



# Common Business Practice on Hydrogen

EASEE-gas

## EASEE Gas Common Business Practice on Hydrogen

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## Summary

In the table below the proposed specification for the EASEE-gas CBP 'Hydrogen specification for dedicated hydrogen pipelines' is presented. The basis for this specification can be found in this report.

*Table 1: Parameters and value EASEE-gas CBP 'Hydrogen in natural gas infrastructure'*

Parameter	Unit	Min	Max
Hydrogen	mol-%	98,0	-
Carbon monoxide	ppm	-	20
Total sulphur content <sup>(1)</sup>	mg S/m <sup>3</sup> (n) <sup>(2)</sup>	-	21 <sup>(3)</sup>
Carbon dioxide	ppm	-	20
Hydrocarbons (including Methane)	mol-%	-	1,5 <sup>(3)</sup>
Inerts (Nitrogen, Argon, Helium)	mol-%	-	2,0
Oxygen	ppm	-	10 <sup>(4,5)</sup>
Total halogenated compounds	ppm	-	0,05
Water dewpoint	°C at 70 bar(a)	-	- 8
Hydrocarbon dewpoint <sup>3</sup>	°C at 1-70 bar(a)	-	- 2 <sup>(3)</sup>
1) Non-odorised hydrogen			
2) normal conditions (1.01325 bar(a), 0 °C)			
3) During the transition period, where the hydrogen composition can be influenced by natural gas residues present in the pipeline system (see Note below the table)			
4) Expressed as a moving 24-hour average			
5) Where the hydrogen can be demonstrated not to flow to installations or end-user applications sensitive to higher levels of oxygen, (e.g. feed stock users or hydrogen storages), a higher limit of up to 1000 ppm may be applied.			
Note:	It is acknowledged that the presence of residues in the pipeline as a result of natural gas transmission, makes it necessary to relax the specification for the total sulphur content, to allow for higher hydrocarbons to be present and to introduce a temporary specification for the hydrocarbon dewpoint.		
Note:	The gas shall not contain constituents other than listed in the table above at levels that prevent its transportation, storage and/or utilization without quality adjustment or treatment.		

# 1 Introduction

In 2019 the EASEE-gas Board agreed to draft a Common Business Practice (CBP) for the harmonisation of the recommended quality specification for hydrogen (non-blended with natural gas, see *Note 1*) flowing through dedicated systems, meaning networks that were originally designed and used for natural gas transmission and after a safety and reliability assessment (see *Note 2*) found suited for conveying hydrogen and newly built hydrogen pipeline systems. The CBP is valid for both the entry as well as the exit points of these dedicated systems

*Note 1: This CBP is not applicable to blends of hydrogen and natural gas.*

*Note 2: This CBP only specifies the recommended hydrogen specification. Before hydrogen can be transmitted through existing European natural gas grids, safety and reliability assessments need to be carried out to prove the suitability of the given grid for the transmission of hydrogen.*

This CBP focusses on 'industrial grade' hydrogen because it is expected that in the coming years, the large-scale production of hydrogen, necessary to operate a pipeline system, will partly take place by chemical conversion of hydrocarbons. In contrast to electrolysis, these processes do not deliver inherent fuel cell quality hydrogen. Possibilities for large scale production of hydrogen via electrolysis are not expected before 2030. Another reason to focus on 'industrial grade' hydrogen is the observation from market forecasts that the industry will take the lion share of the total hydrogen production. Only in the period after 2030, there is a possibility for large scale demand for fuel cell and/or energy production grade hydrogen. Last but not least, no hands-on experience is available on the possible effects of residues in the pipeline resulting from the previous exposure to natural gas on the hydrogen transmitted through such a pipeline. The risk that small amounts of a particular contaminant result in an off-specification at the exit increases with an increase of the minimum hydrogen purity.

## 1.1 Available information

A small literature study in 2018 revealed an ISO and a CEN standard focussing on a hydrogen gas quality specification: ISO 14687:1999/Corr.2:2008 "Hydrogen fuel — Product specification"<sup>1</sup> and EN 17124:2018: Hydrogen fuel - Product specification and quality assurance - Proton exchange membrane (PEM) fuel cell applications for road vehicles.

Based on the specifications for the various grades of 'pure' hydrogen in these standards, there seems to be no specification for 'pure' hydrogen that is suitable as a general specification for the transport of pure hydrogen through a former natural gas network which has been found suitable for conveying pure hydrogen. The hydrogen grade used for Proton exchange membranes refers to hydrogen with a very high purity (minimum 99,97 mol-% H<sub>2</sub>). The expectation is that this high purity hydrogen specification is neither possible to guarantee in an 'old' natural gas network nor necessary for the larger part of the hydrogen end consumers. On the other hand, the lower grade hydrogen specifications don't contain the necessary limit values for parameters normally encountered in natural gas like for example the water dewpoint.

The updated ISO 14687:2019 standard distinguishes several classes for hydrogen and hydrogen-based fuels based on representative applications.

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<sup>1</sup>) ISO 14687 was revised in 2019 and specifies now the minimum quality characteristics of hydrogen fuel as distributed for utilization in vehicular and stationary applications. The scope was also extended to the use as a fuel in other applications than solely fuel cells

Table 2: Hydrogen grades and classes according to ISO 14687:2019 [1]

Type	Grade	Category	Applications	
I (Gas)	A	-	Gaseous hydrogen; internal combustion engines for transportation; residential/commercial combustion appliances (e.g. boilers, cookers and similar applications)	
	B	-	Gaseous hydrogen; industrial fuel for power generation and heat generation except PEM fuel cell applications	
	C	-	Gaseous hydrogen; aircraft and space-vehicle ground support systems except PEM fuel cell applications	
	D	-	Gaseous hydrogen; PEM fuel cells for road vehicles	
	E			PEM fuel cells for stationary appliances
		1		Hydrogen-based fuel; high efficiency/low power applications
		2		Hydrogen-based fuel; high power applications
	3		Gaseous hydrogen; high power/high efficiency applications	

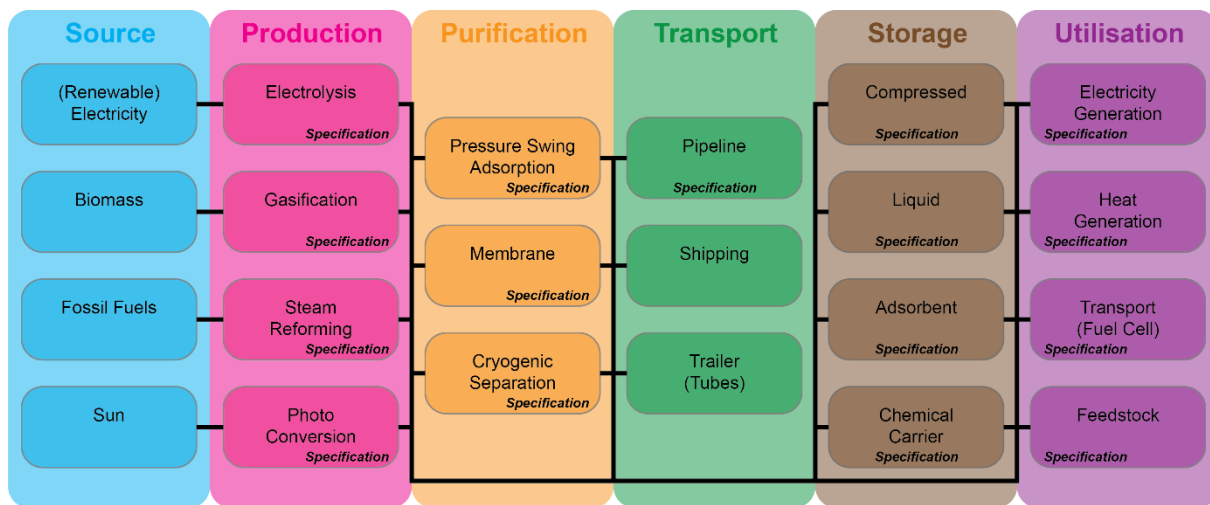
A complete overview of the gas composition requirements for the various grades is given in annex A. Except for grades E1 and E2, the hydrogen content varies between 98,0 mol-% to 99,995 mol-%. Depending on the grade the (trace) contaminants are described in more or less details.

Since the ISO 14687:2019 standard doesn't contain detailed background information on the reason for the choice of the (trace) contaminants and their limit values, it doesn't seem appropriate to make a choice based on this information only.

### 1.2 Approach

In the figure below, an overview is given of the process steps involved in the production, purification, transportation, storage and utilisation of the hydrogen.

Figure 1: Process steps in production, purification, transport, storage and utilisation of hydrogen



For each of the process steps mentioned in the diagram above, 'specifications' are gathered. The end-users participating in the EASEE-gas Gas Quality Harmonisation Working Group which are at least partly familiar with the industrial production of hydrogen from natural gas have contribute to the specification of several of the steps. Another source of information are the studies that have been carried out and still are underway. Furthermore, through liaisons with other organisations like Marcogaz and CEN, it was also possible to receive additional information.

Based on the individual specifications for the various process steps, the market shares of the various hydrogen uses and the ease of upgrading hydrogen to high purities for particular applications such as fuel cells, which needs further investigation, the CBP specification is determined in such a way that is a common denominator.

## 2 Production specification (entry)

Since hydrogen is an energy carrier, there are several processes to produce hydrogen. Depending on the production process the hydrogen content in the end product varies but also the presence and amount of other main constituents and trace components. At the moment the main production methods for producing hydrogen are steam methane reforming and pyrolysis mostly based on natural gas as a feedstock and electrolysis which uses water and electricity as a feedstock.

Long distance transport of hydrogen can also take place in liquid form, in the form of liquified hydrogen or liquid carriers like ammonia or cyclic organic molecules [2].

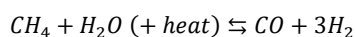
### 2.1 Reforming techniques

There are three general conversion principles to convert natural gas into hydrogen. They will be discussed shortly below, and some key figures will also be given in this part of the report.

#### 2.1.1 Steam Methane Reforming (SMR)

Steam reforming or steam methane reforming is a chemical synthesis for producing syngas (hydrogen and carbon monoxide) from hydrocarbons such as natural gas. This is achieved in a reformer in which steam at high temperature and pressure reacts with methane in the presence of a nickel catalyst. The steam methane reformer is widely used in industry to make hydrogen [3].

The overall chemical reaction for the steam methane reforming process is given by the following equation:



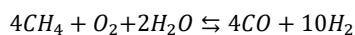
Technology Overview [4]:

- Mature technology and widely used across the refining and petrochemical industries.
- Improvements have included higher performing materials, improved heat recovery, lower pressure drop and higher conversion catalysts.

