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DYNAMIC SIMULATION OF A PROTON EXCHANGE MEMBRANE FUEL CELL SYSTEM FOR AUTOMOTIVE APPLICATIONS

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ABSTRACT

A dynamic model of the PEMFC system is developed to investigate the behaviour and transient response of the fuel cell system for automotive applications. The system accounts for the fuel cell stack with coolant, humidifier, heat exchangers and pumps. Governing equations for fuel cell and humidifier are implemented into the code and are based on adopted mathematical models describing the voltages and current densities and their dependence on operating pressures, temperatures and stoichiometric ratios of the reactant gases. As a result, this model can predict both steady and transient states. The model parameters have been adjusted specifically for a 21.2 kW Ballard stack [1]. This model also incorporates the effects of water cross-over in the fuel cell membrane. Controls for temperatures, pressures, reactant stoichiometry and flows are implemented to simulate the system behaviour for different loads and operating conditions. Simulation results for system start-up and variable loads are discussed. Results for system efficiency, auxiliary power consumption, feed flow effects and water crossover are presented. Transitory effects of liquid water saturation at cathode are also determined. This study can provide sufficient insight for further in-depth analysis of PEMFC and prove to be a basis for efficient control and design methodologies.

Keywords: *Dynamic simulation, PEM fuel cell, water crossover, Control system*

1 INTRODUCTION

Fuel cells are recognized to be one of the future power supply systems. The proton exchange membrane fuel cells (PEMFC) currently appear to be the preferred fuel cell for a variety of mobile applications, mainly due to its relatively low operating temperature, quick start-up, high power density and efficiency, system robustness and low degradation due to corrosion.

Fuel cell operating requirements in vehicles are more inflexible than stationary applications. These systems have to operate at varying conditions related to temperatures, pressures, power load and humidity. All the auxiliary components constitute the balance of plant (BoP). These auxiliary components, such as the air and fuel supply system which include compressors and control valves, and the thermal control system which comprise heat exchangers, coolant pumps and air radiators are essential for the successful operation of the fuel cell system. Therefore, system level dynamic modelling will be a useful tool in analysis of PEMFC systems.

There are quite a few PEM fuel cell models available in the literature. Fuel cell and stack level transient modelling is performed in the dynamic model developed by [2]. A simplistic dynamic model based on cathode kinetics was developed in [3]. A dynamic model in MATLAB/Simulink was developed in [4] to investigate fuel cell transient electrical responses under various operating conditions. Issues related to temperature dynamics are dealt and studied by [5], which could predict the effects of temperature and feed flows on system transient behaviour. [6] proposed a transient model to predict efficiency in terms of voltage output, and a thermal model including heat transfer coefficients and energy balance for the stack. A thermal management system for a PEMFC was designed in [7] which was oriented towards the flow fields within the stack. Start-up behaviour of PEMFC stacks at sub-zero temperatures have been studied and reported by few researchers. [8] conducted experiments and validated their model based on the results while [9] investigated effects of sub-freezing temperatures on fuel cell performance and start-up.

Compared to all these studies, the model presented in this work aims at analysis and investigation of a complete PEMFC system and study its transient response to operating parameters such as temperature, humidity, pressure and reactant mass flows. One of the objectives of this work is to devise a control-oriented dynamic model of the fuel cell stack, accommodating the electrochemical, thermal and feed flow models. Therefore, Aspen Plus Dynamics^{TM} is used to develop a dynamic stack model with liquid coolant circuit incorporated in it, which allows for a detailed analysis of the thermal interaction with the surroundings.

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Moreover, the present model can provide suitable insight to saturated water issues in the fuel cell stack. Two-phase characteristics of concerning material streams are also determined.

2 SYSTEM CONFIGURATION

Figure 1 shows the schematics of fuel cell system analyzed in this study. It includes all the components contained in the system, such as PEMFC stack, air compressor, humidifier, pumps, heat exchangers and radiator for the cooling circuit, flow valves and controllers. Compressed air is cooled and humidified before entering to the cathode of the stack. On the other side, pressurized hydrogen from storage tank is fed to the anode of fuel cell. Since a higher fuel stoichiometry is maintained, anode exhaust is recirculated back to the feed stream via a recirculation pump.

