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# Direct carbon footprint of hydrogen generation via PEM and Alkaline electrolyzers using various electrical energy sources and considering cell characteristics

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## HIGHLIGHTS

- Importance of manufacturing and electrolyte resistance because of high PEM energy consumption sensitivity to cell voltage.
- Predicted emission in 2030 is 5-10 kg CO<sub>2</sub> using PEM/alkaline technology in Italy.
- 18% reduction of national electricity grid CO<sub>2</sub> emission in Australia is predicted. (In 2030 in comparison to 2019)

## ABSTRACT

Hydrogen supplying to industrial users is currently the major hydrogen business worldwide and the demand for hydrogen is almost entirely supplied from fossil fuels. In the last years a widespread interest on hydrogen has grown as energy vector for the decarbonization of multiple sectors, including industry, transport and buildings. Nevertheless, the impact of natural gas and other fossil fuels substitution with hydrogen is highly affected by the mix of different technologies and energy sources applied for hydrogen generation.

The paper aims to investigate current CO<sub>2</sub> emissions related with hydrogen generation in Australia and Italy by means of PEM and alkaline technologies; and to evaluate the potential impact considering cell characteristics variation and 3 scenarios based on energy mix. A sensitivity analysis is performed to identify the critical parameters. Based on experimental data, the energy consumption for hydrogen production using PEM technology is more sensitive to cell voltage compared to current density, which indicates the importance of cell manufacturing and electrolyte resistance. In addition, by performing sensitivity analysis regarding energy sources scenarios it is found that carbon dioxide emission in Australia is more sensitive to renewable energy sources rather than Italy.

## Keywords:

Hydrogen, CO<sub>2</sub>, Electrolysis, Australia, Italy, Renewable energy sources (RES)

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## 1 Introduction

Human population growth and increase in anthropogenic activities have considerably affected overall energy consumption, which is mainly based on fossil fuel sources. Increase in fossil fuel consumption results in more Greenhouse gas (GHG) emissions which cause global warming and climate change. Almost 80% of GHG emissions should be reduced by 2050, in comparison to 1990, to reach the Paris agreement goal, which is limiting the global mean temperature increase to 2°C [1]. Increase in global energy demand, the potential diminishing of fossil fuels in the near future, and fossil fuels' environmental impact led researchers and industries to focus on the transition from fossil fuel sources to low carbon systems and sources of energy. In recent decades, alternative sources of energy generation so-called renewable energies such as solar, wind, and hydropower have considerable contributions to world energy generation. Figure 1 shows the electricity production by various sources in the period of 1985 to 2020. The data are extracted from the BP Statistical Review of World Energy [2]. It can be seen that around 60% of the world's electricity in 2020 was produced by fossil fuels, and this contribution was fluctuating in the range of 60-70% during the mentioned period. However, renewable energies' contribution to the total energy generation of Australia in 2020, according to the Department of Industry, Science, Energy, and Resources, was 24% [3]. While the percentage of renewable energy sources (RES) contribution in Italy in 2019 was 18% [4].

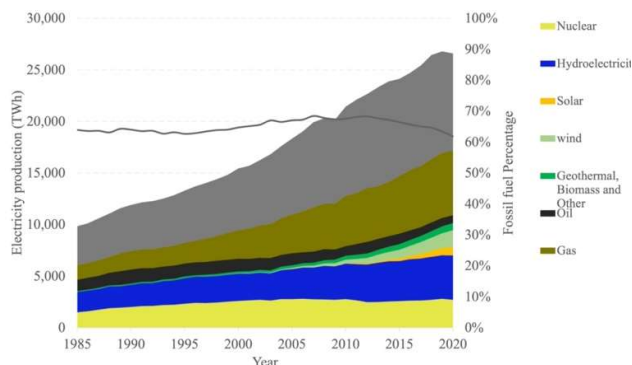


Figure 1 Electricity production by source, World (data from [2]).

RES are intermittent and unpredictable, which causes restriction of contribution in the supply system. To increase the contribution and supply energy demand, it is required to use energy storage systems. There are several challenges for storage systems to be able to supply immediately when it is needed [5]. Hydrogen technology could be a solution to store energy from RES. However, to prove hydrogen technology as a solution to reach net zero emission and an alternative to fossil fuels, various aspects should be assessed, such as hydrogen applications, production, and environmental impact, which are discussed in the following sections. This section describes hydrogen applications, production, cell characteristics and hydrogen yield of PEM and alkaline electrolyzers, energy consumption, and manufacturers to find out the lag of studies which are explained in the scope section. The scope

of this study includes the environmental impact of hydrogen production using PEM and alkaline electrolyser and sensitivity analysis regarding cell characteristics and source of energy which are discussed in section 3 and section 4.

### 1.1 Hydrogen application

Hydrogen can be used as a fuel in internal combustion engines in transport, e.g., hydrogen-fuelled buses, or in fuel cells. It can also be utilized for industrial consumption, such as petroleum refining, metal treating [5], production of ammonia, methanol, pharmaceutical [6], and the food and beverages sector. Power generation, transport sector, and heating in residential are also expected to be the near future applications of hydrogen even if many technical and regulatory gaps are still unsolved [5]. Integration of gas and electricity sectors can be achieved by injection of hydrogen into the natural gas network up to specific values considering legislation in different countries. However, the application in real networks is still hindered due to several challenges such as material degradation, gas leakages check, safety, quality management, and appliance proper and safe performance [7].

One of the main advantages of using hydrogen instead of hydrocarbons is related to the combustion products even if higher combustion temperatures than methane occur requiring special material or combustion control to avoid material degradation. Hydrogen combustion generates large amounts of water and energy, without the release of GHG. Another advantage of the hydrogen industry is related to social impact by creating employment [6].

### 1.2 Hydrogen production

Hydrogen could be considered a source capable of generating direct energy which facilitates energy production [6], although it is not a primary energy source [8]. Hydrogen can be considered a proper zero-emission alternative to fossil fuels as it is the only carbon-free with the highest energy content per kg compared to any known fuel [5].

There are two main categories of hydrogen production regarding the input of hydrogen production systems, conventional and renewable technologies. The conventional category includes the use of fossil fuels and methods of hydrocarbon reforming and pyrolysis. The process could be steam reforming, dry reforming, cracking natural gas, coal gasification, and partial oxidation which are highly energy-consuming processes [5, 6]. The second category covers hydrogen generation using water or biomass. In the case of using water as raw material, it can be split by various methods such as electrolysis, thermolysis, and photo-electrolysis [5]. There are various electrolysis technologies such as Alkaline, PEM, solid oxide electrolysis cells (SOEC), and Anion exchange membrane (AEM). Among these technologies, alkaline and PEM are the most widespread. Currently, 96% of the hydrogen production in the world is based on fossil fuels and the most common hydrogen production technology is the steam methane reforming (SMR) method. SMR is the

cheapest technology for hydrogen production and around 50% of the world's hydrogen is produced by this method [9, 10]. However, Hurtubia et al. [11] stated that the contribution of fossil fuels in 70 Mt of annual hydrogen production is 98%, 75% natural gas or 23% coal, and only 2% is produced by electrolysis. Hydrogen produced through SMR is called grey hydrogen unless its CO<sub>2</sub> emission is captured by carbon capture and storage technologies which results in blue hydrogen. If renewable energy is consumed as the electricity source of hydrogen production, this hydrogen is called green hydrogen. Green hydrogen is the cleanest energy carrier [5].

In terms of emission reduction in hydrogen production, water electrolysis using renewable energy as an energy source offers the most potential [12], however, there are some other methods without GHG emission which are under the early stage of investigation such as microalgae [11].

One of the main challenges in hydrogen production is related to its unavailability in nature in pure form. Hydrogen is only found in compound form. However, low concentrations of the hydrogen molecule in gaseous form can be found in the atmosphere which is not affordable to be captured. An important challenge that has played an essential role over the last two decades is related to policies in investment, market development, and renewable energy-related industries development [9]. Another challenging issue is the cost of hydrogen production. Hydrogen production cost is reported differently in various studies. Kopteva et.al [13] reported that the cost of hydrogen generation approximately ranges from 2 to 5 US dollars per kg. While, in another study, hydrogen production cost from solar thermal, solar PV, nuclear, and wind, in 2010, for electrolysis was reported in the range of 4.15 to 23.27 dollars per kilogram of hydrogen [5, 14]. Considering that 1 kg of hydrogen contains 33.33 kWh primary energy, the mentioned prices will be 0.06 to 0.7 US dollars per kWh which is higher than the price of fossil fuel as an energy source. Janssen et. al [15] projected that the cost of hydrogen production using RES, until 2050, can be less than 2 €/kg in several countries in Europe. Australia aims to reach hydrogen production of under \$2 per kilogram which could be competitive with conventional fuels, although there would be other costs such as compressing, storing, and transporting hydrogen which could cost up to \$2 per kilogram of hydrogen [16]. The prediction of the Australian government for 2030 is A\$2 to A\$4 per kilogram of clean hydrogen [17]. The wide range of hydrogen production costs through electrolysis reflects that the production strongly depends on RES availability.

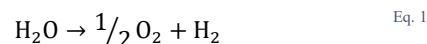
In addition to mentioned issues, it is impossible to blend very high amounts of pure hydrogen into the natural gas network. Only a few countries allow direct injection into the infrastructure, thus, separate distribution infrastructures or suitable hydrogen carriers could be another challenging issue [7].

Thus, suitable methods for affordable clean hydrogen production and efficient distribution network are needed. This study focuses on green hydrogen generation with market-ready technologies, i.e., PEM and alkaline

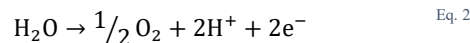
electrolysers, and their operational environmental and GHG impact.

In a PEM electrolyser cell membrane is located at the center of each cell which is the core of the electrolysis cell, membrane material is sulfonated tetrafluoroethylene. The anode and cathode layers are on two sides of the membrane. Iridium and platinum are mostly used as noble metal catalysts in anode and cathode, respectively. The porous transport layer (sometimes called the gas diffusion layer, or current collectors) is the next layer on both sides, commonly titanium is used on the anode side and carbon paper is used on the cathode side. The last layer of each cell on both sides is the bipolar plate, titanium is mostly used as a bipolar plate. Several single cells, considering the desired capacity of the system, could be connected in series, which provide the PEM stack. End plates, bolts, nuts, and sealings are used to assemble cells as a stack [18]. In this study, hydrogen production at the stack level is taken into account.

The overall reaction of water electrolysis is as in Eq. 1, which is an endothermic reaction:



Water is oxidized on the anode side which oxygen is produced while the reduction reaction occurs on the cathode side to produce hydrogen, Eq.2 and Eq.3.



The resulting product of PEM electrolysis could be dry hydrogen with a purity of 99.99% [19] at a pressure of less than 30 bar and a temperature of 323–353 K [20]. The efficiency of the PEM system could be 70 % and the stack energy consumption is 4.2-5.6 kWh/m<sup>3</sup> [20]. Based on Zhao et al. [21] study, considering the electricity generation from a 3 MW wind plant in Denmark and using the ecoinvent database for the emissions, the contribution of electricity consumption to the global warming potential (GWP) index of hydrogen production via the PEM technology is around 90%, which shows the importance of stack operational level investigation.

