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Water availability and water usage solutions for electrolysis in hydrogen production

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A B S T R A C T

Europe is committed to a new growth strategy with no net greenhouse gases emissions by 2050, where hydrogen has a clear role to play. Portugal's strategy for H_2 sets public policies promoting an industry focused on the hydrogen value chain. Considering the production of green hydrogen from renewable sources is key, water electrolysis becomes a priority, and with it, the need to assess the suitability of water sources, which is determined by both quantitative and qualitative factors. This work presents a new approach to assess the suitability of water sources for hydrogen production via water electrolysis by applying a Sustainable Value Methodology for decision-making support, combining economic, environmental and social criteria. The approach is applied to two different sites in Portugal: a semi-urban location on the Atlantic coast (site A) and a rural area far from the coast (site B). For both sites, water sources are evaluated regarding water availability, quality, transport options, abstraction costs, treatment needs and regulation (including environmental constraints) and social acceptance. The resulting sustainable value indicator, aggregator of different levels of information, enables a relative quantitative comparison of the performance of different water sources for electrolysis and the involved costs. It is found that the public grid water is the most suited source of water for electrolysis due to lower risk of supply, lower costs and avoids complex permitting processes. Likewise, seawater and wastewater treatment plant effluent (only in site A) showed to be possible water sources where the factors most affecting suitability are transport costs for water and waste disposal from water treatment.

1. Introduction

Europe is committed to a new growth strategy that will transform the Union into a modern, resource-efficient and competitive economy, aiming for carbon neutrality by 2050 (European Commission, 2018) and for decoupling economic growth from resource use. The European Green Deal is the plan for a sustainable economy in Europe (European Commission, 2019).

In 2020, after the adoption of the European Industrial Strategy, a plan for a future-ready economy, and of proposal of a Circular Economy Action Plan focusing on sustainable resource use, the EU also adopted the strategies on energy system integration (European Commission, 2020a) and on hydrogen (European Commission, 2020b) to pave the way towards a fully decarbonised, more efficient and interconnected energy sector. As stated by the IEA (2019), this is a critical time for hydrogen, which is today enjoying unprecedented momentum. The world should not miss this unique chance to make hydrogen an important part of our clean and secure energy future (Fatih Birol in IEA, 2019). The EU hydrogen strategy foresees at least 6 GW of renewable hydrogen electrolysers deployed up to 2024, producing up to 1 million tonnes of H_2.

Cycles of expectations followed by disillusion are associated to H_2 technologies (Staffell et al., 2019). On the production side, hydrogen can be produced from different sources, namely fossil fuels, biomass, and water electrolysis powered with electricity, naturally with different degrees of impact on the environment (Partidário et al., 2019). For H_2 to make a significant contribution towards the clean energy transition, it needs to be adopted in sectors where it is almost completely absent, such as transport, buildings, and power generation (IEA, 2019).

According to Blank and Molloy (2020), roughly 96% of H_2 produced

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today is from fossil fuels, with the remaining 4% produced through water electrolysis. However, interest in "green" H_2 production via water electrolysis powered with electricity from renewable sources, e.g., solar and/or wind, is growing, mostly due to technological learning effects, which contribute to lower costs and higher performance. Since electricity from renewable sources has zero greenhouse gas emissions, green H_2 is an attractive option for the decarbonisation of energy systems, as concluded by Sgobbi et al. (2016), for the whole EU energy system, and by Blanco et al. (2018) focusing on Power-to-Liquids. It is widely recognized that H_2 has a role to play as new energy vector in the provision of electricity, heat, industry, transport, and energy storage in a low-carbon energy system (Abdin et al., 2020; Staffell et al., 2019). Moreover, the renewable hydrogen value chain can also have synergies with the bioenergy value chain, with biomass being used to produce biohydrogen (Gonçalves et al., 2019).

Nonetheless, there are substantial challenges to be overcome to implement a functioning hydrogen economy regarding technological development (Schmidt et al., 2017), as well as policy and market conditions (Velazquez and Dodds, 2020). Within the policy challenges, it is highlighted the need to ensure that hydrogen production addresses sustainability concerns (Turner, 2004; Dincer and Acar, 2015; El-Emam and Özcan, 2019; Karaca et al., 2020). The first two publications specifically address water use for hydrogen production: Dincer and Acar (2015) qualitatively assess hydrogen production processes considering global warming and acidification potential, social cost of carbon, production cost and energy and exergy efficiencies, looking into resource use as water, biomass and fossil fuels. Turner (2004) compares several production processes and refers that water use for hydrogen production should be substantially lower than for other uses as agriculture. El-Emam and Özcan (2019) present a review on the techno-economics sustainability of "large-scale clean hydrogen production" but they only refer global warming and acidification potential within the environmental dimension. Karaca, Dincer and Gu (2020) apply a Life Cycle Assessment approach to compare nuclear based sustainable hydrogen production options considering the following impact categories: abiotic depletion, acidification, global warming, ozone depletion and human toxicity potential, but they do not refer water resources specifically. Beyond this body of literature assessing sustainability of hydrogen production, there is other work focused on energy consumption for hydrogen generation, as in the review by Christopher and Dimitrios (2012). Finally, Lee et al. (2019) evaluated the impacts of hydrogen fuel cell vehicles deployment on water stress for the USA, but they do not consider types of water sources. In overall terms, the current literature on sustainable hydrogen production is scarce (El-Emam and Özcan, 2019).

Because the overall energy sector (and hydrogen production) is highly dependent on water resources and can be vulnerable to water shortages, an integrated analysis should be done (Howells et al., 2013). This also applies to exploring and evaluating different potential water sources for hydrogen production. Nonetheless, although some studies do address water use in the context of hydrogen production (Dincer and Acar, 2015; Turner, 2004; Lee et al., 2019), to the authors best knowledge there is a lack of work assessing the suitability of different potential water sources and the extent this could influence decision making regarding investing in hydrogen production via electrolysis.

Portugal has become a frontrunner in green H_2 promotion with its national H_2 strategy setting public policies to promote an industrial policy focused on H_2 value chain, namely, in its' production, storage, transport and consumption, including the use of renewable gases in the natural gas grid (Portuguese RCM 63/2020, August 14th). Several initiatives have been identified which are central to unlock the required private investment, namely, (i) regulation of the production of renewable gases; (ii) regulation of the injection of renewable gases into the national natural gas network; (iii) designing mechanisms to support hydrogen production; (iv) implementing a system of guarantees of origin for renewable gases; (v) ensuring that the financial resources available in national and European funds support the production of renewable gases; (vi) set of binding targets by 2030 for the injection of H_2 into the natural gas grid (15% H_2 by 2030); consumption of H_2 as final energy (5% of H_2 in final energy consumption); consumption of H_2 in transport (5% of H_2 in final energy consumption in road transport and implementation of 50–100 refuelling stations for H_2), and H_2 consumption in industry (5% H_2 in final energy consumption in industry). Finally, the Portuguese strategy sets the target to install up to 2.5 GW of electrolysers for green H_2 production by 2030.

