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Modelling and Analysis of Automotive Fuel Cell

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ABSTRACT: More concern is given to climate change and global warming. And the co_2 emissions are worrying. In response a momentous energy revolution is taking place renewable energy sources like wind, as well as new hydrogen and fuel cells technologies are developing now a day to take over from fossil hydro carbons combustion. Fuel cells are electrochemical devices that convert the chemical energy of a gaseous fuel directly to electric energy. This paper proposes a model for the simulation and performance evaluation of a Polymer Electrolyte Membrane (PEM) Fuel Cell generation system. Fuel cell is modeled based on stack voltage model, it includes cell voltage model, anode, cathode flow models and the membrane hydration model. This model includes the finding of open circuit voltage and different over voltages like activation, concentration and ohmic.

KEYWORDS- Fuel Cell, Renewable Energy, Mathematical Model, Clean Environment.

I. INTRODUCTION

Hydrogen is often referred to as an important energy source for the future. The efficient conversion of hydrogen into electrical energy should be done by fuel cells. An important cost factor of a PEFC is the membrane electrode assembly (MEA) by Cleghorn [1]. The efficiency of a fuel cell system is not only influenced by the efficiency of the fuel cell but also by the energy requirements of the auxiliary components, e.g. the air compressor, humidifier and cooling water pump. In particular, the power losses based on the humidification are often underestimated and can reduce significantly the efficiency of a fuel cell system. Fuel cell stack systems are under intensive development for mobile and stationary power applications like particular, Proton Exchange Membrane (PEM) Fuel Cells are currently in a relatively more mature stage for ground vehicle applications. Transient behaviour is one of the key requirements for the success of fuel cell vehicles. Efficient fuel cell system power production depends on proper air and hydrogen feed, and heat and water management. During transients, the fuel cell stack breathing control system is required to maintain proper temperature, membrane hydration, and partial pressure of the reactants across the membrane to avoid degradation of the stack voltage, and to maintain high efficiency and long stack life by Yang et al. [2]. Figure 1 shows a typical automotive fuel cell.

II. FUEL CELL MODEL

The presented model of a fuel cell is based on an approach which can be found in the literature by Lee et al. [3]. The model was changed at several points to make it closer to the reality of the investigated fuel cell stack by Pukrushpan et al. [4]. Fuel cell stack model as shown in Figure-2 contains a cell voltage model, an anode- and cathode flow model and a membrane hydration model. The assumptions on which the model is based are:

- (i) The cathode and anode of the fuel cell are a volume with a constant pressure and temperature
- (ii) All gases behave like ideal gases.
- (iii) The inlet mass flows enter the anode and cathode volume without a pressure drop and the outlet mass flows leave the volumes via a nozzle. If the relative humidity of the water exceeds 100 %, liquid water will condense in the



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anode or cathode volume. Contrary to the basic model, it is possible that the outlet gas flows can transport a limited amount of liquid water, e.g. in the form of droplets.

(iv) The gas diffusion in the gas diffusion layers (GDL) and at the electrode surfaces is neglected

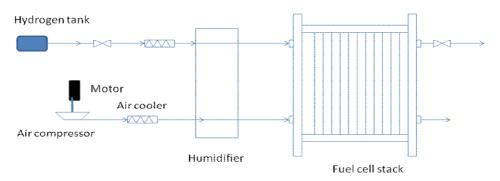


Fig.1. Automotive fuel cell

III. CELL VOLTAGE MODEL

The voltage of a fuel cell is defined as the sum of the theoretical open circuit voltage and the different over -voltages. $V_{FC} = E_0 - V_{act} - V_{ohm} - V_{conc}$. E_0 is the theoretical open circuit voltage and V_{act} , V_{ohm} and V_{conc} are the over-voltages due to the activation losses, the ohmic resistance and concentration losses, which represent losses due to various physical or chemical factors. The energy balance between the reactants and products is used to calculate the open circuit voltage.

