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Mathematical Modelling and Simulation Analysis of Alkaline Water Electrolyser for Stationary Electrolyte in Atmospheric Pressure

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ABTRACT: In recent years, combined hydrogen and oxygen gas (known as brown gas, knall gas and HHO) is introduced in combustion chambers to reduce the emissions of automobiles by reducing NOx and SOx combustion products. The brown gas is produced through water electrolysis in alkaline medium, Potassium hydroxide (KOH) used as electrolyte and nickel used as catalyst. This mathematical approach describes the thermodynamic relations with reversible potential, thermoneutral voltage and taking into account of kinetic Effects on structural parameters (Electrode geometry, activation parameters such as tafel slope and exchange current density) and Effect of operational parameters (temperature, void fraction due formation of bubbles, concentration and conductivity of electrolyte) at anode and cathode compartments of electrolyser even it may not commercially available. This model is able to predict the rate of production, rate of energy consumption and efficiency of electrolyser. The Simulation analysis is done by using Engineering Equation Solver. We observed that efficiency of the cell is optimum at elevated temperatures. For analysis single cell is consider and designed for operating temperatures of 303, 323 and 343 K at atmospheric pressure (1.01325bar).

Keywords:
Alkaline water electrolyser
Thermodynamics
Gas evolution
Electrochemical calculation

INTRODUCTION:

The strong use of fossil fuels causes to air pollution and global warming, it creates utmost urgency of developing a clean and renewable secondary alternative energy. Hydrogen energy is expected to be useful as the secondary energy in near future, For example, fuel for transportation (IC engines), electricity generation in fuel cells and other applications. Unfortunately, the vast majority of hydrogen is being used today produced by fossil-fuel-based processes (steam methane reforming, coal gasification) which may result in gas emissions such as COx, SOx and NOx. These methods violates our original purpose. On the other hand, the fossil-fuel-based hydrogen production processes are both subject to large price fluctuations and a limit

in global supply. The development of renewable, efficient and economical hydrogen production technologies is to replace by Fossil-fuel-based hydrogen production methods is key step towards a sustainable "hydrogen economy" Water electrolysis integrated with nuclear power stations or wind turbines are the most promising methods for large-scale renewable hydrogen production. Photochemical and photoelectrochemical water splitting methods are another promising methods for production of hydrogen. The electrolysis of aqueous alkaline solutions has historically been one of the most popular routes for hydrogen production .Recently, most studies related to alkaline electrolysis emphasize on the development of new advanced electro catalyst materials and the increase in the operating temperature of the Electrolytic cell. Comparatively, the detailed systematically configuration design and Numerical optimum are rare in the current literatures, but they are very important for better understanding the performance, improvement and operating mechanism of an alkaline water electrolyser and worthwhile to be further studied.
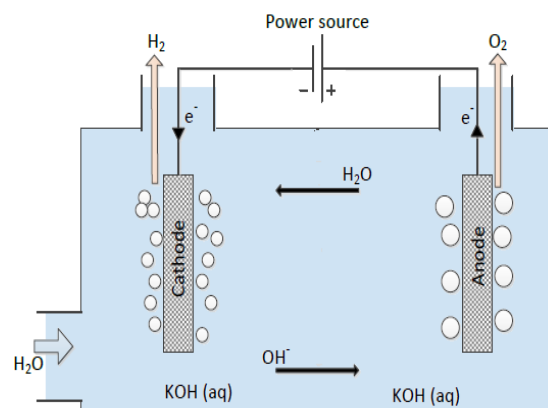

Figure 1. Principle of electrolysis

ALKALINE WATER ELECTROLYSIS: An alkaline electrolysis cell consists of four major components; the electrolyte, which is commonly potassium hydroxide (KOH) in high concentrations (usually 6-7 mol/L or 30%KOH), the cathode, the anode and DC power source. Hydrogen evolution
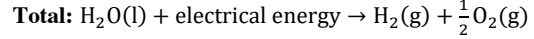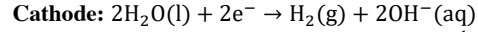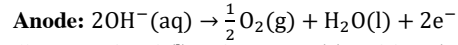
takes place at the cathode, where the electrons are provided for the decomposition of water. The hydroxyl ions are decomposed in to oxygen and water at the anode, where oxygen evolution

Nomenclature:

