
Design of an Alkaline Water Electrolyzer for Hydrogen Production

Chijindu Ikechukwu Igwe^{*}, Chinonso Hubert Achebe, Arinze Everest Chinweze

Department of Mechanical Engineering, Nnamdi Azikiwe University, Awka, Nigeria

Email address:

igwechijindu@gmail.com (Chijindu Ikechukwu Igwe), ch.achebe@unizik.edu.ng (Chinonso Hubert Achebe),

ae.chinweze@unizik.edu.ng (Arinze Everest Chinweze)

^{*}Corresponding author

To cite this article:

Chijindu Ikechukwu Igwe, Chinonso Hubert Achebe, Arinze Everest Chinweze. Design of an Alkaline Water Electrolyzer for Hydrogen Production. *American Journal of Mechanical and Industrial Engineering*. Vol. 7, No. 6, 2022, pp. 89-98. doi: 10.11648/j.ajmie.20220706.12

Received: November 27, 2022; **Accepted:** December 26, 2022; **Published:** January 10, 2023

Abstract: Hydrogen is an excellent energy carrier that is capable of storing excess generated renewable energy. It can be utilised in a fuel cell to produce electrical energy which is a sustainable alternative to conventional energy sources. This paper focuses on the design process of an alkaline water electrolyzer for the production of hydrogen through the electrolysis of water. A single cell, zero-gap, unipolar alkaline water electrolyzer, operating with 30 wt.% KOH solution as electrolyte is designed for a capacity of about 306 g of water. The design of the cell geometry was modified to enable improved hydrogen production. Thermal and stress simulations were performed with Autodesk Inventor Nastran 2019 on some modelled components of the designed electrolyzer cell, with the working temperature at about 80°C to 90°C, while maintaining the operating pressure at about 1.0 bar. Thermal and stress distributions from the results agree with the choice of material for the components, and confirms polytetrafluoroethylene (Teflon), and polypropylene plastic suitable for alkaline electrolyzer construction. Von Mises stress evaluation obtained maximum stress values of 0.143 Mpa and 0.138 Mpa, as well as 0.126 Mpa and 0.157 Mpa, for the endplates and spacers for polytetrafluoroethylene and polypropylene plastics respectively. The stress values are well within the safe limits for both PTFE and PP materials which have yield strength of 35 Mpa and 24 Mpa respectively.

Keywords: Alkaline, Electrolysis, Electrolyzer, Hydrogen, Water

1. Introduction

Hydrogen is the most abundant chemical element in the universe; it makes up more than 90% of all known matter. The hydrogen atom is the lightest known element because it just contains one proton and one electron. Hydrogen is a suitable and desirable fuel for the future due to its abundance on Earth, the low environmental impact of its use, and the need to replace fossil fuels. Hydrogen is rarely found in its pure form, H₂, because its weight is less than that of air, which causes it to ascend in the atmosphere [1].

Hydrogen does not exist naturally in its pure form since it readily forms covalent compounds with most nonmetallic elements; it is locked up in large amounts in compounds of water, hydrocarbons, and other organic matter. Being able to effectively separate hydrogen from its components is one of the difficulties in using hydrogen as a fuel. Steam reforming,

a high-temperature process in which steam combines with a hydrocarbon fuel to produce hydrogen, is one of the various ways of hydrogen extraction. Hydrogen can be produced by reforming a variety of hydrocarbon fuels, such as natural gas, diesel, renewable liquid fuels, gasified coal, and gasified biomass. Approximately 95% of the hydrogen produced today comes from steam reforming natural gas [2]. This method of hydrogen synthesis, according to Kalamaras and Efstathiou [3], results in an efficiency of between 60 and 75% at temperatures between 700 and 1100°C. The technique of electrolysis, in which water is split into oxygen and hydrogen in an electrolyzer, can also be used to create hydrogen from water. An electrolyzer works more like a fuel cell in reverse since it produces hydrogen from water molecules rather than harnessing the energy of hydrogen molecules like a fuel cell does [2]. If the electricity utilised in the reaction process is obtained from renewable energy sources rather than fossil fuel power plants, the process would be less carbon-intensive.

This procedure has a 70–80% efficiency [4].

When used as fuel, hydrogen offers affordable, sustainable, and ecologically friendly options to address the world's energy needs. Water and heat are the only byproducts of the electrochemical reaction when hydrogen is utilised to power a fuel cell; no greenhouse gas is created [5]. It also works well as a medium for storing energy. Until it is consumed, the energy that is held as hydrogen in the form of a gas or liquid is sufficiently conserved. This is not the case for several other energy storage technologies, such as batteries and capacitors, which gradually lose the energy they contain and require routine recharge even while not in use.

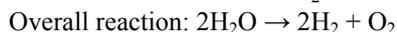
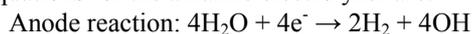
1.1. Electrolysis and Electrolyzers

An electrolyzer is an electrochemical device that conducts electrolytic reactions. An electrolyte acts as a medium between the anode and cathode in an electrolyzer. The concern with electrolyzers is that the process needs electrical energy to be completed. The electrical energy required for the electrolysis reaction should ideally originate from renewable energy sources like hydroelectric, solar, or wind energy. A few benefits of using electrolyzers are the assurance of the hydrogen's purity, the ability to create it right where it will be needed rather than having to first store it, and the fact that it is significantly less expensive than receiving gas in high-pressure cylinders [6]. The slightly varying ways that various electrolyzers operate are mostly determined by the various types of electrolyte material employed.

1.1.1. Types of Electrolyzers

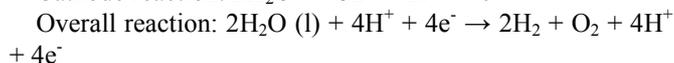
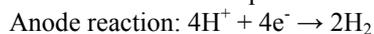
Electrolyzers can be categorised into unipolar and bipolar designs, according to Fuel Cell Store [6]. Alkaline liquids are often used as the electrolyte in unipolar designs, while solid polymer electrolyte membranes are used in bipolar designs. In the past, potassium hydroxide was a widely utilised electrolyte, but nowadays polymer electrolyte membranes are more prevalent.

