VAAL UNIVERSITY OF TECHNOLOGY

FACULTY OF ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING

RESEARCH PROPOSAL ABSTRACT

Modelling of Alkaline electrolyser for hydrogen production using Simulink and artificial neural networks (ANN) for output prediction

Name: Arsene Kalahamba Mahiya

Student number :210133481

Supervisor: Prof Tumisang Seodigeng

Co-Supervisor: Dr John Kabuba Tshilenge

Introduction

The World Bank Progress Indicators have proven that practically every imaginable development aspect of life and society is strongly linked to energy usage (Berrada and Laasmi, 2021).Researchers have been looking for alternative sustainable energy generation methods due to growing concerns over the depletion of fossil fuels and climate change(Ismail et al., 2014). From this vantage point, green hydrogen is one of the most promising alternative energy sources. Hydrogen does not produce toxic gases during its production and combustion process, making it suitable for use in various applications that utilise fossil fuels(Mazloomi et al., 2012). There are several existing or in-development technologies for producing hydrogen from renewable energy sources like solar or wind. These methods include proton exchange water electrolysis (PEM), alkaline water electrolysis (AWE), and solid oxide water electrolysis (SOWE). The most advanced method is alkaline water electrolysis (AWE), which is commercially accessible for large-scale hydrogen production(Amores et al., 2017).

Alkaline water electrolysis

The primary benefit of alkaline water electrolysis over other water electrolysis is that it can be constructed from readily available and affordable materials. Simple Nickel and steel can be used as electrodes to produce oxygen and hydrogen(Stolten, 2010). In a typical AWE, the electrodes are submerged in a strongly alkaline aqueous solution, usually made of 20–40 wt.% concentrated potassium hydroxide. The anode and cathode are separated by a porous solid material (diaphragm) that allows the passage of (OH) ions between the electrodes to prevent mixtures that could result in safety risks and poor faradaic efficiencies. AWE can produce hydrogen gas of great purity (99.9% purity)(Millet and Grigoriev, 2013). On the weak point, Alkaline water electrolysers operate at a modest current density, are not particularly compact, and are not entirely suitable for use with transient power sources(Stolten, 2010). Thus, despite the technology's established maturity, it is still the subject of research and development. For instance, advanced electrocatalysts are being developed to reduce electrode overvoltage. Gap-zero configurations are also exploited for higher current density operation and reduction of ohmic losses(Sanchez et al., 2020). The design and improvement of electrolysis systems can also benefit from modelling and process simulation. Process simulation can help gain insight into the system's performance without the trouble of running experiments(Fragiacomo and Genovese, 2019).

Objectives

This research aims to use artificial intelligence as a cutting-edge technique to optimise process efficiency. However, this paper focuses on Simulink process modelling of the AWE and analysis of the effects of process variables on the electrolysis performance. Mathematical descriptions are used to model the alkaline water electrolyser, and the performance of the process is examined in relation to variables such as current density, temperature, and pressure. Artificial Neural Network is used to prove the effectiveness of AI for prediction and optimisation.

Model conception

Following the study's purpose, only the electrolyser stack is modelled. Simulink is utilised as the modelling software due to its ability to implement visual tools for computational simulations. Simulink provides an extensive library of algorithms and custom function blocks necessary to incorporate mathematical models to build and analyse the process performance. Although Simulink includes an electrolysis component, the latter is rather elementary. It would not allow for a systematic study of the electrolyser's performance. Therefore, a custom electrolyser model has been developed, considering all parameters necessary to satisfy the project's purpose.

The electrolyser model is able to accurately calculate cell voltage(E), current density(I), energy efficiency, faraday efficiency(η), over-voltages and hydrogen yield at various operating conditions. With the ability to operate over a broad range, this model is a valuable tool for studying the effect of parameters such as pressure(p), temperature(T), and current density(I) on the performance of the electrolyser. The suggested model also serves as an effective method to systematically optimise the efficiency of the electrolysis process. The added ANN (artificial neural network) experiment shows that AI can be used to further optimise the process.

Simulink model

As aforementioned, the Simulink model of the alkaline electrolyser is developed to investigate correlations between the process variables and the electrolyser performance in order to improve efficiency.

Cell/stack voltage (E), Faraday efficiency, cell efficiency, polarisation curve, and H2 produced are determined using Electrochemical, thermodynamic and empirical equations for a wide operating range of input variables (power(w), temperature (T), pressure (p), number of cells(N), active area(A)). see figure 1.