#### 2.1.2 Auto Thermal Reforming (ATR)

Auto-Thermal Reforming (ATR) uses pure oxygen<sup>2</sup> for the partial oxidation of the natural gas feed in the flame section, which is followed by a catalyst bed in the steam reforming section of the reactor. The core benefits of this system are that the heat generated by partial oxidation is consumed by the endothermic reforming reaction. This process is inherently energy-efficient, because the reactor operates without an external heat supply. In addition, since the oxidation occurs within the reaction chamber, there is no flue gas produced at this step and carbon dioxide capture is simplified. Modern ATR units have higher reliability / lower unplanned downtime than SMR units, with a ramp up/down rate of 1.5% of the design capacity per minute. Another advantage is that an ATR can be operated at very high pressures (up to and beyond 60 bar, at industrial scale), increasing the capacity of a single ATR unit, and eliminating the need to compress the outlet hydrogen stream. Most ATRs currently in operation are used for ammonia and methanol production [5].

The overall chemical reaction for the auto thermal reforming process is given by the following equation:



Technology overview [4]:

- In the ATR technology, part of the natural gas feed is partially combusted to generate heat for the endothermic reforming reaction. This self-heating ("auto-thermal") mechanism largely eliminates the need for any external heating, which can be met with supplemental hydrogen firing.
- The H<sub>2</sub>/CO ratio from ATR technology is less suited to hydrogen production than SMR, and more suited to Fischer–Tropsch processes, so technology must be "re-optimized" for hydrogen production.
- Numerous ATRs are in operation worldwide, but most operate as secondary reformers in ammonia plants in collaboration with SMR technology. For ammonia plants, stand-alone ATR technology has so far been considered uneconomical. For methanol plants, only a few true standalone ATRs have been realized up to now, but ATR technologies are maturing steadily.

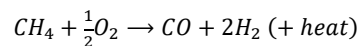
<sup>2</sup>) In some ATR processes air is used instead of pure oxygen.

- The high CAPEX cost of capturing carbon dioxide from SMR flue gas makes the use of ATR more attractive for “blue” hydrogen production, especially if carbon dioxide capture rates above 90% are required.

### 2.1.3 Partial Oxidation (POX)

Partial oxidation (POX) is another type of chemical reaction. It occurs when a sub stoichiometric fuel-air mixture is partially combusted in a reformer, creating a hydrogen-rich syngas which can then be put to further use. Partial oxidation is an exothermic process (it gives off heat). The process is, typically, much faster than steam reforming and requires a smaller reactor vessel. As can be seen in chemical reactions of partial oxidation, this process initially produces less hydrogen per unit of the input fuel than is obtained by steam reforming of the same fuel [6]. Nevertheless, tendency to soot formation and relatively low hydrogen production yield are among the major drawbacks of this method. [3] [7]

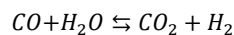
The overall chemical reaction for the partial oxidation process is given by the following equation:



### 2.1.4 Water Gas Shift Reaction (WGSR)

The water gas shift reaction (WGSR) was discovered by Italian physicist Felice Fontana in 1780. The WGSR is an important industrial reaction that is used in the manufacture of ammonia, hydrocarbons, methanol, and hydrogen. It is also often used in conjunction with steam reforming of methane and other hydrocarbons. In the Fischer–Tropsch process, the WGSR is one of the most important reactions used to balance the H<sub>2</sub>/CO ratio. It provides a source of hydrogen at the expense of carbon monoxide, which is important for the production of high purity hydrogen for use in ammonia synthesis [8] and also if the focus is on maximised hydrogen production.

The overall chemical reaction for the water gas shift reaction is given by the following equation:



To produce the maximum hydrogen amount, the SMR, POX and ATR reformer process is always followed by a WGSR to convert the CO present in the product stream of the reformer to hydrogen and CO<sub>2</sub>.

### 2.1.5 Product specifications

Berenschot [9] has published some data on the performance and the resulting hydrogen specification for the various reformer processes. In the processes flow diagram presented in the Berenschot publication a WGSR step is included, so it is assumed that the information given in the table below includes a WGSR process step. Furthermore, it should be noted that the hydrogen is produced at a high pressure of 98 bar.

Table 3: Performance data and hydrogen composition for various reformer processes [9]

Reformer process		SMR		ATR		POX	
<b>Input</b>							
Hi-Cal gas	kg/s	10		10		10	
Air	kg/s	41.4		56		64	
Steam	kg/s	22		22		20	
Thermal input	MWth	478		478		478	
<b>Output stream</b>		<b>CO<sub>2</sub></b>	<b>H<sub>2</sub></b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub></b>	<b>CO<sub>2</sub></b>	<b>H<sub>2</sub></b>
Mass flow	kg/sec	11.0	6.2	20.1	7.4	23.2	6.3
Pressure	bar	60	98	60	98	60	98
Temperature	°C	7	40	7	40	7	40
<b>Components</b>		<b>Vol.</b>					
CH <sub>4</sub>	%	0.0	13.0	0.0	3.2	0.0	0.6
CO <sub>2</sub>	%	99.9	1.0	99.8	1.5	99.9	1.7
N <sub>2</sub>	%	0.0	0.3	0.0	1.3	0.0	1.4
H <sub>2</sub>	%	0.0	84.1	0.0	89.7	0.0	94.0
CO	%	0.1	1.5	0.2	4.3	0.1	2.3
NH <sub>3</sub>	%	0.0	0.1	0.0	0.1	0.0	0.0
H <sub>2</sub> O	%	0.0	0.0	0.0	0.0	0.0	0.0
<b>Output</b>							
Power consumption	MWe	8.0		26.6		31.2	
Plant efficiency	-	83%		82%		78%	
Thermal efficiency	-	85%		87%		83%	
LHV H <sub>2</sub> output	kJ/kg	65664		56028		63415	
H <sub>2</sub> output	t/day	532		637		540	
CO <sub>2</sub> captured	t/day	953		1737		2001	
CO <sub>2</sub> emitted	t/day	1198		-		-	

DNV GL [10] has also published some data on the performance of the various reformer processes which is presented in the table below

Table 4: Hydrogen composition for various reformer processes [10]

Reformer process		SMR + WGSR	ATR + WGSR	POX + WGSR <sup>1</sup>
Components	Vol.	H <sub>2</sub> -stream	H <sub>2</sub> -stream	H <sub>2</sub> -stream
CH <sub>4</sub>	%	3 - 6	0,07 – 0,09	-
CO <sub>2</sub>	%	15 - 25	17	17
N <sub>2</sub>	%	traces	33 - 38 <sup>2</sup>	1
H <sub>2</sub>	%	70 - 80	44 — 49	34
CO	%	0,5 - 3	0,52 – 0,58	48
Ar	%	-	0,39 – 0,45	-

<sup>1</sup>) Although the published information explicitly states that the data for the POX reformer includes a WGSR step, the high CO concentration of vol 48 % suggested otherwise.

<sup>2</sup>) High N<sub>2</sub> content suggests that air is used instead of pure oxygen

Large differences can be observed in the presented hydrogen composition when comparing data of various studies. For example in a not publicly available study the following data were reported for an ATR process configuration which differ considerably from the data presented in table 3 and table 4. These large differences can probably be traced back to the different prerequisites and the diverse goals of the various studies. Another composition for the SMR process without WGSR step can be found in table 11 on page 13.



Table 5: Hydrogen composition for an ATR process

Reformer process		ATR + WGSR
Components	Vol.	H <sub>2</sub> -stream
CH <sub>4</sub>	%	1 – 3
CO <sub>2</sub>	%	-
N <sub>2</sub>	%	0,4
H <sub>2</sub>	%	91 – 98
CO	%	0,5 – 5,0
Ar	%	0,5

ElementEnergy [11] made an overview on the impurities for Steam Methane Reforming, Auto Thermal Reforming with pure oxygen and Electrolysis based on various literature values.

Table 6: Impurity levels of SMR, ATR and Electrolysis [11]

Impurity	SMR (dry mol-%)	ATR (O <sub>2</sub> ) (dry mol-%)	Electrolysis (ppm)
CO	0,1 - 4	0,3-2	n/a
CO <sub>2</sub>	0,35 – 0,7	0,7 – 1,7	0,2 – 5,4
CH <sub>4</sub>	3,5 - 8	0,3 - 3	n/a
N <sub>2</sub>	0 - 0.3	0,7	< 100
Ar	n/a	0,6	n/a
H <sub>2</sub> O	0,2 – 0,4	0,2 – 0,4	< 100
O <sub>2</sub>	n/a	n/a	18 - 500
H <sub>2</sub> S	< 50 x10 <sup>-4</sup>	< 50 x10 <sup>-4</sup>	n/a

As a basis for this Common Business Practice the following general composition resulting from a reforming process including water gas shift reaction step is taken into account. In this table the information presented in this paragraph is summarised.

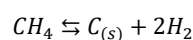
Table 7: General hydrogen composition for a reforming process

General specification		Reforming
Components	Vol.	H <sub>2</sub> -stream
H <sub>2</sub>	%	85 – 98
CH <sub>4</sub>	%	1 – 13
CO <sub>2</sub>	%	-
N <sub>2</sub>	%	0 – 1
CO	%	0,5 – 5,0
NH <sub>3</sub>	%	0 – 0,1
Ar	%	0,5

## 2.2 Pyrolysis

A new approach for utilizing the chemical energy contained in the carbon–hydrogen bonds of methane without the co-production of carbon dioxide in the combustion process is through pyrolysis, namely the thermal treatment of methane in the absence of oxygen. The product of this pyrolysis is solid carbon and gaseous hydrogen but no carbon dioxide.

The overall chemical reaction for the auto thermal reforming process is given by the following equation:



One of the ways envisioned for engineering methane pyrolysis on an industrial scale is inspired by the iron ore blast furnace. In this process, iron ore, coke and limestone are fed into the top of the furnace and molten iron and slag so produced sink and are separated at the bottom of the furnace. A similar processing principle has been proposed for methane pyrolysis, whereby methane is fed into the bottom of a high temperature reactor filled with a molten metal such as lead or a molten metal alloy (Nickel-Bismuth) at 1000 °C. These metallic melts catalyse the formation of solid carbon and gaseous hydrogen. The carbon so formed floats to the top of the melt where it is siphoned off and transferred to a carbon storage tank. Of the co-produced hydrogen (2 mole hydrogen per

mole of methane), 1/3 mole is used to heat the reactor, while the other 5/3 mole is cooled and stored for use as a fuel [12].

Since this new processing route for the conversion of methane into hydrogen is still in the early development phase no detailed information is available on the hydrogen composition.

If due to significant advances in a development of pyrolysis technology there will be new available information at hand related to gas quality parameters of hydrogen produced via pyrolysis then it is recommended to evaluate the current proposed hydrogen specification for the CBP on a non-discriminatory basis.

## 2.3 Electrolysis

There are two commercial principles to produce hydrogen by electrolysis of water which belong to the group of the low-temperature electrolysis: Proton Exchange Membrane (PEM) and Alkaline electrolysis. These two methods will be discussed shortly below. Also, some information is given on two emerging technologies of which one belongs to the group of the low temperature electrolysis, the Anion Exchange Membrane, and one to the group of the high temperature electrolysis, Solid Oxide Electrolysers. Both techniques are not commercially available yet but look promising for the future.