(a) Alkaline Electrolyzers: Aqueous potassium hydroxide (KOH) solution is frequently used as the electrolyte in alkaline electrolyzers. Other frequently used electrolytes include sodium hydroxide (NaOH), sodium chloride (NaCl), and sulfuric acid (H₂SO₄). Operating pressures of 1 to 30 bar and temperatures of 25 to 100°C are ideal for alkaline electrolyzers. Current densities in commercial alkaline electrolyzers range from 100 to 400 mA/cm² [6]. Reaction equations for the alkaline electrolyzer are:



(b) Proton Exchange Membrane Electrolyzers: The proton exchange membrane (PEM) electrolyzer is a widely used technology that is used in a lot of contemporary electrolyzers. An ion-conducting membrane that is thin, and solid, is employed as the electrolyte in place of an aqueous solution. It makes use of a bipolar design and is capable of working in extreme membrane pressure differentials. At the anode, water

reacts to produce positively charged hydrogen ions and oxygen (protons). The hydrogen ions move arbitrarily across the PEM to the cathode as the electrons go through an external circuit. Hydrogen gas is produced at the cathode when hydrogen ions and electrons from the external circuit combine. The reaction equations are as follows:



(c) Solid Oxide Electrolyzers: Solid oxide electrolyzers use a solid ceramic material as the electrolyte to selectively conduct negatively charged oxygen ions (O²⁻) at high temperatures. Hydrogen gas and negatively charged oxygen ions are created when water at the cathode interacts with electrons from the external circuit. Following their passage through the solid ceramic membrane, the oxygen ions react at the anode to produce oxygen gas and electrons for the external circuit.

1.1.2. Alkaline Electrolyzer Cell Configuration

Depending on the electric connection of the electrodes, electrolyzers can be classified into unipolar and bipolar. The unipolar cell design has each of the cell electrodes connected to the electric source. This means that each electrode has the same polarity on its entire surface. In the bipolar design, the electric source is only connected to the two electrodes on the opposite ends of the cell. These electrodes are designated as "terminal electrodes". The unipolar design often uses alkaline electrolytes, whereas the bipolar design uses a solid polymer electrolyte [6]. Therefore, the unipolar cell design is suitable for smaller and less intensive processes where the total electric current flowing through the electrolyzer stack is not extremely high.

An electrolyzer cell configuration can also be gap or zero-gap. In the zero-gap cell design, the porous electrode materials are pressed on each side of the diaphragm, forcing the hydrogen and oxygen gases to exit the electrodes at the back. This method differs from the gap design, in that it has the benefit of reducing ohmic losses. This will enable the cell to operate at higher current densities [7-10].

1.2. Electrolyzer Electrode Technology

An electrode is often a metal substance which conducts current into and out of an electrolytic solution [11]. Electrode materials according to Coutanceau *et al.* [12] need to be resistant to corrosion. One of the most popular electrode materials for the alkaline electrolyzer cell is nickel. According to Scott [13], the development of a commercial electrode for alkaline water electrolysis should take into account four key factors: electrochemical efficiency, stability, scalability, and affordability. Initial requirements for electrode materials include good electrical conductivity, low overvoltage (high electrocatalytic activity), and good corrosion resistance in the alkaline electrolyte at the suggested working temperature. Steel or nickel, which may be activated, serve as the cathode material in typical water

electrolysis. The anode, which is more susceptible to corrosion than the cathode is based on nickel (an example is Ni plated steel or an activated Ni plate or coating).

1.3. Electrolyzer Diaphragm Technology

A diaphragm is a microporous material with typical pore diameters less than 1 μm , according to Coutanceau *et al.* [12]. It allows for the separation of gases and the transfer of water and hydroxyl ions between the anode and cathode compartments. To achieve high cell efficiency, the diaphragm must have high water permeability, high corrosion resistance in strongly alkaline conditions, and high ionic conductivity. To enable the generation of high gas purities and current efficiencies, an electrolyzer diaphragm should isolate oxygen and hydrogen gases and prevent the mixing of catholyte and anolyte.

In an alkaline water electrolysis cell, the function of the separator is to keep the electrodes from shorting out and to keep the evolved hydrogen and oxygen from combining. To do this, the separator must be extremely alkaline stable and highly conductive for the movement of OH^- ions. As the current flows through the liquid electrolyte in the pores of a separator, its porosity and tortuosity play a major role in determining how well it conducts electricity. Additionally, these characteristics affect how dissolved gas is transported through the separator.

Gas crossover in PEM electrolysis models is often explained by a mix of diffusive species transport across the membrane and differential pressure-driven convection. In order to ensure that only diffusional crossover occurs, alkaline water electrolyzers are typically run with equal anodic and cathodic pressures [8]. Inorganic, organic, or composite materials can be used to create separators for industrial alkaline water electrolyzers. The separator for low-temperature electrolyzers can be made of polymer, asbestos, or nickel oxide. At temperatures higher than 120°C , however,

many polymers and asbestos become unstable. Although stabilisation by silicate may be employed, the asbestos diaphragm, which is frequently used in alkaline water electrolyzers, has a rather high electrical resistance and should not be used over 100°C . Additionally, it causes cancer, making its usage in newly constructed electrolyzers illegal [13].

2. Design of the Alkaline Electrolyzer Cell

Many researches have been carried out in this area, and more are still being done. However, this design intends to further improve the existing studies in the following ways:

- (i) Using electrodes for the electrolyzer cell in a zero-gap configuration. From the studied literature, it was discovered that this approach reduces parasitic ohmic resistance while increasing operating current density [7, 8].
- (ii) Design modification of the electrolyzer cell geometry. This prevents electrolytic solution leaking from between component mating surfaces while also distributing compression more evenly throughout the cell.

2.1. Selection of Materials

To determine the best engineering materials for the construction of the alkaline water electrolyzer, suitable materials from the literature review study were evaluated and considered for their attributes. Attribute profiles such as density, strength, toughness, resistance to corrosion, and cost were identified; and compared with those of real engineering materials from the literature review study to find the most suitable match. Ansys Granta 2019 software was used to evaluate material attributes with the aid of material property charts.

Table 1. Selection of materials and components.