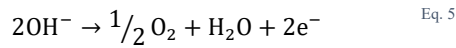
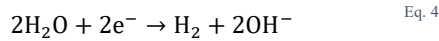
PEM electrolysis plant includes other components to produce pure hydrogen, such as water pump, water purification, ion exchanger, heat exchanger, circulation pump, gas/water separator, demister, and deoxidizer which are not in the scope of this study.

Solid polymer electrolyte is used in the PEM system which leads to eliminating the necessity of circulating aqueous electrolyte and resistance against gas bubbles [21]. The thickness of a PEM cell with high proton conductivity could be around 20–300µm, which is capable of operating at high pressures, above 30 bar. In addition, the operational cost of PEM is smaller in comparison to other electrolysis because it can operate with high energy density, the gases have high purity, and this technology is effective at high voltages [6]. In comparison to alkaline technology, PEM has higher cell efficiency and operates more flexibly regarding load range, which makes this technology more reliable for RES electricity generation [11]. In addition, the

PEM electrolyser can operate with higher current density in comparison to the Alkaline electrolyser [21]. In comparison to SOEC, PEM operates at a lower temperature. In addition, SOEC has some issues in terms of stability and degradation which should be solved before commercialization for large-scale projects [22].

Despite the positive aspects of the PEM electrolyser, it has some drawbacks. The high cost of components such as catalyst materials, system complexity due to high-pressure operation and water purity, low durability, and significant corrosion in systems with high capacity are challenges that profound study is required in future research to find solutions [6, 11].

Alkaline technology is the most mature and oldest method in water electrolysis [23]. The overall reaction of electrolysis in an alkaline electrolyser is the same as PEM electrolyser but the reactions in the cathode and anode are different as follow, equation 4 and 5, respectively [24]:



In general, two configurations of the alkaline cell are available, conventional and zero-gap. In conventional, there is a specific distance between electrodes, while in zero-gap, electrodes are directly pressed to the separator which minimizes ohmic losses in the electrolyte. Various parameters affect the ohmic resistance of the cell such as the ionic conductivity of the separator membrane, the electronic conductivity of the electrode material, the specific conductivity of the electrolyte, and gas bubble effects. The separator can be a ZIRFON product (Agfa) or dense anion exchange membrane, and the most-used type of electrodes are made from nickel. As a result of using nickel as electrodes, there is an overvoltage for reactions which can be diminished by adding catalysts such as iron and molybdenum to anode and cathode reactions, respectively. Potassium hydroxide (KOH, 20-30% at 50-80°C) is mostly used as an electrolyte which is an aqueous solution. Diluted sodium hydroxide can also be used as the electrolyte, although it is cheaper, it has lower conductivity. The purity of hydrogen gas products without additional purification is higher than 99.9 vol.% through alkaline electrolyser while it is between 99.0 to 99.5 vol.% for oxygen. The system performs under 1 to 20 bar pressure and the current density is between 0.05 to 0.7 A.cm<sup>-2</sup> [24]. The operating temperature range is 20-100 °C [25]. However, this range could be up to 150 °C which could be suitable for large-scale hydrogen generation [26]. The efficiency of an alkaline system could be 65-75 % and the stack energy consumption is 4.2-5.9 kWh/m<sup>3</sup> [20]. Based on Zhao et al. [21] study, considering the electricity generation from a 3 MW wind plant in Denmark and using the ecoinvent database for the emissions, the contribution of electricity consumption to the GWP index of hydrogen production via alkaline technology is more than 95%.

Alkaline electrolyser has several advantages such as long-term service life, simple design, relatively low cost (electrodes can be made of inexpensive and abundant materials), limited water purification requirements, and

high reliability in operation. High energy consumption is a challenge in hydrogen production through alkaline electrolyzers which needs improvement [27].

### 1.3 Cell characteristics and hydrogen yield of PEM electrolyser

Studies about PEM electrolysis which included direct or indirect information about cell voltage, current density, and hydrogen yield are represented in Table A.1 and Table A.2 in supplementary file. "Case" term refers to various experimental test conditions in each study.

The range of current density and cell voltage in studies provided in the Table A.1 is 0.5-3 A/cm<sup>2</sup>, and 1.63-2.46 V, respectively. The minimum current density was investigated in Kumar et al. [28], and Millet et al. [29] studies, and the maximum one was assessed by Bareiß et al. [30], Rakousky et al. [31], and Bernt and Gasteiger [32]. The minimum and maximum cell voltage were studied by Kumar et al. [28], and Di Blasi et al. [33], respectively.

In this table power density is the product of cell voltage level and current density. The range of cell efficiency according to the studies provided in Table A.1 is 0.85-6.3. To provide a comparison among studies it is assumed that the experimental units are modular and can be added together to reach 1 MW capacity without any impact on performance. Considering this assumption and power density, the active area for 1 MW in each study is calculated as in Eq. 6:

$$A_A (\text{m}^2) = \text{Capacity}(10^6 \text{W}) / (\text{power density} \left( \frac{\text{W}}{\text{m}^2} \right)) \quad \text{Eq. 6}$$

Where  $A_A$  is the active area (m<sup>2</sup>)

Cell efficiency considering lower heating value,  $\eta_{\text{cell}}$  (LHV), is calculated as follow [30]:

$$\eta_{\text{cell,LHV}} = 1.23 \text{V} / E_{\text{cell}} \quad \text{Eq. 7}$$

Where  $E_{\text{cell}}$  is cell voltage (V).

The range of cell efficiency according to the studies provided in Table A.1 is 0.5-0.75.

Theoretical and experimental energy consumptions for hydrogen production are provided in Table A.1 and Table A.2.

The theoretical hydrogen yield of the cell (l/h) can be calculated by modification of the equation in Atlam and Kolhe [34] study using unit conversion as follow:

$$v_H = v_M \left( \frac{3600 \text{s}}{1 \text{h}} \right) \left( \frac{1}{2F} \right) \quad \text{Eq. 8}$$

Where:

$v_H$  = Theoretical hydrogen yield of cell [l/h];

$v_M$  = one molar volume which can be calculated by ideal gas expression  $v_M = \frac{R(T)}{P}$ ;

$R$  = ideal gas constant 0.08206 [ $\frac{\text{Latm}}{\text{mol.K}}$ ];

$T$  = temperature [K];

$P$  = pressure [atm];



$I$  = current [A] or [C/s], calculated by the product of single cell area and current density;

$F$  = Faraday constant [C/mol], 96,485.332;

Theoretical total hydrogen yield ( $\text{m}^3/\text{h}$ ) is calculated as follow:

$$V_{T,\text{theoretical}} = A_{1\text{MW}} \times \frac{V_H}{\text{cell area}(\text{m}^2)} \times 10^{-3} \quad \text{Eq. 9}$$

Where:

$A_{1\text{MW}}$  = active area for 1MW ( $\text{m}^2$ )

$V_{T,\text{theoretical}}$  = Theoretical total hydrogen yield [ $\text{m}^3/\text{h}$ ];

Theoretical specific energy consumption ( $\text{kWh/kg}$ ) for hydrogen production can be calculated by the following equation, considering that each kg of hydrogen is equal to  $11.1 \text{ Nm}^3$ :

$$E_{c,\text{theoretical}} = (1000 \text{ kW} / V_{T,\text{theoretical}}) \times 11.1 \left(\frac{\text{m}^3}{\text{kg}}\right) \quad \text{Eq. 10}$$

The experimental hydrogen yield of the cell is extracted directly from literature or using the faradaic efficiency and theoretical yield. Experimental total hydrogen yield and experimental specific energy consumption are calculated in the same way as the theoretical one, experimental hydrogen yield of cell is used instead of the theoretical one. Faradaic efficiency is the ratio between the experimental hydrogen yield and the theoretical one. The average theoretical and experimental hydrogen yields in the studies in the Table A.2 are approximately 285 and  $250 \text{ m}^3/\text{h}$ , respectively. The maximum theoretical hydrogen yield is calculated for Millet et al. [29] study,  $323 \text{ m}^3/\text{h}$ , and the maximum experimental was achieved by Di Blasi et al. [33],  $306 \text{ m}^3/\text{h}$ . The range of Faradaic efficiency according to the studies provided in Table A.2 is 83.39-93.81 %.

#### 1.4 Cell characteristics and hydrogen yield of Alkaline electrolyser

Studies including alkaline electrolysis which provided information about electricity consumption for 1 kg hydrogen production and cell efficiency and hydrogen yield are represented in Table A.3. Information about cell voltage and current density provided in these studies is not enough to be shown in the table. The cell efficiency range, referred to LHV, in these studies is 0.5-0.78, and the average experimental hydrogen yield is  $25 \text{ m}^3/\text{h}$ . Since the information on current density is not completely provided in these studies, it is not possible to use eq.8 to calculate the theoretical hydrogen yield.

#### 1.5 Energy consumption

One of the main important concerns regarding hydrogen production is the energy consumption and the source of energy for electricity production. Figure 2 is produced based on the information in Table A.2, using “theoretical specific energy consumption  $\text{kWh/kg}$ ” and “experimental specific energy consumption  $\text{kWh/kg}$  (using Faradaic efficiency or data in articles)” columns, to make a visual comparison of the reviewed literature in terms of energy consumption. Change in Gibbs free energy can be

calculated as the following equation [35], change in Gibbs free energy amount is reported as  $237.22 \text{ kJ/mol}$  by Kumar and Himabindu [22]:

$$\Delta G = \Delta H - T\Delta S \quad \text{Eq. 11}$$

Where:

$\Delta G$  = change in Gibbs free energy,  $\text{kJ/mol}$

$\Delta H$  = change in enthalpy,  $285.83 \text{ kJ/mol}$  [35]

$T$  = temperature in Kelvin

$\Delta S$  = change in entropy  $\text{kJ/mol.K}$

Considering the change of Gibbs free energy in the hydrogen production reaction,  $237.22 \text{ kJ}$  to produce 2 grams of hydrogen, the minimum energy required to produce 1 kilogram of hydrogen is  $32.95 \text{ kWh/kg}$ . This is depicted as the theoretical minimum required energy based on Gibbs free energy in Figure 2 and Figure 3.

To define the theoretical minimum required energy based on enthalpy it is possible to use the change of enthalpy in hydrogen production reaction. The change of enthalpy in this reaction is  $285.83 \text{ kJ}$  to produce 2 grams of hydrogen. Thus, the energy required to produce 1 kilogram of hydrogen is  $39.70 \text{ kWh/kg}$ , which is shown as the theoretical minimum required energy based on enthalpy in Figure 2 and Figure 3.

If the applied voltage to the cell is greater than 1.23 V the required Gibbs free energy is supplied and the thermal energy from the environment helps the water split. A minimum voltage of 1.48 V is necessary to supply the whole reaction enthalpy [30], which is consistent with the voltages shown in Table A.1.