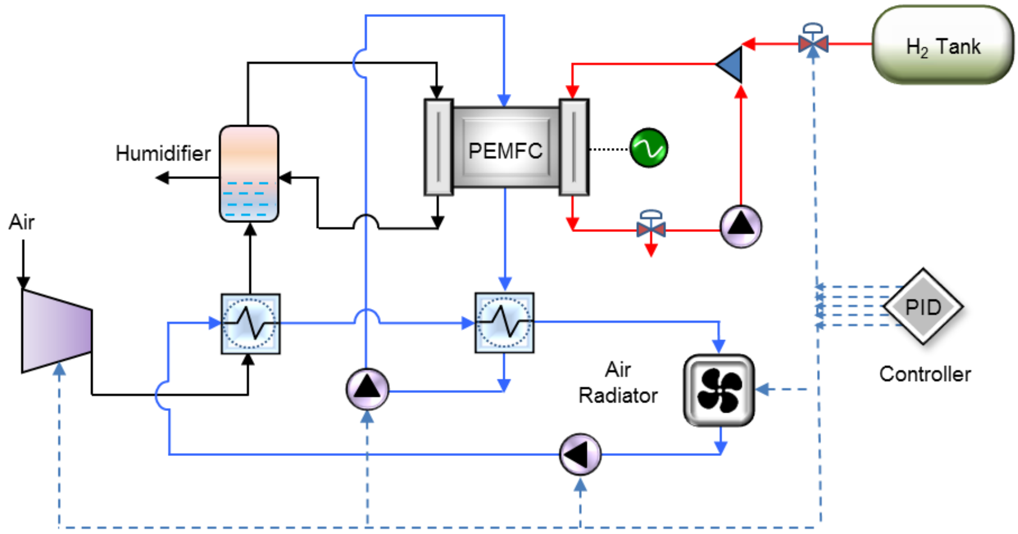

Figure 1. Schematic of a complete PEM fuel cell system with auxiliary components

Heat produced in the stack is absorbed by the coolant which circulates in a circuit associated with the stack and a heat exchanger. An external cooling loop, connected to the aforementioned heat exchanger, in turn cools the water in the internal circuit. This circuit also comprises of a heat exchanger to precool air into the fuel cell and an air radiator for heat rejection. Flow of water is regulated by pumps in the respective circuits.
In this study, a Ballard fuel cell stack [1] has been specifically adapted. The model, which is based on equations adopted by [10], however, contains some parameters which are attributed to the physical characteristics of the system, as well as on operating conditions and membrane properties. Some of these operating conditions for the Ballard stack are shown in Table 1. Current research aims to build up a system which meets the requirements of actual stack running under recommended conditions.

Table 1. Operating conditions for fuel cell stack recommended by manufacturer (Ballard).

Stack power (kW)	Fuel inlet pressure (bar)	Air inlet pressure (bar)	Inlet temperature (°C)	Operating temperature (°C)	Fuel stoichiometry	Air stoichiometry
1.4	1.15	1.08	60	61	6.3	5.1
2.7	1.16	1.10	60	63	3.4	2.4
5.1	1.31	1.17	60	66	2.2	1.8
9.7	1.55	1.38	60	67	1.7	1.8
18.0	2.00	1.80	60	68	1.6	1.8
21.2	2.20	2.00	60	70	1.6	1.8

The fuel cell stack contains 110 cells with the cell area equal of 285 cm^2. Operating temperature of the stack is maintained around 60-70°C. Maximum power produced from the described stack is 21.2 kW

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corresponding to a current of 300A; however it is generally operated at lower current ranges to reduce ohmic and concentration overpotentials and thus higher efficiencies.
Due to the lack of sufficient experimental data, it is assumed that the inlet air flow is optimally humidified after passing through the humidifier. The relative humidity of the air entering the cathode is set to 95% in the calculations; although other values can be chosen. This assumption could be justified as it is very close to the real operational conditions. On the anode side, there is no humidifier and the fuel can reach the desired humidity by means of recirculation and water production at anode exit.
Figure 1 only represents controllable connections initiating from the controller. In calculation as well as reality, the control unit collects information from various temperature, pressure and flow transmitters in addition to current and voltage data from the fuel cell. Here a simplified view of the system is presented.

