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Modeling of The PEM Type Fuel Cells

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ABSTRACT **Population growth, industrialization, and technological developments are increasing the energy requirement of the world every day. Currently, the energy requirement is usually provided by fossil fuels. Fossil fuels are considered to be the main source of global warming due to generating high CO_2 emissions. To reduce the greenhouse gases that threaten the future of the world and humanity, focusing on preference for clean, renewable, and environmentally friendly energy sources is necessary. The intermittent and fluctuating energy production potentials of renewable energy sources require continuous and efficient storage of energy. Fuel cells which are remarkable energy storage systems due to their high specific energy density, also use clean and environmentally friendly hydrogen for energy conversion. Polymer electrolyte membrane fuel cells (PEM) also called Proton exchange membrane (PEM) fuel cell is the most common type of fuel cells. This study modeled PEM fuel cells modeled in MATLAB/Simulink program. The voltage losses, power, and voltage densities of the system were analysed.**

Keywords: Modeling Fuel Cell, PEM Fuel Cell, MATLAB/Simulink Model.

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1. INTRODUCTION

Industrialization, rapid population growth, and human activities such as unconscious consumption increase the amount of greenhouse gases. The greenhouse gases like carbon dioxide, methane, and nitrogen have created the problem of global warming and climate change. The biggest cause of global warming is fossil fuel consumption [1]. Fossil fuels like coal, natural gases, and oil are under threat of extinction due to consumption in less time than the formation process. By Kyoto Protocol, signed in 1997, countries are required to reduce their CO_2 emissions to the level of 1990s [2]. Total greenhouse gas emissions were calculated as 523.9 million tons (mT, CO_2 equivalent) in 2020. These data are compared with 1990, it is seen that there is a 138.5 % increase in CO_2 emission values. 367,6 mT (CO_2 equivalent) energy-related emissions has a big share with 70.2% in 2020 [3]. The Paris Climate Treaty, which entered into force in 2016, also highlighted the need for alternative methods to reduce greenhouse gases in the atmosphere[4]. For all these reasons, a clean, renewable, and environmentally friendly energy policy is needed.

Hydrogen energy is one of the brightest energy sources of the future. Hydrogen is not a natural source it is an energy carrier. Hydrogen energy is an alternative energy source due to its rich reserves, eco-friendly and high gravimetric energy density properties [5]. Nowadays, hydrogen energy has become quite popular as an alternative energy source and energy carrier, and different scenarios have been developed for the use of hydrogen energy in both homes and vehicles [6, 7]. In these scenarios, the energy obtained from renewable energy sources is decomposed into hydrogen and oxygen with the help of an electrolyze, and the energy is stored as hydrogen energy. Hydrogen and oxygen combine again to turn into the water with the help of fuel cells and electrical energy appears. This cycle is commonly referred to as the hydrogen cycle [8, 9].

Fuel cells that convert chemical energy into electrical energy by internal electrochemical reactions are advantageous in point of energy efficiency by comparison to other energy storage systems. The fuel cells can reach a total efficiency of 80% and an electrical efficiency of 40-60% [10]. Fuel cells have wide applications due to their clean and environmentally friendly fuel properties, high energy conversation, easy and fast refueling, and ease of use in stable and portable appliances [11]. Fuel cells are classified according to the electrolyte, alkaline (A), proton exchange membrane (PEM), phosphoric acid (PA), molten carbonate(MC), and solid oxide (SO). The operating temperature and the type of electro catalyst also depend on the electrolyte solution [12].

Polymer electrolyte membrane fuel cells (PEM) also called Proton exchange membrane (PEM) fuel cell is the most common type of fuel cell. PEM fuel cells (PEMFC) use a proton-conducting polymer membrane as the electrolyte and can operate at low temperatures (50-100 ^{o}C) [13]. PEMFC has wide range of fuel options from hydrogen to ethanol to biomass-derived materials. These fuels can either be directly fed into the cell or sent to a reformer for purification of H_2[14]. As a proton exchange membrane in PEMFC, the ionic conductive polymer Nafion is used, which allows the passing of the proton ions in terms of their thermal and physical properties [13]. PEMFC is preferred for fast and portable applications due to its low temperature operation and high energy density Because that the polymer used is expensive and has low catalyst strength, studies have turned to the development of cheaper and more durable systems [11, 14-17].

