

Supplementary Information

Table SI-1 Green hydrogen production and wastewater treatment

<p>1. Synergising green hydrogen production with wastewater treatment</p>	<p>Wastewater-based hydrogen production stands out from other hydrogen production methods due to its ample water supply and the added benefit of converting waste into energy.^{1,2} Technologies for generating hydrogen from wastewater are categorised based on various criteria, including the energy supply method, material resource (water or biomass), and type of process used.^{1,3-6} For example, based on previous studies, Kabir <i>et al.</i>⁶ categorised these methods by primary energy sources: electrical, thermal, photonic, and hybrid, identifying electrical methods as the most energy-efficient (6.15%) but also the highest in production cost, with an average of \$8.26/kg.</p> <p>Some technologies can simultaneously treat wastewater and produce hydrogen gas. These technologies can be further categorised into four types: 1) biological treatment, 2) electrochemical treatment, 3) advanced oxidation processes (AOPs), and 4) solar-driven hydrogen production.⁷ This approach provides a valuable opportunity to utilise wastewater, eliminating the need for high-quality water and thereby reducing additional energy use and costs.</p> <p>Green hydrogen is a sustainable alternative to conventional hydrogen production. Figure SI-1 illustrates a SWOT analysis of green hydrogen, highlighting its strengths, weaknesses, opportunities and threats. Managing uncertainties in renewable energy supply is essential to ensure a reliable green hydrogen supply. By evaluating multiple renewable</p>
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energy sources, Hassan *et al.*⁸ emphasised solar as the most promising source for meeting future demands, wind as a trending source ideal for hybrid systems, geothermal as one of the most reliable sources due to its independence from the surrounding environment, and biomass as a sustainable source recently receiving considerable attention. This study further summarised renewable energy availability for green hydrogen production for different countries and regions.

Assessing Ghana's renewable energy potential, Agyekum⁹ identified the primary strengths in the renewable energy sector as geographical position, the presence of the Renewable Energy Act (Act 832), and political stability, which can be applicable to many countries. The economic potential of hydrogen production in Australia was assessed by Walsh *et al.*,¹⁰ considering both renewable and non-renewable energy sources. The study generated a tool¹¹ to identify the potential H₂ production nationwide. This analysis can be further expanded by considering the utilisation of co-product oxygen in WWTPs, which is the focus of this paper.

Green hydrogen production via water electrolysis is considered more expensive than other methods.⁶ However, utilising the co-produced oxygen from water electrolysis in other industries and services is considered a viable strategy to reduce the cost associated with hydrogen production.¹²⁻¹⁴ Generated oxygen can be harnessed in various stages of WWT through direct oxygen utilisation, as well as for generating ozone and hydrogen peroxide, as discussed in **Section 3** of the main paper. Integrating green hydrogen production with WWT significantly aids in

	<p>decarbonising the wastewater sector.¹⁵ It offers potential for material recovery (oxygen gas), energy recovery (hydrogen gas), and water recovery while enhancing the treatment process and fostering a circular economy.^{6,16-18}</p> <p>The co-location of hydrogen hubs at WWT facilities has recently gained significant attention due to its substantial benefits. According to Woods <i>et al.</i>,² locations with higher renewable energy potential and sufficient space for green hydrogen plants often face water stress conditions. Water electrolysis has been identified as the best technique for co-located hydrogen production.¹⁹ This integration can facilitate self-sufficiency in renewable energy production and utilisation while establishing potential income streams.^{15,20,21} It is worth exploring this co-location further to assess its potential, particularly based on the significance of accessing water.² The proximity of WWT facilities to industrial and residential zones can facilitate higher hydrogen demand and enables easier land approvals for hydrogen facilities, reducing the need for additional land purchase costs.¹⁹</p>
<p>2. Water electrolysis for green hydrogen production</p>	<p>Water electrolysis is a well-established and straightforward method for producing nearly pure hydrogen, currently accounting for around 4% of global hydrogen demand, equivalent to approximately 65 million tons.^{6,22,23} Theoretically, a minimum of 9 kg of water is required to produce 1 kg of hydrogen, and each kilogram of hydrogen co-generates 8 kg of high-purity oxygen, which has great potential for further utilisation.^{2,14,24} The primary methods of water electrolysis include alkaline water electrolysis (AWE), anion exchange membrane water</p>

electrolysis (AEMWE), proton exchange membrane water electrolysis (PEMWE), and solid oxide electrolysis cell (SOEC).^{18,25} Some important information on water electrolysis is provided in **Table SI-2**, while details on the number of case studies of green hydrogen production within the water industry, as reported by Kabir *et al.*,⁶ are illustrated in **Figure SI-3**. Source water quality and quantity are crucial factors for the performance and efficiency of water electrolysis systems. Producing 1 kg of green hydrogen in a PEMWE system can consume up to 11 litres of demineralised water,⁶ considering minor effects from factors such as electrolyser age, operating mode, and climate zone as well.²⁶ Considering associated processes like cooling, the total water consumption can increase to approximately 60–95 kg per kilogram of hydrogen.⁶ However, the effective consumption is only around 15 kg of water per kilogram of hydrogen, as most of the water is returned to the environment.²

