



Production of Hydrogen via Renewable Energy and Investigation of Water Molecular Changes During Electrolysis Process

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ABSTRACT

Studies on renewable energy are essential topics that help find new energy sources to replace fossil sources and promote environment friendliness. Hydrogen is the most practical alternative energy carrier source that meets the mentioned purposes. The mass of hydrogen element in the Earth's water was calculated and found to be about 2.1×10^{20} kg, which is greater than the mass of the world oil reserves by about 9×10^5 times. In addition, essential details of water molecular arrangement were investigated in order to better understand the electrolysis of water. Also, the energy of covalent and hydrogen bonds per molecule of water was theoretically calculated and found to be about 8.17×10^{-19} J/molecule and 3.87×10^{-20} J/molecule, respectively. In the electrolysis process, two stages should be undertaken: the first stage was to break hydrogen bonds between water molecules, in which all water eclectic dipoles would align in the direction of the Applied Electric Field across the electrolysis unit. The second stage was to break water covalent bonds to generate H_2 and O_2 gases. Moreover, the lowest cost to generate one kg of hydrogen (0.4 \$/kg) by electrolysis method using solar energy was about 0.4 \$, which has already been proven, while this value was about 2.8 \$/kg upon considering the average price of electricity of Oman in comparison.

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1. INTRODUCTION

Environmental challenges, availability of energy, and its sustainable development are the most vital issues that are faced by any nation. Most conventional energy sources and continuous environmental deterioration result from inadequate global cooperation. The population of the world will probably be about 9 billion in 2050 and the required power to run this huge population is around 30 TW; about 85 % of this power will be provided from fossil sources at that time [1]. In addition, fossil sources will be depleted with the passage of time. Therefore, in order to bridge this gap in energy sources in the future and to mitigate the environmental risks, the world has started to think seriously in green renewable energy sources such as solar, wind, geothermal, nuclear fusion, magnetic energy, and hydrogen as reliable energy carriers.

After the oil crisis of 1973 [2, 3], the search to find alternatives to fossil sources has exponentially increased and most Western and European countries have begun to invest massive capital in renewable energy sources. Furthermore, transformation to renewable energy will rely on the pace of development in this sensational field and its competitive price to meet the energy demand instead of fossil sources in the future as required. A general vision of the energy supply

sustainability until 2050 for global transformation of the renewable energy sector has been propounded by the International Renewable Energy Agency (IRENA) [4].

In 2019, Zhai reported that within the last decade, the world began to show its concern and fear about the global environment changes because of the greenhouse effect due to fossil fuels combustion and now, they are trying to become a low-carbon world [5]. According to this report, hydrogen has received substantial attention because of its capability to produce water as a byproduct when burning with oxygen, hence eliminating harmful gases and replacing fossil fuels. He also anticipated that the percentage of hydrogen fuel might reach about 18 % of total world energy demand in 2050. Essential details of renewable energy sources, one of which was hydrogen, were investigated by Moosa and Kazem [6]. Globally, around 95 % of hydrogen gas is produced from fossil sources such as natural gas CH_4 , oil, and coal and just about 4 % is produced by water electrolysis method [7]. The serious drawback to using fossil fuels to produce hydrogen gas is environmental pollution with a high percentage of carbon dioxide CO_2 , which then exacerbates the problem of global warming. During 2019, Johan Martens and his co-researchers at KU Leuven in Belgium stated that hydrogen gas could be produced from air moisture using solar panels [8]. Very significant details of hydrogen production in different ways such as electrolysis, hot steam of natural gas CH_4 , photo electrolysis process, plasma cracking, pyrolysis,

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copyrolysis, and thermochemical water splitting routes at a temperature of about 650 °C have been published [9-14]. A comprehensive review of biohydrogen production was reported by Sarvanan et al. in 2020 [15]. They emphasized that biohydrogen and biofuel could be used instead of fossil fuels to resolve their depletion problem over time and with no greenhouse effect. This review includes remarkable details about Microbial Fuel Cells (MFC) and Microbial Electrolysis Cells (MEC). Also, Samsudeen et al. demonstrated that hydrogen could be generated from the distilling of wastewater [16]. They contracted their own compact design of MEC for this purpose. Their results achieved higher efficiency than the conventional route of hydrogen production employing the Microbial electrolysis technique.

To the best of our knowledge and information, the total mass of hydrogen element in the Earth's water as an energy carrier has not been estimated and compared with the world reserve oil so far. In addition, there is a lack of available detail about water molecular structure changes that happen during water electrolysis to produce hydrogen and oxygen gases. The production cost of one kilogram of hydrogen by electrolysis route by utilizing recent solar energy price will be included in the planning of the present work, and it will be compared to the cost of production using the price of electricity in Oman. Furthermore, the authors will focus on using the released byproduct drain-water from air-cooling systems in humid areas to feed the electrolysis cells instead of the water produced by conventional ways to reduce the production cost of hydrogen, which is a new idea in this field.

Depending upon the previous review, the aims and objectives of this article are: (i) Calculating how much the amount of hydrogen is available in the Earth compared with the mass of proven world oil reserves; (ii) devoting very significant attention to hydrogen which is produced using water electrolysis in correlation with some renewable energy sources to generate the required electricity such as solar and wind energy; (iii) comparing the hydrogen production cost when using the present price of electricity in Oman, with the recent price of solar electricity; and (iv) meanwhile, studying the changes that occur for water molecular arrangement during the electrolysis process under the effect of a direct current circuit.