F	Faraday constant (F), 96485 col mol^{-1}
n	Number of moles of electrons for hydrogen
n_{O_2}	Number of moles of electrons for oxygen
n_{H_2O}	Number of moles of electrons for water.
P	Pressure in the cell (P = P_{O_2} = P_{H_2}), bar
P_{O_2}	Partial Pressure of oxygen molecules
P_{H_2}	Partial Pressure of Hydrogen molecules
R	Universal gas constant, 8.31446 j/mol-k
LHV	Lower heating value, 241.83x10^3 j/mol
A	Anode and Cathode surface area, 0.0016 m^2
δ	Thickness of the electrolyte, 0.0015m
T_o	Temperature at standard condition, 298K
T	Absolute temperature of cell, K
I	Total current applied on the cell, A
M_{O_2}	Molar mass or molecular weight of o2, 3.2x10^{-2}kg mol^{-1}
M_{H_2}	Molar mass or molecular weight of h2 2x10^{-3}kg mol^{-1}
ρ_{H_2}	Density of hydrogen molecule, 0.0899 kg m^{-3}
ρ_{O_2}	Density of oxygen molecule, 1.429 kg m^{-3}
h	Height of electrode, m
w	Width of electrode, m
G_o	Gibbs free energy, j mol^{-1}
ΔG_T	Gibbs free energy at temperature T
ΔH_0	Change in enthalpy at standard temperature, j mol^{-1}
ΔH_T	Change in enthalpy with temperature, j mol^{-1}
ΔS_0	Change in entropy at standard temperature J mol^{-1}K^{-1}
ΔS_T	Change in entropy with temperature J mol^{-1}K^{-1}
ΔC_P	Change in specific heat, J mol^{-1}K^{-1}
$C_{P,h2}$	Specific heat of hydrogen gas, J mol^{-1}K^{-1}
$C_{P,o2}$	Specific heat of oxygen gas, J mol^{-1}K^{-1}
$C_{P,h20}$	Specific heat of water, **J mol^{-1}k^{-1}**
S_{h2}	Entropy of hydrogen, J mol^{-1}K^{-1}
S_{O2}	Entropy of oxygen, J mol^{-1}K^{-1}
S_{h2O}	Entropy of water, J mol^{-1}K^{-1}
$U_{rev,T}$	Reversible cell voltage, V
$U_{TH,T}$	Thermo-neutral voltage, V
j_{av}	Average current density (Am^{-2})
j_{o-a}	Anode exchange current density (Am^{-2})
j_{o-c}	Cathode exchange current density (Am^{-2})
η_a	Activation potential losses at anode side
η_c	Activation potential losses at cathode side
U_{OHM}	Ohmic losses due to bubble formation and Resistance of electrolyte
J_{ef}	Current density in presence of bubbles on surface Of electrodes, Am^{-2}
A_{ef}	Effective surface area of electrode, m^2
β_a, β_c	Tafel constants of anode and cathode.mv dec^{-1}
f_g	Average void fraction
α_a, α_c	Transfer coefficients of anode and cathode
HER	Hydrogen evaluation reaction
OER	Oxygen evaluation reaction
R_e	resistance of electrode, Ω
ρ_e	resistivity of electrode,Ωm^{-1}
L	Thickness of electrode, m
K	The specific conductance of electrolyte (S m^{-1})
m	Concentration of solution in mol.L^{-1}
K_e	Effective conductance
ρ_T	Density of the solution at temperature T
μ_T	Viscosity of the solution at temperature T

Takes place.A basic schematic diagram of an alkaline electrolyser along with the most important components is shown in figure.1.The basic reactions of the decomposition of water in an alkaline electrolyser are given by equations. [1]

Anode: $2OH^-(aq) \rightarrow \frac{1}{2}O_2(g) + H_2O(l) + 2e^-$
Cathode: $2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$
Total: $H_2O(l) + \text{electrical energy} \rightarrow H_2(g) + \frac{1}{2}O_2(g)$

The cell voltage, U has to be applied to produce hydrogen and oxygen with a given rate depends on the operating temperature and pressure as well as on a number of other factors such as the electro-catalyst material and microstructure, i.e. a high specific surface area. Furthermore, the right choice of the electrolyte concentration for a specific temperature and proper circulation of the electrolyte are important factors. The losses which occur during the electrolysis process is defined as polarization losses. The polarization further more can be divided into the activation losses at anode and cathode, ohmic losses by conductivity of electrolyte and due to bubble formation on electrodes. In this paper, all operational parameters and kinetic parameters are operated at atmospheric conditions. Figure.1 describes HER and OER occurred on active surfaces of cathode and anode in the electrolyte .Purpose of this paper is to establish a mathematical model by which most important process variables are combined in functional relationship, and describing cell voltage which is required to run the cell and investigate I-V characteristics, activation Potential, reversible potential, ohmic losses by gas evaluation at different temperatures and concentrations. The operating cell parameters are considered for mathematical modelling.