Electrolysers are electricity powered technologies where the reaction of electrolysis, splitting water into hydrogen and oxygen, takes place, according to equation (1) (Shi et al., 2020).

$$H_2O + \text{Electricity (237.2 kJ/mol)} = \text{Heat (48.6 kJ/mol)} + H_2 + 1/2\ O_2 \quad (1)$$

Electrolysis of water is one of the most suitable methods for production of green hydrogen, which uses as inputs electricity, pure water (exothermic reaction) to produce hydrogen and pure oxygen, the sole by-product (Schmidt et al., 2017). From a stoichiometric point of view, the H_2 production via water electrolysis consumes circa 9 kg of water per 1 kg of H_2 (Shi et al., 2020). There are several types of electrolysers with varying technological performance and thus, water consumption levels (Schmidt et al., 2017). Considering some of the electrolyser manufacturers' specifications, slightly higher water needs per kg of H_2 are reported, varying among suppliers and electrolyser type and ranging from 10.01 to 22.40 l per kg of H_2.

The variation in water consumption is also due to different technologies for water electrolysis, namely: (i) alkaline water electrolysis (ii) solid oxide electrolysis (SOE) (iii) microbial electrolysis cells (MEC) and polymer electrolyte membrane (PEM) water electrolysis (Kumar and Himabindu, 2019):

- Alkaline electrolysers operate via transport of hydroxide ions (OH) through the electrolyte from the cathode to the anode with hydrogen being generated on the cathode side. This technology with a 100-year history, is the most mature, durable, and the cheapest. The integration with renewable energy is expected to improve the dynamic of operations.
- SOE electrolysis, which use a solid ceramic material as the electrolyte that selectively conducts negatively charged oxygen ions (O_2-) at elevated temperatures, generate hydrogen in a slightly different way and the technology experiences are being demonstrated, still with relatively high costs (Staffell et al., 2019). See Rashid et al. (2015) for a review.
- MEC technology can be achieved by organic matter, including renewable biomass and wastewaters. This MEC technology is closely related to microbial fuel cells (MFCs), but its' operational principle is reverse of those (Kumar and Himabindu, 2019).
- In a PEM electrolyser, the electrolyte is a solid special polymeric material. Introduced in the 1960s and commercialized in the last decade, these systems have a wider dynamic range (0–200%), more suitable for intermittent power supply. However, capital costs are currently approximately twice of those of alkaline electrolysers, and cell lifetimes need to be improved.

Potential water sources for these electrolysis technologies span from oceans (seawater), estuaries, surface water (creeks, streams, rivers and lakes), ground water, rainwater, water from the public grid, recycled water (treated urban wastewater or industrial wastewater) or from water condensation processes (e.g., cooling towers). Since H_2 has a higher energy content per unit of weight than conventional fuels (according to Abdin et al., 2020, three times that of gasoline), and it can be produced via water electrolysis with lower environmental impacts, H_2 is a very interesting option towards more sustainable energy systems. However, it is essential to explore and evaluate different water sources for H_2 production, since freshwater is a scarce resource (Postel, 2000) and likely to become even scarcer due to climate change (IPCC, 2018). In fact, the EU Water Framework Directive states that member states shall take measures to protect all water bodies considering environmental objectives along with the protection of water bodies for different water uses (European Commission, 2000). Once the selection of the water source is influenced by different quantitative and qualitative factors, the Sustainable Value approach (Catarino et al., 2010), integrating economic with environmental and social issues, has been used as a tool for decision-making support.

This work presents a new approach, applying the Sustainable Value Methodology (Henriques and Catarino, 2015, 2017) to assess the suitability of potential water sources for H_2 production via water electrolysis, combining technologic, economic, environmental, and social criteria. According to the European Standard EN 12973:2020 the value of a study subject can be described as the relationship between the satisfaction of needs (performance) and the resources used in achieving that satisfaction: Value α Satisfaction of needs/use of resources. The approach is implemented using two different sites in Portugal: a semi-urban location along the Atlantic coast with hot summers (site A) and rural area far from the coast with slightly cooler summers (site B). The findings characterise the potential of freshwater, wastewater and seawater sources regarding quantities, quality, treatment needs and accessibility, among others, supporting the decision on H_2 deployment projects and allowing for a comparative analysis of performance and associated costs. Besides this introduction, the paper includes three additional sections: the first details the methodology using Sustainable Value (SV) approach and applying it to the selected case sites. The following section characterises the potential of freshwater, wastewater and seawater sources and presents the results of the most suitable water sources for each of the sites, as it allows a comparative analysis of each water source option's performance and associated costs. Finally, the third section elaborates on the main conclusions and prospects to be further developed.

2. Methodology

2.1. Overview of the approach

The first step for developing the multi-criteria approach to assess the suitability of potential water sources for H_2 production via water electrolysis, combining quantitative and qualitative criteria, was to identify all potential water sources that can input the electrolyser, all the required steps to ensure water supply and how each of these water supply steps (abstraction, transport, treatment, storage) can be translated into a water supply cost (Fig. 1).

As in Fig. 1, nine potential water sources were identified, namely: seawater, estuaries (with different saline concentration from seawater), surface water (aggregating creeks, streams, rivers and lakes), ground water, rainwater, water from the public grid, urban wastewater, industrial wastewater and from cooling towers. Ensuring water supply into the electrolysers involves the following steps: water abstraction/collection, transport to H_2 production plant, water storage, water treatment up to the level required by electrolyser technical specifications, and disposal of residues from water treatment. These water supply steps are not listed sequentially and, in fact, depending on the specific water source site being considered, can be ordered differently (with for example water storage being made before or after water treatment, or both). Each of these steps has associated costs, as well as water losses, which were estimated and are presented in the following sections. We have considered that for some of the sources (namely water from public grid) an infrastructure is already in place that allows delivering water up to the electrolyser. For almost all the other water sources it is necessary to build a whole infrastructure, or parts of it, to abstract, transport, store and treat water. Moreover, each potential water source can be characterised according to the following non-quantitative criteria: reliability of availability, ease of abstraction/collection, existence of concurrent water uses, complexity of transport, complexity of treatment needed, social acceptability and, finally, type of permitting process involved.

The analysis was carried out for the current situation in terms of the present characterization of potential water sources, legal and regulatory framework and existing infrastructures.

Each of the qualitative criteria is detailed further in the following sections.

2.2. Sustainable Value Methodology

The Sustainable Value Methodology was developed by integrating different concepts from distinct subjects such as Value Analysis, ecoefficiency, energy efficiency and cleaner production. Ecoefficiency means "doing more with less", while Value Analysis means satisfying needs using fewer resources. So, the complementarity between those two subjects is clear. Using tools from Value Management (VM), such as Value Analysis and Cleaner Production from ecoefficiency, and profiting from the synergies between them, enabled to develop the SV concept,

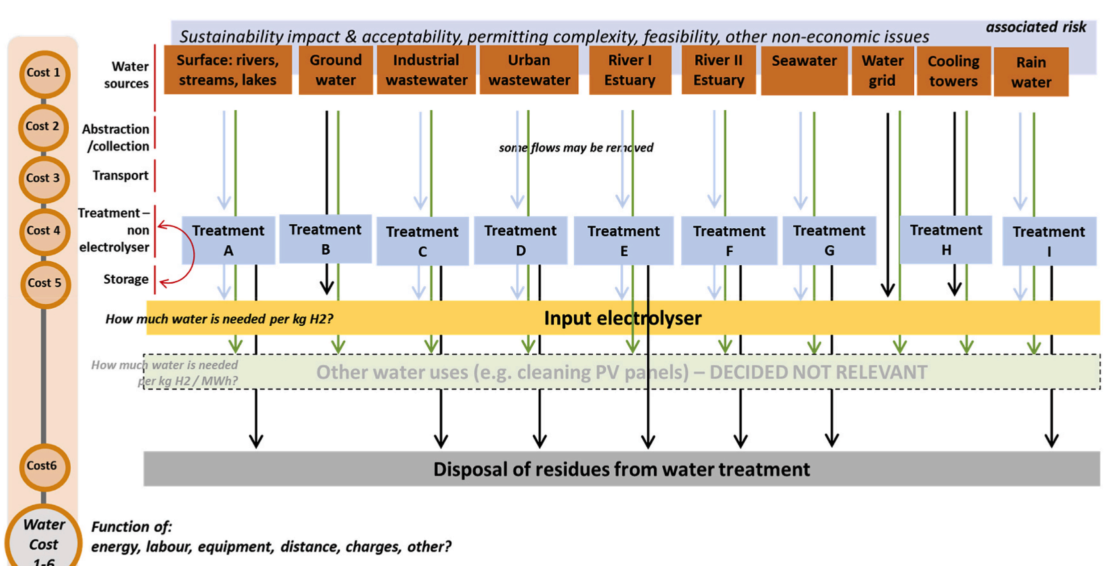

Fig. 1. Overview of considered approach for assessing potential water sources for H_2 production via water electrolysis.