In this study, the structure and operating principle of the PEMFC were studied and calculations were made using theoretical and experimental data of the commercial Ballard Nexa 1.2 kW PEM fuel cell [18, 19].Based on the available data, a current-voltage graph of the PEM fuel cell was created using the MATLAB/Simulink program, and other parameters affecting the output voltage were studied.

2. PRINCIPLE and OPERATIONS of PEMFC

Fuel cell which works according to the principle of redox reactions, consists of three main components: negatively charged electrode(anode),positively charged electrode (cathode), and electrolyte membrane [14]. The basic PEMFC consist of a proton exchange (polymer) membrane, gas diffusion layer (GDL), catalyst, flow field plates, gaskets, and plates. PEM, GDL, and catalyst are sandwiched and called membrane electrode assembly (MEA) [14]. The catalyst layer decomposes the fuel into its ions. Gas diffusion layers(GDL) are e^- conductive layers that provide e^- flow to the oxidizer and fuel. The fuel separates into protons and electrons at the anode.

The positively charged ions (protons) only pass through an electrolyte and the negatively charged ions (electrons) pass through an external circuit that forms a DC current [13]. Molecules cannot state in the ionic state, therefore they recombine with other molecules to return natural state [14]. If the fuel is hydrogen and the chemical is oxygen, they will form water at the cathode while generating electric current in the external circuit [13]. Figure 1 shows the structure and principle of operation of the PEM fuel cell [20].

The redox reactions occurring in the PEMFC can be shown in Equations (1), (2), and (3).

$$Half-reaction\ at\ the\ anode\ side\quad:\quad H_2(g)\rightarrow 2H^+(aq)+2e^- \qquad (1)$$

$$Half-reaction\ at\ the\ cathode\ side:\quad {}^{1}/_{2}\,O_2(g)+2H^+(aq)+2e^- \rightarrow H_2O \qquad (2)$$

$$Overall\ reaction\quad:\quad H_2(g)+{}^{1}/_{2}\,O_2(g)\rightarrow H_2O+El.Enr.+Heat \qquad (3)$$

The heat and water generated as a result of the reactions must be removed from the system.

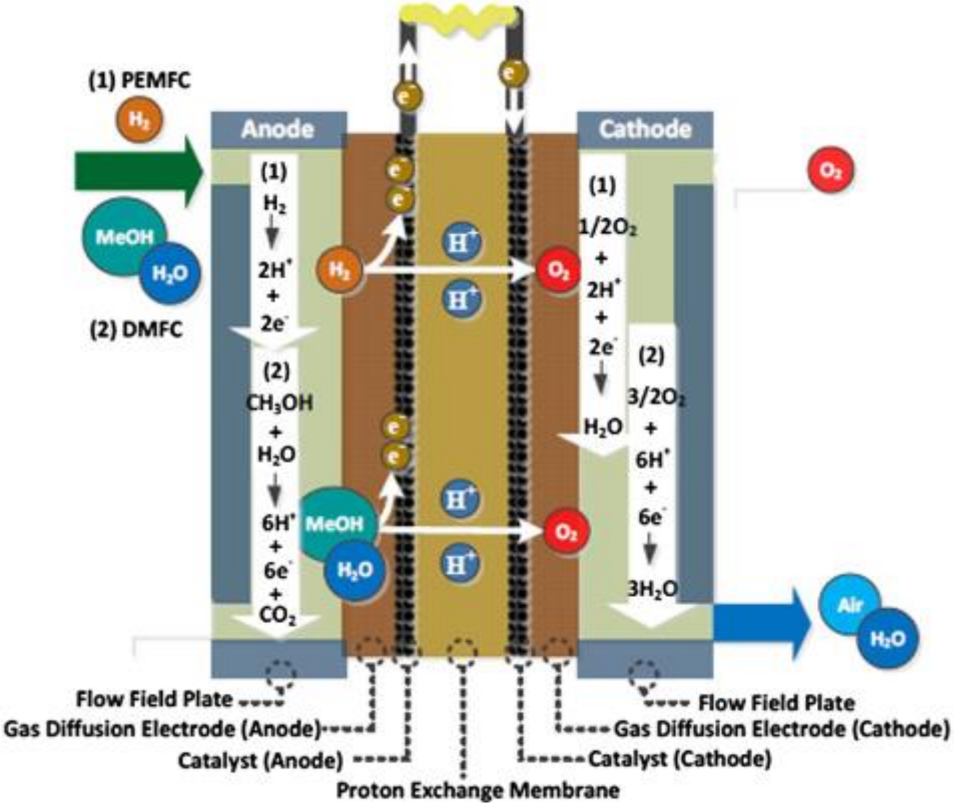

Figure 1. Schematic representation of PEM-type fuel cells [20].

