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Research Article

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Physico-Chemical Factors and Carbon Footprint in Hydrogen Production from Water and Hydrocarbons

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Abstract: The efficiency and competitiveness of hydrogen production technologies are primarily influenced by physico-chemical factors. Water usage is a critical consideration, as it serves as a primary source of hydrogen in most production methods. This paper examines water consumption across various hydrogen production technologies, drawing from both published research and data from operational facilities. Water consumption levels vary based on the quality of the source water, and this should be factored into hydrogen projects to minimize environmental impact. A case study on industrial hydrogen production via steam reforming highlights that 48.88% of the hydrogen is derived from water. Additionally, carbon footprint metrics, which account for greenhouse gas emissions throughout the production process, are becoming increasingly significant. For instance, hydrogen produced through steam reforming emits about 10.03 kg CO2-equivalent per kilogram of hydrogen, while hydrogen from water produces 4.2-4.5 kg CO2-equivalent/kg H2, and hydrogen from methane results in 15.4-15.7 kg CO2-equivalent/kg H2. Thus, nearly half of the hydrogen obtained via steam reforming can be classified as "low-carbon" or "renewable" hydrogen. To make informed decisions, an accurate evaluation of energy and water consumption, supported by system analysis, is essential as hydrogen production expands globally. This growth is expected to place increasing pressure on global water resources and the water cycle.

Keywords: hydrogen production, low-carbon hydrogen, renewable hydrogen, carbon footprint, water consumption in hydrogen production, material balance of hydrogen production.



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Introduction. The growing global use of hydrogen in sectors like energy and transportation requires greater attention to real-world water consumption metrics when developing new projects. Water plays a crucial role in nearly all hydrogen production methods, which vary based on the additional sources of hydrogen such as hydrocarbons or biomass. In energy production, water serves various functions like cooling, refrigeration, and as a working fluid. At the same time, energy is required for water-related infrastructure such as supply systems and desalination. The interrelationship between water and energy is often referred to as the water-energy nexus, which remains a critical area of concern in the context of decarbonization efforts. Water plays a crucial role in energy production, where it is used as a coolant, refrigerant, working fluid, and in the



extraction of fossil fuels. Additionally, energy is required for the functioning of water supply systems, wastewater treatment, desalination, and more [1, 2]. The term "water-energy nexus" is commonly used to describe the interconnection between water usage and energy consumption [3, 4], and finding a balance in this area remains a significant challenge, particularly in the context of decarbonization efforts.

According to the International Energy Agency, energy costs related to this nexus are projected to more than double by 2040. This interdependence becomes even more critical in the hydrogen economy, where increased hydrogen production (primarily from water) significantly impacts water resources. Hydrogen production requires large quantities of water, making water consumption an important factor in the overall growth of low-carbon production. Water is essential in hydrogen production processes that use coal (coal gasification), methane (steam reforming, autothermal reforming, partial oxidation), biomass (biomass gasification), and electricity (electrolysis) [5-8]. Thus, up to 100% of the hydrogen produced originates from water. Whether through carbon-intensive processes like coal gasification or low-carbon ones like electrolysis, water remains the fundamental source of hydrogen. Although hydrogen is predominantly produced from natural gas [9], hydrogen production from water is becoming increasingly important, particularly when renewable energy is used, offering a smaller carbon footprint [10, 11]. The primary objective of this study is to compare water consumption across different hydrogen production methods and quantify the share of hydrogen derived from water in the steam reforming of natural gas, while also assessing the carbon footprint of hydrogen from water and methane based on steam reforming material balances.

Comparing Water Use in Hydrogen Production Technologies: Evaluating hydrogen production from the perspective of energy and water usage requires examining water consumption in detail. As hydrogen production expands, the availability, consumption, and management of water resources will become even more important. Hydrogen project developers must work closely with the water sector to assess the methods and impacts of water use across all types of hydrogen production. A critical success factor will be creating a sustainable approach to selecting water sources and methods for reducing overall water consumption in hydrogen projects [12]. This will help mitigate the negative effects of hydrogen projects on water-scarce communities and prevent exacerbation of existing water security issues. Water quality is also a critical factor in hydrogen production. Water treatment at all stages may result in losses and generate wastewater that requires purification [13]. The processes of obtaining water suitable for electrolysis and steam reforming often involve filtration, desalination, or demineralization, depending on the quality of the raw water. For instance, ultrafiltration can result in up to 10% water loss, while reverse osmosis leads to losses ranging from 15-25% for regular water, 20-30% for wastewater, and 35-40% for seawater. Effluents generated during these water treatment processes must be properly managed to reduce environmental impact, with liquid waste ranging from 7% for ultrafiltration to 21% for reverse osmosis [14]. This research relies on previous studies [15-17] as well as actual data from natural gas steam reforming plants. For hydrogen production through methane steam reforming, the stoichiometric water consumption is 4.5 liters of H2O per kilogram of H2 [18]. However, additional steam and cooling water losses during the steam conversion process must be considered. Producing steam requires 7.35 liters of H2O, and cooling systems demand an additional 38 liters [19]. Factoring in these losses, actual water consumption can vary significantly, ranging from 5.85 to 13.2 liters [20]. This figure is based on the use of demineralized water and its associated losses. To accurately determine water consumption, the amount of waste generated during water treatment must also be considered, as this depends on the quality of the raw water source (e.g., river water, seawater, or water used in methane extraction).



