The Importance of Water in the Emergence of the Hydrogen Rainbow

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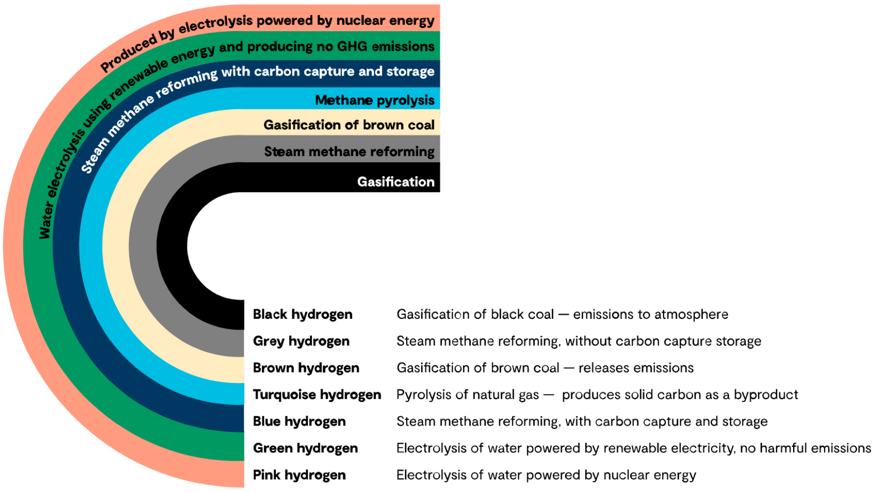
Abstract: Near-zero or zero emissions hydrogen has the potential to make a significant contribution to emissions reduction and decarbonisation in power generation, transportation, and industrial sectors. Rapid exploration and growth are expected into hydrogen as a replacement to conventional energy sources. It will be important for water to be considered and integrated into the developed approach to ensure and enable the realisation of a hydrogen economy in a sustainable manner as directed through the adoption and implementation of the United Nations Sustainable Development Goals (SDGs). It is critical to consider the approach to sourcing and disposing of water, and how to reduce the overall water demand, to avoid exacerbating water security concerns and impacting negatively upon already water-stressed communities. Lessons learnt from real world case studies undertaken have influenced this paper and are used to outline some challenges and opportunities related to water for hydrogen. In addition, potential synergies and reuse opportunities are presented to lower water and power requirements which will assist in the transition to green hydrogen using renewable energy. The focus of this investigation was water consumption, the related challenges and opportunities, environmental impacts including management of waste and brine, and integration within the sustainable water cycle.

Keywords: Hydrogen; Water Requirements; Renewable Energy; Future Energy; Brine Management

Introduction

Hydrogen (H_2) is a versatile energy carrier and feedstock with approximately 120 Mt/a of H_2 currently produced globally; most of this is utilised in refining (39 Mt/a) and ammonia production (33 Mt/a) (IEA, 2019). Approximately 98% of current H_2 production is from reforming methane or gasification of coal (IEA, 2020). H_2 use is expected to increase significantly to replace other energy sources with a large portion via renewable green H_2, as well as blue H_2. Depending on the production method, and carbon intensity of the process, H_2 is assigned a colour label, e.g., 'green' H_2 is produced from water electrolysis via renewable power, whereas 'blue' H_2 is produced via steam methane reforming (SMR) and includes carbon capture and storage (CCS). It is important to reiterate that "hydrogen is hydrogen" and that irrespective of the process used to produce the H_2 and colour label assigned, it is the same product. Hydrogen is the most abundant element, but rarely occurs by itself, it is usually bonded to other elements such as in a water molecule or an organic compound. This requires separation of the H_2 from the other elements for production. Due to the numerous methods of producing H_2, there are many colours, which can be depicted by a "hydrogen rainbow". Figure 1 shows this H_2 rainbow, outlining classification colours with their description. Note that white H_2, is the natural formation found in underground deposits, and not shown in the rainbow as it is naturally occurring and not produced. In the short term, blue H_2 is expected to play a larger role while electrolyser technology continues to become more efficient, affordable, and scalable.