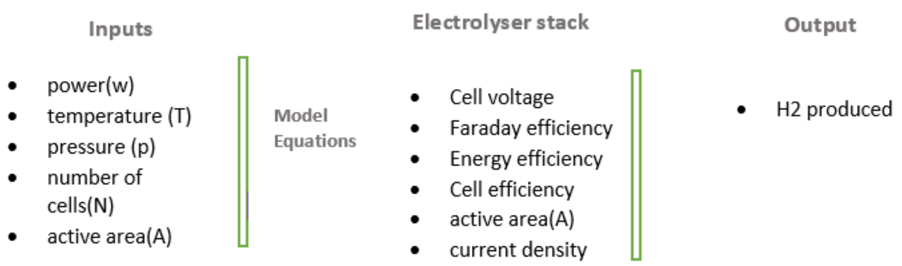

Figure 1 .AWS Simulink model operation flow

Methodology

In Alkaline water electrolysis, water molecules' separation into gaseous oxygen and hydrogen happens when an electrical current (DC) is passed between two electrodes separated by an aqueous electrolyte with strong ionic conductivity (typically KOH ranging from 20 to 40% by weight)(Rashid et al., 2015). The electrolysis process is defined by the dynamics of reactions, thermodynamics, and various transport processes occurring at the electrodes(Santos et al., 2013). Alkaline water electrolysis occurs according to the following reactions:

Anode $4OH^- (l) \rightarrow 0_2 + + 2H_20 + 4e$ requires 0.4V $E^0 = -0.4V$

Cathode $2H_20 (l) + 2e \rightarrow H_2 + 2OH^-$ requires 0.82V $E^0 = -0.83V$

Net $2H_20 (l) \rightarrow 2H_2 + 0_2$ requires 1.24V $E^0 = -1.23V$ (Eq.1)

1.23V is the minimum voltage required for the reaction to take place. It is known as reversible voltage (E_{rev}), measured at standard conditions (1 bar and 25 °C). It can be obtained from the first law of thermodynamics, which states that the amount of electricity (nFE) needed to split a mole of water at equilibrium is equal to the Gibbs free energy change (ΔG^0) of the reaction(Ursua et al., 2011).

$\Delta G^0 = nFE$

$E = \Delta G^0/nF$ (Eq.2)

Where F is the faraday coefficient, and n=2 is the number of electrons transferred
the Gibbs free energy can be calculated from the following equation

$\Delta H (T, 1) = \Delta G (T, 1) + T \cdot \Delta S (T, 1)$ (Eq.3)

ΔH(T,1), ΔSd (T,1) are, respectively, the enthalpy change, the entropy change) at T (25 ^{0}C) and P (1 bar)

The reversible voltage (E_{rev}) can also be calculated using empirical equations under different temperatures and pressure than standard conditions. Empirical equations presented by (Stolten, 2010) are used to calculate E_{rev} as a function of temperature (Eq.4), and (Eq.5) is used to account for both temperature and pressure.

$E_{rev}(T) = 2 F \Delta G(T) = 1.5184 - 1.5421 \times 10^{-3} * T + 9.523 \times 10^{-5} * T * Ln(T) + 9.84 \times 10^{-8} T^2$ (Eq.4)

When taking into account the cell pressure, Erev can be calculated as follow:

$E_{rev} (T, P) = Erev(T) + \frac{3RT}{4F} \ln(P)$ (Eq.5)

However, due to energy losses, the actual cell voltage (E) is always larger than the theoretical one. The actual cell voltage (E) is the sum of reversible voltage (E_{rev}) and overpotentials (ή) (Amores et al., 2017) (see Eq.6).

$E_{cell} = E_{rev} + (ή_{at} + ή_{ohm} + ή_{conc})$ (Eq.6)

ή (overpotential) is the sum of activation, ohmic and concentration overpotentials caused by:

Activation overpotentials: associated with the activation energies for the generation of hydrogen and oxygen on the surface of electrodes.

Ohmic overpotential: refers to the sum of transport resistance due to gas bubbles, ionic transfer in the electrolyte, and membrane resistivity, together with the electrical resistance of various components, such as electrodes and current collectors.

Concentration overpotentials: caused by mass transport restrictions that arise at high currents on the surface of the electrodes(Amores et al., 2017).

The overpotentials are represented on the polarisation curve in figure 2. The polarisation curve is used to establish the electrolysis kinetics reactions. It allows for determining the ideal cell voltage and current density(Ursua et al., 2011).