According to the estimates of the International Energy Agency, energy costs here will more than double by 2040^{*}. The dependence between water and energy is particularly relevant for the hydrogen economy considering the impact of increased hydrogen production (primarily from water) on water resources and systems.

Hydrogen production is associated with the consumption of a significant amount of water, and therefore the influence of this factor on the overall growth rate of low carbon footprint production is important. Hydrogen production involves the mandatory use of water as a raw material and its reduction to hydrogen using coal (coal gasification), methane (steam reforming, autothermal reforming, partial oxidation), biomass (biomass gasification) and electricity (electrolysis) [5-8]. As a result, up to 100 % of hydrogen is formed from the water. Water is the only source of hydrogen for processes diametrically opposite in terms of carbon footprint, such as coal gasification and electrolysis. Despite the dominance of hydrogen produced from natural gas in industry [9], hydrogen production from water is gaining momentum; provided that renewable energy is used, it can result in a relatively small carbon footprint [10, 11].

The main purpose of this study is to compare water consumption for various hydrogen production methods, as well as determine the proportion of hydrogen produced from water during steam reforming of natural gas, and estimate the carbon footprint of hydrogen from water and methane based on data from the material balance of hydrogen production by steam reforming.

Comparison of water consumption for various hydrogen production technologies. The assessment of hydrogen in terms of energy and water costs requires verification in terms of water consumption. With the growth of hydrogen production, the factor of provision, consumption and management of water resources will become more important. The initiator of hydrogen projects needs a comprehensive interaction with the water sector in terms of evaluating the methods and consequences of using water in the production of all types of hydrogen. A key success factor is the formation of a sustainable approach to the choice of sources and methods of water utilization, as well as reducing the overall water consumption for hydrogen projects [12]. The implementation of this approach will eliminate the negative impact of hydrogen projects on communities experiencing water scarcity, as well as prevent the aggravation of current water security problems.

An important factor is the requirements for water quality used in the production of hydrogen. At all stages of water purification, losses and the formation of polluted effluents requiring purification are possible [13]. The process of obtaining water of the required quality for electrolysis and steam reforming can be associated with filtration, desalination and/or demineralization (depending on the type and quality of available water sources). During the process of ultrafiltration water losses can reach 10 vol.%, and for reverse osmosis, they amount to 15-25 % for ordinary water, 20-30 % for wastewater, 35-40 % for seawater. Liquid effluents generated during the water treatment process should be disposed of in order to minimize the negative impact on the environment. Their value can range from 7 % for ultrafiltration to 21 % for reverse osmosis [14].

The research uses publications on this topic [15-17], as well as actual data from listed additional indicators, the real value of water consumption in the production of hydrogen, depending on the water source, may, according to various data, be 13-40 liters of H2O per 1 kg of H2 produced [21-22].

Water consumption indicators of alternative natural gas conversion technologies (partial oxidation, autothermal reforming) may initially be lower. For autothermal reforming this value approaches 7.4 liters of H2O per 1 kg of H2 produced [23]. The full use of the carbon-containing feed potential to achieve maximum hydrogen yield requires a water-gas shift reaction between carbon monoxide and water steam, i.e. an additional amount of water steam consumption. The



actual water consumption in hydrogen production by these methods will be comparable, and in some cases even higher than the same indicator for the steam reforming process^{*}.

Thus, when obtaining "low-carbon" hydrogen (with CO2 capture), the actual consumption increases by 85 %^{**} [24] and, taking into account CO2 capture, steam compression and water cooling can be 18-44 liters of H2O per 1 kg of H2 produced [21].

