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Hydrogen fuel quality — Product specification

Qualité du carburant hydrogène — Spécification de produit

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Foreword

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The procedures used to develop this document and those intended for its further maintenance are described in the ISO/IEC Directives, Part 1. In particular, the different approval criteria needed for the different types of ISO document should be noted. This document was drafted in accordance with the editorial rules of the ISO/IEC Directives, Part 2 (see www.iso.org/directives).

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For an explanation of the voluntary nature of standards, the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the World Trade Organization (WTO) principles in the Technical Barriers to Trade (TBT), see www.iso.org/iso/foreword.html.

This document was prepared by Technical Committee ISO/TC 197, *Hydrogen technologies*.

This second edition cancels and replaces the first edition (ISO 14687:2019), which has been technically revised.

The main changes are as follows:

- a new Grade of hydrogen quality for internal combustion engine (Grade F) applications has been added in Informative Annex F;
- rationale for each Grade D specification has been moved from ISO19880-8 to this document;
- each specification for each Grade has been modified reflecting recent research work and change in industrial needs.

Any feedback or questions on this document should be directed to the user’s national standards body. A complete listing of these bodies can be found at www.iso.org/members.html.

Introduction

In recent years, the landscape for using hydrogen as a fuel has changed significantly in response to its potential to contribute to the reduction of greenhouse gas emissions. This shift is influenced by challenges on both the hydrogen supply side, such as production technologies and supply chain infrastructure, and also the hydrogen energy usage side, including advancements in fuel cell and combustion technology. To address these changing conditions, the hydrogen fuel specifications in this document have been updated.

The hydrogen fuel specifications for proton exchange membrane (PEM) fuel cell applications in this document are primarily based on research, development and data on the following items [2][3][4][5][6][7][8][9][10][11][12][13][14]:

- PEM fuel cell catalyst and fuel cell tolerance to hydrogen fuel impurities;
- effects/mechanisms of impurities on fuel cell power systems and components;
- impurity detection and measurement techniques for laboratory, production and in-field operations;
- fuel cell vehicle demonstration and stationary fuel cell demonstration results.

Grade D and grade E in this document are intended to apply to PEM fuel cells for road vehicles and stationary appliances, respectively. These aim to facilitate the provision of hydrogen of reliable quality balanced with acceptable lower cost for the hydrogen fuel supply.

In addition, Grades F-1 and F-2 are newly specified in this edition to apply to hydrogen internal combustion engines for use in vehicular and stationary applications, respectively. The new Grades were placed in an informative annex (Annex F) to allow experience to be gained with this fuel quality prior to inclusion in the normative text.

While this document reflects the state-of-the-art at the date of its publication, the rapid development of quality requirements for hydrogen technology applications would necessitate future revisions in response to technological progress.

Hydrogen fuel quality — Product specification

1 Scope

This document specifies the minimum quality characteristics of hydrogen fuel as distributed for utilization in residential, commercial, industrial, vehicular and stationary applications.

This document is applicable to hydrogen fuelling applications, which are listed in Table 2.

2 Normative references

The following documents are referred to in the text in such a way that some or all of their content constitutes requirements of this document. For dated references, only the edition cited applies. For undated references, the latest edition of the referenced document (including any amendments) applies.

ISO 19880-8, *Gaseous hydrogen — Fuelling stations — Part 8: Fuel Quality Control*

ISO 19880-9, *Gaseous hydrogen — Fuelling stations — Part 9: Sampling for fuel quality analysis*

ISO 21087, *Gas analysis — Analytical methods for hydrogen fuel — Proton exchange membrane (PEM) fuel cell applications for road vehicles*

3 Terms, definitions and abbreviations

For the purposes of this document, the following terms and definitions apply.

ISO and IEC maintain terminological databases for use in standardization at the following addresses:

- ISO Online browsing platform: available at http://www.iso.org/obp
- IEC Electropedia: available at http://www.electropedia.org/

3.1 Terms and definitions

3.1.1
boundary point
<proton exchange membrane *fuel cell* (3.1.7) for stationary applications> point between the *hydrogen fuel supply equipment* (3.1.13) and the PEM *fuel cell power system* (3.1.9) at which the quality characteristics of the hydrogen fuel are to be determined

3.1.2
constituent
component (or compound) found within a hydrogen fuel mixture

3.1.3
contaminant
impurity that adversely affects the components within the *fuel cell system* (3.1.8), the *fuel cell power system* (3.1.9) or the hydrogen storage system

Note 1 to entry: An adverse effect can be reversible or irreversible.

3.1.4
customer
<proton exchange membrane *fuel cell* (3.1.7) for stationary applications> party responsible for sourcing hydrogen fuel in order to operate the *fuel cell power system* (3.1.9)

3.1.5
detection limit
lowest quantity of a substance that can be distinguished from the absence of that substance with a stated confidence limit

3.1.6
determination limit
lowest quantity which can be measured at a given acceptable level of uncertainty

3.1.7
fuel cell
electrochemical device that converts the chemical energy of a fuel and an oxidant to electrical energy (DC power), heat and other reaction products

3.1.8
fuel cell system
<proton exchange membrane *fuel cell* (3.1.7) for road vehicle applications> power system used for the generation of electricity on a fuel cell vehicle

Note 1 to entry: The fuel cell system typically contains the following subsystems: fuel cell stack, air processing, fuel processing, thermal management and water management.

3.1.9
fuel cell power system
<proton exchange membrane *fuel cell* (3.1.7) for stationary applications> self-contained fuel cell assembly used for the generation of electricity which is fixed in place in a specific location

Note 1 to entry: The fuel cell power system typically contains the following subsystems: fuel cell stack, air processing, thermal management, water management and automatic control system. It is used in applications such as: distributed power generation, back-up power generation, remote power generation, electricity and heat co-generation for residential and commercial applications.

Note 2 to entry: For the purposes of the applications, the fuel cell power system does not contain a fuel processing system due to the location of the *boundary point* (3.1.1).

3.1.10
gaseous hydrogen
hydrogen under gaseous form

3.1.11
hydrogen-based fuel
<proton exchange membrane *fuel cell* (3.1.7) for stationary applications> gas containing a specified concentration of hydrogen used in PEM fuel cells for stationary applications

Note 1 to entry: The concentration of hydrogen in the gas is specified in tables in this document (ISO 14687).