$$E_0 = 1.229 - 8.5*10^4 (T_{FC} - 29815) + 4.3085*10^5 T_{FC} [\ln P_{H_2} + \frac{1}{2} \ln P_{O_2})]$$

where the fuel cell temperature T_{FC} is expressed in Kelvin, and reactant partial pressures P_{H_2} and P_{O_2} are expressed in atm. The activation losses are caused by the processes of the chemical reaction. On the catalysts surfaces the bonds in the hydrogen and oxygen molecules were broken and new bonds were formed to produce water. This breaking and forming of bonds needs energy and causes a voltage drop [5]. The activation over-voltage rises very rapidly at low current densities and increases almost linearly at high current densities. This behavior is described by Tafels law[6,7]. The Tafel equation may be approximated by the following equation

 $V_{act} = V_0 + V_a (1 - e^{-c_1 i})$ The activation overvoltage depends on temperature and oxygen partial pressure[8,9].

where V_0 is the voltage drop at open circuit V_a is the rising of the activation losses and c_1 is a constant. The ohmic overvoltage, $v_{\it ohm}$, arises from the resistance of the polymer membrane to the transfer of protons and the resistance of the electrodes and collector plates to the transfer of electrons. The drop in voltage is proportional to the stack current.

 $V_{ohm} = i * R_{ohm}$ The resistance, R_{ohm} , depends on membrane humidity[10] and temperature of the cell[11].

The concentration over-voltage is caused by a limited transportation velocity of the reactants to the electrodes[13]. The concentration losses can be approximated by[12].

$$V_{conc} = i(c_2 \frac{i}{i_{max}})^{c_3}$$
 where c_2 , c_3 and i_{max} depend on temperature and reactant partial pressure and can be

determined empirically.

The mass balance for the cathode is



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$$\frac{dm_{o_{2}}}{dt} = W_{o_{2},in} - W_{o_{2},out} - W_{o_{2},reacted}$$

$$\frac{dm_{N_{2}}}{dt} = W_{N_{2},in} - W_{N_{2},out}$$

$$\frac{dm_{W,ca}}{dt} = W_{v,ca,in} - W_{v,ca,out} + W_{v,ca,gen} + W_{v,membr}$$

and, the simpler mass balance for the anode is

Fig.2. Fuel cell stack block diagram

IV ANODE AND CATHODE FLOW MODEL

$$\frac{dm}{dt}_{v,an,in} = W_{v,an,in} - W_{v,an,out} - W_{v,membr}$$



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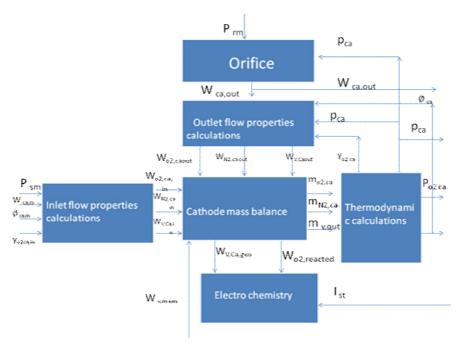


Fig.3. Cathode flow model

The consumed oxygen and hydrogen and the produced water can be calculated by Faraday's law. The membrane hydration model is used to calculate the water flux across the membrane. The rate of water flow at inlet is calculated in reference to the absolute humidity of the gas. It is assumed that without any drop in pressure, gas enter the anode and cathode. The gas leaves the outlet via a nozzle and can be calculated by a linear nozzle equation

 $W_{out} = k_{nozzle}(P_{up} - P_{down})$ where k_{nozzle} is a constant, P_{up} is the pressure in the anode or cathode volume and P_{down} is the pressure behind the anode or cathode volume.

