grade D	Limit value Grade A	Limit value Grade D	Limit value Grade A	Limit value Grade D
Material		Cast iron, steel		Plastic, (steel)		Plastic	
Cleaning/pigging possible		no		no		no	
relevant substance groups/components	Hydrocarbons	🟩	🟥	🟩	🟥	🟩	🟩
	Water	🟩	🟨	🟩	🟨	🟩	🟩
	Sulphur compounds	🟩	🟨	🟩	🟥	🟩	🟩
	Inert gases + O_2	🟩	🟩	🟩	🟨	🟩	🟩
	CO, CO_2, methane	🟩	🟩	🟩	🟩	🟩	🟩
	Other	🟩	🟩	🟩	🟥	🟩	🟩
relevant substance groups after conversion	Hydrocarbons	🟩	🟥	🟩	🟥	🟩	🟩
	Water	🟩	🟨	🟩	🟨	🟩	🟨
	Sulphur compounds	🟩	🟨	🟩	🟥	🟩	🟩
	Inert gases + O_2	🟩	🟩	🟩	🟨	🟩	🟩
	CO, CO_2, methane	🟩	🟩	🟩	🟩	🟩	🟩
	Other	🟩	🟩	🟩	🟨	🟩	🟨

Overall, however, it can be summarised that the distribution of an H_2 quality of Group A is also possible in the distribution network.

Estimating the duration of a conversion phase is somewhat speculative. However, it will always be a matter of months or years; short periods of weeks or a few months seem unrealistic according to current knowledge.

6.2 Other components in the hydrogen network

Odorisation is a special case; however, in Germany it is practised mainly in the distribution networks. According to current regulations, hydrogen must be odourised for supply in public spaces. Current odorants, whether sulphur-free or not, interfere with individual users such as PEM-FC and would be removed accordingly prior to such applications. At the moment, there is consensus in the European natural gas industry that the odorisation measure is also necessary for hydrogen as a safety measure vis-à-vis the public gas customer, although central odorisation will continue to be carried out in the transport network on a European scale. There are two possibilities to solve this problem:

1. use of minimal quantities of the sulphurous odorants deodorisation before the customer
2. development of suitable sulphur-free odorants

Another special case would be the transport of hydrogen to Germany in the form of ammonia. This is then catalytically converted into hydrogen and nitrogen. Plants for this are in the prototype phase; thus no conclusive statements can yet be made about the residual ammonia and nitrogen content. However, according to BASF, a high H_2 purity analogous to Group D quality or $H_2 \geq 99.97$ mol % can be expected.

6.3 Site recommendations for gas purification and treatment under consideration of the network topology

The need for gas purification and treatment in the hydrogen network as well as the requirements for the feeders and the available hydrogen purities for the users depend largely on the purity targeted in the gas network. Here, a distinction is made between the two hydrogen purities defined in DVGW Code of Practice G 260 (A), Group A ($\geq$ 98 mol % H_2)and Group D ($\geq$ 99.97 mol-% H_2), taking into account the component-specific limits (see Table 20 and Table 21).

Within the framework of this work package, it will be worked out which gas processing plants are required at which points in the system for the two hydrogen units in the hydrogen network as well as which variant is realistically feasible and advantageous from an economic perspective.

To simplify matters, the following boundary conditions are assumed in this project phase:

- We consider the target system in which the gas networks have already been converted to hydrogen and expanded by new construction to meet demand.
- The actual network structure is not taken into account; we assume a closed system with almost the same H_2 quality from which the sectors are supplied.

6.3.1 Factors influencing achievable/desirable hydrogen purities in the hydrogen network

The answer to the question of the optimal design of the future hydrogen system in terms of targeted hydrogen purity and required processing effort depends on the three areas presented in more detail below and analysed in terms of requirements and achievable hydrogen purity.

1. Hydrogen sources
2. Hydrogen transport and distribution
3. Hydrogen sinks

Simplified, the issue can be reduced to the question: Is the hydrogen processed to the purity required by customers at the feed-in point or only before use?

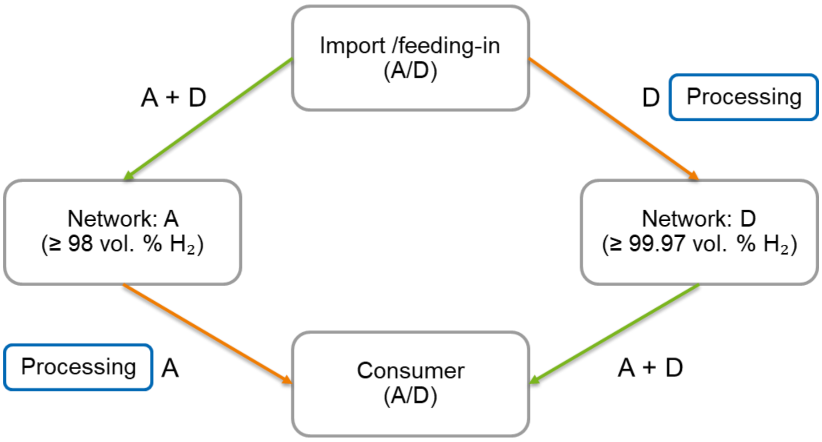

Figure 22: Basic concept for sites Gas treatment

This question can be discussed for the entire system. However, beyond that, intermediate solutions in which areas of the network are supplied with hydrogen quality that deviates from the main system are also conceivable.

6.3.1.1 Hydrogen sources of the gas network

Hydrogen generation: The purity of the hydrogen that can be fed into the hydrogen networks and imported depends on the respective generation technology and the gas treatment that may be required (see Table 16). Hydrogen from electrolysis plants meets the requirements of Group A: With integrated gas treatment, all technologies can achieve both Group A and, with increased effort, Group D.

Hydrogen import: In addition to the technologies, another key focus with regard to possible hydrogen purification units is the coordination of H_2 delivery qualities at European level. This has a considerable influence on the hydrogen qualities to be transported in European and national transmission networks. Normative coordination at the CEN level is currently in preparation.

Hydrogen storage: The third potential source of hydrogen is fed in from hydrogen underground gas storage (H_2 UGS). The hydrogen units of the different storage types that can be fed out are shown in Chapter 5, Table 19. Gas drying at the storage tank is required in any case; the treatment requirement beyond that depends on the requirements and the qualities of the individual storage tanks available.

The production and feeding-in of hydrogen is ultimately always linked to gas treatment processes, the scope and location of which vary.

6.3.1.2 Hydrogen transport and distribution

On the part of the hydrogen networks, there are no special requirements for the hydrogen quality when complying with the DVGW regulations. There are qualitative requirements for gases to be transported (e.g. restrictions on dust or condensation behaviour) to protect the overall system – both in the German and the European framework. With regard to hydrogen, the requirements in the European framework have yet to be defined.

In the run-in target state of the hydrogen system, the following sources of influence on the hydrogen purity are to be expected on the part of the network

- Work on the network (repairs, maintenance, pigging, other work (e.g. sampling), and new connections) and operation of the network (e.g. oil slippage through compressors)
- Integration of new pipeline sections from new construction or conversion
- Introduction of impurities from converted pipelines (see Section 6.1)

When working on the network, the work itself (i.e. contamination of the new pipeline sections, possible purging processes with inert gas and the (re)commissioning[24]) can lead to the introduction of nitrogen/air, water, and contamination from welding or drilling work.

Work on the network: Welding or drilling work can lead to contamination with particles; these can be removed by filters (e.g. in the following GDRA).

New construction and conversion: The introduction of non-hydrogen gases can lead to “bubbles” in the network with a gas composition that deviates from the target purity. The size of the bubble depends, among other things, on the size of the affected pipe section; the amount of deviation from the target value can be influenced by the design of the flushing process. According to DVGW G 466-1, when flushing pipe sections with inert gas (nitrogen), an oxygen content < 1 vol. % must be verified; a flushing process with hydrogen must be considered separately, taking into account the operating parameters. An update and adaptation of the underlying DVGW rules and regulations is necessary and sensible depending on the purity targeted for hydrogen.

Entry from converted lines: Possible impurities from converted pipeline sections can be introduced for many years after the conversion. An overview of the substances that can be introduced is shown in Section 6.1. The existing pipelines can be roughly divided into the following classes: transmission and distribution network and the generations

- Existing until approx. 1980/90 (operation with mains gas, metallurgical gas)
- Existing; operation with natural gas only (concerns only the transport network level)
- existing, operation with natural gas and other components (odourisation, biomethane)

with different substance groups from the historical operation and different possibilities for cleaning.

In all cases of conversion of existing pipelines, hydrocarbons from transport and distribution of natural gas and sulphur compounds are still to be expected after conversion – even after possible pigging. In pipes where biogas has been distributed, other components such as terpenes or additional sulphur compounds such as CS_2 may be present.

