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Modeling and Simulation of Solid Oxide Fuel Cell System

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Abstract

Fuel cell technology is a relatively new energy-saving technology that has the potential to compete with the conventional existing generation facilities. Among the various onsite generation or distributed generation or localized generation technologies available, fuel cells are being used as a potential source of electricity because they have no geographic limitations and can be placed anywhere. Fuel cells have number of benefits which make them superior than other technologies. The continuous power supply to the load as per the demand is provided by the integration of the fuel cell system. In this paper, the characteristic of Solid Oxide Fuel Cell (SOFC) is studied and model has been developed based on the physical and chemical equations. In this work, the steady state and dynamical operation of SOFC technologies has been analysed.

Keywords: *SOFC, Physical and chemical equations, Steady State, Dynamic Operation*

1. INTRODUCTION

The power is generated by the fuel cells through the electrochemical reaction between hydrogen and oxygen. The conversion efficiency is high and leaves only water and heat as the by-products, which is the main motivation for the increasing the interest in this technology [6]. Fuel Cells offer lower emission and higher efficiency than Diesel Engine but are likely to be expensive for many applications. The first fuel cell unit was discovered and developed by SirWilliam Grove 1842 [12] with the use of four primitive cells utilizing hydrogen and oxygen. However, it was not used practically until the 1960's when NASA demonstrated a potential fuel cell application. After such demonstrations, commercial companies became interested in this technology because of its power quality, high efficiency, modularity and the environmental benefits.

Fuel cells could potentially replace the internal combustion engine and many other energy generation devices used today. Reduced emissions of greenhouse gases and increased efficiency are two of the major reasons that fuel cells are being seriously researched as a replacement to the internal combustion engine.

A fuel cell (FC) is an electrochemical energy conversion system, where chemical energy is directly converted into the electrical energy and heat. The main advantages of this technology are high efficiency almost at partial load, low emissions, and noiselessness (due to nonexistence of moving parts), and free adjustable ratio (50 kW to 3 MW) of electric and heat generation. The basic structure of fuel cells consists of a pair of electrodes, one positive and negative, and an electrolyte. The fuel used in the fuel cell is usually hydrogen, but fuel cell also requires oxygen. The hydrogen is supplied to the anode where the fuel is oxidized, liberates the electrons, which directed through the external circuit. At the cathode, the oxidant is reduced, consuming electrons from the external circuit. Ions are traveled through the electrolyte to balance the flow of electrons through the external circuit. The anode-cathode reactions and the composition and direction of the flow of the mobile ion vary with the type of fuel cell.

All fuel cells generate a direct current only, the voltage depending on cell voltage and the number of cells connected in series. Furthermore, the voltage varies with the load and also to some extent with time as the fuel cell stack ages. To obtain AC current, the fuel cell equipment should have power conditioning equipment such as inverter to handle DC to AC conversion and current, voltage, and frequency control. Fuel cells have high reliability as the number of moving parts is low. It consists of auxiliary equipment such as fans and pumps. The target for life length of fuel cells is usually given as 40000 h for the stack and at least twice the number of hours for the system. This target has been reached for a minimum number of fuel cells but in general it still remains to be proven.

2. SOLID OXIDE FUEL CELL

Solid Oxide Fuel Cell (SOFC) is one type of high temperature fuel cell that appears to be one of the most promising technology to provide the efficient and clean energy production for wide range of applications (from small units to large scale power plants). Solid oxide fuel cell is based on the concept of oxide ion migration through an oxygen ion conducting electrolyte from the oxidant electrode (cathode) to fuel electrode (anode) side. Figure 1 shows the basic elementary of the SOFC. It operates at temperatures in the range of (600-1000) ºC, which makes them highly efficient as well as fuel flexible. In case of SOFC the electrolyte is a dense solid material that involves ceramic materials like Yttrium-stabilized zircon dioxide whose function is to prevent electrons from crossing over while allowing passage to the charged oxygen ions.