For coal based hydrogen production, the actual water consumption can be 30-70 liters of H2O per 1 kg of H2 produced for hard coal and 25-60 liters of H2O per 1 kg of H2 produced for lignite coal due to its higher humidity. It takes about 12 liters of water directly to carry out the reaction [25, 26]. For steam conversion of biogas, the stoichiometric indicator of water consumption is equal to the same indicator of the steam conversion process of natural gas (4.5 liters of H2O per 1 kg of H2). However, taking into account the heat losses for removing CO2 from biogas before reforming, the actual water consumption may be 15-40 liters of H2O per 1 kg of H2 produced [27]. The biogas production itself is very water-intensive in addition [28]. The stoichiometric indicator of water consumption for the water electrolysis process is 9 liters of H2O per 1 kg of H2, which is twice as high as the same indicator for the steam conversion of natural gas. Additional factors affecting the water consumption indicators of the water electrolysis process should also be indicated, which are often omitted or not fully taken into account when conducting a feasibility study of projects [29, 30]:

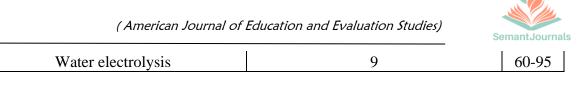
- ➤ water cooling of electrolyzers the one of the key reasons for the decrease in the efficiency of electrode battery during the service life (8-10 years) is additional heating, and therefore the cooling load on the electrolyzer during operation can increase by 40-70 %. The effect of this factor on the water consumption index is 30-40 liters of H2O per 1 kg of H2 *** [31];
- water cooling of related equipment, such as compressors to compress hydrogen to the pressure required for storage/application;
- purification of the source (raw) water depending on the quality of the source water, the amount of waste (effluents) of the purification process can be 20-40 %;
- wastewater disposal an increased concentration of impurities in the composition of wastewater in most cases prevents the discharge of these wastewater into the environment in its pure form; additional purification or dilution may be required for wastewater disposal.

The actual water consumption for water electrolysis process, taking into account the listed additional factors, may be 60-95 liters of H2O per 1 kg of H2. At the same time, 60-70 % of the total amount of water consumed falls on the recharge of water cooling systems. The general scheme of the water consumption in the process of water electrolysis process is shown in Figure^{***} [31].

The above water consumption indicators are possible when using relatively good quality fresh water as a feedstock. For water with high salinity, seawater or industrial wastewater, raw water consumption and the amount of process effluents may increase significantly [32].

| | Water consumption, liters of H2O per 1 kg of H2 | |
|---------------------------------------|---|--------|
| Production method | Stoichiometric | Actual |
| Steam methane reforming | 4.5 | 15-40 |
| Steam methane reforming + CO2 capture | 4.5 | 18-44 |
| Steam biogas reforming | 4.5 2 | |
| Hard coal gasification | Depending on C:H ratio and ~ | |
| Lignite coal gasification | on coal humidity | ~60 |

