Mathematical modelling of solid oxide fuel cell using Matlab/Simulink

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***Abstract*— This paper explicates a phenomenal approach for computer modeling of a single cell solid oxide fuel cell where transfer function model is implemented for the calculation of partial pressures of hydrogen, oxygen and water. Activation, concentration and ohmic losses are also considered to obtain better characteristics of fuel cell. Steady state characteristics of fuel cell are obtained at different fuel flow rates ranging from 31ml/sec to 51ml/sec at two different operating temperatures 800^{o}C and 850^{o}C. It is observed that the limiting current density of fuel cell increases with the increase in fuel flow rate. Results are validated with the experimental data. The software that has been incorporated in designing is MATLAB/SIMULINK.**

Keywords—Solid Oxide Fuel Cell, simulation, transfer function model

I. INTRODUCTION

The Energy consumption of the world is voracious and it is known that fossil fuels are depleting very fast. Also, they are toxic to atmosphere. Due to the concern for environmental safety and evolution in the technology, reliance on renewable energy has taken vast leaps in the current decade. Few of such abundantly available and prolific sources are solar energy, wind energy and fuel cells as they are inexhaustible and very benign to the atmosphere unlike fossil fuels. Power generation from solar and wind is unpredictable because solar power depends on the availability of sun light and wind energy system depends on the wind. Since fuel cells have no geographical limitations, they are preferred for small scale power generation. Power generation in fuel cells depends on the hydrogen input which is available in abundance. Further, fuel cells are known for their low to zero emissions, high efficiency and high reliability because of the absence of moving parts.

Fuel cell is an electrochemical device that converts hydrogen and oxygen to electricity and water. Having water as its by-product, it is absolutely harmless. The effectiveness of the fuel cell depends on the type of electrolyte employed. Based on the type of electrolyte, fuel cells are categorized as molten carbonate, polymer electrolyte membrane, phosphoric acid, solid oxide etc. [1-2]. Solid oxide fuel cells (SOFC) are predominantly used in small scale power generation on consumer side because of their higher operating temperature (800-1000^{o}C). SOFCs produce large amount of heat due to the chemical reaction, can be utilized for cogeneration and internal reforming of hydrogen. Hence emphasis is laid in modeling the solid oxide fuel cells.

As the real systems are high-priced, a simulator is essential for experimentation. Hence mathematical models are developed in order to reduce the risk during testing. Mathematical modeling refers to represent an application in tractable mathematical formulae whose numerical analysis would provide answers for the given application. Modeling is useful for experimenting new ideologies and to analyze the hypothetical behavior of the real system. The entire setup of the fuel cells is very expensive and not flexible. Any damage during testing would arrive at a great loss. Hence it necessitates the development of simulator of fuel cell which would turn out to be very useful for the upcoming researches. To develop the simulator, fuel cell has to be modeled accurately. Hence authors of this paper have focused on the modeling of SOFC in MATLAB/SIMULINK.

Many approaches on SOFC modeling are available and they are found to be very intricate because of the inclusion of numerous parameters [3-6]. In [7] and [8], a parallel RC circuit for partial pressure calculation is developed. In [9] and [10] transfer function modeling is used for partial pressure calculation but none of the losses are involved. Perfect characteristics of a fuel cell are obtained only when all the losses are considered. This paper considers the transfer function for modeling of partial pressures as well as various losses i.e. activation, concentration and ohmic losses.