Table 1
Overview of water treatment needs per potential water source.

Water source	Main water pollutants and treatment parameters	Considerations on water quality	Unitary Treatment Operations Needed
Surface: rivers, streams, lakes	Suspended solids (TSS), BOD_5	Good quality water, flow rate abundant in the closest river, capability to provide water all year round. In Site A the water stream can be dry in summertime	Fine screening, coagulation/ filtration + reverse osmosis pumping with moderate elevation (20 m) distance to evaluate (assumed here 10 km)
Groundwater	Dissolved solids	Generally, of very good quality due to soil filtration. May contain specific ions (carbonates or metals as iron/manganese). Solution feasible at Site A, due to the good aquifers, needing permit. In Site B the availability of ground water must be checked.	Depend on composition. May be necessary to remove some ions which can be also ensured via Reverse Osmosis. Authorisation requires payment of a yearly fee of about 750 €. Pumping costs may be high (assuming NPSH - Net Positive Suction Head of 200m)
Treated Industrial wastewater	Depends on the industry, suspended solids, BOD_5, COD, toxicity	Depends on the industry, can have organic pollution or not. May be problematic to ensure flow rate throughout the whole year.	Tertiary treatment (coagulation + filtration) + reverse osmosis
Urban wastewater	Suspended solids, BOD_5, COD, toxicity	Usually in Portugal the treatment degree is secondary or secondary with nutrient removal. Thus, additional tertiary pre-treatment (coagulation/ filtration) before reverse osmosis can be necessary	Tertiary treatment (coagulation + filtration) + reverse osmosis
Seawater	Salinity 36–37‰	Seawater is used when no other sources are accessible. Contains high dissolved solids (chloride and sulphate) availability is great but the distance can be forbidding.	Fine screening + Membrane for desalination (reverse osmosis). Pumping elevation and distance may be high.
Estuary	Salinity 33–34‰ Algae, suspended solids	Estuarine water has high salinity, algae e variable composition. The uptake can be complicated (more costly) due to the tide level fluctuations.	Fine screening + Membrane for desalination (reverse osmosis) Elevation and distance may be high.
Water supply network	Dissolved solids	Good quality water. Depends on a contract with the company.	Reverse osmosis. The amount requested may be too high and not available
Cooling towers	Dissolved and suspended solids	May be difficult or costly to collect and condensate the water vapours. If these waters are of good quality most probably, they are condensed and reused in the respective industry. The amount available must be checked	Collect the water and condensate. Reverse osmosis
Rainwater	Some dissolved solids, BOD_5, TSS	Rainwater is usually of good quality bringing some compounds due to gas absorption when falling in the air or due to drainage in the soil. The use of this water requires large storage for ensuring water availability throughout the whole year. It eventually could be combined with agriculture activities (in Site B) to reduce costs.	Fine filtration + reverse osmosis. Requires storage and pumping

Notes: BOD_5 stands for Biochemical Oxygen Demand and is used as a surrogate of the degree of organic pollution of water. COD stands for Chemical Oxygen Demand and is used as a proxy for organic matter in water. TSS stands for Total Suspended Solids.

which integrates the three aspects of sustainability (economic, environmental and social) in the Sustainable Value concept (Henriques et al., 2008; Henriques and Catarino, 2015, 2017).

In the last centuries, the business world has been using the concept of Value with different meanings and scopes and more recently several authors differently introduced the concept of Sustainable Value (see Hahn et al., 2007; Kuosmanen and Kuosmanen, 2009).The SV approach, as considered in this paper, is based on the Value definition in Value Management (European Standard EN 1325, 2014), in which “Value” is the relationship between the satisfaction of needs and the resources used to achieve it and explicitly takes into account the three dimensions of sustainability (equation (2)).

$$Sustainable\ Value\ (SV)\ \alpha\ \frac{Performance}{Resources\ (costs)} \tag{2}$$

According to EN 1325–1:1996 standard, this concept of Value is relative, and may be viewed differently by different parties in differing situations. The symbol α in the equation means that the relationship between needs and resources is only a representation and that trade-offs from one against the other can result in the most beneficial balance. The optimization is achieved by balancing the amount to which needs are satisfied against the resources utilized. If, in the terms of this relationship, economic, social, and environmental aspects are considered, in a systematic and objective way, then we are talking about what we have defined as Sustainable Value. VM methods and tools, namely Value Analysis (VA), considered mainly economic aspects in Value quantification, but nowadays to lead towards creation of Sustainable Value, VM methods must also integrate environmental and social aspects. Improved value may be achieved by changing the way in which processes are carried out so that the same outcome is obtained or improved, for example, using fewer resources. “Value” is therefore an indicator that, by considering different aspects as referred above, enables to

Table 2
Relevant unitary water treatment options, energy needs, water losses and waste production from water treatment.

Unitary treatment operation	Description	Energy Needs	Water losses	Waste production
Fine screening	Used to retain solids found in the influent (waste) water to the treatment plant. The main purpose of screening is to remove solid materials. Typical opening sizes are of 1.5–6 mm [a]	*0.5-1.5* Wh/m^3 [b]	negligible	Wet sludge
Coagulation-flocculation & filtration	common water treatment for removing particulates and turbidity from water. A coagulant (most commonly iron or aluminium salts with polymeric materials) is added and mixed with the water to be treated. The coagulant adsorbs onto the impurities and forms larger particles (flocs) which are then removed by filtration (this could be with sand, anthracite coal, or both)[c] (Plappally and Lienhard V, 2012).	$<$*0.05* kWh/m^3	negligible	Wet sludge
Ultrafiltration	is an alternative that uses membranes and is more cost effective with more compact design, lower maintenance requirements, lower waste production and cheaper operating costs (Plappally and Lienhard V, 2012).	*0.025-0.1* kWh/m^3	10%	7% of water input sludge type saline concentrate
Reverse osmosis	a partially permeable membrane is used to remove ions, unwanted molecules, and larger particles from water. An applied pressure is used to overcome osmotic pressure which is driven by chemical potential differences of the solvent. A large plant processes at least 10 000 m^3/day.	*3-6* kWh/m^3 [d]	15–25% groundwater 20–30% wastewater 35–40% seawater	14% groundwater 21% wastewater Brine concentrate - high-saline solution (dissolved solids)

[a] EPA - Wastewater Technology Fact Sheet - Screening and Grit Removal https://www3.epa.gov/npdes/pubs/final_sgrit_removal.pdf.
[b] HUBER https://www.huber.de/solutions/energy-efficiency/wastewater-collection-and-treatment/mechanical-pre-treatment.html.
[c] Turner et al. (2019). Potential Alternative Reuse Pathways for Water Treatment Residuals: Remaining Barriers and Questions—a Review. Water, Air, & Soil Pollution, 230(9), 227. https://doi.org/10.1007/s11270-019-4272-0.
[d] Kim, J., Park, K., Yang, D. R., & Hong, S. (2019). A comprehensive review of energy consumption of seawater reverse osmosis desalination plants. Applied Energy, 254, 113652. https://doi.org/10.1016/j.apenergy.2019.113652.

compare the initial solution with improvement proposals, resulting from the methodology application, and finally to choose the one with a higher value, within the scenario considered during the study, or just to be used for a comparative purpose.