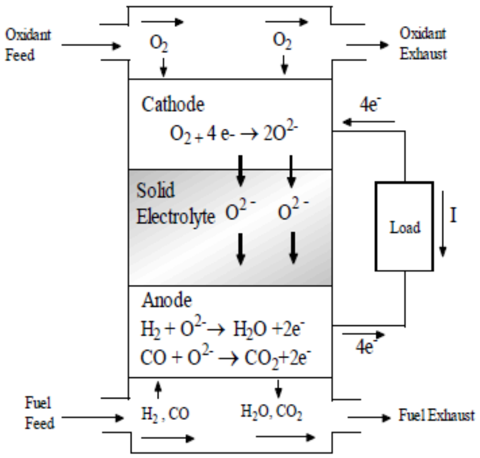

Figure 1 Basic Electrochemistry of an SOFC

The reduction reaction is carried out at the cathode where molecular oxygen reacts with the electrons supplied from external circuit to the produce oxide ions. The oxygen ions travel through the solid electrolyte to anode. In the anode side, they combine with the hydrogen molecule to produce the water, carbon-di-oxide and electrons. The electrons flow through the externally connected circuit to reach the cathode and producing electrical energy in the process. Water is produced by the recombination of oxygen ions and electrons with hydrogen at the anode, as opposed to PEMFCs where water is produced at the cathode. Under operation, either an oxygen ion-conducting electrolyte or a proton conducting electrolyte can be used by the SOFC. Here the SOFC with the oxygen ion-conducting electrolyte ($SOFC\text{-}O^{2-}$) has been considered rather than with proton-conducting electrolyte ($SOFC\text{-}H^+$) as Solid Oxide fuel cells are based on concept of an oxygen ion conducting electrolyte. The high temperature operation of SOFC enables it to work with hydrogen as well as hydrocarbon-based gases as fuel. In addition, SOFCs has the high tolerance to fuel impurities such as natural gas. They permit internal reforming, and also use less expensive catalysts for the dissociation of the oxidant. The chemical reactions placed inside the SOFC which are directly involved in the production of electricity are as follows.

At anode (fuel electrode):

$$H_2 + O^{2-} = H_2O + 2e^- \qquad (1)$$

$$CO + O^{2-} = CO_2 + 2e^- \qquad (2)$$

At cathode (air electrode):

$$O_2 + 4e^- = 2O^{2-} \qquad (3)$$

Overall cell reaction:

$$H_2 + ½\, O_2 = H_2O \qquad (4)$$

3. MODELING OF SOFC

Solid Oxide Fuel Cells (SOFC) are particularly attractive because they are the most efficient in terms of fuel input to electricity output. This technology is best applicable in the MG. The high operating temperature produces heat suited well to cogeneration applications. SOFC do not contain noble metals and do not utilize liquid electrolytes which can cause problems and be expensive [10]. The stack model will be based on the following assumptions.

- The gases are ideal.
- The stack is fed with hydrogen and air. If the natural gas is used as the fuel, the dynamics of the fuel processor must be added in the model, upstream of the hydrogen inlet, as a first-order transfer function [2]. The transfer function gain should reflect the changes in composition occurring during the process.
- The channels that transport the gases along the two electrodes have a fixed volume, but their lengths are small, so that it is only necessary to define one single pressure value in their interior.
- The exhaust of each channel is via a single orifice. The ratio of pressures between the interior and exterior of the channel is large enough to consider that the orifice is choked.
- The temperature is stable at all times.
- The only source of losses is ohmic, as the working conditions of interest are not close to the upper and lower extremes of current.
- The Nernst equation can be applied.

By Nernst’s equation output fuel cell dc voltage V_{fc} across stack of the fuel cell [5] at current I_{fc} is given by the

$$V_{fc} = N_0\left(E^0 + \frac{RT}{2F}\ln\left(\frac{P_{H_2} P_{O_2}{}^{0.5}}{P_{H_2O}}\right)\right) - rI_{fc} \qquad (5)$$

Where,
V_{fc}-Fuel cell stack voltage(V),
N_0-Number of cells in stack,
E_0-Standard reversible cell potential(V),
I_{fc}-Stack Current(A)
r-Internal resistance of the stack(Ω),
R-Universal gas constant(J/molK),
T-Stack Temperature(K),
F-Faraday’s constant(C/mol).

The expression for partial pressure of hydrogen as [5]

$$P_{H_2} = \frac{1/K_{H_2}}{1+\tau_{H_2} s}\left(q_{H_2}^{in} - 2K_r I_{fc}\right) \qquad (6)$$

Where, τ_{H_2} is the value of system pole associated with the hydrogen flow, expressed in seconds and is given as

$$\tau_{H_2} = \frac{V_{an}}{K_{H_2} RT}$$

The partial pressure for the reactant, oxygen and product, water can be expressed as follows,

$$P_{O_2} = \frac{1/K_{O_2}}{1+\tau_{O_2} s}\left(q_{O_2}^{in} - K_r I_{fc}\right) \qquad (7)$$

$$P_{H_2O} = \frac{1/K_{H_2O}}{1+\tau_{H_2O} s}\left(2K_r I_{fc}\right) \qquad (8)$$

Where

K_{H_2O} -Valve molar constant for water [kmol/(s atm)]