### 2.3.1 Proton Exchange Membrane (PEM) Electrolysers

Hydrogen electrolysis with PEM (Proton Exchange Membrane) offers rapid dispatchability and turn down to follow the energy output from renewables and is therefore ideal for pairing with wind farms for low-carbon hydrogen production or the provision of rapid response to the grid. Typical output pressure is 2 – 3 MPa, but work is underway to attempt to increase this to 8 MPa and higher to allow for direct injection into transmission systems. [4]

### 2.3.2 Alkaline electrolysis

Hydrogen production by alkaline electrolysis is a proven technology with almost 90 years of operational experience. The largest plant to date is rated at 90MW (electrical energy input) [currently mothballed] and produced around 1,200 kg/hr hydrogen for ammonia fertiliser production. Typical output pressure is 2 – 3 MPa, whilst there is work currently ongoing to increase the output pressure it is not expected to exceed 6 MPa. Therefore, an additional compression step will always be needed for alkaline electrolyser plants which are injecting into the transmission system. [4]

### 2.3.3 Anion Exchange Membrane (AEM) Electrolysers

Anion Exchange Membrane electrolysis is also known as alkaline PEM. One of the major advantages of AEM water electrolysis is the replacement of conventional noble metal electrocatalysts with low cost transition metal catalysts. AEM electrolysis is still a developing technology; therefore, with a view to using it to eventually achieve commercially viable hydrogen production, AEM electrolysis requires further investigation and improvements, specifically regarding its power efficiency, membrane stability, robustness, ease of handling, and cost reduction [13].

### 2.3.4 Solid Oxide Electrolysers

High temperature solid oxide electrolysis (SOE) is an immature production technology with the potential to be a future large-scale production method. The advantage of SOE is the ability to make use of industrial sources of waste heat to improve the overall efficiencies. Indeed, if the energy cost of the waste heat is not included in the calculation, SOE electrical efficiencies can exceed 100%. SOE is not currently commercially available and demonstration cells are nowhere near the scale of PEM or Alkaline. There is still considerable development required to get a commercially ready, scalable system with an acceptable stack replacement life. They currently have a short life due to the high operating temperatures in the process. The largest systems installed to date are in the 10 to 100kW range and these have been installed as proof of principle units rather than as truly commercial offerings. [4]

### 2.3.5 Product specifications

Shell has published some information [14] on the various types of electrolyzers which can be found in the table below.

*Table 8: Performance data and hydrogen composition for various types electrolyzers [14]*

Electrolyser type		AE	PEM	AEM	SOE
Temperature	° C	60 - 80	60 -80	60 - 80	700 – 900
Electrolyte	-	Potassium hydroxide	Solid state membrane	Polymer membrane	Oxide ceramic
Plant size	m <sup>3</sup> H <sub>2</sub> /h (n)	0,25 - 760	0,01 - 240	0,1 - 1	Laboratory
	kW	1,8 – 5.300	0,2 – 1.150	0,7 – 4,5	
Purity H <sub>2</sub>	%	99,5 – 99,9998	99,9 – 99,9999	99,4	N/A
Efficiency	%	65 – 82	65 - 78	N/A	85
Lifespan	H	60.000 – 90.000	20.000 – 60.000	N/A	1.000
Maturity level	-	Commercially used in industry for the last 100 years	Commercially used for medium and small applications	Commercially available for limited applications	Experimental stage

As a basis for the Common Business Practice, the following general composition resulting from an electrolyser is considered. In the table below the information on electrolysis presented in this paragraph is summarised.

*Table 9: General hydrogen composition for an electrolyser*

General specification		Electrolysis
Components	Vol.	H <sub>2</sub> -stream
H <sub>2</sub>	%	99,5 – 99,9999
O <sub>2</sub>	ppm	< 500
H <sub>2</sub> O	ppm	< 100

Hydrogen is also produced as a “by-product” during the manufacturing of chlorine by the electrolysis of a sodium chloride solution (brine), which is also known as the Chlor-Alkali process. The production of chlorine results in the co-products caustic soda (sodium hydroxide) and hydrogen gas. These two products, as well as chlorine itself, are highly reactive. Chlorine can also be produced by the electrolysis of a solution of potassium chloride, in which case the co-products are hydrogen and caustic potash (potassium hydroxide) [15]. In hydrogen produced by a Chlor-Alkali process, chlorine is present as a trace component.

## 2.4 Other hydrogen production processes

Currently, new processes to produce hydrogen are in the research and development phase. The conversion of biomass by torrefication into hydrogen and ‘green’ carbon is such an example. Since no compositional data is available yet for these processes, they are not further taken into account in this report. However, it is expected that since the CBP specification is based on the requirements of the end users, the CBP specification is also valid for these novel processes.

## 2.5 Hydrogen production shares

At this moment there is a significant amount of uncertainty with respect to possible future hydrogen production shares between three main production technologies (Pyrolysis, SMR/ATR, electrolysis)

In the Hydrogen Roadmap [16] two scenarios are defined to predict the amount of hydrogen produced by SMR/ATR and by electrolysis.

In the water-electrolysis-dominant scenario, water electrolysis will almost exclusively supply transportation demand from the start. Other industries will rely on water electrolysis and SMR in equal parts until about 2030. After 2030, no new SMR capacity is installed as electrolysis becomes the source of hydrogen with the lowest costs. All existing reforming capacity is gradually retrofitted with CCS. For power generation, buildings, and industry, this scenario results in a mix of about 70% centralized water electrolysis, approximately 20% decentralized water electrolysis, and 5% SMR in 2050. For transportation, an even more electrolysis-centred split is assumed, with 95% of the hydrogen generated with water electrolysis, half of which uses decentralized water

electrolysis. Important conditions to this scenario include having enough renewable power capacity and electrolyser capacity in the EU, and a significant drop in the costs of electrolysis and renewable power.

The SMR-/ATR-dominant scenario, relies primarily on SMR and completes the hydrogen production portfolio with smaller shares of electrolysis. For utility scale power generation, heating and power for buildings and industrial use, this scenario assumes 85% of hydrogen from SMR/ATR in 2050 and 10% via central electrolysis. For transport applications, it is projected that SMR would contribute about half of the hydrogen supply, with the other half from water electrolysis.

According to a study carried out by Pöyry [17] pyrolysis makes up 55% of hydrogen production, while SMR with CCS supplies 30%, and electrolysis 15% in 2050.

A summary of the possible hydrogen production shares divided into electrolysis, SMR/ATR, Pyrolysis and as a by-product of other production processes is given in the table below.

*Table 10: Possible hydrogen production shares [16] [17]*

<b>Production shares [%]</b>		<b>Electrolysis</b>	<b>SMR/ATR</b>	<b>Pyrolysis</b>	<b>By-product</b>
Water electrolysis dominant	2030	30 %	55 %		15 %
	2050	80 %	15 %		5 %
SMR/ATR dominant	2030	10 %	75 %		15 %
	2050	20 %	75 %		5 %
Pyrolysis dominant	2050	15 %	30 %	55 %	

### 3 Utilisation specification (exit)

The required hydrogen quality from the perspective of the end user strongly depends on the end user's application. In general, the required specification for hydrogen fired in traditional applications is usually less strict compared to the use of hydrogen as a feedstock or as an energy source for fuel cells.

In the following paragraphs an analysis is made per user category.

#### 3.1 Fuel cell

For PEM fuel cells which are among other application used in road vehicles, information is available regarding the effect of the contaminations on their performance and durability [6]: The effects of fuel quality on PEM fuel cell performance and durability must be considered within the larger context of the causes and mechanisms of PEM fuel cell degradation, that is, the gradual decline in power output during operation in road vehicles. According to Borup et al., who conducted a comprehensive review of the research and literature on this topic, these mechanisms include degradation of mechanical properties due to dissolution and sintering of platinum particles, thinning of the membrane, and corrosion of carbon support materials. Borup et al. [7] cite a delicate balance between maximizing fuel cell performance and durability while reducing cost and complexity and consider the presence of contaminants in the fuel stream as one of the conditions of the operation, along with temperature, voltage, current, pressure, and duty cycle that affect performance and durability. Borup et al. [7] state that "the causes of the gradual performance decline are not completely understood, especially the degradation mechanisms that occur in the fuel cell's different components and the relative contribution of each component's degradation to the degradation of the entire fuel cell."

In the conclusions of the report of the U.S. Energy Department [6] it is stated that "Because testing for all of the non-hydrogen constituents included in the ISO and SAE standards would be too time-consuming and extremely expensive, the team defined a subset of those constituents that are likely to be the major technical and economic drivers of the trade-offs between fuel quality and cost, as discussed above. After much discussion among the team members, industry, and other ISO and SAE working group members, the team identified "critical constituents" upon which to focus the testing, modelling, and analysis: carbon monoxide (CO), sulphur (S) species, ammonia (NH<sub>3</sub>), methane (CH<sub>4</sub>) and other inert gases, and particulate matter (PM) under 10 microns in diameter. These constituents are those most likely to affect PEM fuel cell performance and durability as well as the cost of hydrogen produced by SMR and purified by PSA to the levels required by the ISO and SAE standards."

The effect of the various contaminants on the performance of a fuel cell are described in ISO 14687:2019 [1] and can be found in Annex B of this document.

In the report of the U.S. Energy Department [6] an analysis was made on the relative difficulty of removing contaminant species. Helium, which is found in some natural gas sources in the United States, cannot be removed using PSA. CO has the highest "purification ratio for SMR," perhaps providing a basis for its serving as a "canary" for other contaminant species, i.e., the amount of CO in the fuel stream may serve as an indicator of the likely presence and concentrations of the other critical constituents (except PM). The team established a relationship between CO concentration with respect to PSA breakthrough properties of other critical constituents (NH<sub>3</sub>, S species, CH<sub>4</sub>, etc.) and estimated a rough order of magnitude of breakthrough of these constituents in relation to CO concentration for the baseline system. The results of this analysis can be found in table 11. The original table (table 2-1 [6]) referred to the ISO FDIS 14687:2012 whereas in table 11 reference is made to ISO 14687:2019 [1] Grade D. The main difference is the value for methane which has been changed from 2 ppm including the other hydrocarbons to 100 ppm for only methane and 2 ppm for the other hydrocarbons.