The SV methodology was used in this work, with some of the methodological steps applied in a succinct way, to estimate Value, namely global inventory, and functional analysis. The function to be satisfied is providing water for electrolysis, while performance is characterized with technical, environmental and social criteria and quantified by performance levels. Associated costs (CAPEX and OPEX) were used to quantify the denominator resources as in equation (2).

2.3. Potential water sources and treatment needs

High purity water is necessary as an input to the electrolysers, since impurities can affect the reaction by depositing in the electrolysers, on the electrode surfaces and/or in the membrane (Zeng and Zhang, 2010). Water quality requirements vary across electrolyser manufactures, but typically deionised water is necessary, such as water Type I or II, as defined by the American Society for Testing and Materials (ASTM)[1] or slightly less demanding with a conductivity of <5 μS/cm. Most electrolysers in the market thus include a deionisation step as part of the equipment.

For the purpose of this study, values of 10.00–11.11 l per kg produced H_2 are considered as required to input the electrolyser solely for the reaction (for PEM and Alkaline electrolysers, respectively). The values are based on information publicly available from five electrolyser suppliers (Kraftanlagen München GmbH, Thyssenkrupp Uhde Chlorine Engineers GmbH, Hydrogenics, GreenHydrogen.dk and H-Tec Systems GmbH).

Additionally, if 10% water losses are considered (due to evaporation, leaks, etc.) and 25% more water is assumed to be needed for cleaning the equipment, then the water consumption to be input into the electrolyser is estimated to be of 13.50–15.00 L water/kg H_2. Table 2 summarises "average" unitary water needs considered in this section, as well as corresponding daily and annual estimates, which naturally depend on the capacity of electrolyser, its load and technology type. Note that for

[1] Type I ASTM water is known as Ultrapure and has a resistivity of >18 MΩ-cm, a conductivity of <0.056 μS/cm and <50 ppb of Total Organic Carbon (TOC). Type II ASTM water has a resistivity of >1 MΩ-cm, a conductivity of <1 μS/cm and <50 ppb of TOC. www.astm.org.

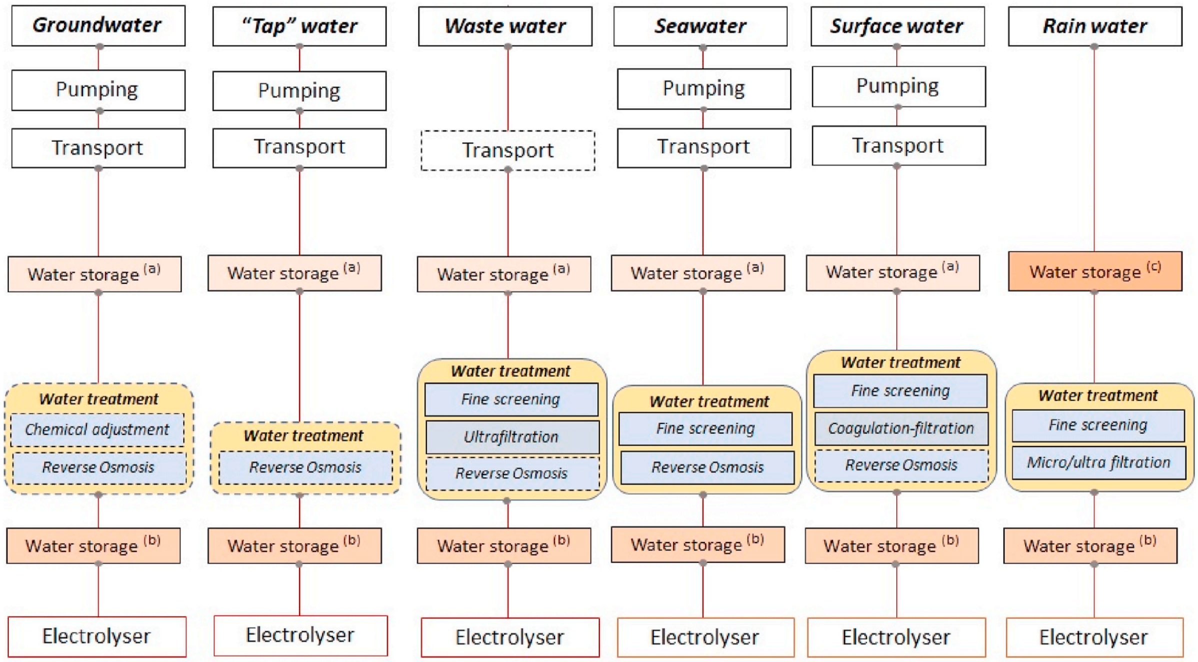

Fig. 2. Water abstraction/collection supply steps per potential source including necessary treatment. Dotted line represents optional processes depending on water quality of the specific source. (a) Water storage in small tank 100 m^3 300 €/m^3; (b) Water storage in tank of 1000 m^3 200€/m^3; (c) Water storage in lagoon of 90000 m^3 circa 3–5 m height (6 months storage) 40 €/m.^{3}.