Table 1. Operating cell information:

Operating parameters	values
Operating voltage per cell	2.5-3 V
Operating pressure (P)	1.01325 bar
Operating temperatures (T)	303.15,323.15,343.15 K
Electrical power	2.5W-3W

Thermodynamic calculations: thermodynamic calculation provides functional relations of Reversible voltage, thermoneutral voltage and change in Gibbs free energy with temperature. To calculate the thermodynamic effects in electrolytic reaction, it is convenient to assume hydrogen and oxygen gases partial pressure are equal to water pressure. Which is operated at atmospheric pressure. The minimum work is required dissociation water is equal to Gibbs free energy is given by [2]

$$G_O = \Delta H_0 - T_0 \Delta S_0 \qquad (1)$$

In which, G_o, ΔH_o, ΔS_o are Gibbs free energy, enthalpy Change and entropy change at standard temperature (T_o) and atmosphere pressure (P). Eq. (2), Eq. (3) represents enthalpy change and entropy change at standard conditions. [2]

$$\Delta H_O = H_{h2} + \frac{1}{2}H_{02} - H_{h2O} \qquad (2)$$

$$\Delta S_O = S_{h2} + \frac{1}{2}S_{O2} - S_{h2O} \qquad (3)$$

Change in specific heat with temperature T is given by the following equation [2]

$$\Delta C_P = C_{P,h2} + \frac{1}{2}C_{P,O2} - C_{P,h20} \qquad (4)$$

Table.2
Thermodynamic parameters for the reactant/products at 1.01325bar, where (g) and (l) represents gas phase and liquid phase, respectively [3]

Properties	H_2 (g)	O_2 (g)	H_2O (l)
$G_o(T_0)$,**J mol^{-1}**	-38,960	-61,120	-306,690
$H_o(T_0)$ **J mol^{-1}**	0	0	-285830
$S_o(T_0)$ **J mol^{-1}k^{-1}**	130.68	205.00	69.95
C_{p}, **J mol^{-1}k^{-1}**	27.28+0.00326*T +50000/T^2	29.96+0.00418*T -167000/T^2	75.44

Substituting the thermodynamic data as in Table.2 in to the Eq. (4). Change in specific heat with various temperatures is shown in Eq. (5)

The temperature dependent change in specific heat is obtained by substituting the thermodynamic parameters in eq.4. This is given by

$$\Delta C_P = -33.18 + 5.35 \times 10^{-3}T - 33500/T^2 \quad (5)$$

Change in enthalpy with temperature is given by Eq. (6) [2]

$$\Delta H_T = \Delta H_O + \int_{298}^{T} \Delta C_P dT \quad (6)$$

To express temperature dependent enthalpy change, substituted specific heat in Eq.6 and integration with temperature. Applying limits from 298 to T,

$$\Delta H_T = 295367.673 - 33.18T + 2.675 \times 10^{-3}T^2 + 33500/T \quad (7)$$

Change in entropy with temperature can be written as

$$\Delta S_T = \Delta S_0 + \int_{298}^{T} \left(\frac{\Delta C_P}{T}\right) dT \quad (8)$$

For the change in entropy with temperatures, substitute Eq. (3), Eq. (5) and integrating with temperature in the limits 298 K to T as shown in Eq. (9)

$$\Delta S_T = 349.612 + 5.35 \times 10^{-3}T - 33.18 \ln T + 16750/T^2 \quad (9)$$

Gibbs free energy at operating temperature T is given by Eq. (10)

$$\Delta G_T = \Delta H_T - T\Delta S_T \quad (10)$$

Substituting Eq. (7) and Eq. (9) in Eq. (10) the available energy at various temperatures at 1 .0325 bar is given as Eq. (11)

$$\Delta G_T = 295367.67 - 382.792T - 2.675 \times 10^{-3}T^2 + 33.18T \ln T + \frac{16750}{T} \quad (11)$$

U_{rev} (reversible cell voltage) is the minimum cell voltage to drive the splitting of water with various temperature is given In Eq. (12)

$$U_{rev,T} = \frac{\Delta G_T}{nF} = 1.5306 - 1.9836 \times 10^{-3}T - 1.3862 \times 10^{-8}T^2 + 1.7194 \times 10^{-4}T \ln T + \frac{0.0868}{T} \quad (12)$$

Thermoneutral voltage (U_{th}) is voltage at which neither endothermic nor exothermic reaction takes place, it is shown in Eq. (12)

$$U_{TH,T} = \frac{\Delta H_T}{nF} = 1.5306 - 1.7194 \times 10^{-4}T + 1.3862 \times 10^{-8}T^2 + \frac{0.1736}{T} \quad (13)$$

