MODELLING AND SIMULATION OF SINGLE CELL SOLID OXIDE FUEL CELLS

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ABSTRACT

Over the last decade, fuel cells and hydrogen energy technologies have received attention in power generation and automobile industries. Use of the fuel cells in these sectors has remarkable advantages like high efficiency, zero emission, no noise and low heat transmission. A fuel cell is an environmentally friendly device which is capable of converting chemical energy obtained from fuel into electrical energy and produces fewer pollutants (water and heat). Therefore, fuel cells are considered as low pollution power source among other power conversion technologies. A fuel cell system is, inherently, multidisciplinary because it is composed of interacting subsystems or parts from different engineering disciplines requiring an integration of chemical engineering, process engineering, mechanical engineering, electrical engineering and control engineering. Bond graphs provide a unified approach to the modelling and analysis of dynamic systems and are ideally suited for modelling fuel cell systems because the coupling between different domains can be easily modelled. A bond graph model of a solid oxide fuel cell is presented in this paper. The constitutive relations of a C-field for two species of gases are formulated in order to model the cathode and the anode channels of the fuel cell. For given values of system operating pressure, the air source and hydrogen source pressures, the outlet pressures and the inlet gas compositions, the fuel utilisation (FU) and air utilisation are interpreted in terms of the partial pressures of the gases in the anode channel and cathode channel. The developed model satisfactorily captures all the essential dynamics of the SOFC system.

KEYWORDS

Hydrogen, Fuel cell, Bond graph model, Software packages, Electrochemical phenomena

1. INTRODUCTION

The electric potential of a single cell is weak (less than 1V at Open Circuit Voltage). So, to make it more suitable for real applications, different cells are assembled (in series from an electrical point of view and in parallel for the fluids) in order to form a stack. However, like in every series system, when one element in the chain is out of order, all the complete assembly is in failure mode. This is clearly a problem for the application of the FC technology in transportation systems for which high availability rates are required. Furthermore, transport operating conditions to be applied on FC generators are characterized by severe constraints in terms of reliability and life time. FC operation is subject to inherent uncertainty in various material and control parameters, which causes performance variability and impacts the reliability of the cells [1].

Awaiting successful commercialisation, solid oxide fuel cells are subject to extensive research and development activities. Detailed physical models are used during component design and performance evaluation involving multi-dimensional distributed representations at cell level. They can help overcome technological challenges such as choosing appropriate materials for

membranes, and estimating correct dimensions of gas flow channels; all reducing the need for and supporting the choice of required physical testing. The goal is to increase efficiency and durability of SOFCs to a competitive level. Heavy computational efforts are needed to solve complex thermofluid and electrochemical phenomena, and such models are regarded superfluous when investigating system integration. Wang et al. [2] points out the value of such models for SOFCs since there is a lack of experimental data available. Important contributions to modelling part-load performance of solid oxide fuel cells on a fairly detailed level, while still allowing for system integration, can be found in for example [3] and [4].

At the other end of the scale are dynamic models applied for controller development. Most are based on lumped approaches, treating each gas channel or solid membrane as volumes with uniform physical properties [5], [6], [7]. In some cases fuel cells are simply modelled as an equivalent electric circuit. Parameters and dynamic response of such models must be verified against measurements or more detailed models.

Models investigating properties of specific phenomena occurring in solid oxide fuel cells are for example [8], presenting models for chemical reaction rates, or [9] who uses impedance measurements to establish an equivalent circuit for the electrochemical reactions. In Todd and Young [10] the accuracy and reliability of methods applied to predict properties of SOFC gas mixtures are evaluated.

Above publications show how distributed characteristics have grate influence on SOFC dynamic behaviour. Models including such characteristics easily become computationally heavy, and decoupling of dynamics or ignoring physical phenomena of less importance to the ones studied are common approaches.