Overall, the number of possible sources of contamination of the hydrogen by the hydrogen network is limited. In principle, they can occur at all points in the network. The expected order of magnitude of the proportions of relevant substance groups in the hydrogen after conversion is so high that operation of the converted networks with Group D quality can be guaranteed only to a limited extent or not at all, especially in the distribution network. These restrictions do not apply to newly constructed lines. They are nevertheless relevant and must be taken into account in a network consisting of both converted and newly constructed line sections. In contrast, the requirements for hydrogen of Group A quality (≥ 98 mol %) can most likely be met in all variants.

Even in newly constructed pipelines, ensuring Group D can be challenging, especially with regard to the limit

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[24] DVGW Code of Practice G 465-2 (previously applicable only to natural gas) or G 466-1

value for water. There is a lack of experience in how far the water content in these networks can be kept at a low level.

A purity of 99.99 vol. % H_2 is guaranteed for a privately operated H_2 network in the US. However, the extent to which this can be transferred to a much larger hydrogen network with many operators is currently difficult to estimate.

6.3.1.3 Hydrogen sinks

The hydrogen sinks in the form of customer/gas applications define the required hydrogen purities through their processes. These must be achieved either from the network or through gas treatment upstream of the customer. Further requirements result from the H_2 UGS and downstream networks (European and national transmission networks, distribution networks). The challenges here are primarily on the part of the customers/gas applications.

6.3.2 Possible configurations for a future hydrogen network

The considerations in Section 3 have shown the following:

- The provision of hydrogen from production and feeding-in can be carried out with either Group A or Group D depending on the processing effort.
- The requirements for the purity of hydrogen at the European level still require coordination; this then influences the European and national hydrogen networks (coordination at the CEN-TS level)
- The requirements on the part of H_2 UGS for the hydrogen purity depend, among other things, on the storage type; the withdrawal and feeding-in into the hydrogen networks requires processing in any case. This includes at least one drying and, if necessary, further gas treatment plants depending on the requirements and boundary conditions of the respective storage facility.
- The hydrogen network in itself does not place any special requirements on hydrogen purity. However, the planned conversion of existing pipelines leads to the potential introduction of various substance groups from historical operation.
- On the user side, there is a differentiated picture with regard to the requirements for hydrogen purity.

Accordingly, the converted network components of the hydrogen network limit the guaranteed purity of the hydrogen in the system to Group A. However, operation with Group D is conceivable in separate (sub-) networks that are either newly constructed or, in the case of conversion, appropriately cleaned and tested.

In the following, the two borderline cases “A network” and “D network” are presented as examples, whereby A or D defines the gas transported in the leading system (transmission networks). The differences lie mainly in the location, number, and performance of the treatment plants required for the respective configuration. This can be broken down again to the basic question of “centralised” (at the point of feeding-in) or “decentralised” gas processing. Beyond that, however, there are essential points that must be taken into account in both variants. This is, on one hand, the gas treatment when feeding out the H_2 UGS and, on the other hand, the handling of inputs from pipeline sections polluted by historical operation that are converted for an H_2 network. Both require case-by-case considerations depending on the specific challenge.

The challenge for an A network is to purify the gas to Group D as required upstream of the respective user or downstream of networks that are operated with Group D quality. In this case, gas processing is mainly decentralised with considerably more and therefore smaller plants. These will have a higher investment volume in terms of specific plant costs and will have to be integrated into the overall system in a more energy-intensive way. For this purpose, only that a portion of the hydrogen needed for the application is processed as far as possible.

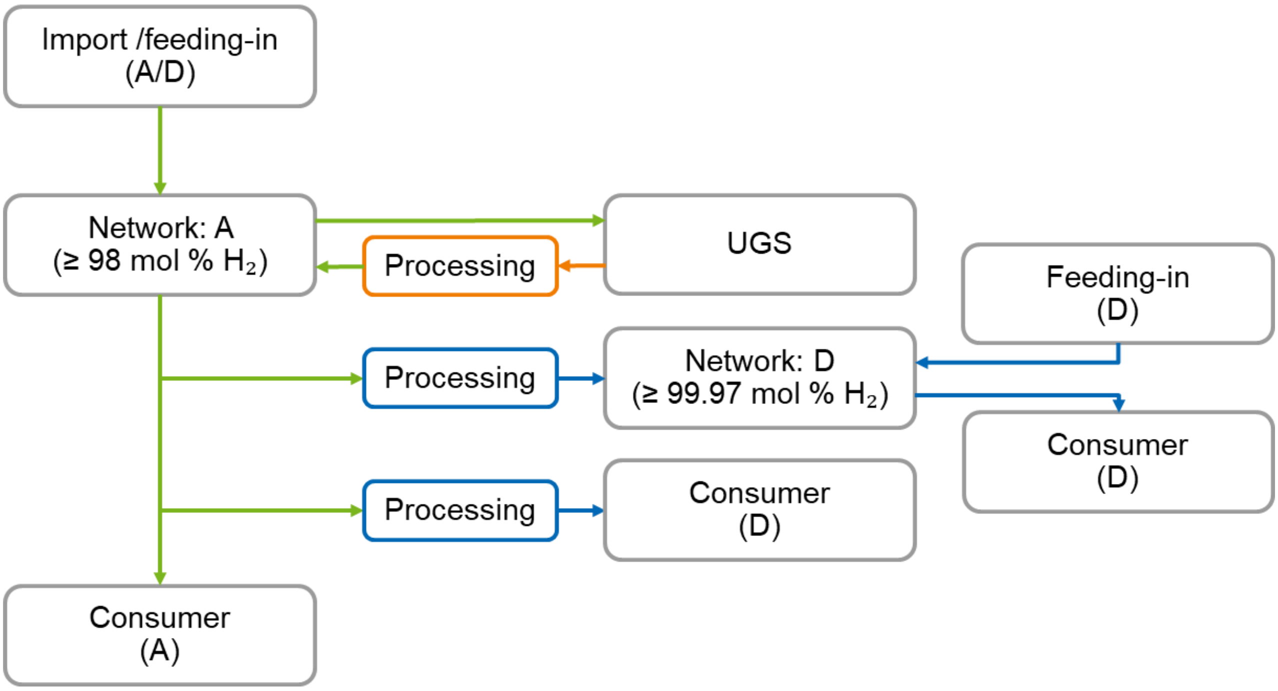

Figure 23: Concept: A network

On the other hand, the D network is based on central processing at the hydrogen feed-in point and feeds into the overall network with Group D quality. It can be understood both as a complete system and as a subset of the A network to provide Group D on a local or regional basis. Here, the restrictions described above with regard to switched lines must be taken into account.

In this variant, gas processing is carried out mainly centrally at the feed-in point so that fewer but larger plants are needed. In addition, the entire quantity of hydrogen is purified/processed here to Group D – even for those applications that would cope with Group A quality.

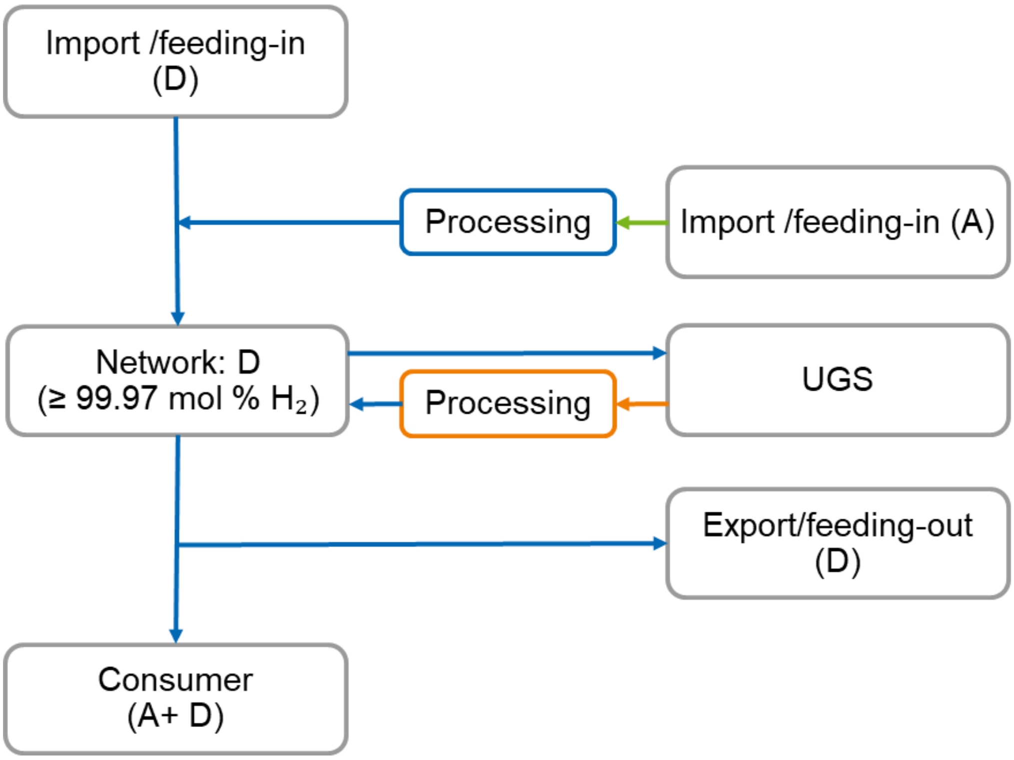

Figure 24: Concept: D network

As a further variant for a system based on existing pipelines, a network can also be fed with high-purity hydrogen (Group D) so that the processing effort can still be carried out centrally at the feed-in point with only a few larger plants. The possible introduction from the existing pipelines can then be removed with relatively simple and inexpensive gas purification systems. These would have to be placed upstream of the consumers with corresponding hydrogen requirements or upstream of sub-networks based on new construction.

