Chapter 6

Conclusion

While fuel cell is a unique and fascinating system, the accurate system selection, design, and modeling for prediction of performance are needed to obtain optimal performance and design. In order to make strides in performance, cost, and reliability, one must possess an interdisciplinary understanding of electrochemistry, materials, manufacturing, and mass and heat transfer. Accurately modeling the PEM layer can help improve the properties of future membrane materials.

There are many types of PEM models, and choosing the right one depends upon the end goals and resources available. In order to have an accurate model, mass, energy, and charge balances must be written for the fuel cell membrane layer. In addition to these, using an empirical relationship for membrane water content may save time when creating a model. The requirements for the membrane include high ionic conductivity, adequate barrier to the reactants, and chemically and mechanically stable and low electronic conductivity. There are many choices for the PEM in the fuel cell, and the decision regarding the type chosen must depend upon many factors including, most importantly, cost and mass manufacturing capabilities. Understanding the reactions at the fuel cell anode and cathode is critical when modeling fuel cells.

Usage of a mathematical model to define the useful terms of fuel cell and its components helps one to derive the use full modeling foundation. According the research which is done on hydrogen and fuel cell describes under three sections as given below.

1) The chapter 3 covered the basic electrochemistry needed to predict electrode kinetics, activation losses, currents, and potentials in a fuel cell. The electrochemical reactions control the rate of power generation and are the main cause of activation voltage losses. The activation overvoltage is the voltage loss due to overcoming the catalyst activation barrier in order to convert products into reactants. The equations presented in this chapter help to predict how fast the reactants are converted into electric current, and how much energy loss occurs during the actual electrochemical reaction.

    I. Accordingly derived here are the following issues for designing of improved and better fuel cells. Basically electrolysis of water effectively any and efficiently into H2 and O2 at low cost is specific. It was so justified here.
    II. Basic electro kinetic concepts have been established. Here the actual reactions proceed through many steps and intermediate species. Anodic reaction is specific.

$$H_2 \leftrightarrow H_{ad} + H_{ad}$$

$$H_{ad} \leftrightarrow H^+ + e^-$$

III. Activation loss, Ohmic Loss and Voltage losses are next important factors established.

$$V_{act} = -b * \log\left(\frac{i}{i_0}\right) \quad where \quad b = \frac{R * T}{2 * \propto * F}$$

$$V_{Ohmic} = -(i * r)$$

$$V = E_{Nernst} + V_{act} + V_{ohmic} + V_{conc}$$

Accordingly simulation was carried out for the given real time data as shown in Example 3.1 in page 33. According to the above situation, its useful to study about the electrochemistry of fuel cell as it helps to identify the electrical behavior of Fuel cell. The simulated polarization curve of FC voltage loss describes how the electrical energy is drawn from the fuel cell, the actual cell voltage drops from the theoretical voltage due to several irreversible loss mechanisms such as activation polarization, ohmic polarization and concentration polarization. Therefore, the operating voltage of the cell can be represented as the departure from ideal voltage caused by these polarizations. To develop the better and efficient output, the gap between operating voltage and ideal voltage should be reduced.

Modeling catalyst layer is also established (Table 3.2), together with the following parameters and the steps are given below. Likewise, reliable parameters were established for the modeling of catalyst layer .Thus, assumptions are also satisfied

- The first step is to calculate the Nernst voltage and voltage losses
- The partial pressure of hydrogen and Oxygen
- The voltage losses will now be calculated
- The ohmic losses (see Chapter 4) are estimated using Ohm's law
- The Nernst voltage can be calculated using the following equation

$$E_{Nernst} = -\frac{G_{f,liq}}{2 \times F} - \frac{R \times T_k}{2 \times F} \times \ln\left(\frac{P_{H_2O}}{P_{H_2} \times P^{1/2}{}_{O2}}\right)$$

- The actual voltage is the addition of the Nernst voltage plus the voltage losses

$$V = E_{Nernst} + V_{act} + V_{ohmic} + V_{conc}$$

- The calculation of effectiveness factor is extracted as a justification of the search

$$E = \frac{1}{3\emptyset^2}(3\emptyset \coth(3\emptyset) - 1)$$

Modeling of Effectiveness factor due to the mass transfer and reaction of H2 and O2 versus current density also shows how the behavior of effectiveness of H2 and O2 with reference to the current density is. The effectiveness factor deals with the actual rate of reaction of particular fuel with the rate of reaction with losses as mentioned above. To normalize the effectiveness factors of fuel cell the modeling and simulation are highly helpful. In the meanwhile the power curve represents the abnormal behavior in the increase in current density. That is also due to the several irreversible mechanisms in fuel cell. It was clearly demonstrated here.

