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Hydrogen technologies — Methodology for determining the greenhouse gas emissions associated with the production, conditioning and transport of hydrogen to consumption gate

Annex K

Hydrogen purity

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Annex K
(informative)

Hydrogen Purity

K.1 Background

In practice, hydrogen production facilities are likely to produce gas streams that are not 100% hydrogen because they contain traces of impurities (i.e., gases that are not hydrogen). A high purity hydrogen can be considered to be practically pure if impurities have negligible impact on the greenhouse gas emissions intensity calculation of hydrogen. A purity level of 99% mole fraction of hydrogen (1% impurities) may at most add 0.22 $kgCO_2e/kgH_2$ or < 2 gCO_2e/MJ H_2.

For most hydrogen applications, the purity level requirement exceeds 99%. The following are examples of the gaseous hydrogen (Type I) fuel quality specification in the ISO 14687 for various stationary and vehicle applications with purity specification ≥99%: grade B (99.9% purity); grade E, category 3 (99.9% purity); grade C (99.995% purity); and grade D (99.97% purity). Grade A and F have purity specification ≥98%.

For hydrogen purity below 99% mole fraction, the purity of hydrogen becomes significant for calculating hydrogen carbon intensity (CI) considering two important factors:

(1) the amount of impurities (e.g., x% by mole) impacts the life cycle functional unit of hydrogen, typically a mass unit of 1 kg, especially when considering the much smaller molecular weight of hydrogen compared to most impurities (e.g., N_2, CO, CO_2, etc.) For example, 1% of CO_2 impurity (mole basis, i.e., 99% H_2 purity) in 1 kg of the product stream will represent 18% of CO_2 by mass, thus only 0.82 kgH_2 is the share of H_2 in the product stream by mass instead of the assumed 1 kg of H_2 product if such impurity is ignored on its small share per mole basis.

(2) If the impurity contains carbon in its chemical composition (e.g., CO, CO_2, CH_4), such impurities will add to the CI of H_2 assuming oxidation of the carbon containing impurity to CO_2 before being emitting to atmosphere. Considering the previous example, each 1% of non-biogenic CO, CO_2 or CH_4 (by mole) in the product stream will add 0.22 kg of CO_2 to the CI of H_2. Thus, it is important to pay attention and quantify the impact of impurities on the CI calculations of H_2 product ($kgCO_2e/kgH_2$). The methodology described below provides details on how the CI of hydrogen in $kgCO_2e/kgH_2$ can be calculated, considering the two factors mentioned above.

K.2 Method

The following example describes how to account for impact of carbon containing and non-carbon impurities on the CI calculation of H_2 product. In this example, the hydrogen production facility emits y $kgCO_2e$/kg-gas, where the kg-gas includes both H_2 and impurities at the production gate, resulting in well-to-gate emissions (i.e., including GHG emissions upstream of H_2 plant) of Y $kgCO_2e$/kg-gas. In this example, the purity of the hydrogen is a% moles H_2/moles-gas with an impurity content of b% CH_4, c% CO, d%, N_2, and e% H_2O. The well-to-gate (WTG) CI of H_2 in units of $kgCO_2e/kgH_2$ can be calculated as follow:

$$Y\,\frac{kgCO2e}{kg\ gas}\ X\ \frac{1\ kg}{1000g}\ X\ \frac{a\ mol\ H2\ X\ \frac{2\ grams}{mol} + b\ mol\ CH4\ X\ \frac{16.04\ grams}{1\ mol} + c\ mol\ CO\ X\ \frac{28.01\ grams}{1\ mol} + d\ mol\ N2\ X\ \frac{28\ grams}{1mol} + e\ mol\ H2O\ X\ \frac{18.02\ grams}{1mol}}{100\ mol\ gas}\ X\ \frac{100\ mol\ gas}{a\ mol\ H2}\ X\ \frac{1\ mol\ H2}{0.002\ kg\ H2} +$$

$$[\frac{b\ mol\ CH4}{100\ mol\ gas}\ X\ \frac{1\ mol\ C02}{1mol\ CH4}\ X\ \frac{0.044\ kg\ C02}{1\ mol\ CO2}\ x\ \frac{1\ mol\ gas}{0.002\ kgH2} + \frac{c\ mol\ CO}{100\ mol\ gas}\ X\ \frac{1\ mol\ C02}{1mol\ C0}\ X\ \frac{0.044\ kgCO2}{1\ mol\ CO2}\ X\ \frac{1\ mol\ gas}{0.002\ kgH2}] \qquad \text{(K1)}$$

= *WTG CI of* H_2 *in* $kgCO_{2e}/kg_{H2}$

The above formula requires that the hydrogen production facility measures the mass flow rate of the (H_2 + impurities) gas stream (e.g., via Coriolis meter) and the chemical composition (mol%) of each impurity in the hydrogen product gas stream, including that of hydrogen (mol%) (e.g., via gas analyzer). The hydrogen production facility will measure or calculate the GHG emissions rate for the same production period. Then dividing the GHG emissions rate by the product mass flow rate provides the *y* $kgCO_2e$/kg-gas mentioned above.

Depending on the energy feedstock and other H_2 production process inputs, the upstream emissions associated with these inputs can be calculated and added to *y*, with the resultant sum representing WTG emissions *Y* $kgCO_2e$/kg-gas for use in the above formula. We note that the last term in the above formula (between square brackets) can be ignored if carbon balance (for non-biogenic carbon) is calculated around hydrogen production facility, i.e., assuming all carbon in feedstock and other inputs supplied to facility minus all carbon sequestered (via CCS or otherwise) will be emitted as CO_2.

Bibliography

[1] ISO 14687:2019, *Hydrogen fuel quality — Product specification*