Table 11: Relative difficulty of removing selected contaminants species from hydrogen produced by SMR and PSA

Species	Adsorption Force (PSA)	ISO 14687 Class D Specification <sup>1</sup>	SMR Mol-%	Purification Ratio for SMR	Overall Effect
Helium (He)	Zero	100 ppm (total inert) <sup>1</sup>	500 ppm	5	Not Possible
Hydrogen (H <sub>2</sub> )	Weak	99,97 %	75 – 80 %		
Oxygen (O <sub>2</sub> )		5 ppm			Impacts PSA Recovery & Capital Cost
Argon (Ar)		100 ppm (total inert)	500 ppm	5	Impacts PSA Recovery & Capital Cost
Nitrogen (N <sub>2</sub> )		100 ppm (total inert)	1000 ppm	10	Impacts PSA Recovery & Capital Cost
Carbon Monoxide (CO)		0,2 ppm	0,1 – 4 %	200.000	Impacts PSA Recovery & Capital Cost
Methane (CH <sub>4</sub> )		100 ppm <sup>1</sup>	0,5 – 3 %	15.000	Impacts PSA Recovery & Capital Cost
Carbon Dioxide (CO <sub>2</sub> )		2 ppm	15 – 18 %	90.000	Relative Easier to Remove
Total Hydrocarbons		2 ppm	0,5 %	2.500	Relative Easier to Remove
Ammonia (NH <sub>3</sub> )	Strong	0,1 ppm	Low ppm		Relative Easier to Remove
Total Sulphur (S)	Strong	0,004 ppm			Relative Easier to Remove
Halogenates	Strong	0,05 ppm			Relative Easier to Remove
Water (H <sub>2</sub> O)	Strong	5 ppm	Dew Point		Relative Easier to Remove

<sup>1)</sup> The original table referred to ISO FDIS 14687:2012. In this table the values are taken from ISO 14687:2019 for Class D

### 3.1.1 User Requirements – fuel cell

A small literature scan shows that current hydrogen specifications used for fuel cells underlies fact-based information. The important contaminants influencing the performance and durability of a fuel cell are carbon monoxide (CO), sulphur (S) species, ammonia (NH<sub>3</sub>), methane (CH<sub>4</sub>) and other inert gases, and particulate matter (PM). As a basis for the Common Business Practice the following general user requirements for fuel cells are originating for ISO 14687:2019 (grades D and E-3) considered:

Table 12: General hydrogen specification for a fuel cell

End use application		PEM Fuel Cell
Components	Vol.	H <sub>2</sub> -stream
H <sub>2</sub>	%	99,9 - 99,97
H <sub>2</sub> O	-	Non-condensing at any ambient condition
CO	ppm	0,2
Total sulphur species	ppm	0,004
NH <sub>3</sub>	ppm	0,1
CH <sub>4</sub>	ppm	100
Inert Components	ppm	300 - 1000
Particulate Matter	mg/kg	1

## 3.2 Industry

### 3.2.1 Ammonia production

In the Netherlands, the hydrogen for ammonia is produced in dedicated SMR's using natural gas as a feed stock. These SMR's produce a mixture of hydrogen and nitrogen in the 3:1 molar ratio required for ammonia. Other components are not allowed or not preferred like for example oxygen containing components (e.g. H<sub>2</sub>O or CO<sub>2</sub>) will poison the ammonia catalyst. The presence of inerts (e.g. Ar or CH<sub>4</sub>) will reduce the efficiency of the reaction due to the larger recycle streams and thus to higher costs. The hydrogen/nitrogen mixture from the SMR is pressurized to about 200 bars where it reacts to ammonia at 400-500 °C. The ammonia synthesis section of an ammonia plant can be fed with a mixture of hydrogen and nitrogen [5].

### 3.2.2 Methanol production

Methanol (CH<sub>3</sub>OH) is produced from synthesis gas (syngas), which main constituents are hydrogen, carbon monoxide and carbon dioxide. Synthesis gas is usually obtained by reforming natural gas, but other, even solid feedstocks can be used as well through gasification to obtain synthesis gas. Methanol is typically produced in two steps. The first step is to convert the feedstock (natural gas) into syngas. The process normally used for this step is steam methane reforming and a water-gas shift reaction to convert CO and H<sub>2</sub>O in more CO<sub>2</sub> and H<sub>2</sub>. As described in more details in paragraph 2.1.1. The second step entails the catalytic synthesis of methanol from the syngas, mostly using copper and zinc oxide (ZnO) on an alumina support as a catalyst. For both steps a variety of technologies exist. The reaction takes place at temperatures ranging from 300 to 400 °C and at pressures between 50 – 300 bar.

### 3.2.3 Refinery usage

Hydrogen is used in refinery operations for various hydrotreating operations. Hydrotreating is a (hydrogenation) process used to remove contaminants such as nitrogen-, sulphur- and/or oxygen containing components, and metals from petroleum fractions. These contaminants may not only affect the quality of the final refined products negatively, but also have detrimental effects on the refining equipment and the used catalysts. Next to hydrotreating, hydrocracking is another process frequently used in refineries to break heavier, higher boiling-point petroleum fractions into more desirable and valuable products (lower fractions such as gasoline and diesel). (Hydro)cracking is usually done after hydrotreating to reduce the sulphur compounds.

### 3.2.4 User requirements – Industry

In the DNV GL HyQuality study an overview is presented of the specific hydrogen requirements for various industrial processes which use hydrogen as a feedstock or as an energy carrier.

Table 13: General hydrogen specification for industrial usage (mostly feedstock) [10]

End use application Components	Industrial usage (mostly feedstock)							
	Refinery <sup>1</sup>	Ammonia <sup>2</sup>	Methanol <sup>3</sup>	Steel production	Hydrogen bromide	Hydrogen peroxide	Gas turbines <sup>4</sup>	Fisher Tropsch
Hydrogen H <sub>2</sub> (vol-%)	99,5	98,5 99,9	74	99,9	99,95	99,9	70	60
Total sulphur (ppb)		1	50			< 1000		< 100
Halides (ppb)		1	1				Low <sup>5</sup>	10
Oxygen (ppm)				ppm-level		< 10		
Carbon Monoxide (ppm)	10 – 50		20 vol-%		ppb-level	< 1		30 vol-%
Carbon Dioxide (ppm)	10 - 50					< 2		inert
Iron (ppb)			5					
Nickel (ppb)			5					
Hydrogen chloride (ppb)			2					
Water (ppm)						< 10		
Nitrogen (ppm)		reactant	0,5 vol-%			< 2000		50 ppb
Methane (ppm)	inert	inert	3 vol-%		ppb-level	< 10		inert
Argon / Helium (ppm)		inert				< 2000		inert

<sup>1)</sup> For crude oil desulphurisation, lower purity hydrogen (~98 vol-%) can be used  
<sup>2)</sup> Hydrogen purity requirements differ per ammonia producer. While some producers allow for CO/CO<sub>2</sub> concentration up to 10.000 ppm (~ 1 vol-%), others have CO/CO<sub>2</sub> fully removed and thus require higher purities.  
<sup>3)</sup> Methanol can be directly made from syngas as CO/CO<sub>2</sub> are reactants. Typical hydrogen concentrations in syngas (SMR+WGS) are ~70 vol-% or higher.  
<sup>4)</sup> Gas turbines can be engineered using hydrogen concentrations down to 70 vol-% (the remainder being nitrogen) to lower combustion temperatures and therewith NO<sub>x</sub> emissions. Once the turbine has been designed for a certain concentration, the hydrogen purity (quality) needs to be within strict limits (typically a Wobbe-range of +/- 5%).  
<sup>5)</sup> Low (as low as possible) typically means below 2%.

### 3.3 Appliances

Appliances for use with 'pure' hydrogen are currently under development. Therefore, it is not possible to formulate the requirements based on information of appliances provided by the manufactures. In the United Kingdom, a specification for 'pure' hydrogen is defined in the UK Hy4Heat project [11]. The specification is aimed at manufacturers developing prototype hydrogen appliances and during their subsequent demonstration, as part of the Hy4Heat programme. Since, the hydrogen will be distributed through the existing distribution grid, this specification is based on the natural gas regulation in the United Kingdom (GSMR:1996). This can be clearly observed in the traditional 'natural gas' parameters water dewpoint, hydrocarbon dewpoint and Wobbe-index.



Table 14: Hydrogen Purity Specification Hy4Heat UK [11]

Content or characteristic	Value	Rationale
Hydrogen fuel index (minimum mole fraction)	98 %	Aim is to have a threshold value that meets user requirement.
CO	20 ppm	A practical engineering limit based on achievable production limits and to meet long term exposure limits HSE EH/40)
H <sub>2</sub> S	≤ 3.5 ppm	These values are taken from GS(M)R:1996 as any detrimental effects would be similar for hydrogen and natural gas.
Total sulphur content (including H <sub>2</sub> S)	≤ 35 ppm	
O <sub>2</sub>	≤ 0.2 % (molar)	
Hydrocarbon dewpoint	-2 °C	Complies with GSMR:1996 and EASEE-gas
Water dewpoint	-10 °C	
Sum CH <sub>4</sub> , CO <sub>2</sub> and total hydrocarbons	≤ 1% (molar)	No combustion impacts and to reduce carbon emissions
Sum Ar, N <sub>2</sub> and He	≤ 2% (molar)	To avoid transporting inert gases and to limit the impact on Wobbe Number
Wobbe Index	42 – 46 MJ/m <sup>3</sup>	Range and percentage variation based on natural gas range in GS(M):R1996
Other impurities	Shall not contain solid, liquid or gaseous material that might interfere with the integrity or operation of pipes or any gas appliance, within the meaning of regulation 2(1) of the Gas Safety (Installation and Use) Regulations 1998, that a consumer could reasonably be expected to operate	

### 3.4 Hydrogen end user markets shares

Besides the hydrogen quality requirements for the different processes and applications, it is necessary to know their current and future market share. It is obvious that there is a large uncertainty with respect to the expected future market shares, especially for those sectors which are currently under development. Furthermore, it is the expected that market shares will be dependent on the local situation and as a result can be different in the various European Member States. However, to be able to estimate the size of the markets for the different hydrogen grades data, relevant information for the European Union is presented in this chapter.

An overview of the various segments using hydrogen today is given in the Hydrogen Roadmap [16]. The purity specification presented in table 15 are taken from table 13.

Table 15: Use of hydrogen today in the EU [TWh] [16]

Market segment	Purity [vol-%]	Usage [TWh]	Share [%]
Refining <ul style="list-style-type: none"> <li>Hydrocracking</li> <li>Hydro-treating (e.g., fuel desulfurization)</li> <li>Biorefinery</li> </ul>	99,5	153	45
Ammonia <ul style="list-style-type: none"> <li>Production of ammonia (for urea and other fertilisers)</li> </ul>	98,5 – 99,9	129	38
Methanol <ul style="list-style-type: none"> <li>Production of methanol and derivatives</li> </ul>	74	27	8
Other chemicals <ul style="list-style-type: none"> <li>Other chemicals (e.g., polymers, polyurethanes, fatty acids)</li> </ul>	N/A	3	1
Processing <ul style="list-style-type: none"> <li>Heat treating of steel</li> <li>Welding of metals</li> <li>Forming and blanketing gas</li> <li>Glass production</li> </ul>	N/A	13	4
Liquified Hydrogen <sup>1</sup> <ul style="list-style-type: none"> <li>Rocket fuel</li> <li>Automotive fuel</li> <li>Semiconductor industry</li> </ul>	N/A	14	4
<b>Total</b>		<b>339</b>	<b>100</b>

Hydrogen Europe has also made a forecast of the hydrogen consumption in 2030 and 2050 using two scenarios *business as usual (bau)* and *ambitious (amb)*.