3.1.12
hydrogen fuel index
mole fraction of a fuel mixture that is hydrogen

3.1.13
hydrogen fuel supply equipment
equipment used for the transportation or on-site generation of hydrogen fuel, and subsequently for the delivery to the *fuel cell power system* (3.1.9), including additional storage, vaporization and pressure regulation as appropriate

3.1.14

irreversible effect

effect, which results in a permanent degradation of the *fuel cell system* (3.1.8) or the *fuel cell power system* (3.1.9) performance that cannot be restored by practical changes of operational conditions and/or gas composition

3.1.15

liquid hydrogen

hydrogen that has been liquefied, i.e. brought to a liquid state

3.1.16

particulate

solid or liquid such as oil mist that can be entrained somewhere in the production, delivery, storage or transfer of the hydrogen fuel to a *fuel cell system* (3.1.8) or a *fuel cell power system* (3.1.9)

3.1.17

reversible effect

effect, which results in a temporary degradation of *the fuel cell system* (3.1.8) or the *fuel cell power system* (3.1.9) performance that can be restored by practical changes of operational conditions and/or gas composition

3.1.18

slush hydrogen

hydrogen that is a mixture of solid and liquid at the eutectic (triple-point) temperature

3.1.19

system integrator

<proton exchange membrane *fuel cell* (3.1.7) for stationary applications> integrator of equipment between the PEM *fuel cell power system* (3.1.9) and the hydrogen supply

3.2 Abbreviated terms

Table 1 — Abbreviated terms

Abbreviated term	Definition
PEM	proton exchange membrane
FCEV	fuel cell electric vehicle

4 Classification and application

4.1 Classification

Hydrogen fuel shall be classified according to the following types and grade designations:

a) Type I (grades A, B, C, D, E and F): gaseous hydrogen and hydrogen-based fuel;

b) Type II (grades C and D): liquid hydrogen;

c) Type III: slush hydrogen.

4.2 Application

Table 2 characterizes representative applications of each type and grade of hydrogen fuel.

Table 2 — Hydrogen and hydrogen-based fuel classification by application

Type	Grade	Category	Applications	Clause
I Gas	A	—	Gaseous hydrogen; residential/commercial combustion appliances (e.g. boilers, cookers and similar applications)	7
	B	—	Gaseous hydrogen; industrial fuel for power generation and heat generation except PEM fuel cell applications	7
	C	—	Gaseous hydrogen; aircraft and space-vehicle ground support systems except PEM fuel cell applications	7
	D[a,b,c]	—	Gaseous hydrogen; PEM fuel cells for road vehicles	5
	E	PEM fuel cells for stationary appliances		6
		1	Hydrogen-based fuel	
		2	Gaseous hydrogen	
	F[c]	Internal combustion engine applications		Annex F
		1	Gaseous hydrogen; internal combustion engine vehicular applications	
		2	Gaseous hydrogen; internal combustion engine stationary applications	
II Liquid	C	—	Aircraft and space-vehicle on-board propulsion and electrical energy requirements; off-road vehicles	7
	D[a,b,c]	—	PEM fuel cells for road vehicles	5
III Slush	—	—	Aircraft and space-vehicle on-board propulsion	7

[a] Grade D may be used for other fuel cell applications and internal combustion engines in vehicular and stationary applications, including on and non-road vehicles.

[b] Grade D may be used for PEM fuel cell stationary appliances alternative to grade E category 2.

[c] Fuel cells can be contaminated by lower grade hydrogen. Protection against misfuelling with Grade F is ensured by the nozzle/receptacle geometry. These geometries are specified in ISO 17268-1 [15]. Care should be taken to ensure cross contamination does not occur in the supply chain nor when dispensing into vehicles or other systems.

NOTE Biological and other sources of hydrogen can contain additional constituents (e.g. siloxanes or mercury) that can affect the performance of the various applications, particularly PEM fuel cells. However, these are not included in most of the following specifications due to insufficient information.

5 Hydrogen quality requirements for PEM fuel cell road vehicle application

5.1 Fuel quality specification

The quality of hydrogen at dispenser nozzle for grade D hydrogen (see Table 2) shall meet the requirements of Table 3. The fuel specifications are not process-dependent or feed-stock-specific. Non-listed contaminants have no guarantee of being benign.

Annex A provides the rationale for the selection of the impurities specified in Table 3.

Table 3 — Fuel quality specification for PEM fuel cell road vehicle application

Constituents [a] (assay)	**Type I, Type II** **grade D**
Hydrogen fuel index [b] (minimum mole fraction)	99,97 %
Total non-hydrogen gases (maximum)	300 µmol/mol
Maximum concentration of individual contaminants	
Water (H_2O)[c]	5 µmol/mol
Hydrocarbons except methane [a,d] (C1 equivalent)	2 µmol/mol
Methane (CH_4)	100 µmol/mol
Oxygen (O_2)	5 µmol/mol
Helium (He)	300 µmol/mol
Nitrogen (N_2)	300 µmol/mol
Argon (Ar)	300 µmol/mol
Carbon dioxide (CO_2)	2 µmol/mol
Carbon monoxide (CO)[e]	0,2 µmol/mol
Sulfur compounds [a,f] (S1 equivalent)	0,004 µmol/mol
Formaldehyde (HCHO)[e]	0,2 µmol/mol
Ammonia (NH_3)	0,1 µmol/mol
Halogenated compounds [a,g] (Halogen equivalent)	0,05 µmol/mol
Maximum particulate concentration [h]	1 mg/kg

[a] For the constituents that are grouped, such as hydrocarbons except methane, sulfur compounds and halogenated 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] The allowable water content is based upon a HRS operating at 70 MPa nominal pressure and -40 °C hydrogen pre-cooling. The allowable water content may be allowed to increase to 7 µmol/mol H_2O for a station only dispensing at a nominal working pressure of 35 MPa and a precooling temperature of -26 °C or warmer. The change should be confirmed by the hydrogen quality plan as discussed in ISO 19880-8 to ensure that no water condensate can form. The potential temperatures and pressures in the FCEV should be considered.

[d] Hydrocarbons except methane include oxygenated organic species (for example, formic acid). Hydrocarbons except methane which can potentially be in the hydrogen gas should be determined by the hydrogen quality control plan discussed in ISO 19880-8. Hydrocarbons except methane shall be measured on a C1 equivalent (µmol/mol).