It can be seen in Figure 2 and Figure 3 that all studies' results are in the mentioned range or above it. By comparing these figures, it can be realized that, in general, PEM electrolyzers consume less energy than alkaline electrolyzers to produce 1 kg hydrogen.

#### 1.6 Manufacturers

There are several manufacturers all around the world that produce PEM and alkaline electrolysis systems. Information about power consumption is available in the public datasheet. However, attention should be given to the fact that several additional components are installed to ensure proper operations of the electrolyzers like, for example, but not limited to water pumps, cooling fans, and control system components that contribute to the total power consumption. As the best knowledge of the authors and the availability of data, Table B.1 in supplementary file is provided. The reported range of energy consumption is  $42.2$  to  $65.6 \text{ kWh/kg}$  of hydrogen which is generally higher than the experimental values represented in Figure 2 and Figure 3. This difference might be due to various characteristics of stack, scaling and balance of plant, and the system efficiency. The average energy consumption for PEM technology and alkaline technologies is 53 and  $54.7 \text{ kWh/kg}$ , respectively.

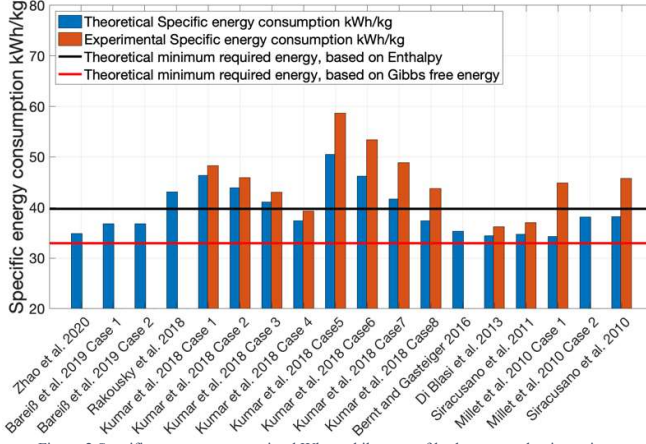


Figure 2 Specific energy consumption kWh per kilogram of hydrogen production using PEM electrolyser

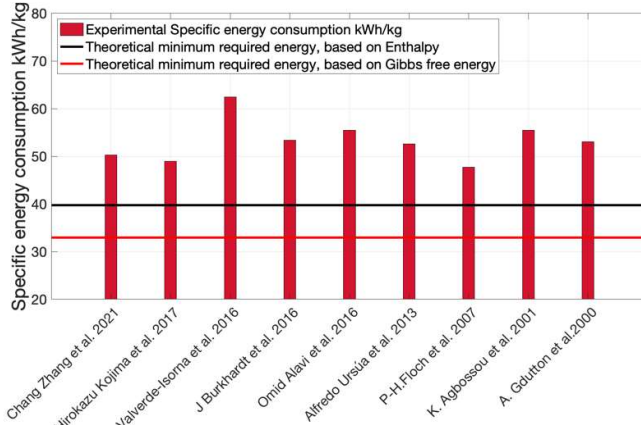


Figure 3 Specific energy consumption kWh per kilogram of hydrogen production using Alkaline electrolyser

## 1.7 Scope of the study

The focus of previous studies was mainly on the techno-economic analysis [22], life cycle assessment of hydrogen production, and determination of the most contributor among the components and procedures of hydrogen production. In addition, the main comparison which has been made in publications includes a review of the materials, methods, and components [36]. Considering the different characteristics of electrolyzers and the variety of input energy sources in different countries there is a lack of comprehensive comparative assessment of environmental impact and sensitivity analysis of cell characteristics and energy sources, which will be discussed in this study.

The objectives of this study are 1) the assessment of the minimum amount of various fuel types for hydrogen generation via PEM and alkaline technologies and their carbon dioxide emission, 2) the estimation of the carbon dioxide emission to produce 1 kg hydrogen using PEM and alkaline technologies in Europe and Australia by means of the current electricity generation condition, 3) prediction of the carbon dioxide emission to produce 1 kg hydrogen using PEM and alkaline technologies in Europe and Australia in 2030, 4) sensitivity analysis of energy consumption for hydrogen generation via PEM and alkaline regarding cell characteristics, and 5) sensitivity

analysis of energy consumption for hydrogen generation via PEM and alkaline regarding various energy scenarios.

In this study, carbon dioxide emissions regarding the fuel type and the location of energy generation for the current situation and prediction for 2030 are assessed. In addition, sensitivity analysis regarding cell characteristics and energy sources is performed by providing empirical equations to define the most effective cell characteristics and the impact of the transition from fossil fuels to renewable energy in hydrogen production via PEM and alkaline electrolysis.

## 2 Methodology

### 2.1 Environmental impact

In this study environmental impact of hydrogen production at the stack level using PEM and alkaline electrolyzers is investigated including the emission regarding energy sources and the location of energy generation.

#### 2.1.1 Energy sources

The electrical energy input to produce hydrogen can be provided by means of various types of fuel and RES. Energy content of various fuels according to the Australian government, Department of Industry, Science, Energy, and Resources [37] is provided in Table C.1 in the supplementary file.

By using the energy content column in Table C.1 and “experimental required energy” reported in studies in Table A.2 and Table A.3 in supplementary file, the minimum required amount of each fuel to produce 1 kg hydrogen can be calculated as in Eq.12:

$$F_m = \frac{E_{esc} \times (0.0036 \text{ (GJ)/1 kWh})}{E_c} \times \frac{1000 \text{ (kg)}}{1 \text{ (t)}} / \quad \text{Eq. 12}$$

$F_m$  = Minimum required fuel (kg)

$E_{esc}$  = Experimental specific energy consumption (kWh)

$E_c$  = Energy content (GJ/t)

$\eta_f$  = Thermal to power energy conversion efficiency of fuel kind

Thermal to power energy conversion efficiency of fuel kind varies with the process of electricity generation, types of fuel, and the type of generator. For simplification, a combined gas/steam turbine with an average efficiency of thermal to mechanical energy of 50% [38] is assumed for all kinds of fuel, and 98% is considered as the mechanical to electrical conversion efficiency. Therefore, thermal to power energy conversion is considered 49% for the calculations.

It is assumed that 100% of fuel and energy is used to produce hydrogen, energy consumption in other parts of the plant is not considered.

#### 2.1.2 Carbon dioxide emission based on fuel type

The emission factor of various fuels according to the Australian government, Department of Industry, Science, Energy, and Resources [37] is provided in Table C.1 in the

supplementary file. By using the emission factor values and the experimental required energy reported in studies in Table A.2 and Table A.3, the amount of CO<sub>2</sub> emission from the production of 1 kg of hydrogen using different fuel sources can be calculated as follow:

$$E_{fuel} = F_m(\text{kg}) \times \frac{1(t)}{1000(kg)} \times E_c \times E_f \quad \text{Eq. 13}$$

Where:

$E_{fuel}$  = Carbon dioxide emission regarding fuel type (kg CO<sub>2</sub>)

$E_f$  = Emission factor (kg CO<sub>2</sub>/GJ)

### 2.1.3 CO<sub>2</sub> emission of electricity generation for hydrogen production, Australia states, current situation

Due to the high potential of Australia in hydrogen production using RES and its geographical location that can supply the hydrogen demand of Asian countries a part of this study is allocated to CO<sub>2</sub> emission of electricity generation for hydrogen production in this country. Scope 2 and Scope 3 Electricity emission factors since 1989 are provided by the Australian government, Department of Industry, Science, Energy, and Resources [37] for various states in Australia and the whole country. The last estimate of the combination of CO<sub>2</sub> emission for Scope 2 and Scope 3 in Australia is used to estimate the carbon dioxide emission in Australia based on the required energy for electrolysis represented in Table A.2 and Table A.3.

### 2.1.4 CO<sub>2</sub> emission of electricity generation for hydrogen production, Europe, current situation

Considering the importance of Europe in terms of hydrogen production using RES and reaching net zero emission, the same method, as for the Australian states, is applied to European countries by using electricity generation CO<sub>2</sub> emission factor and studies in Table A.2 and Table A.3. The emission estimation is performed on EU28 countries. In addition, CO<sub>2</sub> emission of 1 kg hydrogen production in seven European countries is investigated to present the possible range of emission.

### 2.1.5 CO<sub>2</sub> emission of electricity generation for hydrogen production, Australia, 2030 Prediction

Efforts have been made to reduce CO<sub>2</sub> emissions to reach the Paris agreement goals. According to the Australian government, Department of Industry, Science, Energy, and Resources [39], the emission reduction target in Australia up to 2030 is 26% to 28% below 2005 levels. By using electricity emission factors since 1989 provided by the Australian government, Department of Industry, Science, Energy, and Resources [37], it is possible to define the trend of CO<sub>2</sub> emission for hydrogen production over the years. This information can be used to predict CO<sub>2</sub> emissions in the future.

Prediction of CO<sub>2</sub> emission in 2030 by using a linear trend is provided in Table 1. The most significant reduction trend is related to South Australia. The negative value for

Tasmania means that the emission is predicted to increase. This could be due to an inappropriate linear trend for this state. Tasmania electricity has been supplied by Victoria in some periods, which could be the reason for the inappropriate linear trend as this supply was not constant. 18% reduction in CO<sub>2</sub> emission in Australia in total is predicted in 2030 in comparison to 2019. This could be achievable by changing the source of electricity generation and using more efficient technologies.

State	Scope 2 and 3 prediction for 2030 kg CO <sub>2</sub> e/kWh	reduction respect to 2019
New South Wales and Australian capital territory	0.777	9%
Victoria	0.847	15.3%
Queensland	0.804	12.6%
South Australia	0.003	99.0%
Western Australia-south west interconnected system (SWIS)	0.447	35.2%
Tasmania	0.218	-36.3%
Northern territory	0.490	15.6%
Australia	0.664	18.0%

Table 1 Prediction of CO<sub>2</sub> emission in 2030

### 2.1.6 CO<sub>2</sub> emission of electricity generation for hydrogen production, Europe, 2030 Prediction

The same procedure is applied to the European countries to predict the emission factor in 2030. The predicted emission factors and required energy for electrolysis represented in Table A.2 and Table A.3 are used in this study to predict the carbon dioxide emission for hydrogen production by means of PEM and alkaline electrolyzers in 2030.

## 2.2 Sensitivity analysis

Sensitivity analysis regarding cell characteristics and energy sources is performed in this study. For the energy sources sensitivity analysis, sources in Australia and Italy are considered due to their potential in hydrogen production using RES and their strategic geographical position which can allow supplying hydrogen to numerous countries.