Water electrolysers are sensitive to water quality, making it essential to meet stringent quality requirements to achieve optimal performance, high hydrogen quality, and a long system lifespan.²⁷ To meet these requirements, standards for water quality are specified as ASTM D1193-06 Type I or II,^{26,28,29} or ISO 3696 Grade 2 water (especially low-temperature water electrolysis technologies),^{27,30,31} as detailed in **Table SI-3**.

Consequently, understanding the impurities in treated wastewater and the necessary purification pathways to meet water electrolysis quality requirements is crucial. **Table SI-4** summarises various impurities in feed water and their impacts, highlighting how cationic, anionic, organic, and

inert impurities can adversely affect different electrolyser systems, leading to issues such as catalyst poisoning, corrosion, unintended byproduct generation, and performance degradation.²⁷

Methods such as the Sustainable Value Methodology²⁸ can be utilised to assess water source suitability for electrolysis, while techniques including Scanning Electron Microscopy, Energy Dispersive X-ray Spectroscopy, X-ray Photoelectron Spectroscopy, Electron Probe Microanalysis, and Attenuated Total Reflectance–Fourier Transform Infrared Spectroscopy are used for impurity testing.²⁷

Multiple membrane-based treatment processes have been analysed as pre-treatment technologies to achieve the required water quality for water electrolysis. Ultrafiltration (UF) is one of the methods that can be utilised to achieve the required water quality.^{32,33} Reverse osmosis (RO) treatment is also recommended as a viable treatment option to achieve the intended treatment goals when implemented after chemical tertiary treatment or ultrafiltration.^{18,28}

Besides membrane-based technologies, non-membrane-based technologies like advanced oxidation processes (AOPs) and ozone-biological activated carbon process (ozone/BAC) are also applicable for producing high-quality water.^{32,34}

Further research is encouraged on electrolysers to assess the methods of recovering from poisoning, ensuring the stability and solubility of balance-of-plant materials in ultra-pure water, and developing methods to evaluate long-term stability against impurities in a shorter time frame.²⁷

<p>3. Enhanced decision-making and feasibility assessment</p>	<p>Defining the water sector's role in this innovative sector coupling approach and assessing the potential for co-location and co-product utilisation are crucial for establishing a sustainable and circular economy. Strategies and innovative approaches should be developed to ensure responsible hydrogen production that does not disrupt existing water demands, thereby preventing potential water stress.² A comprehensive feasibility assessment can aid in better decision-making by ensuring a sustainable water-energy nexus, considering various integration avenues. While many studies explore the techno-economic and environmental feasibility of green hydrogen, further research is needed from the water industry's perspective, focusing on co-location benefits and utilisation of hydrogen co-products.</p> <p>A sustainability analysis incorporates four pillars: energy, efficiency, society, and environment.⁶ As the initial step in this multi-step analysis, a study could be conducted to determine the amount of treated effluent available for hydrogen production in the wastewater treatment facility, which can be later compared with the required water quantity for the intended amount of hydrogen production. This should be done in a way that does not compete with existing demands for treated wastewater, such as by reusing effluent that was previously discharged to a sea outfall.^{2,35}</p> <p>A market analysis is crucial for evaluating the potential of green hydrogen, its utilisation options, and the social and political views towards hydrogen. Further, conducting a SWOT analysis for green hydrogen is also advantageous for evaluating its strengths, weaknesses, opportunities, and threats (see Figure SI-1).^{6,35} Technical feasibility can be assessed by</p>
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considering key parameters associated with electrolysis technology, such as water input, the electrolyser system, hydrogen production and storage, co-product oxygen separation, and the power supply source.^{35,36} At this stage, it is crucial to determine the method of supplying the thermal energy required for the electrolyser system and the method of cooling water supply by considering different cooling systems to assess their technical feasibility.