[e] The sum of measured CO and HCHO shall not exceed 0,2 µmol/mol.

[f] Sulfur compounds which can potentially be in the hydrogen gas (for example, H_2S, COS, CS_2 and mercaptans, which are typically found in natural gas) should be determined by the hydrogen quality control plan discussed in ISO 19880-8. Sulfur compounds shall be measured on a S1 equivalent (µmol/mol).

[g] Halogenated compounds which can potentially be in the hydrogen gas [for example, hydrogen chloride (HCl) and organic chlorides (R-Cl)], should be determined by the hydrogen quality control plan discussed in ISO 19880-8. Halogenated compounds shall be measured on a halogen equivalent (µmol/mol).

[h] Particulate includes both solid and liquid particles and may be comprised of oil mist. Large particulates can cause issues with vehicle components and should be limited by using filter as specified in.[14] No visible oil shall be found in fuel at a nozzle.

5.2 Analytical method

The analytical laboratories measuring the constituents should follow industry approved practices, such as ISO/IEC 17025. For Grade D hydrogen, the analytical methods used shall be validated according to the requirements in ISO 21087.

5.3 Sampling

Sampling procedures shall be in accordance with ISO 19880-9. ISO 19880-9 outlines requirements for sampling from hydrogen refuelling stations for samples taken at the dispenser.

5.4 Hydrogen quality control

The means of assuring that the hydrogen quality meets the specification in 5.1 shall be in accordance with ISO 19880-8.

6 Hydrogen and hydrogen-based fuel, quality requirements for PEM fuel cell stationary applications

6.1 Fuel quality specification

The quality of hydrogen and hydrogen-based fuel, supplied to stationary PEM fuel cell appliances, shall meet the requirements of Table 4 at the boundary point set between the hydrogen fuel supply equipment and the PEM fuel cell power system.

NOTE 1 Annex B provides guidance for the selection of the boundary point.

NOTE 2 Annex C provides the rationale for the selection of the impurities specified in Table 4.

Type I, grade E hydrogen and hydrogen-based fuel, for PEM fuel cell applications for stationary appliances, specify the following subcategories in order to meet the needs of different stationary applications, depending on the requirements specified by the manufacturer:

- Type I, grade E, category 1 (hydrogen-based fuel);
- Type I, grade E, category 2 (gaseous hydrogen).

Table 4 — Fuel quality specification for PEM fuel cell stationary applications

Constituents [a] **(assay)**	**Type I, grade E**	
	Category 1	**Category 2**
Hydrogen fuel index [b] (minimum mole fraction)	50 %	99,9 %
Total non-hydrogen gases (maximum mole fraction)	50 %	0,1 %
Water (H_2O) [c]	Non-condensing at any ambient conditions	Non-condensing at any ambient conditions
Maximum concentration of individual contaminants[d]		
Hydrocarbons except methane [a,e] (C1 equivalent)	10 µmol/mol	2 µmol/mol
Methane (CH_4)	5 % (mole fraction)	100 µmol/mol
Oxygen (O_2)	200 µmol/mol	50 µmol/mol
Sum of nitrogen (N_2), argon (Ar) and helium (He)[a] (mole fraction)	50 %	0,1 %
Carbon dioxide (CO_2)	Included in total non-hydrogen gases	2 µmol/mol
Carbon monoxide (CO)	10 µmol/mol	0,2 µmol/mol[f]
Sulfur compounds [a,g] (S1 equivalent)	0,004 µmol/mol	0,004 µmol/mol
Formaldehyde (HCHO)	3 µmol/mol	0,2 µmol/mol[f]
Ammonia (NH_3)	0,1 µmol/mol	0,1 µmol/mol
Halogenated compounds [a,h] (halogen equivalent)	0,05 µmol/mol	0,05 µmol/mol
Maximum particulate concentration	1 mg/kg	1 mg/kg
Maximum particle diameter	75 µm	75 µm

[a] For the constituents that are grouped, such as hydrocarbons except methane, sulfur compounds and halogenated 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] 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.

[d] The maximum concentration of impurities against the total gas content shall be determined on a dry basis.

[e] Hydrocarbons except methane include oxygenated organic species. Hydrocarbons except methane which can potentially be in the hydrogen gas should be determined by the hydrogen quality control plans referred to in ISO 19880-8. Hydrocarbons except methane shall be measured on a C1 equivalent (µmol/mol).

[f] The sum of measured CO and HCHO shall not exceed 0,2 µmol/mol.

[g] Sulfur compounds which can potentially be in the hydrogen gas (for example, H_2S, COS, CS_2 and mercaptans, which are typically found in natural gas) should be determined by the hydrogen quality control plans referred to in ISO 19880-8. Sulfur compounds shall be measured on a S1 equivalent (µmol/mol). On the purpose to avoid the degradation of the fuel cell performance, the threshold level of 0,000 1 µmol/mol may be used for sulfur compounds.

[h] Halogenated compounds which can potentially be in the hydrogen gas [for example, hydrogen chloride (HCl) and organic chlorides (R-Cl)] should be determined by the hydrogen quality control plans referred to in ISO 19880-8. Halogenated compounds shall be measured on a halogen equivalent (µmol/mol).

6.2 Quality verification

6.2.1 General requirements

Quality verification requirements shall be determined at the boundary point using the sampling methods specified in 6.3.

The selection of relevant fuel contaminants for analysis as specified in Table 4 should be carried out based on the hydrogen production method.

All analyses conducted under this document shall be undertaken using gaseous calibration standards (or other calibration devices) that are traceable to the International System of Units (SI) via national standards, where such standards are available.

NOTE ISO 21087 provides guidance for analytical methods.

6.2.2 Analytical requirements of the qualification tests

The frequency of testing and analytical requirements for the qualification tests shall be defined. Consideration shall be given to the consistency of hydrogen supply in determining the test frequency and constituents to be tested.

Annex D provides a recommended practice of the quality assurance for steam methane reforming (SMR) hydrogen production processes using pressure swing adsorption (PSA) purification.

6.2.3 Report results

The detection limits and the determination limits for analytical methods and instruments used shall be reported along with the results of each test and the date the sample was taken.