3. MODELLING of PEM TYPE FUEL CELLS

Modeling of the PEMFC needs to be considered many perspectives. Cell temperature, fuel-oxidizer temperatures, fuel or oxidizer pressure, cell potential, mass ratios of reactants should be considered while modelling [14]. Kinetic and thermodynamic aspects of PEMFC modeling, there are studies on gas-liquid mass transfer in porous layers, suitable operating conditions for liquid-vapor phases, mathematical modeling of diffusion and convection in gaseous diffusion layers in the literature [12]. Recently, when modeling, three-dimensional, steady-state voltage characteristics are usually selected [14].

Theoretically calculated voltage value in a fuel cell unfortunately cannot obtained possibly. Losses are observed in the system due to reasons such as slowing down of the chemical reaction seen in the system, electrolyte resistance, and concentration losses [10]. Given these losses, the cell potential is calculated as in Equation (4). In Equation 4; V_{act} is activation losses, V_{ohm} is ohmic losses, and V_{con} is concentration losses expressed [10].

$$V_{cell} = E_{nernst} - V_{act.} - V_{ohm.} - V_{con.} \tag{4}$$

PEM fuel cell modeling studies were carried out taking into account the technical characteristics of the *Ballard Nexa 1.2 kW* commercial fuel cell. Table 1 shows the technical characteristics of the fuel cell system [19].

Table 1. Characteristic of Ballard Nexa 1.2 kW commercial fuel cell [19].

Outputs	**Requirement**	**Definition**	**Quantity**
Power	Rated power	Capacity at standard conditions, BOL	1200 W
	Voltage	Operating voltage range	22 V to 50 V
		The voltage at rated power	26 V
	Start-up time	Minimum time to achieve rated power from a cold start	2 minutes
Emissions	Water	The maximum quantity of liquid water produced at Rated Power	870 mL/hour
	Noise	Maximum noise emission at 1meter	72 dBA
Physical	Dimensions	L x W x H	56 x 25 x 33 cm
	Mass	Total system mass	13 kg
Lifetime	Operating life	Minimum number of operating hours before EOL	1500 hours
	Cyclic life	Minimum number of start-up & shut-down cycles before EOL	500
	Shelf life	Minimum storage (non-operation) before EOL	2 years
Inputs	**Requirement**	**Definition**	**Quantity**
Fuel	Purity	Lowest acceptable concentration of hydrogen is 99.99%	99.99 % (vol.)
	Pressure	The allowable range of inlet supply pressure	70 – 1720 kPa(g)
	Consumption	Maximum fuel consumption at rated power	<18.5 SLPM
DC Power Supply	Voltage	The allowable range of input voltage	18 V to 30 V
	Power	Maximum power draw during start-up	60 W
Operating Environment	Temperature Range	Range of acceptable ambient, cooling air, and oxidant air temperatures	3 ºC – 40 ºC
	Relative Humidity Range	Range of acceptable ambient relative humidity	0%-95%

3.1. Determination of Nernst Equation

The ideal performance in fuel cells is determined theoretically by the level of voltage generated. This potential voltage is known the reversible cell voltage which is defined by the Nernst equation as in Equation (5) [13].

$$E_{Nernst} = E^0 - \frac{RT}{2F} ln\left(\frac{P_{H2O}}{PH_2 * Po_2^{0.5}}\right) \quad (5)$$

In Equation (5) E^0 is the standard cell potential and 25 °C and 1 atm. conditions hydrogen-oxygen fuel cell the value of $E^0 = 1.229$ V [14]. Other parameters necessary for calculations are also given in Table 2.

Table 2. The parameters for calculations [21].