Even though the utilisation of solar energy-based systems (e.g. parabolic trough collectors (PTCs) based solar farms) for thermal energy supply for the electrolysis process results in a high levelized cost of hydrogen (LCOH) due to their high capital cost compared to fossil energy-based systems (e.g. preheaters), the environmental benefits associated with reducing fossil energy usage are much more substantial.³⁷ As the principal water consumer, the cooling systems will demand the largest amount of water, which varies depending on the cooling technology (e.g. once-through cooling, evaporative cooling, or air cooling) and the climate.²⁶ However, instead of dissipating heat to the environment, it can be repurposed for thermal energy-based advanced WWT processes that produce high-quality water.^{15,38}

A cost-benefit analysis can be conducted by considering capital expenditures (e.g., equipment and land costs), operating expenditures (for factors such as energy, raw materials, maintenance, labour, and waste management), as well as revenue schemes for the WWT facility.^{6,35} By integrating green hydrogen production with WWT, the revenue schemes can include hydrogen sales³⁵ as well as co-product oxygen sales^{13,21}.

Furthermore, determining the emissions savings from the integrated model is crucial to demonstrate feasibility from an environmental perspective.³⁹

Modelling and simulating the integrated system can aid in identifying and analysing different scenarios, providing valuable insights for feasibility assessment and resulting in informed outcomes for decision-making. However, finding a simulation tool capable of simulating the intended integration of green hydrogen production and WWT together presents a significant challenge.¹³ Various tools are available for the modelling and simulation of electrolyser systems for hydrogen production, including TRNSYS, MATLAB/Simulink, Aspen Custom Modeler, Aspen Plus, INSEL, EDGAR, EnergyPLAN, ANSYS Fluent, and COMSOL Multiphysics.^{13,40}

Wastewater treatment modelling is beneficial for understanding the treatment process and predicting the behaviour of the plant, either at the planning and design stage of a new plant or for providing necessary upgrades or modifications for an existing plant.^{41,42} This can aid in addressing challenges related to a variety of vital factors, including energy, cost, water quality & quantity, and resource recovery, while enhancing the economic and operational efficiencies of the plant.⁴³

Process-based mechanistic WWT models are more useful than the empirical models (which are based on observed data and statistical relationships without explicit consideration of the underlying processes) when a deep understanding of underlying mechanisms is required. Scientific research that relies on the underlying physical, chemical, or

biological processes that especially focus on mass balance can use analytical models or mechanistic models for decision-making purposes.^{42,44}

According to Nemcik *et al.*,⁴² an analytical WWTP model can be subcategorised into four main types: hydraulic model, biological treatment model, oxygen transfer model, and settling tank model. The Activated Sludge Models (ASM1, ASM2, ASM2d, and ASM3), developed by the International Water Association (IWA), are widely regarded as robust representations of the biological processes within activated sludge systems.^{41,42} With the complexity of mechanistic models, which aim to capture the underlying mechanisms and dynamics of a system, strong computational tools like BIOWIN, GPS-X, AQUASIM, SUMO, SIMBA, and WEST are used in practice for WWT modelling.⁴¹ The data-driven models that are based on machine learning have attracted considerable attention recently over mechanistic models because of their capability for making better predictions and minimal errors.⁴³

General-purpose simulators, such as MATLAB/Simulink⁴¹ and Aspen Plus⁴⁵, are recognised as suitable for WWT process modelling, providing the flexibility to integrate with processes beyond WWT. However, it has been highlighted that the model developer is required to specify system parameters and the reactions while generating the model, unlike using dedicated WWT simulators or spreadsheet-based tools.⁴⁵ Anaerobic digestion-based biogas production and its utilisation, aerobic activated-sludge treatment lagoons, and reverse osmosis treatment have been modelled and simulated using Aspen Plus software to generate important

outcomes such as mass-energy balances, process economics, profitability, and commercial viability of the application.^{46,47}

Hönig *et al.*¹³ describe a simulation tool, GHOST (Green Hydrogen Oxygen Simulation Tool), version 1, designed to simulate the integration of green hydrogen production and WWT for technoeconomic analysis, where the co-product oxygen is utilised in the aeration stage in this project. This tool was developed using Visual Basic for Applications (VBA) in Microsoft Excel, providing the flexibility to incorporate additional information as well. Developing a common simulation platform is essential for assessing the comprehensive integration needed to unlock the full potential of the green hydrogen and WWT nexus.

Table SI-2 Water electrolysis for green hydrogen production

Water electrolysis	<p>Even though multiple technologies for green hydrogen production exist, the current methods are predominantly limited to water electrolysis, with many others still in the early development stages.^{1,13,18,48} However, there are significant attempts to assess other technologies, such as alternative water-splitting methods.^{2,48} According to Nicita <i>et al.</i>,¹⁴ the environmental friendliness of the water electrolysis method further enhances its applicability. However, de Kleijne <i>et al.</i>⁴⁹ demonstrated that excluding the life-cycle emissions of renewable energy sources, hydrogen leakage, and component production creates a deceptive impression that electrolyser-based green hydrogen production and transportation have minimal emissions.</p>
Global contribution	<p>Water electrolysis is a well-established technology for generating hydrogen gas.^{2,6,7,50} It is popular due to its straightforward method of producing nearly pure hydrogen.^{1,32} Analysing 193 case studies on water electrolysis for hydrogen production in the water industry, Kabir <i>et al.</i>⁶ identified that the highest percentage, 62.69%, of active projects are located in European countries, while the lowest rate, 0.51%, is in African countries (see Figure SI-3). With technological advancements and integration into industries such as WWT, more projects are expected to be developed worldwide.</p>
Hydrogen production	<p>In the water electrolysis process, electricity breaks down water molecules into hydrogen gas at the cathode and oxygen gas at the anode, as described in Eq. SI-1.²³</p>