6.3 Sampling

6.3.1 Sample size

Where possible, the quantity of hydrogen in a single sample container should be sufficient to perform the analyses for the hydrogen fuel quality specification. If a single sample does not contain a sufficient quantity of hydrogen to perform all of the analyses required to assess the quality level, additional samples from the same lot shall be taken under similar conditions. A large sample or sample with a greater pressure, where applicable, may be required if multiple tests are to be conducted.

6.3.2 Selection of the sampling point

A boundary point shall be established so that gaseous samples are representative of the hydrogen supplies to the PEM fuel cell power systems.

NOTE Annex B provides guidance to assist in the identification of the party responsible for the quality of hydrogen at the boundary point and also the selection of the boundary point.

6.3.3 Sampling procedure

Gaseous hydrogen samples shall be representative of the hydrogen supply, withdrawn from the boundary point through a suitable connection into an appropriately sized sample container. No contamination of the hydrogen fuel shall be introduced between the boundary point and the sample container (a suitable purge valve may be used).

The residual gases inside the sample container shall be evacuated to ensure that the sampled hydrogen is not contaminated. If evacuation is not possible, the sample container shall be cleaned using repeated purge cycles.

Sampled gases are flammable. Measures shall be taken to avoid hazardous situations. Guidance is given in[16].

6.3.4 Particulates in gaseous hydrogen

Particulates in hydrogen shall be sampled from the boundary point, using a filter, if practical, under the same conditions (pressure and flow rate) as employed in the actual hydrogen supplying condition. Appropriate measures shall be taken for the sample gas not to be contaminated by particulates coming from the connection device and/or the ambient air.

7 Hydrogen quality requirements for applications other than PEM fuel cell road vehicle and stationary applications

7.1 Fuel quality specification

The quality of hydrogen supplied to the example specifications for applications other than PEM fuel cell road vehicles and stationary applications shall meet the requirements of Table 5. A blank indicates no maximum limiting characteristic. The absence of a maximum limiting characteristic in a listed quality level does not imply that the component is or is not present, but merely indicates that there is no limitation regarding this component for compliance with this document.

NOTE Other specifications can be equally suitable for these applications. CEN/TS 17977[17] details a comprehensive specification for the quality of hydrogen delivered to user applications through rededicated gas systems, which is anticipated to be suitable for many applications covered by the Grades A and B below.

Table 5 — Fuel quality specification for applications other than PEM fuel cell road vehicle and stationary applications

Constituents [a] (assay)	Type I			Type II	Type III
	Grade A	Grade B	Grade C	Grade C	
Hydrogen fuel index [b] (minimum mole fraction)	98,0 %	99,90 %	99,995 %	99,995 %	99,995 %
Para-hydrogen (minimum mole fraction)	—	—	—	95,0 %	95,0 %
Impurities (maximum content)					
Total non-hydrogen gases	2 % (mole fraction)	1 000 µmol/mol	50 µmol/mol	50 µmol/mol	—
Water (H_2O)	250 µmol/mol [c] 60 µmol/mol [c]	250 µmol/mol [c] 60 µmol/mol [c]	[d]	[d]	—
Hydrocarbons except methane [e] (C1 equivalent)	100 µmol/mol	Non-condensing at all ambient conditions	[d]	[d]	—
Oxygen (O_2)	[f]	100 µmol/mol	[g]	[g]	—
Argon (Ar)	[f]	—	[g]	[g]	—
Nitrogen (N_2)	[f]	400 µmol/mol	[d]	[d]	—
Helium (He)	—	—	39 µmol/mol	39 µmol/mol	—
Carbon dioxide (CO_2)	[f]	—	[h]	[h]	—
Carbon monoxide (CO)	20 µmol/mol	—	[h]	[h]	—
Sulfur compounds (S1 equivalent)	7 µmol/mol [i]	10 µmol/mol	—	—	—
Permanent particulates	[j]	[k]	[k]	[k]	—

[a] For the constituents that are grouped, such as hydrocarbons except methane and sulfur 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] To prevent condensation under expected temperature condition range, the value is 250 µmol/mol at maximum operating pressures ≤1 MPa and 60 µmol/mol at maximum operating pressures > 1 MPa.

[d] Combined nitrogen, water and hydrocarbon: maximum 9 µmol/mol.

[e] Hydrocarbons except methane include oxygenated organic species and shall be measured on a C1 equivalent basis (µmolC/mol).

[f] Combined oxygen, nitrogen, argon and carbon dioxide: maximum mole fraction of 1,9 % (19 000 µmol/mol).

[g] Combined oxygen and argon: maximum 1 µmol/mol.

[h] Combined CO_2 and CO: maximum 1 µmol/mol.

[i] Sulfur compounds excludes any sulfur from odorants and shall be measured on a S1 basis (µmolS/mol).

NOTE Odorisation is considered as a safety issue dealt with at the national level. National requirements can permit amount fractions higher than 7 µmol/mol.

[j] The hydrogen shall not contain dust, sand, dirt, gums, oils or other substances in an amount sufficient to damage residential/commercial combustion appliances.

[k] To be defined as appropriate for each application.

7.2 Quality verification

7.2.1 General requirements

The supplier shall assure, by standard practice, the verification of the quality level of hydrogen. The sampling and control procedures are described in 7.3.

NOTE 1 Annex E provides the rationale for the selection of the impurities specified in Table 5.

NOTE 2 ISO 21087 can be used as guidance for validation protocol for analytical methods for the contaminants in Table 5.

7.2.2 Production qualification tests

Production qualification tests are a single analysis or a series of analyses that shall be performed on the product to assure the reliability of the production facility to supply hydrogen of the required quality level. This production qualification can be achieved by verifying the analytical records of product from the supplier, or, if required, by performing analyses of representative samples of the product from the facility at appropriate intervals as agreed between the supplier and the customer. Production qualification tests can be performed by the supplier or by a laboratory agreed upon between the supplier and the customer.

7.3 Sampling

7.3.1 Sample size

The quantity of hydrogen in a single sample container shall be sufficient to perform the analyses for the fuel quality specifications. If a single sample does not contain a sufficient quantity of hydrogen to perform all of the analyses required to assess the quality level, additional samples from the same lot shall be taken under similar conditions.