K_{H_2} -Valve molar constant for hydrogen [kmol/(s atm)]

Ko_2 -Valve molar constant for oxygen [kmol/(s atm)]

Fuel utilization is the ratio between the fuel flow that reacts and the input fuel flow. Hence, we have

$$U_f = q_{H_2}^{r} / q_{H_2}^{in} \qquad (9)$$

It has been shown that the fuel utilization ranging from 0.8 to 0.9 provides the better performance and prevents overused and underused fuel conditions. Considering the above specified fuel conditions, $U_f > 0.9$ can cause permanent damage to the cell because of fuel starvation and $U_f < 0.7$ leads to higher cell voltage rapidly. For the definite hydrogen input flow, the demand current of fuel cell system can be limited in the range given as:

$$\frac{0.8 q_{H_2}^{in}}{2K_r} \le I_{in} \le \frac{0.9 q_{H_2}^{in}}{2K_r} \qquad (10)$$

The optimum utilization factor assumed for this model is 0.85[17]. The fuel utilization can be set at this value by regulating the input fuel flow depending on the real output current recorded in the fuel cell system. Therefore, the value of fuel input flow, depending on fuel cell output current is given as

$$q_{H_2}^{in} = \frac{2K_r I_{fc}}{0.85} \qquad (11)$$

From the overall fuel cell reaction (4), the stoichiometric ratio of hydrogen to oxygen is 2 to 1. Oxygen excess is always taken to let hydrogen react with the oxygen more completely. Their simulation in fuel cell system shows that rH-O should be kept around 1.145 in order to keep the fuel cell pressure difference below 4 kPa under normal operation.

The chemical reaction is modeled as a first-order transfer function with a 5S time constant because of the fuel processor is usually slow as it is associated with the time to change the chemical reaction parameters after a change in flow reactions. The electrical response time in the fuel cells is generally fast and mainly associated with the speed at which the chemical reaction is capable of restoring the charge that has been drained by the load. This is also modeled as a first-order transfer function but with a 0.8 s time constant.

Based on [8] and the above discussions, the SOFC system dynamic model which is proposed by [14] is summarized in (11) and (12).

$$I_{ref} = \begin{cases} q_{H_2}^{in} \dfrac{U_{\max}}{2K_r}, if ------\rightarrow \bar{I} > q_{H_2}^{in} \dfrac{U_{\max}}{2K_r} \\ q_{H_2}^{in} \dfrac{U_{\min}}{2K_r}, if ------\rightarrow \bar{I} > q_{H_2}^{in} \dfrac{U_{\min}}{2K_r} \\ \bar{I} = \dfrac{P_{ref}}{V_{fc}}, otherwise \end{cases} \qquad (11)$$

The block diagram of dynamic model of a SOFC is shown in Figure 2.The different model parameters such as maximum fuel utilization, minimum fuel utilization, optimum fuel utilization fuel system response time, and electrical response time and so on as mentioned in Table 1. The power produced by the fuel cell is then given by the following relation:

$$P_{fc} = V_{fc} I_{fc} \qquad (12)$$

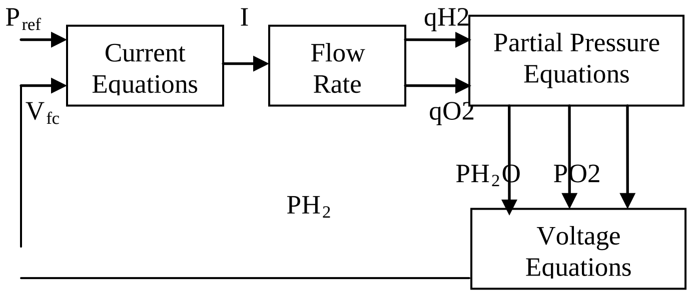

Figure 2 Block diagram for dynamic model of SOFC

Table 1 Parameters of the SOFC

Variable	Representation	Value
T	Absolute temperature	1273K
F	Faraday's constant	96487C/mol
E_0	Standard reversible cell potential	1.18V
N_o	Number of cells in stack	384
K_r	Constant	0.996×10^{-6}
U_{max}	Maximum fuel utilization	0.9
U_{min}	Minimum fuel utilization	0.8
U_{opt}	Optimum fuel ratio	0.85
K_{H_2}	Value molar constant for hydrogen	$8.43X10^{-04}\left(Kmol/s\quad atm\right)$
K_{O_2}	Value molar constant for oxygen	$2.52X10^{-03}\left(Kmol/s\quad atm\right)$
K_{H_2O}	Value molar constant for water	$2.81X10^{-04}\left(Kmol/s\quad atm\right)$
τ_{H_2}	Response time for hydrogen flow	26.1s
τ_{H_2O}	Response time for water flow	78.3s
τ_{O_2}	Response time for oxygen flow	2.91s
R	Ohmic loss	0.126Ω
T_e	Electric response time	0.8s
T_f	Fuel processor response time	5s
rHo	Ratio of hydrogen to oxygen	1.145
R	Universal Gas Constant	8314 J/(kmolk)

