Mathematical Synthesis of Water Electrolysis: Driving Cost Reduction in Hydrogen Production.

Hugo Andrade Cerqueira

Abstract. Hydrogen is increasingly recognized as a key renewable fuel in the global energy economy. Currently, the two primary methods for hydrogen production are steam methane reforming (SMR) and water electrolysis. While SMR has a negative environmental impact due to carbon dioxide emissions, water electrolysis offers a cleaner alternative by using electric energy to split H_2O molecules into hydrogen and oxygen. However, the main barrier to the widespread adoption of electrolysis is its cost, driven by expensive materials and high energy requirements. The electrolysis process depends on multiple variables, such as electrolyte conductivity, water volume, and the electrical current supplied, all of which influence both efficiency and expense. This paper presents a mathematical synthesis of the water electrolysis system, offering a set of equations that optimize these variables to enhance system efficiency and reduce production costs, making electrolysis a more viable solution for clean hydrogen production.

Keywords. Hydrogen, Renewable energy, Electrolysis, Mathematical formula, Synthesis

1. Introduction

The use of hydrogen as fuel and renewable power source is one of the optimal and healthier options for the global energy industry. Hydrogen is present in many abundant substances and materials, however, the production of hydrogen has many obstacles. The main two methods for hydrogen production are the Steam Methane Reforming (SMR) and the electrolysis of water (splitting H2O molecules into hydrogen and oxygen). For the SMR method of hydrogen production a couple of undesirable residues of carbon dioxide are produced along with the hydrogen product, increasing the impact of the factors that cause global warming.

But in spite of that, the electrolysis of water does not produce harmful side products (if a proper electrolyte is used for the electrolytic system), it can be the cleanest way of production, it is very malleable and its results depend on its process model. The main problems with the use of electrolysis to fabricate hydrogen gas is its pricing. The materials necessary for the process can be very expensive and the energy used for the production can be very high, nevertheless, the electrolysis system is defined by many variables: the amount of water and electrolyte in the electrolysis tank, the conductivity and quality of the electrolyte, the material and size of the electrodes, the amount of current and voltage is used in the process, and many more variables.

To synthesize the modelling and planning of the electrolysis system, with the objective of increasing efficiency and lower the cost of hydrogen production through electrolysis, a mathematical representation of all the interactions and variables of the chemical process will be shown in this research paper

2. Research methods

2.1 The main functions and variables of the electrolysis system:

The electrolysis of water can take many forms, as it involves numerous variables, qualities, and quantities that significantly modify the process. To develop a precise mathematical formula that allows for the calculation of any (or most) electrolysis device models, an organization of the key processes and their variables is necessary. By arranging these elements, mapping the interactions between them becomes much more feasible and easier to understand.

2.2 The logical synthesis of oxy-hydrogen production:

Firstly, the mathematics behind the generation of hydrogen and oxygen gas through electrolysis have a simple structure and line of thought. To calculate the amount of oxy-hydrogen gas produced in an electrolysis system under a certain amount of electric charge a couple of steps must be followed. Faraday's first law of electrolysis defines that for every amount of substance produced through electrolysis an equivalent amount of charge must be spent for the production [1]. Accordingly, two simple equations can be formed to represent the amount of moles of oxygen and hydrogen produced under a specified amount of charge.

Faraday's second law of electrolysis describes the essence of the following equations [1]. To make 1 mole of hydrogen gas molecules (H_2) 2 moles of charge must be spent, to calculate the amount of charge a battery delivers into a electrolytic system we multiply the amount of current (in amps) the electric source delivers by the amount of time the process will happen (in seconds).

$$Q = i \times t \ (1)$$

After determining the total amount of charge, the calculation of the oxy-hydrogen moles produced in the electrolysis system can be made with the following equations:

$$F = 96485 \text{ C/mol} \ (2)$$

$$N_{H2} = \frac{Q}{2F} \ (3)$$

$$N_{O2} = \frac{Q}{4F} \ (4)$$

Where "N_{H2}" is the number of moles of hydrogen gas (H_2) and "N_{O2}" is the number of moles of oxygen gas (O_2), both of those variables are calculated by dividing the amount of charge sent to the system by two faraday's to calculate the amount of hydrogen gas moles, and by four faradays to calculate the amount of oxygen moles produced. Since the amount of charge that enters the system is the same amount of charge that exits it, returning to the electric source, the charge (Q) used in the formulas is the total amount of charge that enters the system and that exits it. That will translate to the amount of moles produced in the cathode (H_2) and the anode (O_2).