2. HYDROGEN MASS AS EARTH COMPONENT

The hydrogen mass in the Earth can be calculated in proportion to the Earth's water. Table 1 includes different estimated water reservoirs in the Earth. It is very difficult to access mantle water which can be found at the depth ranges of about 400-600 km [17]. Therefore, other amounts of water will be counted to calculate approximately the mass of hydrogen in the Earth: $(1.37 \times 10^{21} \text{ kg} + 5 \times 10^{20} \text{ kg}) = 1.87 \times 10^{21} \text{ kg}$. From Table 1, the volume of the Earth's water (V_{water}) is approximately $5.87 \times 10^{18} \text{ m}^3$ after using the pure water density of $1 \times 10^3 \text{ kg/m}^3$ at 1 Atm. pressure and 25 °C to calculate the volume of the water ($V_{\text{water}} = m/\rho_{\text{water}}$). The volume of the Earth is about $1.1 \times 10^{21} \text{ m}^3$ ($V_{\text{Earth}} = 4/3\pi r^3$, $r = 6.37 \times 10^6 \text{ m}$); therefore, the volume of the Earth's water is around 0.53 % of Earth's volume.

The mass of hydrogen in the water contained in the Earth without mantle water can be calculated as follows:

The molar mass of the water H_2O is $\sim 18 \text{ g/mol}$ and the total number of moles of H_2O in Earth's water is:

$$\begin{array}{l} \frac{\text{No. of mole}}{1 \text{ mol H}_2\text{O}} \quad \frac{\text{Mass}}{18 \text{ g}} \\ x \quad 1.87 \times 10^{24} \text{ g} \rightarrow x = \frac{(1 \text{ mol H}_2\text{O})(1.87 \times 10^{24} \text{ g})}{18 \text{ g}} \\ = 10.39 \times 10^{22} \text{ mol} \approx 10.4 \times 10^{22} \text{ mol} \end{array}$$

Each mole of H_2O contains 2 moles of H element so that the total mass of the H element in the water is:

$$\text{Mass of the H element} = (\text{No. of mol H}_2\text{O})(2)(\text{molar mass of H}) = (10.4 \times 10^{22} \text{ mol})(2)(1.008 \text{ g/mol}) \approx 2.1 \times 10^{23} \text{ g} \approx 2.1 \times 10^{20} \text{ kg} \quad (1)$$

Similarly, the number of H_2O moles in one kg of water is:

$$\begin{array}{l} \frac{\text{No. of mole}}{1 \text{ mol H}_2\text{O}} \quad \frac{\text{Mass}}{18 \text{ g}} \\ x \quad 1000 \text{ g} \rightarrow x = \frac{(1 \text{ mol H}_2\text{O})(1000 \text{ g})}{18 \text{ g}} = 55.55 \text{ mol} \end{array}$$

Therefore, the mass of the H element in one kg of H_2O is:

$$\text{Mass of the H element} = (\text{No. of mol H}_2\text{O})(2)(\text{molar mass of H}) = (1 \text{ kg})(55.55 \text{ mol})(2)(1.008 \text{ g/mol}) \approx 112 \text{ g}$$

Table 1. Different reservoirs of the Earth's water [17]

Type of reservoir	~ Mass (kg) [17]	~ Volume m^3 $V = m/\rho_{\text{water}}$	of Earth's volume %
Oceans	1.37×10^{21}	1.37×10^{18}	0.1245 %
Ice and snow, Atmospheric moisture, Rivers, Groundwater, Sedimentary rocks, Lakes, Soils	5×10^{20}	5×10^{17}	0.0454 %
Mantle water	4×10^{21}	4×10^{18}	0.3636 %
Total	5.87×10^{21}	5.87×10^{18}	~ 0.53 %

Another approach to determining the hydrogen and oxygen amount per kilogram of water is as follows:

$$\% \text{ elem. in a comp.} = \frac{n(\text{molar mass of the elem.})}{\text{molar mass of the comp.}} \times 100 \quad (2)$$

where n is the number of atoms of the counted element in the compound. Afterwards, the mass of the element can be calculated at a certain amount of any compound as follows:

$$\text{Mass of elem. in a comp.} = \text{mass of the elem. in the comp.} \times \text{percent of the elem. in the comp.} \quad (3)$$

Hence, the % H and % O in one kg of water:

$$\% \text{ H} = \frac{2(\text{molar mass of H})}{\text{molar mass of H}_2\text{O}} \times 100 \% = \frac{2(1.008 \text{ g/mol})}{18 \text{ g/mol}} \times 100 \% = 11.2 \%$$

$$\% \text{ O} = \frac{1(\text{molar mass of O})}{\text{molar mass of H}_2\text{O}} \times 100 \% = \frac{1(16 \text{ g/mol})}{18 \text{ g/mol}} \times 100 \% = 88.88 \%$$

Thus, the masses of H and O in one kg of water are:

$$\begin{aligned} \text{Mass of H in 1 kg of water} &= \text{watermass} \times \text{percent of H} \\ &= (1 \text{ kg})(0.112) = (1000 \text{ g})(0.112) = 112 \text{ g} \end{aligned}$$

$$\begin{aligned} \text{Mass of O in 1 kg of water} &= \text{watermass} \times \text{percent of O} \\ &= (1 \text{ kg})(0.8888) = (1000 \text{ g})(0.8888) = 888.8 \text{ g} \end{aligned}$$

The total mass of H and O is 100.8 g; the slight difference results from the rounding process of the molar masses of H, O, and H₂O. From these calculations, it can be concluded that the generated mass of O is much higher than that of H by about 8 times. This result should be considered environmentally and economically for a massive quantity of oxygen mass as a byproduct of the electrolysis process. Fortunately, this byproduct oxygen gas can be used in many industrial and health sectors. Furthermore, it is expected that the mentioned gas will reduce the level of carbon dioxide CO₂ in the atmosphere to a greater extent upon turning to global-scale renewable energy rather than fossil fuels. This matter must be considered in advance by environment specialist scientists to guess the environmental changes that will result from the use of many renewable energy sources instead of fossil fuels.