3 METHODOLOGY

The characteristics of the PEMFC system described above are implemented in Aspen Plus Dynamics ™ which is a simulation tool for process modelling and energy system analysis. The program contains a vast library of components and controls for standard energy processes. The PEMFC stack model presented in this study is based on a model developed by [10]. Concentration losses are neglected in the present study, which is justified by the fact that the system does not run at such high current densities where the concentration overpotentials becomes significant. Models for fuel cell and humidifier are also implemented into the code and are based on adopted mathematical models describing the voltages, current densities and their dependence on operating pressures, temperatures and stoichiometric ratios of the reactant gases. This model which incorporates governing equations for cell electrochemical, polarization overpotentials, heat transfers and water diffusion across the membrane is implemented into Aspen Plus Dynamics and system controls are implemented in order to ensure stable operation of the plant during load changes. The thermodynamic efficiency and net power of the system are determined by current drawn and voltage produced by the stack. The total energy into the fuel cell is consumed by the electrical power output, heat removed by the coolant, heat loss at the stack surface and energy stored by the stack itself. In the current model, a lumped thermal model proposed by [6] is considered. The subordinate components in the BoP, i.e. anode recirculation and water pumps, air compressor, mixers and heat exchangers are modelled using the default mathematical models provided in Aspen Plus Dynamics.

4 CONTROL SYSTEM

This section presents methodology of controlling system parameters and operating conditions for the system to have a stable operation. Classic proportional-integral (PI) controllers, which are widely used in industrial control systems, are employed to regulate different components and flow streams. Key parameters to be controlled in the proposed system are reactant inlet stoichiometries, inlet pressures, coolant inlet and operating temperatures of the stack.
As shown in Table 1, the recommended fuel and air stoichiometries for the selected fuel cell stack and their inlet pressures, temperature difference between stack inlet and outlet need to be controlled. It can be seen that at low current loads, high amounts of excess reactant flows are desired. This is due to the fact that at low power consumption and low pressures, water formed due to the reaction in the cathode side of the cells needs to be ejected out of the stack, which is done by supplying high amounts of air. Therefore, an algorithm based on the above figure is developed to be the process variable for the PI controller, which regulates the compressor power in order to maintain the desired oxygen ratio. Similarly, an algorithm for controlling hydrogen flow is devised along with a PI controller, which regulates the control valve opening for optimal fuel supply.
Thermal management in PEMFC systems is of vital importance, basically due to the fact that heat produced in the selected fuel cell cannot be dissipated by convection and radiation through the stack surface. A consistent and stable operation of around 70°C thus requires a cooling system, preferably with a liquid coolant. Since the operating temperature of the fuel cell is not very high, a low temperature difference with the ambient requires having a large heat transfer surface. Therefore, an efficient thermal control system becomes of substantial importance to ensure optimum system performance. In this case, the temperature in the stack can be controlled by the coolant flow rate which acts as an input signal and is controlled by the PI controller. Based on Ballard recommendations, an algorithm for start-up, shut-down and normal operations is thus developed which sets the process variable for the controller. Coolant flow is manipulated by sending

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output signals to the driving pump. Temperature of the coolant entering the stack can similarly be controlled by the flow of water in the external circuit. Control signal to the associated pump regulates the electrical power of the pump and hence the coolant inlet temperature into the stack. In a similar fashion, the temperature of water in the external circuit is dependent on radiator fan speed. PI controllers are used to regulate the fan speed as well.