Table 16: Future use of hydrogen in the EU (business as usual and ambitious scenarios) [16]

Market segment	Usage [TWh]					
	Scenario	2015	2030 bau	2030 amb	2050 bau	2050 amb
Existing industry feedstock		325	427	427	391	391
New industry feedstock				62	1	257
Industry energy				8	53	237
Heating and power for buildings			25	33	207	579
Transportation			4	70	85	675
Power generation, buffering			25	65	43	112
<b>Total hydrogen</b>		<b>325<sup>1</sup></b>	<b>481</b>	<b>665</b>	<b>780</b>	<b>2.251</b>
<b>Final energy demand</b>		<b>14.100</b>	<b>11.500</b>	<b>11.500</b>	<b>9.300</b>	<b>9.300</b>

<sup>1)</sup> The amount specified for 2015 in the previous table (table 15) and this table (table 16) differ by an amount of 14 TWh probably being the liquid hydrogen segment.

By combining the information of the current and expected size for the various market segments and the required hydrogen purity for the given segment, it is possible to make an estimate of the sizes of the different hydrogen classes in time. For the market segments *Existing industry feedstock* and *New industry feedstock*, the required hydrogen quality is subdivided based on usage share in 2015 for the sub segments *Refining*, *Ammonia* and *Methanol* (see table 15). This results for both *industry segments* in a 50% usage share for the hydrogen quality 99 % - 99,9 % range, a 42% usage share for the hydrogen quality 98 % - 99 % range and finally a 8% usage share for the hydrogen quality range  $\leq 98$  %. A hydrogen quality range  $\leq 98$  % is allocated to the market segments *Industry energy*, *Heating and power for buildings* and *Power generation, buffering*. A hydrogen quality range  $\geq 99,9$  % is allocated to the market segment *Transportation*.

Table 17: Future classification of hydrogen in the EU (business as usual and ambitious scenarios) [10] [16]

Hydrogen classification	Usage [TWh]					
	Scenario	2015	2030 bau	2030 amb	2050 bau	2050 amb
Hydrogen (vol-%) $\leq 98$ <sup>1</sup>		26	84	145	334	980
98 < Hydrogen (vol-%) $\leq 99$ <sup>2</sup>		137	179	205	165	272
99 < Hydrogen (vol-%) $\leq 99,9$ <sup>3</sup>		163	214	245	196	324
Hydrogen (vol-%) $> 99,9$ vol-% <sup>4</sup>		0	4	70	85	675

<sup>1)</sup> Industry energy, Heating and power for buildings, Power generation, buffering (burners, turbines), Existing and new industry feedstock (8% usage share)  
<sup>2)</sup> Existing and new industry feedstock (42% usage share)  
<sup>3)</sup> Existing and new industry feedstock (50% usage share)  
<sup>4)</sup> Mobility (fuel cell)

From this table, it can be concluded that the hydrogen classes with a purity range between 98 – 99 vol-% and 99 – 99,9 vol-% will possess the largest sizes in the coming years until 2030. The market for high purity hydrogen ( $> 99,9$  vol-%) is strongly depending on the chosen scenario. In the ambitious scenario, the size of this market segment will be comparable to the total market for 98 – 99,9 vol-% hydrogen in 2050. However, in the business as usual scenario the size of the high purity hydrogen market will only be 22% of the total market for 98 – 99,9 vol-% hydrogen in 2050. The market for low purity hydrogen will only develop from 2030 and onwards. Depending on the scenario, the market share for  $\leq 98$  vol-% purity hydrogen varies in 2030 between 10% (business as usual) and 16% (ambitious) of the overall H<sub>2</sub> market and in 2050 between 39% (business as usual) and 41% (ambitious).

In summary, the information provided in the table above, shows that the different market segments have distinctive purity requirements and that depending on the chosen scenario, all defined hydrogen purity classes could have a significant market share.

## 4 Purification

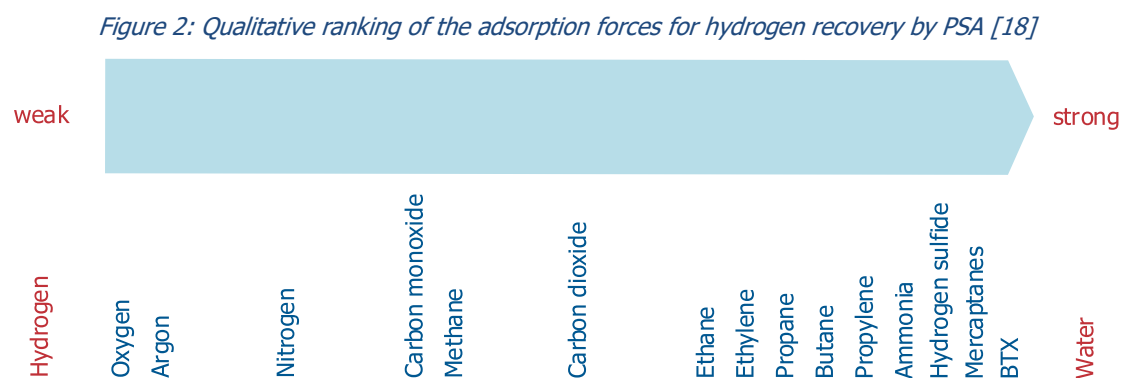
The reason to apply purification to a hydrogen containing gas stream can be two folded. One reason to use a purification step is to enrich the hydrogen content of the gas stream to upgrade the hydrogen class of the processed gas stream. Another reason is to remove unwanted, harmful (trace) component from the hydrogen rich gas stream to make it suitable for transport, distribution and/or end use application.

### 4.1 Enrichment of hydrogen content

Various purification techniques are available to 'upgrade' the hydrogen content of a gas stream. Drawback of a purification step is the emergence of a residual product (purge gas) lean in hydrogen content and rich in the other constituents of the feed gas.

At the moment, Pressure Swing Adsorption (PSA) is the most widely applied technology (> 85% [10]) followed by membranes. The separation effect of PSA is based on differences in binding forces to the adsorbent material. Highly volatile components with low polarity, such as hydrogen, are practically non-adsorbable as opposed to molecules as N<sub>2</sub>, CO, CO<sub>2</sub>, hydrocarbons and water. Consequently, these components, which are qualified as impurities, can be adsorbed from a hydrogen containing stream and high purity hydrogen is recovered. During the PSA process, the hydrogen is recovered and purified at a pressure close to the feed pressure, while adsorbed impurities are removed by lowering the pressure resulting in a PSA purge gas stream.

In a brochure from Linde on hydrogen recovery by pressure swing adsorption [18], a qualitative ranking of the adsorption forces is given. This ranking looks similar to the ranking provided in table 11 but in the figure below some additional components are shown.



In the DNV GL HyQuality study [10] the following comparison is given of the different techniques. The hydrogen recovery is the ratio of the quantity of hydrogen from the feed that is recovered in the product. Recovery is influenced by product purity, feed composition (nature and quantity of impurities) and pressure conditions. The minimal hydrogen content specifies the minimum hydrogen concentration in the feed which can be processed by the given purification technique.

Table 18: Comparison of key characteristics for hydrogen enrichment techniques [10]

Feature	PSA	Membrane	Cryogenic	Electro-chemical
H <sub>2</sub> Purity	98 – 99.9999%	90 – 98%	95 – 99%	>99.9%
H <sub>2</sub> Recovery	75 – 92%	85 – 95%	90 – 98%	>90 – 100%
Min. H <sub>2</sub> content	> 40%	>25 – 50%	> 10%	>8 – 100%
Typical Capacity [m <sup>3</sup> H <sub>2</sub> /hr (n)]	< 400,000	< 50,000	10,000 – 75,000	1 – 1,000
Operating Pressure [bar]	10 – 40	20 – 200	20 – 50	Very high pressure (up to 600 bar)
Operating Temperature [°C]	Room temperature	0 – 100	-180	20 – 80
Pre-treatment	No	Minimal, H <sub>2</sub> S removal	CO <sub>2</sub> and H <sub>2</sub> O removal	Sulphur removal
Start-up Time	Minutes	Minutes	Hours	Minutes
Availability	Traditional method	Traditional method	Traditional method	Early stage of commercialization
Reliability	High	High	Average	High, no moving parts
Typical Impurities	CO <sub>2</sub> , H <sub>2</sub> O, CH <sub>4</sub> , (HCs), CO	Hydrocarbons, CO	Hydrocarbons	H <sub>2</sub> O
Comments	The recovery is relatively low as hydrogen is lost in the purging step. Purging results in tail gases.	He, CO <sub>2</sub> and H <sub>2</sub> O may also permeate the membrane	Pre-purification step necessary to remove CO <sub>2</sub> , H <sub>2</sub> S and water	Sulphur-containing compounds poison the electro-catalysts

## 4.2 Reduction of the impurity content

Although the enrichment of the hydrogen stream also reduces the amount of impurities, some impurities require specific treatment. In the public literature limited information can be found regarding this specific aspect. In the Hy4Heat project an overview is given of the purification techniques needed to guarantee the given specification (see table 14). It should be taken into account that Hy4Heat specification is at the lower end of the range with a minimum hydrogen content of 98 vol-% and therefore the results are only partly useable if a higher-grade hydrogen needs to be purified.

Table 19: The Hy4Heat standard from a production and end-user perspective [11]

Impurity	Level	Production/Purification Impact	End-user	Justification
CO	20 ppm	Both methanation and PSA can reach.	Not suitable for PEMFC	Meets HSE long term exposure limit without ruling out potentially cheaper purification option
Water dewpoint	-10 °C	Met with PSA if CO standard met. Drying required with methanation.	Further purification required for PEMFC	Complies with GSMR:1996 and EASEE-gas
Total Sulphur	35 ppm	Met by production with no further purification.	Not suitable for PEMFC or SOFC	May be present at these levels initially in the grid. Used as a warning to be review with time.
Oxygen	≤ 0.2 %	Met by production with no further purification.	Not suitable for PEMFC	GSMR:1996
Sum of methane, CO <sub>2</sub> , total hydrocarbons	≤ 1 %	Met with a PSA reaching CO spec. Rules out methanation with an SMR, but could be used with careful ATR design.	Not suitable for PEMFC and potential SOFC issues.	Restriction must be applied for boiler design. Lowest restriction applied
Sum of inerts	≤ 2 mol %	Met by SMR with no purification. Met with PSA meeting CO standard.	Small impact on PEMFC – could be managed	To avoid transporting inert gases with no calorific value and to limit the impact on Wobbe Number (see below)

## 5 Pipeline specification

The Common Business Practice to be developed is targeting the harmonisation of 'pure' hydrogen flowing (partially) through dedicated hydrogen pipelines. In case an existing natural gas pipeline is upgraded to the level to allow the transportation of pure hydrogen transportation, possible contaminations during the 'natural gas' life of the pipeline need to be taken into account. Since natural gas pipelines are designed, built and operated with the transmission of (natural) gas in mind, the effect of exposure of the pipeline to hydrogen is a main point of attention.