7.3.2 Gaseous samples

Gaseous samples shall be representative of the hydrogen supply. Samples shall be obtained using one of the following procedures.

a) Fill the sample container and delivery containers at the same time, on the same manifold and in the same manner.

b) Withdraw a sample from the supply container through a suitable connection into the sample container.

c) For safety reasons, the sample container and sampling system shall have a rated service pressure at least equal to the pressure in the supply container.

d) Connect the container being sampled directly to the analytical equipment using a suitable pressure regulator to prevent over-pressurizing this equipment.

e) Select a representative container from the containers filled in the lot.

7.3.3 Liquid samples (vaporized)

Vaporized liquid samples shall be representative of the liquid hydrogen supply. Samples shall be obtained using one of the following procedures:

a) by vaporizing, in the sampling line, liquid hydrogen from the supply container;

b) by flowing liquid hydrogen from the supply container into or through a suitable container in which a representative sample is collected and then vaporized.

CAUTION — Due to the high expansion ratio for liquid hydrogen, extreme caution shall be used to avoid overpressure within the sample container.

Annex A
(informative)

Rationale for the selection of hydrogen impurities for PEM fuel cell road vehicle application

A.1 General

This annex gives a brief description of the impact of impurities on the stack, fuel cell components and the complete fuel cell powertrain. Detailed information can be found in the relevant literature and journal publications. It shall be noted that this annex refers to known impurities and their effects on the fuel cell powertrain at the time of publication. It cannot be excluded that other impurities exist. Furthermore, in most cases only the impact of a single impurity has been investigated and there is still the need for fundamental research regarding the impact of a combination of the different impurities on the fuel cell powertrain.

A.2 Inert gases

The main effect due to the presence of inert gases such as Ar and N_2 is to lower the cell voltage due to the dilution effect of the inert species (dilution of the hydrogen gas) and inertial (diffusion) effects. Nevertheless, under consideration of the threshold value current stack designs, fuel cell components and fuel cell powertrains are not adversely affected by inert constituents. High inert gas concentrations will lead to power losses, increased fuel consumption, and loss of efficiency. Furthermore, H_2 starvation caused by high inert gas concentrations can lead to permanent damage of the fuel cell stack or vehicle stop. Inert gases will accumulate in the anode loop and can affect venting and recycle blower control. Further sources report that the presence of N_2 hinders desorption of adsorbed CO from the surface of the anode catalyst. It should also be noted that inert gases can affect the accuracy of mass metering instruments for hydrogen dispensing.

A.3 Oxygen

Oxygen can have a detrimental effect on the fuel cell anode, but the concentration where this effect occurs is not fully known. Higher levels of oxygen can have an impact on metal hydride storage materials.

A.4 Carbon dioxide

The contamination effects of CO_2 depend on the concentration, fuel cell operation conditions, and anode catalyst composition. Firstly, CO_2 dilutes the hydrogen gas and can affect venting and recycle blower control of the fuel cell powertrain. Furthermore, very high concentrations of CO_2 can be catalytically converted via a reverse water gas shift reaction into CO which in consequence poisons the catalyst. In addition, co-occurrence of CO and CO_2 in hydrogen has an accumulated influence on cell performance. CO_2 can adversely affect on-board hydrogen storage systems using metal hydride alloys.

A.5 Carbon monoxide

Carbon monoxide causes severe catalyst poison that adversely affects the performance of the fuel cell powertrain. CO binds strongly to Pt sites, resulting in the reduction of the effective electrochemical surface area available for H_2 adsorption and oxidation. The catalyst poison effect is strongly related to the concentration of CO, the exposure time, the cell operation temperature and anode catalyst types. Although the effects of CO on the fuel cell can be reversed through mitigating strategies, such as material selection of membrane electrode assembly, system design and operation, the life time effects of CO on performance is a strong concern. The lower catalyst loadings needed for cost optimization and longer hydrogen protection times especially lead to more severe poisoning effects. Therefore, CO needs to be kept at very low levels in hydrogen fuel.

A.6 Methane

Methane is one of the very few hydrocarbons that does not contaminate PEM fuel cells. It does not react with the catalyst, so dilution is the major effect that shall be considered with methane gas.

A.7 Water

Water is an issue for hydrogen dispensing systems, in the on-board vehicle tank system or fuel cell components due to the formation of ice. Excess water can exist in a liquid state and can cause corrosion of metallic components. Low quantities can lead to severe impacts on the components. Furthermore, water affects the function of the stack. Water provides a transport mechanism for water-soluble impurities, especially as a solvent for cations like Na^+, K^+, Ca^{2+}, Cs^+ and NH_4^+ when present as an aerosol. The cations absorb to and block the functional groups of the ionomer thereby reducing the proton conductivity of the membrane. Water is only a concern for the stack in very large quantities. It can lead to water management issues that limit the current and cause an increase in over-potential. Water should remain gaseous throughout the operating conditions of system. It is believed that water affects the metal hydride life cycle due to exothermic reactions.

A.8 Sulfur compounds

Sulfur containing compounds are severe catalyst poisons that at even very low levels can cause irreversible degradation of fuel cell performance. The specific sulfur compounds that are addressed are in particular: hydrogen sulfide, sulfur dioxide, carbonyl sulfide, carbon disulfide, methyl mercaptan. Beside these specific compounds further sulfur compounds can exist. The adsorption of the sulfur-containing species to the active sites of the catalyst prevents the hydrogen from adsorbing at the catalyst surface resulting in a significant drop in performance. The reactions of the adsorbed sulfur compounds result in the formation of the very stable platinum sulfide which makes it impossible to recover the fuel cell catalyst from contamination. Lower catalyst loadings are particularly susceptible to catalyst poisoning contaminants.

A.9 Ammonia

Ammonia contamination causes some irreversible fuel cell performance degradation by reducing the proton conductivity of the ionomer. NH_3 migrates into the membrane and reacts with protons to NH_4^+ which then absorb to and block the functional groups of the ionomer. The level of deterioration depends on both the NH_3 concentration and exposure time. Performance decay is also attributed to the adsorption of ammonia on the catalyst surface blocking the active sites.

A.10 Hydrocarbons

Different hydrocarbons have different effects on fuel cell performance. The main effect is the adsorption on the catalyst layer, reducing the catalyst surface area and thereby decreasing the cell performance. The severity of the effect depends on the type of hydrocarbon. Generally aromatic hydrocarbons, acid and aldehydes adsorb more strongly on the catalyst surface than other hydrocarbons inhibiting access to hydrogen and degrade performance. Phthalates, squalene and erucamide which can be found in seals and hoses will cause problems on the stack side. CH_4 is considered an inert constituent since its effect on fuel cell performance is to dilute the hydrogen fuel stream (see A.6).