The total world oil reserve on 31st December 2018 was about 1,663,331 million barrels, around 50 % of which is produced in the Middle East countries. The top 10 reserves holders range from Venezuela (302,809 million) all the way to Libya (48,363 million) [18]. The volume of the oil barrel is approximately 42 gallons and the volume of one gallon is about 0.003785 m³ so that the volume of one barrel of oil is around 0.159 m³. The average of crude oil density is about 900 kg/m³ which is dependent on the production zone [19] and so, the mass of crude oil barrel is about 143 kg ($m = \rho V$). The whole mass of the world oil reserves ($M_{\text{res.oil}} = \text{no. barrels} \times 143 \text{ kg}$) is around $2.38 \times 10^{14} \text{ kg}$. Therefore, the mass of the hydrogen element (M_{H}) in the Earth as calculated above ($\sim 2.1 \times 10^{20} \text{ kg}$) is much greater than the mass of the world crude oil reserves by about 9×10^5 times:

$$\frac{M_{\text{H}}}{M_{\text{res.oil}}} = \frac{2.1 \times 10^{20} \text{ kg}}{2.38 \times 10^{14} \text{ kg}} = 8.8 \times 10^5 \approx 9 \times 10^5$$

3. ENERGY STORED IN HYDROGEN FUEL

The stored energy in hydrogen fuel is in the range of 120-143 MJ/kg, while it is much less in the case of fossil fuels, e.g., is around 54 MJ/kg and 46 MJ/kg in the liquefied natural gas and automotive diesel, respectively [1, 14]. Also, fossil fuels will surely come to an end in the coming future, even if the Earth is entirely turned into fossil fuels. Therefore, researchers and policy-makers should seriously consider hydrogen as a promising energy carrier and other renewable energy sources to replace fossil fuels in many energy sectors. Table 2 includes the energy density (MJ/kg) for different types of fossil fuels and hydrogen.

4. SIGNIFICANCE OF HYDROGEN

- Representing the future source of energy carrier that can replace fossil fuels.
- Being the source of solar energy, as the Sun is almost a plasma of hydrogen ions and electrons confined by a very strong magnetic field to keep the Sun in its present form and

activity [6]. Therefore, the hydrogen element is the basis of life on the Earth because the Sun is the main source of energy.

- Generally, there is no water on the Earth without the existence of hydrogen element [20]. The water is the main component of the human body (around $\frac{3}{4}$ of the human body consists of water on average), plants, and other organisms. Hydrogen is one of the elements that forms the water molecules and the water is the basic substance to maintain life on our planet beside the Sun.
- Petroleum materials mainly consist of carbon and hydrogen, which are extremely important sources of energy that ensure the continuity of life on the Earth, in addition to the renewable energy contribution by a small proportion, nowadays, and in the near future.
- It has been very successfully used in the production of very strong Rare Earth Permanent Magnets (REPM) worldwide since 1978 employing the Hydrogen Decrepitation (HD) process. In this process, hydrogen could be fragmented to cast Rare Earth ingots of Sm-Co and Nd-Fe-B when exposed to hydrogen gas to get very friable hydride, which is easy to mill to the required particle size prior to magnets production [21].

Table 2. Energy density of different fuels in [1] and [14]

Fuel	Energy density (MJ/kg), [14]	Energy density (MJ/kg), [1]	Av. energy density (MJ/kg)
Hydrogen	120	143	131.5
Liquefied natural gas	54.4	54	54.2
Propane	49.6	-	-
Aviation gasoline	46.8	-	-
Automotive gasoline	46.4	44	44.8
Automotive diesel	45.6	46	45.8
Ethanol	29.6	-	-
Methanol	19.6	20	19.8
Coke	27	24	25.5
Wood (dry)	16.2	16	16.1
Biogases	9.6	-	-

5. WATER FOR ELECTROLYSIS PROCESS

Freshwater is the main substance in the electrolysis of water to produce hydrogen gas. Production of freshwater from rivers, groundwater, and desalination of seawater is very costly according to the world standard level. Producing water for electrolysis at a low cost is one of the significant factors in reducing hydrogen production expenditure. Consequently, encouraging the world to use it as an alternative source of energy carrier instead of fossil fuels.

All sources of natural freshwater come to being with the formation of atmospheric moisture as water vapor by solar energy everywhere in the world. Subsequently, the hydrologic cycle (water cycle) starts to circulate itself as a natural system between the atmosphere and the Earth until the end of the Sun's epoch because the Sun is not an endless source of energy [6]. Generally, about 97.5 % of the Earth's water is briny. Around 2.5 % is freshwater, 70 % of it is ice at the polar caps, and about 30 % is atmospheric moisture. Thus, only < 1 % of the water is ready for direct use [22]. In fact, even the main cause of the natural freshwater formation on the Earth is hydrogen ions in the Sun, which consists of plasma of hydrogen ions and electrons as mentioned above. All-natural freshwater is formed by the condensation of water vapor in the

atmosphere as rainwater. Generally, the cheapest freshwater provided by electrolysis or any other methods involves a process in which water generates hydrogen, which can be summarized as follows:

- Direct rainwater collection and storage.
- Collection of drain water out of cooling air-conditioning units given that this water is a byproduct in humid areas [23]. It was found to be almost distilled water with a pH of about 7, very low electrical conductivity, and low TDS [24]. Table 3 reveals some chemical and physical parameters of the drain water released from Air Cooling systems in three Provinces of Oman, even though the TDS can be greatly reduced by filtration.
- Condensation and precipitation of water vapor take place in coastal and agricultural places worldwide, which are characterized by relatively high humidity zones, through any cooling system technique in correlation with solar or wind energy [25, 26]. Figure 1 shows monthly mean values of Relative Humidity (RH %) in the year 2019 in Sohar, which is one of the coastal cities in Oman. The trend of the curves is almost the same; the maximum value of the three curves is in July which represents the peak of summer in Oman. Also, there is a valley shape in the spring season from March to May in Oman. The mean value of the RH % in the year 2019 is about 67 %, which is too high to exploit to produce freshwater for various uses.