### 5.1 Pipeline contaminations

Depending on the lifetime and the nature of the transported gas, a natural gas pipeline will often contain liquid and solid contaminants:

- Black powder is a generic term for corrosion products that are made up of iron sulphide and/or iron oxides. Also, other particles such as sand and debris can be found as solids.
- Liquid contaminants in gas streams can include water, glycols, hydrocarbon condensates as well as compressor oils.
- Gaseous elementary mercury present in some natural gas can be present at or in the inner layer of the pipeline wall as a result of ad- and/or absorption processes.
- Odorants, often containing sulphur components, tend to partly adsorb to the pipeline wall. The amount adsorbed will depend strongly on the nature of the odorant.

#### 5.1.1 Cleaning natural gas pipelines

To avoid the contamination of the hydrogen by the residual natural gas components in the pipeline, cleaning the internal surfaces of the pipeline system seems to be a sensible option. Nowadays, several techniques are available to clean natural gas pipelines, however, now no information is available on the effectiveness for the abovementioned components. Especially the behaviour of components adsorbed at or absorbed in the pipeline wall, like odorants and mercury is unclear. Further investigations are needed to define the best procedure to convert a pipeline from natural gas to hydrogen operation and which steps should be taken in that process.

### 5.2 Natural gas pipeline requirements for conveying hydrogen

Reusing natural gas pipelines for the transmission of 'pure' hydrogen is studied intensively by many institutes since this offers a solution to decarbonise the energy system without having to invest massively in new energy infrastructure<sup>3</sup>. Currently in CEN TC234 'Gas infrastructure' a Technical Report is drafted in which the consequences of the introduction of hydrogen both as a mixture with natural gas as well as 'pure' hydrogen on the various standards within CEN TC234 is compiled. As part of this process CEN TC234/WG3 'Gas transportation' is looking into the effect of hydrogen on the pipeline.

In a position paper of Gasunie and OGE [19] the effect of hydrogen on an existing natural gas pipeline is described:

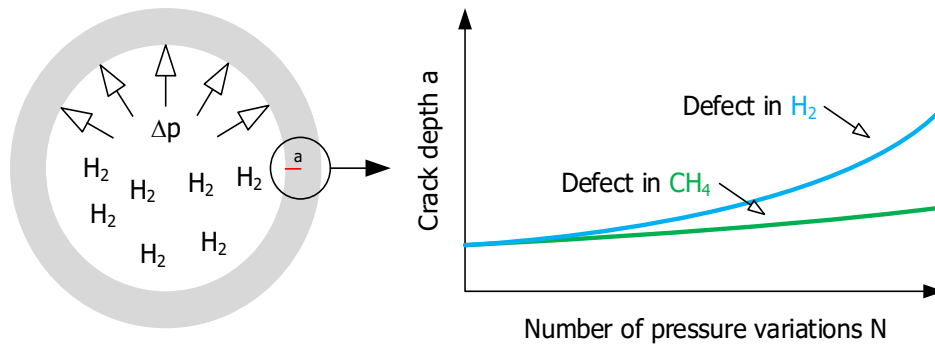
Gas pipelines are usually designed so that stresses are below the specified minimum yield strength and fatigue loading is also usually not relevant considering the compressibility of gas. This situation can be compared with the tensile test, where no hydrogen effects are to be expected. However, pipelines are welded structures and weldments can contain a variety of defects, including crack-like defects. In this situation, a fracture toughness test might be relevant. This test involves a constantly increasing load, meaning continuous plastic straining at the crack tip in the presence of hydrogen. Pipelines might be stressed by settlements, but existing pipelines are settled without hydrogen being present. Fatigue loading due to daily demand differences in combination with crack-like defects is a situation comparable to the fatigue crack growth tests.

So, where hydrogen gas is transported in pipelines at ambient temperatures and moderate pressures, the relevant hydrogen degradation mechanism is hydrogen-enhanced fatigue crack growth: existing crack-like defects in a pipeline, e.g. weld defects, may grow faster in hydrogen gas than in natural gas under a fatigue loading due to pressure cycles.

<sup>3</sup>) The costs for retrofitting of a natural gas network are depending on the technical characteristics and can vary significantly for different networks.

At newly created steel surfaces, hydrogen molecules dissociate and are absorbed in the steel. Around the plastic zone of a growing crack-like defect, hydrogen atoms interact with the steel enhancing the crack growth, see figure below.

Figure 3: Illustration of the hydrogen-enhanced fatigue crack growth in pipelines



### 5.2.1 Measures to diminish hydrogen-enhanced fatigue crack growth

Hydrogen-enhanced fatigue crack growth can be diminished in the presence of other gases such as  $O_2$ ,  $CO$ ,  $COS$ , and  $H_2O$  [20] [21]. It was found that, with oxygen, the crack growth rate in hydrogen was the same as in nitrogen gas. Experiments carried out in Naturalhy project confirmed this phenomenon. One mechanism is that, at newly formed crack surfaces, iron reacts with gases thereby hindering the dissociation process of the hydrogen molecules.

At the moment it is not clear what amount of oxygen, if any, would be needed to safeguard the natural gas pipeline for hydrogen-enhanced fatigue crack growth. This is strongly depending on the pipeline material, the fatigue loading due to pressure cycles and other factors. In the literature [21], the effect of an oxygen concentrations of 100 ppm and 500 ppm is shown. Since a concentration of 500 ppm is not completely mitigate the effect of hydrogen-enhanced fatigue crack growth a concentration of 1000 ppm (0,1 mol-%) is suggested.

The presence of oxygen to safeguard the natural gas pipeline against hydrogen enhanced fatigue cracking seems to be in contradiction to most of the user requirements which specify very low oxygen contents in the ppb to ppm range. However, it seems to be possible to remove the oxygen in an efficiency way by a catalyst at low temperatures [22]: *Catalytic recombination or deoxygenation is used to remove oxygen ( $O_2$ ) impurities. The process is also known as a 'deoxo' process. The oxygen reacts with the hydrogen to form water vapor, which can then be removed by a dryer if necessary. The catalysts that are used are based on platinum group metals (PGM). A typical system could handle up to 3%  $O_2$  in  $H_2$  in the feed and reduce the  $O_2$  content to less than 1 ppm.*

## 6 CBP specification

The current CBP regarding the Harmonisation of Natural Gas Quality [23] prescribes the following parameters and values.

*Table 20: Parameters and value EASEE-gas CBP 'Harmonisation of Natural Gas Quality' [23]*

Parameter	Unit	Min	Max	Recommended implementation date
WI	kWh/m <sup>3</sup>	[13.60]	15.81	1/10/2010
d	m <sup>3</sup> /m <sup>3</sup>	0.555	0.700	1/10/2010
Total S	mg/m <sup>3</sup>	-	30	1/10/2006
H <sub>2</sub> S + COS (as S)	mg/m <sup>3</sup>	-	5	1/10/2006
RSH (as S)	mg/m <sup>3</sup>	-	6	1/10/2006
O <sub>2</sub>	mol %	-	0.001*	1/10/2010
CO <sub>2</sub>	mol %	-	2.5	1/10/2006
H <sub>2</sub> O DP	°C at 70 bar (a)	-	- 8	See note**
HC DP	°C at 1- 70 bar (a)	-	- 2	1/10/2006
<p>*) Limit is &lt;0.001 mol%, daily average. However, cross border point daily average levels up to 0.01 mol% will be accepted if these are the result of the prudent operation of UGS's, existing in 2006, which use oxygen for desulphurisation purposes. (Based on the full CBP Wobbe range).</p> <p>**) At certain cross border points, less stringent values are used than defined in this CBP. For these cross-border points, these values can be maintained, and the relevant producers, shippers and transporters should examine together how the CBP value can be met in the long run. At all other cross border points, this value can be adopted by 1st October 2006.</p>				

### 6.1 Hydrogen content

The required hydrogen content strongly depends on the application and differ greatly from one another. In literature often three quality grades are distinguished:

- Fuel cell quality – ISO 14687:2019 Grade C and E-3 [1].
- Industrial quality<sup>4</sup>
- Heating quality<sup>5</sup>

The Common Business Practice will focus on 'industrial quality' hydrogen. The reason is:

- In the coming years, it is expected that large scale production of hydrogen will take place through the conversion of methane. In contrast to electrolysis, these conversion processes do not deliver inherent fuel cell quality hydrogen. Possibilities for large scale production of hydrogen via electrolysis are not expected before 2030.
- Market forecasts show that the industry will take the lion part of the total hydrogen demand. Only in the period after 2030, there is the possibility for large scale demand for fuel cell and/or energy production grade hydrogen.
- No hands-on experience is available on the possible effects of residues in the pipeline resulting from the previous exposure to natural gas on the hydrogen transmitted through such a pipeline. This effect is expected to be neglectable but the higher the hydrogen grade the larger the risk that small amounts of a particular contaminant can result in an off-specification situation at the exit.

From the inventory carried out in this document, it has become clear that it is not possible to define a minimum hydrogen value that suits all stakeholders. A minimum hydrogen concentration of 98 mol-%<sup>6</sup> seems to be a good compromise to be used in the CBP. This minimum requirement is achievable with reforming processes without complex and expensive purification and is well suited for use in heating applications. The minimum hydrogen concentration of 98 mol-% doesn't fulfil the requirements of several feedstock processes. However, given the requirements those processes require with respect to the presence of some of the trace components, like sulfur, oxygen and/or nitrogen, a local purification step at the end user site seems to be necessary for those processes

<sup>4</sup>) Industrial quality hydrogen is hydrogen used in the industry as a feedstock and/or in chemical processes (see chapter 3.2)

<sup>5</sup>) Heating quality hydrogen is hydrogen used for generating heat in domestic, commercial & industrial applications i.e. boilers, furnaces.

<sup>6</sup>) Although in most data sources vol-% is used, it is from an analytic chemistry point of view better to use mol-%. Since there is no significant difference between vol-% and mol-% no conversion factor is applied.

before those users can use the hydrogen. For the application in fuel cells a very high grade hydrogen ( $\geq 99,97$  mol-% ISO 14687:2019 Grade D) is required. Conveying such a very high grade hydrogen through repurposed natural gas infrastructure could result in off-specification at the exit because of the uptake of small amounts of contaminants from the pipeline. Furthermore, the market for such a very high grade hydrogen is relatively small and the upgrading of hydrogen produced by reforming processes costly. A minimum hydrogen concentration of 98 mol-% is also specified in ISO 14687:2019 as Grade A<sup>7</sup>.

Depending on the developments in the hydrogen production, i.e. a strong increase in electrolysis and/or pyrolysis, and advances in the market, i.e. large market for fuel cells, it is recommended to reassess the current proposed value of 98 mol-% and hydrogen specification for the CBP after a few years. An additional advantage is that more information will be available on the behaviour of the residues in the pipeline which can be considered in a revised version of the CBP.

## 6.2 Transition Phase

The scope of this CBP is a recommended quality specification for hydrogen (non-blended with natural gas, see Note 1) flowing through dedicated systems, meaning networks that were originally designed and used for natural gas transmission and after a safety and reliability assessment (see Note 2) found suited for conveying hydrogen and newly built hydrogen pipeline systems. *After the pipeline is switched over from natural gas to hydrogen there is a period in which the hydrogen composition can be influenced by natural gas residues still present in the pipeline system.* This period is referred to by the term 'transition period'. During this transition period, for some of the constituents present in the hydrogen temporary deviating values are valid. The duration of the transition period is unknown and is also depending on the given constituent.