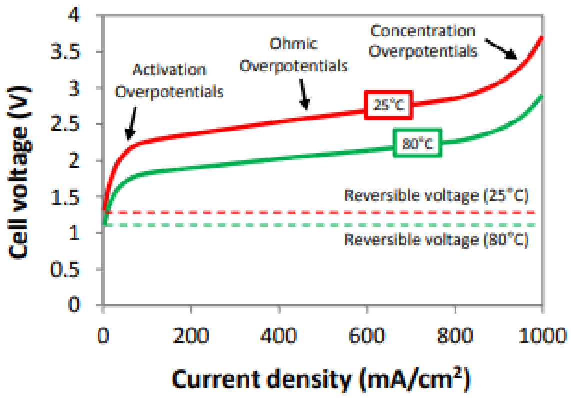

Figure 2 alkaline electrolysis polarisation curve at 25 and 80 ^{0}C

A semi-empirical approach (Eq. 7) introduced by (Ulleberg, 2003) and further modified by (Sanchez et al., 2020) has been used to calculate the cell overpotential (E_{cell}) for the model. The equation relates temperature(T), pressure(p) and current density(i) to the polarisation curve. concentration overpotential is omitted from the equation as it only occurs at high current density, passed the operating range of the model.

$E_{cell} = Erev + [(r1 + d1) + r2.T + d2.p] + S.\log\left[\left(t1 + \frac{t2}{T} + \frac{T3}{\mathrm{T2}}\right) i + 1\right]$
(Eq. 7)

Another critical parameter for evaluating AWE performance is the faraday efficiency (Eq. 8). It represents the ratio of the experimental hydrogen gas produced to the theoretical value. It refers to the amount of current transformed in the reaction and the energy lost due to losses(Santos et al., 2013).

$\eta F = \frac{\mathrm{nH2\ prod}}{\mathrm{nH2th}}$ (Eq. 8).

Much like the polarisation curve, Faraday's efficiency has also been modelled using the empirical equation proposed by (Ulleberg, 2003).

$\eta F = \left(\frac{\mathrm{i2}}{\mathrm{f11+f12.T+I2}}\right).(f21 + f22.T)$ (Eq.9)

There is a direct correlation between the flow of electrons (current) and the production rate of hydrogen (Faraday's Law). The electrochemical behaviour of the cells influences the rate of hydrogen generation at the cathode. Hydrogen production at the cathode was computed using a derived equation of the Faraday efficiency

$nH2prod = \eta F \frac{\mathrm{I}}{\mathrm{z.F}}.N$ (Eq.10)

The electric input power is determined using ohm's law

$W_{stack} = E_{stack}.I = (E_{cell}.N).(I.\ Acell)$ (Eq.11)

With N the quantity of cells in the stack.

Figure 3 shows the electrolyser model developed using Simulink.

