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Hydrogen Fuel Quality for Fuel Cell Vehicles			

RATIONALE

This document has been revised to incorporate changes reflecting progress of the fuel cell and automotive industries have made in the determination of acceptable levels of contaminants and to account for advances in the methodologies used to verify those levels.

Since the previous TIR publication, proposals have been introduced to the Interface Working Group (IWG) by members of the energy and specialty gas industries seeking to modify the values of contaminants contained in Table 1. These proposals were intended to bring the values into conformance with current established norms for hydrogen production and delivery. These proposals have been discussed at length within the IWG and, by consensus, have been accepted. Acceptance of these proposals also dictates that the values of the Hydrogen Fuel Index and the Total allowable non-hydrogen, non-helium, non-particulate constituents contained in Table 1 be updated.

This revision also contains clarifications of works in progress pursuant to the enhanced test methodologies under development and coordinated through ASTM D03.

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TABLE OF CONTENTS

1.	SCOPE.....	3
1.1	Purpose.....	3
1.2	Field of Applicability	3
1.3	Relationship of SAE Standard to ISO and ASTM Standards	3
2.	REFERENCES.....	3
2.1	Applicable Publications	3
2.1.1	ASTM Publications.....	3
2.1.2	EPA Publications.....	4
2.1.3	JIS Publications.....	4
2.1.4	NIOSH Publication	5
2.1.5	SCAQMD Publication.....	5
3.	DEFINITIONS	5
4.	HYDROGEN QUALITY SPECIFICATION	6
4.1	Threshold Limits.....	6
4.2	Sampling	7
5.	NOTES	9
5.1	Marginal Indicia	9
APPENDIX A	ADDITIONAL DEFINITIONS.....	10
APPENDIX B	R/Y/G CHART SUPPORTING THE DEVELOPMENT OF SAE 2719.....	11
APPENDIX C	RESEARCH PAPERS SUPPORTING THE DEVELOPMENT OF SAE 2719	13
TABLE 1	HYDROGEN FUEL QUALITY SPECIFICATION.....	8

1. SCOPE

This Standard provides background information and a hydrogen fuel quality standard for commercial proton exchange membrane (PEM) fuel cell vehicles. This Report also provides background information on how this standard was developed by the Hydrogen Quality Task Force (HQTf) of the Interface Working Group (IWG) of the SAE Fuel Cell Standards Committee.

1.1 Purpose

The purpose of this hydrogen fuel quality standard is to specify hydrogen fuel quality requirements for all commercial hydrogen fueling stations for PEM fuel cell vehicles (FCVs). Hydrogen quality is defined as the quality measured at the dispenser nozzle using a suitable adapter and methodology developed by the ASTM D03 (Gaseous Fuels) Committee.

1.2 Field of Applicability

This hydrogen quality standard is applicable to PEM FCVs at the point of interface between the fueling station and the vehicle. The specification of hydrogen quality is intended to meet the requirements of FCVs, and will meet or exceed the requirements of ICEVs to the extent that they have been determined. Information considered in the specification of the fuel quality includes:

- Applicable standard chemical analysis methods to quantify the presence of identified H₂ impurities
- Infrastructure sources of contaminants and cost related to production, distribution, storage and handling of H₂
- Fuel cell systems, specifically, levels of contaminants that adversely impact performance and/or durability
- On-board hydrogen storage and delivery systems

1.3 Relationship of SAE Standard to ISO and ASTM Standards

The content of this standard was coordinated with ISO TC197/WG12 (H₂ Fuel – Product Specification Working Group) as well as the ASTM D03 (Gaseous Fuels) Committee and is consistent with ISO 14687 Part2.

2. REFERENCES

2.1 Applicable Publications

The following publications define this specification to the extent specified in this Standard. Unless otherwise indicated, the latest versions of publications apply.

2.1.1 ASTM Publications

Available from ASTM International, 100 Barr Harbor Drive, P.O. Box C700, West Conshohocken, PA 19428-2959, Tel: 610-832-9585, www.astm.org.