5 RESULTS AND DISCUSSION

Reliability of the suggested model has been verified and validated against experimental data by [10], where the characteristics of the model were studied at various operating temperatures and power loads. As suggested by the manufacturer, stack temperature range of 60-70°C has been used in the simulations of the current system. In case of PEMFC, dynamic behaviour of a start-up is of particular importance to ensure a short start-up time and an efficient operation. In current simulations, the initial temperature of the stack is assumed to be 25°C. Other parameters and operating conditions are selected from section 2.

Here, results for a start-up case are summarised, when a current corresponding to a specific power load is drawn from the stack. As can be seen in the Fig. 2a, when the stack is started at current of 60 A, it takes approximately 300 seconds to reach stable operating temperature. At start, the flow in cooling circuits is set to the lowest value since it is desired to raise the stack temperature to its optimal operation. Coolant flow in the internal circuit is fixed to 290 kg/hr as recommended by the manufacturer. Flow in the internal cooling circuit increases, once the stack temperature difference increases by 15°C. Flow in external circuit is regulated to maintain stack inlet temperature of internal cooling circuit. Air flow in radiator starts to maintain temperature of external cooling loop to around 50°C. It can be observed that the voltage reduces abruptly when simulation time is around 155 seconds. At this stage, the decrease in cell temperature and voltage is caused by the sudden increase in coolant flow into the stack, which aims to maintain the stack operating temperature.

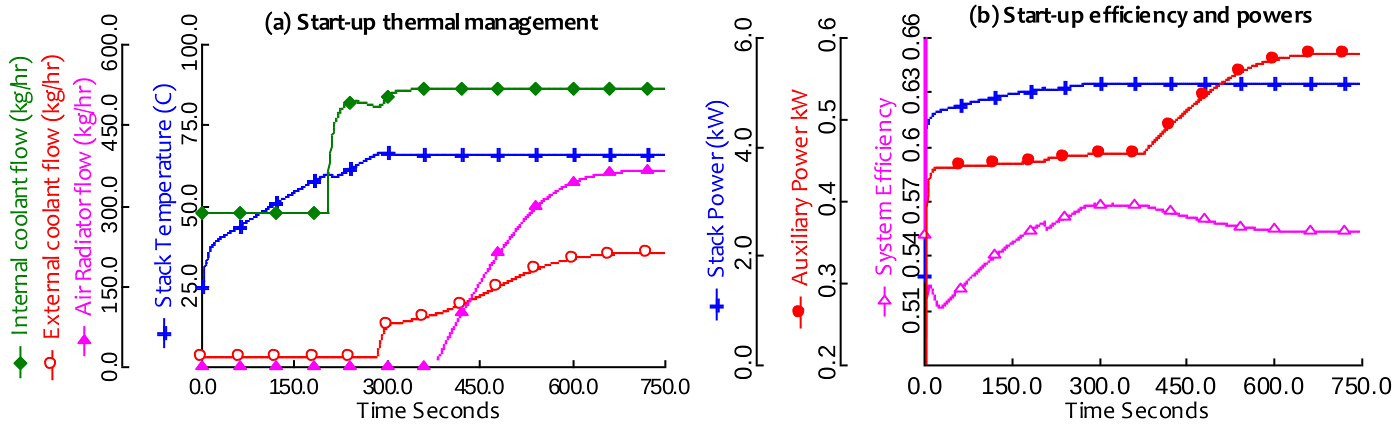

Figure 2. System start-up (a) Stack temperature and corresponding coolant flows at current of 60A, (b) System efficiency, stack power output and power consumed by auxiliary components

Overall efficiency of the system is as much affected by compressor and fan, as by the fuel cell stack itself. Is can be observed from Fig. 2b, that power produced by the stack increases with operating temperature untill it reaches steady-state conditions. Also, power consumed by the air compressor becomes constant after a few seconds into the start. Although, efficiency of the system follows a similar trend, it decreases once the radiator fan is turned on at around 370 seconds. Together, air compressor and radiator consume 10% to that of stack power, whereas a coolant and recirculation pumps account for 1.0-1.3% of it. This is also noticed in figures above; increase in internal and external coolant flows at time 200 and 370 seconds respectively, elevates the auxiliary power consumption to a very small extent as compared to air compressor and radiator.