S/N	Components	Material Choice	Reasons
1	Endplates	Teflon (PTFE), and Polypropylene plastic	1) Tough, ductile, resistant to shock and vibration, and possess high tensile and compressive strength. 2) Resistant to oxidation and corrosion.
2	Electrodes	Nickel	1) Good electric conductor. 2) Corrosion-resistant. 3) Stable in alkaline media.
3	Sealing gaskets	Silicone rubber	1) Good electrical insulator. 2) Vibration and shock-resistant. 3) Long term chemical stability and excellent sealing capability.
4	Diaphragm	Zirfon (Agfa Zirfon Perl UTP 500), and PP geotextile fabric.	1) High ionic conductivity. 2) Resistive to atomic oxygen produced on the anode electrode.
5	Spacers	Teflon, and PP plastic	1) Good impact resistance and resistive to chemical corrosion. 2) Availability and low cost.
6	Bolts and nuts	Stainless steel	High torsional and fatigue strength.
7	Electrolyte tubing	Silicone rubber	1) Resistant to ageing, temperature, and chemical corrosion. 2) Flexible, strong, and resilient.
8	Electrolyte reservoir	Polypropylene plastic	1) Very dense. 2) Readily available and cheap. 3) Hard, durable, and excellent tensile strength.
9	Electrolyte	KOH solution	High ionic conductivity.
10	DC power supply	12V DC bench power source	12V, 5 A DC bench power supply.

2.2. Design Operations

The design of a single-cell alkaline water electrolyzer for hydrogen production is based on parameters such as cell size, electrolyte concentration, operating pressure, process temperature, current density, conductivity, load range, and production capacity.

2.2.1. Current Efficiency

According to Faraday's law, 0.336 g of water is split into 0.418 dm³ H₂ and 0.209 dm³ O₂ (at 273.15 K, 1.013 bar) by an electric charge of 3,600 C, which is equivalent to an electric current of 1 A flowing through an electrolyzer for one hour (1 Ah). Therefore, in theory, it takes 2.39 kWh to generate 1 m³ H₂ and 0.5 m³ O₂. The real current efficiency for water electrolysis at atmospheric pressure is quite close to 99%. This indicates that a water molecule is divided into two molecules, H₂ and O₂, using practically all of the electric current flowing through the cell. The missing 1% results from both the infiltration of the generated hydrogen into the anode compartment and the presence of parasitic currents in bipolar electrolytic stacks [14].

2.2.2. Energy Consumption

According to Hnát *et al.* [14], the amount of electric power (P in Watt) required to decompose water through electrolysis is determined as:

$$P = U_j * I \quad (1)$$

Substituting the theoretical, reversible cell voltage ($U_{\text{cell,rev}}$) for U_j and current to produce 1 m³ H₂ (at 273.15 K, 1.013 bar) in 1 h, the minimum energy consumption is equal to 2.94 kWh Nm⁻³ H₂ (32.93 kWh kg⁻¹ H₂). However, the actual energy consumption is much higher; this is primarily because of the real cell voltage and partially because of the current efficiency loss. Depending on the technology, materials, and operational conditions employed, 3.8 to 5.6 kWh of energy can be achieved.

2.2.3. Heat Generation

In accordance with the first law of thermodynamics, the electric energy provided to the electrolyzer is used to decompose water and to generate heat. Recall that $U_{\text{cell,rev}}$ equals 1.23 V, however, U_j is higher. The electric energy (W_{el}) measured in watts supplied to the electrolyzer is given by Hnát *et al.* [14] as:

$$W_{\text{el}} = P = Q + q \quad (2)$$

In other words, W_{el} equals the total of the heat produced by the electrolyzer Q (W), and the theoretical heat produced by the combustion of the gases generated by electrolysis of water q (W). At temperatures below 100°C, this assumption is considered valid.

Faraday's law stipulates that $q = 1.48$ when utilizing current I (A or C s⁻¹). I (W) (by combustion of 1 mol H₂ and 0.5 mol O₂, heat of 286 kJ is released, considering liquid water as the final product). The electrolyzer's heat

production (W) can be represented as follows when Q from equation (2) is expressed and the appropriate values are substituted:

$$Q = U_j \cdot I - 1.48 \cdot I = I \cdot (U_j - 1.48 \text{ V}) \quad (3)$$

Water can be electrolyzed without producing or releasing heat at parameters of T = 298 K, p = 1.013 bar, and $U_j = 1.48$ V. This voltage is referred to as the water electrolysis thermoneutral voltage (U_{TN}). The standard thermodynamic parameters at 298.15 K and 1.013 bar are $\Delta H = 286 \text{ kJ mol}^{-1}$, $\Delta S = 163 \text{ J mol}^{-1} \text{ K}^{-1}$. In an ideal situation, the amount of electric energy needed for water electrolysis is related to ΔG . The additional energy which equals T ΔS is considerably more cost-effective to be supplied in the form of heat. If both energies are supplied as electric energy, the theoretical voltage of the cell is thus increased by $U_{\text{T}\Delta S} = \frac{T\Delta S}{n * F} = 0.252 \text{ V}$ (T = 298 K, p = 1.013 bar). The summation of $U_{\text{cell,rev}}$ and $U_{\text{T}\Delta S}$ therefore gives 1.48 V.

2.2.4. Electrolyzer Construction

For this work, unipolar electrolyzer cell designs are adopted and designed. This cell configuration requires less precision during manufacturing. They work better in smaller, less demanding processes with moderate overall electric current-density flows through the electrolyzer stack. In this work, an alkaline water, single-cell unipolar electrolyzer of zero-gap cell configuration, working at 300 Am⁻² below 3.0 V is to be developed.

2.2.5. Electrolyzer Geometry

The electrolyzer cell cross-section is chosen to measure 190 mm x 150 mm. The polypropylene plastic (or Teflon) endplates and spacers are chosen to measure 190 mm x 150 mm x 20mm, and 150 mm x 150 mm x 20 mm respectively. The nickel electrodes measure 90 mm x 90 mm x 1 mm. The zirfon UTP 500 (or polypropylene fabric) diaphragm measures 150 mm x 150 mm, and the silicone rubber gaskets are chosen to measure 150 mm x 150 mm x 3 mm. The cell will be held in uniform pressure by stainless steel bolts and nuts of size M8.