II. MODELLING OF SOLID OXIDE FUEL CELL

Modeling of fuel cell voltage [7] constitutes four voltages. Fuel cell voltage is obtained after subtracting activation (V_{act}), concentration (V_{conc}) and ohmic losses (V_{ohmic}) from the open circuit voltage E_{nernst} . It is given by equation (1). Figure.1 shows the simulink model of a single cell fuel cell.

$$V_{fc} = E_{nernst} - V_{act} - V_{conc} - V_{ohmic} \quad (1)$$

II.1 Nernst Reversible Voltage (E_{nernst})

E_{nernst} is often termed as thermodynamic potential of the fuel cell or open circuit voltage when current density (I_{fc}) is made

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zero[7]. E_{nernst} depends on the partial pressures of the individual species and is shown in equation (2).

$$E_{nernst} = E_O + \frac{RT}{F}\left(\frac{P_{H2}P_{O2}^{0.5}}{P_{H2O}}\right) \quad (2)$$

Where E_O is the standard potential, R is the universal gas constant, T is the operating temperature, F is the faraday's constant, P_{H2}, P_{O2}, P_{H2O} are the partial pressures of the respective species [9]. Values of all the constants are mentioned in Table 1.

$$P_{H2} = \left(\frac{\frac{1}{K_{H2}}}{1+\tau_{H2}}\right)\left(q_{H2} - 2K_r I_{fc}\right) \quad (3)$$

$$P_{O2} = \left(\frac{\frac{1}{K_{O2}}}{1+\tau_{O2}}\right)\left(q_{O2} - 2K_r I_{fc}\right) \quad (4)$$

$$P_{H2O} = \left(\frac{\frac{1}{K_{H2O}}}{1+\tau_{H2O}}\right)\left(2K_r I_{fc}\right) \quad (5)$$

$$q_{H2} = \frac{2K_r}{U_{opt}}\left(\frac{1}{1+\tau_f s}\right) \quad (6)$$

$$q_{O2} = \frac{q_{H2}}{r_{OH}} \quad (7)$$

Where q_{H2} is the fuel flow rate, q_{O2} is the oxygen flow rate, K_{H2} , K_{O2} , K_{H2O} are the molar valve constants of hydrogen, oxygen and water respectively, τ_{H2}, τ_{O2} , τ_{H2O}, are the response times of hydrogen, oxygen and water respectively, τ_f is the fuel response time in seconds, U_{opt} is the optimum fuel utilization, r_{OH} is the ratio of hydrogen to oxygen given in Table.1. Figure.2 shows the simulink model of E_{nernst}.

II.2. Activation loss (V_{act})

Activation loss is the energy required to overcome the energy barriers for the electro-chemical reactions to proceed. It is expressed using butler-volmer equation [7,8]. Here α_1 is made equal α_2 to for implementation purpose. I_O is the exchange current density. Equations (8) and (9) describe all. Figure.3 shows the simulink model for activation loss.

$$I_{fc} = I_O\left(e^{(\alpha_1 F/RT)V_{act}} - e^{(\alpha_2 F/RT)V_{act}}\right) \quad (8)$$

$$V_{act} = \frac{RT}{n\alpha F}\ln\left(I_{fc}/2I_O + \sqrt{(I_{fc}/2I_O)^2 + 1}\right) \quad (9)$$

II.3. Concentration loss (V_{conc})

The significance of the concentration loss [2] is when current density nears the limiting current density(I_L) of the fuel cell. I_L is the maximum possible current density of the cell at a given flowrate. It is given by equation (10). Figure.4 shows the simulink model of concentration loss.

$$V_{conc} = -\frac{RT}{nF}\ln\left(1 - \frac{I_{fc}}{I_L}\right) \quad (10)$$

II.4. Ohmic loss

There will always be a resistance for flow of ions in electrolyte and also for the flow of electrons through the electrodes. All these losses together constitute to ohmic loss. The inherent resistance of the cell depends on the temperature and is given by equation (11)

$$V_{ohmic} = \left(\gamma \exp\left[\beta\left(\frac{1}{T_O} - \frac{1}{T}\right)\right]\right) I_{fc} = rI_{fc} \quad (11)$$

where γ=0.2ohm and β=-2870K are the constant coffiencients of fuel cell, T_O=973K, T is the operating temperature of fuel cell, r is the internal resistance.