	$H_2O + \text{Electricity (237.2 kJ/mol)} + \text{Heat (48.6 kJ/mol)} \rightarrow H_2 + \frac{1}{2}O_2 \text{ (SI - 1)}$
Power source	<p>The water electrolysis process can utilise renewable energy as the power source, including solar, wind, hydro, biomass, geothermal and nuclear.^{1,6}</p> <p>This makes the process environmentally friendly, delivering valuable green hydrogen gas resulting in zero-carbon emissions.^{6,51,52} The water electrolysis process is applicable for remote locations without grid access, as it can harness renewable energy sources.⁵³ This method effectively manages renewable energy by converting it into chemical energy and enhancing its storability.¹³</p>
Microbial electrolysis	<p>Microbial electrolysis cells (MECs) have also been considered in multiple studies as a bio-electrochemical method for hydrogen production.^{3,25}</p>
Electrolysis methods	<p>AWE and PEMWE are well-established low-temperature electrolysis processes popular in the industry. PEMWE is emerging as favourable for renewable energy-based systems due to its capability to operate dynamically with quick response times.²⁶ AWE operates at temperatures ranging from 30°C to 80°C⁶ with current densities less than 1 A cm⁻², while PEMWE operates at temperatures from 20°C to 80°C with higher current densities greater than 1 A cm⁻².⁵⁴</p> <p>Solid Oxide Electrolysis Cells (SOECs) are high-temperature electrolysis processes that operate at temperatures ranging from 500°C to 900°C.^{23,50,54}</p> <p>Even though this technology is still in the experimental stage of using wastewater as the feedstock, unlike low-temperature electrolyzers, SOECs do not require high-quality water for the electrolysis process because this method utilises evaporated water by significantly separating it from</p>

	<p>impurities and salts.⁵⁴</p> <p>However, while AWE, PEMWE and high-temperature water electrolysis show higher daily hydrogen production rates in terms of utilising biogas-based electricity and sewage sludge obtained from a municipal wastewater treatment plant, exergetic efficiencies are higher for dark fermentation biohydrogen production and high-temperature steam electrolysis.⁵⁵</p>
Electrical efficiency	<p>According to Mazloomi and Sulaiman,⁵⁶ the key factors affecting the electrical efficiency of water electrolysis include electrolyte quality, temperature, pressure, electrolyte resistivity, electrode and separator materials, and applied voltage.</p>
Water consumption	<p>The water consumption for hydrogen production depends on the source water quality, water treatment process, hydrogen production method, cooling system, and hydrogen conversion method. Assessing the water footprint of green hydrogen is essential to determine its sustainability and appropriateness for global use. While water is directly consumed as a feedstock or cooling aid in the production phase and carrier conversion,²⁶ water is indirectly consumed for other processes as well, such as renewable energy generation and feedstock production (e.g., pre-treatment and the manufacturing of other chemicals). Additionally, water is used in the supply chain, including transportation and water and wastewater management.</p>
Cooling water	<p>The greatest direct water requirement for the water electrolysis process is cooling water, and the amount significantly varies depending on the cooling process (e.g., evaporative cooling and once-through cooling) and the climate.²⁶ The same study determined that a once-through cooling system</p>