Table 3. Some physical and chemical analysis of drain-water released from air cooling unit in three provinces in Oman [24]

Parameters	Results: mean value of 3 samples of collecting drain-water		
	Muscat	Sohar	Al-Buraimi
Temperature (°C)	20.7	22	19.1
Turbidity (NTU)	0.57	0.94	2.1
pH	7.01	6.9	7.01
Electrical Conductivity, EC (µS/cm)	25.29	40.44	45.68
TDS (Total Dissolved Solids) (mg/L)	16.44	25.29	29.69
Chloride Cl ⁻ (mg/L)	6.17	3.7	4.68
Total alkalinity (mg/L)	12.6	17	20.33
Calcium hardness (mg/L)	2.8	2.46	7.53
Total Hardness (mg/L)	4.13	3.33	7.8
NO ⁻³ (mg/L)	1.03	0.39	1.42
SO ₄ ⁻² (mg/L)	2.47	1.73	5.82

6. PRODUCTION OF HYDROGEN BY ELECTROLYSIS USING RENEWABLE SOURCES

6.1. Production process

One of the objectives of this research is to focus on the production of hydrogen via water electrolysis as the easiest method and using renewable energy sources for electricity generation to feed the electrolysis cells. In countries where

high solar intensity is abundant such as all Middle East countries, in which 90 % of the days are sunny per year. Accordingly, solar energy is the best and cheapest option for long-term plans to provide the required electricity for hydrogen production. This idea has been strongly recommended by the authors of the current article [6, 24].

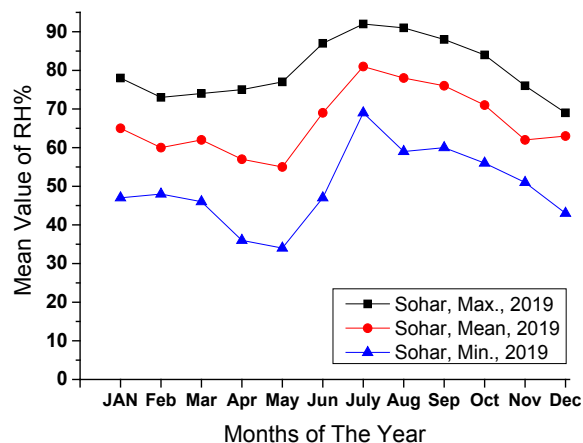


Figure 1. Monthly mean values of RH % vs. the months of 2019, Sohar, Oman

The electrolysis process of water can be defined as chemical-physical actions to split the water molecule into its hydrogen and oxygen elements by applying a direct current through the electrolysis unit. It is a chemical process because the water molecule decomposes into H and O elements and it is also a physical process because electrical energy must be provided to the electrolysis unit to generate H₂ and O₂ gases at its electrodes (cathode and anode) at room temperature. Commonly, electrodes are made of Platinum, Nickel, or Stainless Steel to avoid corrosion.

Electrolysis of water is a very practical method to produce hydrogen in correlation with the most available renewable energy sources such as PV solar panels and wind turbines. The production of hydrogen utilizing renewable energy was reported by Levene et al., Badea et al., and Bca'kova' et al. [27-29]. Historically, the electrolysis of water method to generate hydrogen gas has been known for 223 years, with its first discovery dating back to 1797 by Troostwijk and Deiman [30].

The advantages of using electrolysis route for hydrogen production over other adopted production methods include (i) being the easiest approach which can be run at room temperature, (ii) non-requirement for highly sophisticated technology, (iii) higher efficiency, and (iv) zero greenhouse gas byproduct in the case of using solar or wind energy. Figure 2 illustrates the electrolysis unit together with solar panels and wind power mill setting to provide the required electricity. The efficiency of hydrogen gas production reaches about 75 % through electrolysis [31].

According to Figure 2, the pressure of H₂ gas is twice O₂ gas pressure, because each molecule of water contains two atoms of hydrogen and one atom of oxygen and the volume of H₂ is twice the O₂ volume according to the ideal gas law:

$$P_H V_H = n_H RT \rightarrow P = \frac{n_H RT}{V_H} \quad (4)$$

where n is the number of moles and in the case of the water electrolysis, the produced moles of H₂ are twice that of O₂.