Black hydrogen	Gasification of black coal — emissions to atmosphere
Grey hydrogen	Steam methane reforming, without carbon capture storage
Brown hydrogen	Gasification of brown coal — releases emissions
Turquoise hydrogen	Pyrolysis of natural gas — produces solid carbon as a byproduct
Blue hydrogen	Steam methane reforming, with carbon capture and storage
Green hydrogen	Electrolysis of water powered by renewable electricity, no harmful emissions
Pink hydrogen	Electrolysis of water powered by nuclear energy

Figure 1 Hydrogen classified according to colour, depending on its production pathway (Potts & Coertzen, 2022)

It is estimated that the 2050 world H_2 demand will be >580 Mt/a, and it is expected two thirds of this will be supplied from renewable H_2 (IRENA, 2021). Another estimate predicts that within Europe 270 Mt/a of green H_2 will be required to meet net zero energy systems by 2050 resulting in an investment in infrastructure required of 18 billion Euro (approx. $27 billion AUD) (Ram et al., 2020). It is expected that the Australian hydrogen export could reach 1 Mt/a by 2030 (ACIL Allen Consulting for ARENA, 2018), and even up to 45 Mt/a by 2050, equivalent of $90 billion AUD (Murray, 2021). In addition to H_2 for export, Australia will have domestic uses including integration with natural gas networks, fuel cells used in transportation, energy storage to generate electricity in remote communities, and as an industrial chemical feedstock to produce ammonia, fertiliser, and steel (Australian Government, 2020). This is estimated to be a demand of up to 230 Mt/a (Pendlebury, et al., 2021).

The movement toward green hydrogen production aligns with numerous UN SDGs and is critical in the transition to affordable clean energy (SDG 7), responsible consumption and production (SDG 12), and acting against climate change (SDG 13) through the development of key partnerships (SDG 17) between water, community, energy, transport and end users. As the hydrogen economy continues to emerge this will drive economic growth in Australian through investment and job promotion (SDG 8) and allow Australia to transition away from the exportation of fossil fuels through industry, innovation and infrastructure (SDG 9). There are numerous export agreements established or being developed between Australia and other countries, including Germany, Japan and South Korea. There are also potential future buyers looking to transition away from fossil fuels for energy including India who are looking to secure their energy future and transport industry due to large population increases (Sontakke & Jaju, 2021). The current attention directed towards hydrogen production is driven through decarbonisation, with Australia well placed to capitalise based on capacity for renewable energy production and established resource export industry capability and infrastructure. To achieve implementation however water availability and use challenges will need to be appropriately managed. This is crucial to manage potential implications for sustainable water management and to ensure that water communities are not further stressed through drought or arid conditions.

Both green and blue H_2 production are dependent on demineralised water (typically conductivity <0.5 uS/cm) which depending on the water source often requires desalination using two-pass reverse osmosis (RO) and further demineralisation process units. As for any desalination process, a major consideration is the complexity relating to brine management. Based on water balances developed for Australian H_2 production, large volumes of water can be required; it is important to strive to reduce this, particularly in non-coastal locations with limited water availability, to mitigate against risks associated with declining water security and drought. Another aspect of water treatment for use in electrolysers and evaporative cooling to produce green hydrogen is the waste streams created (e.g. pre-treatment and brine wastes). It is critical to understand and optimise the synergies between water and H_2 production to create a shared sustainable future, aligning with United Nations SDGs requirements, before significantly increasing H_2 production capacity around the globe.

Depending on feed water sources, pre-treatment (produces various wastes) and desalination (produces a brine waste) are often required prior to demineralisation to achieve the required electrolyser feed quality. These streams require management and disposal in a manner that does not impact waterways or the wider environment. Key issues relating to water treatment for hydrogen production include the impact of hydrogen plant siting, water security (many readily available sources require desalination), feed water chemistry and cooling requirements as outlined in Table 1.

Table 1 Challenges and opportunities related to water treatment for hydrogen production

Challenge/Opportunity	Description
Location Siting	• Proximity to various water sources, hydrogen export location, feed stock methane, and energy sources • Cooling considerations
Water Security and Feed Water Chemistry	• Water security and feed water availability (e.g. may already be allocated to drinking water, agriculture, or environmental flows) • Feed water quantity and quality uncertainty (e.g. groundwater). Many available sources but challenging to treat (e.g. brackish, contain oil) • Regulations related to water access and allowable end-uses • Feed water chemistry data (e.g. number of samples, representative samples across seasons, correct sampling method)
Brine Management Strategy	• Many readily accessible water or waste streams require desalination • Desalination produces a considerable waste stream that is challenging (e.g. costs, regulations, environment) to treat, manage, and dispose • Optimisation of beneficial reuse opportunities (e.g. salt recovery)
Recycling of Waste Streams	• At water constrained locations there are drivers to maximise plant recovery and minimising waste discharge • Waste stream recycling from hydrogen production can be challenging due to quality and lack of information available
Steam Reuse Applications	• Potential to use blue hydrogen production steam to drive thermal desalination • Potential to use green hydrogen electrolyser to drive thermal desalination
Waste Heat Recovery	• Waste heat can be used for desalination, brine management, air water generation and overall heat management (e.g. cooling)
Cooling Water Requirements	• Air versus water cooled dependent on local climate, interplays with siting • Seawater once through cooling versus seawater cooling tower (although small number of cycles and expensive materials) • Adiabatic cooling requirements at hot inland locations such as inland Australian due to local humidity and ambient temperature conditions
Oxygen Reuse Opportunities	• Reuse the oxygen generated from the electrolyser for water treatment process e.g. aeration of the wastewater treatment processes