### 2.2.1 Sensitivity analysis- Cell characteristics

The first step to perform the sensitivity analysis in this study is the determination of the parameters in Table A.1, which have a logical relationship with experimental energy consumption that can later be used to determine the general equation for sensitivity analysis. Figure 4 and Figure 5 show experimental energy consumption for 1 kg hydrogen production through a PEM electrolyser versus “cell voltage, cell efficiency, and current density” and “cell faradaic efficiency”, respectively. The linear trendline is provided for each parameter in Figure 4. It can be seen that cell voltage and current density have almost linear relationships with experimental energy consumption with the coefficient of determination of 0.77 and 0.57, respectively. It is seen that, for all 3 parameters, the



maximum residual (different between actual value and trendline) occurs around 45 kWh/kg energy consumption. As it is mentioned in eq.7, the cell voltage is the denominator of the cell efficiency equation, thus, it is rationalship when cell voltage has a linear relationship with experimental energy consumption there would not be a linear relation between cell efficiency and experimental energy consumption. Figure 5 shows that there is not a specific relation between cell faradaic efficiency and experimental energy consumption. Therefore, for the sensitivity analysis, cell voltage, and current density are considered as parameters to find the general linear equation. However, there is a sudden drop in the faradaic efficiency at around 45-50 kWh/kg which could be used as a condition to have two clusters to formulate the estimated experimental specific energy including faradaic efficiency. But it needs more investigation and is not considered in this study.

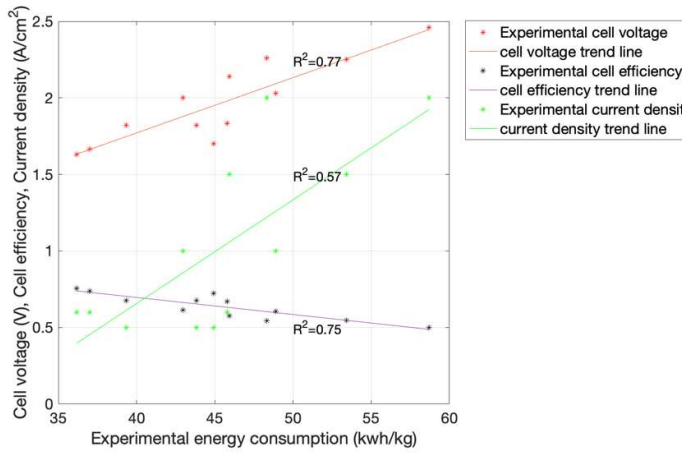


Figure 4 Experimental energy consumption for 1 kg hydrogen production by means of PEM electrolyser versus cell voltage, cell efficiency and current density

Based on the information provided in Table A.1 and Table A.2, the relation between current density, cell voltage, and experimental specific energy consumption for 1 kg hydrogen production through the PEM electrolyser is achieved as in eq.14 ( $R^2=0.82$ ). This equation is created by applying multiple regression in python, using pandas and sklearn libraries. The correlation coefficient is 0.91 which is depicted in Figure 6. This figure shows the relation between the experimental and estimated energy consumption. The black line is the linear trendline and it can be seen that the maximum residual occurs around 45 kWh/kg experimental energy consumption.

$$E_{e,experimental,PEM} = -6.90 \times I_{density} + 35.63 \times E_{cell} - 17.59 \quad \text{Eq. 14}$$

where:

$E_{e,experimental,PEM}$  = Estimated experimental specific energy consumption for 1 kg hydrogen production (kWh) by means of PEM electrolyser

$E_{cell}$  = cell voltage (V)

$I_{density}$  = current density ( $A/cm^2$ )

Eq.14 can be modified by combination with eq.7 as follow:

$$E_{e,experimental,PEM} = \frac{44.07}{\eta_{cell,LHV}} - 6.90 \times I_{density} - 17.59 \quad \text{Eq. 15}$$

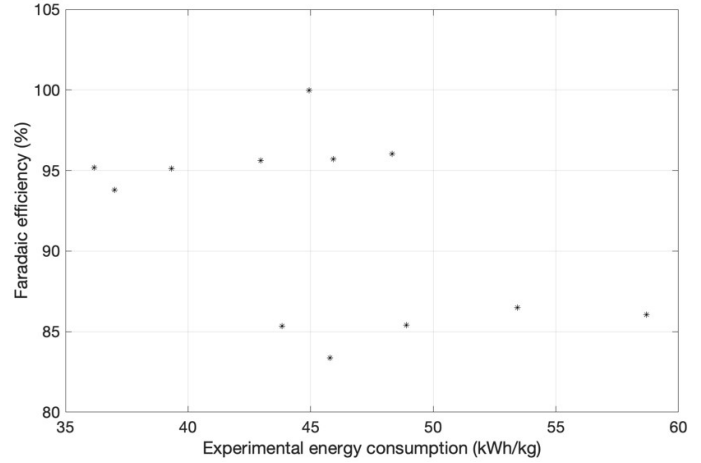


Figure 5 Experimental energy consumption for 1 kg hydrogen production by means of PEM electrolyser versus cell faradaic efficiency

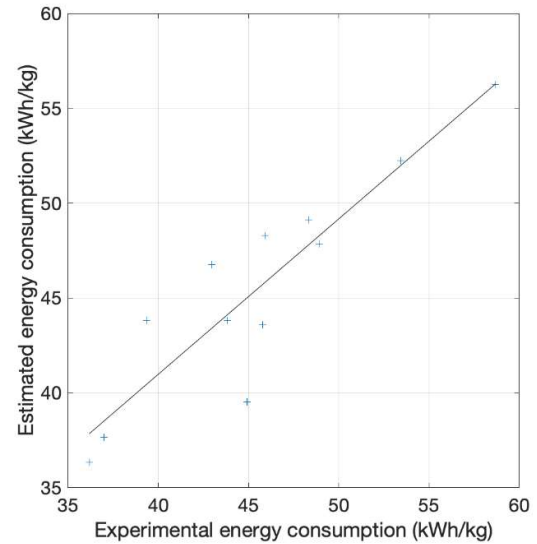


Figure 6 correlation between experimental and estimated energy consumption for 1 kg hydrogen production by means of PEM electrolyser

To perform the sensitivity analysis of estimated energy consumption, the average current density and cell voltage are considered as initial values, 1.025 ( $A/cm^2$ ) and 1.967 (V) respectively (12 cases with information about experimental energy consumption, current density, and cell voltage). Cell efficiency related to the cell voltage equal to 1.967V is %62.5. For each sensitivity analysis regarding the desired parameter, the second parameter in eq.14 and eq.15 is considered as the fixed parameter, and -30% to 30% tolerance is applied to the desired parameter.

The same procedure as in PEM sensitivity analysis is applied to alkaline, but in this case, the only available information is cell efficiency and experimental energy consumption. The equation between estimated experimental energy consumption and cell efficiency is shown in eq.16 ( $R^2=0.64$ )

$$E_{e,experimental,alkaline} = -53.16 \times \eta_{cell,LHV} + 88.33 \quad \text{Eq. 16}$$

where:

$E_{e,experimental,alkaline}$  = Estimated experimental specific energy consumption for 1 kg hydrogen production (kWh) by means of alkaline electrolyser

Considering that this equation has only one variable and and coefficient of determination is low it seems that it is not reliable to perform the sensitivity analysis with this equation. It needs in-depth research which could be covered in future studies.

### 2.2.2 Sensitivity analysis- Energy source

In this section sensitivity analysis of carbon dioxide emission regarding renewable energy sources including solar, wind, and hydro energies in Australia and Italy is assessed. For this purpose, the median values of CO<sub>2</sub> emission for hydrogen production by means of PEM and alkaline technologies in Australia and Italy are extracted from Figure 13 and Figure 14. The median emissions for PEM technology in Italy and Australia were 13.15 and 38.1 kg CO<sub>2</sub>/kg hydrogen, respectively. And the median emissions for alkaline technology in Italy and Australia were 15.4 and 43.01 kg CO<sub>2</sub>/kg hydrogen, respectively.

Several scenarios were considered as follow:

- 1) Constant share of wind and hydro, and replacement of the other sources with solar
- 2) Constant share of solar and hydro, and replacement of the other sources with wind
- 3) Constant share of solar and wind, and replacement of the other sources with hydro

Based on the IPCC report, 2018, Annex III, table AIII.2, carbon dioxide emissions for 1MWh electricity generation by solar (utility), wind (onshore), and hydropower are 48, 11, and 24 kg respectively [40]. According to the Department of Industry, Science, Energy, and Resources, renewable energies contribution to total energy generation in Australia in 2020, was 24% (Solar 9%, wind 9%, hydro 6%) [3]; While the percentage of RES contribution in Italy in 2019 was 18 % (Solar 1.7%, wind 1.4%, hydro 3.4%, other renewable sources 11.5%) [4].

To estimate the average emission of the other sources of carbon dioxide emission the following equation is used:

$$E_T = E_{consumption} \times (C_s \times E_s + C_w \times E_w + C_h \times E_h + C_o \times E_o) \quad \text{Eq. 17}$$

Where:

$E_T$  = Total carbon dioxide emission, (kg CO<sub>2</sub>)

$E_{consumption}$  = Average electricity consumption for 1 kg hydrogen generation, (kg CO<sub>2</sub>/MWh)

$C_s$  = solar contribution, (percentage of the total, in MWh)

$E_s$  = electricity generation carbon dioxide emission by means of solar energy, (kg CO<sub>2</sub>/MWh)

$C_w$  = wind contribution, (percentage of the total, in MWh)

$E_w$  = electricity generation carbon dioxide emission by means of wind energy, (kg CO<sub>2</sub>/MWh)

$C_h$  = hydro contribution, (percentage of the total, in MWh)

$E_h$  = electricity generation carbon dioxide emission by means of hydro energy, (kg CO<sub>2</sub>/MWh)

$C_o$  = other energies contribution, (percentage of the total, in MWh)

$E_o$  = electricity generation carbon dioxide emission by means of other sources of energy, (kg CO<sub>2</sub>/MWh)

Based on the studies in Table A.2 and Table A.3 the average electricity consumption in PEM technology is 45.44 kWh/kg hydrogen and 53.29 kWh/kg hydrogen for alkaline technology. Table 2 is provided to define the contribution of other sources and their average carbon dioxide emission based on equation 17 and average electricity consumption.

	Italy (PEM)	Australia (PEM)	Italy (alkaline)	Australia (alkaline)
$E_T$ (kg CO <sub>2</sub> /kg Hydrogen)	13.15	38.1	15.4	43.01
$C_s$	1.70%	9.00%	1.70%	9.00%
$E_s$ (kg CO <sub>2</sub> /MWh)	48	48	48	48
$C_w$	1.40%	9.00%	1.40%	9.00%
$E_w$ (kg CO <sub>2</sub> /MWh)	11	11	11	11
$C_h$	3.40%	6.00%	3.40%	6.00%
$E_h$ (kg CO <sub>2</sub> /MWh)	24	24	24	24
$C_o$	93.50%	76.00%	93.50%	76.00%
$E_o$ (kg CO <sub>2</sub> /MWh)	307.6	1094.37	307.16	1053.08

Table 2 Contribution of energy sources and average emission of sources

To perform the sensitivity analysis, considering the defined scenarios, contribution increments are applied to each source (reduction of  $C_o$  at the same time) and the carbon dioxide emission is calculated based on equation 17.