2.2.6. Zero-Gap Cell Design

The alkaline electrolyzer will be constructed using a zero-gap cell configuration. The porous electrode materials are pressed on each side of the diaphragm in the zero-gap cell design, forcing the hydrogen and oxygen gases to exit the electrodes at the back. This method differs from the conventional in that it has the benefit of reducing ohmic losses in the electrolyzer system and the impact of gas evolution on the efficiency of the cell. Comparing the cell to the traditional finite gap design, this will enable the cell to run at higher current densities.

2.2.7. Electrolyte

Since water typically has poor electrical conductivity, electrolysis cells often use an alkaline solution to boost the solution's specific conductivity. The electrolyte's ionic

conductivity is primarily influenced by two variables: temperature and concentration. The efficiency of the electrolytic cell as a whole is impacted by the relationship between ionic conductivity and electrolyte resistance. The alkaline electrolyzer cell uses 30 wt.% KOH solution as electrolyte. According to Schalenbach *et al.* [15], and Philips and Dunnill [16], Ohms law is used to express the voltage drop across an electrolytic solution as shown below:

$$IR = \frac{Id}{AK} = \frac{jd}{K} \quad (4)$$

I represents the current in amperes; the current density in $A.m^{-2}$ is represented by j; d represents the electrode spacing in m; A represents the cross-sectional area of the conducting electrode in m^2 ; and K represents the conductivity in $S.m^{-1}$.

2.2.8. Electrolyzer Power and Cell Efficiency

The power and efficiency calculation of the electrolyzer cell is important to appreciate and better evaluate the performance of the system. De Silva and Middleton [17] gave the following relationships in their study.

Total Power: The product of the total current (I) and cell voltage (V) determines the total power of an electrolytic cell.

$$P_{total} = I \times V \quad (5)$$

Ohmic Power: This is determined by the product of the square of the total current and the ohmic resistance. In general, ohmic resistance is directly proportional to the distance between the cell electrodes. Hence, it can be reduced by shortening the distance between the electrodes.

$$P_{ohmic} = I^2 \times R_{ohmic} \quad (6)$$

Electrolysis Power: This power is determined by the difference of the total power to the ohmic power.

$$P_{electrolysis} = P_{total} - P_{ohmic} \quad (7)$$

Electrolysis Efficiency: This is determined by the ratio of the electrolysis power of the cell to the total power.

$$\eta_{cell} = \frac{P_{electrolysis}}{P_{total}} \times 100\% \quad (8)$$

Cell Energy Efficiency: This is determined by the ratio of the theoretical EMF to the cell voltage.

$$\eta_{energy} = \frac{Theoretical\ EMF}{Cell\ Voltage} \times 100\% \quad (9)$$

The effectiveness of the electrolysis process can also be expressed in different ways; the ratio of the energy content of one mole of hydrogen to the total energy input determines the usable energy output for the entire cell while it is functioning exothermically. This is the amount of electrical energy that the power source provided to create that single mole of hydrogen.

$$\eta_{H_2} = \frac{HHV_{H_2}}{W_{in}} = \frac{286\ kJ}{I * V * t} \quad (10)$$

HHV_{H_2} represents the higher heating value of a mole of

hydrogen; I represents the current; the cell voltage is represented with V, and t represents the time taken to produce a mole of hydrogen.

Furthermore, the efficiency relationship below makes a comparison of the actual measured amount of energy required to split a mole of water to the theoretical amount of energy.

$$\eta = \frac{W_t}{W_a} = \frac{V_t * I * t}{V_{cell} * I * t} = \frac{V_t}{V_{cell}} \quad (11)$$

Here, the theoretical energy required to split a mole of water is represented with W_t , and the actual energy required by the electrolyzer cell is represented with W_a . The theoretical voltage (V_t) of the electrolyzer cell, also known as the thermoneutral voltage (V_{TN}), is given as:

$$\eta = \frac{V_{TN}}{V_{cell}} = \frac{1.48\ V}{V_{cell}} \quad (12)$$

Faraday Efficiency: This efficiency is defined as the hydrogen generation efficiency. It compares the real volume of hydrogen produced by the electrolyzer cell, to the ideal volume of hydrogen expected for a particular operating condition. According to Chakik *et al.* [18], Faraday efficiency is expressed as:

$$V_{H_2Ideal} = \frac{I * V_M * t}{2 * F} \quad (13)$$

V_{H_2Ideal} represents the ideal volume of hydrogen generated; I represents the current (A); V_M represents the molar volume of hydrogen in ideal state (24.47 L/mol); t represents time (s), and F represents the Faraday constant (96,485 A.s/mol).

$$V_{H_2Real} = V_{H_2Measured} * \frac{T_{standard}}{T_{measured}} \quad (14)$$

V_{H_2Real} represents the actual volume of generated hydrogen; $V_{H_2Measured}$ represents the volume of hydrogen obtained via experimentation, and $T_{standard}$ and $T_{measured}$ represent the reference temperature (298.15 K) and the average temperature (K) measured during electrolysis respectively.

$$\eta_H = \frac{V_{H_2Ideal}}{V_{H_2Real}} = \frac{\frac{I * V_M * t}{2 * F}}{V_{H_2measured} * \frac{T_{standard}}{T_{measured}}} \quad (15)$$

2.2.9. Energy Requirement of the Electrolyzer Cell

The molecular mass of water (H_2O) is about 18 g/mol. Thus, every 18 g of water contains 2 g of hydrogen.

A litre of water, which is equivalent to 1000 cm^3 weighs about 1000 g at standard conditions. The volume of the spacers in the electrolyzer cell sums up to 306 cm^3 , which would weigh about 306 g.

306 g of water contains $(306 \times \frac{2}{18}) = 34$ g of hydrogen. If 18 g of water per 1 g/mol is 18 mol, and 306 g of water per 1 g/mol is 306 mol. Then, the ratio of the volumes is $\frac{306}{18} = 17$ mol.

Gibbs Free Energy of formation of water gives that each mole of water requires about 237 kJ/mol of energy to

electrolyze. This gives that 17 mol of water will require about 4,029 kJ or 4 MJ of energy to electrolyze.