For large production projects seawater desalination may be the most viable sustainable water source. Seawater desalination can introduce additional environmental approvals, waste and energy management, and social license issues which can affect project environmental and planning approvals and timeframes. All desalination methods require consideration of brine management and disposal. Thermal brine treatment processes are effective but are energy intensive, have very high associated capital expenditure (e.g. materials and equipment) and operating costs (e.g. energy requirements and maintenance needs) compared to RO. However, these technologies are likely one of the key technologies for inland H_2 projects where desalination is required with associated brine minimisation. Feed water chemistry can be challenging for many of the more accessible water sources such as the often-complex chemistry of inland groundwater, produced water sources, and high salinity sources and recycled water from treated sewage is prone to specific scaling and biofouling challenges. Additionally, for inland projects, storage ponds increase risks associated with algae contamination and consequential additional water quality problems. Recycling of waste streams such as cooling tower blowdown often requires complex treatment and needs careful consideration to minimise overall project costs.

As outlined, the water requirements for H_2 vary depending on project related factors such as water quality, technology selected, cooling method and H_2 production type. Therefore, it is important to determine appropriate tools during the design phase for managing the various challenges and capitalising on opportunities. To make informed decisions, the correct analysis tools should be employed, such as process modelling of the water treatment and interlinked cooling water make-up/blowdown process, and process chemistry modelling. Results can be used for concept engineering design (involving lab and pilot testing), cost estimation including determination of net present costs (NPC) or even internal rate of return (IRR) for the overall project and multi criteria analyses (MCAs) for hydrogen production siting, technology selection and brine management decisions.

The treatment process that would typically be used for the water treatment for hydrogen includes appropriate pre-treatment (e.g., microfiltration / ultrafiltration) prior to RO (likely two stage) prior to feeding a CEDI (continuous electro deionisation) unit for further pollutant removal prior to feeding an electrolyser. Waste from the initial pre-treatment, CEDI, brine from the RO, and any cooling / electrolyser waste are collated and require disposal if not recycled for reprocessing through the water treatment plant. Figure 2 provides a block flow diagram with simplistic water balance, outlining the water demands for a brackish water fed green hydrogen system.

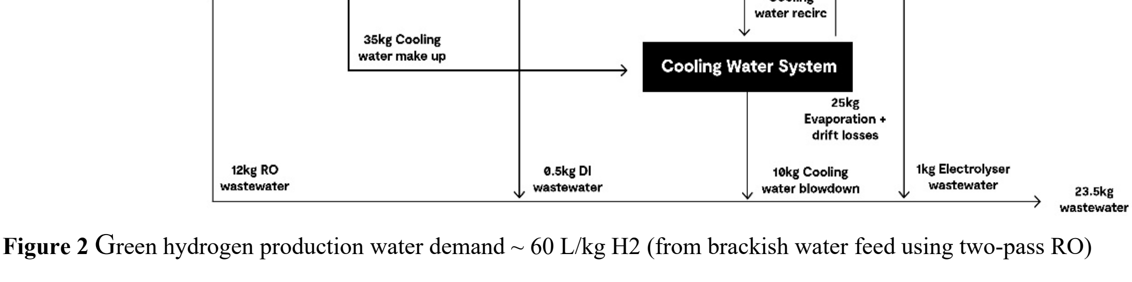


Figure 2 Green hydrogen production water demand ~ 60 L/kg H2 (from brackish water feed using two-pass RO)

Method

The following work describes the methodology used to assess water requirements and waste steam production for various hydrogen pathways. This was done for real world case studies within Australia for both inland brackish water demands, and seawater demands to compare to the stoichiometric values. This comparison allowed for the various colours of hydrogen to be compared on a water demand basis irrespective of the hydrogen carrier selected for transport. The development of water treatment for hydrogen should be undertaken in the following steps:

1. Water quality sampling: Sampling should occur over an as long as practicable period to ensure data is representative and seasonal variation is observed. All analytes important for design need to be analysed. It is essential that all parameters are tested that may affect design.
2. Process selection and design including process simulation: Preliminary designing and sizing should be undertaken using process simulation software. EVS: Water was used to inform the initial concept design, for rapid development of multiple alternative treatment schemes whilst accounting for process chemistry and costs.
3. Brine management strategy development: Determination of the brine volume minimisation approach (if required), disposal/beneficial use route and end of life management are key considerations for the desalination process. For inland sites, the determination of brine chemistry behaviour (GHD used OLI Stream Analyzer for this work) and integration with water balance modelling is useful for prediction of bulk crystallisation timing. Different options are compared on an NPC basis.
4. Cost estimation: Often paired with an MCA as cost comparison to influence the decisions made from both a technical proficiency and a cost to the organisation to find a compromise between cost and performance. Additionally, cost estimation assists in determining project feasibility which is critical in the emerging hydrogen market due to current uncertainties. Typical cost estimation occurs through NPC analysis which feeds into the overall project IRR.
5. Multi Criteria Analysis (MCA): Used to compare all facets of an engineering design e.g. cost, technical, environmental, and social considerations. Commonly used for siting selection (important for space constrained coastal projects), technology selection (e.g., pre-treatment) and brine management strategy decisions including pond storage vs thermal treatment or comparison of complete strategies.
6. Lab or pilot test work: In addition to water quality testing, jar testing, lab testing of technology and even pilot plant testing can be required to determine or prove feasibility of technologies that may be novel.

Through these steps, the water demand is determined for the respective pathway and can be repeated for various hydrogen pathways, water sources, treatment arrangements and cooling technologies to determine the L/kg of H_2 required. For this study this was determined using “good quality” brackish raw water e.g., water free of oil, grease, and high levels of hydrocarbons or organics, which would require additional treatment processes to remove. The water demand for each hydrogen production method was then determined for maximum and minimum ranges to compare to the stoichiometric requirements. This was repeated using seawater as the feed water source to complete the comparison of hydrogen production method and water quality demands. Whilst hydrogen is a low energy density fuel, it can be difficult to transport and store either via compression, liquefying or chemically combining (e.g. ammonia).

Results and Discussion

Typical H_2 production processes require significant total water volumes per kg of H_2 produced. This is larger than the often-quoted stoichiometric needs as outlined in Table 2 for various production methods including additional process operations. Note the values below report only the water required to produce H_2. Therefore, it does not include the water requirements associated with the energy source used in production (e.g. requirements associated with nuclear energy generation, for pink H_2 or in the manufacture of solar panels), or water for carrier methods. The study is based on using H_2 gas carrier and does not include additional water demands necessary for liquefication cooling, or chemical conversion to ammonia which can be significant.

Table 2 Hydrogen production – water demand

H_2 production pathway	Stoichiometric demand (L/kg H_2)	Total demand (L/kg H_2), assuming good quality raw water import	Total demand (L/kg H_2), assuming seawater as raw water import
Natural gas reforming (grey H_2)	4.5	15*-40	38-100
Natural gas reforming with carbon capture (blue H_2)	4.5	18*-45	45-110
Biogas reforming (other green H_2)	4.5	20*-45	50-115
Coal gasification (black H_2 and brown H_2)	Dependent on coal C:H ratio and moisture	70	175-350
Biomass gasification (can be classed as green H_2)	Dependent on biomass C:H ratio and moisture	60	150-300
Water electrolysis (green H_2)	9	60-95	50*-120
Water electrolysis via nuclear energy (pink H_2)	9	102**	50*-220
Methane pyrolysis (turquoise H_2)	0	0	0

Note: *Includes some air cooling, **Running an electrolyser at 75% efficiency

Overall water requirements for hydrogen production from various energy sources generally significantly exceed the stoichiometric needs (e.g. green hydrogen's 9 L/kg H_2), resulting in total water demands that are significantly higher (e.g. green hydrogen's 60-95 L/kg H_2) depending upon water source and quality, hydrogen process selection and cooling needs. Replacing blue with green H_2 for example could potentially lead to an increase in water consumption of approx. 35% to 100% per kg of H_2.

Putting water consumption into perspective, a 10 MW green H_2 electrolyser unit creates roughly 4 tpd H_2, requiring approx. >0.24 ML/day of raw water. A 1 GW unit increases this demand to >24 ML/day, producing 400 tpd of green H_2; assuming typical stack power consumption of 51 kWh/kgH_2, an operating capacity of 85%, WTP recovery of 60%, and 100% evaporative cooling. H_2 is typically converted to a carrier after production e.g., liquefied H_2, liquid organic carriers, or ammonia via the Haber-Bosch process, accounting for 1.2% of global carbon emissions (D'Angelo et al., 2021). Conversion requires additional water demand and to reduce this demand for green H_2, the focus should be on cooling water make-up demand. The individual water demands for carrying the hydrogen need to be considered from an overall water balance but should not be used as the main factor in selecting the carrier, with economics and hydrogen loss more important. Air cooling is an alternative that can significantly reduce overall water needs; however, applicability is subject to location and climate and impacted by cost, footprint, and power demand. Air cooling is limited to 40-50°C ambient and may need to be augmented by evaporative cooling, refrigeration or adiabatic cooling, therefore is not always a suitable substitute.