## 3 Result and discussion

### 3.1 Environmental impact

#### 3.1.1 Energy sources

Based on Eq.12 the amount of fuel to produce 1 kg of hydrogen using PEM and alkaline electrolyzers at stack level is calculated and shown in Figure 7 and Figure 8. Considering the assumption, the required amount of fuel, in reality, is more than the reported values in Figure 7 and Figure 8. By comparing Figure 7 and Figure 8 it can be recognized that the required fuel amount in Alkaline technology is higher than in PEM.

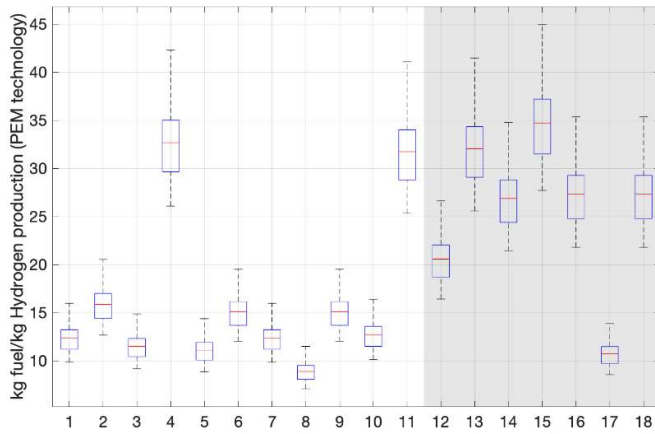


Figure 7 Minimum required fuel to produce 1 kg hydrogen (based on experimental energy values) by means of PEM technology, numbers in the x axis is the fuel row number in Table A.1. Highlighted part is related to zero emission fuels.

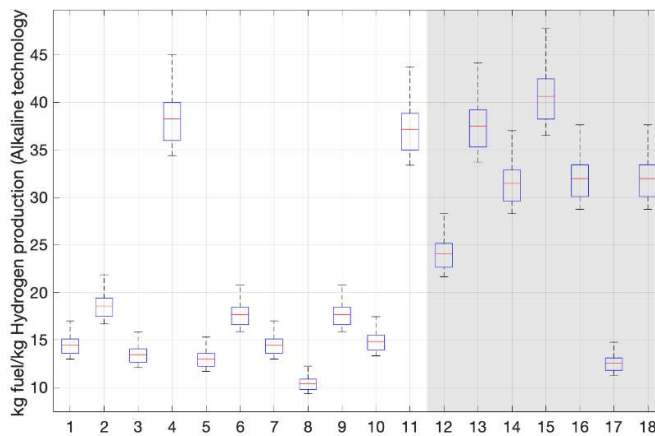


Figure 8 Minimum required fuel to produce 1 kg hydrogen (based on experimental energy values) by means of Alkaline technology, numbers in the x axis is the fuel row number in Table A.1. Highlighted part is related to zero emission fuels.

The boxplot of each number in the horizontal axis shows the results based on studies in Table A.2 and Table A.3, and using the relevant fuel type in Table A.1. In Figure 7 and Figure 8, in general, the required mass of fuels with an emission factor of zero is considerably higher than fuels with non-zero emission, except some fuels, such as brown coal, non-biomass municipal materials, if combusted to produce heat or electricity, and charcoal. Coal tar amount is the minimum one, however, its emission is significantly high. Among the fuels with zero emission factor, charcoal is the fuel with the minimum weight required to produce 1 kg of hydrogen due to its high energy content. However, the amount of fuel consumption is not related only to the fuel type and its energy content but also to the technology. For example, as can be seen in Figure 7, the minimum fuel amount of dry wood with zero emission is around 15 kg fuel/kg hydrogen which is almost equal to or less than the maximum values of bituminous coal, sub-bituminous coal, coal briquettes, coal coke, “Solid fossil fuels other than those mentioned in the items above”, and “industrial materials and tyres that are derived from fossil fuels, if recycled and combusted to produce heat or electricity”. In other words, charcoal is not the only zero-emission fuel with a low amount of fuel consumption if charcoal is sourced from sustainably managed biomass.

### 3.1.2 Carbon dioxide emission based on fuel type

Carbon dioxide emission corresponding to the type of fuel to produce 1 kg hydrogen using PEM and alkaline electrolyzers at stack level is shown in Figure 9 and Figure 10. Zero emission fuels, fuels 12 to 18, do not emit carbon dioxide. If non-zero emission fuels are used in hydrogen production, CO<sub>2</sub> emission at stack level, assuming 100% efficiency of burning fuels, will be around 25-40 kg for 1 kg of hydrogen production via PEM technology and approximately 30-40 kg for alkaline, except coal coke which is a bit higher. Coal coke has the highest carbon dioxide emission, while coal tar and “industrial materials and tyres” have the lowest values among the non-zero fuels. The mentioned range is related only to burning fuel, without consideration of other emissions such as extraction and transport. It is seen that the carbon dioxide emission associated with alkaline technology is approximately 5 kg higher than PEM technology.

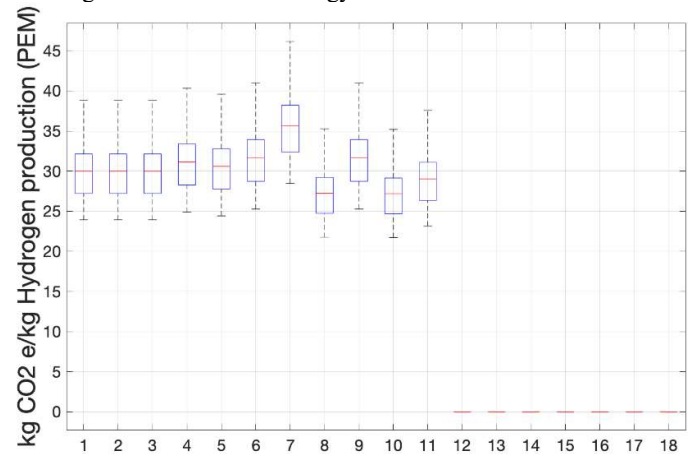


Figure 9 CO<sub>2</sub> emission of 1 kg hydrogen production only from fuel burning (based on experimental energy values) by means of PEM technology, numbers in the x axis is the fuel row number in Table A.1.

### 3.1.3 Australia states, current situation

The last estimate of the combination of CO<sub>2</sub> emission for Scope 2 and Scope 3 in Australia and its states based on studies represented in Table A.2 and Table A.3 are provided in Figure 11 and Figure 12. By using these figures, it is possible to recognize the range of CO<sub>2</sub> emission in Australia and each state to produce 1 kg of hydrogen using PEM and alkaline electrolyser at the stack level.

It is seen that the values related to the alkaline technology are higher than PEM. The overall range of carbon dioxide emission to produce 1 kg hydrogen, using electricity from the grid, in the current situation, is approximately 30-45 and 38-50 kg CO<sub>2</sub> via PEM and alkaline technologies, respectively. However, the difference between carbon dioxide emission of states is considerable. NSW and capital territory, Victoria and Queensland have higher emission in comparison to the average emission of the country, while WA, Northern territory, South Australia and Tasmania have lower quantities. Among the Australian states, Tasmania has the lowest emission intensity and Victoria has the highest one. These differences could be

due to the technologies and energy sources which are used in each state regarding the authorities' strategies.

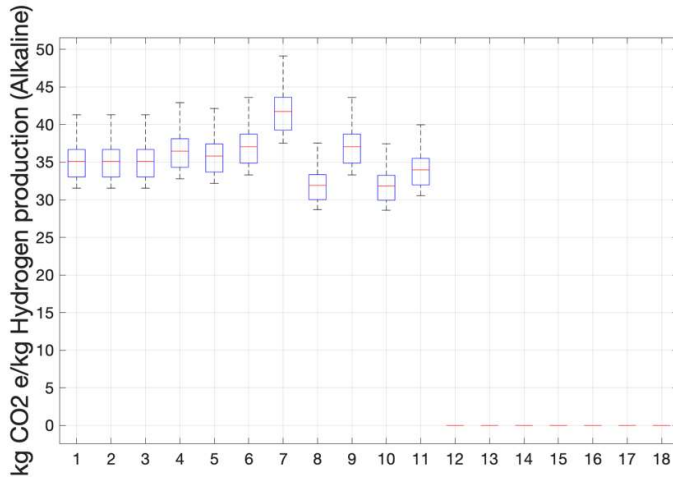


Figure 10 CO<sub>2</sub> emission of 1 kg hydrogen production only from fuel burning (based on experimental energy values) by means of Alkaline technology, numbers in the x axis is the fuel row number in Table A.1.

There is a considerable difference between the range in “Figure 9 and Figure 10 “ and “Figure 11 and Figure 12” which could be due to the consumption of other types of fuel and the efficiency of the powerplants, in addition, Figure 9 and Figure 10 are based only on the emission of fuel combustion, not other emissions such as transport and extraction. Thus, if the technologies represented in Table A.2 and Table A.3 be used, the CO<sub>2</sub> emission for 1 kg of hydrogen production in Australia could be around 30 to 40 kg and 40-50 kg, at stack level, via PEM and alkaline technologies, respectively.

According to the council of Australian government (COAG) energy council report, annually around 350 kt hydrogen is produced in Australia, including export to other countries such as Japan and Korea [41]. Only 55 t of produced hydrogen in Australia is clean hydrogen [17]. If zero-emission fuels and RES are not 100% used as energy sources, the results would be 10.5 to 14 Mt of CO<sub>2</sub> emission for PEM technology and 14 to 17.5 Mt of CO<sub>2</sub> emission for alkaline technology. If the required energy represented in the manufacturer list in Table C.1 is used instead of the experimental required energy, CO<sub>2</sub> emission could be closer to the upper boundary of this range, since the required energy in the manufacturer list is closer to the maximum values in experimental tests. Therefore, it can be expected to have annually 17.5 Mt of CO<sub>2</sub> emission due to hydrogen production using PEM and alkaline technology in Australia.

#### 3.1.4 Europe, current situation

Based on studies represented in Table A.2, Table A.3 and the greenhouse gas emission factor of the electricity sector for the production of electricity, extracted from the ISPRA report [42], the current situation of CO<sub>2</sub> emission for 1 kg hydrogen production by means of PEM and Alkaline in Europe and main countries is calculated which is depicted in Figure 13 and Figure 14. For the sake of comparison, Australia is included in these figures.

