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"Quality specification and safety in hydrogen production, commercialization and utilization"

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ABSTRACT

For decades, the issue of hydrogen quality specification has been a source of complexity and confusion in particular for end users, especially because of the jargon spoken by different providers and clients in varied and diverse areas of application. Virtually every requirement was established within the customer–supplier relationship.

The rise of new hydrogen technologies, the emergence of new devices like fuel cells and the spread of knowledge, together with the growing need for uniformity has pushed the specialists to solve this problem. As a result, standardization seems to be the key to accomplish with quality goals at the lowest cost possible. This article discusses the traditional concepts used in the past, the current situation, the standards used today and future developments in hydrogen quality requirements to simplify and facilitate the use and the applications of hydrogen and blends with a careful respect for the quality of the product and safety.

1. Introduction

When defining the purity of a gas, reference is made to the contents of a particular species and the absence of other pollutants, or substances that could be considered unwanted constituents. Traditionally, a high degree of purity is associated with a low content of other gases, or their absence. However, a high purity gas is considered better in terms of quality and the cost is higher.

In general, between manufacturers and their customers, the term "number of nines" is colloquially used to indicate the purity with the final concentration of the gas followed by a decimal value. In other words, three nines means 99.9 percent purity or 0.999 or 3.0 in abbreviated decimal fraction (ADF), while six nines indicates a purity of 99.9999 percent or 6.0. Finally, the expression 4.6 indicates a four nines purity followed by a 6 i.e. 99.996 percent. This means that the process of expressing the purity is obtained indirectly through a subtraction process, subtracting from one hundred the sum of all impurities or contaminants remaining within the gas. The sum of pollutants includes those which are determined or those that fail because determination have no appropriate methods or the accuracy of the determination technique is not good enough to provide definitive final values.

Table 1 presents a comparison of different methods of expressing the purity of industrial gases, among which is hydrogen.

Analyzing the table for purity of gases is noted that the purity or grade of a gas such as hydrogen can be expressed by the level of impurities (I) in ppm (parts per million) contained by such a gas. However, the actual degree must take into

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Table 1 – Purity expressions for hydrogen and other industrial gases.

Nines	Impurities	Purity %	Alternative expressions			
			N	Fraction	ADF	I ppm
One nine	10^{-1}	90%	1	0.9	1.0	100,000
Two nines	10^{-2}	99%	2	0.99	2.0	10,000
Three nines	10^{-3}	99.9%	3	0.999	3.0	1000
Four nines	10^{-4}	99.99%	4	0.9999	4.0	100
Five nines	10^{-5}	99.999%	5	0.99999	5.0	10
Six nines	10^{-6}	99.9999%	6	0.999999	6.0	1
Seven nines	10^{-7}	99.99999%	7	0.9999999	7.0	0.1
Eight nines	10^{-8}	99.999999%	8	0.99999999	8.0	0.01
Nine nines	10^{-9}	99.9999999%	9	0.999999999	9.0	0.001
Nine nines	$5 \cdot 10^{-9}$	99.99999995%		0.9999999995	9.5	0.005

account not only the level of impurities which owns the gas, but what are the individual components that integrate the total level of impurities. Each application may require a particular level depending on the specific requirements and limitations of the technology. This is the reason to make reference to those standards defining such aspects. It is not economically correct specify a gas purity much higher than actually necessary in every application, or even worse that exceeds the analytical capabilities of control. Such sort of specifications can be technically inconsistent or detrimental to the advancement and dissemination of new technologies, or both. For the specific case of quality of hydrogen fuel, the ISO 14687 series of standards must be the reference at global level [1–3].

2. Hydrogen quality standards

Hydrogen standards derived from the work of ISO TC 197 use the concept of Hydrogen fuel index (HFI) to indicate the purity of the hydrogen fuel as a fraction or percentage of a fuel mixture that is hydrogen. Therefore the HFI can be obtained subtracting the total non-hydrogen gases from 100%.

HFI (mole fraction) = 100% − $\sum$NHG% (Sum of all non-hydrogen gases)

In addition to this concept, all non-hydrogen gases should be individually specified and the maximum admissible concentration of individual contaminants should be indicated.

Hydrogen fuel for internal combustion engines, PEM fuel cell applications for road vehicles, space vehicle programs and many other applications are classified according to the types and grade designations shown in Table 2.

3. Hydrogen purity for delivery and fuel cell utilization systems

The delivery and utilization system of hydrogen as shown in Fig. 1 comprises different stages in the production process of hydrogen until final utilization, in this case in transportation vehicles.

Each of these steps can be carried out by different actors and therefore the product quality and safety aspects should take such circumstances into account. It would be established which impurities or contaminants can be found into the product, but previously it should be considered what are the sources where such impurities are originated.

It should be known if the impurities are present in some raw materials, if they come from production process, if they result from materials or metals used, if they are incorporated during operations of compression, transfer or some others

Table 2 – Fuel hydrogen types and grades and their applications according to the standard ISO 14687 [all parts].

Fuel	Type	Grade	Applications		Purity
Gaseous	I	A	Internal combustion engines for transportation; residential or commercial appliances. (All applications, except fuel cells)		98.0
	I	B	Industrial fuel, for use e.g. in power generation or as a heat energy source		99.90
	I	C	Aircraft and space-vehicle ground support systems		99.995
	I	D	Fuel cells for vehicles		99.97
	I	E	Fuel cells for stationary applications	Category 1	50.0
				Category 2	50.0
				Category 3	99.9
Liquid	II	A	Aircraft and space-vehicle on board propulsion systems and electrical energy requirements; land vehicles except fuel cells		99.995
	II	B	Fuel cells for transportation		99.97
Slush	III		Aircraft and space-vehicle on board propulsion systems		99.995

Purity is expressed as Minimum mole fraction.