The production equation for hydrogen and oxygen gases by electrolysis route is given below:

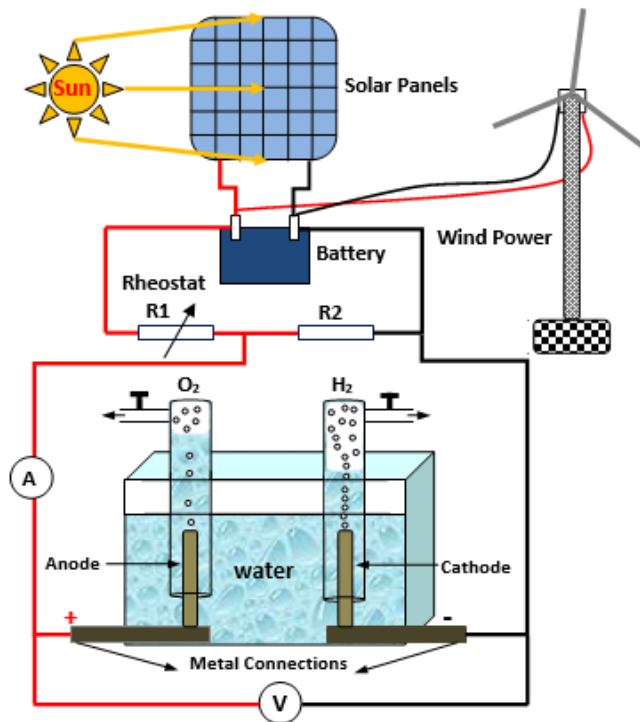
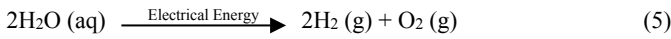


Figure 2. General proposed schematic setting of electrolysis unit of water using solar and wind power

Electricity provided by some renewable energy sources could help to provide vast amounts of hydrogen for different uses with no harmful environmental impact [32], particularly in countries that receive high solar intensity, as in the Middle East and African countries. Most territories of these countries are unused Sahara areas with very high solar intensity. As a logical consequence, such countries will likely be exporters of electricity from solar fields and of hydrogen produced by solar energy.

In Europe and other countries that have wide agricultural areas as well as those with long coastal lines, wind energy is the dominated option for hydrogen production, because different regions in such countries are characterized by pressure differences (ΔP s) and high relative humidity RH % because of water evaporation and plants transpiration process. The ΔP s will cause the formation of wind which can be utilized for electricity generation. The higher RH % value helps collect an immense quantity of water by condensation process, thus augmenting the production of green hydrogen using renewable energy. Germany in Europe is the best example of widely using wind energy on a large scale [33], and Oman in the GCC countries has a very long coastline with a length of about 3160 km and high RH % and also receives a very high solar intensity [6]. The most important factor in the production of hydrogen is electricity price, which has significant influence on the hydrogen sale price.

To understand what happens over the electrolysis process, much meditation must be given to changes to the water molecular structure. The water molecule is polar and consists of 2 H atoms and O atom, forming two electric dipoles with an angle of about 105° , as shown in Figure 3.

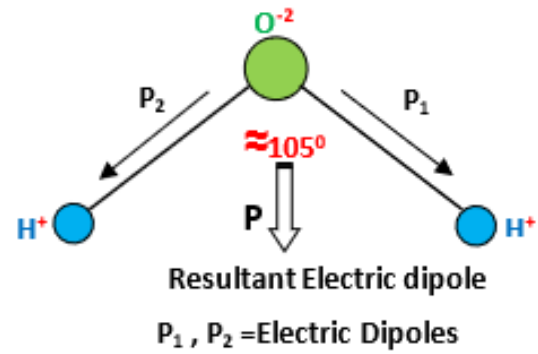


Figure 3. Ionic structure of water molecule with 2 electric dipoles P_1 and P_2

The bonds between H and O atoms in the water molecule are covalent, because the first orbit of H atom is saturated by 2 electrons and the second orbit of O atom is saturated by 8 electrons. These bonds are weak and can be broken by slight energy, of about 492 kJ/mol [34]. Meanwhile, this sort of water molecular structure will lead to formation of another type of bonds, called hydrogen bonds, due to the electrostatic reaction between the positively charged hydrogen and the negatively charged oxygen of the water molecules. These bonds are very weak within the range of 23.3 kJ/mol [34]. By using these values of energy densities and after dividing them on the Avogadro's number ($\sim 6.022 \times 10^{23}$ atom or molecule/mole), the energy per molecule of covalent and hydrogen bonds is about 8.17×10^{-19} J/molecule and 3.87×10^{-20} J/molecule, respectively.

To generate hydrogen by electrolysis of water; covalent and hydrogen bonds of the water molecules must be broken by applying enough external electric field across the electrolysis cell. This process will occur in two stages:

Stage one

At this stage, the water dipoles will be aligned in the direction of the Applied Electric Field (\mathbf{E}) due to the electrical effect between \mathbf{E} and the electric charges of H^+ and O^{2-} of each dipole. As a result, electric force \mathbf{F} is exerted on each charge of the electric dipoles ($\mathbf{F} = q \mathbf{E}$), \mathbf{F} and \mathbf{E} are written as bold letters because they are vector quantities. Consequently, the dipoles will orient according to the direction of \mathbf{E} , as illustrated in Figure 4. The angle between the dipoles of H-O certainly will decrease because of the net forces exerting on H^+ and O^{2-} of each molecule. This stage represents the phase of the hydrogen bonds disjointing within a certain limit of \mathbf{E} , which must be enough to align all water molecules, as shown in Figure 4. The magnitude of \mathbf{E} across the electrolysis cell can be controlled by adjusting the distance d between the cathode and the anode of the cell, and the applied external potential difference V , ($E = V/d$), where \mathbf{E} is directly proportional to V and inversely proportional to d .