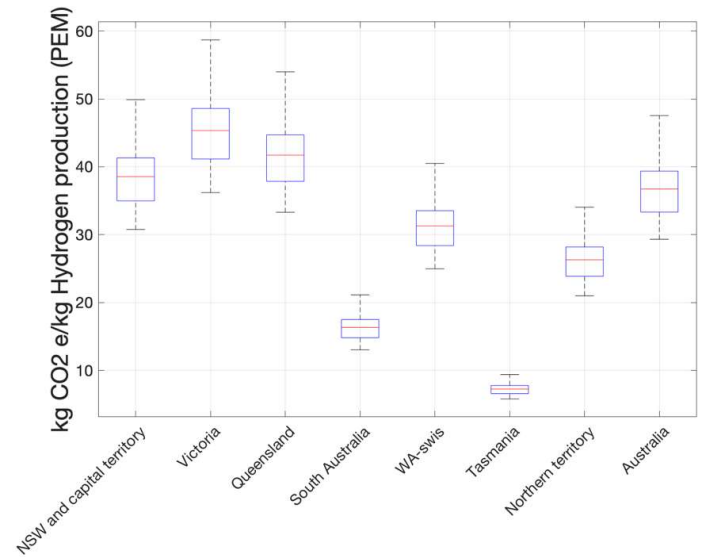


Figure 11 Scope 2 and Scope 3 combination CO<sub>2</sub> emission of 1 kg hydrogen production in Australia and its states based on studies represented Table A.2 (last estimate after 2019), PEM technology

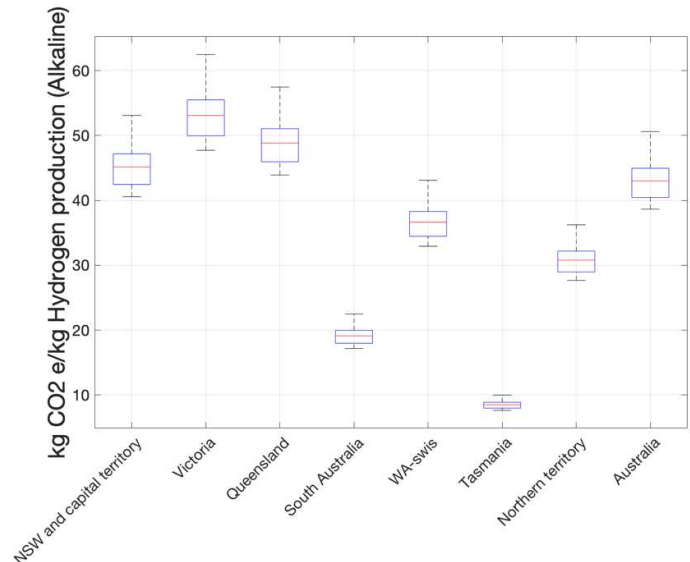


Figure 12 Scope 2 and Scope 3 combination CO<sub>2</sub> emission of 1 kg hydrogen production in Australia and its states based on studies represented in Table A.3 (last estimate after 2019), Alkaline technology

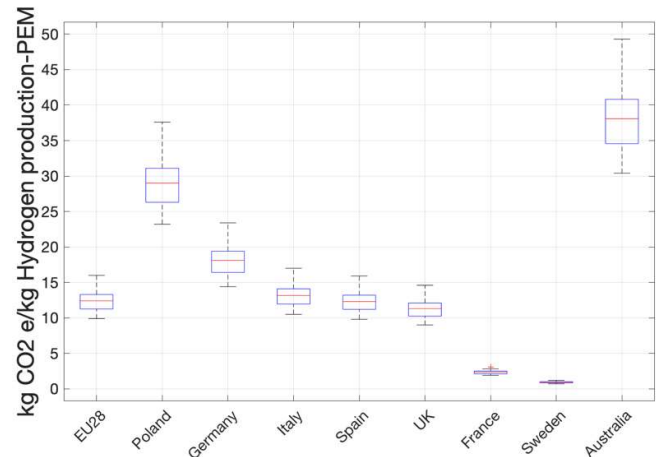


Figure 13 CO<sub>2</sub> emission of the production of 1 kg hydrogen in Europe and Australia based on studies represented in Table A.2, PEM technology



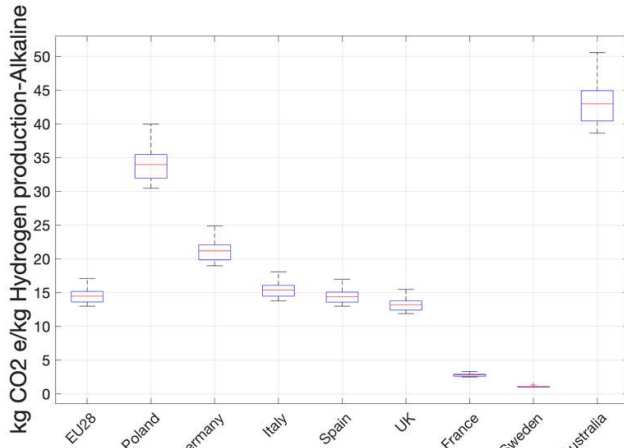


Figure 14 CO<sub>2</sub> emission of the production of 1 kg hydrogen in Europe and Australia based on studies represented in Table A.3, Alkaline technology

It is seen that the amount of carbon dioxide emission to produce 1 kg hydrogen in EU28 is around 10-15, and 12-17 via PEM and alkaline technologies, respectively. Germany, Italy, Spain, and UK have emission close to the average value of EU28 while Poland, France and Sweden have considerable difference with the average EU28. Australia has significantly higher CO<sub>2</sub> emissions compared to European countries on average; the difference is approximately 25 and 30 kg carbon dioxide emission via PEM and alkaline, respectively. Despite the considerable difference between EU28 and Australia, it is seen that some countries like Poland could have high emission close to Australia's emission, while countries like Sweden and France could have significantly low CO<sub>2</sub> emission for hydrogen production by PEM and Alkaline.

### 3.1.5 Australia, 2030 prediction

Based on the predicted values and energy consumption in the represented studies in Table A.2 and Table A.3, predicted CO<sub>2</sub> emission for 1 kg hydrogen production using PEM and alkaline technology in Australia if electricity is drawn from the national and State grids in 2030 is provided in Figure 15 and Figure 16.

It can be seen that CO<sub>2</sub> emission for 1 kg of hydrogen production in Australia using the PEM electrolyser at stack level is predicted to be around 25-35 kg in 2030 and 30-40 kg for Alkaline technology. It is seen that NSW and capital territory, Victoria, and Queensland could have higher emission in comparison to the average Australia, while other states could have lower carbon dioxide emission to produce 1 kg hydrogen in 2030. According to the Council of Australian Government (COAG) energy council report, hydrogen production in Australia in 2030 is projected to be around 1 Mt per year [41], resulting in 25 to 35 Mt of CO<sub>2</sub> emission and 30 to 40 Mt of CO<sub>2</sub> for PEM and Alkaline technologies, respectively, if the trend is the same as projected values. According to Figure 15 and Figure 16, it is predicted that, in 2030, South Australia could almost reach zero emission hydrogen generation while Victoria would have the highest carbon dioxide emission for hydrogen generation. Therefore, energy generation patterns and management in South Australia could be

applied as a guide to other states to reduce the overall carbon dioxide emission in Australia.

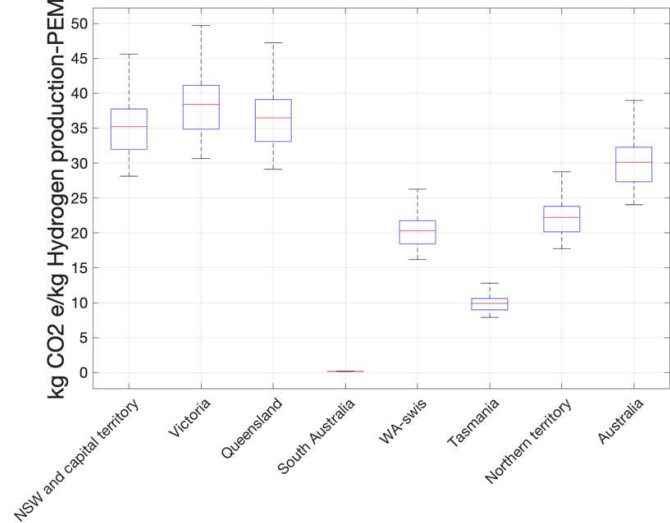


Figure 15 Emission for 1 kg hydrogen production using PEM technology (based on experimental energy values)-2030 prediction, Australia states

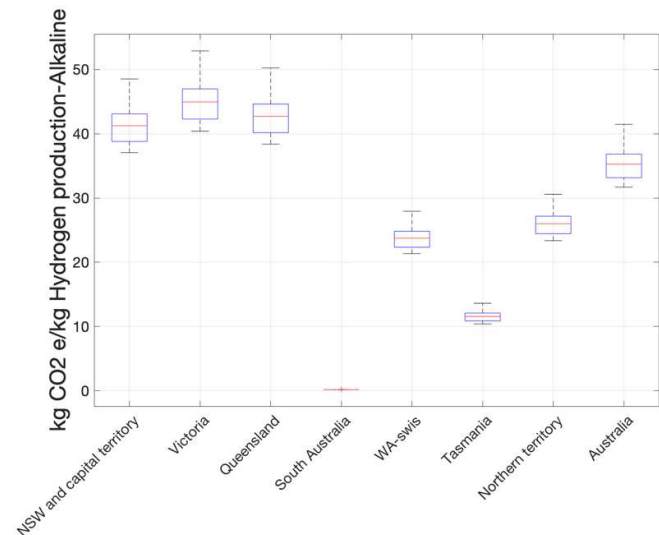


Figure 16 Emission for 1 kg hydrogen production using alkaline technology (based on experimental energy values)-2030 prediction, Australia states

### 3.1.6 Europe, 2030 prediction

The predicted CO<sub>2</sub> emission in 2030 in European countries is provided in Figure 17 and Figure 18. For the sake of comparison, these figures include predicted emission related to Australia.

In 2030, the average carbon dioxide emission to produce 1 kg hydrogen via PEM and alkaline technology is predicted to be approximately 7-12, and 10-13 kg CO<sub>2</sub>, respectively. It is seen that Australia might have significantly higher emission for hydrogen production using PEM and alkaline electrolyzers in comparison to European countries and Poland might have the highest emission among European countries. Thus, it is necessary to make proper decisions in countries like Australia and Poland to be able to reach the Paris agreement objective. The emission difference between Australia and EU28 in



2030, would be approximately 20 and 25 kg carbon dioxide via PEM and alkaline, respectively; which is almost 5 kg less than the difference in the current situation.