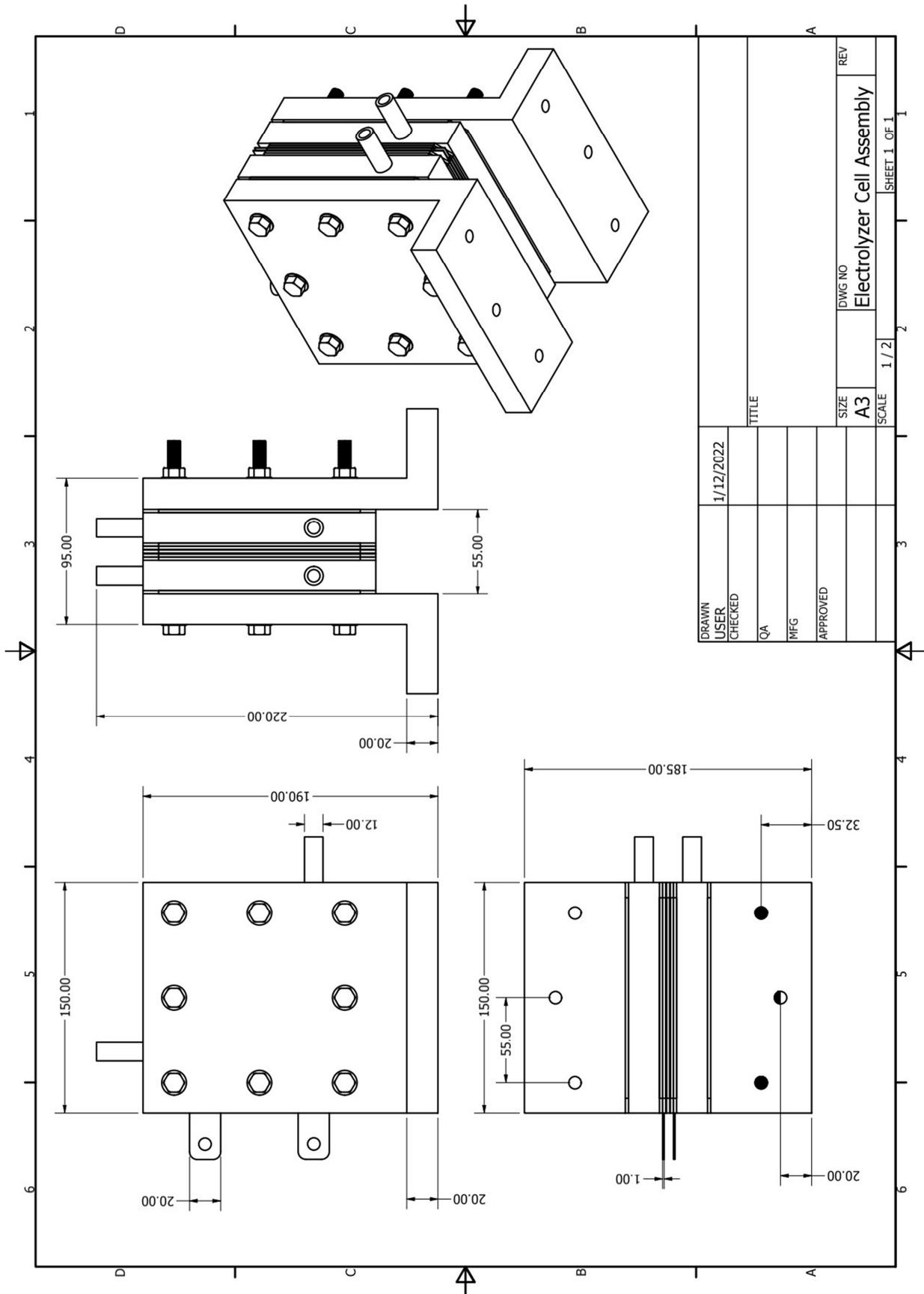


Figure 1. Orthographic drawing of the electrolyzer cell.