Voltage efficiency is defined as energy content of hydrogen to electrical energy supplied to the cell. This also call energy efficiency.

$$\eta_{energy} = \frac{U_{TH,T}}{U} \quad (14)$$

Electrochemical calculations:
Total cell voltage U is sum of the reversible, activation losses and ohmic voltages due to bubble formation and resistivity of electrolyte [5]

$$U = U_{rev,T} + \eta_a + \eta_c + U_{Ohm} \quad (15)$$

Activation polarisation at cathode and anode:
tafel expressions is used to determine the activation over potential losses at anode and cathode,which is defined as follow

$$\eta_a = \beta_a \log \frac{j_a}{j_{0-a}} \quad , \quad \eta_c = \beta_c \log \frac{j_c}{j_{0-c}} \quad (16)$$

bubble formation on electrodes is reduces active surface area,this results in change current density on surface of electrode. the active surface area is replaced with effiective active surface area. The effective current density can be written as Eq(17)

$$J_{ef} = \frac{I}{A_{ef}} \quad (17)$$

By applying bubble effect to activation over potential Eq.(16) changes in to Eq.(18),Eq. (19)[5]

$$\eta_a = \beta_a \log \left(\frac{j_{av}}{j_{0-a}}\right) - \beta_a \log(1 - \theta) \quad (18)$$

$$\eta_c = \beta_c \log \left(\frac{j_{av}}{j_{0-c}}\right) - \beta_c \log(1 - \theta) \quad (19)$$

which η_a, η_c are anodic and cathodic overvoltage. β_a, β_c is the tafel slopes for anode and cathode respectively. j_{0-a} and j_{0-c} are exchange current densities at anode and cathode. β_a, β_c are computed by using the Eq.(21)[6]

$$\beta_a = \frac{2.303RT}{\alpha_a nF}; \quad \beta_c = \frac{2.303RT}{\alpha_c nF} \quad (20)$$

j_{av} is the average current density with absence of bubble effect. J_{ef} is current density with bubble effect and A_{ef} is the effective area [6]

$$A_{ef} = A(1 - \theta) \quad (21)$$

according to experimental work of ketnz and The bubble rate coverage as function of current density and temperature.[5]

$$\theta = \left(-97.25 + 182\left(\frac{T}{298}\right) - 84\left(\frac{T}{298}\right)^2\right)\left(\frac{j}{j_{Lim}}\right)^{0.3} \quad (22)$$

H.Vogt and R.J balzer [11] suggested the limiting current density value is 300KA/m^2.Hammoudi [5] proposed temperature dependent correlation for anodic transfer coefficient(α_a) and cathodic transfer coefficient(α_c) given as Eq.(23)&Eq.(24)
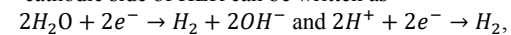
$$\alpha_c = 0.1175 + 0.00095(T - 273) \quad (23)$$

$$\alpha_a = 0.0675 + 0.00095(T - 273) \quad (24)$$

Electrode kinetics: HER, OER reaction are determines the reaction rate of each step.for obtaining higher efficiency proper electro-catalyst must be selected by reducing the cathode and anode overpotentials.
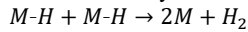
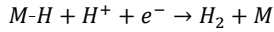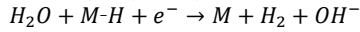**Hydrogen evalution reaction(HER):**
cathodic side of HER can be written as
$2H_2O + 2e^- \rightarrow H_2 + 2OH^-$ and $2H^+ + 2e^- \rightarrow H_2$,
HER starts with volmer step ,which involves hydrogen ion is bonding the near metal site M.
$$M + H_2O + e^- \rightarrow M\text{-}H + OH^- \quad \text{This is fast step,}$$
$$M + H^+ + e^- \rightarrow M\text{-}H$$
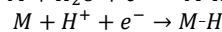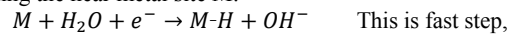
The rate determining step is slow step, which inhibits the rate of reaction. It's shown by tafel reaction

$$M\text{-}H + M\text{-}H \rightarrow 2M + H_2$$

Or by Heyrovsky reaction

$$H_2O + M\text{-}H + e^- \rightarrow M + H_2 + OH^-$$
$$M\text{-}H + H^+ + e^- \rightarrow H_2 + M$$