7 WP 6: Definition of process chains and reprocessing requirements

The supply of potential H_2 customers requires the supply of Group D quality in various cases. In the hydrogen network, this can be offset by the somewhat lower quality of Group A. Gas treatment is therefore necessary; the extent of this depends on the following factors:

- Composition of the 2% “residual component” (if Group A was fed in)
- Condition and age of the transport network as well as the possibly integrated distribution network
- Intermediate storage of the hydrogen
- Customer requirements (chemical, H_2 filling station, household, commercial, stationary fuel cells, PtX processes)

In addition, any necessary processing steps could be carried out spatially separately. This results in many possible scenarios, the evaluation of which must be carried out from a technical, ecological, and financial point of view.

In order to show the considerable differences in terms of the effort, scope, and ultimately also the costs of such process chains, three different scenarios are evaluated below. It is shown that different purification methods exist and that the costs depend on the necessary purification cascade. These scenarios are intended to exemplify the range of different potential treatment costs in this study.

The following results of the calculations can be summarised:

- There are no treatment costs for the network operator if the electrolyser is equipped with treatment and the hydrogen is transported to the customer via new pipelines.
- The costs of a gas treatment vary greatly; in the calculated cases, from €0.15 /kg H_2 to €1.09/kg H_2. These additional costs are to be added to the production costs of Group A quality hydrogen. The cases considered are not comparable with each other; some cases are shown as examples.
- Decisive for the costs are the throughput of the treatment plant as well as the operating costs (OPEX). The aim is to continuously operate a treatment plant (e.g. at a transfer point) – ideally to supply several consumers.
- The OPEX can be quite high for PSA (treatment of Group A to Group D quality) because of the hydrogen losses during the desorption phase. It would have to be examined whether such processes can be avoided (e.g. by taking over a Group D H_2 purity unit, using membrane processes, or supplying customers with lower H_2 quality requirements).

7.1 Scenario 1: Electrolysis direct supply

The most common case is currently the construction of an electrolysis plant with the hydrogen produced being piped directly to a customer. Group D hydrogen is required at the customer’s site. This application could be an H_2 filling station.

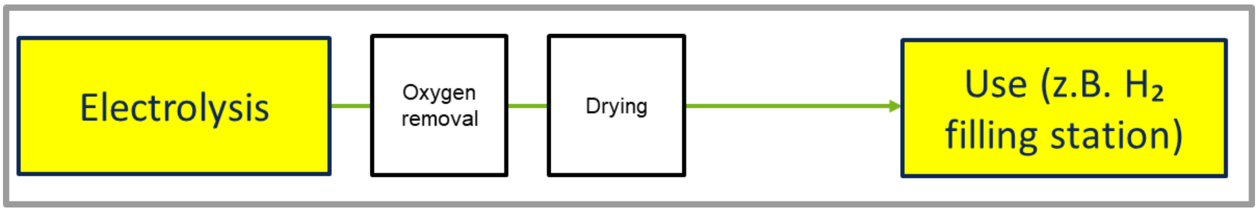

Figure 25: Scenario 1, Direct supply to a customer from electrolysis with new pipeline

This case can be seen as a complete unit; the electrolysis supplies an H_2 filling station directly. Gas treatment is necessary and coupled to the electrolysis. The research showed that the gas treatment required here (oxygen removal and drying) is a standard component of electrolysis. Oxygen removal is always included in the scope of delivery of an electrolysis. A market survey from January 2022 [29] confirms that almost all electrolyser manufacturers guarantee a hydrogen quality of ≥ 99.99 mol %. Group D quality can be taken over directly by the network operator; in this case, the costs of processing would be included in the hydrogen purchase price. There is no change in this gas quality in the new pipeline.

In a few cases of electrolyser manufacturers, a quality of "only" 99.9 mol % is guaranteed because of a higher water content [29]; a further drying stage is thus necessary in order to achieve a quality of 99.97 mol %.

In the following, this case is considered from a calculatory point of view; an additional drying stage for the production of Group D quality is built and operated. 1,000 m^3 of hydrogen/h are produced and transported at a pressure of 8 bar_a. In this case, green hydrogen is produced from wind power, and 5,000 full-load hours per year of electrolysis operation are assumed according to the usual wind load profiles.

7.2 Scenario 2: H_2 filling station

A hydrogen filling station is supplied as a user with an H_2 demand of approx. 500 m^3/h via an existing pipeline converted to hydrogen. The distribution takes place at 16 bar; the hydrogen comes from a UGS. The hydrogen quality of Group D (99.97 mol %) was fed into this. The necessary H_2 quality for the filling station is defined as Group D.

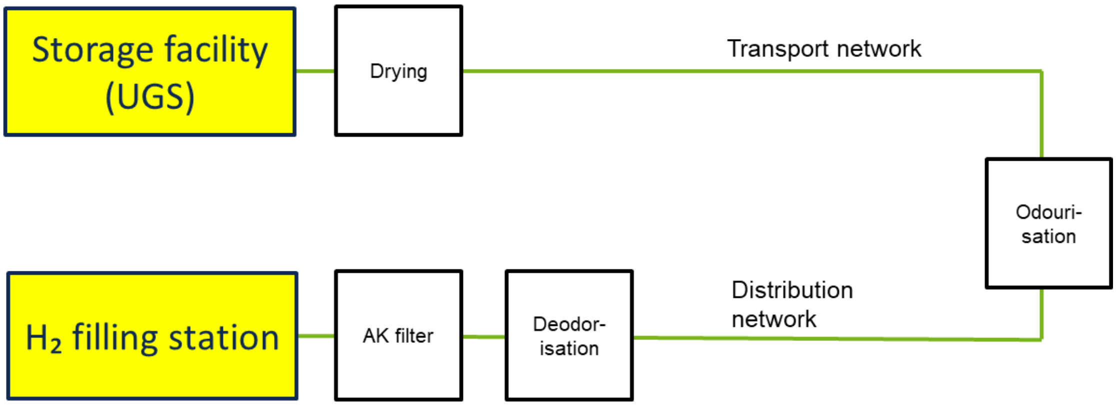

Figure 26: Scenario 1 of hydrogen use, filling station supply

The following expenditure is necessary for the gas preparation:

- at the UGS, the drying process is changed. Instead of a TEG drying system, a molecular sieve drying system is installed, thereby resulting in higher operating costs.
- A deodoriser (e.g. in the form of an adsorber filled with a molecular sieve). A sulphur-containing odorant is used.
- An activated carbon filter to retain hydrocarbons desorbed from the hydrogen network.

In this scenario, no desulphurisation is necessary at the storage tank. It is assumed that the transport and distribution network are dried; drying to the required 5 ppmv H_2O per m³ before the filling station is not necessary.

This is a relatively simple scenario; the necessary treatment stages are also currently used for natural gas.

The integration of a storage facility is advocated by companies in the chemical industry for reasons of redundancy and security of supply. An example of this is the statement made by Linde at the Leuna site to the consortium of the “Bad Lauchstädt Energy Park” lighthouse project.

7.3 Scenario 3: Supply of a customer in the chemical industry

The supply of a chemical plant also requires at least H_2 quality of Group D. The starting point is the adoption of Group A quality by the hydrogen network operator. Extensive gas treatment (

Figure 27) with 10,000 m³/h of hydrogen to be purified is planned. This corresponds, for example, to the scale of the current “Bad Lauchstädt Energy Park” project in which an electrolysis plant will produce approx. 6,000 m³ of H_2 per hour and deliver it to a customer in the Leuna Chemical Park.