V. MEMBRANE HYDRATION MODEL

The membrane hydration model captures the effect of water transport across the membrane .Both water content and mass flow are assumed to be uniform over the surface area of the membrane, and are functions of stack current and relative humidity of the gas in the anode and cathode. The water transport across the membrane is achieved through two distinct phenomena. First, the electro- osmotic drag phenomenon is due to the water molecules dragged across the membrane from anode to cathode. The gradient of water concentration across the membrane results in 'back-diffusion' of water, usually from cathode to anode. The water concentration, c_{ν} is assumed to change linearly over the membrane thickness, t_{m} . The flow of water from anode to cathode is

$$W_{v,membr} = M_{v} A_{FC} n \left(\frac{n_{d} I_{st}}{F} - \frac{D_{w} (c_{v,ca} - c_{v,an})}{t_{m}} \right)$$

The coefficients n_d and D_w vary with membrane water content, λ_m , which is calculated from the average of the water content at the anode (λ_{an}) and cathode (λ_{ca}) λ_{an} and λ_{ca} are calculated from the membrane water activity,



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$$a_{i} = \frac{y_{v,i}P_{i}}{P_{sat}} = \frac{P_{v,i}}{P_{sat,i}} : i \in [an, ca]$$

$$\lambda_{i} = 0.043 + 17.81a_{i} - 39.85a_{i}^{2} + 36a_{i}^{3} \qquad (0 < a_{i} <= 1)$$

$$= 14 + 1.4(a_{i} - 1), (1 < a_{i} <= 3)$$

$$n_{d} = 0.0029\lambda_{m}^{2} + 0.05\lambda_{m} - 3.4 * 10^{-19} \text{ and}$$

$$D_{w} = D_{\lambda} \exp(2416(\frac{1}{303} - \frac{1}{T_{FC}})) \qquad \text{Where}$$

$$D_{\lambda} = 10^{-6} \qquad \lambda_{m} < 2$$

$$= 10^{-6}(1 + 2(\lambda_{m} - 2)) \qquad 2 <= \lambda_{m} < 3$$

$$= 10^{-6}(3 - 1.67(\lambda_{m} - 3)) \qquad 3 <= \lambda_{m} < 4.5$$

$$= 1.25 * 10^{-6} \qquad \lambda_{m} >= 4.5$$

and T_{FC} is the fuel cell temperature. The water concentration at the membrane surfaces, $c_{v,ca}$ and $c_{v,an}$, are functions of water content on the surface, λ_{ca} and λ_{an} Specifically,

$$c_{v,i} = \frac{\rho_{m,dry} \lambda_i}{M_{m,dry}}, \qquad i \in [an, ca] \qquad \text{where } \rho_{m,dry} \text{ (kg/cm}^3 \text{)is the dry membrane density and } M_{m,dry} \text{ (kg/mol)is}$$

the membrane dry equivalent weight.

These equations are developed based on experimental results measured for Nafion 117 membrane, PEM membranes have evolved tremendously and the empirical equations 17 may no longer be a good representation of the new membrane properties.

VI RESULTS AND CONCLUSION

A model was presented which can determine the average conditions in a PEFC. The open circuit voltage of a fuel cell is calculated from the energy balance between chemical energy in the reactants and electrical energy. Three main types of losses in the fuel cell are explained. It is suitable to indicate the influence of changes in the operating parameters, especially of the inlet gas flows, on the fuel cell performance.

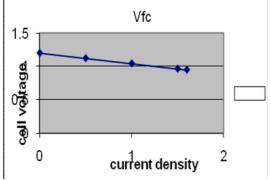


Fig.4. voltage drop caused by ohmic losses only

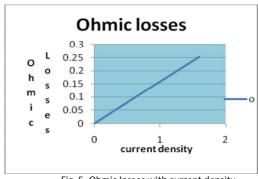


Fig. 5. Ohmic losses with current density



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The figure 4 shows how fuel cell voltage is decreasing with current density due to ohmic losses only. Figure 5 shows the voltage drop due to ohmic losses with current density. Figure 6 shows how the activation losses are varying with current density.

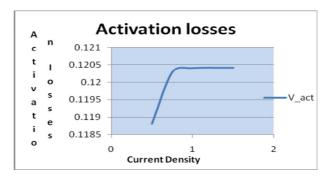


Fig. 6. Activation losses with current density

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