Oxygen evalution reaction(OER): hydroxide ions are diffused through anode side where oxygen evolution reaction takesplace.the reactions can be written as

$$OH^- + M \rightarrow M\text{-}OH + e^-$$
$$M\text{-}OH + OH^- \rightarrow M\text{-}O + H_2O + e^-$$
$$M\text{-}O + M\text{-}O \rightarrow O_2 + 2M$$
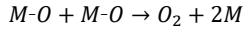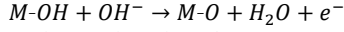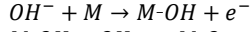
Selection of Material is very important aspect for modelling of electrolysers. High activation energy material has less activation losses. Platinum is a highest active material among all materials for HER and Poor activity towords OER due to formation of platinum oxide film. IrO_2 is the one of the best stable electrode for OER in acidic medium but it suffers less activation. RuO_2 is known as most active metal oxide toword OER however it suffers instabilty. Improve stabilty and activation is very costly process. Reasercher are shifted focusing on devolping cost effective, chemically stable materials. Untill now wide range of material devolped for higher activation and stability. Ni and Ni-base electrodes are among the best materials used for alkaline water electrolysis because of good activation energy and excellent chemical stabily and cost effective.Activity is decrease with purity of electrolyte decreases,even small traces of Fe (0.5-1 ppm) in solution results in increase in tafel slope(β). Table.3 shows the tafel perameter for higher over potential for HER and OER [7][9].

Table.3
Tafel perameter of HER and OER on Ni electrode in 30Wt%KOH solution for over potentials (high)at different temperatures [7][9]

Temperature(K)	$β_c$(mV)	$i_{o\text{-}c}$ (A/cm²)
303	115	3.55×10^{-5}
323	111	4.47×10^{-5}
343	104	7.08×10^{-5}
Temperature(K)	**$β_a$(mV/dec)**	**$i_{o\text{-}a}$(A/cm²)**
303	130	0.11×10^{-3}
323	150	0.38×10^{-3}
343	159	0.93×10^{-3}

Voltage lose due to electrode resistance :(Re) the resistance could be expected to increase with increase in temperature Thus a fractional change in resistance for nickel electrode is can be defined as function of T. resistance for two electrodes defined by

$$R_e = \frac{2}{\sigma_{Ni}} \frac{L}{S}$$
(23)

Above relation defined by considering, the thickness of electrodes (L) and cross section area of electrode(s) is same. Where L is in m and S is in m². Electrical conductivity (σ_{Ni}) in S cm⁻¹, of the Ni defined as a function of temperature [6]

$$\sigma_{Ni} = 6000000 - 279650(T - 273) + 532(T - 273)^2 - 0.38057(T - 273)^3$$
(24)

Voltage loss due to electrode resistance defined as, in V

$$V_R = IR_e$$
(25)

Voltage losses due to electrode resistance on the electrolyser performance can be neglected.

Table.4
Electrolyser model parameters

Symbols	descriptive	values
A	contact surface area of anode and cathode	0.0049m²
h	electrode height	0.07m
w	Width of electrode	0.07m
δ	thickness of elctrolyte	0.0025m
L	thickness of electrode	0.0015m
S	surface area of electrodes	0.0049m²
Electrolyser's components		**materials**
Anode		nickel(99.97%)
Cathode		nickel(99.97%)
Electrolyte		aq. KOH

Voltage losses due to bubble formation:
The evolution of gases during reaction at cathode and anode in the electrolyte. These gases are formed in bubbles and ascending in vertically upward direction. Since bubble have negligible electrical conductivity, the flow of current path is restricted then polarisation losses are increased. Bruggeman correlation [2] is used to describe voltage drop due bubble formation. It can be expressed as ratio of effective conductance to specific conductance. [2]

$$V_{OHM} = \frac{j_{av} \delta}{K_e} \quad ; \quad \text{Where} \quad K_e = K(1 - f_g)^{3/2}$$
(26)

V_{OHM} is voltage losses due to bubble formation and K_e is the effective conductance and f_g is the gas void fraction. This correlation does not affect the bubble size, collision and it is applicable to uniform void distribution throughout the cell. It can be expressed as $f_g = \left(\frac{2}{3}\right)\theta$[5]. I is the applied current in A and J_{av} is the average current density in A/cm², P is **power** required for operating the single cell.

$$P = I.U$$
(27)

R.J.gilliam proposed a correlation for Specific conductivities of potassium hydroxide solutions is function of concentrations and temperatures [10] is expressed by

$$K = \left[-2.041M - 0.0028M^2 + 0.005332MT + \frac{207.2M}{T} + 0.001043M^3 - 3.0 \times 10^{-7}M^2T^2 \right] \times 100$$
(28)

K is specific conductivity of KOH solution in S/m, M is the concentration of solution in mol/L is defined as [10]

$$M = \frac{\%wt \times \rho_T}{56.105 \times 100}$$
(29)