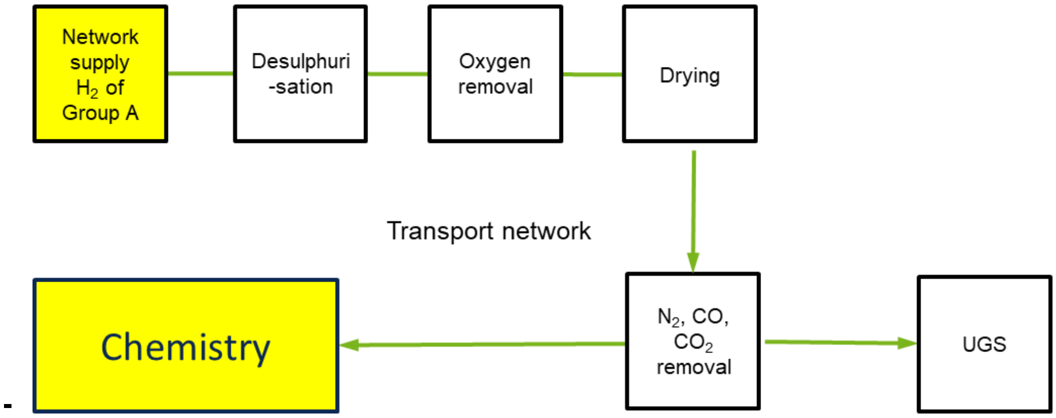

Figure 27: Scenario 3 of hydrogen use, supply of chemical plant

The following processing effort is incurred:

- A desulphurisation unit removes hydrogen sulphide
- Catalytic oxygen removal is necessary. The resulting water is retained in a molecular sieve adsorber.
- Other components must be removed from the 2% range by means of pressure swing adsorption – specifically N_2 and CO_2.

There is no need for an additional activated carbon filter to remove hydrocarbons from the hydrogen network; this task is performed by the existing adsorbers. Odorisation and thus subsequent deodorisation is not necessary in the transport network. These treatment steps would also be necessary to fill an underground gas storage tank with the recommended H_2 quality.

7.4 Economic consideration of the different gas treatment variants

7.4.1 Scenario 1

Electrolysis requires an additional drying stage, and the dried gas is fed to the user via a new pipeline.

Output parameters:

- Gas flow: 1.000 m^3/h = 84.1 kg/h
- Pressure: 8 bar(a)
- Plant running time h/a: 5,000 h (factor in year 0.57)
- Hydrogen kg/a 420,050 (at 5,000 h)

Fixed economic parameters:

- Inflation: 2%/a
- Cross WACC WS: 5%/a
- Depreciation period: 20 a
- Energy costs 0.17 €/kWh

The hydrogen production price in its range from grey to green hydrogen is not relevant for the cost calculation in this case.

The CAPEX include only adsorptive gas drying; the molecular sieve is regenerated. Regeneration takes place without the loss of hydrogen. First, an adsorber is charged with moist hydrogen. In the product gas line (dry hydrogen), the dew point is monitored by means of a humidity sensor. If the water content in the product gas increases, the moist hydrogen is automatically switched to the second adsorber. For regeneration, part of the reactant gas flow is branched off via a throttle valve, heated, and passed over the adsorber to be regenerated. The hot humid gas is cooled, and any condensate is separated. The cooled gas is then fed to the main gas stream and thus to the adsorber for drying. This process is reciprocally operated. Because of this mode of operation, there are no gas losses. Operating costs result from the heat required to desorb the water as well as maintenance and support of the plant. The investment costs of the plant amount to approx. €530,000 (CAPEX) and the operating costs (OPEX) to €25,960/a

The following costs were determined.

Costs:

• CAPEX (€/kg H_2)	€0.084
• OPEX (€/kg H_2)	€0.060
Total	€0.144

This results in additional costs of €0.147/kg for the hydrogen in addition to the calculated cost price.

To show the range within a scenario, the full load hours were reduced by 20%, and the electricity price was increased to €0.25/kWh:

• CAPEX (€/kg H_2)	€0.126
• OPEX (€/kg H_2)	€0.091
Total (€/kg H_2)	€0.217

It should be emphasised again at this point that the investor (network operator, stakeholder) usually buys an electrolyser, including complete treatment; the gas treatment costs are covered by the purchase of the electrolyser as a complete package. The additional treatment costs then amount to zero. In the event that fine drying at the electrolysis is dispensed with, additional costs in the order of €0.15–0.22/kg H_2 arise.

The following figure shows the dependence of treatment costs on various factors for Case 1 (sensitivity analysis). The starting point and centre of the figure are the mean calculated cost range (€ 0.18/kg H_2) and the mean electricity cost range (€0.21/kWh)

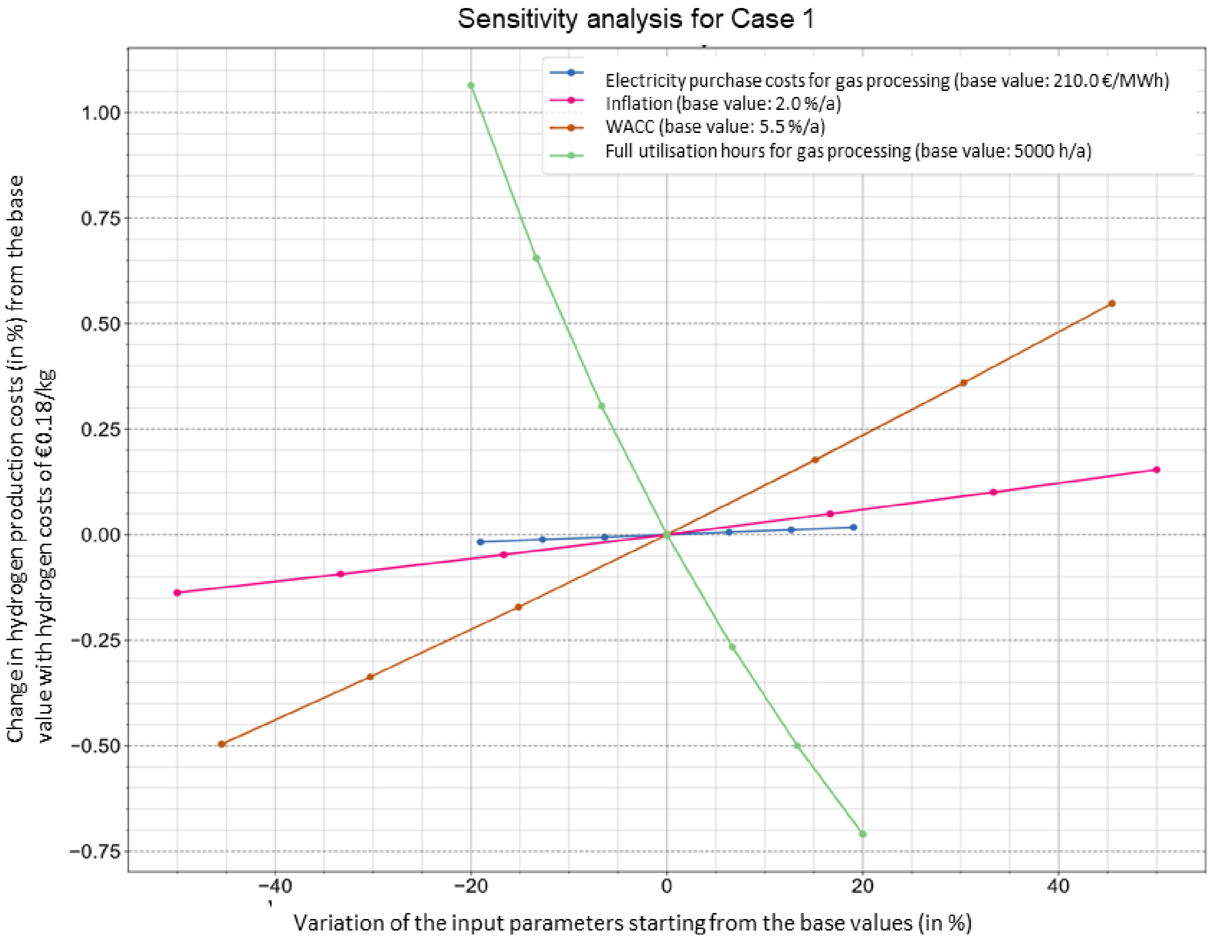

Figure 28: Sensitivity analysis of cost calculation for Scenario 1

The electricity purchase costs are of little relevance: The operating hours of the treatment should ideally be quite high; this would speak in favour of linking treatment plants.

7.4.2 Scenario 2

Hydrogen is fed out of a UGS, and the hydrogen is transported to a hydrogen filling station via a converted former natural gas pipeline. Before this, a preparation is necessary.

The following boundary conditions are used for the cost estimate:

- Gas drying at the storage tank is carried out by means of a molecular sieve, redundant, thermal regeneration of the adsorbers, withdrawal rate approx. 1,000 m³/h H_2 (this makes it a small plant)
- Deodorisation is carried out with an adsorbent; this adsorption capacity with respect to THT is approx. 4 mass %. There is no regeneration.
- The activated carbon adsorber retains higher hydrocarbons; the activated carbon is changed and disposed of. Approx. 10 mg/m³ of hydrocarbon mix is introduced with the hydrogen from the distribution network.

Measurement technology is required only to a limited extent. Random samples are sufficient to check the gas quality; moisture and oxygen content are checked by means of a sensor at the filling station.