Being a tool for multi-domain modelling, bond graphs should be well suited for fuel cell modelling at a system level, particularly for control-plant models. Examples of bond graph implementations of fuel cell models are [11], [12], [13] and [14]; all for PEM fuel cells. Saisset, Turpin et al [15], [16] and [17] apply bond graphs to modelling of a SOFC. All the bond graphs are fairly consistent when it comes to modelling the electrochemical and electrical phenomena in the fuel cells.

More difficult it seems to agree upon a consistent way of treating the exchange of energy between thermofluid and electrochemical domains. When multiple gas components and phases are present the models become rather specialised for assumptions such as the ideal gas approach. In this paper, we have modelled the behaviour of the conversion energy systems. This study illustrates the importance of using simplified bond graph model properly account for the reduce simulation time in comparison with the available software package.

2. PROCESS DESCRIPTION

A PEMFC converts the chemical energy of a fuel, just as the hydrogen (H2), and an oxidizer, just as the oxygen (O2), in electrical energy. The outline of a typical PEMFC is illustrated in figure (1). On a side of the cell, referred as the anode, the fuel is supplied under certain pressure. The fuel for this model is the pure gas H2, although other compositions of gases can be used. In these cases, the hydrogen concentration should be determined in the mixture. The fuel spreads through the electrode until it reaches the catalytic layer of the anode where it reacts to form protons and electrons, as shown below in the reaction [18], [19]:
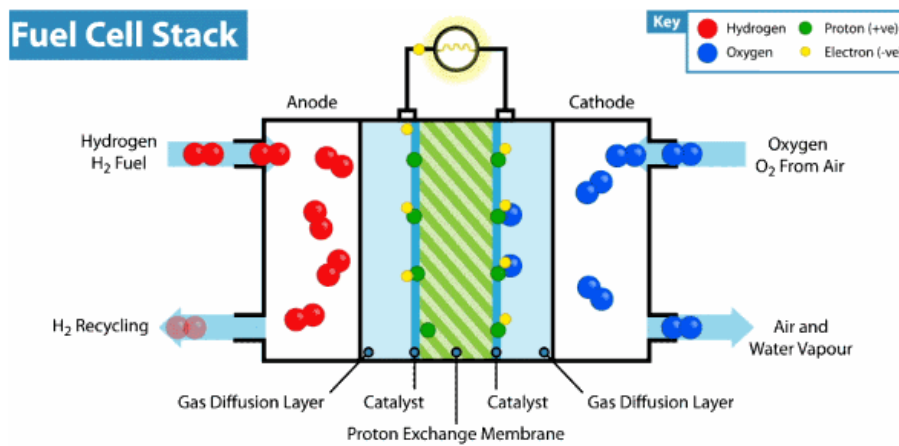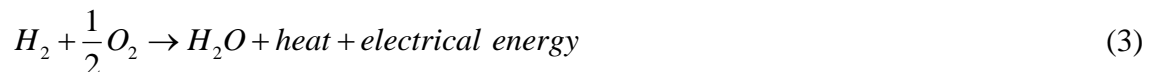
$$H_2 \rightarrow 2H^+ + 2e^- \tag{1}$$

Figure 1. Fuel cell stack

The protons are transferred through the electrolyte (solid membrane) to the catalytic layer of the cathode. On the other side of the cell, the oxidizer flows through the channels of the plate and it spreads through the electrode until it reaches the catalytic layer of the cathode. The oxidizer used in this model is air or O2. The oxygen is consumed with the protons and electrons and the product, liquid water, is produced with residual heat on the surface of the catalytic particles. The electrochemical reaction that happens in the cathode is:

$$2H^+ + 2e^- + \frac{1}{2}2O_2 \rightarrow H_2O + heat \tag{2}$$

Then, the full physical-chemical FC reaction is:

$$H_2 + \frac{1}{2}O_2 \rightarrow H_2O + heat + electrical\ energy \tag{3}$$

3. MODELING OF PROCCES

3.1. Gas Supply Model

At the anode side fuel is supplied as a gas flow between the tubes, and steam, carbon dioxide and heat is transported away as products of the reactions. In addition to electrochemical reactions the reforming reaction and the shift reaction will change the gas composition in the anode gas flow. At the cathode side the ADT supplies heated air at the bottom of the tube. Air transports oxygen to the reactions as well as provide cooling for the stack.