Density of KOH solution can be expressed as a function of temperature (T) and concentration (%wt in 'w') and correlation is obtained from experimental data of r.j.gilliams and drawn plot in three dimensional. The functional correlation was obtained by using polynomial regression technique, R-square value adjusted to 1 and RMSE value is 0.9984. This is defined as
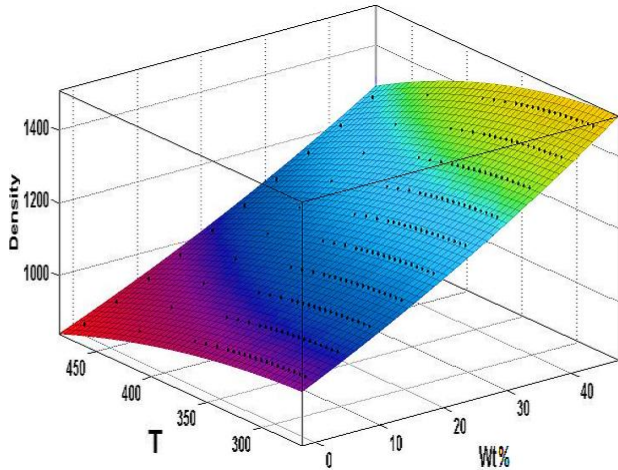
Figure 2.Representation of density of aq.KOH is function of temperature (K) and concentration (wt %).

$$\rho_T = 868.1 + 6.81w + 1.137T + 0.04391w^2 + 0.0138wT - 0.002487T^2 + 0.0001279w^3 - 2.547 \times 10^{-5}w^2T - 2.644 \times 10^{-5}wT^2 \tag{30}$$

Above functional correlation is can be applicable for 275.15-473.15K and 0-45%Wt KOH

Mass flow rate calculation:

The rate of production of hydrogen gas and oxygen gas in mol/sec are expressed as [3]

$$N_{h2,out} = \frac{J_{av}A_{ef}}{2F}, \quad N_{o2,out} = \frac{J_{av}A_{ef}}{4F} \tag{31}$$

Rate of production of gas in lit/hr for hydrogen and oxygen is given by following eq.

$$V_{H_2} = \frac{J_{av}A_{ef}M_{H_2}}{2F\rho_{H_2}}, \quad V_{O_2} = \frac{J_{av}A_{ef}M_{O_2}}{4F\rho_{O_2}} \text{ in m}^3/\text{s} \tag{32}$$

Total gas flow rate is given by

$$V_T = (V_{H_2} + V_{O_2}) \times 3600 \times 1000 \text{ in lt/hr} \tag{33}$$

Quantity of heat produced in the cell is product of current and over voltage is defined as joule effect in W

$$Q_J = I(\eta_a + \eta_c + V_{OHM}) \tag{34}$$

Efficiency of system is $\quad \eta_{SYS} = \frac{N_{h2,OUT}LHV}{P} \tag{35}$

Simulation of mathematical model:

Mathematical model is developed and programmed in Engineering Equation Solver in order to integrate model parameters and generate simulation for different operating conditions such as temperature, current density and bubble fraction, etc. The characteristic of electrolyser is studied at different temperatures and summarised in graphs.

Fig .3 indicates the temperature does not gives considerable effect on thermoneutral voltage. But reversible voltage reduces with increase in temperature. In this paper, the temperature dependent reversible voltage and thermoneutral voltages are derived in atmospheric pressure. These correlations are suggested up to water in liquid state.
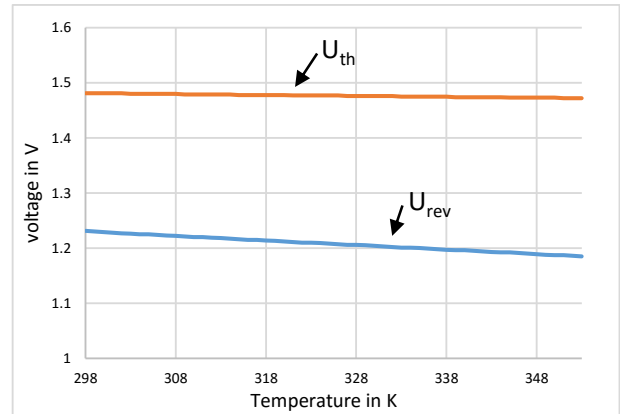

Figure 3. Thermoneutral voltage (U_{th}) and reversible voltage (U_{rev}) vs temperature for water electrolysis
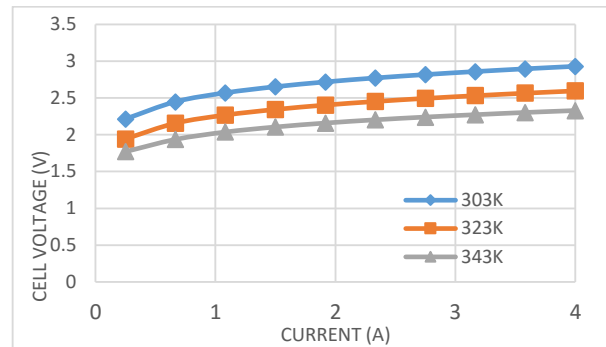

Figure 4. Change in cell voltage with current for different temperatures.