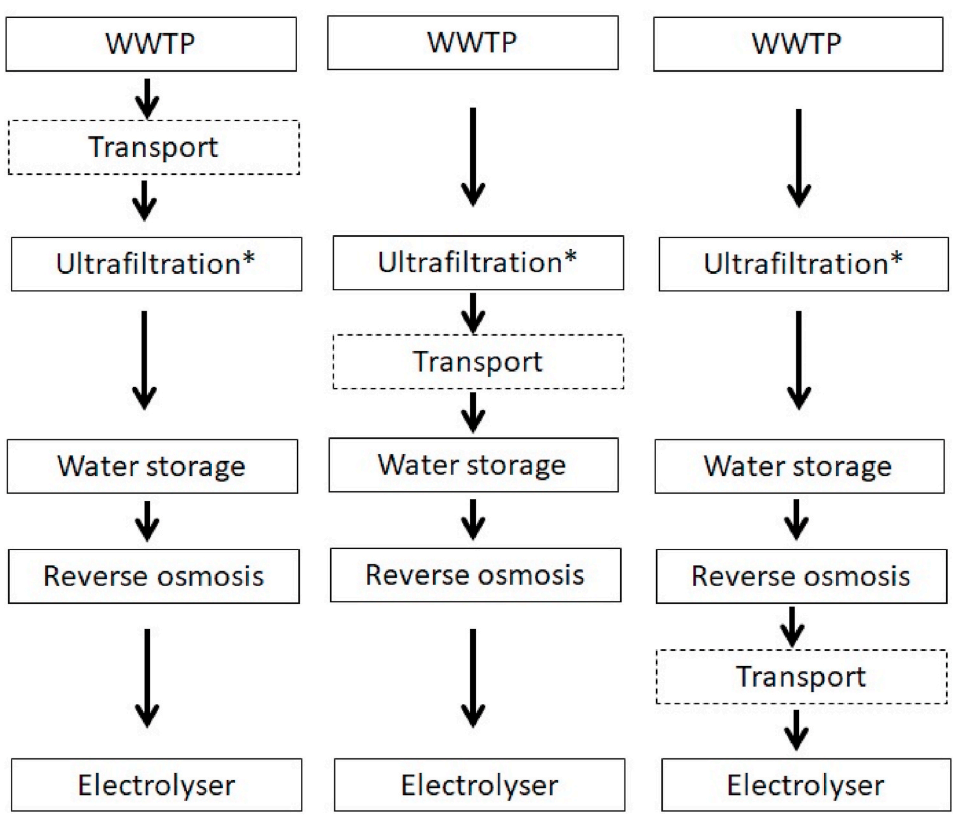

Fig. 3. Possible configurations for location of treatment operations. (*) can be replaced by chemical treatment depending on water quality parameters for each specific water source.

this paper we have assumed that for a 60 MW electrolyser circa 389-386 m^3 water are needed per day (for an optimistic continuous operation over a 24-h period), corresponding to circa 25,920-28,560 kg H_2 produced. Assuming an electrolyser load of 60% of the year, annually this would translate in circa 85,147-84,438 m^3 water and circa 5,677-6,255 t of produced H_2. The range in values reflects estimates for alkaline and PEM electrolysers, respectively. These values do not consider losses for supplying water up to the electrolyser, namely those occurring during abstraction/collection, transport, and treatment.

Fig. 2 shows the processes required for water supply up to the electrolyser, from water abstraction/collection to water use, for each of the potential water sources. In this figure, the dotted lines identify the processes that may not be necessary depending on the specific characteristics of the water source to be used (i.e. groundwater and tap water characteristics vary even for the same country).

Table 1 presents an overview of the potential water sources for the two sites, as well as the considered needed unitary water treatment options vis-à-vis the required by the electrolysis technology.

Table 2 summarises the main water treatment operations that may be required with indication of their respective energy needs, water losses and waste production. It is assumed that the de-ionisation treatment step is part of the electrolyser “black-box” and thus it is not detailed here.

The sum of total water needs for the electrolyser are of circa 85% on top of the water needs for the stoichiometry of the electrolysis reaction. This value includes 5% water losses in abstraction/collection, 10% losses in transport, 15–40% losses depending on the type of water treatment, 10% losses due to evaporations/leaks at the electrolyser input, as well as 25% more water that is assumed to be needed for cleaning and finally an additional 10% water for minimising shortage risks.

The configuration of water treatment operations can vary depending on who is responsible for the different treatment steps. There are several possible configurations regarding which of the treatment steps can take place within/outside the wastewater treatment plant (WWTP) site, which depends on business model and interest of water treatment companies as outlined in Fig. 3.

Of all the identified options for water sources, special attention has been paid to the reuse of wastewater from WWTP due to current concerns with water scarcity in Portugal and to the existing policies on wastewater reuse (Portuguese Decree-Law 119/2019 of August 21st). The current goal is set for the reuse of 10% of each WWTP output (before 2025), which is a difficult goal to meet, as WWTP flows are very high. The daily volumes required by H_2 production via electrolysis are much smaller than the daily output of most WWTP in urban areas (for example, in the site A area WWTPs have an output of circa 2,000 m^3/day with a small WWTP treating circa 400 m^3/day). In rural areas (as in site B), smaller WWTP units exist with flows below 400 m^3/day. Because of these volumes there seems to be no major problems with reliability of wastewater supply, although in any case a selection of most adequate WWTP sources should be done.

So far, wastewater reuse for H_2 production via water electrolysis has not yet been identified as a possibility in the regulation, but it seems an interesting option. Nonetheless, treating wastewater up to electrolyser quality requirements is not part of the “core business” of WWTP companies. Volumes of 600-400 m^3/day, as needed for electrolysis, are substantially higher than what is currently reused and thus, a cheaper price for water supply could probably be foreseen within a long-term contract with H_2 producers. It is not entirely clear who should bear the additional wastewater treatment costs – this would depend on the policy makers and existence of incentives for using wastewater for H_2 production.

2.4. Qualitative performance of water sources for electrolysis

Each of the potential water sources (Table 1) was qualitatively assessed for each site adopting a functional value approach where the function is to supply water for hydrogen production. For this, the following criteria were identified:

a) Short-term reliability of availability (effect of weather factors on water source as droughts);
b) Long-term reliability of availability which can affect authorisation on water use by environmental authorities (perceived future impact of climate change on water source);
c) Reliability of supply (possibility for non-weather-related intermittencies, such as maintenance pauses, that could damage ensuring continuity of water supply);
d) Competition with other uses (at water abstraction/collection level);

Table 3
Criteria for Sustainable Value analysis (qualitative assessment) of water sources.

Criteria	Weight	Performance level			
		1	2	3	4
Reliability of availability (short time: weather)	1	Highly dependent on weather factors (water source not available throughout the whole year)	Medium dependent on weather factors (annual water source flow can vary and can be lower than needed by electrolyser)	Low dependence on weather factors (annual water source flow can vary but will not be lower than needed by electrolyser)	Not dependent on weather
Reliability of availability (climatic effect)	1	High climate change impact expected	Medium climate change impact expected	Low climate change impact expected	No climate change impact expected
Reliability of availability (continuity of supply)	1	Strong possibility of interruptions in supply	Medium possibility of interruptions in supply	Light possibility of interruptions in supply	No interruptions in supply
Competition with other uses [water collection]	1	Competition with human water supply and/or agricultural uses	Competition with agricultural uses	Competition with other uses	Without expected competition
Complexity of abstraction/ collection	1	Very difficult and with potential unexpected complications	Requires permit and payment of charges	Requires negotiations and eventually payment of charge/tariff	Freely accessible
Transport distance	1	Long distance	Medium	Short distance	*In situ*
Treatment needed	1	Very high [fine screening (or microfiltration) + coagulation/ filtration (or ultrafiltration) and reverse osmosis]	High [microfiltration (or ultrafiltration)]	Medium [fine filtration (or fine screening) and ultrafiltration]	Light [fine filtration (or fine screening) and ultrafiltration]
Social acceptance	1	Difficult acceptance due to the possibility of exhaustion of the resource	Weak acceptance due to the possibility of rejection of brines in the ecosystem	Possibly difficult acceptance due to impact on water availability	No anticipated problems with acceptancy
Complexity of permitting process	1	High complexity	Medium complexity	Low complexity	Permit not necessary

e) Complexity of abstraction/collection (number of involved entities and existence of previous experience with this type of water for a similar use);
f) Transport distance from water source to H_2 production plant site;
g) Degree of water treatment needed up to electrolyser input requirements;
h) Social acceptance;
i) Complexity of the permitting process required (number of involved entities and existence of previous experience with this type of water for a similar use, including transport).

The performance of each water source can be classified according to the identified criteria using a four-level scale where 1 is worse performance and 4 is best performance as in Table 3. At the current stage, all criteria have the same weight of 1, since it was assumed that all criteria have same weight.