Output parameters:

• Gas flow:	500 m³/h = 42.05 kg/h
• Pressure:	16 bar(a)
• Plant running time h/a:	2,920 h (factor in year 0.33)
• Hydrogen kg/a	122,786 (at 2,920 h)

Fixed economic parameters:

• Inflation:	2%/a
• Cross WACC WS:	5%/a
• Depreciation period:	20 a
• Energy costs	0.17 €/kWh

The hydrogen production price is also not relevant for the cost calculation in this case.

For technical reasons, no H_2 losses from a treatment process need to be taken into account in this scenario either. Compression steps or temperature control of the gas are not necessary except for the regeneration of the molecular sieve adsorber.

The calculatory integration of the storage is problematic. A UGS is designed for feeding-out volumes ≥ 100,000 m³/h, and such volumes are to be expected in the long term. In this way, the investment costs (CAPEX) are distributed among several customers. In order to enable a presentation nevertheless, two cases were calculated:

- Case 1: without drying at the storage facility (CAPEX €303k)
- Case 2: the costs of drying from Scenario 1 are added, but the OPEX are calculated down to the real throughput. (CAPEX €687k)

Costs:

	Case 1 (without drying)	**Case 2 (with drying)**
• CAPEX (€/kg H_2)	€0.115	€0.262
• OPEX (€/kg H_2)	€0.116	€0.158
Total (€/kg H_2)	€0.237	€0.426

With a 40% increase in the CAPEX and an increase in electricity costs to 0.25 €/kWh, the treatment costs rise in total to 0.60 €/kg H_2 in Case 3 and to 1.09 €/kg H_2 in Case 4.

The investment costs for the storage facility itself (e.g. cavern expansion, cushion gas, and drilling) are not included in the scenario. These costs are added to the price of hydrogen by the storage facility operator. So far, no cost estimates from storage facility operators are available.

The following is an example of a sensitivity analysis for Scenario 2 in relation to various cost components. The starting point or centre of the figure is a mean cost range of Case 1 and 2 (€0.38/kg H_2), mean investment costs and the mean electricity cost range (€0.21/kWh).

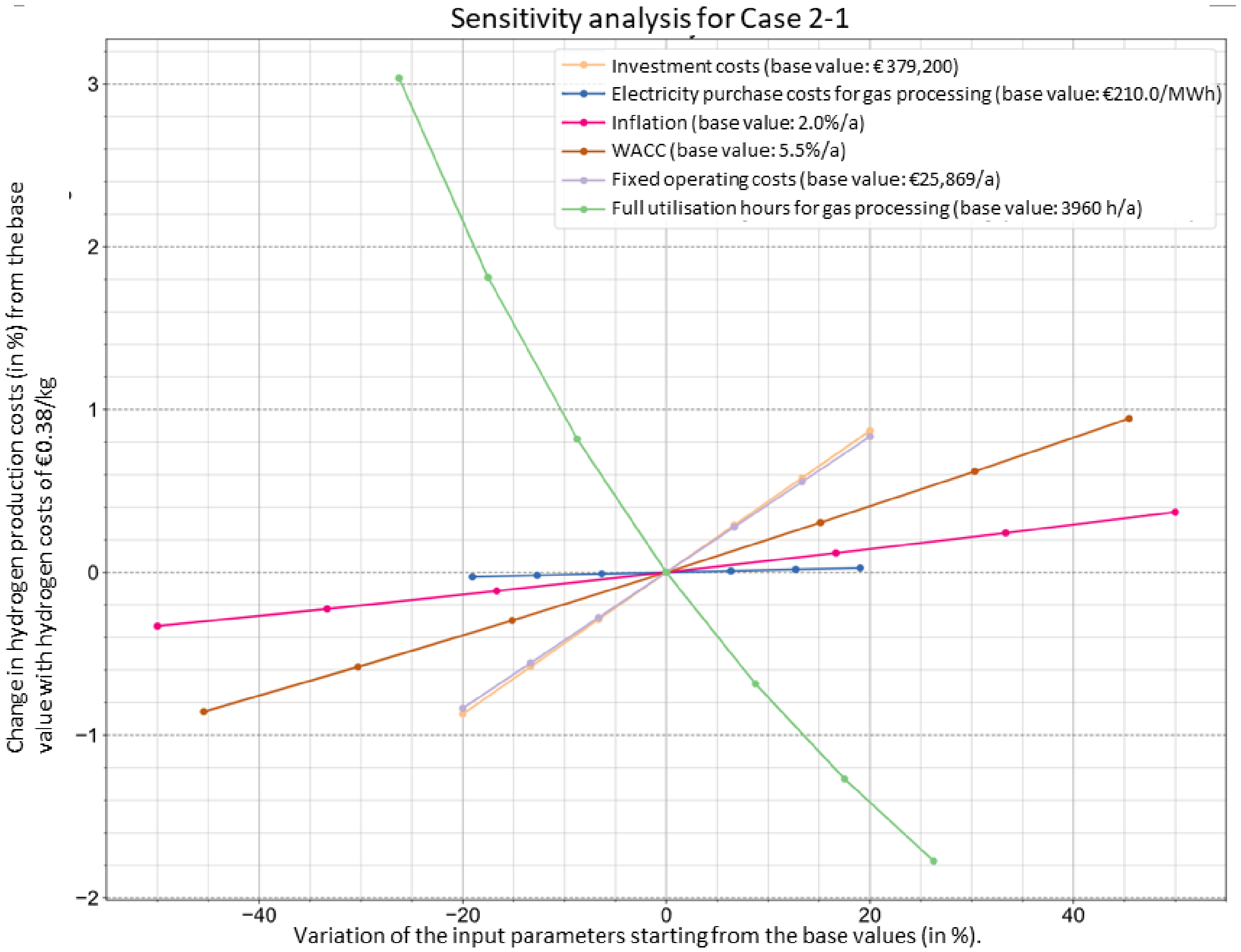

Figure 29: Sensitivity analysis of cost calculation for Scenario 2

7.4.3 Scenario 3

A Group A hydrogen must be brought to Group D quality. Multi-stage gas treatment is necessary.

The following boundary conditions are used for the cost estimate:

- Desulphurisation takes place adsorptively; the hydrogen sulphide is converted to sulphur via the oxygen content in the gas. This provides a high adsorption capacity; the adsorbent is exchanged.
- Oxygen removal takes place catalytically at low temperatures. The moist hydrogen is then dried over a molecular sieve.
- Downstream are two adsorbers that remove the residual CO_2 in the order of 1 mol %. This is a PSA. There are no plans to use the purge gas after treatment, and any costs for the emission of CO_2 have not been taken into account.

Additional measurement technology is planned to control the H_2 quality. After the PSA, a calibrated quantity measurement is necessary to record the H_2 losses metrologically. Two cases were calculated again:

Output parameters:

•	Gas flow:	10.000 m³/h = 841 kg/h
•	Pressure:	30 bar(a)
•	H_2 production price: variable, depending on production process	
•	Plant running time h/a:	8,585 h (factor in year 0.98)
•	Hydrogen kg/a	7,219,817

Fixed economic parameters:

•	Inflation:	2%/a
•	Cross WACC WS:	5%/a
•	Depreciation period:	20 a
•	Energy costs	0.17 €/kWh

For technical reasons, H_2 losses from a treatment process need to be taken into account in this scenario. The cases of 2% and 10% loss of hydrogen were assumed as examples. The OPEX thus vary depending on the hydrogen production costs. The following table therefore shows the OPEX without hydrogen losses.

For CAPEX in the amount of €7,146k, the following processing costs result: The following costs were determined.

Costs:

		Case 1 **2% H_2 loss**	**Case 2** **10% H_2 loss**
	CAPEX (€/kg H_2)	€0.078	€0.078
•	OPEX, without gas losses (€/kg H_2)	€0.045	€0.046
	Total (€/kg H_2)	€0.123	€0.124
	plus costs of gas losses (€/kg H_2)	*€0.009–0.07*[25]	*€0.046–0.36*

With a 40% increase in CAPEX and an increase in electricity costs to €0.25/kWh, the sum values CAPEX + OPEX without including gas losses in Case 1 and 2 increase from €0.12/kg H_2 to €0.20/kg H_2.

The following is an example of a sensitivity analysis for Scenario 3 in relation to various cost components. The starting point or centre of the figure is a mean cost range of all four cases considered, this is recognisable by the mean investment costs of the figure.