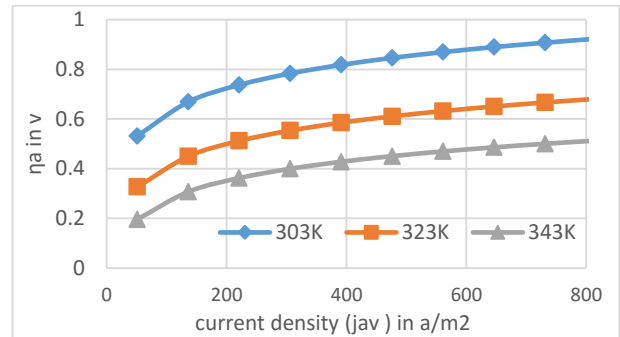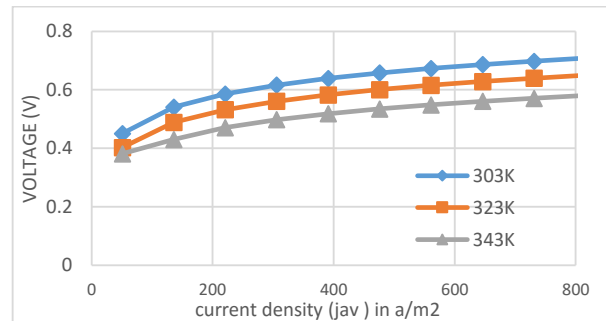Figure 5.Change in Anodic activation losses with current density

Figure 6. Change in Cathode activation losses with Current density at different temperatures.
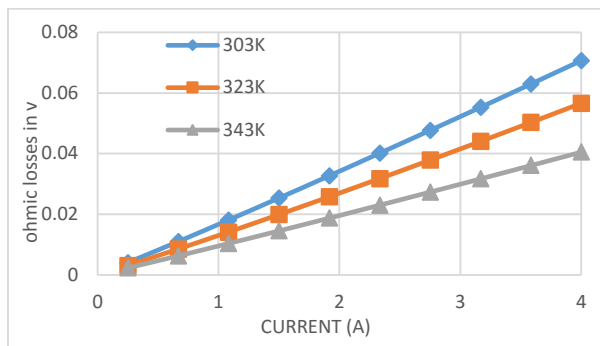
Figure 7. Change in Ohmic losses due to bubbles and electrolyte resistance with current
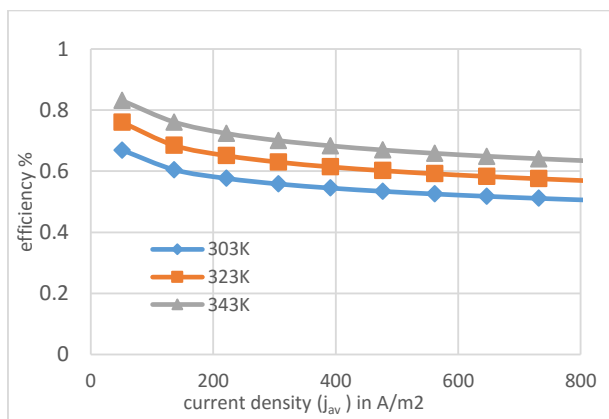

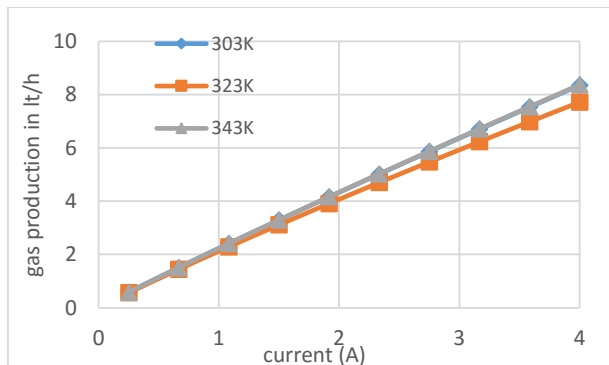*Figure 8. Predicted efficiency losses with current density*

Figure 9. Predicted gas production with current at different temperatures.