The assessment of performance of the water sources according to each criterion, relied on literature review and on interviews with the following sources of: (i) Portuguese water policies and regulations on strategic water uses, water management plans, and permitting processes; (ii) Portuguese environmental authorities in charge of water (re) use permitting (i.e. APA the Portuguese Environment Agency); (iii) (two) waste water treatment companies; and (iv) weather and climate change information from IPMA, the Portuguese Meteorological Institute. Thus, there is some degree of subjectivity, but nonetheless the assessment is based on transparent and objective information for the two sites and all potential water sources.

2.5. Water costs estimation

All costs (abstraction/collection, transport and additional treatment needs, as well as permitting process) must be quantified to estimate the resources associated for the Sustainable Value Indicator calculation. For the preliminary assessment of the current cost of water, all identified water sources for Site A and Site B were considered.

The water costs (€ per cubic meter of processed water) were disaggregated into capital costs (CAPEX) for abstraction/collection, water transport, water treatment, storage and disposal of water treatment waste), and operations costs (OPEX), namely for abstraction/collection, for disposal of water treatment waste, for electricity (pumping, transport, treatment, and other), for water charges and finally for labour. Note that for transport costs, the actual distance between the water source and the H_2 plant site must be considered. Two transport options were assessed, trucks and pipeline.

A water flow of ca. 700 m^3/day (255 500 m^3/year), including water losses, and a plant operation time of 365 days/year (8760 h) was used as a base case for calculation, regardless of the plant location. This value departs from the previously mentioned 389-386 m^3 water per day plus water losses with abstraction/collection, transport and treatment (that is, 85% more). For both CAPEX and OPEX cost components, some assumptions were considered and are briefly summarized in the Annex 1.

3. Results and discussion

This section presents the results obtained for assessing the potential water sources suitability for two potential H_2 production plant sites in Portugal (A and B) to supply water to electrolysis processes regarding the water sources performance on the mentioned qualitative criteria, the estimated water supply costs and a combination of both (the Sustainable Value Indicator estimated for each water source).

3.1. Water sources performance on qualitative criteria

The performance of potential water sources was evaluated according to the qualitative criteria and corresponding level of performance for both site A and site B. When the volume of the water source was considered insufficient for H_2 production via electrolysis, it was considered that the viability of the source was of special concern (see for Site A, columns: industrial wastewater, cooling towers and rainwater; and for Site B, columns: industrial wastewater, treated urban wastewater and rainwater). The results of the qualitative criteria are shown in Table 4, in which the grading (1–4 points) follows the criteria presented in Table 3.

The best qualitative water source performance was obtained for "tap" water from the water grid, followed by treated urban wastewater for the two sites. This is followed by industrial wastewater, rainwater, and water from cooling towers, for site A, and for site B by industrial wastewater, surface waters and rainwater. The water options with lower performance values for site A are surface waters, which includes estuary, and ground water. For site B the worst performing option is groundwater.

Portuguese regulatory entities in charge with permitting water management supply make a fine screening of the potential water uses across different sources, considering the various factors involved in the process of supplying water, and considering needs for specific water reserves to manage future risks of supply considering available water scarcity forecasts. This is herein accounted for and contributes to the comparative advantage of the water grid source in this analysis. Note that the better performance of tap water reflects the current situation in Portugal, where, both in site A and site B, there is no risk of supply of both water grids. This can change for other sites and for the future, due to competition among water uses and due to increased water scarcity (as mentioned by Mehmeti et al., 2018).

The good performance of **urban wastewater** as a source of water for electrolysis is caused not just because there is a good social acceptance for wastewater reuse, but also because: (i) this source does not compete with other water uses and (ii) its availability is less vulnerable to weather effects and climate change impacts. Because site A is in a large urban area, a continuous supply is ensured for this site, on the contrary of site B, located within a rural area with a small population.

For the case of **industrial wastewater**, there are concerns with reliability of supply since this source could be affected by both weather and climate change impacts. Moreover, agri-food industries also contribute with effluents and their activity is seasonal and can be highly affected both by weather and climate change. Furthermore, industrial wastewater can carry many pollutants, some of them needing different and specific treatments prior usage for electrolysis. The difficulty of abstraction/collection is higher in site A since there are many factories with different characteristics, while in site B the few industrial facilities are all within the same activity sector (agri-food). Within the industrial sector, water from the **cooling towers** appears as a candidate source. Potentially, this solution may have problems related with water supply since this source is strongly dependent on variable weather conditions (as cold spells), impact of climate change (temperature increase) and continuity of supply as the operation of cooling towers depends on the place of industrial operation which could be affected with maintenance stops, changes in production or other. Furthermore, there is a substantial difficulty for the water abstraction, leading to a bad performance of this water source.

Surface waters (rivers, streams, lakes) and **groundwater** have lower levels of overall performance, especially groundwater, because they provide water for other concurrent water uses, especially water for human consumption (especially in site A) and agriculture. Using these water sources requires a complex permitting process and has a potential rather low social acceptance, since these (especially groundwater) are perceived as strategic reservoirs allowing to cope with future water shortages. The water reliability of availability in what concerns effects of weather conditions, climate change impacts and continuity of supply is relatively low, especially for site A located in a dryer region of Portugal. The same concerns with reliability of availability apply to **estuary waters**, which are of very high relevance for protecting wildlife and ecosystems and were thus considered with a bad performance for

Table 4
Performance of water sources according to qualitative assessment of selected value analysis criteria.

Criteria/water source	Site A									Site B					
	Surface: rivers, streams, lakes	Groundwater	Industrial wastewater	Treated urban wastewater	Seawater	Estuary	Water grid	Cooling towers	Rainwater	Surface: rivers, streams, lakes	Groundwater	Industrial wastewater	Treated urban wastewater	Water grid	Rainwater
Reliability of availability (short time: weather)	1	2	2	4	4	2	4	1	1	3	2	2	4	4	1
Reliability of availability (climatic effect)	1	2	3	4	3	1	4	2	1	2	2	3	4	4	1
Reliability of availability (continuity of supply)	2	2	1	4	3	2	4	1	1	3	2	1	2	4	1
Competition with other uses [water collection]	1	1	4	4	4	3	4	4	4	1	1	4	4	4	4
Complexity of abstraction/ collection	2	2	2	3	1	1	4	1	1	2	2	3	3	4	1
Transport distance	2	3	2	2	1	1	4	2	4	3	3	2	2	4	4
Treatment needed	1	2	1	3	1	1	4	3	3	3	2	1	3	4	3
Social acceptance	2	1	4	4	2	2	4	4	4	4	1	4	4	4	4
Complexity of permitting process	2	1	3	3	1	1	4	3	3	2	1	3	3	4	3
Total points	**14**	**16**	**22**	**31**	**20**	**14**	**36**	**21**	**22**	**23**	**16**	**23**	**29**	**36**	**22**
Total classification (%)	**39**	**44**	**61**	**86**	**56**	**39**	**100**	**58**	**61**	**63**	**44**	**64**	**81**	**100**	**61**

Table 5
Water supply costs with and without reverse osmosis (€/m^3).