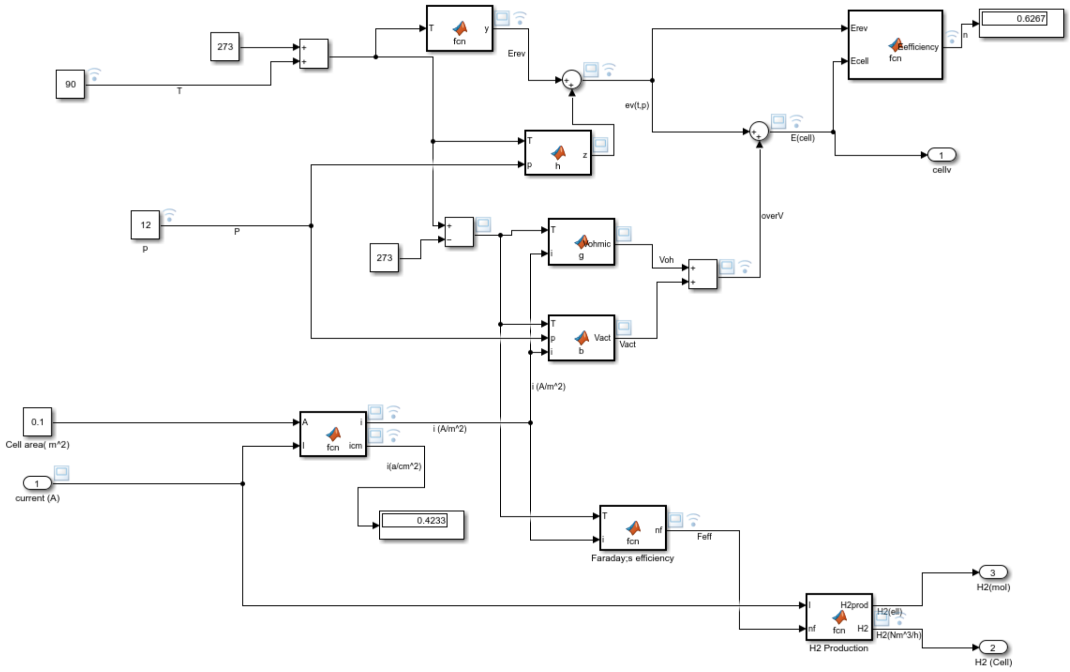

Figure 3: alkaline cell electrolysis Simulink simulation

ANN (artificial neural network) predictive model

One of the most used AI modelling techniques in chemical engineering is ANN (Dutta and Upreti, 2021). Figure 4 shows the setup used for configuration, which consists of a three-layer system with three neuron inputs (temperature (T), power (P), and pressure (P), a hidden layer with ten nodes, and six output layers (cell efficiency, faraday efficiency, hydrogen yield, energy efficiency, current density, and cell voltage). BP-ANN trains the algorithm using a first-order gradient descent technic(Maier et al., 2000). The Marquardt-Levenberg BP learning approach was selected as the back-propagation method(Banza and Rutto). The log-sigmoid transfer function for all data sets in ANN (log sig) was employed in the hidden layers(Senthil Kumar et al., 2012). ANN is used to demonstrate that the process can be modelled and optimised using AI

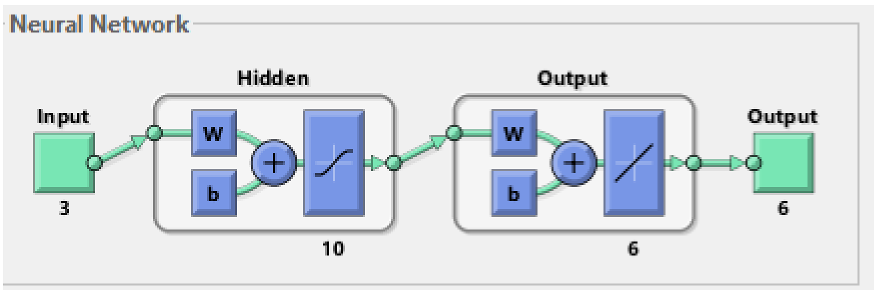

Figure 4:ANN architecture

Results and Discussion

The model is developed using Simulink to study the effects of pressure, temperature, and current density on cell performance. The insight gained will serve as a base to further optimise the process using artificial intelligence.

Influence of temperature and on the polarisation curve

Figure 5 shows the polarisation curve and the effect of temperature (25 ^{0}C-100 ^{0}C). It's observed that a rise in input power increases the current density and cell voltage. As discussed in Eq.11 current density (I/A) is proportional to the power delivered to the electrolyser. Therefore, an increase in the input power results in a higher current density, Cell voltage increases due to overvoltages caused by a higher current density (Eq. 7)
. On the other hand, the cell voltage decreases as the temperature drops due to the decrease in the reversible voltage (Eq.4), which should subsequently lead to a reduction in input power.