A.11 Formaldehyde

Formaldehyde (HCHO) has a similar effect on fuel cell performance as carbon monoxide. HCHO adsorbs on the anode electrocatalyst and degrades the fuel cell performance, but its adsorption strength is weaker than CO. Contamination due to HCHO can be recovered by changing the cell voltage and by purging with pure hydrogen. Therefore, HCHO can be considered as a reversible contaminant with the same impact on the fuel cell as for CO. Lower catalyst loadings are particularly susceptible to catalyst poisoning contaminants.

A.12 Halogenated compounds

Halogenated compounds adsorb on the catalyst layer, reduce the catalytic surface area, and decrease the cell performance. The performance degradation caused by halogenated compounds is an irreversible effect. Potential sources include seawater electrolysis, chloralkali production processes, refrigerants used in processing, and cleaning agents. Chloride for example promotes the dissolution of Pt by the formation of soluble chloride complexes and subsequent deposition in the fuel cell membrane.

A.13 Helium

The main effect due to the presence of helium is to lower the cell potential due to the dilution effect of the inert species (dilution of the hydrogen gas) and inertial (diffusion) effects. It should be considered that hydrogen sensors show interference with helium. Higher inert gas concentrations may also affect the venting and recycle blower control. Current stack designs are not adversely affected by higher inert gas concentrations. Nevertheless, higher inert gas concentrations will lead to power losses, increased fuel consumption, and loss of fuel cell efficiency.

A.14 Solid and liquid particulates (aerosols)

Aerosols are dispersed solid and/or liquid particles in a gas. These particulates may be introduced in the production, storage, or delivery of hydrogen fuel. A maximum solid and liquid particle concentration is specified to ensure that filters are not clogged and/or solid and liquid particles do not enter the fuel system and affect operation of fuel system components and fuel cell stacks. A maximum particulate size diameter is not specified yet but should be addressed in a fuelling station standard and/or future revision of Grade D of ISO 14687. Particulate sizes should be kept as small as possible.

There are various effects of station operating fluids and solid particulates on the stack, fuel cell components, and the complete fuel cell powertrain. These particulates originate from the operation of hydrogen fuelling stations and show severe impacts. This group of substances comprises cleaning agents, oils, lubricant oils, siloxanes, ionic liquids, decomposition products of ionic liquids, additives, metals, metal oxides, and metal ions. One effect of these substances is the adsorption to the active site of the fuel cell catalyst which prevents the hydrogen from adsorbing at the catalyst surface resulting in significant performance drop. Other effects are the reduction of the proton conductivity of the membrane, impact on storage systems, and interference of H_2 sensors. Generally, the use of operating fluids should be minimized as far as possible. If the use of operating fluids is necessary, means should be provided by the hydrogen fuelling station to hinder these operating fluids from contaminating the vehicle fuel cell powertrain.

The contamination due to aerosols is of extreme importance as illustrated by the following example using SnO_2, the oxide of the tetravalent tin as a model substance. This heavy metal oxide is present in the solid state of matter with a molar mass of $M_{SnO2} = 150{,}69\ \text{g} \cdot \text{mol}^{-1}$ and a density of $\rho_{SnO2} = 6{,}95\ \text{g} \cdot \text{cm}^{-3}$ at 20 °C. Under the assumption of a spherical particle shape with a diameter of $d_{\text{particle}} = 0{,}1\ \mu\text{m}$ and under consideration of the Avogadro constant $N_A = 6{,}022 \cdot 10^{23}\ \text{mol}^{-1}$ the number of SnO_2-molecules n_{SnO2} in the particle can be calculated as follows:

$$n_{SnO_2} = \frac{\pi \cdot d_{\text{particle}}{}^3 \cdot \rho_{SnO_2}}{6 \cdot 10^{15} \cdot M_{SnO_2}} \cdot N_A \qquad \text{(A.1)}$$

$$n_{SnO_2} = 1{,}45 \cdot 10^7 \qquad \text{(A.2)}$$

These 14,5 million SnO_2 molecules can lead to irreversible impacts in microelectronic structures. Therefore, it is necessary to filter out any solid and liquid particles close to the fuelling nozzle to prevent any impact on the fuel cell powertrain.

Annex B
(informative)

Guidance on the selection of the boundary point for PEM fuel cell stationary applications

B.1 Purpose

The following guidance is provided to assist in the identification of the boundary point and who is responsible for the quality of hydrogen at the boundary point.

B.2 Hydrogen production guidance

Hydrogen, and hydrogen-based fuel, can be produced in a number of ways, including reformation of fossil fuels or other hydrocarbons, the electrolysis of pure water or alkaline water, and numerous biological methods. Hydrogen, and hydrogen-based fuel, can be generated on-site, in relatively small quantities, or in a larger scale production system off-site, then transported under pressure or as a liquid to the point of use.

B.3 Identification of the party responsible for hydrogen quality at the sampling point

It is recognized that provision of hydrogen to a fuel cell power system may involve numerous parties.