Stage two

Stage two represents the rupture between water covalent bonds by increasing the applied external voltage gradually until bubbles of hydrogen and oxygen gases start to appear around the cathode and the anode of the electrolysis cell. In this period, the magnitude of \mathbf{E} must be greater than the dielectric strength of the used water. Generally, the dielectric strength represents the maximum of \mathbf{E} that the dielectric substance can withstand before its breakdown. The pure water is a dielectric substance with dielectric constant of 80.4 at

room temperature and dielectric strength of 6.5×10^7 V/m [35]. Figure 5 clarifies the idea of forming H_2 and O_2 gases through electrolysis route. Water with low electrical conductivity and TDS is preferred to be used in the electrolysis process to avoid the formation of some compounds on the cathode and the anode. Therefore, as noted in Table 4, the collected and released drain water from cooling air-conditioners as a byproduct is ready to be used in electrolysis cells for hydrogen production [24].

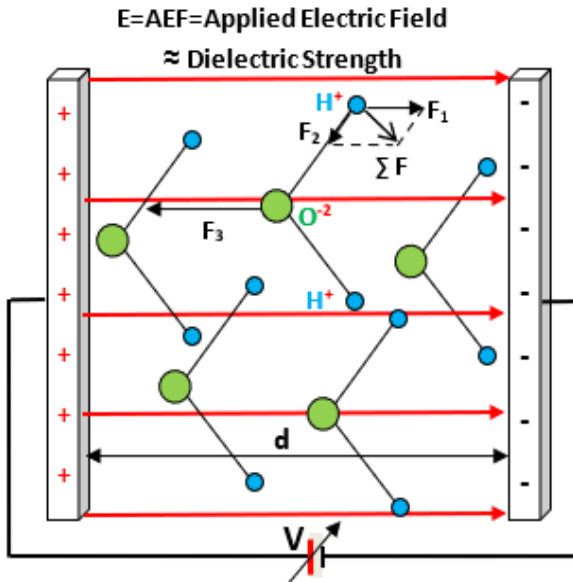


Figure 4. Full alignment of the water dipoles under the influence of E

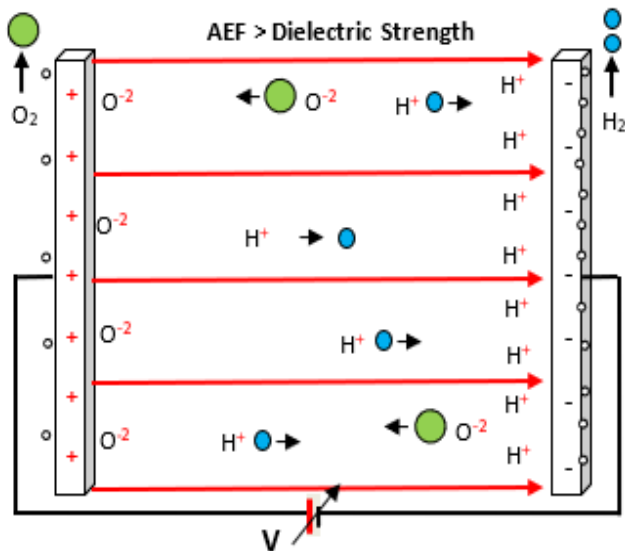


Figure 5. Splitting the molecules of the water into hydrogen and oxygen by electrolysis method

7. DETERMINING REQUIRED ENERGY TO DECOMPOSE ONE KILOGRAM OF WATER INTO OXYGEN AND HYDROGEN

7.1. Using domestic electricity

The required electricity to decompose one kilogram of H_2O can be calculated as follows:

- The total energy to break the covalent and hydrogen bonds of the water is:

$E = 492 \text{ kJ/mol} + 23.3 \text{ kJ/mol} = 515.3 \text{ kJ/mol}$, as mentioned in the above information [34].

- Each kilogram of H_2O contains about 55.55 mole of water molecules; hence, the total required energy for electrolysis one kg of water is:

$$E = (515.3 \text{ kJ/mol})(55.55 \text{ mol}) \approx 28625 \text{ kJ}$$

- Energy unit factor is converted as follows:

$$1 \text{ kWh} = 3.6 \times 10^3 \text{ kJ}$$

- Therefore, the energy (kWh) for electrolysis of one kg of water is:

$$1 \text{ kWh} = 3.6 \times 10^3 \text{ kJ}$$

$$x \quad 28625 \text{ kJ} \quad \rightarrow \quad x = \frac{(1 \text{ kWh})(28625 \text{ kJ})}{3.6 \times 10^3 \text{ kJ}} \approx 8 \text{ kWh}$$

- Given that the energy price of one kWh in Oman is 15 Pisa on average in Oman, the cost of converting one kg of water into H_2 and O_2 gases is ($8 \text{ kWh} \times 15 \text{ Pisa/kWh} = 120 \text{ Pisa} = 0.12 \text{ RO}$, RO = Rial Omani). Each kilogram of water contains about 112 g of hydrogen and about 888 g of oxygen; therefore, the cost of producing one kg of hydrogen by electrolysis route is as follows:

Mass of H	Cost in RO
112 g	0.12 RO

$$1000 \text{ g/kg} \quad x \quad \rightarrow \quad x = \frac{(0.12 \text{ RO})(1000 \text{ g/kg})}{112 \text{ g}} \approx 1.07 \text{ RO/kg}$$

1 Rial Omani equal 2.6 US Dollar as an average of 2020; thus, the cost to produce one kg of hydrogen in the US Dollar is $1.07 \text{ RO/kg} \times 2.6 \text{ \$/RO} = 2.78 \text{ \$/kg}$. These are theoretical calculations; however, in practice, the cost may be much more or less depending on the experimental work and electricity price during the production stage. Also, the almost pure byproduct oxygen gas that is generated during the electrolysis process will be definitely used in industrial and health sectors instead of the industrial one.