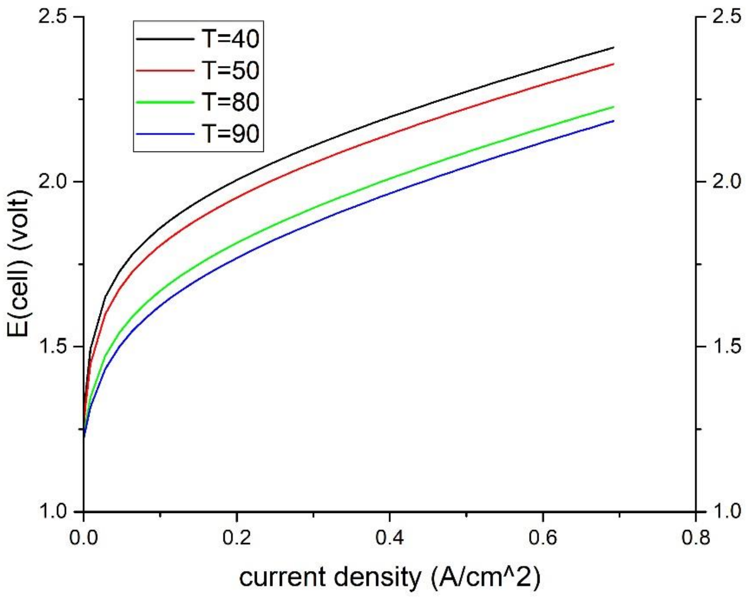

Figure 5: effect of temperature and current density on cell potential

Influence of temperature and current density on efficiency and hydrogen yield

Figure 6 and 7 shows hydrogen flow rate and cell efficiency at different temperatures and current density. Hydrogen production increases with a rise in current density. The phenomenon is in line with faraday's 1st law of electrolysis, which states that the quantity of hydrogen produced is directly proportional to the input current. The faraday efficiency (Eq.9) is closer to 1 at a higher current density. The cell efficiency, on the other hand, decreases with increased current density. Cell efficiency is related to input power and hydrogen yield. At higher current density, more energy loss occurs due to overvoltages leading to lower efficiency. The increase in temperature, however, results in higher efficiency since the reversible voltage diminishes at a higher temperature eq. Hydrogen yield decreases slightly at higher temperatures due to the drop in the faraday efficiency.

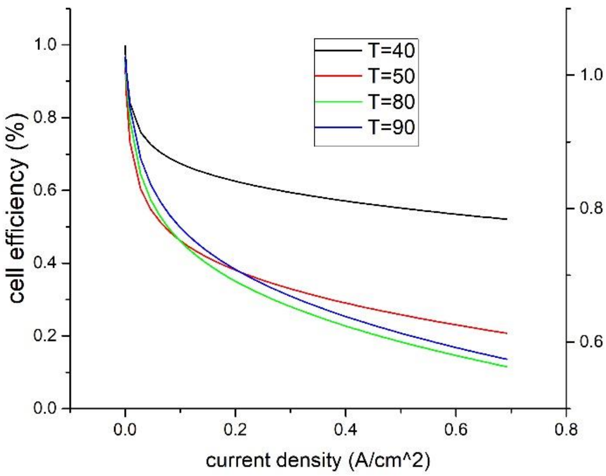

Figure 7:effect of temperature and current on cell efficiency

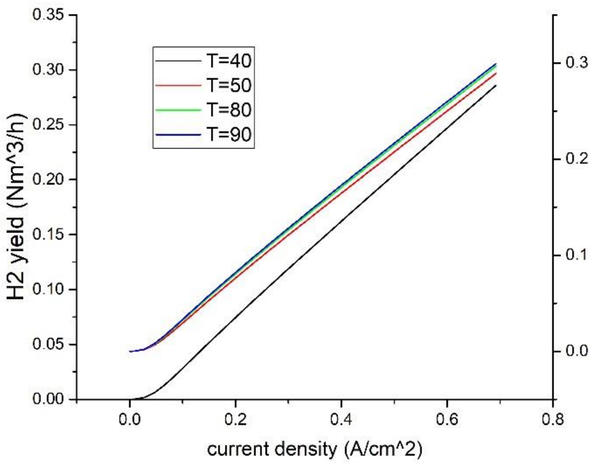

Figure 6:effect of temperature and current on H2 yield

Temperature and pressure optimisation

Figures 8 and 9 show the effects of temperature and pressure on hydrogen production as well as cell efficiency, identified as essential parameters for electrolyser optimisation (Lubitz and Tumas, 2007). Pressure and temperature could be used to optimise the process when input power is lower than the desired value. It shows that when the current density is lower, efficiency and hydrogen production can be kept at the desired value by lowering the pressure and increasing the temperature

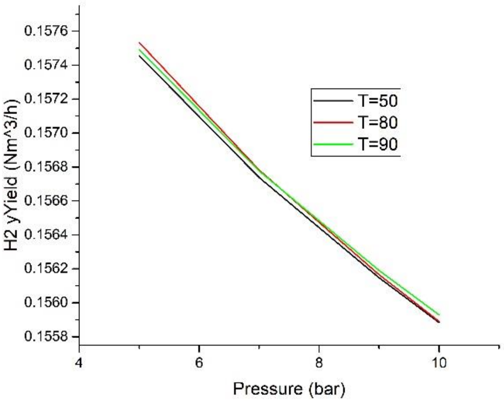

Figure 9:effect of pressure and temperature on H2 yield

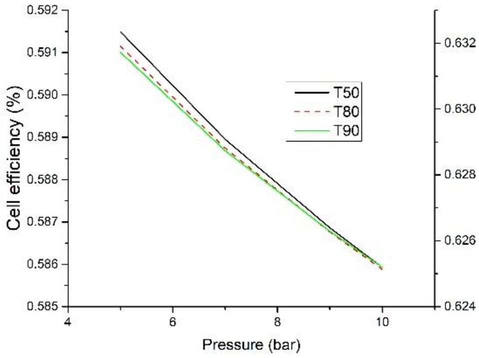

Figure 8:effect of pressure and temperature on efficiency

ANN model and prediction

figure 10. shows the way the network and data interact. The correlation coefficient for training, testing, validation and all data is 1. It entails that the ANN predict the output data with almost perfect accuracy