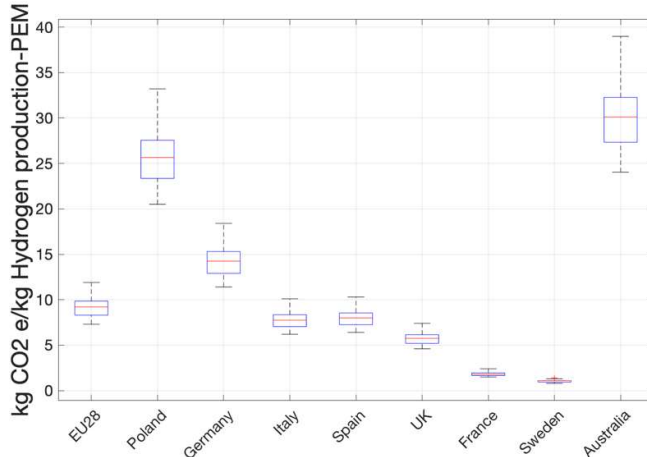


Figure 17 Emission for 1 kg hydrogen production using PEM technology (based on experimental energy values)-2030 prediction, European countries and Australia

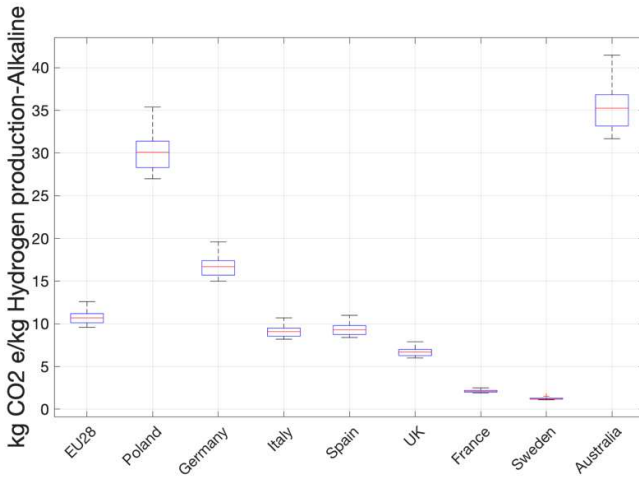


Figure 18 Emission for 1 kg hydrogen production using Alkaline technology (based on experimental energy values)-2030 prediction, European countries and Australia

## 3.2 Sensitivity analysis

### 3.2.1 Sensitivity analysis- Cell characteristics-PEM technology

The result of the sensitivity analysis of estimated energy consumption for 1 kg hydrogen production through the PEM electrolyser is depicted in Figure 19. It can be seen that energy consumption for hydrogen production is more sensitive to the cell voltage and cell efficiency, which are related concepts as shown in eq.7, while its sensitivity to current density is very low. The variation of estimated energy consumption is approximately -46 to 46%, 65 to -35%, and 4.6 to -4.6% for cell voltage, cell efficiency, and current density variation respectively. It can be realised that the impact of cell voltage is almost 10 times higher than the current density impact with an inverse direction.

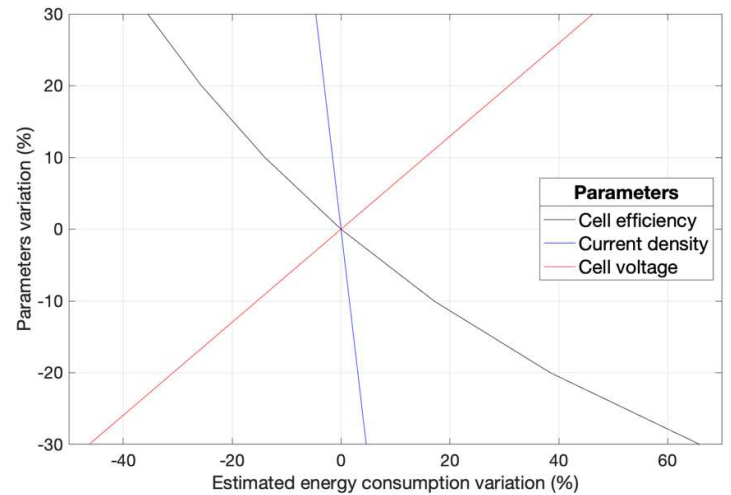


Figure 19 variation of parameters (-30 to 30%) and variation of estimated energy consumption for 1 kg hydrogen production by means of PEM electrolyser

According to Faraday's 1st law, the quantity of produced hydrogen is proportional to the current density, not the cell voltage. The result of sensitivity analysis, based on experimental studies, shows higher sensitivity of energy consumption to cell voltage in comparison to current density. This result indicates the importance of cell manufacturing and electrolyte resistance that could result in lower faradaic efficiency due to undesirable reactions or electrolyte impurities.

### 3.2.2 Sensitivity analysis- Energy source

The result of sensitivity analysis based on energy source is shown in Figure 20 for Italy and Figure 21 for Australia. The maximum amount of contribution increment is determined based on the  $C_0$  values.

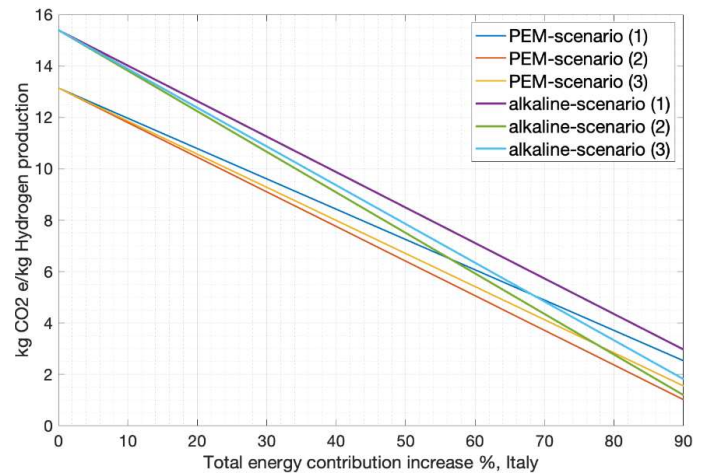


Figure 20 variation of energy source contribution and impact on CO<sub>2</sub> emission for 1 kg hydrogen production by means of PEM and alkaline electrolyser in Italy.

It can be seen in Figure 20 that the result of a 90 % increment of renewable sources contribution could be emission reduction from approximately 13-15 kg of carbon dioxide to around 1-3 kg CO<sub>2</sub>/kg hydrogen generation. The minimum carbon dioxide emission could be reached by scenario 2 using PEM technology, however, the most significant change is related to scenario 2 with alkaline technology (considering the slope of lines).

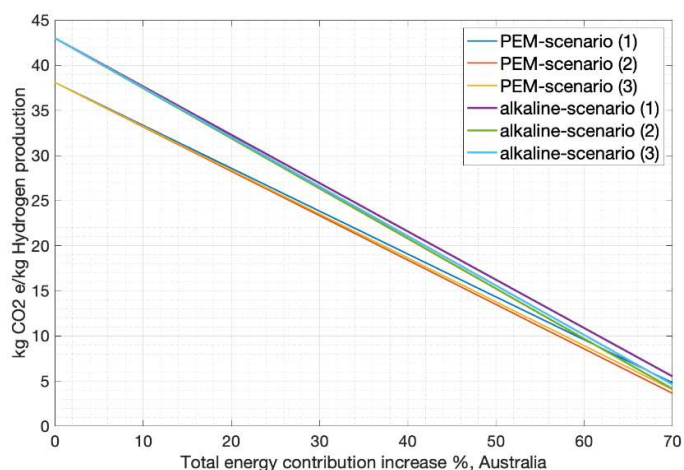


Figure 21 variation of energy source contribution and impact on CO<sub>2</sub> emission for 1 kg hydrogen production by means of PEM and alkaline electrolyser in Australia.

In addition, by comparing the line slopes it is seen that scenario 1 via PEM technology has the lowest sensitivity. The result of 70% increment of renewable sources in Australia could be 3.5-5.5 kg CO<sub>2</sub>/kg hydrogen generation and the minimum emission and most significant change are like Italy. By comparing the line slopes which show the result of sensitivity analysis, it can be realized that emission in Australia is more sensitive to RES rather than in Italy. By comparing the carbon dioxide emission considering the maximum contribution percentage in Australia, 70 %, it is seen that the emission range for both countries would be 3.5-6 kg CO<sub>2</sub>. It should be noted that Australia can reach this point with an initial amount of around 40 kg CO<sub>2</sub> emission, while Italy's initial emission value is approximately 14 kg CO<sub>2</sub> emission. Considering that the lower amount of carbon dioxide emission would be desirable, scenario 2 using PEM technology could be the best choice, while alkaline scenario 1 is the worst choice in both countries for any increment of RES contribution.

Considering the 2050 net zero emission goal of Australia, a complete transition will be required from fossil fuels to renewable energies in hydrogen production. This transition could be achievable, considering 262,000 square kilometers of land suitable for hydrogen production using renewable electricity, which is about 3% of Australia's total land area [16].

#### 4 Conclusion

Hydrogen production using PEM and alkaline electrolyzers and their potential carbon dioxide emission are assessed in this study. The minimum energy required

to produce 1 kilogram of hydrogen based on the Gibbs free energy and enthalpy is 32.95 kWh/kg and 39.70 kWh/kg, respectively. However, the experimental values and values provided by manufacturers are higher due to differences in stack configuration and efficiency of the system. The range of energy consumption reported by manufacturers is 42.2 to 65.6 kWh/kg of hydrogen. Various fuel sources with different CO<sub>2</sub> emissions can be used to provide electricity for water electrolysis. Considering the current consumption of various fuel types in Australia, if PEM and alkaline technologies represented in Table A.2 and Table A.3 are used, the CO<sub>2</sub> emission for 1 kg of hydrogen production in Australia could be around 30 to 40 kg and 40 to 50 kg, at stack level, via PEM and alkaline technologies, respectively. Considering the current amount of hydrogen production in Australia, if it was produced by the PEM electrolyser the emission equivalent is to be 10.5 to 14 Mt of CO<sub>2</sub> and 14 to 17.5 Mt of CO<sub>2</sub> emission for alkaline technology. It is predicted that in 2030 in comparison to 2019 there will be a reduction of around 18% in CO<sub>2</sub> emission of the national electricity grid in Australia, which would have resulted in around 25 to 35 kg CO<sub>2</sub> emission for 1 kg of hydrogen production by PEM technology and 30-40 kg for Alkaline technology. The current CO<sub>2</sub> emission for 1 kg hydrogen production in Italy is approximately 12 to 15 kg CO<sub>2</sub> and the predicted emission in 2030 is 5 to 10 kg CO<sub>2</sub> using PEM or alkaline technologies. To overcome the problem of CO<sub>2</sub> emissions, the transition from fossil fuels to RES is necessary. A sensitivity analysis is performed to identify the critical parameters regarding energy consumption and carbon dioxide emission. The result of sensitivity analysis, based on experimental data, regarding cell characteristics shows higher sensitivity of PEM energy consumption to cell voltage in comparison to current density. It could be due to undesirable reactions or electrolyte impurities that amplify the importance of cell manufacturing and electrolyte resistance. In addition, by performing sensitivity analysis regarding energy sources scenarios it is concluded that carbon dioxide emission in Australia is more sensitive to renewable energy sources rather than in Italy.

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#### Conflict of interest

"The authors declare no conflict of interest."