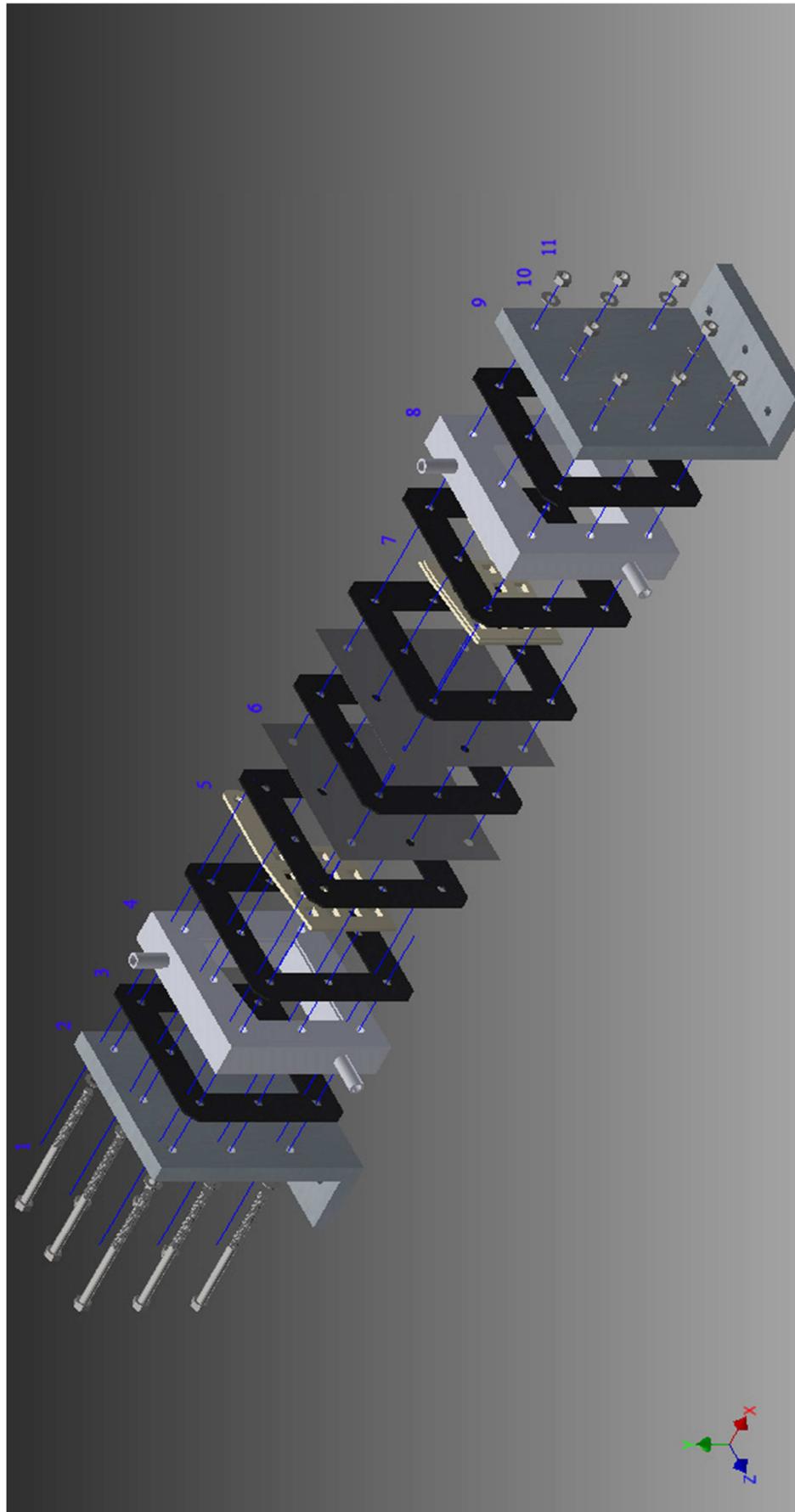


Figure 2. Exploded view of the electrolyzer cell.

2.2.10. The Working Principle of the Alkaline Water Electrolyzer Cell

The alkaline water electrolyzer cell uses 30 wt.% KOH solution as electrolyte. The 12 V DC power source supplies a voltage and current density of below 3.0 V and 300 A.m⁻² respectively. The operating temperature is maintained at 50°C, and the operating pressure, at 1.0 bar. Given that water molecules can traverse the membrane to the other side, the alkaline electrolyte penetrates both the anode and cathode regions on both sides. Water molecules in the electrolyte mix with electrons in the cathode part of the cell to make hydrogen and hydroxide ions, and in the anode region, the hydroxide ions lose electrons to form oxygen and water. This process occurs when the cell is powered by the supply of electric current. The membrane keeps the generated hydrogen and oxygen gases separated for collection through their separate channels.

- 1 – Bolts; 2 – Endplate 1; 3 – Sealing gasket; 4 – Spacer 1;
- 5 – Anode electrode; 6 – Diaphragm; 7 – Cathode electrode;
- 8 – Spacer 2; 9 – Endplate 2; 10 – Washers; 11 – Nuts.

3. Thermal and Stress Simulations of the Modeled Electrolyzer Cell Components

The thermal and stress simulations of the modelled electrolyzer cell components were performed in Autodesk Inventor Nastran 2019 software. To perform these simulations; the models of the cell spacers and endplates were subjected to extreme operating temperature obtainable for alkaline water electrolysis which is around 90°C (363 K) [19, 20].

- Two essential thermal loads were applied on the components:
- 1) Heat from the electric power supply to the nickel electrodes (363 K).
 - 2) Convection heat which is the temperature of the surrounding of the system (293.15 K; with convective coefficient of 0.00321 mW/mm²K).

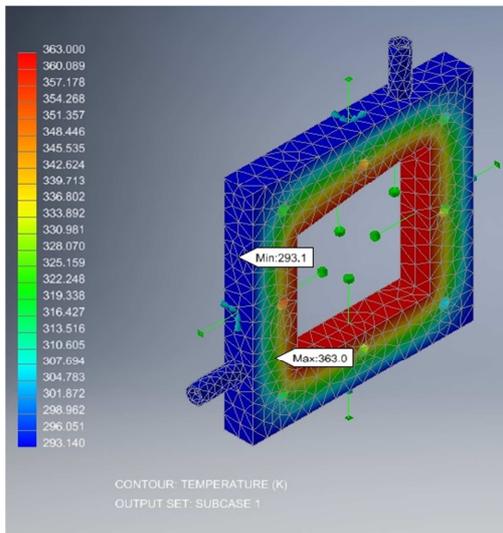


Figure 3. Thermal simulation of the modelled PTFE plastic electrolyzer spacer.

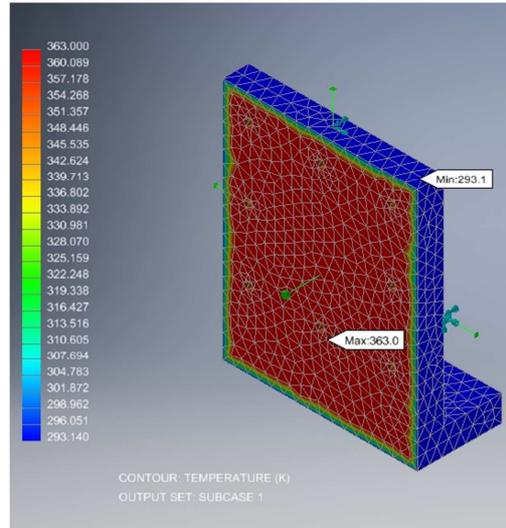


Figure 4. Thermal simulation of the modelled PTFE plastic electrolyzer endplate.

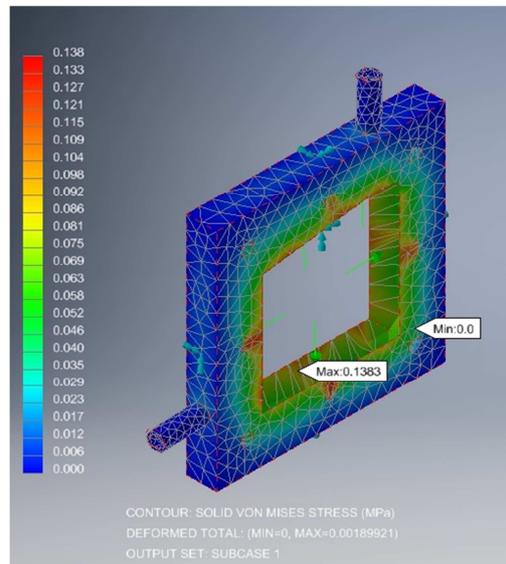


Figure 5. Stress simulation of the modelled PTFE plastic electrolyzer spacer.