III. TABLE AND SIMULINK MODELS

Table.I. constants and parameters involved in modeling

Parameter	Value	Unit
E_O	1.1	V
R	8.314	KJ/Kmol.K
F	98486	C/mol
K_{H2}	$8.43\text{x}10^{-4}$	Kmol/atm
K_{O2}	$2.81\text{x}10^{-4}$	Kmol/atm
K_{H2O}	$2.52\text{x}10^{-3}$	Kmol/atm
τ_{H2}	26.1	seconds
τ_{O2}	2.91	seconds
τ_{H2O}	78.3	seconds
τ_f	5	seconds
U_{opt}	0.85	-
r_{OH}	1.145	ohm

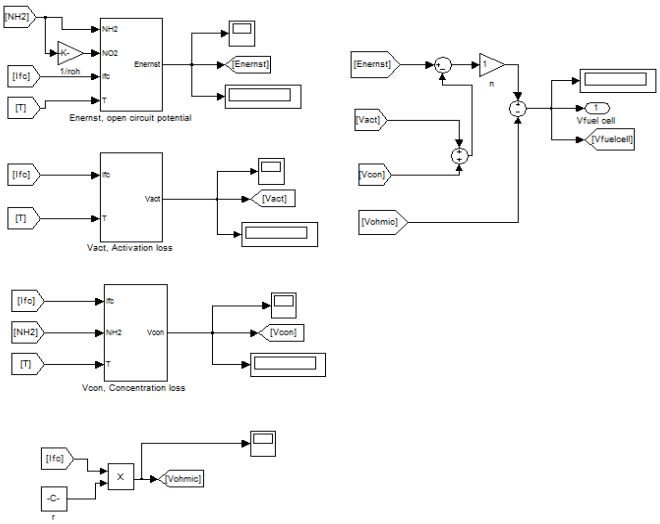


Fig.1 simulink model of solid oxide fuel cell

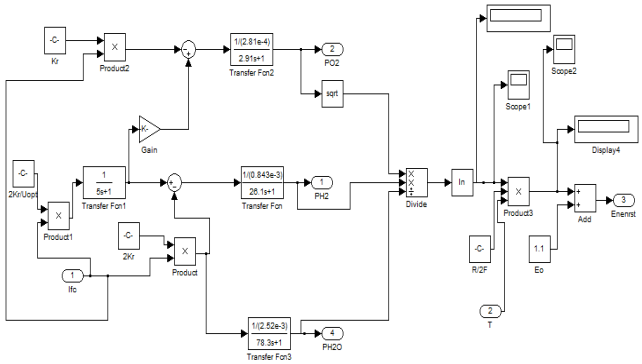


Fig.2 simulink model for E_{nernst}

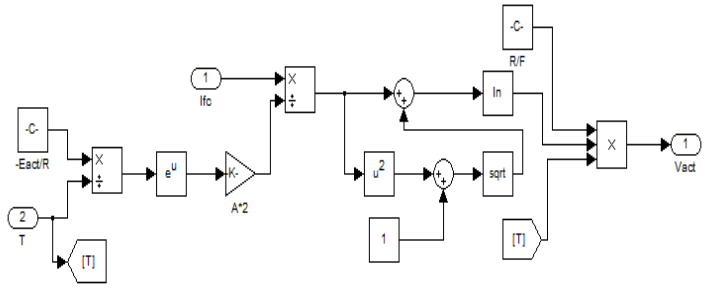


Fig.3 simulink model for Activation loss

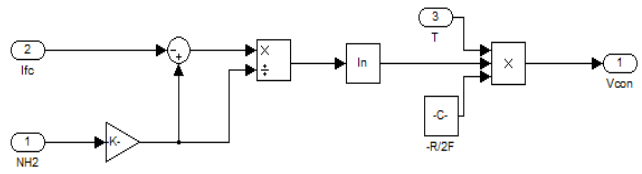


Fig.4 simulink model for Concentration loss

III. RESULTS AND DISCUSSION

A single cell SOFC is modelled using MATLAB/SIMULINK software. Fuel cell exhibits several characteristics when subjected to different flow rates and operating temperatures as shown in Figure.5 to Figure.12. With the change in temperature, the exchange current density of the cell changes and thus reflecting in activation drop. Depending on the concentration of products and reactants, the limiting current density changes resulting in concentration drop. V-I characteristics are plotted for flow rates 31ml/sec, 36ml/sec, 41ml/sec, 51ml/sec and two different operating temperatures 800^{o}C and 850 ^{o}C. It can be seen from the graphs that cell voltage is same in all. Figures 1 and 2 are the characteristic graphs at flow rate 31ml/sec and temperatures 800^{o}C and 850^{o}C respectively. It can be noticed that limiting current density I_L in this case is 3A. Figures 3 and 4 are for flow rate 36ml/sec and temperatures 800^{o}C and 850^{o}C respectively. I_L in this case is observed as 3.5A. Figures 5 and 6 are for flow rate 41ml/sec, temperatures 800^{o}C and 850^{o}C respectively and I_L is 4A. Figures 7 and 8 are for the flow rate 51ml/sec, temperatures 800^{o}C and 850^{o}C respectively. In this case limiting current is 4.9A. Experimental results are considered from the reference paper [7] for validation.