7.2. By using solar electricity

In Oman, the Authority for Electricity Regulation (AER) in March 2018 has approved the grid-connected PV incentives. Any surplus power exported back into the grid will be remunerated at prevailing Bulk Supply Tariffs (BST), which are higher than the electricity tariffs for residential customers – a feature designed to incentivize the rollout of rooftop solar capacity under the Authority’s “Sahim” initiative.

The cost of energy is calculated based on the “Sahim” initiative. The costs of Grid-Connected Photovoltaic (GCPV) systems specified by the AER are as follows: 0.879, 0.805, and 0.776 USD for 1-10 kWp, 10-100 kWp, and 100-500 kWp, respectively. Table 4 shows the Cost of Energy (CoE) compared with studies in Oman. It is worth mentioning that the cost specified by the AER is relatively high.

From Table 4, the calculated revenue for grid-connected PV systems in different sites of Oman is promising for PV system installation due to the higher solar energy available than that in other sites. In addition, it is noted that the authors of [36-40] did not consider the production reduction due to system age. In other words, the CoE in these researches could be higher than the stated one in the case of considering this important issue.

Table 4. PV systems' cost of energy comparison

Ref.	Year	Location	PV power	Cost of generated kWh (\$)	Cost of generated kWh (RO)
[36]	2011	Oman	10 kW	0.2100	0.081
[37]	2011	Oman	5 MW	0.3270	0.125
[38]	2012	Oman	50 kW	0.2060	0.079
[39]	2017	Oman	1 MW	0.2258	0.086
[40]	2019	Oman	1.4 kW	0.0450	0.017
AER CoE	2018	Oman	-	0.7760	0.298

Therefore, using solar energy, the production cost of hydrogen is calculated:

$$\frac{\text{Mass of H}}{112 \text{ g}} \quad \frac{\text{Cost in RO}}{0.298 \text{ RO}}$$

$$1000 \text{ g/kg} \quad x \rightarrow x = \frac{(0.298 \text{ RO})(1000 \text{ g/kg})}{112 \text{ g}} \approx 2.66 \text{ RO/kg}$$

However, this cost is relatively high since it depends on the selling of electricity to the grid. If a standalone solar system is used and is dependent on the highest and lowest costs published by [37] and [40], respectively, the cost will be as follows:

$$\frac{\text{Mass of H}}{112 \text{ g}} \quad \frac{\text{Cost in RO}}{0.125 \text{ RO}}$$

$$1000 \text{ g/kg} \quad x \rightarrow x = \frac{(0.125 \text{ RO})(1000 \text{ g/kg})}{112 \text{ g}} \approx 1.11 \text{ RO/kg}$$

This value in [37] is in good agreement with our calculation above when using the domestic electricity price.

$$\frac{\text{Mass of H}}{112 \text{ g}} \quad \frac{\text{Cost in RO}}{0.017 \text{ RO}}$$

$$1000 \text{ g/kg} \quad x \rightarrow x = \frac{(0.017 \text{ RO})(1000 \text{ g/kg})}{112 \text{ g}} \approx 0.151 \text{ RO/kg}$$

The last value in [40] (0.151 RO/kg is about 0.4 \$/kg) points to a very promising method to produce hydrogen using solar energy and is probably reduced over long-term use. This value represents the lowest cost of hydrogen production worldwide.

8. THE FUTURE VISUALIZATION OF USING HYDROGEN AS AN ENERGY CARRIER

The great advantage of using hydrogen as a future energy carrier fuel is two-fold: its high availability in the Earth's water and its burning with oxygen yields water as a byproduct. Also, the hydrogen fuel cell automobiles are classified by zero harmful greenhouse gases emission. It appears that hydrogen as an alternative energy carrier has the following advantages over the fossil fuels:

- It is very environment friendly as its combustion feedback is water byproduct.

- The byproduct water can be reused to generate hydrogen gas again and consequently; the hydrogen production cycle repeats itself using many renewable energy sources.
- Globally, more abundant than any other element can be used as an energy carrier fuel.
- Hydrogen energy density is greater than that of fossil fuels by about 2.4 times (Please see Table 2). It is characterized by the highest energy density among other energy sources.
- It can be produced using many methods and different energy sources, either renewable or ordinary.
- Hydrogen contributes to solving energy scarcity problems worldwide in intermediate- and long-term scenario plans, say 2040-2050.
- The production cost will decrease upon reducing renewable energy price with the passage of time such as solar and wind energy.
- It can be used as liquid or gas in many domestic sectors and industry such as power generation or fuel cells that convert chemical energy into electrical energy to run engines such as trucks, trains, cars, etc.

Figure 6 accentuates a general idea about hydrogen production by electrolysis route using condensed water from atmospheric moisture and electricity generated by solar or wind energy.

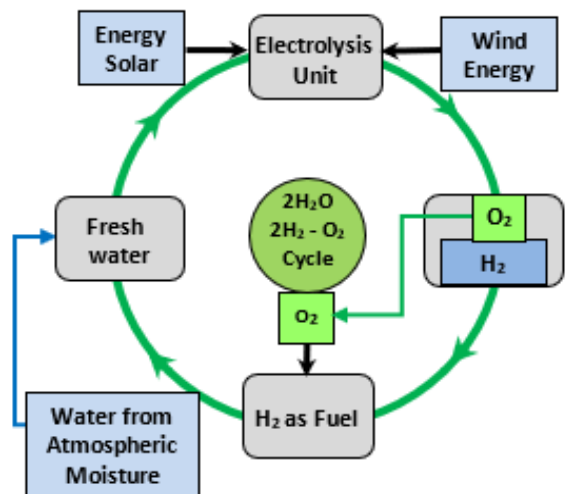


Figure 6. A general scheme of water-hydrogen-oxygen-fuel cycle by electrolysis together with solar and wind energy