	<p>consumes the most water, whereas evaporative cooling requires makeup water due to losses in the process. Considering a total life cycle analysis, the water footprint of hydrogen production for 3.2 Gkg of hydrogen production in 2040 shows that a solar-based system requires 136 GL (around 43 L of water per 1kg of hydrogen).² In contrast, wind-based systems have a footprint of 55 GL (around 17 L of water per 1kg of hydrogen).⁵⁷</p>
<p>Standard specifications</p>	<p>High-purity water is necessary for current water electrolysis systems.^{27,28}</p> <p>The exact water quality requirements can vary depending on the type of electrolyser and the manufacturer. Academic researchers generally use the American Society for Testing and Materials (ASTM) D1193-06²⁹ Type I ultra-pure water for water electrolysis.²⁷ While Simoes <i>et al.</i>²⁸ recommend both Type I and Type II deionised water for water electrolysis, Arup Australia Pty Ltd²⁶ specifically highlight ASTM Type II demineralised water as suitable for a PEMWE system, noting that AWE systems are less sensitive to water quality than PEMWE systems. Electrolyser manufacturers typically recommend that the water feedstock have a conductivity of less than 1 $\mu\text{S}/\text{cm}$.^{18,27} For low-temperature water electrolysis technologies, the European Union harmonised protocols from the Joint Research Centre³¹ specify the use of ISO 3696 Grade 2 water (conductivity $<1.0 \mu\text{S}/\text{cm}$).^{27,30}</p> <p>According to some studies, a conductivity of less than 5 $\mu\text{S}/\text{cm}$ is still considered acceptable for water electrolysis.^{28,58} Many electrolysers available in the market include a deionisation step to further ensure these quality levels.²⁸</p>

<p>Water impurities</p>	<p>Reclaimed water quality can significantly vary depending on the original wastewater source and the treatment process. It is crucial to assess the gap between relevant water quality parameters of the treated wastewater and the requirements for the water electrolysis process to identify the advanced treatment requirements, which essentially require additional cost and energy. According to Chauhan and Ahn,³² turbidity and total dissolved solids (TDS) are important parameters to consider, whereas Arup Australia Pty Ltd²⁶ recommend assessing the conductivity or total dissolved solids. Other than those parameters, levels of organic matter, algae, alkalinity, silica, minerals like calcium and magnesium, and metal solids are also identified as important parameters, as they can cause issues such as fouling and scaling in industrial water systems.²⁶</p> <p>Effluents from WWTPs are challenging to utilise as the feedstock for hydrogen production due to the presence of impurities such as organics, nitrogen, dissolved and suspended solids, microbial contaminants, and metals.³² Becker <i>et al.</i>²⁷ define these impurities as exogenous impurities. The impurity levels vary depending on the extraction point, such as the treatment plant's primary, secondary, or tertiary effluent.³²</p>
<p>Cooling water quality</p>	<p>Further, specific water quality requirements exist depending on the type of cooling system utilised. According to Arup Australia Pty Ltd,²⁶ water quality is not a crucial factor in a once-through cooling system due to minimised evaporation, which allows the use of raw water sources with minimal treatment. However, based on the same study, water quality is a</p>

	<p>significant concern in evaporative cooling, as increased concentrations of dissolved solids can lead to corrosion and fouling in the system.</p>
<p>Impurity testing</p>	<p>According to Simoes <i>et al.</i>,²⁸ the Sustainable Value Methodology^{59,60} can be used to determine the suitability of a water source for the water electrolysis process. Further, various techniques can be used for impurity testing and impact identification. These testing methods include half-cell or single-cell approaches and are conducted in situ, in an operating device, or off-site (ex-situ).²⁷ Based on the review by Becker <i>et al.</i>,²⁷ the related information is summarised as follows. Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS) enable combining detailed imaging and element mapping. Detecting impurities at low concentrations using Electron Probe Microanalysis (EPMA) and conducting surface-sensitive analysis with techniques like X-ray Photoelectron Spectroscopy (XPS) are also highlighted in this study. The impact of contaminants can be further assessed using Attenuated Total Reflectance–Fourier Transform Infrared Spectroscopy (ATR-FTIR). Furthermore, many additional techniques are available for investigating impurities. Identifying the impacts of impurities and degradation mechanisms aids in enhancing device robustness, leading to extended lifetimes and lower operating costs.</p>
<p>Pre-treatment technologies</p>	<p>Chauhan and Ahn³² examined the possibility of using AWE systems to utilise lower-grade wastewater for hydrogen production, assessing the impacts of organics, nitrogen, and other impurities. This study identified increased turbidity and total dissolved solids (TDS) values as significant challenges for hydrogen production and recommended tertiary effluent</p>

ultrafiltration (UF) to achieve the required water quality. It has been identified that SOECs have the ability to use low-quality water to generate green hydrogen, ensuring no liquid waste with high pollutant concentrations is produced in the process.⁵⁴ Ayyaru and Ahn³³ also proposed a novel high-strength ultrafiltration-based process for producing advanced treated water from wastewater.³²

Arup Australia Pty Ltd²⁶ have provided information on implementing a system to improve the reclaimed wastewater quality (TDS < 800 mg/L), suggesting a sequential process: 1) Forming chloramine by adding sodium hypochlorite and/or aqueous ammonia to reduce biofouling in the ultrafiltration membranes, 2) ultrafiltration membrane treatment (adding coagulants to improve filtration and colour removal), 4) pH adjustment, chlorine removal, and antiscalant dosing, 5) reverse osmosis (RO) treatment (two passes recommended where cooling water can be extracted after the first pass), and 6) Electro deionization (EDI). In this process, clarification is optional and can be used if the water contains higher amounts of algae and solids. Another study analysing seven different treatment processes based on ultrafiltration and reverse osmosis processes determined that the application of two-pass membrane systems is suitable for treating recycled municipal wastewater to achieve the intended quality levels for water electrolysis (conductivity < 5 μ S/cm).⁵⁸