- | | |
|---------------|---|
| ASTM D7550-09 | Standard Test Method for Ion Chromatography Based Determination of Cations in Hydrogen and Other Fuel Cell Feed Gases; |
| ASTM D7650-10 | Standard Test Method for Sampling of Particulate Matter in High Pressure Hydrogen used as a Gaseous Fuel with an In-Stream Filter |
| ASTM D7651-10 | Standard Test Method for Gravimetric Measurement of Particulate Concentration of Hydrogen Fuel |
| ASTM D7653-10 | Standard Test Method for Determination of Ammonia and Trace Water in Hydrogen and Other Gaseous Fuels by Infrared Spectroscopy |

ASTM D7649-10	Standard Test Method for Determination of Trace Contaminants in Hydrogen and Related Fuel Cell Feed Gases
ASTM D7634-10	Standard test method for microscopic measurement of particulates in hydrogen fuel
ASTM D7606-11	Standard Practice for Sampling of High Pressure Hydrogen and Related Fuel Cell Feed Gases
ASTM D7652-11	Standard Test Method for Determination of Trace Hydrogen Sulfide, Carbonyl Sulfide, Methyl Mercaptan, and Carbon Disulfide in Hydrogen Fuel by Gas Chromatography and Sulfur Chemiluminescence Detection
ASTM D1945-03	Standard Test Method for Analysis of Natural Gas by Gas Chromatography
ASTM D7675-11	Determination of Total Hydrocarbons (C1 basis) in Hydrogen by Total Hydrocarbon Analyzer (THC)

2.1.2 EPA Publications

Available from EPA/NSCEP, P.O. Box 42419, Cincinnati, OH 45249-0419, Tel. 800-490-9198, www.epa.gov/ncepihom/ordering.

EPA Method T012	Listing Background Document for the Chlorinated Aliphatics Listing Determination (Final Rule)
EPA Method T015	Hazardous Air Pollutant Emissions for Miscellaneous Coating Manufacturing
EPA Method 200.7	Determination of Metals and Trace Elements in Water and Wastes by Inductively Coupled Plasma-Atomic Emissions Spectrometry
EPA Method 11	Determination of Hydrogen Sulfide Content of Fuel Gas Streams in Petroleum Refineries
EPA 625/R-96/010A	Compendium of Methods for the Determination of Toxic Organic Compounds in Ambient Air—Second Edition
EPA Method 5i	Determination of Low Level Particulate Matter Emissions

2.1.3 JIS Publications

Available from Japanese Standards Association, 4-1-24 Akasaka Minato-ku, Tokyo 107-8440, Japan, Tel: +81-3-3583-8005, www.jsa.or.jp.

JIS K0101:1998	Testing Methods for Industrial Water
JIS K0114:2000	General Rules for Gas Chromatographic Analysis
JIS K0123:1995	General Rules for Analytical Methods in Gas Chromatography Mass Spectrometry
JIS K0124:2002	General Rules for High Performance Liquid Chromatography
JIS K0127:2001	General Rules for Ion Chromatographic Analysis
JIS K0225:2002	Testing Methods for Determination of Trace Components in Diluent Gas and Zero Gas
JIS K0804:1998	Gas Detector Tube Measurement System (Length-of-Stain Type)

2.1.4 NIOSH Publication

Available from National Institute for Occupational Safety and Health, Tel: 800-356-4674, www.cdc.gov/niosh.

NIOSH 2541:1994 Formaldehyde by GC

2.1.5 SCAQMD Publication

Available from South Coast Air Quality Management District, 21865 Copley Drive, Diamond Bar, CA 91765, Tel: 909-396-2000, www.aqmd.gov.