In addition to the start sequence of the aforementioned model, transitory effects under variable load are investigated as well. An instance of load change, when current is ramped from 60 A to 100 A at a rate of 20 Amperes per second and vice versa, is presented in Fig. 3a and its effect on cell voltage is examined. Decline in voltage potential at increase of current density is a well-established fact. However, it is also noticed that cell voltage is also a function of operating temperature and pressure. Since, pressures of the reactants are already regulated to be at the optimum; here we will discuss temperature dependency of developed potential differences in the cell. Voltage decreases steadily with the decrease in operating temperature. This fact is due

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to the reason being fast reaction kinetics at the electrodes of individual cell sites. The opposite could also be observed when the current is reduced back to 60A.

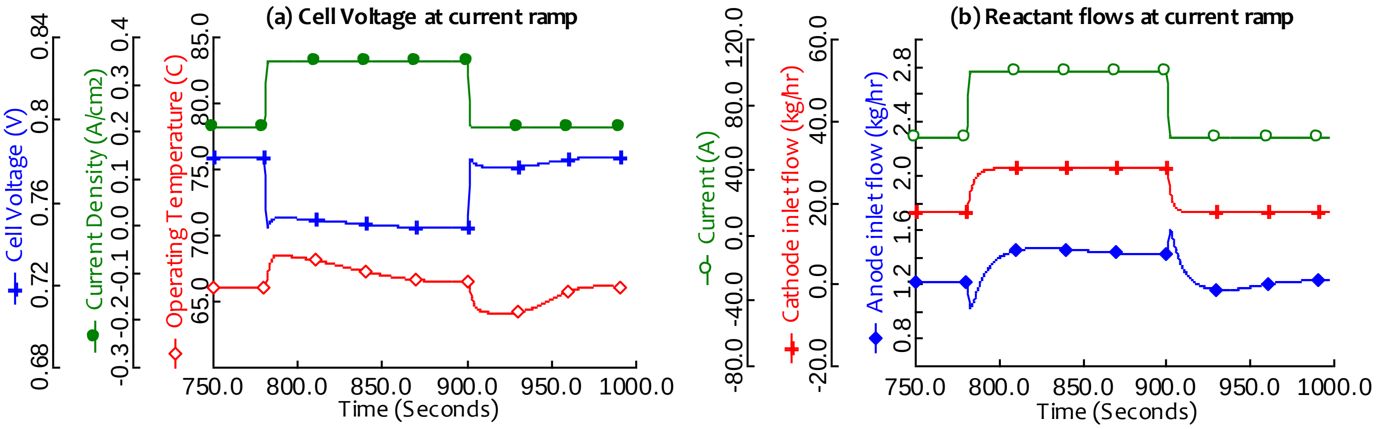

Figure 3. Current ramp-up from 60-100A and vice versa: (a) Changes in cell voltages and operating temperature, (b) Variations in fuel and air inlet flows

Fig. 3b depicts the variations in reactant inlet flows when the load on fuel cell is varied. As expected, the air flow into the cathode, regulated by a controller, increases when the current is ramped up and steadies along with the system. It is however interesting to notice the fluctuations in the anode inlet. Since anode inlet is supported by recirculation from anode exhaust, the changes within the stack influence it considerably. Although, anode flows also tend to increase as the current is increased, they are affected by the water content in the anode outlet (70% mass fraction), which depends on the net water crossover within the cell. Initial peaks at both load changes are attributed to the electro-osmotic drag which is a function of current density.