Assessing the water recovery from membrane-based systems is important to determining the total quantity of reclaimed water needed. It has been determined that a total of 5.2 ML of Class A recycled water is needed to

produce 1 ML of ASTM Type II water and 1 ML of cooling water, whereas 2.1 ML of advanced treated water (Class A water + reverse osmosis) is required to produce the same amounts of ASTM Type II water and cooling water using the proposed membrane-based treatment technologies by.²⁶ Moreover, handling the generated waste streams (e.g., brine, supernatant, and solid waste), amounting to 3.2 ML and 0.1 ML respectively, is very important in both cases. In this study, the clarified sludge and waste from the filter were pumped for thickening, then dewatered and disposed of, with the dewatering effluent directed to the head of the plant. Additionally, brine from the reverse osmosis process and electro-deionisation can be directed to a brine tank and pumped for disposal, used for filter backwash, or directed to further treatment, depending on its quality.

Producing ultrapure water from reclaimed water requires improvements in traditional processes such as ion exchange, granular activated carbon (GAC), ultraviolet (UV) irradiation, and reverse osmosis, as these methods are not effective in removing small molecular organics like urea.³⁴ They propose a new technology based on advanced oxidation processes to achieve the required quality levels. Zhang *et al.*³⁴ identify advanced oxidation processes using ozone and H₂O₂ as potential options for removing urea while emphasising the significance of further research. Interestingly, this review focuses on utilising co-generated oxygen from green hydrogen production to effectively generate oxidants for ozonation and advanced oxidation processes, which can also aid in producing high-purity water for water electrolysis, further enhancing the system's circularity.

Table SI-3: Standard specifications for water quality for water electrolysis^{29,30}

Parameter	ASTM Type I	ASTM Type II	Parameter	ISO 3696:1987 Grade 2
Conductivity (max.) at 25 °C in $\mu\text{S}/\text{cm}$	0.056	1	Conductivity (max.) at 25 °C in $\mu\text{S}/\text{cm}$	1
Resistivity (min.) at 25 °C in $\text{M}\Omega.\text{cm}$	18	1	Oxidisable matter oxygen content (max.) in mg/L	0.08
TOC (max.) in $\mu\text{g}/\text{L}$	50	50	Absorbance at 254 nm and 1 cm optical path length (max.) in absorbance units	0.01
Sodium (max) in $\mu\text{g}/\text{L}$	1	5	Residual after evaporation on heating at 110 °C (max.) in mg/kg	1
Total Silica (max) in $\mu\text{g}/\text{L}$	3	3	Silica (max.) in mg/L	0.02
Chloride (max) in $\mu\text{g}/\text{L}$	1	5		

Table SI-4: Various impurities in feed water and their impacts²⁷

Impurity Type	Components get affected	Degrading mechanisms	Impacts of the Impurities
Cations e.g. Fe ³⁺	PEMWEs: Catalyst, ionomer, membrane, and the amount of metallic components in the system presenting endogenous sources	<ul style="list-style-type: none"> • Replacement of existing protons in the membrane and ionomer. • Adsorption and deposition • Facilitate unfavourable reactions 	<ul style="list-style-type: none"> • Lower the conductivity of the membrane • Catalyst poisoning • Lower the ionomer conductivity • Reduced rate of hydrogen evolution reaction
	AWEs and AEMWEs: Anode and cathode Cations do not directly impact like in PEMWE systems.	<ul style="list-style-type: none"> • Adsorption and deposition 	<ul style="list-style-type: none"> • Possibility to improve the oxygen evolution reaction and the hydrogen evolution reaction • Catalyst poisoning • Increase surface area • Develop dendrites at negative potentials • Issues in mass transport due to deposition
Anions e.g. Cl ⁻	PEMWEs: Cell components, anode and cathode	<ul style="list-style-type: none"> • Changed reactions • Adsorption and fouling 	<ul style="list-style-type: none"> • Corrode cell components • Catalyst poisoning • Unintended byproduct generation • Enhanced dissolution