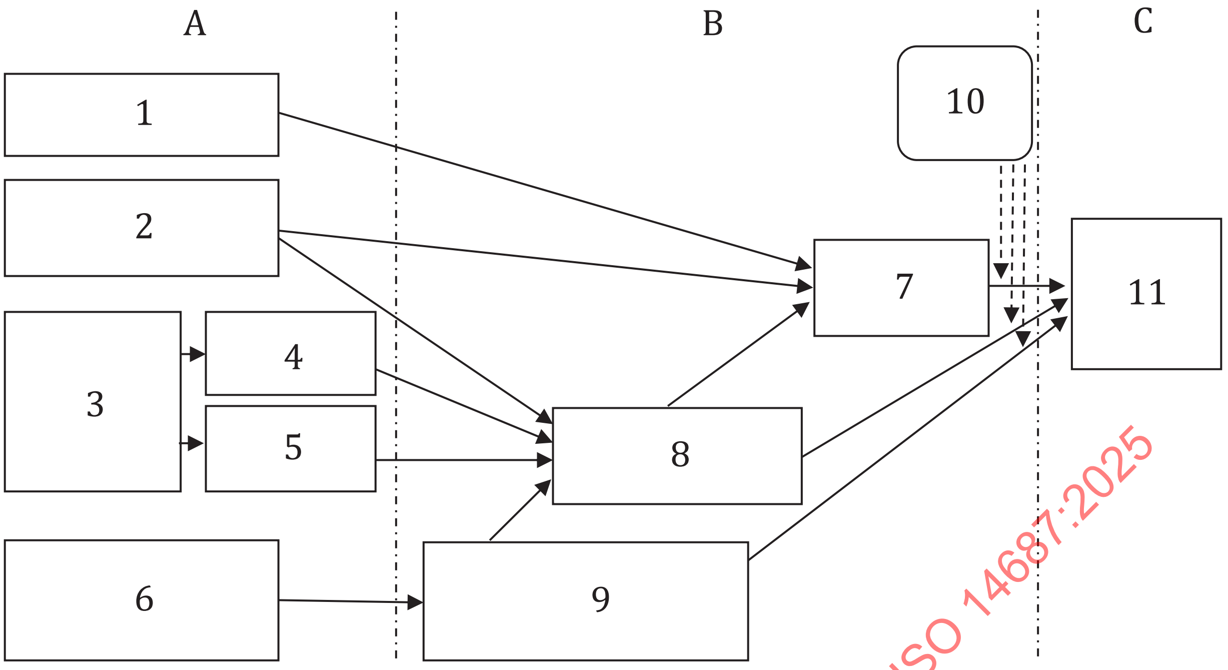
The following text and figure provide examples for information purposes, but are not intended to be comprehensive. Hydrogen delivery systems that incorporate different equipment or hydrogen feedstock should use these examples as a basis for determining the responsibility for the quality of hydrogen at the boundary point and, if appropriate, additional sampling points.

The following are examples of parties involved in and responsible for the supply of hydrogen:

- gaseous hydrogen supplier (for example, cylinders, bundles or tube trailers);
- filtration/purification system;
- liquid hydrogen supplier;
- hydrogen via pipeline distributor;
- reformer manufacturer;
- electrolyser manufacturer.

Depending on the form of the hydrogen supply, there may be a requirement for system integrators to provide equipment between the source of the hydrogen and the inlet to the fuel cell power system. Such equipment may comprise, as applicable, the following, shown in Figure B.1:

- pressure regulators;
- liquid hydrogen storage, cryogenic pumps and vaporizers;
- gaseous hydrogen buffer storage;
- additional manifolds from hydrogen source to fuel cell power system inlet.



Key

A	hydrogen supply
B	system integration
C	fuel cell power system
1	delivery by pipeline
2	delivery by cylinder or tube trailer
3	utility supply (natural gas, electricity, water, etc.)
4	fuel processing system
5	electrolyser
6	delivery by truck (liquid hydrogen)
7	pressure regulator
8	gaseous hydrogen buffer
9	liquid hydrogen storage, cryogenics pump, vaporizer
10	boundary point (for sampling)
11	PEM fuel cell power system

Figure B.1 — Examples showing the supply of hydrogen to a fuel cell power system and position of the boundary point

It should be recognized that the system integrator is responsible for the quality of hydrogen at the boundary point, immediately prior to the inlet of the fuel cell power system. If the system integrator and fuel cell power system operator are the same party, one or more appropriate alternative sampling points for meeting hydrogen quality characteristics should be determined by an agreement between the hydrogen supplier and the customer.

In some cases, the system integrator can also be the hydrogen supplier, in which case the responsibility for the hydrogen quality characteristics at the boundary point is that of the hydrogen supplier unless otherwise specified by an agreement between the hydrogen supplier and the customer.

Where the system integrator and hydrogen supplier are different parties, the responsibility for the hydrogen quality characteristics at the boundary point is that of the system integrator. In such cases, the analytical requirements (periodicity, impurities and appropriate interface test point) for the hydrogen supply should be determined by an agreement between the hydrogen supplier, the system integrator and the customer.

It can also be the case that the hydrogen supplier provides some aspects of on-site system integration but does not directly interface with the fuel cell power system. In such cases, the hydrogen supplier is responsible for meeting the hydrogen quality characteristics at the supplier interface to the additional equipment that connects to the fuel cell power system, while the integrator interfacing with the fuel cell power system is responsible for the analytical requirements of the hydrogen quality at the boundary point. The analytical requirements (periodicity, impurities) at any additional sampling points appropriate to the system should be specified by an agreement between the system integrator and the hydrogen supplier.

Where system maintenance is to be carried out by an additional party, the requirements for hydrogen quality assurance following the completion of such maintenance should be determined by an agreement between the system integrator, the party responsible for maintenance and the fuel cell operator.

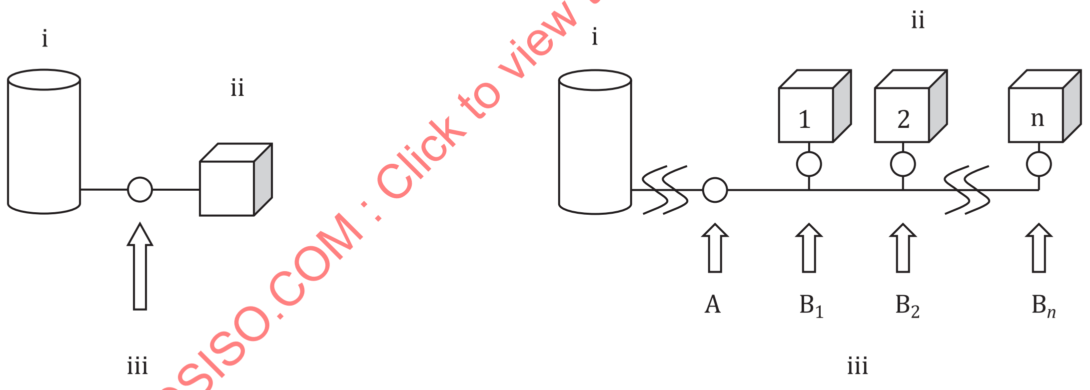
B.4 Selection of the sampling point

In the case of a single fuel cell power system, as shown in Figure B.2 a), the boundary point should be as close as practical to the fuel inlet to the fuel cell power system.