## 6.3 Main constituents

### 6.3.1 Carbon monoxide

If the production of hydrogen gas takes place by reforming, carbon monoxide is one of the constituent's present. The requirements regarding the carbon monoxide content for the various industrial processes and appliances show a wide range of values but most of them are in the ppm range.

For the CBP a maximum carbon monoxide content of 20 ppm is proposed because this limit value is appropriate for most end user applications, for example refineries require a limit value between 10 – 50 ppm carbon monoxide (see Table 13). This value is a compromise between the hydrogen production and the usability by the various end user categories. In the Hy4Heat study [11], which was the basis for the BSI PAS 4444 standard, a similar conclusion was drawn.

### 6.3.2 Sulphur components (non-odorised hydrogen)

A source of sulphur components, like hydrogen sulphide and mercaptans, is the (natural) gas used in a reforming process. Since sulphur components are poisoning the catalysts used in the various types of reforming processes, the sulphur components will be removed from the (natural) gas before the actual reforming process takes place and thus the resulting hydrogen is almost free of sulphur components. In table 6 a value of maximum 5 ppm hydrogen sulphide is mentioned in the product stream for a SMR or ATR process.

In some countries, it is necessary to odorize the hydrogen before it is allowed to be transmitted and/or distributed. Most commercial available odorants used for (natural) gas contain sulphur components but there are also sulphur free odorants available. Because of all these uncertainties regarding odourisation, this CBP will only specify the maximum sulphur content for the non-odorised hydrogen.

Another source of sulphur components could be the residue left in the pipeline. During the transition period, which ends for sulphur at the moment no sulphur components are released anymore from the pipeline debris, the total sulphur shall not be more than 21 mg S/m<sup>3</sup> (n). This value corresponds to the specification mentioned in European EN 16726 standard for H-gas [24].

<sup>7)</sup> The maximum concentrations specified in ISO 14687:2019 for the trace components deviate, in some instances even substantially, from the values that were found in this analysis and therefore it is no option to adopt the ISO 14687:2019 Grade A as a suitable specification for hydrogen in repurposed natural gas infrastructure.



After the transition period, the maximum amount of total sulphur is expected to be much lower since most of the existing hydrogen production processes are known to produce virtual no sulphur components. However, since no accurate data is available, no maximum value for the total sulphur content after the transition phase is specified.

### 6.3.3 Carbon dioxide

If the production of hydrogen gas takes place by reforming, carbon dioxide is also one of the constituent's present. Like for carbon monoxide, the requirements regarding the carbon monoxide content for the various industrial processes and appliances show a wide range of values but most of them are in the ppm range.

For the CBP a maximum carbon dioxide content of 20 ppm is proposed because this limit value is appropriate for most end user applications, for example refineries require a limit value between 10 – 50 ppm carbon dioxide (see Table 13). The value of 20 ppm is for carbon dioxide also a good compromise between the hydrogen production costs and the usability of the hydrogen by the end users.

### 6.3.4 Hydrocarbons

#### 6.3.4.1 Methane

Methane will be mostly present in the hydrogen gas if a chemical conversion process is used for its production. In most of the industrial feedstock applications, methane does not take part in the chemical reaction and is considered as an inert. However, the presence of a higher concentration of methane in the hydrogen feedstock can result for processes in which part of the feed stream is recycled to larger recycle- and vent streams and thus to higher costs. On the other hand a higher hydrocarbon (methane) specification facilitates the use of methanation as a purification method for hydrogen production. The methanation step converts carbon monoxide and carbon dioxide into methane.

#### 6.3.4.2 Other hydrocarbon species

During reforming most of the other hydrocarbon species present in the (natural) gas will be converted into hydrogen resulting apart from methane in the absence of other hydrocarbon species in the product stream<sup>8</sup>.

Another source of hydrocarbons could be originating from the residue present in the pipeline after cleaning the pipeline.

#### 6.3.4.3 CBP value for hydrocarbons

The amount of hydrocarbons shall not be more than 1,5 mol-%. Various end users prefer to have separate specifications for the maximum allowed amount of methane and the other (heavier) hydrocarbons because of the different effects on their processes. Since no accurate data is available at the moment it is not possible to come up with a proposal for such a split.

### 6.3.5 Hydrocarbon Dewpoint (During Transition Period)

During the transition process of a pipeline system from (natural) gas to hydrogen, it cannot be fully excluded that in the beginning hydrocarbons from the pipeline residue are taken up by the hydrogen passing along. To limit the maximum allowable concentration hydrocarbons, during this transition, a hydrocarbon dewpoint specification is in force. The specification of  $\leq 2$  °C at any pressures between 1 and 70 bar(a) is taken from the European standard EN 16726 for H-gas [24].

### 6.3.6 Inerts

#### 6.3.6.1 Argon

Argon can be found as a constituent in the hydrogen gas if it is produced via an Auto Thermal Reforming or Partial Oxidation process. Being one of the noble gases it does not take part in any chemical reaction and behaves as a perfect inert component.

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<sup>8)</sup> A purification step based on pressure swing adsorption will preferably remove the higher hydrocarbons because of their affinity to the adsorbent.

### 6.3.6.2 Helium

Some natural gases contain helium and therefore helium can be found as a constituent in the produced hydrogen gas via a reforming process. Since helium is not trapped in a Pressure Swing Adsorption purification step, the helium present in the natural gas will appear unchanged in the hydrogen. Like argon, helium is also one of the noble gases and does not take part in any chemical reaction and behaves too as a perfect inert component.

### 6.3.6.3 Nitrogen

Nitrogen will only be found in the hydrogen gas if it is produced via an Auto Thermal Reforming or Partial Oxidation process. Apart from the ammonia production, nitrogen does not take part in the chemical reaction and is therefore also categorised as an inert.

### 6.3.6.4 CBP value for inerts

The fraction inerts consists of argon, helium and nitrogen. The specification ( $\leq 2$  mol-%) is complementary to the hydrogen specification ( $\geq 98$  mol-%). Like with the hydrocarbons, large amounts of inerts can result for processes in which part of the feed stream is recycled to larger recycle- and vent streams and thus to higher costs. On the other hand, a higher maximum allowed concentration of inerts avoids the use of Pressure Swing Adsorption as a purification method for hydrogen production by reforming.

### 6.3.7 Water

The current specification for natural gas specifies a water dewpoint of  $-8$  °C at a pressure of 70 bar(a). According to the Michell Instruments Humidity calculator [25], this would result for hydrogen in a water content of 48 ppm (v). With this value the specified water content does not fulfil the requirements for fuel cells ( $< 5$  ppm) and the production of hydrogen peroxide ( $< 10$  ppm). Since both applications require a higher hydrogen concentration<sup>9</sup> as specified in this CBP, a water dewpoint specification of  $-8$  °C at a pressure of 70 bar(a) can be maintained in the CBP.

### 6.3.8 Halogenated compounds

Halogenated compounds can be present in the hydrogen gas if produced by electrolysis of a sodium chloride solution or theoretically by reforming of gas originating from a landfill. However, the latter is not very realistic because this requires an extensive cleaning of the gas before it can be used in a reformer. Furthermore, in the required purification step, which is probably based on pressure swing adsorption, halogenates will preferably be trapped. For the CBP a maximum value of 0,05 ppm for halogenated components is proposed. This value is based on the requirement stated in ISO 14687:2019 for Grade D and Grade E [1]

### 6.3.9 Oxygen

For (natural) gas, according to the European standard EN 16726 [24], a maximum level of 10 ppm, expressed as a moving 24-hour average, is specified for sensitive users. The production of hydrogen, both by reforming as well as electrolysis can fulfil this requirement without requiring complex process steps and thus high costs. Especially industrial feedstock users require an oxygen content in the lower ppm range because oxygen can poison the catalysts used in those chemical processes. However, where the hydrogen can be demonstrated not to flow to installations or end-user applications sensitive to higher levels of oxygen, , e.g. feed stock users or hydrogen storages, a higher limit of up to 1000 ppm may be applied.

For the CBP a maximum value of 10 ppm, expressed as a moving 24-hour average, for oxygen is proposed.

### 6.3.10 Other components

Since it is impossible to specify maximum value for alle components that could possibly be encountered in the hydrogen a general statement is added to the CBP stating "*The gas shall not contain constituents other than listed in the table above at levels that prevent its transportation, storage and/or utilization without quality adjustment or treatment.*"

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<sup>9)</sup> It is common to enrich the hydrogen concentration by a pressure swing adsorption purification step. Since water is a polar substance, it will be trapped effectively by the adsorbent.

### 6.3.11 Wobbe-index

Based on the limit values specified for individual components or groups of components, the Wobbe-index is only influenced by the amounts of inerts (nitrogen, helium and/or argon) and methane present at various hydrogen levels. Since the carbon dioxide concentration is limited to a maximum value of 20 ppm, the presence of carbon dioxide might not influence the Wobbe-index.

In the table below the Wobbe-index is calculated for combinations of inerts (nitrogen, helium and/or argon) and methane at various hydrogen levels.

Table 21: Wobbe-index variation as function of different concentrations of nitrogen and methane

H <sub>2</sub> [mol-%]	N <sub>2</sub> [mol-%]	CH <sub>4</sub> [mol-%]	WI [MJ/m <sup>3</sup> (n)]	ΔWI [MJ/m <sup>3</sup> (n)]
100			48,34	
99	1		45,05	3,29
99	0,5	0,5	46,37	1,97
99		1	47,74	0,60
98	2		42,25	6,10
98	1,5	0,5	43,43	4,91
98	1	1	44,66	3,68
98	0,5	1,5	45,92	2,42

The only combination resulting in a larger reduction of the Wobbe-index is the combination of 98 mol-% hydrogen with 2 mol-% nitrogen. In case of this "extreme" mixture of 98 mol-% hydrogen and 2 mol-% nitrogen, two limit values need to be controlled simultaneously by the process operator without having any margin at all to accommodate for variation in the process conditions or small changes in the feedstock used. Thus in practice, it will only be possible incidentally to operate an installation at this specific composition. Since, it is not possible to have large variations in the Wobbe-index for a longer period of time, it was decided not to include the Wobbe-index in this CBP. However, a remark is made in the CBP that the largest difference in Wobbe-index occurs for a composition existing of 98 mol-% hydrogen and 2 mol-% nitrogen and using ISO 6976 results in a maximum shift of 6,1 MJ/m<sup>3</sup> (n), or equivalently, in a maximum reduction in WI of 12,6 %.

## 6.4 CBP 'Hydrogen in former natural gas networks'

Combining all the information on the above information results in the following CBP table.