		<ul style="list-style-type: none"> • Corrosion 	
	AWEs and AEMWEs: Anode	<ul style="list-style-type: none"> • Charge carrier substitution • Adsorption 	<ul style="list-style-type: none"> • Nickel corrosion (except in specialised configurations)
Organic impurities	PEMWEs: Anode and cathode	<ul style="list-style-type: none"> • Adsorption and dissolution 	<ul style="list-style-type: none"> • Enhanced dissolution • Catalyst poisoning • Unintended byproduct generation
	AWEs and AEMWEs: Anode and cathode	<ul style="list-style-type: none"> • Oxidation 	<ul style="list-style-type: none"> • Catalyst poisoning
Inert impurities	PEMWEs: Anode and cathode	<ul style="list-style-type: none"> • Deposition 	<ul style="list-style-type: none"> • Blocks and issues in mass transport
	AWEs and AEMWEs: Separator, membrane or conductivity		

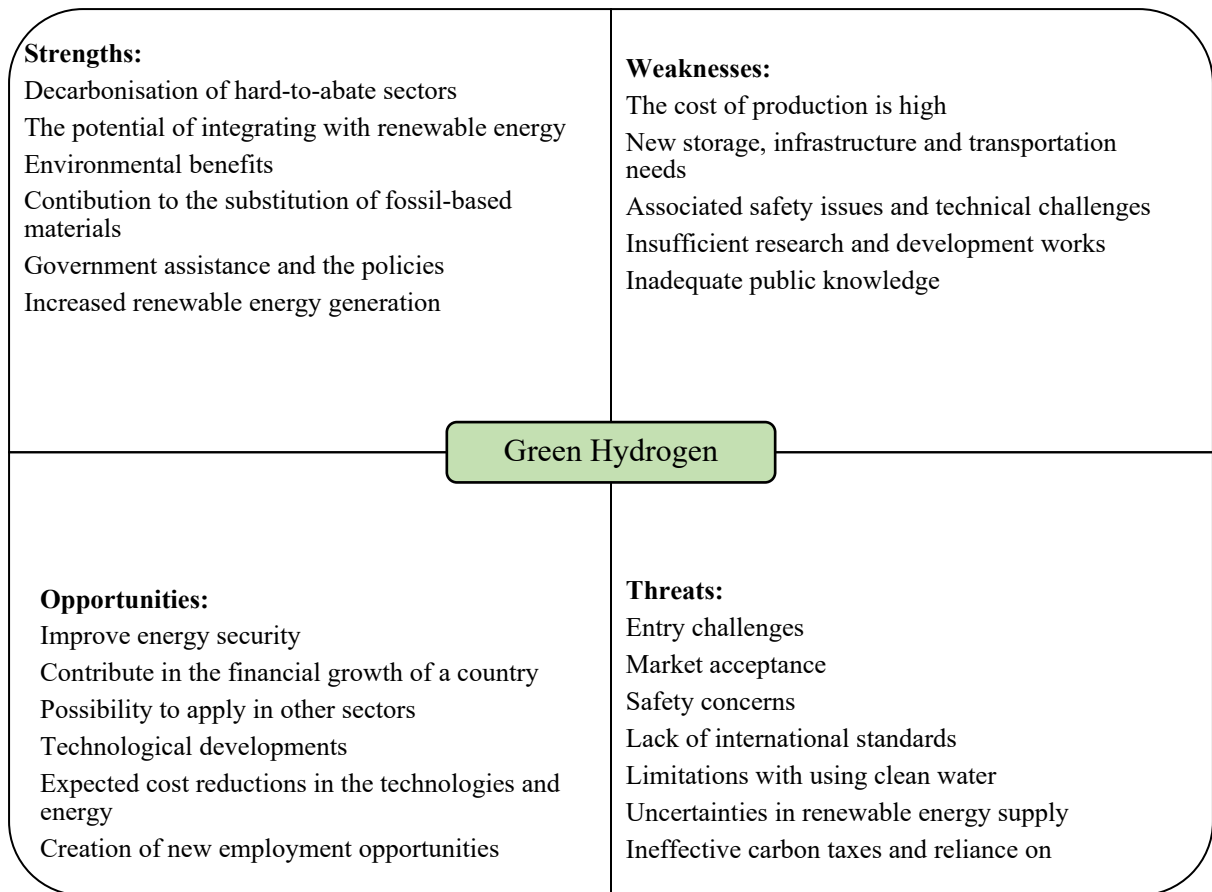


Figure SI-1: SWOT analysis (Based on Donald & Love¹⁵, Rahimirad & Sadabadi⁶¹ and Simões & Santos⁶²)