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[25] Two borderline cases of H_2 production costs of €0.50/kg H_2 and €4/kg H_2 were assumed for illustration purposes

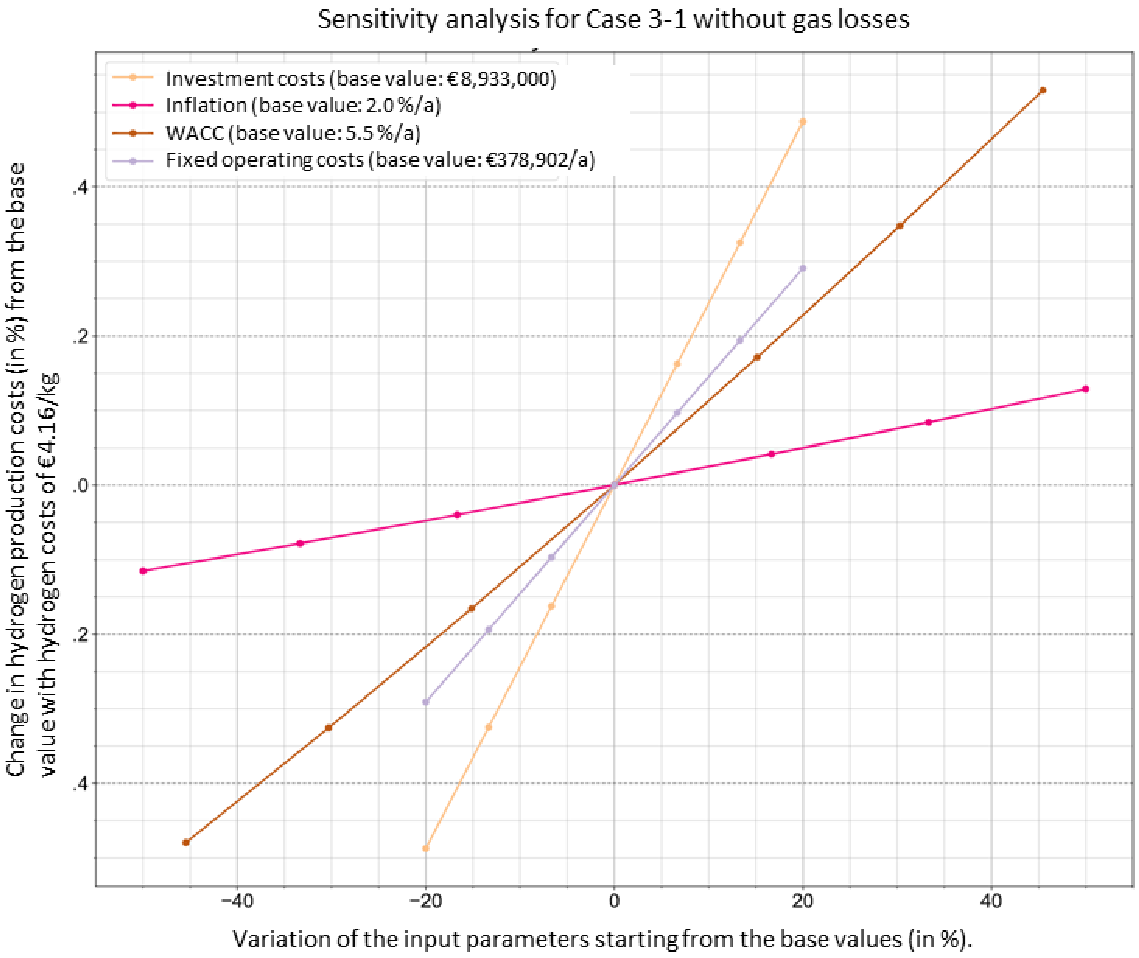

Figure 30: Sensitivity analysis of cost calculation for Scenario 3

As expected, potential H_2 losses are price drivers: Especially in the case of green hydrogen production, 10% gas losses through gas treatment should be avoided in any case. Analogous to case 2, the treatment costs are also strongly influenced by the investment costs.

8 WP 6: Definition of further steps – recommendations for action for Germany

In this study, the focus is on hydrogen quality as well as the effects on and requirements for gas quality caused by the various processes and system components. This includes, among others, storage operation, gas processing, and networks. The questions still open are summarised below.

8.1 Evaluation of the study results and listing of the existing knowledge gaps

8.1.1 Uncertainties regarding future quantities of hydrogen

In Chapter WP 1: Estimation of the H_2 requirement2, a sufficiently robust and granular hydrogen quantity framework in the “target scenario” 2045 was determined for the purposes of this short study. Further refinements are required to specify the conceptual design of a hydrogen system:

- **Hydrogen demand**: Various studies currently cover a wide range of expected quantities of hydrogen. In industry and power generation, a considerable role for hydrogen is undisputed. In the mobility and building sectors in particular, however, it is still unclear which technologies will be dominant; forecasts regarding the resulting hydrogen demand are thus fraught with uncertainty. However, it is already foreseeable that the structure of a sensible hydrogen network will differ from the current natural gas network (e.g. because of the change in use and decentralised feeding-in).
- **Hydrogen production/origin**: For the design of a hydrogen network, the question of origin also arises (both of the hydrogen itself and of the hydrogen downstream products needed in Germany).
    - In principle, it can be assumed that a considerable proportion of the hydrogen used in Germany will be imported. However, it is still unclear from which countries, on which transport route, and in which quality the hydrogen will reach Germany. All these factors may have implications for the overall system (e.g. the requirements for processing plants or for the quality of domestic hydrogen production).
    - In addition to imports, the interaction with complementary distribution instruments (e.g. lorries, trains, and ships) will also influence the design of the German hydrogen network. Depending on how the regional distribution of hydrogen production and demand develops, the requirements for a hydrogen network can vary considerably.
    - Because of their higher energy density and good transport properties, hydrogen derivatives are generally suitable for import from abroad. However, there are also various national projects for PtX production that will have to be supplied with hydrogen in order to enable the intended technological pioneering role of Germany in the hydrogen economy.
    - So if, in addition to demand, the production and origin of hydrogen and hydrogen derivatives are also taken into account, further complexities arise with regard to the future design of a hydrogen system; these must therefore be investigated.

- **Regional distribution**: Furthermore, this short study has not yet taken a detailed look at the likely regional distribution of hydrogen production (or landfall/boundary crossing) and hydrogen consumption. Further analyses of the regional distribution of hydrogen consumption and production will be required to specify the design of hydrogen networks.
- **Market ramp-up**: In addition, the consideration in this short study focuses on hydrogen use in 2045 as the “target scenario” for climate neutrality. In order to prepare decisions on the prioritisation and chronology of the development of a hydrogen network, a more detailed understanding of the hydrogen demand (and generation) in the transformation phase up to 2045 is needed beyond the 2045 target scenario. Regarding the quality design of pure hydrogen networks, the focus of this short study, an understanding of the expected market ramp-up is particularly relevant if different ramp-up rates are expected between sectors with different hydrogen quality requirements and tolerances to blending of hydrogen and natural gas.

8.1.2 Ambiguities in the area of hydrogen production and use

In Chapter 3, it was shown that the various hydrogen production processes are capable of producing high quality hydrogen (Group D) with appropriate processing. For H_2 production or transport processes not yet in use, there are gaps in the understanding of the scope and type of gas treatment. In the area of H_2 use, there are sometimes considerable fluctuations in the statements of potential users on the necessary gas quality. It is necessary to look at the following topics in depth:

- **Hydrogen production**: The production of turquoise hydrogen via methane pyrolysis is in the pilot phase. There is a lack of information on the type and extent of possible added gases in order to be able to estimate the effort required for processing to Group D quality. With regard to the production of hydrogen from ammonia, no practical experience on the residual ammonia content was obtained. It must be specified which contamination is to be expected from which manufacturing process.
- **Hydrogen application**: There are large discrepancies in the hydrogen quality requirements of potential H_2 users; these can be seen in the discussions on normative drafts regarding quality requirements in Europe. It is necessary to specify the various sources in terms of informative value and background and to go into more specific detail on technologies to be defined as well as their specific requirements.
- **Application tolerance**: At the moment, the trend is to maximise H_2 quality requirements. However, from a chemical/technical point of view, it is clear that higher proportions of individual accompanying components do not lead directly to damage to devices such as fuel cells but rather to an acceleration of ageing processes. It would have to be considered which added gases this concerns and to what extent an economic optimisation is possible.
- **Fluctuation of hydrogen quality**: The problem of fluctuating H_2 concentrations was only briefly touched upon in this short study. Statements on fluctuations usually refer to considerably greater changes than between Group A and Group D. For catalytic processes and fuel cells, fluctuations in H_2-quality in this range are, in principle, less decisive than the proportion of particularly critical impurities.

8.1.3 Knowledge gaps regarding gas treatment

The available treatment processes were described in Chapter 4, and estimates of the costs of individual process chains were made in Chapter 7. Necessary treatment technologies are available; however, unresolved issues also emerged in this area.