Table 22: Parameters and value EASEE-gas CBP 'Hydrogen in natural gas infrastructure'

Parameter	Unit	Min	Max
Hydrogen	mol-%	98,0	-
Carbon monoxide	ppm	-	20
Total sulphur content <sup>(1)</sup>	mg S/m <sup>3</sup> (n) <sup>(2)</sup>	-	21 <sup>(3)</sup>
Carbon dioxide	ppm	-	20
Hydrocarbons (including Methane)	mol-%	-	1,5 <sup>(3)</sup>
Inerts (Nitrogen, Argon, Helium)	mol-%	-	2,0
Oxygen	ppm	-	10 <sup>(4,5)</sup>
Total halogenated compounds	ppm	-	0,05
Water dewpoint	°C at 70 bar(a)	-	- 8
Hydrocarbon dewpoint <sup>3</sup>	°C at 1-70 bar(a)	-	- 2 <sup>(3)</sup>
1) Non-odorised hydrogen			
2) normal conditions (1.01325 bar(a), 0 °C)			
3) During the transition period, where the hydrogen composition can be influenced by natural gas residues present in the pipeline system (see Note below the table)			
4) Expressed as a 24-hour average			
4) Where the hydrogen can be demonstrated not to flow to installations or end-user applications sensitive to higher levels of oxygen, (e.g. feed stock users or hydrogen storages), a higher limit of up to 1000 ppm may be applied.			

Note:	It is acknowledged that the presence of residues in the pipeline as a result of natural gas transmission, makes it necessary to relax the specification for the total sulphur content, to allow for higher hydrocarbons to be present and to introduce a temporary specification for the hydrocarbon dewpoint.
Note:	The gas shall not contain constituents other than listed in the table above at levels that prevent its transportation, storage and/or utilization without quality adjustment or treatment.

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## Annex A: Various hydrogen specifications in ISO 14687:2019

Constituents* (assay)	Maximum concentration of individual contaminants <sup>1</sup>			grade E			
	Grade A	Grade B	Grade C	Grade D	Category 1	Category 2	Category 3
Hydrogen fuel index (minimum mole fraction) <sup>b</sup>	98,0 %	99,90 %	99,995 %	99,97 %	50 %	50 %	99,9 %
Total non-hydrogen gases (maximum)	0,20 %	0,10 %	0,01 %	0,03 %	50 %	50 %	0,1 %
Maximum concentration of individual contaminants <sup>1</sup>							
Water (H <sub>2</sub> O)	Non-condensing at all ambient conditions <sup>c</sup>	Non-condensing at all ambient conditions		5 µmol/mol	Non-condensing at any ambient conditions <sup>b</sup>	Non-condensing at any ambient conditions <sup>b</sup>	Non-condensing at any ambient conditions <sup>b</sup>
Total hydrocarbons	100 µmol/mol	Non-condensing at all ambient conditions	k				
Total hydrocarbons except methane (C1 equivalent)			k	2 µmol/mol <sup>e</sup>	10 µmol/mol <sup>e</sup>	2 µmol/mol <sup>e</sup>	2 µmol/mol <sup>e</sup>
Methane (CH <sub>4</sub> )				100 µmol/mol	5 %	1 %	100 µmol/mol
Oxygen (O <sub>2</sub> )	j	100 µmol/mol	l	5 µmol/mol	200 µmol/mol	200 µmol/mol	50 µmol/mol
Helium (He)			39 µmol/mol	300 µmol/mol			
Nitrogen (N <sub>2</sub> )	j	400 µmol/mol	k	300 µmol/mol	50 %	50 %	0,1 %
Argon (Ar)	j		l	300 µmol/mol			
Carbon dioxide (CO <sub>2</sub> )			m	2 µmol/mol	Included in total non-hydrogen gases	Included in total non-hydrogen gases	2 µmol/mol
Carbon monoxide (CO)	1 µmol/mol		m	0,2 µmol/mol <sup>d</sup>	10 µmol/mol	10 µmol/mol	0,2 µmol/mol <sup>e</sup>
Total sulphur compounds (S1 equivalent)	2,0 µmol/mol	10 µmol/mol		0,004 µmol/mol <sup>e</sup>	0,004 µmol/mol <sup>e</sup>	0,004 µmol/mol <sup>e</sup>	0,004 µmol/mol <sup>e</sup>
Formaldehyde (HCHO)				0,2 µmol/mol <sup>d</sup>	3,0 µmol/mol	0,2 µmol/mol	0,2 µmol/mol <sup>e</sup>
Formic acid (HCOOH)				0,2 µmol/mol <sup>d</sup>	10 µmol/mol	0,2 µmol/mol	0,2 µmol/mol <sup>e</sup>
Ammonia (NH <sub>3</sub> )				0,1 µmol/mol	0,1 µmol/mol	0,1 µmol/mol	0,1 µmol/mol
Halogenated compounds (Halogen ion equivalent)				0,05 µmol/mol <sup>f</sup>	0,05 µmol/mol <sup>f</sup>	0,05 µmol/mol <sup>f</sup>	0,05 µmol/mol <sup>f</sup>
Maximum particulate concentration	o	n	n	1 mg/kg <sup>g</sup>	1 mg/kg	1 mg/kg	1 mg/kg
Maximum particle diameter					75 µm	75 µm	75 µm
Mercury (Hg)		0,004 µmol/mol					

a) For the constituents that are additive, such as total hydrocarbons and total sulphur compounds, the sum of the constituents shall be less than or equal to the acceptable limit.

b) The hydrogen fuel index is determined by subtracting the "total non-hydrogen gases" in this table, expressed in mole percent, from 100 mole percent.

c) Total hydrocarbons except methane include oxygenated organic species. Total hydrocarbons except methane shall be measured on a C1 equivalent (µmol/mol).

d) The sum of measured CO, HCHO and HCOOH shall not exceed 0,2 µmol/mol

e) As a minimum, total sulphur compounds include H<sub>2</sub>S, COS, CS<sub>2</sub> and mercaptans, which are typically found in natural gas.

f) All halogenated compounds which could potentially be in the hydrogen gas [for example, hydrogen chloride (HCl) and organic chlorides (R-Cl)] should be determined. Halogenated compounds shall be measured on a halogen ion equivalent (µmol/mol).

g) Particulate includes solid and liquid particulates comprises of oil mist. Large particulates can cause issues with vehicle components and should be limited by using filter as specified in ISO 19880-1. No visible oil shall be found in fuel at a nozzle.

h) Each site shall be evaluated to determine the appropriate maximum water content based on the lowest expected ambient temperature and the highest expected storage pressure.

i) The maximum concentration of impurities against the total gas content shall be determined on a dry basis.

j) Combined water, oxygen, nitrogen and argon: maximum mole fraction of 1,9 % (19 000 µmol/mol).

k) Combined nitrogen, water and hydrocarbon: maximum 9 µmol/mol.

l) Combined oxygen and argon: maximum 1 µmol/mol.

m) Total CO<sub>2</sub> and CO: maximum 1 µmol/mol.

n) To be agreed between the supplier and the customer.

o) The hydrogen shall not contain dust, sand, dirt, gums, oils or other substances in an amount sufficient to damage the fuelling station equipment or the vehicle (engine) being fuelled.

## Annex B: Effect of hydrogen impurities (ISO 14687:2019)

### *Water content*

Water (H<sub>2</sub>O) generally does not affect the function of a fuel cell; however, it provides a transport mechanism for water-soluble contaminants such as K<sup>+</sup> and Na<sup>+</sup> when present as an aerosol. Both K<sup>+</sup> and Na<sup>+</sup> are recommended not to exceed 0,05 µmol/mol for category 3. In addition, water can pose a concern under sub-zero ambient conditions and affect valves. Thus, water must remain gaseous throughout the encountered ambient temperature conditions.

### *Total hydrocarbon content*

Different hydrocarbons have different effects on fuel cell performance. Generally aromatic hydrocarbons adsorb more strongly on the catalyst surface than alkanes, inhibiting access to hydrogen. Methane (CH<sub>4</sub>) is considered an inert gas since its effect on fuel cell performance is to dilute the hydrogen fuel stream.

### *Oxygen content*

Oxygen (O<sub>2</sub>) in low concentrations does not adversely affect the function of the fuel cell power system; but high concentration oxygen causes degradation of the fuel cell.

### *Helium, nitrogen and argon contents*

Inert constituents, such as helium (He), nitrogen (N<sub>2</sub>) and argon (Ar) do not adversely affect the function of fuel cell components or a fuel cell power system. However, they dilute the hydrogen gas.

### *Carbon dioxide content*

Carbon dioxide (CO<sub>2</sub>) does not typically affect the function of fuel cells. It dilutes the hydrogen fuel thereby affecting the efficiency of the fuel cell power system. Furthermore, concentrations of CO<sub>2</sub> higher than 25 % in mole fraction can be catalytically converted via a reverse water gas shift reaction into CO, which in consequence poisons the catalyst. However, under normal operating conditions, such high levels of CO<sub>2</sub> are highly unlikely to be present in the anode.

### *Carbon monoxide content*

Carbon monoxide (CO) is a severe catalyst poison that adversely affects fuel cell performance and thus needs to be kept at very low levels in hydrogen fuel. While the impact on performance can be reversed by changing operating conditions and/or gas composition, these measures may not be practical. In reformat applications (categories 1 and 2), the impact of the inherently higher CO levels is mitigated through material selection, and/or system design and operation, nonetheless the long-term effect of CO on fuel cell durability is a concern, specifically for low anode catalyst loadings.

### *Total sulphur concentration*

Sulphur-containing compounds are catalyst poisons that at even very low levels can cause some irreversible effects on fuel cell performance. The minimum specific sulphur compounds that need to be included in the testing are: hydrogen sulphide (H<sub>2</sub>S), carbonyl sulphide (COS), carbon disulphide (CS<sub>2</sub>), mercaptans (e.g. methyl mercaptan), which may be found in hydrogen reformed from natural gas. The total sulphur concentration should be monitored. Lower catalyst loadings are particularly susceptible to catalyst poisoning contaminants.

### *Formaldehyde and formic acid contents*

Formaldehyde (HCHO) and formic acid (HCOOH) have a similar effect on fuel cell performance as CO and are thus considered as contaminants which cause reversible effects. The effect of HCHO and HCOOH on fuel cell performance can be more severe than that of CO due to slower recovery kinetics and their specifications are lower than that for CO. Lower catalyst loadings are particularly susceptible to catalyst poisoning contaminants.



### *Ammonia content*

Ammonia (NH<sub>3</sub>) causes some irreversible effects on fuel cell performance by contaminating the proton exchange membrane/ionomer and reacting with protons in the membrane/ionomer to form NH<sub>4</sub><sup>+</sup> ions. Test data for ammonia tolerance should include ion exchange capacities of membrane and/or electrodes. Lower catalyst loadings imply lower ion exchange capacities within the electrode.

### *Total halogenated compounds contents*

Halogenated compounds cause irreversible effects on performance. Potential sources include chloralkaline production processes and refrigerants used in processing and cleaning agents.

### *Particulates*

A maximum particulate concentration and size are specified to ensure that filters are not clogged and/or particulates do not enter the PEM fuel power system and affect the operation of valves and fuel cell stacks. Potassium and sodium ions present in aerosols cause irreversible effects on performance by contaminating the proton exchange membrane/ionomer. Iron-containing particulates, even at very low concentrations, cause severe membrane/ionomer degradation.