SCAQMD Method 301-91 Identification of Particles by Microscopy

3. DEFINITIONS

Hydrogen fuel as defined in this Standard consists of hydrogen gas and trace impurities. The impurities consist of both inert and reactive contaminants. Inert contaminants, generally, do not permanently affect the performance of a fuel cell. Inert contaminants may affect the performance of the fuel cell system including hydrogen storage tanks, regulators etc. Reactive contaminant effects can be reversible, partially reversible or irreversible in their impact on the performance and/or life of the fuel cell. Additional related definitions are noted in Appendix A.

3.1 CONSTITUENT

A component compound or element found within a hydrogen fuel mixture

3.2 CONTAMINANT

An impurity that adversely affects the components within the fuel cell system or the hydrogen storage system by reacting with its components or that reduces the energy content of the fuel through dilution. An adverse effect can be reversible or irreversible.

3.3 DILUENT

An impurity that reduces the concentration of hydrogen, and may be a contaminant or non-reactive in nature.

3.4 FUEL CELL SYSTEM

A power system producing electrical energy which typically includes the fuel cell stack, equipment for air processing, fuel processing, thermal management, water management, and the balance of plant.

3.5 HYDROGEN FUEL INDEX

The hydrogen fuel index is the value obtained when the amount of aggregate impurities, as, expressed as percent ($\mu\text{mole}/\mu\text{mole}$), is subtracted from 100%.

3.6 INERT GAS

Non-reactive gases such as argon, helium, krypton, neon, radon, and xenon.

3.7 IMPURITY

A non-hydrogen constituent in hydrogen fuel.

3.8 IMPURITY LIMIT

The concentration limit of each specific impurity analyzed in a hydrogen fuel. Impurity limits are designated in micromoles per mole of fuel ($\mu\text{mol/mol}$) with the exception of particulates, which are designated by mass concentrations (milligrams per kilogram of hydrogen fuel).

3.9 PARTICULATE

A solid or aerosol particle that may be entrained or introduced in the production, storage, delivery, or use of hydrogen fuel. Particulates are specified by mass concentration (milligrams per kilogram of fuel).

3.10 SUBLIMATE

An impurity that may undergo a phase-change from solid to gaseous state in the production, delivery, storage or use, of hydrogen fuel.

3.11 TRACER

An easily detected inert substance introduced into a fuel stream.

3.12 THRESHOLD LIMITS

The concentration threshold level of each specific impurity analyzed in a hydrogen fuel. Thresholds are designated in micromoles per mole of fuel ($\mu\text{mol/mol}$) with the exception of particulates, which are designated by size (in micrometers) and mass concentrations (milligrams per kilogram of hydrogen fuel).

4. HYDROGEN QUALITY SPECIFICATION

Development of this standard is based upon consideration of technical presentations given to and discussions with the IWG by industry, universities and other organizations, such as NEDO/JARI, DOE national laboratories, CaFCP, U.S. Fuel Cell Council (USFCC) and ASTM International. The hydrogen quality specification resulting from consensus agreement between the various stakeholders is shown in Table 1, Hydrogen Quality Specification. Particulate concentration should be minimized to avoid contamination, clogging, and erosion of fuel system components. The fuel should be processed with a filter rated at 10 micron nominal (i.e., 98% efficiency) particle size.

4.1 Threshold Limits

The limits in Table 1 were derived by consensus by national and academic laboratories whose work was sponsored by the Japanese government through NEDO and the US government through DoE EERE. Appendix B gives guidance on the rationale for selecting the compounds listed in the table. Appendix C lists the papers that supplied the test data supporting the various limits.

The analytical methods listed in Table 1 are not intended for use as process control or field verification methods. They are intended for use as a resource in for the generation of process equipment calibration gases, field sampling methodology validation and as a method for resolving third party disputes. It is expected that process control and field verification methodology will evolve under the leadership of the fuel providers and applicable federal and state agencies.

Some constituents are listed in terms of family of compounds associated with the total accepted threshold limit per family, as well as example constituents in the particular family. The list is not intended to be totally inclusive. Although there may be more (or less) speciation per each family, the data presented here reflect the current knowledge of constituents of concern.