3.2. Gas Flow

Each gas volume is modelled by the pseudo-bond C-field. Control volumes modelled as C-fields set the pressure, temperature and concentration of the gas flows. Pseudo-bond R-fields are implemented to model the flux of mass and energy in and out of each control volume, as shown in figure (2). In SOFCs the gases flow at low velocities and can thus be modelled as plug flows with no gas dynamics included.
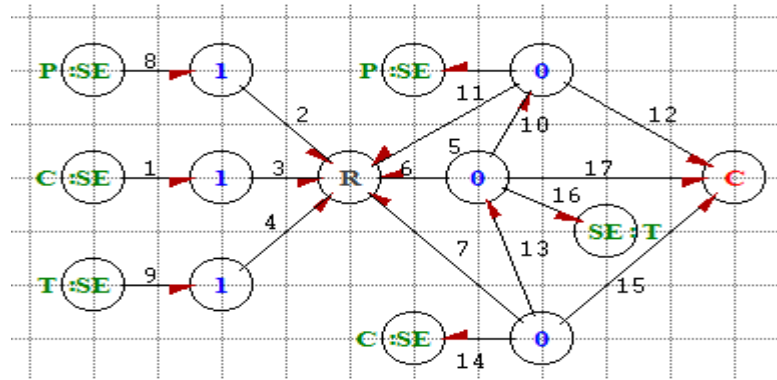
Figure 2. Pseudo-bond graph description of gas flow

3.2.1. Change in Gas Composition

The reforming rate of methane can be modelled using the same approach. Inside the SOFCs this reaction occurs on the anode surface catalyzed by nickel-cermet materials. In literature there is described some uncertainty regarding this reforming rate as discussed in [10]. The empiric relation most frequently referred to, based on Arrhenius law and developed by [13], is adopted here. A is the active area of the fuel cell.
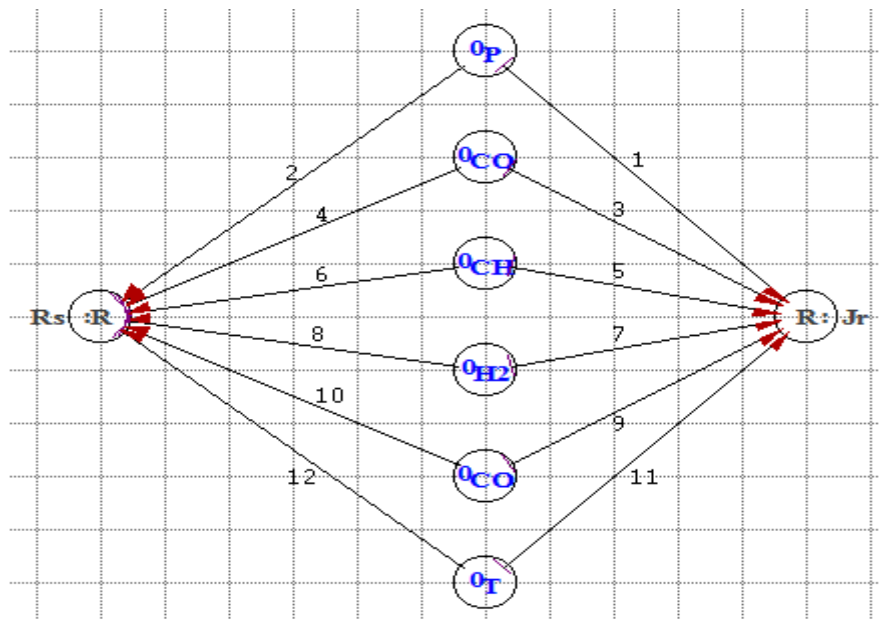

Figure 3. Chemical reactions in anode channel

R-fields attached to the zero junctions of the control volume C-fields are used to model the change in gas composition caused by chemical reactions, figure (3). The R-field calculates and sets the rate of a chemical reaction based on the current temperature, pressure and gas composition in the volume. The reforming reaction is endothermic and the shift reaction is exothermic. No work or heat transfer to the surroundings is caused directly by these chemical reactions, and the change in free energy is accounted for by the enthalpy flow in and out of the control volume. Zero energy therefore flow on the thermal bonds of figure (3). Conservation of mass for each reaction can be controlled by monitoring the bonds representing net mass flow into the R-fields.