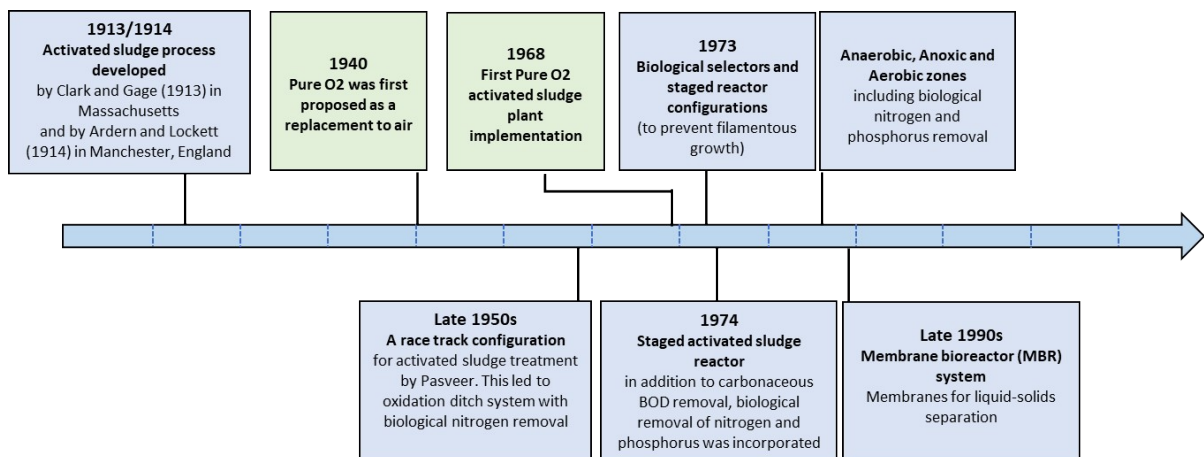
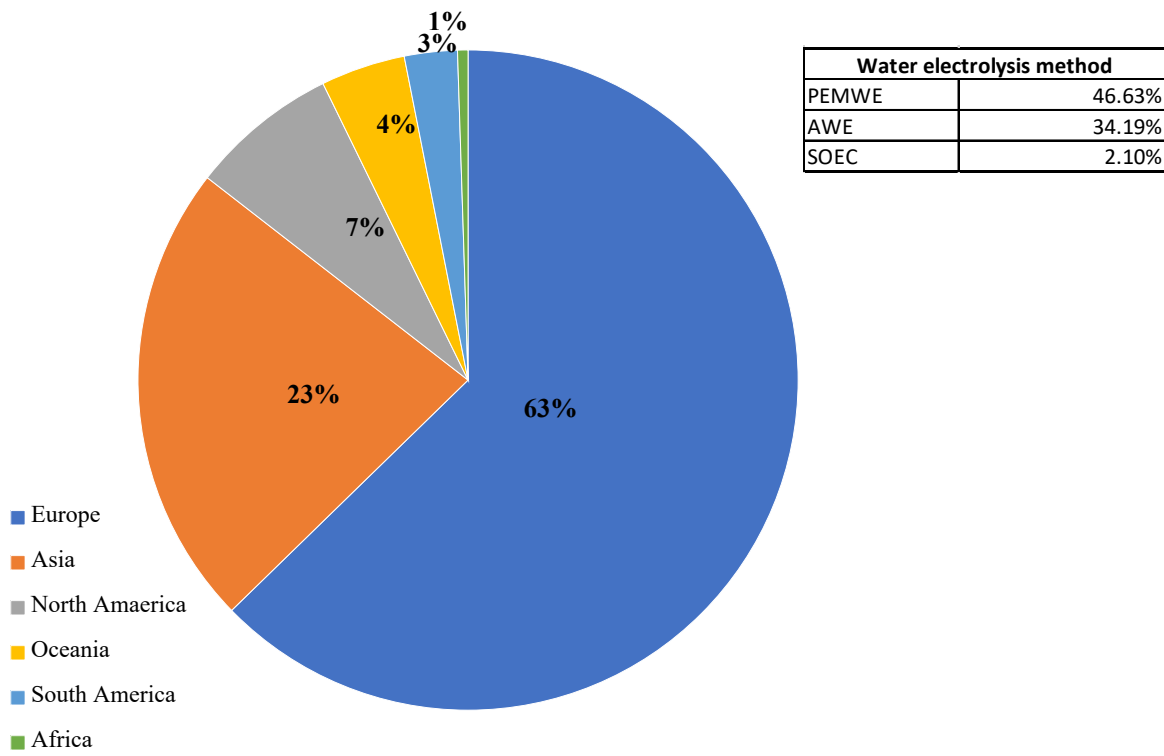


Figure SI-2: Activated sludge treatment process development and introduction of pure oxygen to the process (Based on Metcalf & Eddy⁶³ and Skouteris *et al.*⁶⁴)



Water electrolysis method	
PEMWE	46.63%
AWE	34.19%
SOEC	2.10%

Figure SI-3: Recent case studies of green hydrogen production in the water industry - figure generated from the data in the analysis by Kabir *et al.*⁶

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