The analytical methods and limits of detection contained in Table 1 are based on available ASTM Standards or upon ASTM Standards documented as under development. Although for many constituents the public analytic techniques satisfy the requirements for testing hydrogen fuel used in demonstration projects, hydrogen sold commercially is likely to require lower contaminant detection than has been validated for these methods. The limits for constituents in Table 1 are the same as the detection limits in some cases. As a result these constituents will require methods with detection limits validated one or more orders of magnitude below the listed limits.

Subsequent revisions of this standard may include additional constituents as supported by data. In addition, the constituent list addresses a wide range of constituents not all of which are expected to be present in every source of hydrogen.

Requirements for filtering of particulate matter from the fuel stream are contained in fueling dispenser construction documents (e.g., CSA HGV 4.1. ISO 20100). Total hydrocarbons on a C1 basis is a methodology where total carbon is calculated and all of the hydrocarbons are assumed to have only a single carbon atom. Therefore, if the total carbon on a C1 basis calculates out to 1 μ mole hydrocarbon/mole of hydrogen and the hydrocarbon was methane (CH_4), there would be 1 μ mole of methane/mole of hydrogen. However, if the hydrocarbon were benzene (C_6H_6), 1 μ mole hydrocarbon/mole of hydrogen calculates out to 0.17 μ mole benzene/mole of hydrogen.

Alternative commercially accepted analytical methods may be used if they are suitable to detect the impurity at or below the limit and the seller and the buyer (or the Authority Having Jurisdiction) concur.

These requirements are a reflection of the current level of published knowledge on this topic. Limits will be revised as additional information on long-term impacts and mechanisms of fuel cell impact are explored and understood. Test methodology will be updated as it becomes available from ASTM.

4.2 Sampling

It is recommended that samples taken to determine the gaseous components in Table 1 conform to ASTM D7606-11.

It is also recommended that samples taken to determine the particulates in Table 1 conform to ASTM D7650-10.

Alternative commercially accepted sampling methods may be used if they are suitable for the task and the seller and buyer (or the Authority Having Jurisdiction) concur.

TABLE 1 - HYDROGEN FUEL QUALITY SPECIFICATION

- Units are $\mu\text{mol/mol}$ unless otherwise specified
- All limits are subject to revision after additional testing under operational conditions and improved standardized analytical procedures
- Limits are upper limits except for the hydrogen which is a lower limit.
- Gaseous sampling uses procedures in ASTM D7606-11

Constituent	Chemical Formula	Limits	Laboratory Test Methods to Consider and Under Development ^e	Minimum Analytical Detection Limit
Hydrogen fuel index	H ₂	> 99.97%		
Total allowable non-hydrogen, non-helium, non-particulate constituents listed below		100		
Acceptable limit of each individual constituent				
Water ^a	H ₂ O	5	ASTM D7653-10, ASTM D7649-10	0.12
Total hydrocarbons ^b (C ₁ basis)		2	ASTM D7675-11	0.1
Oxygen	O ₂	5	ASTM D7649-10	1
Helium		300	ASTM D1945-03	100
Nitrogen, Argon	N ₂ , Ar	100	ASTM D7649-10	5
Carbon dioxide	CO ₂	2	ASTM D7649-10, ASTM D7653-10	0.1
Carbon monoxide	CO	0.2	ASTM D7653-10	0.01
Total sulfur ^c		0.004	ASTM D7652-11	0.00002
Formaldehyde	HCHO	0.01	ASTM D7653-10	0.01
Formic acid	HCOOH	0.2	ASTM D7550-09, ASTM D7653-10	0.02
Ammonia	NH ₃	0.1	ASTM D7653-10	0.02
Total halogenates ^d		0.05	(Work Item 23815)	0.01
Particulate Concentration		1 mg/kg	ASTM D7650-10, ASTM D7651-10	0.005 mg/kg