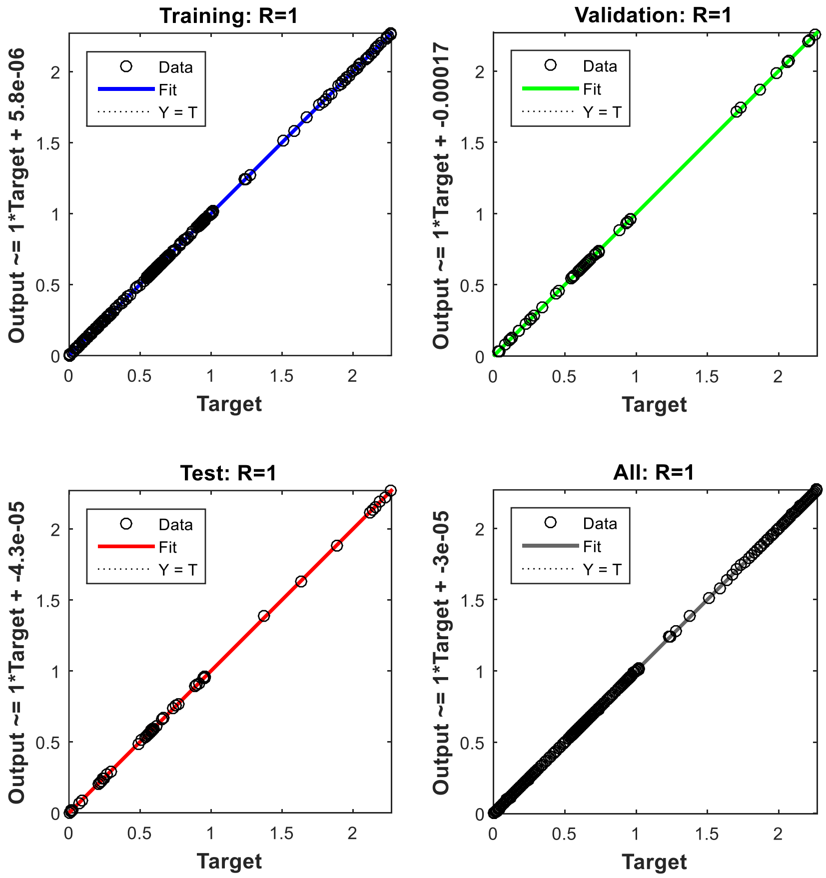

Figure 10: neural network regression analysis

conclusion

This paper proposes a Simulink model of an alkaline electrolyser with the objective of studying the influence of the process parameters such as pressure, temperature and current density on the electrolyser performance.

The developed stack electrolyser model is able to generate a polarisation curve, faraday efficiency, cell efficiency and hydrogen yield at various temperatures and pressures.

Analysis of the model data shows that at higher current density, the efficiency of the electrolyser decreases due to overvoltages. However, hydrogen yield increases since it is proportional to the current density in the cell. An increase in temperature can improve efficiency by reducing the cell voltage. Currently, the cell temperature of alkaline electrolysers is restricted to a maximum of (100^0C-130^0C) due to corrosion of components under high temperature alkaline medium. It has been observed that at lower values (5-10 bar), pressure has a negligible effect on the hydrogen yield. The cell efficiency, on the other hand, decreases with increased pressure due to the increase in potential energy. Nonetheless, running the electrolyser at higher pressure reduces the energy needed to compress hydrogen for storage.

For process optimisation, finding a proper equilibrium between cell efficiency and hydrogen yield while considering the constraints related to high temperature, pressure, and current density should allow for better optimisation of the electrolyser performance. At reduced input power, the efficiency of the electrolyser could still be maintained by lowing the pressure and increasing the temperature.

The implementation of ANN(artificial neural network) successfully proved that AI could be used to model and further optimise the process. the ANN has been trained Levenberg BP learning approach and was able to predict the output data with very high accuracy(R=1)

The knowledge gained from this work will be used to build a data driven algorithm for improved process control and optimisation.

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