The fig .4 shows that cell voltage is increases with increase in current, this results increase in current density. Therefore more water molecules dissociate in to hydrogen and oxygen on cathode and anode compartments. Besides heat is also generated inside the electrolyser by joule heating phenomenon, this heat is absorbed by electrolyte and increases its temperature and decreases operating cell voltage or increase in rate of reaction by withdrawn more electrons. This is occurred only in stagnate electrolytes.

In alkaline water electrolysis, reactions does not occurs at reversible voltage. Cell needs more energy to initiate reaction. Because inactivity of electrode, resistance in the electrolyte and

due to bubble formation. Activation losses major losses that occurs in reaction on cathode and anode. The tafel expression clearly shows the polarization losses directly depends upon tafel slope and exchange current density are shown in fig.6 and fig.5. Anode and cathode losses shows significant effects on electrolyser voltage can be reduced by proper selection of electrodes. Fig.7 represents combined ohmic losses due to bubble formation and losses in conductivity of electrolyte are changed with current. It shows ohmic losses increase with increase in current, besides losses are decreased with increase in temperature. Ohmic losses are developed due of bubble formation on both electrodes. These bubbles are reduces contact surface area of electrode to electrolyte. This results increase in current density of electrode surface. These losses can be reduced by operating electrolyser in high temperatures and providing more surface area. Fig.8 and Fig .9 shows the efficiency and production rate of gases at different temperatures. Both efficiency and production rate are increased by operating temperatures.

Conclusion:

New thermodynamic correlation are developed in atmospheric pressure and compared with standard values [1]. At standard condition U_{rev} = 1.229V and U_{th} =1.482V. The temperature dependent correlation are developed in this paper shows U_{rev}=1.231V and U_{th}=1.481V. At 80ºC, these two voltages decreases slightly U_{rev} = 1.184V and U_{th}=1.473V, but correlations proposed in this paper shows U_{th}=1.185V and 1.472V. By comparing these results, there is a negligible difference in reversible voltage and thermoneutral voltage. Correlation shows influence of temperature on efficiency and production rate is observed. A mathematical model for an advanced alkaline electrolyser has been developed by combining effects of thermodynamic, electrochemical empirical correlation in engineering equation solver. This model permits only to extract current-voltage characteristics curve, production rates with current in temperature differences.

BIBLIOGRAPHY:

[1] Ulleberg, Øystein. "Modeling of advanced alkaline electrolyzers: a system simulation approach." International Journal of Hydrogen Energy 28.1 (2003): 21-33.

[2]. Goodridge, F., and Kenneth Scott. Electrochemical process engineering: a guide to the design of electrolytic plant. Springer Science & Business Media, 2013.

[3]. Zhang, Houcheng, Guoxing Lin, and Jincan Chen. "Evaluation and calculation on the efficiency of a water electrolysis system for hydrogen production." international journal of hydrogen energy 35.20 (2010): 10851-10858.

[4]. Zhang, Houcheng, et al. "Configuration Designs and Parametric Optimum Criteria of an Alkaline Water Electrolyzer System for Hydrogen Production." Int. J. Electrochem. Sci 6 (2011): 2566-2580.

[5]. Hammoudi, M., et al. "New multi-physics approach for modelling and design of alkaline electrolyzers." international journal of hydrogen energy 37.19 (2012): 13895-13913.

[6]. Henao, Christian, et al. "Simulation tool based on a physics model and an electrical analogy for an alkaline electrolyser." Journal of Power Sources 250 (2014): 58-67.

[7]. Huot, J-Y. "Hydrogen Evolution and Interface Phenomena on a Nickel Cathode in 30 w/o KOH I. Kinetics Parameters and Electrode Impedance Between 303 and 363 K." Journal of The Electrochemical Society 136.7 (1989): 1933-1939.

[8]. Kibria, M. F., M. Sh Mridha, and A. H. Khan. "Electrochemical studies of a nickel electrode for the hydrogen evolution reaction." International journal of hydrogen energy 20.6 (1995): 435-440.

[9]. Kibria, M. F., and M. Sh Mridha. "Electrochemical studies of the nickel electrode for the oxygen evolution reaction." International journal of hydrogen energy 21.3 (1996): 179-182.

[10]. Gilliam, R. J., et al. "A review of specific conductivities of potassium hydroxide solutions for various concentrations and temperatures." International Journal of Hydrogen Energy 32.3 (2007): 359-364.

[11]. Vogt, H., and R. J. Balzer. "The bubble coverage of gas-evolving electrodes in stagnant electrolytes." *Electrochimica Acta* 50.10 (2005): 2073-2079.