3.2.2. Heat Transfer Model

Figure (4) shows the bond graph model implemented for the control volume. Heat flows are output from R-elements, calculated based on temperature inputs from each side. The implementation assures a positive heat flow from warm to cold independent of power bond directions. The heat capacities are included in C-elements setting the temperature and fixing the causality of the model.
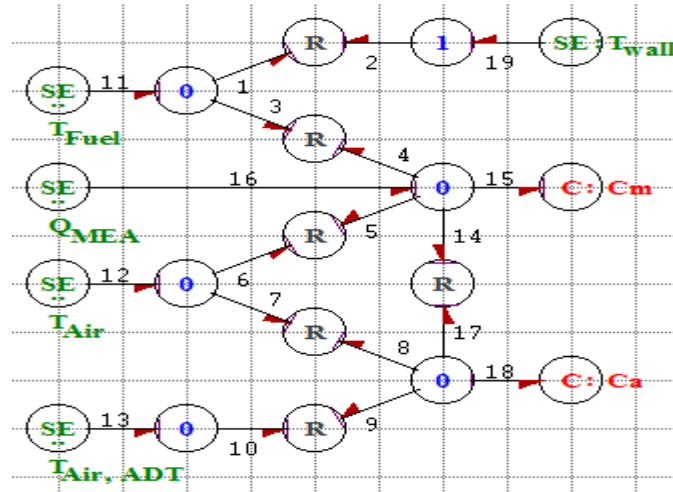

Figure 4. Bond graph of heat flows through MEA and ADT

3.2.2. Electrochemical Model

As introduced earlier, the power from a fuel cell is produced through electrochemical reactions at the triple phase boundaries. There is a net transport of mass (oxygen ions) from the cathode side to the anode side, as well as a net energy transport from both gas volumes.
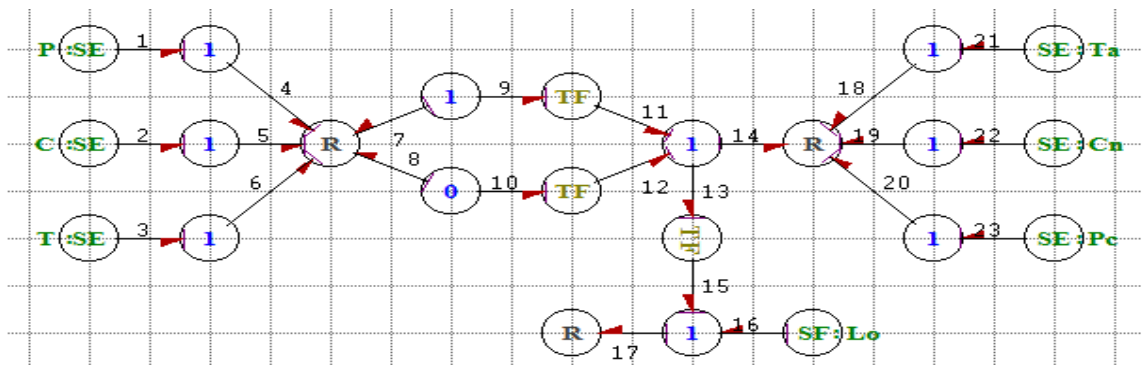

Figure 4. Bond graph of electrochemical reactions

The transfer between pseudo-bond variables and chemical potential are as described for the R-field. This is implemented in the same R-field as the diffusion losses for transport through the membranes. The loss of entropy from the reaction is added to the diffusion losses, and represented by thermal bonds out of the R-fields on the anode and cathode side. TA and TC are the surface temperatures of the anode and the cathode. Ohmic losses are shown at the electrical side, while the activation losses are left out for now. Ways to implement the three main losses in a fuel cell model is outlined below.