Water source	*Assuming reverse osmosis only for sea/estuary*				*Assuming reverse osmosis for all sources where applicable (except rainwater)*			
	Site A		Site B		Site A		Site B	
	CAPEX	OPEX	CAPEX	OPEX	CAPEX	OPEX	CAPEX	OPEX
River/creeks	0.577	1.553	1.674	1.570	0.856	1.753	1.953	1.770
Groundwater	1.769	1.615	1.769	1.632	1.908	1.799	1.908	1.816
Ind. WW	1.544	1.585	2.702	1.604	1.823	1.785	2.981	1.803
Urban WW	1.727	1.757	1.971	1.604	2.006	1.785	2.250	1.803
River	-	–	1.419	1.560	–	–	1.670	1.755
Estuary 1	1.687	1.746	–	–	1.687	1.746	–	–
Estuary 2	2.113	1.748	–	–	2.113	1.748	–	–
Seawater	4.648	4.183	–	–	4.648	4.183	–	–
Water grid	1.574	1.715	1.574	1.347	1.825	1.910	1.825	1.543
Cooling towers	1.391	1.520	–	–	1.642	1.716	–	–
Rainwater	2.793	0.440	2.793	0.459	2.793	0.440	2.793	0.459

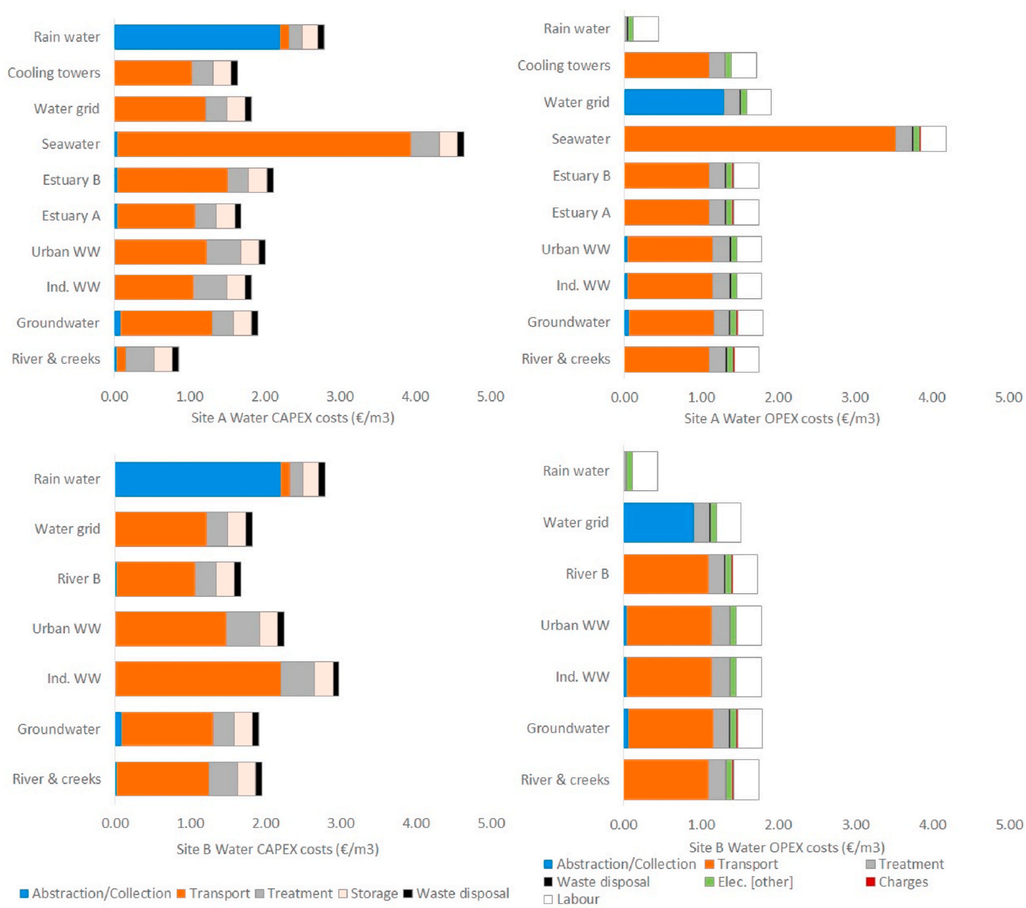

Fig. 4. CAPEX (left) and OPEX (right) water supply cost estimates in €/m^3 for sites A (top) and B (bottom).

competing water uses. Estuary waters usage also entails a very complex permitting process due to the many organisations involved.

Seawater has a good performance in the three criteria related with reliability of availability but is more than 32 km away from site A. Its abstraction and collection will be difficult due to terrain characteristics and it requires a more complex treatment to remove salts before use in hydrogen production. Its permitting process is highly complex with many entities involved in coastal zone planning.

Rainwater has a very good social acceptance, its use for electrolysis is not competing with other water uses, and if collected in site, it does not require water transport. However, it has a low reliability of availability, as it is highly dependent of precipitation very affected by both weather conditions and climate change leading to a problem of continuity of supply. A similar qualitative assessment of rainwater use was made by (Nápoles-Rivera et al., 2013).

It should be noted that the results obtained in the qualitative analysis have a degree of subjectivity and reflect the current situation and the assumption that all criteria have the same relative importance (weight). Moreover, they are location specific, for both Site A and Site B and could naturally vary for other sites. This is in line with what is mentioned by (Lee et al., 2019), since the impacts of water consumption are location specific due to different freshwater supply and demand balances in different regions.

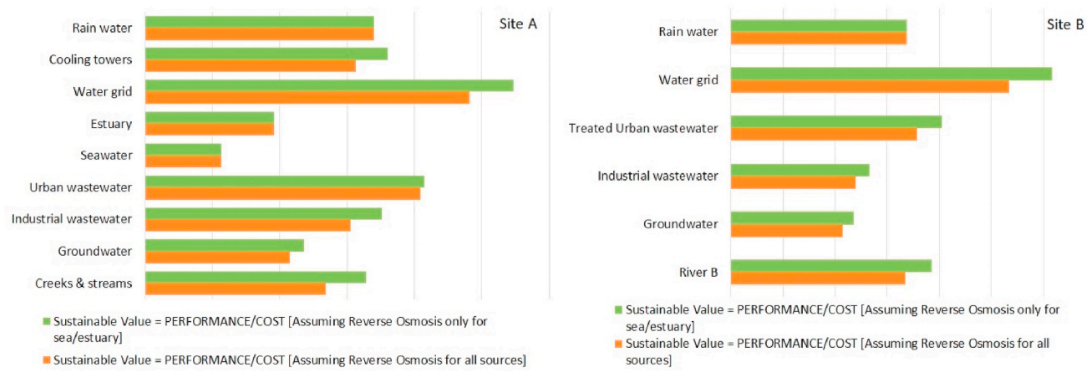

Fig. 5. Overview of "Sustainable Value Indicator" for all potential water sources for site A (left) and B (right).

3.2. Water sources supply costs

Table 5 shows the estimated potential costs for the various water supply cost components, for 700 m^3/day of processed water, assuming reverse osmosis is needed for all sources (except rainwater). The values shown in Table 5, represent the worst-case scenario in terms of very high degree of water purity to input the electrolyser. Complementarily, an alternative cost estimate was made where reverse osmosis was considered only for sea and estuary water sources, representing a situation where water quality requirements for electrolyser input are slightly less demanding (Fig. 4, see also Annex 2).

The CAPEX and OPEX cost estimates obtained for all potential water sources for sites A and B in what concerns abstraction/collection, transport, treatment, disposal of waste from water treatment. OPEX costs include also waste disposal costs, electricity costs for water treatment operation and for pumping for water transport, water charges and labour costs.

The effect of the distance between water sources and site very significantly affects CAPEX and OPEX for both sites, especially in the case of seawater (for site A) where the transport (and treatment) needs are higher. The importance played by water transport costs across overall water supply costs is recognized by other authors, namely by (Gude, 2016) that refers that up to 60% of the water supply costs are due to water transport (for desalinated water supply). Abstraction/collection costs are particularly relevant for rainwater's CAPEX, as large water storage facilities (lagoon) are built, as well as for the OPEX of the water grid source, since water is bought from the supplier.