## Reference

- [1] C. Wulf and M. Kaltschmitt, "Life cycle assessment of hydrogen supply chain with special attention on hydrogen refuelling stations," *international journal of hydrogen energy*, vol. 37, pp. 16711-16721, 2012.
- [2] BP, "Statistical Review of World Energy," 2021. [Online]. Available: <https://www.bp.com/en/global/corporate/energy-economics/statistical-review-of-world-energy.html>. [Accessed January 2022].
- [3] "Australian electricity generation - fuel mix," Department of Industry, Science, Energy, and Resources, 2020. [Online]. Available: <https://www.energy.gov.au/data/australian-electricity-generation-fuel-mix>. [Accessed January 2022].
- [4] L. Jensen, "Climate action in Italy Latest state of play," 2021. [Online]. Available: [https://www.europarl.europa.eu/RegData/etudes/BRIE/2021/690663/EPRS\\_BRI\(2021\)690663\\_EN.pdf](https://www.europarl.europa.eu/RegData/etudes/BRIE/2021/690663/EPRS_BRI(2021)690663_EN.pdf). [Accessed 15 August 2022].
- [5] A. P. Pavlos Nikolaidis, "A comparative overview of hydrogen production processes," *Renewable and Sustainable Energy Reviews*, vol. 67, pp. 597-611, 2017.
- [6] K. G. d. Santos, C. T. Eckerta, E. D. Rossi, R. A. Baricatti, E. P. Frigo, C. A. Lindino and H. J. Alves, "Hydrogen production in the electrolysis of water in Brazil, a review," *Renewable and Sustainable Energy Reviews*, vol. 68, pp. 563-571, 2017.
- [7] L. M. Romeo, M. Cavana, M. Bailera, P. Leone, B. Peña and P. Lisbona, "Non-stoichiometric methanation as strategy to overcome the limitations of green hydrogen injection into the natural gas grid," *Applied Energy*, vol. 309, p. 118462, 2022.
- [8] J. Lu, A. Zahedi, C. Yang, M. Wang and B. Peng, "Building the hydrogen economy in China: Drivers, resources and technologies," *Renewable and Sustainable Energy Reviews*, vol. 23, pp. 543-556, 2013.
- [9] S. M. Alirahmi, E. Assareh, N. N. Pourghassab, M. Delpisheh, L. Barelli and A. Baldinelli, "Green hydrogen & electricity production via geothermal-driven multi-generation system: Thermodynamic modeling and optimization," *Fuel*, vol. 308, p. 122049, 2022.
- [10] T. Longden, F. Beck, F. Jotzo, R. Andrews and M. Prasad, "Clean' hydrogen? – Comparing the emissions and costs of fossil fuel versus renewable electricity based hydrogen," *Applied Energy*, Vols. Volume 306, Part B, p. 118145, 2022.
- [11] B. Hurtubia and E. Sauma, "Economic and environmental analysis of hydrogen production when complementing renewable energy generation with grid electricity," *Applied Energy*, vol. 304, p. 117739, 2021.
- [12] M. Delpierre, J. Quist, J. Mertens, A. Prieur-Vernat and S. Cucurachi, "Assessing the environmental impacts of wind-based hydrogen production in the Netherlands using ex-ante LCA and scenarios analysis," *Journal of Cleaner Production*, vol. 299, p. 126866, 2021.
- [13] A. Kopteva, L. Kalimullin, P. Tcvetkov and A. Soares, "Prospects and Obstacles for Green Hydrogen Production in Russia," *Energies*, vol. 14, no. 3, p. 718, 2021.
- [14] J. R. Bartels, M. B. Pate and N. K. Olson, "An economic survey of hydrogen production from conventional and alternative energy sources," *International Journal of Hydrogen Energy*, vol. 35, no. 16, p. 8371-84, 2010.
- [15] J. Janssen, M. Weeda, R. Detz and B. v. d. Zwaan, "Country-specific cost projections for renewable hydrogen production through off-grid electricity systems," *Applied Energy*, vol. 309, p. 118398, 2022.
- [16] A. Government, "State of Hydrogen 2021, Australia's pathway for a clean hydrogen future," Australian Government, Department of Industry, Science, Energy and Resources, 2021. [Online]. Available: <https://www.industry.gov.au/data-and-publications/state-of-hydrogen-2021-australias-pathway-for-a-clean-hydrogen-future>. [Accessed February 2022].
- [17] A. Government, "State of Hydrogen 2021-Hydrogen industry development," Australian Government, Department of Industry, Science, Energy and Resources, 2021. [Online]. Available: <https://www.industry.gov.au/data-and-publications/state-of-hydrogen-2021/hydrogen-industry-development>. [Accessed 1 February 2022].
- [18] E. Schropp, G. Naumann and A. M. Gaderer, "Life Cycle Assessment of a Polymer Electrolyte Membrane Water Electrolysis," in *In Progress in Life Cycle Assessment*, Springer, Cham, 2019, pp. 53-66.
- [19] O. Schmidt, A. Gambhir, I. Staffell, A. Hawkes, J. Nelson and S. Few, "Future cost and performance of water electrolysis: An expert elicitation study," *international journal of hydrogen energy*, vol. 42, pp. 30470-30492, 2017.
- [20] B. Lee, H. Lee, J. Heo, C. Moon, S. Moon and H. Lim, "Stochastic techno-economic analysis of H2 production from power-to-gas using a high-pressure PEM water electrolyzer for a small-scale H2 fueling station," *Sustainable energy and fuels*, vol. 3, p. 2521, 2019.
- [21] G. Zhao, M. R. Kraglund, H. L. Frandsen, A. C. Wulff, S. H. Jensen, M. Chen and C. R. Graves, "Life cycle assessment of H2O electrolysis technologies," *international journal of hydrogen energy*, vol. 45, pp. 23765-23781, 2020.
- [22] S. Kumar and V. Himabindu, "Hydrogen production by PEM water electrolysis – A review," *Materials Science for Energy Technologies*, vol. 2, no. 3, pp. 442-454, 2019.
- [23] D. M. Santos, C. A. Sequeira and a. J. L. Figueiredo, "Hydrogen production by alkaline water electrolysis," *Química Nova*, vol. 36, pp. 1176-1193, 2013.
- [24] J. B. a. T. Turek, "Alkaline Water Electrolysis Powered by Renewable Energy: A Review," *Processes*, vol. 8, no. 248, 2020.
- [25] M. Rashid, M. A. Mesfer, H. Naseem and M. Danish, "Hydrogen production by water electrolysis: a review of alkaline water electrolysis, PEM water electrolysis and high temperature water electrolysis," *International Journal of Engineering and Advanced Technology*, 2015.
- [26] R. Bhandari, C. Trudewind and P. Zapp, "Life cycle assessment of hydrogen production via electrolysis—a review," *Journal of cleaner production*, vol. 85, pp. 151-163, 2014.
- [27] N. Kuleshov, V. Kuleshov, S. Dovbysh, S. Grigoriev, S. Kurochkin and P. Millet, "Development and performances of a 0.5 kW high- pressure alkaline water electrolyser," *International journal of hydrogen energy*, vol. 44, p. 29441e29449, 2019.
- [28] S. S. Kumar, S. U. B. Ramakrishna and D. B. & V. Himabindu, "Preparation of Ru/Pd-xO2 electrocatalysts for the oxygen evolution reaction (OER) in PEM water electrolysis," *Ionics*, vol. 24, pp. 2411-2419, 2018.
- [29] P. Millet, R. Ngameni, S. A. Grigoriev, N. Mbemba, F. Brisset, A. Ranjbari and C. Etiévant, "PEM water electrolyzers: From electrocatalysis to stack development," *International Journal of Hydrogen Energy*, vol. 35, no. 10, pp. 5043-5052, 2010.
- [30] K. Bareiß, C. d. I. Rua, M. Möckl and T. Hamacher, "Life cycle assessment of hydrogen from proton exchange membrane water electrolysis in future energy systems," *Applied Energy*, vol. 237, pp. 862-872, 2019.
- [31] C. Rakousky, G. P. Keeley, K. Wippermann, M. Carmo and D. Stolten, "The stability challenge on the pathway to high-current-density polymer electrolyte membrane water electrolyzers," *Electrochimica Acta*, vol. 278, pp. 324-331, 2018.
- [32] M. Bernt and H. Gasteiger, "Influence of Ionomer Content in IrO2/TiO2 Electrodes on PEM Water Electrolyzer Performance," *Journal of The Electrochemical Society*, vol. 163, no. 11, p. F3179, 2016.
- [33] A. D. Blasi, L. Andalaro, S. Siracusano, N. Briguglio, G. Brunaccini, A. Stassi, A. S. Aricò and V. Antonucci, "Evaluation of materials and components degradation of a PEM electrolyzer for marine applications," *International Journal of Hydrogen Energy*, vol. 38, no. 18, pp. 7612-7615, 2013.
- [34] O. Atlam and M. Kolhe, "Equivalent electrical model for a proton exchange membrane (PEM) electrolyser," *Energy Conversion and Management*, vol. 52, pp. 2952-2957, 2011.
- [35] C. Zhang, J. Wang, Z. Ren and Z. a. W. P. Yu, "Wind-powered 250 kW electrolyzer for dynamic hydrogen production: A pilot study," *International Journal of Hydrogen Energy*, vol. 46, no. 70, pp. 34550-34564, 2021.
- [36] A. Dutton, J. Bleijs, H. Dienhart, M. Falchetta, W. Hug, D. Prischich and A. and Ruddell, "Experience in the design, sizing, economics, and implementation of autonomous wind-powered hydrogen production systems," *International Journal of Hydrogen Energy*, vol. 25, no. 8, pp. 705-722, 2000.
- [37] C. Yilmaz and M. Kanoglu, "Thermodynamic evaluation of geothermal energy powered hydrogen production by PEM water electrolysis," *Energy*, vol. 69, pp. 592-602, 2014.

- [38] M. Carmo, D. L. Fritz, J. Mergel and D. Stolten, "A comprehensive review on PEM water electrolysis," *international journal of hydrogen energy*, vol. 38, p. 4901e4934, 2013.
- [39] d. o. I. S. E. a. R. Australian government, "NATIONAL GREENHOUSE ACCOUNTS FACTORS, Australian National Greenhouse Accounts," 2021. [Online]. Available: <https://www.industry.gov.au/sites/default/files/August%202021/document/national-greenhouse-accounts-factors-2021.pdf>. [Accessed January 2022].
- [40] M. M. Kostic, "Energy: Global and Historical Background," in *Encyclopedia of Energy Engineering and Technology, Second Edition*, Taylor & Francis, 2007.
- [41] A. Government, "Australia's emissions projections 2021," Australian Government, Department of Industry, Science, Energy and Resources, 6 October 2021. [Online]. Available: <https://www.industry.gov.au/data-and-publications/australias-emissions-projections-2021>. [Accessed 1 February 2022].
- [42] T. B. (Germany), L. F. (USA), E. H. (Austria/Norway), A. M. (UK/Germany), D. P. (Argentina), J. R. (India), R. S. (Brazil), S. S. (Germany), R. S. (. Zealand) and P. S. (UK), "Technology-specific Cost and Performance Parameters," IPCC, 2018. [Online]. Available: [https://www.ipcc.ch/site/assets/uploads/2018/02/ipcc\\_wg3\\_ar5\\_annex-iii.pdf](https://www.ipcc.ch/site/assets/uploads/2018/02/ipcc_wg3_ar5_annex-iii.pdf). [Accessed 10 August 2022].
- [43] "Taskforce, COAG Energy Council" – "National Hydrogen Strategy", "Deloitte, Australian and Global Hydrogen Demand Growth Scenario Analysis," COAG Energy Council, 2019.
- [44] (ISPRA) and A. Caputo, "Fattori di emissione atmosferica di gas a effetto serra nel settore elettrico nazionale e nei principali Paesi Europei," ISPRA, Rome, 2020.