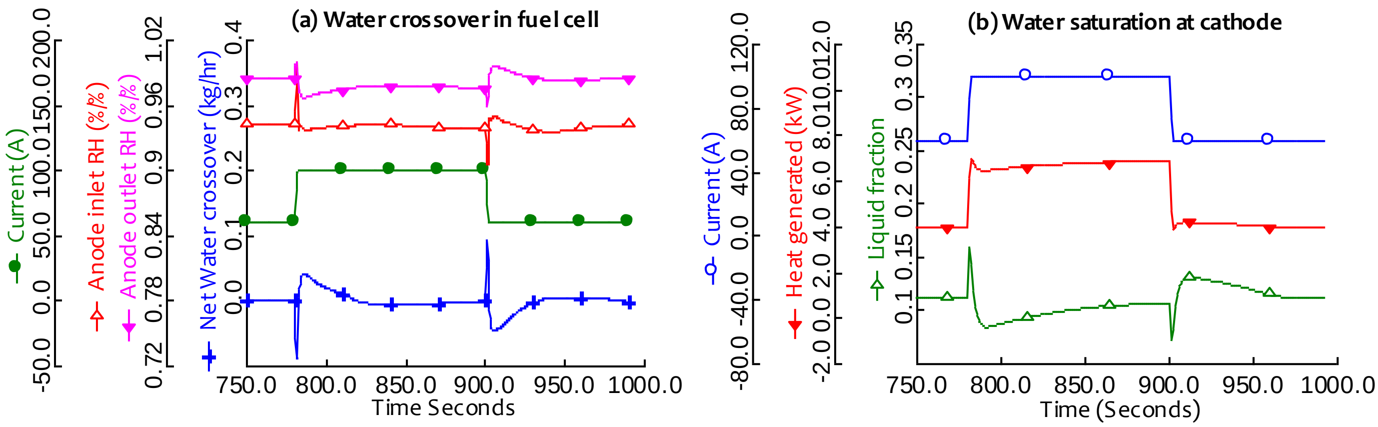

Figure 4. Current ramp-up from 60-100A and vice versa: (a) Amount of liquid water at cathode outlet, (b) Variation in net water crossover and anode RH.

Water management is a critical issue since the performance of PEM fuel cell is strongly influenced by its internal water distribution. As discussed above, water crossover within the cell influences anode inlet stream. Fig. 4a shows net water diffusion in the cell when the current is changed from 60A to 100A and back. At high currents, more water is produced in the cathode which supports back-diffusion towards the anode until the system reaches back to steady-state and there is almost no net water crossover. The peaks observed at the start of current change are due to electro-osmotic drag as mentioned above. Effect of water distribution can also be observed in anode inlet and outlet relative humidities. Whereas for the cathode, since it is assumed that air enters at a constant relative humidity of 95%, the outlet humidity is always above 100%. Therefore, results for only anode are discussed here.

Removal of water from the cathode is dependent on stack temperature and pressure drop. Temperature is the more critical factor, since at high temperature the water will be in the vapour state and easier to remove. Inlet humidities also contribute to liquid water saturation in the fuel cell, which is reported in [11]. It can be seen in Fig. 4b, that the amount of liquid water at cathode decreases at high currents. Heat produced by cell reactions elevates the stack temperature, thereby reducing saturated water at the outlet. On the other hand, reduction in stack current and temperature increases the liquid water. Therefore, at low temperatures and currents, water removal is the dominant factor and stoichiometries are determined by the minimum flow rates required for water removal which in the present case are more than adequate to provide the necessary concentrations. Moreover, condensation of water at cell sites produces additional heat which requires higher coolant flows to maintain the stack operating temperature, though it does not affect the system efficiency to a greater extent, since liquid pumps do not consume that much power.

6 CONCLUSIONS

This work has presented a comprehensive dynamic model of a fuel cell system along with the BoP. The model is oriented towards the control of associated operating conditions for the fuel cell module. Main contributions of the proposed model are attributed to the system response methodology, which incorporates stack thermal behaviour in addition to fuel cell electrochemistry and flow mass and energy balance. Emulation of the presented system shows that the results are in good agreement with the manufacturer's data. It is observed that voltage system efficiency increase with operating temperature. Air radiator does not affect system start-up, though consumes 10% of stack power together with the air compressor. Furthermore, water crossover in the stack affects the flows and humidity in anode recirculation. Also, removal of liquid water from cathode is dependent on operating temperature. Further analysis is required to study water diffusion in the cell, however based on these results; this model can be used for optimizing and designing operational strategies for PEMFC systems for automotive applications.

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