Symbol	***Parameter***	***Value***	***Unit***
R	İdeal gases constant	8.314	J/molK
F	Faraday constant	96,485	C/mol
T	Temperature	80	C°
PH_2O	Partial pressure of H_2O	2.03	Atmospher
PH_2	Partial pressure of H_2	1.265	Atmospher
PO_2	Partial pressure of O_2	2.527	Atmospher
n_h	Number of cells	90	-

A_h	Surface area of cell	100	cm^2
R_{ohm}	Electrolyte internal resistance	0.19	Ohm/cm^2
α	Transfer coefficient	0.5	-
I_0	Current density change	$10^{-6.912}$	A/cm^2
I_L	Current density limit	1.4	A/cm^2
σ	Electrolyte conductivity	0.1	Ω^{-1}.cm^{-1}
L_{elek}	Electrolyte thickness	0.005	cm
E_0	Ideal standard potential	1.229	V

The E_{Nernst} given by Equation (5) has been simulated in the MATLAB/Simulink environment and is shown in Figure 2.

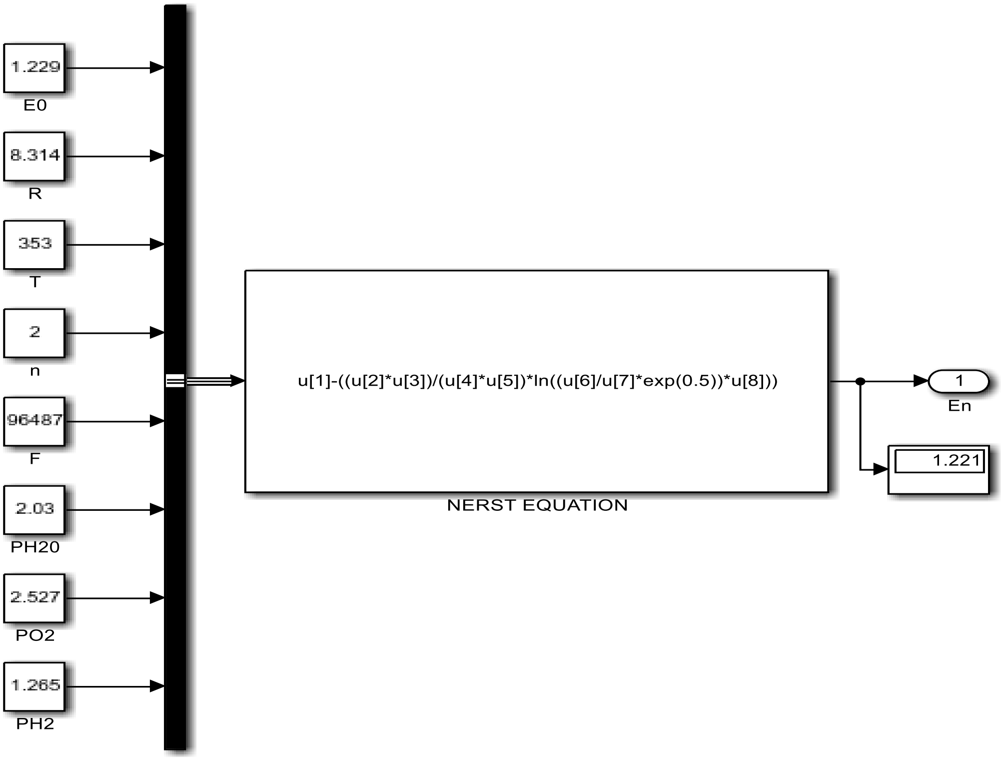

Figure 2. MATLAB/Simulink simulation of PEMFC Nernst equation.

3.2. Determination of Activation Losses

The activation losses are observed when the rate of the electrochemical reaction is controlled by the slow step. The ratio of voltage lost due to resistance in the reaction kinetics increases with current density. The activation losses expressed by Equation 6 [13, 22].

$$V_{ac} = \frac{RT}{n\alpha F} ln\left(\frac{I}{I_0}\right) \qquad (6)$$

Where; V_{act}: Activation losses, *R:* İdeal gases constant, *T:* Temperature, *F:* Faraday constant, *n*: number of electrons per molecule (H_2 = 2 electrons /molecule), *I:* Current density, I_o: Current density change and *α:* transfer coefficient.