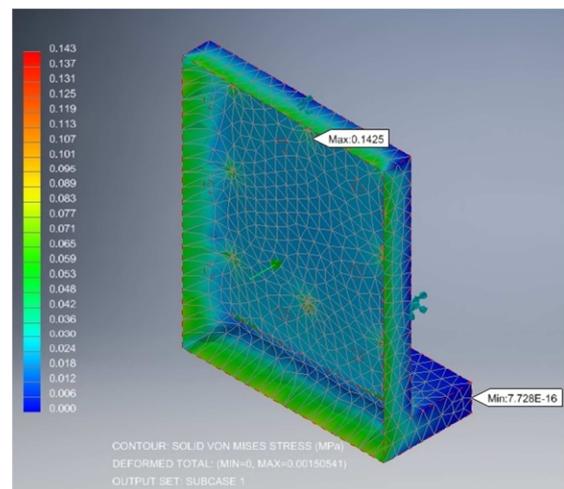


Figure 6. Stress simulation of the modelled PTFE plastic electrolyzer endplate.

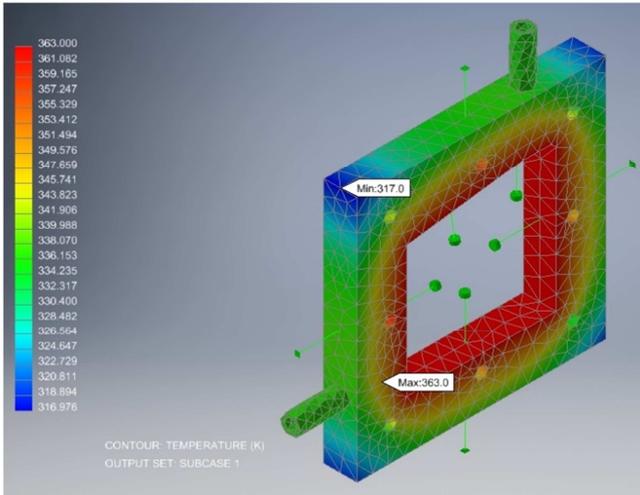


Figure 7. Thermal simulation of the modelled PP electrolyzer spacer.

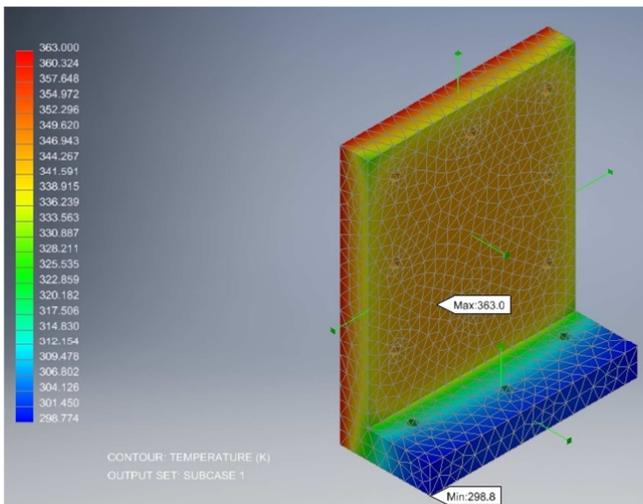


Figure 8. Thermal simulation of the modelled PP electrolyzer endplate.

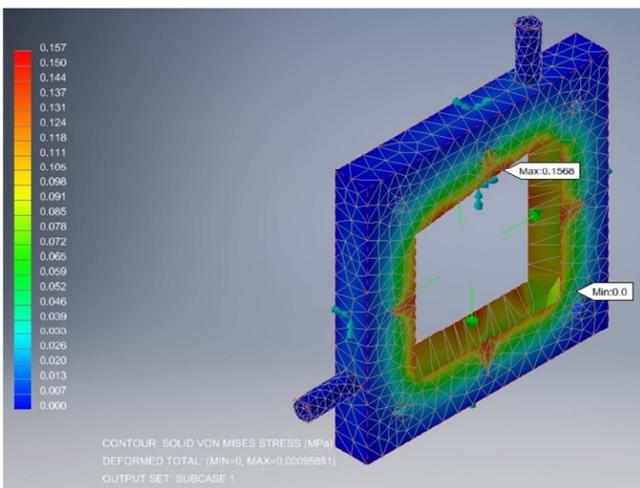


Figure 9. Stress simulation of the modelled PP electrolyzer spacer.

The results of the thermal simulations are shown in Figures 3, 4, 7, and 8. The thermal distribution with their resulting temperature ranges are represented with several colour codes. The regions with maximum temperatures (363

K) and minimum temperatures (293.1 K for the PTFE plastic endplate and spacer), and (298.8 K for the PP plastic endplate and 317 K for the PP plastic spacer) are shown and highlighted. The results equally show temperature ranges of the amount of heat the components are going to develop while in operation, the ranges of temperatures from the results are well within safe limits. The results of the simulations, thus do agree with the design of the chosen materials (polytetrafluoroethylene plastic, and polypropylene plastic) as being suitable for the desired purpose.

Stress simulations on the modelled components were performed by subjecting the components to the load of the pressure acting within the electrolyzer system, maintained at 1.0 bar (0.1 MPa). Again, the results of the stress simulations are shown in Figures 5, 6, 9, and 10. The stress distribution over the components evaluated using Von Mises stress highlights regions of the components that are highly stressed and the regions that experience minimal stress. The maximum stress values of 0.143 MPa and 0.138 MPa (PTFE plastic), as well as 0.126 MPa and 0.157 MPa (PP plastic), for the endplate and spacer respectively, are well within the safe limits for the chosen materials. The yield strength of polytetrafluoroethylene (PTFE) and polypropylene (PP) plastics are 35 MPa [21], and 24 MPa respectively [22].

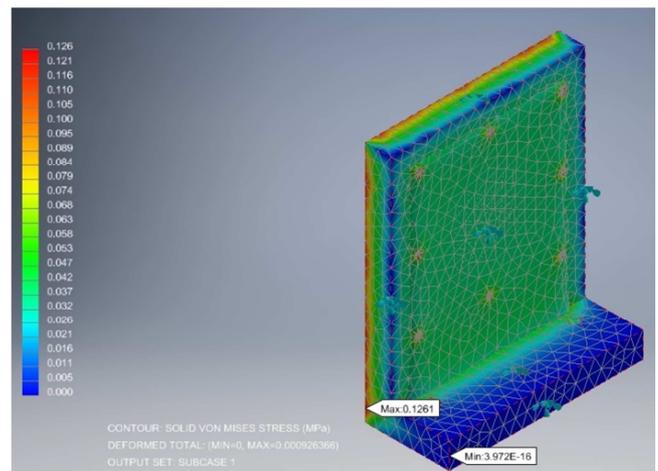


Figure 10. Stress simulation of the modelled PP electrolyzer endplate.