Voltage loss as a function of cell area clearly shows how important the fuel cell membrane area is. According to the graph, it is clean that voltage loss is directly proportional to the area of the membrane. To avoid the voltage loss the less area of fuel cell membrane can be used to gain high output.

2) The study of thermodynamics and its relation to fuel cells is very important for predicting fuel cell performance. The determination of fuel cell potential and efficiency depends heavily on the evaluation of thermodynamic properties. Some of the important properties explored in the chapter 4 include the enthalpy, specific heat, entropy, Gibbs free energy, reversible voltage, net output voltage, and the fuel cell efficiency. The following factors for modeling were searched and established were as follows with the heat transfer calculations given in the Table 4.1.

1. Entropy of H2, O2, and water in the PEM cell
2. Heat transfer of fuel cell
3. Energy balances for fuel cell layers

The geometrical model for Gas Diffusion layer (GDL) is extremely helped for modeling of interior heat distribution. These thermodynamic concepts allow one to predict states of the fuel cell system, such as potential, temperature, pressure, volume, and moles in a fuel cell. Learning and applying these concepts are the bases of all fuel cell modeling and analysis, and is essential for understanding the remainder of this thesis.
The basic behavior of heat inside the fuel cell is very complicated to understand as the heat produced in FC reaction is negligible. But when the FC system comes as a large, the heat behavior is considerable. In such a situation the modeling of heat transfer inside the fuel cell is highly valuable. In FC technology the only output which can be consider as non environmental friendly is heat. Therefore the simulation of FC interior is help full to eliminate the heat distribution in side in it. In such a situations external cooling systems or self cooling agents can be introduced for better output.

3) In many fuel cell types, the flow fields are usually arranged as a number of parallel flow channels; therefore, the pressure drop along a channel is also the pressure drop in the entire flow field. In a typical flow channel, the gas moves from one end to the other at a certain mean velocity. The pressure difference between the inlet and outlet drives the fluid flow. By increasing the pressure drop between the outlet and inlet, the velocity is increased. In such a situations the modeling of FC channel properties, the pressure drop can be simulated to identify the flow fields. Fuel flowing manner inside the channel is highly important in FC output. In such a situation the external pressure controlling unit can be introduced to control and regulate the fuel flow.

The pressure drop calculation as a justification is done with the following equation extracted, with the help of relevant parameters.

$$\Delta P = f\frac{L_{chan}}{D_H}\rho\frac{\bar{V}^2}{2} + \sum K_L\rho\frac{\bar{V}^2}{2}$$

4) The chapter 5 highlights the real world applications and experimental data. Under this chapter basic proton exchange membrane fuel cell stack principle is discussed with the real time experimental details alone with the solar hydrogen FC basic model and Fuel cell concept model vehicle. Cost estimation for solar hydrogen fuel cell basic model for home is discussed.

The basic FC concept is new to the Srilanka as well as to the southern region of Asia. It is really important to identify the reasons why the FC technology is not absorbed by this region. According to the nature of environmental condition in southern region of Asia, it is obvious that the input resource can be generated easily. The major input resource; hydrogen can be easily electrolyzed by using the solar power or wind power. Therefore the only impossible target is the membrane material (Nifion). As the Nifion is a chemical polymer it is so costly to produce or buy. Other than to that the developer can turn in to the possible substitute for the said material. Established here are the following factors for the comparison between batteries and fuels cells

- Fuel cell power systems have around 40-60% efficiencies depending on the type of electrolytes and independent of size. Battery power systems themselves have high energy efficiencies, but their overall system efficiencies from raw fuel (mostly coal or nuclear) through the batteries to converted ac power are reduced to below 30%.The actual efficiency of the cell is then the actual voltage divided by these values, or

  $$\text{Cell Effciency} = \frac{V_c}{1.48}\ 100\%\ (\text{ with reference to HHV})$$

  The Figure 5.1 shows why the Fuel cell efficiency does not reach 100%.

- Fuel cells have an advantage over storage batteries in the respect of operational flexibility. Batteries need several hours to be taken for recharging after they are fully discharged. Fuel cells, on the other hand, do not undergo such material changes. The fuel stored outside the cells can quickly be replenished, so they do not run down as long as the fuel can be supplied

- The history of fuel cell equipment costs has shown that the price of fuel cells has dropped significantly as the commercial market grows and the manufacturing technology becomes mature.

Basing on the above issues mathematically, the practical model was designed basically to justify that the fuel cell system is possible partially as a substitute for fuel crisis in world.