Regarding other components of the CAPEX estimate, clearly storage, treatment, and waste disposal have a less importance in total costs, especially for treatment costs for sources water grid, river and cooling towers, whose water quality is better and thus requires fewer adjustments.

The OPEX labour costs are almost constant for the different alternatives, and mainly determined by the treatment needs. Energy needs for treatment, waste disposal, transport and other activities are also not negligible components in OPEX for both sites.

3.3. Sustainable value of the potential water sources

The Sustainable Water Value Indicator is calculated by the ratio of the qualitative performance and the assessed costs. By combining these costs with the qualitative index, previously presented (Table 4), it is possible to obtain a proxy water value as in Fig. 5. This "Sustainable Water Value Indicator" combines water costs (with and without reverse osmosis) with the qualitative index for the two studied sites, resulting in an index combining qualitative performance (from 0 to 100) and the estimated cost (in €/m^3).

Therefore, the most suitable water sources are presented in Fig. 5. According to the SV methodology approach, currently water from the water grid is the best option for both studied sites. This is mainly because the entity responsible for water grid supply has especially favourable water supply charges (which are the water prices charged to each consumer) and water quality levels for industrial uses (as H_2 production via electrolysis). For other sites in Portugal, namely in the south of the country where grid water has already some dissolved salts and is currently a scarce result, this water source would have a lower performance. Near urban areas, treated urban wastewater is another potentially adequate source of water for H_2 production via electrolysis, while in rural locations the second-best water source is surface water from a nearby river, since treated urban wastewater may not guarantee the amount of water required for electrolysis.

Among all the assessed potential water sources, seawater (only relevant for site A) is found to be the least suited water source, due to the distance from the coast to the site and the complexity of legislative and techno-economic issues. However, seawater could rank higher in the Sustainable Value Indicator for electrolyser sites located closer to the seacoast, if this option would imply lower transport needs that could compensate administrative constraints and water treatment costs. As Portugal has a wide Atlantic coast, environmental and natural constraints associated with water shortages are substantially less important when considering the use of seawater.

4. Conclusions and prospects

Green H_2 is currently believed to be one of the essential vectors for the transition to a decarbonised economy, even though several required steps for the implementation of this vision are still being developed. This paper contributes to this end by proposing a framework for a comprehensive analysis of different potential water sources when it comes to the selection of alternative H_2 production plant sites via electrolysis of water. This is herein exemplified with the application to two concrete cases in the Portuguese territory, a semi-urban location near the seacoast (site A) and a rural location distant from the sea (site B). The approach provides elements to support decision-making regarding most suitable water inputs for H_2 production from water electrolysis, namely: quality and reliability of water sources, treatment needs, complexity of the permitting process and associated costs.

A novel approach for assessing water sources was implemented calculating a Sustainable Value Indicator which acted as an aggregator of qualitative information regarding the performance of possible sources of water for electrolysis of water and the costs involved, leading to differentiated values for the two studied potential electrolysers' locations. All identified potential water sources were studied, with environmental and social criteria addressed in a qualitative way and with an estimate of potential costs leading to an integrative indicator showing which is the most adequate water sources for the two cases. The results have shown that, currently, given the high levels of water purity requirements and the distance between the water origin and its final use for H_2 production, the preferred available option, in both cases, is the public grid water, which has lower risk of supply, lower supply costs and does not require complex permitting processes. However, the authors acknowledge that there is a degree of subjectivity in the qualitative analysis, even though the qualitative assessment followed a structured and rigorous methodology.

Because the Sustainable Water Value is a relation of performance with associated resources, this indicator could be improved by an increase in performance or by an associated reduction in resources use, or both. The results of each of the case studies are only valid for the respective circumstances here analysed, showing the hierarchy of values for the present moment and having in mind that any Sustainable Value Indicator may result differently, depending on the how technical achievements or political decisions occur in time. For example, the higher Sustainable Value of using water from the public grid for H_2 production can change in the medium-term, since public and governmental perception of suitability of such water type use can change with the expected increasingly severe impacts of climate change on water availability. Thus, in the medium term, other sources of water, such as seawater or treated wastewater, can perform differently to what was now obtained. Moreover, the results presented refer to the water needs for one single 60 MW electrolyser. If for a location several 60 MW electrolyser are deployed, the unitary water supply costs could increase, and the qualitative performance of water sources could change since some of the sources could potentially not be able to supply larger amounts and/or there could be competition with other water uses (as well as different performance along the several qualitative performance criteria). Such modifications in the ranking of water sources are not foreseen for a duplication in water volumes, but could occur for higher volumes (e.g. 10 times).

Nonetheless, despite its limitations, this proposed approach enables a clearer communication for decision-making, highlighting all different components that should be considered when selecting water inputs for H_2 production via electrolysis. The approach is relatively straightforward to implement, and it can be tailored and adapted to other contexts, for example by changing the weights of each qualitative criteria, instead of assuming that all are equally relevant.

Future development of this work includes expanding the approach to include more H_2 production sites (for example industrial areas) and/or other H_2 production technologies of different sizes. In methodological terms the presented approach could be improved by using expert elicitation methods to attribute and vary the weights of each qualitative criterion. Other future improvements include complementing the short-term analysis with a prospective analysis for the qualitative criteria to better accommodate climate change impacts on water availability and foreseen regulatory changes (eventually with scenarios).

CRediT authorship contribution statement

Sofia G. Simoes: Conceptualization, Validation, Formal analysis, Writing – original draft, Writing – review & editing, Supervision. **Justina Catarino:** Investigation, Methodology, Writing – original draft, Writing – review & editing. **Ana Picado:** Writing – original draft, Writing – review & editing. **Tiago F. Lopes:** Formal analysis. **Santino di Berardino:** Investigation. **Filipa Amorim:** Formal analysis, Writing – original draft, Writing – review & editing, Data curation. **Francisco Gírio:** Investigation. **C.M. Rangel:** Investigation, Writing – review & editing. **Teresa Ponce de Leão:** Funding acquisition, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jclepro.2021.128124.

Table of Abbreviations

μ_c	Fluid viscosity in Pa·s
A	Water use from public domain
B′ and J	Constants
BOD_5	Biochemical Oxygen Demand
CAPEX	Capital costs
COD	Chemical Oxygen Demand
$C_{pumping}$	Pumping costs
D_i	Internal diameter of the pipe
E	Efficiency of the motor and pumps
EU	European Union
GHG	Greenhouse gas
H_2	Hydrogen
H_2O	Water
H_y	Hours of operation per year
I	Extraction of sand and other inert materials
IPMA	Portuguese Meteorological Institute
K	Cost of electrical energy
MEC	Microbial electrolysis cells
MFC	Microbial fuel cells
O	Occupation of the public domain of the State
O_2	Oxygen
OH	Hydroxide ions
OPEX	Operations costs
PEM	Polymer electrolyte membrane
q_f	Fluid volumetric flow rate
S	Sustainability of urban water services
SOE	Solid oxide electrolysis
SV	Sustainable Value
TOC	Total organic carbon
TSS	Total suspended solids
U	Usage of water
VA	Value Analysis
VM	Value Management
W	Wastewater disposal
WWTP	Wastewater treatment plant
Yr	Year
ρ	Fluid density

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