In 2019, very essential details of production routes and the future of using hydrogen in many energy sectors were almost fully reported by the IEA (International Energy Agency) [41]. In April 2020, Bill Ireland urged the world seriously to adopt hydrogen as a future green fuel to overcome the global greenhouse effect [42]. According to the recent report of the International Renewable Energy Agency in September 2019, the production cost of hydrogen utilizing solar and wind energy will be very competitive to fossil fuels during the coming five years. The report also revealed that the cost of green hydrogen would be less than that produced from fossil fuels in the period of 2030-2040 [43]. Figure 7 projects the general view of hydrogen production cost via solar and wind energy up to 2050, from which it could be seen that the cost is always less upon using wind energy. Generally, the production cost decreases with time for the two cases because of technological development in these two important fields of renewable energy applications.

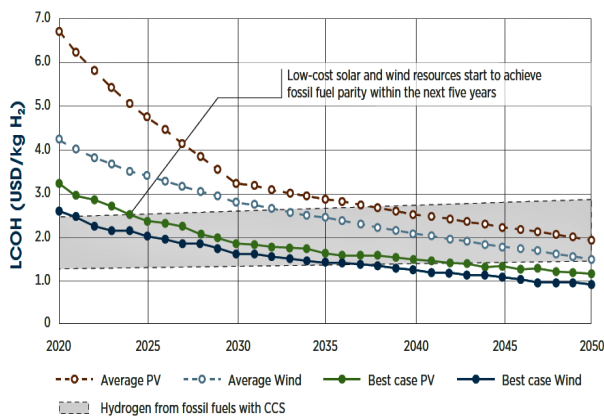


Figure 7. The production cost of hydrogen with years using solar and wind energy; LCOH: Levelized Cost of Hydrogen; CCS: Carbon Capture and Storage [43]

Very important visions about hydrogen as a renewable source of energy were proposed by Pareek et al. in 2020 [44]. They confirmed that hydrogen was the most attractive option of renewable source to replace fossil fuels, that are inevitably declining with time, in addition to no environmental harm when using green-hydrogen as a fuel.

9. RESULTS AND DISCUSSION

Hydrogen, as the most abundant Earth element, has been theoretically estimated depending on the whole water reserves in the Earth, excluding the mantle water, which is very deep into the Earth's crust. The obtained result showed that the quantity of hydrogen of the Earth was much greater than the world oil reserves by about 5×10^5 times. Economically, this finding is remarkable and it makes hydrogen ready as an energy carrier to ensure its adoption as the alternative to fossil fuels when required. In addition, some important features of hydrogen are summarized to highlight the research of this field.

It is proven that finding freshwater with low price, or free of charge, as a byproduct from any physical activities is very essential to reduce the production cost of hydrogen and oxygen gases by electrolysis technique. Therefore, using the byproduct-gained water from any air-cooling system in humid areas certainly will reduce the production cost of hydrogen in any way. Technically and comparatively, using almost distilled water, as shown in Table 3, is more reliable than wastewater, used in the biohydrogen method to generate hydrogen [15, 16].

A deeper study on the electrolysis of water to produce hydrogen and oxygen gases is still very necessary for researchers in this field to demonstrate the physical water structure variations via the influence of DC current. The energy to split water molecules into hydrogen and oxygen after breaking the covalent and hydrogen bonds of the water was theoretically calculated, which is a very important attempt to understand the electrolysis process better.

The cost of producing one kilogram of hydrogen by water electrolysis method through the proposed theoretical framework of ours and based on the present price of electricity in Oman was determined to be about 2.8 \$/kg. This cost is quite reasonable compared with those in other relevant researches [27, 37, 40]. Furthermore, this study proved the lowest cost of hydrogen production so far by using recent

solar energy price in Oman, which was about 0.4 \$/kg as a very significant novel result.

The general conclusion is that hydrogen is a very encouraging energy carrier to replace the fossil fuels, which are already depleting with time. Meanwhile, using hydrogen in different sectors on a large scale will contribute to the reduction of greenhouse harm gases and global enhancement of the environmental quality.

10. CONCLUSIONS

The novelty of the article can be given as follows:

- (i) The whole hydrogen mass of the Earth's water without mantle part was calculated and found to be much greater than the world oil reserves by about 9×10^5 times.
- (ii) Much attention was given to the production of green hydrogen by water electrolysis and using solar and wind energy as a very promising energy carrier instead of fossil fuels.
- (iii) The water molecular structure and its change were thoroughly investigated under the influence of the AEF during the water electrolysis process.
- (iv) The production cost of hydrogen utilizing normal electricity of Oman and solar electricity was studied for comparison purposes. A production cost of one kg of hydrogen gas by electrolysis method was calculated and found to be about 0.4 \$/kg, depending on recent information about price of solar energy. However, using the present electricity price of Oman showed a reasonable value of around 2.8 \$/kg.

Also, the following general findings can be concluded:

- Hydrogen is a very reliable energy carrier as an alternative to fossil fuels presently and in the future.
- Solar and wind energy is recommended to be utilized to provide the required electricity to run the electrolysis cells to generate H_2 and O_2 .
- The byproduct oxygen gas of the electrolysis method certainly will be used in industrial and health sectors.
- Production cost of hydrogen will be reasonable in long-term plans using renewable energy sources with much less greenhouse effect.
- The required water for electrolysis process could be produced from atmospheric moisture in different ways such as the byproduct drain water of air-conditioner units in humid places, leading to a decrease in the production cost of hydrogen.

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