To speculate the mass of the substances produced, the conversion of moles to the exact mass of each substance produced can be done to create an approximate value of the mass of oxy-hydrogen gas produced in a specified environment/process.

$$m_{H2} = N_{H2} \times MM_{H2} \ (5)$$

$$m_{O2} = N_{O2} \times MM_{O2} \ (6)$$

$$m_{total} = m_{H2} + m_{O2} \ (7)$$

However, the current and tension configuration of the energy source, does not translate to the amount of current that the electrolytic system receives. Because the path of the charge coming through the electric source to the electrolytic system presents a resistance, to calculate the resistance of the path of the current the two Ohm's laws must come into account to approximately determine the conductive path's electrical resistance. Being the two equations the following:

$$U = R(\Omega) \times I(A) \text{ or } I = \frac{U}{R} \text{ or } R = \frac{U}{I} \ (8)$$

$$R(\Omega) = \rho \times \frac{L}{A} \ (9)$$

As an example, when a battery delivers a current of *10A* (amps) with a tension of *10V* (volts) to an electrolysis system through a conductive metal that presents a resistance of *1,5*Ω (Ohms). Given the following scenario, the calculation to determine the reduction in the tension or current can be done this way:

$$6{,}6A = \frac{10}{1{,}5} \text{ (Real current received) } (10)$$

Ohm's first law is used to discover the real current received by the electrolysis system after the resistance of the conductive path. Meaning, the energy deducted from the final current value most probably was converted into heat during the current transportation. Ohm's second law (9) can be used to define the conductor's resistance, if it has not been determined yet, for that the resistivity of the conductor's material must be determined first to the calculation. The resistivity of a material is an experimental property; there are many online databases, books and research papers that list the approximate resistivity of any conductor or semiconductor and the most common materials for first class conductors [2].

2.3 The calculation of conductivity of the electrolytic solution:

The electrolytic solution, the main component of the electrolysis system, is the heart of the entire process. The quality of the production is a dependent value of the conductivity of the electrolytic solution. To develop a formula that, by assigning the values of the properties of a specified electrolysis system, can calculate the conductivity of the entire solution a collection of calculations must be done to group every contributing factor. The main mathematical representations of the process are:

$$\sigma = \sum_{i} \lambda_i \times c_i \ (11)$$

$$c_i = \frac{mi}{Mi \times V} \ (12)$$

$$\sigma = \sum_{i} \lambda_i \times \frac{mi}{Mi \times V} \ (13)$$

$$\sigma_{\text{solution}} = \frac{1}{V} \times \left(\sum_{i} \lambda i \times \frac{mi}{Mi} \right) (14)$$

To determine the conductivity of the electrolytic solution of the system a couple of variables must be defined: the concentration of the electrolyte (*i*) represented by the letter "*c*"; the electrolyte's mass in grams (m_i); the molar conductivity of each present ion in the solution (λ_i); the volume of the whole solution in liters (*V*) and the molar mass of the electrolyte's substance (M_i). Firstly, when it comes to determining the molar conductivity of the ions present in the solution, it must be stated that this value is an experimental property, and needs to be researched on literature or online databases to define each ion's conductivity. One way to determine circumstantially the molar conductivity of one ion in the solution, is if you use the following equation and have already defined the molar conductivity of the solution and the conductivity of one of the ions:

$$\lambda_s = \lambda^0_+ + \lambda^0_- \ (15)$$

If the "λ_s" is already known and also one of the two ionic molar conductivity ($\lambda^0_+ \, or \, \lambda^0_-$), the value of the other could be immediately determined by subtracting from the total molar conductivity of the solution by the already known molar conductivity of one of the ions in it. Secondly, the concentration of the electrolyte in the solution can be determined using the equation number twelve (12). The concentration of the electrolyte is determined by dividing the mass of the electrolyte, in grams (m_i) by the product of the molar mass of the electrolyte used, in grams (M_i), and the volume of the entire solution (*V*). The equation number thirteen (13) is the more detailed instance of the first equation, that defines the conductivity of the entire electrolytic solution by multiplying the sum of the ion's molar conductivity by the concentration of the electrolyte in the solution, that can be written as the division of the electrolyte's mass by the product of the electrolyte's molar mass and the entire volume of the solution.

To assemble a more objective and simplified formula, for the calculation of the solution's conductivity, the equation fourteen (14) is a more broad and objective conglomerate of all the other equations.

3. Conclusions

The electrolysis of water is a promising energy production technology that, if correctly planned and invested, could be an innovative and efficient solution for the renewable energy global economy. When each process and detailed technical properties of the electrolysis system is synthesized using mathematics, the system planning becomes much more direct and precise. With it, the researcher does not need to physically experiment every hypothesis related to electrolysis, it could verify its theoretical base and develop the logic of the research more efficiently. The area of study of electrolysis is somewhat superficial when it comes to simple experiments, but the inner workings of the entire process can be very deep and complicated. Since it shares electrodynamics, conductometry, ionized solutions, molar conductivity and many more technical technical subjects, the research of the area can be very interesting and tackles many areas of knowledge. There's still more descriptive mathematical representations that could be added into this research, however, this has the objective of synthesizing the logical operations and reasonings that build the understanding of the electrochemical subject of electrolysis.

4. References

[1] John B. Russel. *General chemistry*. McGraw-Hill College. New York, London. 1992. Volume 2. 1064 pg.

[2] John Newman, Karen E. Thomas-Alyea. *Electrochemical systems*. John Wiley & Sons, Inc., Hoboken, New Jersey. 2004. 672 pg.