- **Treatment technology:** The treatment of hydrogen from 98 mol % to 99.97 mol % can cause high operating costs depending on the component to be removed as shown in the example of a pressure swing adsorption (PSA). There are alternatives; among other things, the development of membrane technology should be pursued. With regard to sulphur, it remains to be demonstrated that the various adsorption processes achieve the limit value of 4 ppb.
- **Costs and procedural adjustments:** The short study draws in part on experience in the chemical industry; however, somewhat different gas compositions or concentration ratios are handled in comparison to the tasks at hand. This has implications for plant design and treatment costs.
- **Impurities**: In general, knowledge about the type and extent of the expected contamination is incomplete. This also applies to the time course of desorption from pipelines (referred to in this study as the run-in phase).

Research projects are currently being carried out to answer various questions of a technical and economic nature; the results of these are to be evaluated and form the basis for more concrete statements in the more detailed framework.

8.1.4 Knowledge gaps in underground storage

8.1.4.1 Cavern UGS

There currently is no storage facility for pure hydrogen in Germany. Regarding the completion of the borehole, there has not yet been any investigation on hydrogen compatibility to a large part of the materials (e.g. API steels for tubings and casings and elastomers). In addition, there are questions that specifically concern the quality of hydrogen:

- **Standardisation, setting of limit values:** The feeding-in of natural gas and hydrogen into a UGS is already subject to special qualitative requirements. The extent to which Group A hydrogen quality may be fed into “clean” hydrogen caverns must be clarified. The consequence of this would be component-flexible requirements for gas treatment.
- **Previous use**: Without exception, planned practical cavern projects currently deal with caverns that have not yet been used for natural gas and are under water (brine). With the integration of old or existing caverns, the quantification of contamination from previous use is necessary (conversion of natural gas and petroleum caverns/mineral oil as residual blanket). Concrete cases, including possible outgassing from the brine, must be considered. The possibilities of using different cushion gases and resulting quality changes are to be evaluated.
- The **conversion process of** existing caverns itself is not considered in this short study.
- The state of knowledge on **biological activity** should be expanded on a European scale; practical experience beyond Germany should be evaluated.

The conversion of existing caverns will become the norm in the long term; this quality-relevant process must therefore be considered in greater depth.

8.1.4.2 Pore UGS

Worldwide, about 75% of underground gas storage capacity is provided by pore storage[26]; especially in Ukraine, the European country with the largest gas storage capacity (and the third largest in the world), only pore storage exists. Against this background, it is necessary to assess pore storage facilities with regard to associated gas substances because it must be assumed that these added gases enter the network and UGS in Germany during gas imports (natural gas and, prospectively, hydrogen).

Pore storage systems were not the subject of this study; nevertheless, the following decisive quality-relevant challenges can be summarised:

- **Interaction:** Evaluation and investigation of possible interactions of hydrogen with the mineralogical, geochemical, petrophysical, and microbiological conditions of the reservoir and overburden. The possible alteration of the pore structure (porosity and permeability) and associated impurities of the storage gas must also be evaluated
- The **interaction between hydrogen and natural gas, the distribution as a gas mixture**, and the solubility of H_2 and natural gas in water are to be investigated in particular. Although there are selective studies, there are no generally valid statements or mathematical descriptions. The time course of the conversion of an existing pore UGS from natural gas to hydrogen must be considered.
- Possibility of a **generally valid qualification** of pore storage tanks for suitability for hydrogen storage. It should be investigated whether exclusion criteria exist for such a conversion.

8.1.5 Uncertainties regarding future hydrogen networks

So far, the gas industry has no practical experience with the conversion and cleaning of existing networks to hydrogen. In principle, it is possible to feed H_2 with high purity into the network and then separate the individual components introduced through the pipelines and operation in a demand-oriented and cost-efficient manner. Experience in the chemical and refinery industry shows that hydrogen can be transported in high quality via new hydrogen networks. However, there is a consensus in the gas industry that the conversion from natural gas to hydrogen lines will be necessary.

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[26] With an inverse ratio of approx. 75% of gas storage capacity in cavern storage facilities, Germany represents an international individual/special case.

The lack of experience results in an increased need for investigation:

- **Impurities**. The components that can lead to hydrogen impurity are known. This varies depending on the previous use and operating time of the pipelines.
    - The concentration of these components must be determined in connection with the history of the pipeline. Statements on concentration are essential for the design of a gas treatment system.
    - The duration of the “conversion phase” is open. This can be made more precise using practical examples. For individual components (e.g. water from North Stream I), a more detailed statement is already conceivable if measurement data are made available.
- **Local gas treatment**: This is currently already being done before fuel cells or natural gas filling stations. A further evaluation of these small plants (e.g. service life, material, or costs) enables a precise assessment of the treatment directly before an application (e.g. H_2 filling station or an H_2 fuel cell).
- **Time frame and conversion scenarios:** With the deepening of knowledge on hydrogen demand and market ramp-up (WP 1), scenarios can be specified with regard to the quality to be distributed as well as the spatial location of the qualitative requirements. The allocation to the different pipeline systems (transport network, distribution network) with different gas treatment efforts would be conceivable.

It should be noted (as in 8.1.2) that for some application processes not all Grade D requirements need to be met. The consequence of this finding and how to take this into account in an overall network is yet to be determined.

8.2 Summary and recommendations for action

The existing natural gas infrastructure in Germany can be converted for the transport and storage of hydrogen. Because of the future energetic and considerably higher expected material use of hydrogen in almost all industrial, municipal, and private sectors, the provision of a suitable quality from a transport and distribution network is a central basis for the energy transition. The short study has presented the relevant quality-relevant processes.

Several quality ranges for the required hydrogen can be defined with regard to the **requirements**. These are the energetic quality range and are comparable with the H_2 quality of Group A of DVGW Code of Practice G 260, the catalytic quality range, and the requirement range for fuel cells (quality of Group D of DVGW G 260). Group A is not sufficient for the catalytic quality range, which covers the requirements of the chemical industry, the refinery industry, and future PtX processes. On the other hand, not all quality requirements of Group D for catalytic quality have to be fulfilled; the requirements for individual added gases may differ.

The evaluation of existing studies shows that high quality hydrogen (catalytic and fuel cell) will take a considerable portion of the total in 2045. Depending on the import possibilities and quantities of Power-to-X (PtX) products, this can amount to up to 30–40% of the necessary hydrogen demand in Germany. Within the scope of the study, it was shown that all of today’s relevant hydrogen **production processes**, combined with the existing treatment processes, are capable of producing hydrogen for all future areas of application. This also explicitly applies to the highest quality requirement: the use in PEM fuel cells

A reduction of the manufacturing effort by simplifying the gas treatment at the manufacturer to meet the somewhat lower requirements of H_2 of Group A quality (98 mol %) is both conceivable and technically feasible. If the gas treatment effort is reduced as part of the production process, this effort may become necessary for the distribution network or storage operator or the end customer.

For the **transport of** hydrogen, the quality-influencing changes in storage and pipeline transport were presented. For the storage of hydrogen in the salt caverns available in Germany, it is expected that, in addition to moisture absorption, microbial processes will also lead to the formation of impurities that can be separated by adsorptive processes. In any case, a specific consideration of the previous use is necessary when converting old caverns. The use of pore storage was not considered in this study. It is to be expected that case-by-case considerations will be necessary here.

It can be assumed that the imports of hydrogen also do not fulfil the high quality of Group D in every case. The reason for this could be other legal situations or the integration of pore storage facilities outside of Germany into the transport system.

There are technologies can remove these impurities. The extent of the necessary gas treatment varies. Conceivable locations for treatment are transfer points in the hydrogen network. Hydrogen purification can also be installed directly in front of the end customer. The processing effort will lead to an increase in the cost of hydrogen with processes involving hydrogen losses (e.g. PSA) incurring higher costs than for simple adsorption.

The upcoming step-by-step transformation process of power supplies and storage units is unprecedented in terms of existing quality requirements. Accordingly, this study has identified a number of **knowledge gaps** in addition to the facts mentioned above. It is recommended that these gaps be closed in the coming years. This can be done by involving potential users, using the experience of ongoing research projects, and deepening the research work beyond the national scale.