4. SIMULATION RESULTS

It is assumed that the stand-alone SOFC system is operating with constant rated voltage 333.8 Volts and power demand 70 kW. All parameters of the system are the same as in Table 1.

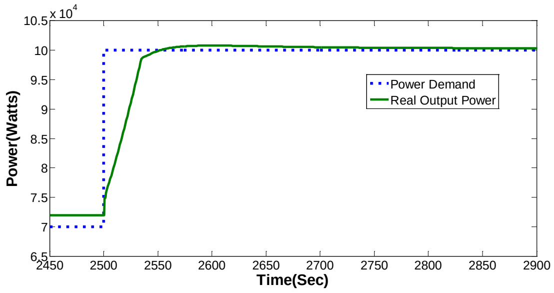

Figure 3 Response of SOFC when increasing power demand from 70KW to 100KW

At t = 2500 sec, there is a step increase of the power demand from 70 kW to 100 kW. Figure 3 shows the dynamic response of this system. Figure 4 shows the dynamic response of the SOFC when there is a decreasing in power demand from 70 kW to 40 kW.

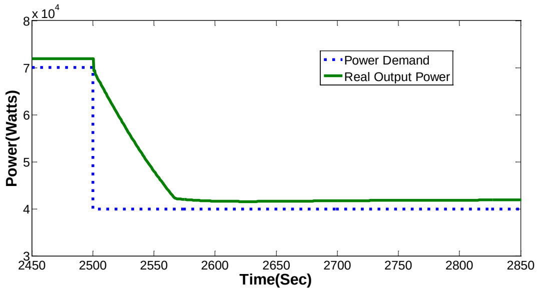

Figure 4 Response of SOFC when decreasing power demand from 70KW to 40KW

Results show that the SOFC has some slow dynamic response, so that using SOFC alone may be not suitable for systems that need a fast dynamic response.

Figure 5 illustrates the response of the fuel cell pressure difference between hydrogen and oxygen. We can notice that it increases to the peak value of 3.5 kPa when the power demand increased from 70KW to 100KW, which is less than the maximum safety pressure difference 8 kPa. It can return to the normal operating pressure difference value around 0 kPa.

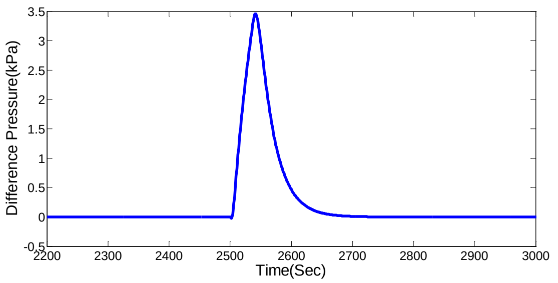

Figure 5 Response of pressure difference between hydrogen and oxygen

In Figure 6 the fuel utilization response is presented, due to increase in the power demand, the fuel utilization increases to the maximum fuel utilization *U*max in about 2500 s. After staying at *U*max for about 25 s, it decreases to optimal fuel utilization Uopt.

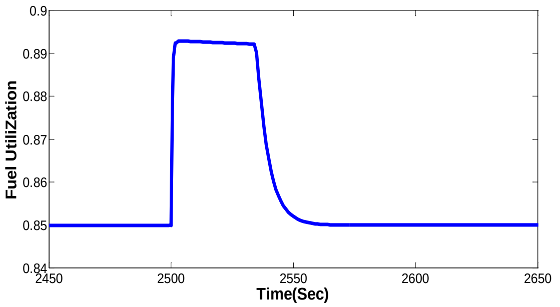

Figure 6 Response of Fuel Utilization

5. CONCLUSIONS

Modeling and simulation study of a SOFC power system is investigated in this paper. The response of the system to step changes in load demand are presented along with the analysis of the simulated results. A validated SOFC dynamic model is used to model the fuel cell system. The model can be used in future applications for the analysis of hybrid power systems. A hybrid power system consists of a combination of two or more power generation technologies to do the best use of their operating characteristics and to obtain higher efficiencies than those can be obtained from a single power source.

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