Finding sustainable water sources and managing waste is critical in developing a sustainable H_2 industry to drive world decarbonisation. Options include fresh water, brackish groundwater, industrial wastewater, sewage effluent, and seawater. Utilising fresh water has the lowest treatment cost but is not preferred as this diverts scarce and valuable water from other valuable societal use. H_2 hubs will typically be located with other industrial activities and larger populations where significant volumes of sewage and industrial wastewater are available but with the need for higher levels of treatment and overall consumption due to the factors explained.

Given the projected dramatic growth in demand to >580 Mt/a H_2 by 2050, water consumption could be as high as 55,000 GL/a. This is a relatively small proportion of global water use when compared to 2,800,000 GL/a for global agriculture, 800,000 GL/a for industrial and 470,000 GL/a for municipal use (FAO & UN, 2011). However, the challenge is not solely solved by the water balance, rather by the availability of water availability in proximity to the locations where suitable energy source availability and demand for hydrogen or transport and export infrastructure exists or can be developed. In the transition away from fossil fuels water resources currently utilised may be released but may not be accessible to locations economically suitable for hydrogen production. Rather it is often the case that in suitable locations water scarcity is already increasing pressure on water resources and difficult choices may be needed to support a change to application in hydrogen production.

There are other low-carbon production methodologies that could form part of the hydrogen production rainbow. Production of hydrogen from biomass or biogas, or turquoise hydrogen production (natural gas pyrolysis to produce hydrogen and carbon black) could contribute to the overall hydrogen supply. While these production pathways could have lower water demand for the process itself, there are other issues to overcome. The main challenges with these processes are technology development, capital cost investment required and the constraints in ability to supply large enough volumes of feedstock to centralised production points. Currently, there are few demonstration facilities in place. One of the strengths of this hydrogen production pathway is that it typically utilises what is considered a waste or zero-value product to generate energy.

The analysis completed catalogues the various viable production methods for hydrogen use different feed sources and have different water demand, with some advantages and disadvantages outlined below:

- Green H_2 – Advantage: renewable energy usage. Disadvantage: electrolyser technology development, higher cooling load and associated water demand, cost
- Blue H_2 – Advantage: less water required, assists in transition from fossil fuel, established and scalable. Disadvantage: carbon intensity, CCS efficiency dependent
- Pink H_2 – Advantage: nuclear pairs well with electrolysers, low carbon intensity. Disadvantage: water usage, electrolyser technology development
- Turquoise H_2 – Advantage: minimal water requirement, only cooling water. Disadvantage: not sustainable process due to fossil fuel feedstock
- Grey H_2 – Advantage: low cost, large scale H_2 production and most used globally. Disadvantage: not sustainable process due to fossil fuel feedstock

- Brown/Black H_2 – Advantage: low cost, produces solid carbon by-product, largest water demand. Disadvantage: unsustainable process as fossil fuel feedstock.

Conclusions

As the green hydrogen industry develops as a part of the energy transition, water for H_2 is and will become an increasingly important part of the water industry globally. Today's typical H_2 production processes all require a significant amount of water, with optimisation of demand being a critical need in enabling industry development. Water treatment for green and blue hydrogen projects, whether inland or coastal, all have scenario specific challenges and opportunities. However, many of these are common between projects and there are potential integration opportunities to create complementary designs that are advantageous for both water treatment and hydrogen production plants. Harnessing these opportunities to lower the overall water demand of sites will reduce risks and align with SDGs and sustainable water security targets. This will assist in maintaining social license and reducing environmental concerns associated with the emerging green hydrogen industry. Technology selections (e.g., water treatment, cooling systems, heat recovery, brine management) are crucial with synergies between these processes necessary for long term project success. If green H_2 plants can encompass full evaporative cooling and effectively utilise waste heat in thermal desalination or thermal brine treatment processes this will result in lower water requirements and carbon footprint of hydrogen production facilities. This further reiterates the importance of water in the transition away from fossil fuels towards a new energy system across Australia and the world and will assist with the lowering of hydrogen costs towards the aimed "H_2 under 2 (dollars)" set by the Australian government from the current approximate cost of 8 AUD/kg (Fowler, 2020).

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