In the case of multiple fuel cell power systems in parallel, as shown in Figure B.2 b), the location of the boundary point should be determined by an agreement between the system integrator and the fuel cell operator.

Examples for the location of the sampling point may include:

- boundary point A - the supply for fuel cell power systems 1 to *n*;
- a single boundary point between B_1 and B_n, representing the worst case:
- all boundary points B_1 through B_n.



a) Single fuel cell power system

b) Multiple fuel cell power systems in parallel

Key

i	hydrogen and hydrogen-based fuel supply equipment
ii	PEM fuel cell power system(s)
iii	boundary point(s)

Figure B.2 — Positioning of sampling point

Annex C
(informative)

Rationale for the selection of hydrogen impurities to be measured for PEM fuel cell stationary applications

C.1 Water

Water (H_2O) generally does not affect the function of a fuel cell; however, it provides a transport mechanism for water-soluble contaminants such as potassium and sodium ions when present as an aerosol. 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.

C.2 Hydrocarbons

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_4) is considered an inert gas since its effect on fuel cell performance is to dilute the hydrogen fuel stream.

C.3 Oxygen

Oxygen (O_2) 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.

C.4 Helium, nitrogen and argon

Inert constituents, such as helium (He), nitrogen (N_2) 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.

C.5 Carbon dioxide

Carbon dioxide (CO_2) 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_2 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_2 are highly unlikely to be present in the anode.

C.6 Carbon monoxide

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 reformate applications (category 1), 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.

C.7 Sulfur compounds

Sulfur-containing compounds are catalyst poisons that at even very low levels can cause some irreversible effects on fuel cell performance. The minimum specific sulfur compounds that need to be included in the testing are: hydrogen sulfide (H_2S), carbonyl sulfide (COS), carbon disulfide (CS_2), mercaptans (e.g. methyl mercaptan), which can be found in hydrogen reformed from natural gas. The total sulfur concentration should be monitored. Lower catalyst loadings are particularly susceptible to catalyst poisoning contaminants.

C.8 Formaldehyde

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

C.9 Ammonia

Ammonia (NH_3) 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_4^+ 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.

C.10 Halogenated compounds

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

C.11 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.

Annex D
(informative)

Pressure swing adsorption and applicability of CO as an indicator for PEM fuel cell stationary applications

D.1 Indicator: major impurities from different H_2 production and purification processes

For SMR-PSA production and purification, CO can serve as an indicator for the presence of other impurities listed in Table 4 because it has the highest probability of presence in a fuel produced by the given process. Confirmation that CO content is less than its specified limit indicates that other impurities, except inert impurities, are present at less than their specified limits.

The maximum content of inert impurities in the product can be estimated by using the maximum content of inert impurities in the feedstock specified by the supplier and the flow increase in the SMR system and the flow decrease in the PSA system. The flow increase in the SMR system and the flow decrease in the PSA system can be calculated from the feedstock composition, steam to carbon ratio and the hydrogen conversion rate.

D.2 In-line monitoring of the indicator

In-line monitoring of CO is strongly recommended to show that its content in the hydrogen fuel is less than the specification on a real-time basis, which indicates that other contaminants are less than their specifications on a real-time basis. For this purpose, commercially available infrared CO analysers can be used. In the case of an SMR-PSA system, the analyser should be placed just after the SMR-PSA system to avoid contamination of the equipment downstream.

D.3 Batch analysis

For back-up of in-line monitoring of CO content, batch sampling of product hydrogen and laboratory analyses of all impurities constituents as listed in Table 4 are also recommended. The batch sample should be taken at the boundary point. The frequency of sampling and analysis is determined by the hydrogen supplier. The quality assurance and sampling methods as described in 6.2 and 6.3 should be applied.

Annex E
(informative)

Grade A: Gaseous hydrogen for applications other than PEM fuel cell road vehicle and stationary applications — rationale for parameter selection and value specifications

E.1 Hydrogen fuel index

Hydrogen fuel index is required to determine fuel properties such as calorific value and the Wobbe index. Various hydrogen production methods are available that are capable of producing hydrogen of varying purity content. Higher purity of hydrogen can be achieved by the means of purification units.

E.2 Water

Water can be present due to specific hydrogen production mechanisms (e.g., electrolysis of water) and can also be present in existing infrastructure used for natural gas. The rationale for limiting its content is because water can condense under certain temperature and pressure conditions found within appliances. Water in contact with iron/steel can cause corrosion, especially in the presence of ‘acidic’ gases such as carbon dioxide which dissolve to form an acid. Oxygen will also cause corrosion in the presence of water. If water is prevented from condensing, these issues are avoided. Thus, water content is specified based on pressure conditions to ensure it remains gaseous throughout all possible ambient temperature conditions.

E.3 Total non-hydrogen gases

This specifies the combined total impurity gases (exclusive of hydrogen) content within the hydrogen. Gases other than hydrogen can be present due to hydrogen production and transportation mechanisms. The rationale for limiting its content is to prevent dilution of the hydrogen. Individual gaseous impurities are specified separately within Table 5 in cases where effects of that impurity are significant.

E.4 Hydrocarbons

Hydrocarbons can be present in hydrogen at trace levels due to production mechanisms and also transportation of hydrogen in repurposed natural gas infrastructure. The rationale for limiting its content is to prevent condensation of hydrocarbons within grade A applications, as liquid hydrocarbon content can lead to process failures. Hydrocarbons except methane include oxygenated organic species and shall be measured on a C1 equivalent basis (µmol/mol).

E.5 Oxygen, carbon dioxide, nitrogen and argon

These gases can be present due to specific production and transportation mechanisms. The rationale for limiting their combined content is to prevent dilution of the hydrogen. This limits the content of gases with no calorific value being used within processes and limits carbon emissions from process exhausts.

Oxygen specific rationale: Oxygen can be present due to specific production mechanisms and the possibility of air ingress during gas transport. The rationale for limiting oxygen content is to prevent explosive mixtures being generated in the presence of hydrogen and to reduce corrosion of equipment in the presence of water. The limiting oxygen concentration for flame propagation is in the region of 4 cmol/mol to 5 cmol/mol (inclusive of pressures of 100 kPa to 10 000 kPa and temperatures of 20 °C to 100 °C). The limit of 19 000 µmol/mol for the combined content of oxygen, carbon monoxide, nitrogen and argon ensures that the limiting oxygen concentration is not exceeded.