Table 1. Water consumption for various hydrogen production methods



Water consumption in the process of water electrolysis

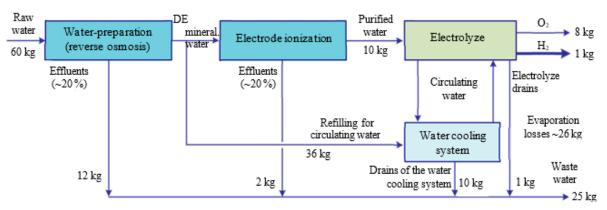


Table 1 summarizes water consumption indicators for different types of hydrogen production according to the current color classification. With the expected growth in hydrogen production, water consumption in this sector could increase by 35-100%. Considering the projected hydrogen demand (70 EJ), by 2050, the total water consumption for hydrogen production could reach 35-55 thousand tons annually, potentially increasing pressure on water resources and posing a heightened risk to water security in several countries. One of the major challenges in advancing the hydrogen economy is optimizing hydrogen storage and delivery to end users. In addition to liquefaction, other potential transportation methods include liquid organic hydrogen carriers (LOHCs) and using hydrogen in a chemically bound form (e.g., ammonia). Each method is linked to technologies that require steam, demineralized, and/or cooling water. Although water consumption is not a primary factor when choosing hydrogen storage and transport methods, it should still be factored into planning new hydrogen projects. When planning to reduce water use in future hydrogen projects, particular attention should be given to minimizing the consumption of make-up cooling water. This is the main contributor to overall water use and includes losses from evaporative cooling in cooling towers (~75%), cooling system blowdown (~15%), and other minor losses [33-35]. Water consumption for different hydrogen production methods also depends on the quality of the water source. In addition to water use optimization, the effectiveness of hydrogen projects depends on the type of water resource used. There are three main water sources for hydrogen production: freshwater, seawater, and industrial wastewater. While freshwater is the least expensive, it may not always be the best option, as it could be used more efficiently in other sectors of the economy and society. Hydrogen production facilities are often located near other industrial plants or settlements, allowing them to use industrial and domestic wastewater. Although this increases water treatment costs, it offers benefits such as shorter water pipelines, lower transportation costs, and reduced raw water expenses [33-35]. Seawater is often the only practical water source for large-scale hydrogen production plants. However, using seawater significantly increases overall water consumption compared to using freshwater [14, 36, 37]. Desalinating seawater places an additional environmental burden, requiring environmental assessments, permits, and approvals, which can increase both the time and investment required for hydrogen projects. Furthermore, the energy required for desalination adds to the energy consumption of hydrogen production, as water purification is energy-intensive [14]. Desalination plants typically consume about 0.5 kWh per kilogram of hydrogen, a relatively minor figure compared to the ~50 kWh per kilogram of hydrogen used during electrolysis. However, in some cases, desalination energy costs can range between 7 and 20 kWh per kilogram of hydrogen [31]. The most widespread desalination process today is reverse osmosis, though thermal desalination (distillation) is also widely used, especially in the Middle East. Other



methods, including direct osmosis, membrane purification, ion exchange, and electrodialysis, are at different stages of commercialization and research. Improving and optimizing desalination technologies will be crucial to the future efficiency of hydrogen projects. Table 2 compares water consumption for hydrogen projects using freshwater (the preferred option) versus seawater (the least favorable). Interestingly, freshwater consumption for hydrogen production is comparable to that of the method with the highest carbon footprint (coal gasification) and the one with the lowest (electrolysis using green electricity). However, using seawater leads to record-high water consumption. When industrial or domestic wastewater is used as a source, water consumption is expected to fall between the best and worst-case scenarios.

| | Water consumption, liters of H2O per 1 kg of H2 | | |
|--|---|----------------------------------|--|
| Production method | Freshwater, evaporative cooling | Seawater, evaporative cooling | |
| | cooning | cooning | |
| Steam methane reforming | 15-40 | 38-100, occasional up to 200 | |
| Steam methane reforming + CO2 capture | 18-44 | 45-100, occasional up to 220 | |
| Steam biogas reforming | 20-45 | 50-113, occasional up to 225 | |
| Hard coal gasification | ~70 | 175-350 | |
| Lignite coal gasification | ~60 | 150-300 | |
| Water electrolysis | 60-95 | 150-238, occasional up to 475 | |

| Table 2. Water consumption for various hydrogen production methods depending on the |
|---|
| quality of the source water |

The carbon footprint estimation for hydrogen production via steam reforming of methane is based on the material balance data from an operational plant. Hydrogen production from water is often labeled as "renewable" hydrogen, as water is a primary source. However, water also plays a crucial role in steam methane reforming (SMR), one of the most widely used industrial methods for hydrogen production. In the SMR process, methane reacts with steam in the presence of catalysts in two stages:

1. • CH4+H2O→CO+3H2, ΔH298∘=+206 kJ/mol

2• CO+H2O→CO2+H2, Δ H298∘=-41.2kJ/mol

The overall reaction CH4+2H2O \rightarrow CO2+4H2, where half of the produced hydrogen comes from water and the other half from methane, confirming a roughly 50/50 ratio. Material balance data from a real production facility show that 48.88% of hydrogen is derived from water, validating that around half of the hydrogen produced in SMR is "low-carbon" from water, with a significantly reduced carbon footprint. The findings show that, when comparing energy and water consumption, SMR is more efficient in terms of water usage than electrolysis. Additionally, approximately 50% of hydrogen from SMR can be considered "low-carbon" due to the water used in the process. However, as global hydrogen production shifts toward water as a feedstock, this could have increasing implications for the water cycle and water resources globally.

In conclusion, the comparative analysis conducted in this study demonstrates that water consumption in hydrogen production via steam reforming is considerably lower than in production through electrolysis. Data from an operational hydrogen plant reveal that nearly 50% of the hydrogen produced through traditional steam reforming can be classified as "renewable" and "low-carbon," based on the use of water and the associated carbon footprint. However, as the



hydrogen economy expands and global hydrogen production from water increases, the impact of this sector on the water cycle and global water resources is expected to grow significantly.

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