Activation losses were calculated according to the values in Table 2 using the program created in the MATLAB/Simulink software. The change in activation losses observed at different temperature values of different current densities and constant current density at constant temperature is shown in Figure 3.

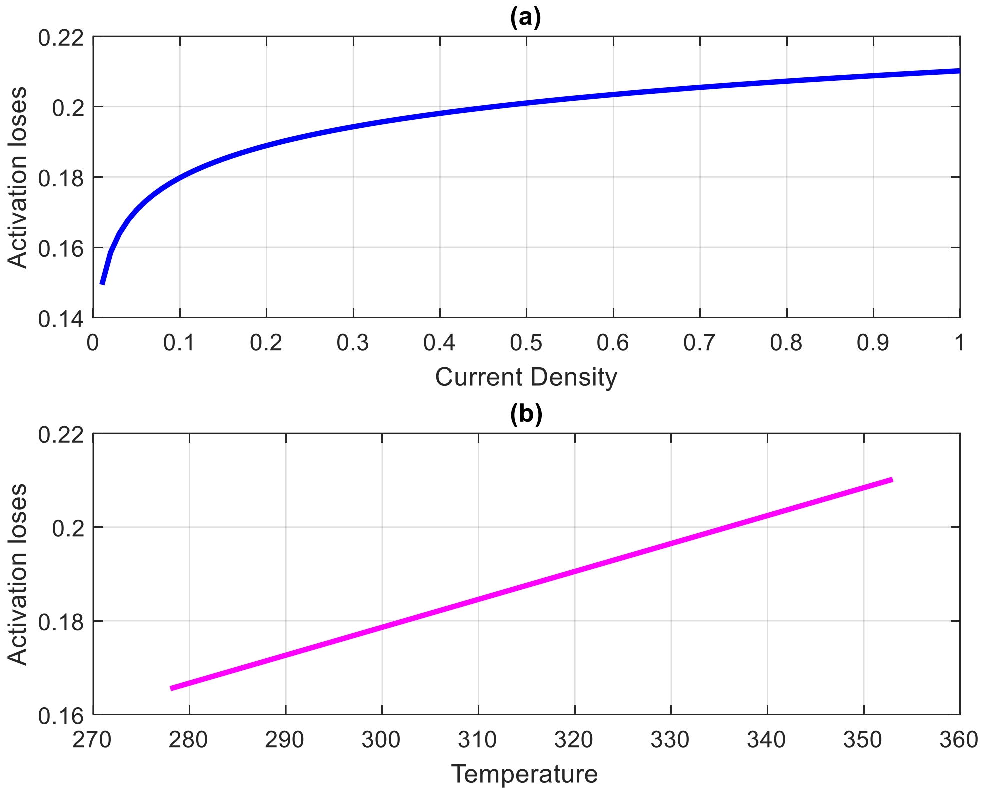

Figure 3. (a) Activation loses of constant temperature-variable current density, **(b)** Activation loses of variable temperature-constant current density.

When the activation losses due to current density and temperature are plotted as a surface graph in a MATLAB software, Figure 4 is obtained.