^a Due to water threshold level, the following constituents should not be found, however they should be tested for if there is a question on water content:

Sodium (Na⁺) @ < 0.05 $\mu\text{mole/mole H}_2$ or < 0.05 $\mu\text{g/liter}$

Potassium (K⁺) @ < 0.05 $\mu\text{mole/mole H}_2$ or < 0.08 $\mu\text{g/liter}$

or Potassium hydroxide (KOH) @ < 0.05 $\mu\text{mole/mole H}_2$ or < 0.12 $\mu\text{g/liter}$

^b Includes, for example, ethylene, propylene, acetylene, benzene, phenol (paraffins, olefins, aromatic compounds, alcohols, aldehydes). THC may exceed 2 micromoles per mole due only to the presence of methane, in which case the summation of methane, nitrogen and argon is not to exceed 100 ppm.

^c Includes, for example, hydrogen sulfide (H₂S), carbonyl sulfide (COS), carbon disulfide (CS₂) and mercaptans.

^d Includes, for example, hydrogen bromide (HBr), hydrogen chloride (HCl), chlorine (Cl₂) and organic halides (R-X).

5. NOTES

5.1 Marginal Indicia

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PREPARED BY THE SAE INTERFACE WORKING GROUP OF THE SAE FUEL CELL STANDARDS COMMITTEE

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APPENDIX A - ADDITIONAL DEFINITIONS

The objective of this appendix is to document the terms used when discussing hydrogen fuel quality from the perspective of the members of the IWG-HQTF working on this topic.

Terms not defined herein follow the definitions found in standard dictionaries or in SAE J2574.

A.1 DEFINITIONS

A.1.1 CONDENSABLE

An impurity that may undergo a phase-change from gas to liquid or solid at any point during the delivery, storage, or use of the hydrogen fuel.

A.1.2 HYDROGEN QUALITY

A description of hydrogen fuel that includes the hydrogen fuel index and the concentration of specific impurities.

A.1.3 IRREVERSIBLE EFFECT

The degradation of the fuel cell power system performance that cannot be restored by practical changes of operational conditions and/or fuel composition.

A.1.4 NON-CONDENSABLE

An impurity that that may not undergo a phase-change from gas to liquid or solid in the delivery, storage, or use of the hydrogen fuel.

A.1.5 NON-REACTIVE

Not engaging in chemical reactions such as bonding, debonding, adsorbing and absorbing.

A.1.6 REVERSIBLE EFFECT

The degradation of the fuel cell power system performance that can be restored by practical changes of operational conditions and/or fuel composition.

APPENDIX B - R/Y/G CHART SUPPORTING THE DEVELOPMENT
OF SAE 2719

Species	On PEM Stack	On BOP	On Storage
Helium	H ₂ dilution effect only	May affect venting and recycle blower control	Unknown
Inert Gases (Argon, Nitrogen, etc)	H ₂ dilution effect only	May affect venting and recycle blower control	Unknown - Believed to affect MeH Cycle life
Hydrocarbons	Aromatics, acids, aldehydes, etc. degrade performance	Unknown	Unknown - Believed to affect MeH Cycle life
Oxygen	Tolerant to > 500 ppm	May form ice	Exothermic reactions - Believed to affect MeH Cycle life
Carbon Monoxide	Reacts with catalyst, degrades performance	No effect expected	Believed to affect MeH Cycle life

Species	On PEM Stack	On BOP	On Storage
Carbon Dioxide	Tolerant at ≤ 100 ppm, limited CO back shifting	May affect venting and recycle blower control	Believed to affect MeH Cycle life
Formaldehyde	Reacts with catalyst, degrades performance	Unknown	Unknown
Formic Acid	Reacts with catalyst, degrades performance	Unknown	Unknown
Sulfur Compounds	Reacts with catalyst, degrades performance	Unknown	Believed to affect MeH Cycle life
Ammonia	Degrades membrane ionomer conductivity	Unknown	Unknown