4. Conclusion

The single cell alkaline water electrolyzer device was designed with consideration to some of the existing designs from the reviewed literatures. It was intended to modify some of the geometric features of existing designs, as well as the adoption of the zero-gap cell configuration. Furthermore, another important aspect of this design is the choice of material function. The material specifications for this design, through due studies, intend to serve better functionality, and offer a much improved production output. Simulation results obtained in this study confirms that the recommended materials and designs are suitable for the alkaline water electrolyzer. Furthermore, given the current high rate of global energy demand, depleting fossil fuel reserves, and

concerns with greenhouse gas emissions; this design study is beneficial to researchers, institutes, and energy industries for a wide adoption and utilisation of hydrogen as a sustainable alternative energy source/carrier. It is therefore essential to subject this developed alkaline water electrolyzer design to some necessary experimental tests to determine its performance.

References

- [1] Altork, L. N. and Busby, J. R. (2010). Hydrogen fuel cells: part of the solution. *Technology & Engineering Teacher*, 70 (2) 22-27.
- [2] U. S. Department of Energy (2020). Hydrogen and fuel cell technologies office. *Energy Efficiency & Renewable Energy*. Retrieved from <https://www.energy.gov/eere/fuelcells/hydrogen-and-fuel-cell-technologies-office> on June 26, 2021.
- [3] Kalamaras, C. M. and Efstathiou, A. M. (2013). Hydrogen production technologies: current state and future developments. *Conference papers in energy*, 2013: 1-9. Retrieved from <https://www.hindawi.com/journals/cpis/2013/690627/> on April 10, 2020.
- [4] Stolten, D. (2016). *Hydrogen Science and Engineering: materials, processes, systems and technology*. John Wiley & sons (898).
- [5] Campbell, R. J. (2020). Hydrogen in electricity's future. Congressional Research Service. CRS Report, R46436. June 30, 2020.
- [6] Fuel Cell Store (2017). Introduction to electrolyzers. Retrieved from <https://www.fuelcellstore.com/blog-section/introduction-to-electrolyzers> on June 27, 2021.
- [7] Amores, E., Rodriguez, J. and Carreras, C. (2014). Influence of operation parameters in the modeling of alkaline water electrolyzers for hydrogen production. *International Journal of Hydrogen Energy* (39) 13063-13078.
- [8] Haug, P., Kreitz, B., Koj, M. and Turek, T. (2017). Process modeling of an alkaline water electrolyzer. Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr, Germany. *International Journal of Hydrogen Energy*, 1-19.
- [9] Kuleshov, V. N., Kuleshov, N. V., Grigoriev, S. A., Udris, E. Y., Millet, P. and Grigoriev, A. S. (2016). Development and characterization of new nickel coatings for application in alkaline water electrolysis. *International Journal of Hydrogen Energy* 41, 36-45.
- [10] Brauns, J. and Turek, T. (2020). Alkaline water electrolysis powered by renewable energy: a review. Institute of Chemical and Electrochemical Process Engineering, Clausthal University of Technology, Leibnizstr, Germany (8) 248.
- [11] Britannica (2011). Electrode electronics. The Editors of Encyclopedia Britannica. Retrieved from <https://www.britannica.com/science/electrode> on August 4, 2021.
- [12] Coutanceau, C., Baranton, S. and Audichon, T. (2018). Chapter 3 – Hydrogen production from water electrolysis. In *Hydrogen Energy and Fuel Cells Primers*, Hydrogen Electrochemical Production, Academic Press, 17-62.
- [13] Scott, K. (2017). *Hydrogen production and water electrolysis. Sustainable and Green Electrochemical Science and Technology*, First Edition. Published by John Wiley & Sons Ltd.
- [14] Hnát, J., Paidar, M. and Bouzek, K. (2020). Hydrogen production by electrolysis. Current Trends and Future Developments on (Bio-) Membranes. Department of Inorganic Technology, University of Chemistry and Technology Prague, Czechia.
- [15] Schalenbach, M., Kasian, O. and Mayrhofer, K. (2018). An alkaline water electrolyzer with nickel electrodes enables efficient high current density operation. *International Journal of Hydrogen Energy*, 1-7.
- [16] Phillips, R. and Dunnill, C. W. (2019). Zero gap cell design for alkaline electrolysis. A PHD Thesis, Energy Safety Research Institute, Swansea University Prifysgol Abertawe.
- [17] De Silva, Y. S. K. and Middleton, P. H. (2020). Design of an alkaline electrolysis stack. Faculty of Engineering and Science, University of Agder.
- [18] Chakik, F., Kaddami, M. and Mikou, M. (2017). Effect of operating parameters on hydrogen production by electrolysis of water. Faculty of Science and Technology, University Hassan I, Settat, Morocco. *International Journal of Hydrogen Energy*.
- [19] Mittelsteadt, C., Norman, T., Rich, M. and Willey, J. (2015). PEM electrolyzers and PEM regenerative fuel cells industrial view. *Electrochemical Energy Storage for Renewable Sources and Grid Balancing* (159-181). Retrieved from <https://www.sciencedirect.com/topics/engineering/electrolyzer-technology> on June 27, 2021.
- [20] Chisholm, G. and Cronin, L. (2016). Hydrogen from water electrolysis. School of Chemistry, University of Glasgow, United Kingdom. (16) 315-339.
- [21] Matmatch (2022). Polytetrafluoroethylene (PTFE) datasheet. Retrieved from <https://matmatch.com/materials/mbas023-polytetrafluoroethylene-ptfe-> on June 04, 2022.
- [22] Barbosa, L. G., Piapia, M. and Ceni, G. H. (2017). Analysis of impact and tensile properties of recycled polypropylene. *International Journal of Materials Engineering* 2017, 7 (6): 117-120.