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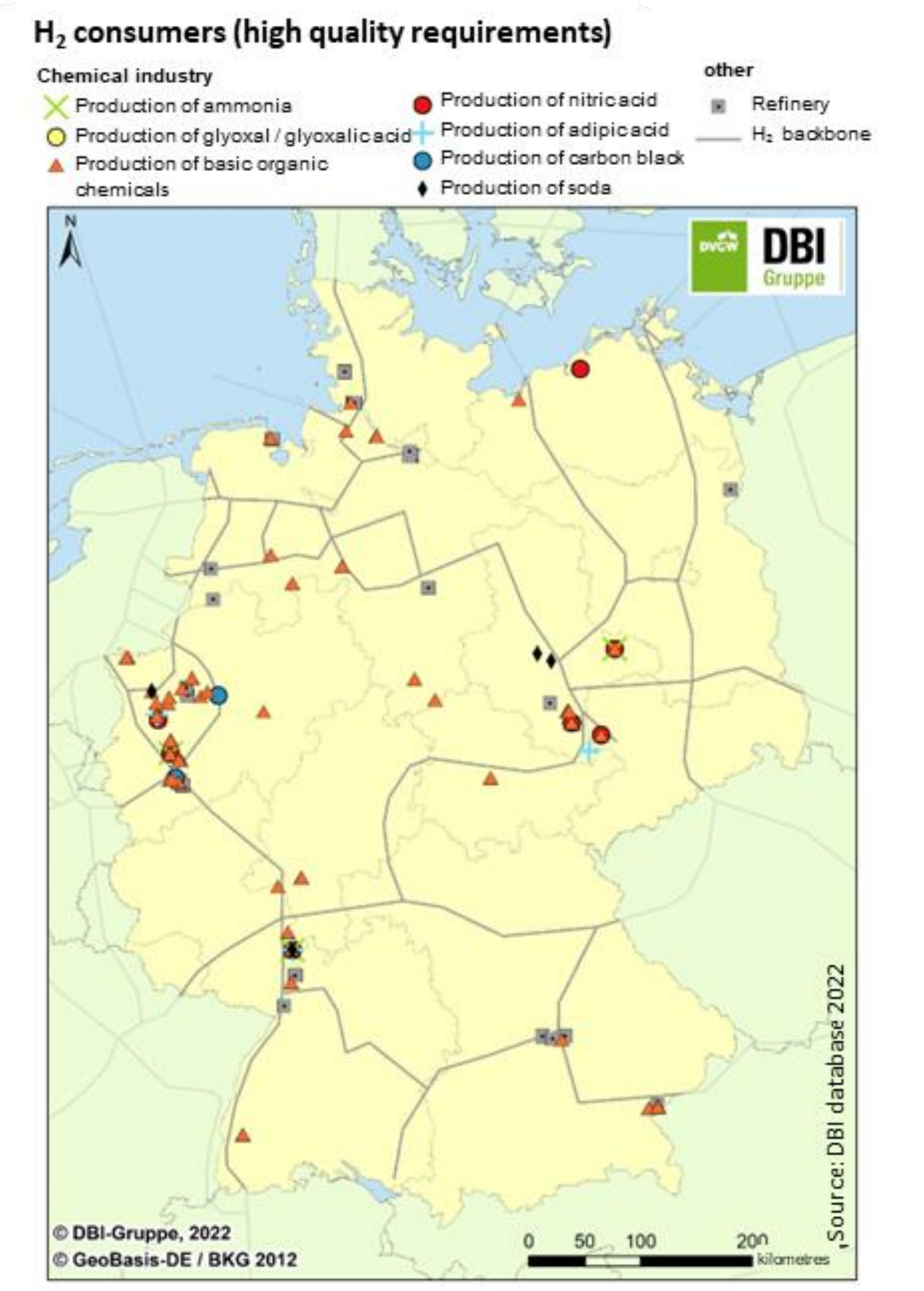
Appendix

Appendix 1: H_2 consumer sites, high quality requirements, informative



Appendix 2: List of the hydrogen (admixture) volumes of the German cavern UGS with corresponding injection and withdrawal rates

Location	0 vol. % H_2	1 vol. % H_2	5 vol. % H_2	20 vol. % H_2	100 vol. % H_2	100 vol. % H_2	100 vol. % H_2	Max. withdrawal rate	Max. injection rate
	million m³ i.N.	million m³ i.N.	million m³ i.N.	million m³ i.N.	million m³ i.N.	t	TWh	1,000 m³/h i.N.	1,000 m³/h i.N.
Bad Lauchstädt	654	650	624	566	444	39,940	1.33	920	Not specified
Bernburg	898	893	856	777	610	54,841	1.82	1,000	Not specified
Bremen-Lesum-Storengy	152	151	145	132	103	9,283	0.31	360	91
Bremen-Lesum-Wesernetz	21	21	20	18	14	1,282	0.04	160	5
Empelde	378	376	360	327	257	23,085	0.77	510	161
Epe-ENECO	94	93	90	81	64	5,741	0.19	400	342
Epe-innogy, H-Gas	388	386	370	336	263	23,695	0.79	870	Not specified
Epe-innogy, L-gas	178	177	170	154	121	10,871	0.36	400	181
Epe-innogy, NL	296	294	282	256	201	18,077	0.60	500	174
Epe-KGE	186	185	177	161	126	11,359	0.38	400	150
Epe-NUON	300	298	286	260	204	18,321	0.61	600	259
Epe-Trianel	190	189	181	164	129	11,603	0.39	600	301
Epe-Uniper	1,916	1,905	1,827	1,659	1,301	117,011	3.89	2,900	1,200
Etzel-EGL 1 and 2	1,170	1,163	1,116	1,013	794	71,453	2.37	1,320	770
Etzel-EKB	895	890	853	775	608	54,658	1.82	800	446
Etzel-ESE	1,912	1,901	1,823	1,655	1,298	116,767	3.88	2,250	116

Location	0 vol. % H_2	1 vol. % H_2	5 vol. % H_2	20 vol. % H_2	100 vol. % H_2	100 vol. % H_2	100 vol. % H_2	Max. withdrawal rate	Max. injection rate
Etzel-FSG Crystal	390	388	372	338	265	23,818	0.79	600	197
Harsefeld	110	109	105	95	75	6,718	0.22	300	90
Huntorf	308	306	294	267	209	18,810	0.63	450	335
Jemgum-astora	760	755	725	658	516	46,414	1.54	930	365
Jemgum-EWE	366	364	349	317	249	22,352	0.74	250	202
Katharina	347	345	331	300	236	21,192	0.70	900	Not specified
Kiel-Rönne	62	62	59	54	42	3,786	0.13	100	21
Kraak	257	255	245	222	175	15,695	0.52	400	177
Krummhörn	154	153	147	133	105	9,405	0.31	280	Not specified
Nüttermoor	1,311	1,303	1,250	1,135	890	80,064	2.66	1,780	178
Peckensen	367	365	350	318	249	22,413	0.74	895	309
Reckrod	110	109	105	95	75	6,718	0.22	100	50
Rüdersdorf	100	99	95	87	68	6,107	0.20	140	39
Staßfurt	645	641	615	558	438	39,391	1.31	650	306
Xanten	172	171	164	149	117	10,504	0.35	320	Not specified
Total	**15,087**	**14,996**	**14,386**	**13,060**	**10,244**	**921,374**	**30.62**	**22,085**	**6,465**

Appendix 3: Specific differences between pore and cavern UGSs

	Pore UGS	**Cavern UGS**
Geology		
Structure	Mainly porous rock such as sandstone and limestone	Salt rock, mainly halite
Overlying rock	Layer of dense, impermeable rock, mainly clay	Reservoir rock itself (salt)
Storage volume	dependent on the extent of the formation, its structure, depth, porosity, and permeability	dependent on the extent of the salt formation; theoretically expandable through the construction of further caverns
Cushion gas volume	High	Low, but variable (depending on the size of the caverns)
Erection		
Bores	Several operating wells:	One (or two) boreholes per cavern
	Depending on the structure, faults, storage horizons, and their hydraulic communication	
	Productivity/injectivity index of the boreholes	
	Possibly different depths if the reservoir has different storage layers	
Initial gas filling (GEB)	-	Additional equipment for GEB, extraction, and disposal of brine from the brine process.
Cushion gas	Exhausted fields: Remaining hydrocarbons (mainly natural gas), CO_2, and the like	The use of media other than storage gas is currently being investigated.
	Aquifers: Proportion of the storage medium, typically 40% by volume of the total gas volume	
Max. pressure	In accordance with formation pressure gradient + safety factor (dependent on depth) According to the pressure gradient in the formation + safety factor (depending on the depth)	
Min. pressure	Depends on pore size, permeability, and capillary pressure.	Cushion gas volume maintains minimum pressure: Preventing too rapid a creep rate and reducing cavern size
Injection and withdrawal rates	Depending on permeability and current reservoir pressure	Depending on the tubing size and the max. permissible pressure change in the cavern (typically 10 bar/d)
	In most cases, decreasing over the production period.	

	Pore UGS	**Cavern UGS**
	Verify through injection and production tests as well as borehole simulation models	
	Can differ from borehole to borehole (and from layer to layer)	
Operation		
Gas treatment	Gas drying: Always	Gas drying: Always
	Desulphurisation: if required, may result from microbial processes in the reservoir in the case of H_2	Removal of hydrocarbons if a cavern was filled with (diesel) oil as blanket, residual amounts of natural gas that was not removed during flooding
	Removal of hydrocarbons: required for use of former reservoirs or converted natural gas UGS	
Injection and withdrawal cycles	Once per year	Several times per year
Monitoring	Sometimes additional observation wells in the reservoir or in the upper layers:	Monitoring of ground movements (as a result of convergence of caverns)
	Pressure monitoring → detection of fluid flows in edge areas and upper layers of the UGS	
	Water inflow monitoring and gas analysis	