3.2.3. Electric Output Power

As the cells are coupled in series in a fuel cell stack the same current flows through each of the individual cells. One cell can only deliver a small voltage set up by the membranes, and a summation of these contributions results in the stack output voltage. In bond graph notation the power from a cell stack can be represented by figure (6).
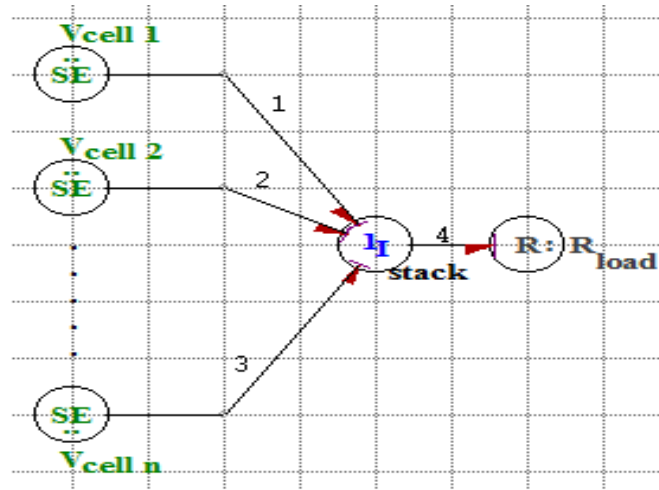
Figure 6. Bond graph of electric power flow in stack

4. SIMULATION RESULTS

4.1. Behaviour of Single Cell Models

The immediate voltage drop in figure (7) is caused by the increase in fuel utilisation and the corresponding decrease in Nernst voltage. An increased number of reactions occur and more thermal energy is released. The following increase in output voltage is caused by the increased temperature that reduces losses, and the slow stabilisation is caused by the long stabilisation times for the temperatures.
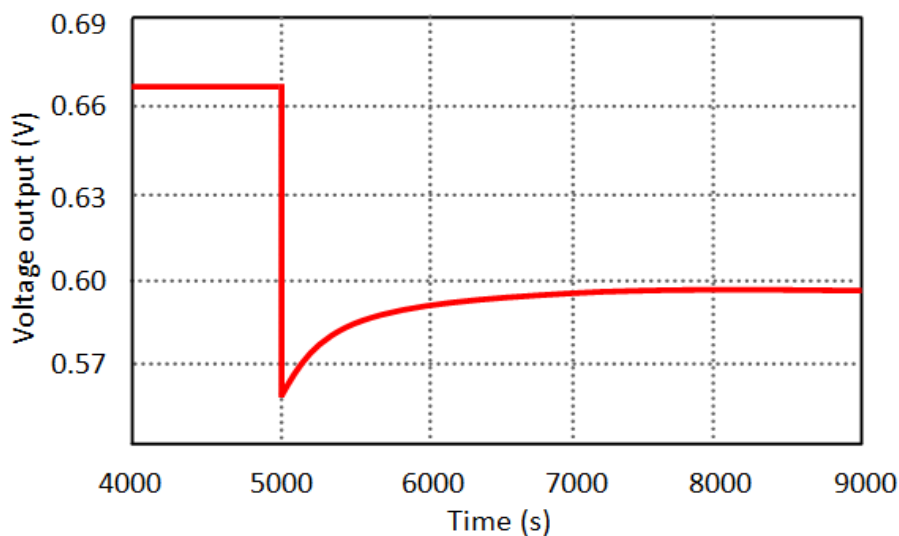
Figure 7. Voltage output, load increase of 60 A at 5000 s