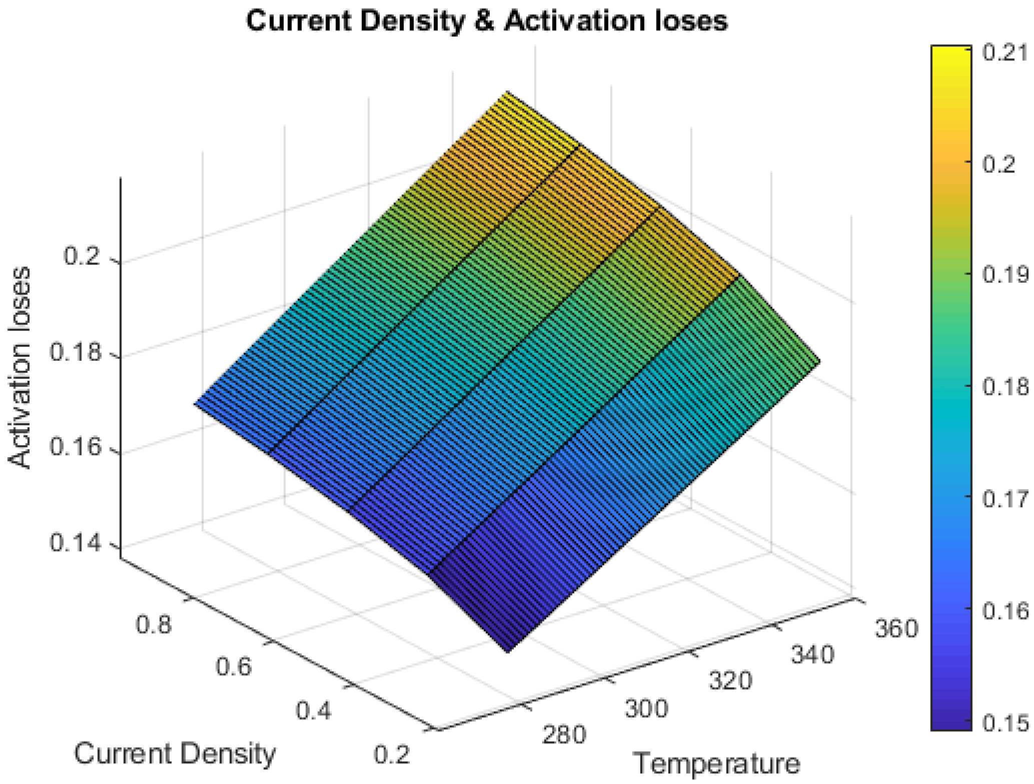

Figure 4. Activation loses connected to current density and temperature.

3.3. Determination of Ohmic Losses

Ohmic losses are caused by the resistance of the electrolyte liquid to the ion transition. The ohmic losses depend on the humidity and temperature of the membrane, and by that, the membrane ionic resistance is considered as R_{ohmic} [13].

$$V_{ohmic} = i \ x \ R_{ohmic} \qquad (7)$$

Common methods of reducing ohmic losses include making electrolytes as thin as possible, and employing high conductivity materials that are well connected to each other [14].

Since the electrical resistance in fuel cells is usually expressed in conductance (σ) as in Equation 8.

$$\sigma = \frac{i}{R_{ohmic}} \text{ and } \qquad R_{ohmic} = \frac{L_{cond.}}{\propto A_{cond.}} \qquad (8)$$

Where L_{cond} is the length (cm) of the conductor, $A_{cond.}$ is the cross-sectional area (cm^2) of the conductor, and α is the electrical conductivity (ohm^{-1} x cm^{-1}). The current density is j, (A/cm^2), can be defined as;

$$j = \frac{i}{A_{cell}} \qquad (9)$$

The ohmic over potential for the fuel cell is mainly due to ionic resistance in the electrolyte, this can be expressed as;

$$V_{ohmic} = ixR_{ohmic} = j \ A_{cell}\left(\frac{L_{cond.}}{\propto A_{cond.}}\right) \qquad (10)$$

Ohmic losses were calculated with the values of Table 2 and created in the MATLAB software. The observed change in ohmic losses at different electrode thickness values is indicated in Figure 5.