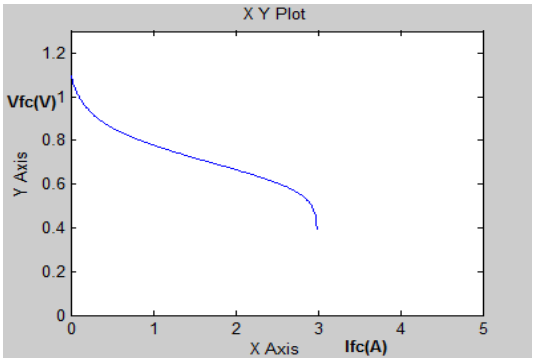


Fig.5 Flow rate=31ml/sec, T=973K

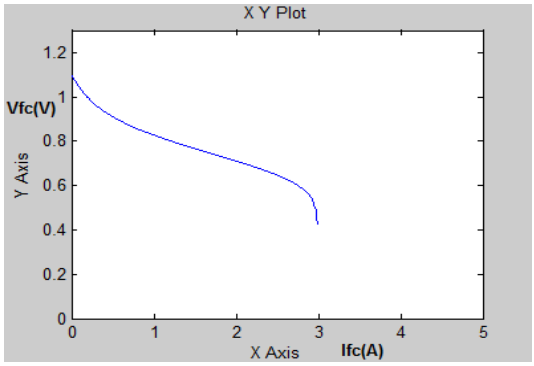


Fig.6 Flow rate=31ml/sec, T=1023K

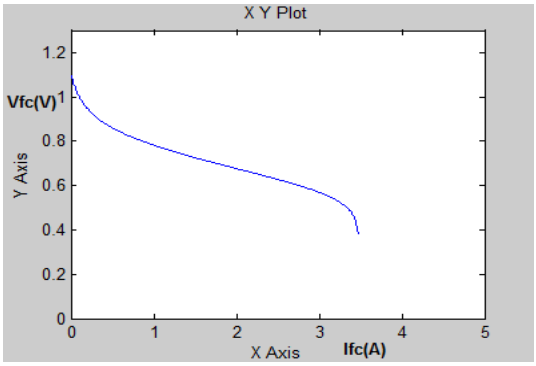


Fig.7 Flow rate=36ml/sec, T=973K

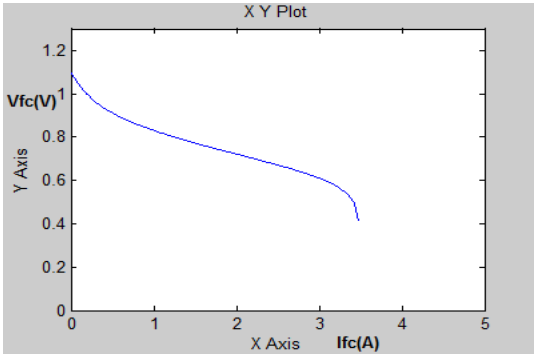
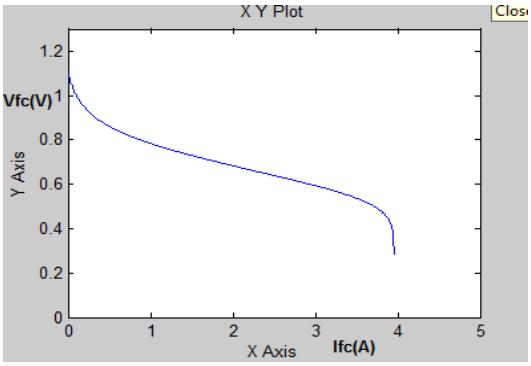


Fig.8 Flow rate=36ml/sec, T=1023K



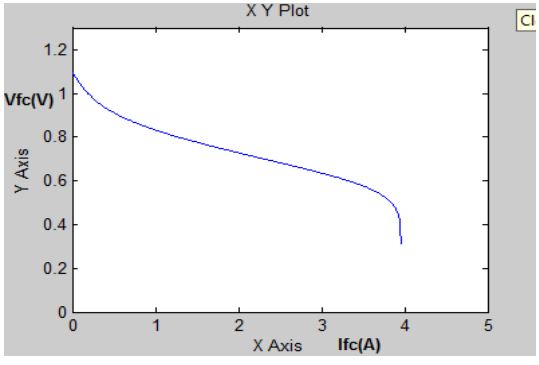


Fig.10 Flow rate=41ml/sec, T=1023K

Fig.9 Flow rate=41ml/sec, T=973K

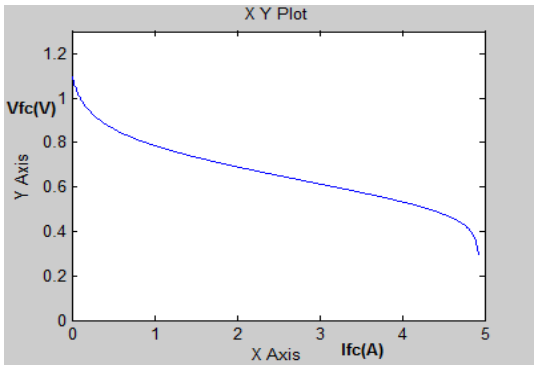


Fig.11 Flow rate=51ml/sec, T=973K

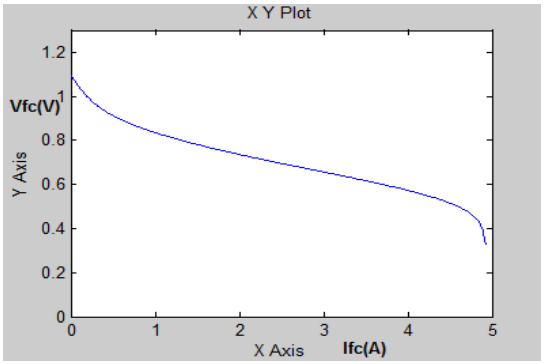


Fig.12 Flow rate=51ml/sec, T=1023K

IV CONCLUSION

In this paper transfer function model of Nernst reversible voltage and all the losses are included for modeling. Steady state response of single cell fuel cell is obtained at different flow rates and temperatures. It is observed that as the flow rate is increased, the limiting current value has also increased. The maximum limiting current is observed at fuel flow rate 51ml/sec. Results are validated from the experimental results in the reference paper [7].

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