Figure (8) shows the temperature development for the anode gas control volumes of the two models. It shows a time to steady state at around 3000 s, and a time constant of about 600 s.
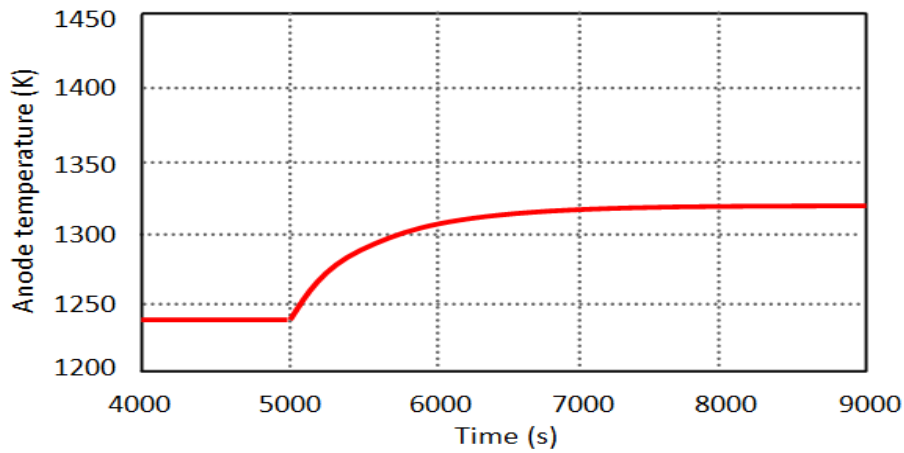

Figure 8. Temperature in anode channel, load increase of 60 A at 5000 s

Material properties for the MEA (density and heat capacity) were slightly different, but changing to similar values had minimal effect. However, increasing the inlet pressure to obtain the same gas velocity reduced the time constant, and the results were comparable.

In addition to the magnitude of gas flowing through the system, the material properties and heat transfer coefficients will influence temperature dynamics.

Voltage losses due to activation are strongly affected by temperatures, reactant concentration and current density. Figure (9) shows the development in the first and last section along the fuel cell model when load is increased from 190 A to 250 A. The immediate response is caused by increased current, and the long term decrease is caused by higher temperatures. The corresponding current distribution between the two sections is shown in figure (10), the temperature increase in figure (11).
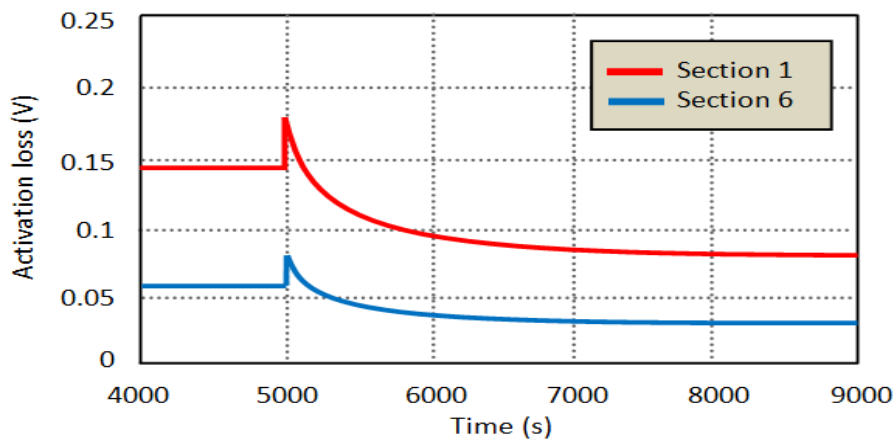

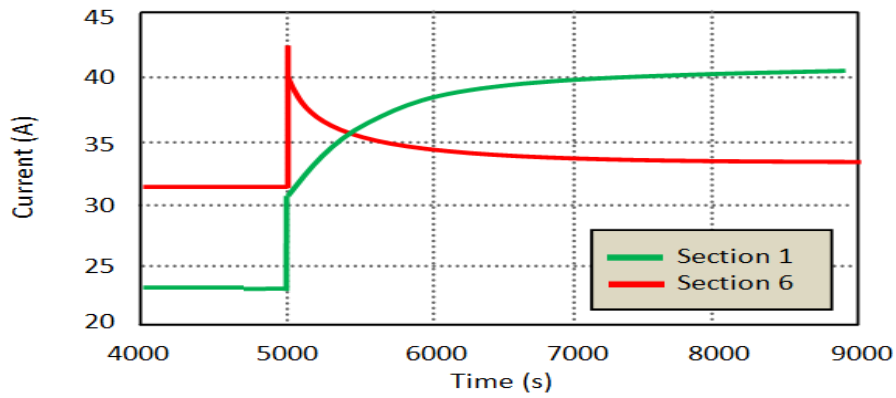Figure 9. Activation losses at anode during load increase