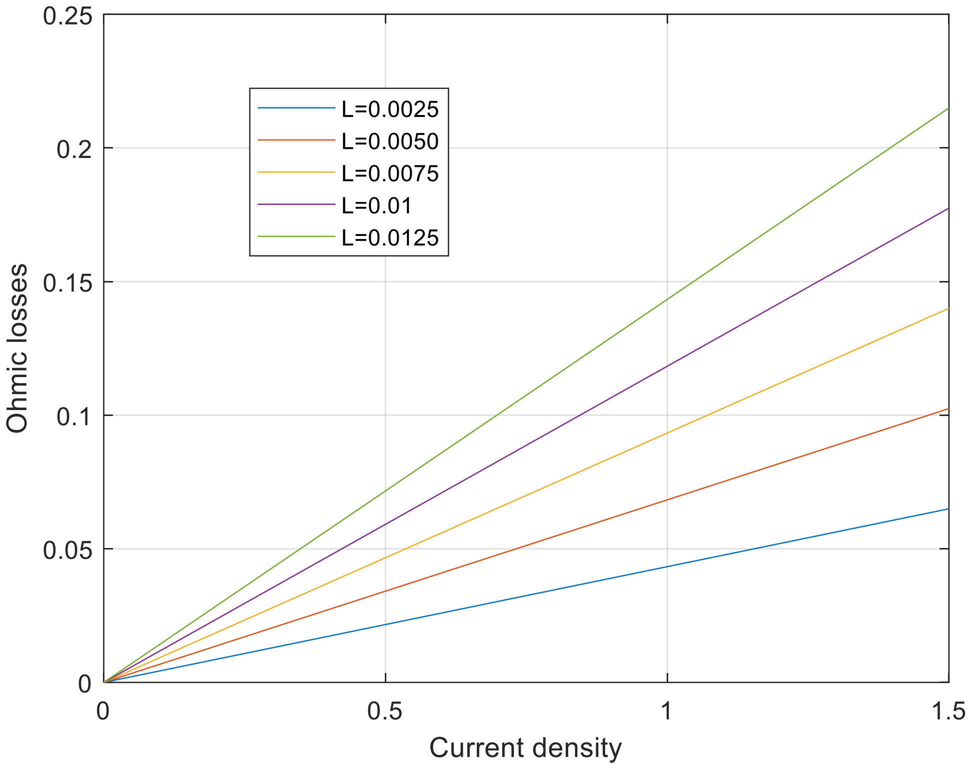

Figure 5. Change of ohmic losses and current density with electrode thickness.

When ohmic losses are calculated depending on the current density and electrode area according to Equation 10, the surface graph in Figure 6 is obtained.

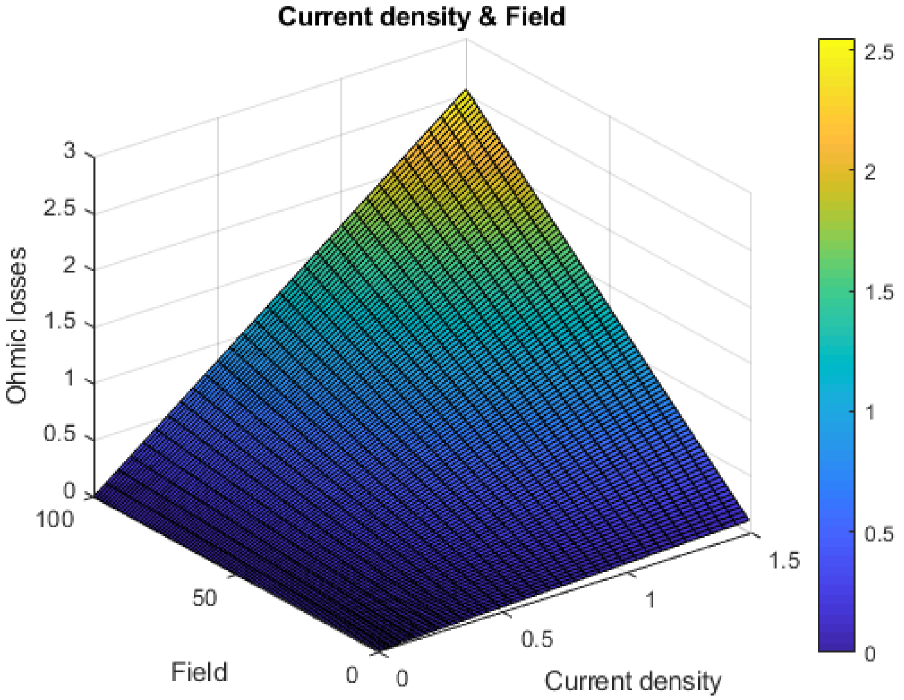

Figure 6. Current density and field-dependent variation of ohmic losses.

3.4. Determination of Concentration Losses

The fuel consumption rate increases with the current density increment. When the volume flow rate exceeds the diffusion rate of the reactants to the catalyst surface on the electrode surface, the same reactant concentration cannot be observed all over the electrode surface. In this case, the reactants cannot fully reach the reaction sites and transition limitations are observed. Cell potential mass-transition limitations, which are more often observed at high current densities, lead to activation losses [10, 13, 22]. Concentration losses are expressed by Equation 11.

$$V_{con} = \frac{RT}{nF}\ln\left(\frac{I_L}{I_L - I}\right) \tag{11}$$

The values in the expression I_L: current density is the limit value, I: current density, T: temperature, R: ideal gases constant, F: Faraday constant, n: number of electrons per molecule (H_2 = 2 electrons /molecule)
The concentration losses of the examined system were calculated in the MATLAB software according to the values in Table 2. As a result of the calculation, it was found that the losses incurred in the system were at a negligible level.

3.5. Determination of System Voltage and Power

The values obtained as a result of modeling studies of the PEM fuel cell system were combined and the voltage of the system was determined according to Equation 4. As a result of the calculations performed in the MATLAB software, the output voltage curve depending on the current density of the system was obtained as in Figure 7 (a).

Depending on the number of cells in the PEMFC and the output voltage, the output power of the system can be calculated according to Equation 12 by values in Table 2. The relationship between current density and output power has been plotted in MATLAB software as shown in Figure 7(b). *P* is the power of the system, *V* is the output voltage of the system, n_h is the number of cells, *I* is the current density, and A_h is the cell surface area in Equation 12.

$$P = V\, n_h\, A_h\, I \qquad (12)$$

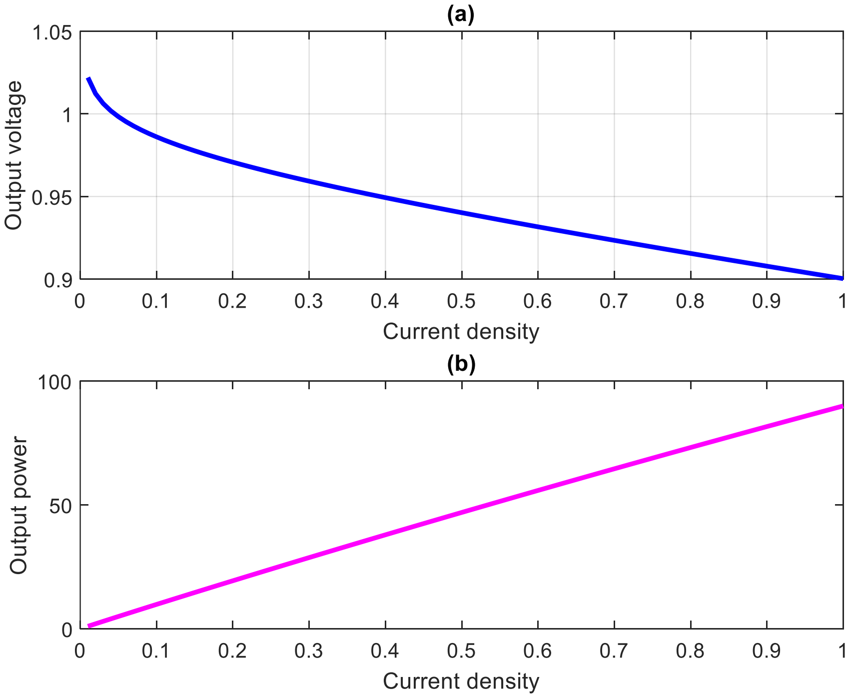

Figure 7. Output voltage curve (a), output power curve (b), depending on the current density of the system.

4. CONCLUSION

Within the scope of PEM fuel cell modeling studies, Ballard Nexa 1.2 kW commercial fuel cell model was modelled. The modelling and calculations were performed in MATLAB software. Improve the cell performance and determine voltage changes in PEM fuel cells various factors need to be considered. Unfortunately, it is not possible to actually obtain the theoretically calculated voltage value in a fuel cell. Losses are observed in the system due to reasons such as slowing down of the chemical reaction seen in the system, electrolyte resistance, and concentration losses. Within the scope of the modeling studies using the data of Ballard Nexa 1.2 kW commercial fuel cell, the voltage losses of the fuel cell were examined. Activation losses, ohmic losses and concentration losses were calculated in the MATLAB software. As a result of the calculations, it was observed that the activation losses increase depending on the temperature and current density. The value of ohmic losses depends on the electrode thickness. The ohmic losses values has increased with the increasing electrode thickness. Concentration losses have neglected because they are too low for take into consideration. In the current density determination, as the current density increased, the output voltage was decreased. The power of the system has increased linearly with the increasing current density. Increasing interest in renewable and clean energy sources increases the importance of fuel cells and hydrogen technology. The investigation of the parameters that affecting the cell voltage in fuel cells and studies for reduction of losses are promising for usage of fuel cells.

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