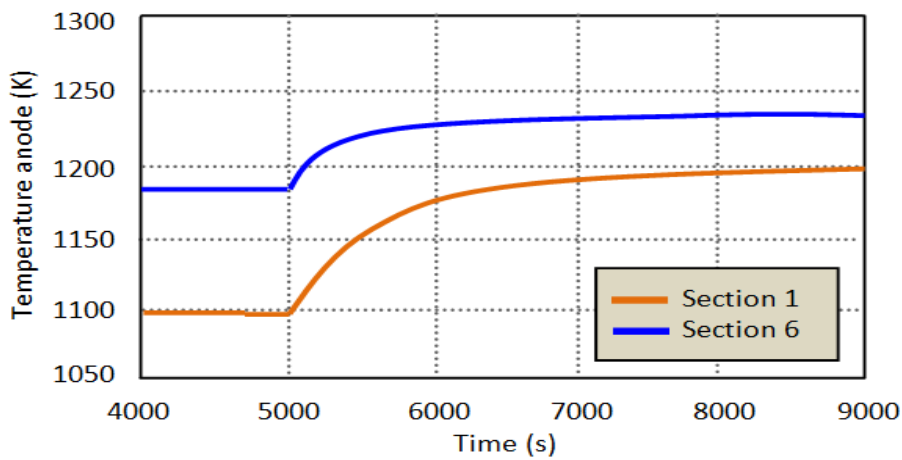Figure 10. Current in section 1 and 6 during load increase

Figure 11. Temperature in section 1 and 6 during load increase

Figure (12) shows the voltage current density plot for a single cell. It is assumed that the reformers are placed in-between the fuel cells and receive heat from the whole length of the cells. The reformer consists of a supply tube transporting the fuel internally from the bottom of the stack to the top allowing counter flow between the anode gas and the reformer gas. The exchange of heat between the supply tube and the outer tube is not included in the model.
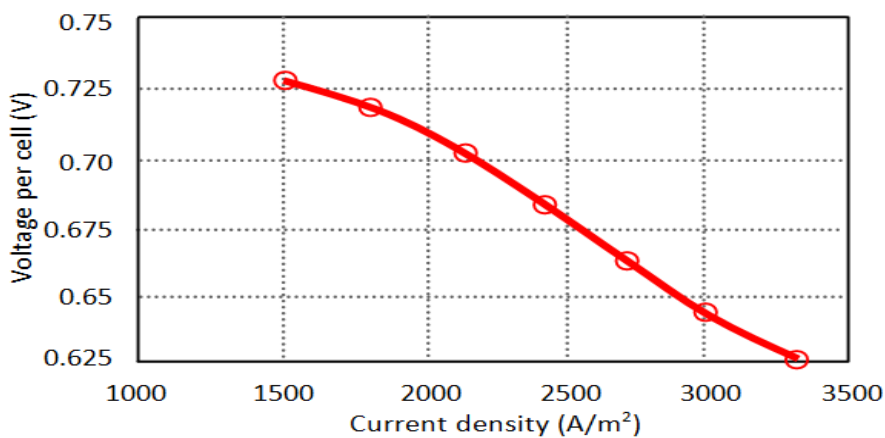

Figure 12. Voltage-current density plot for a single cell

5. CONCLUSIONS

Bond graphs were identified as a good tool for the multi-domain nature of fuel cell modelling. Pseudo-bond graphs were chosen to model thermofluid properties while true bond graphs were the choice for electrochemical and electrical domains. A new R-field was developed enabling a straight forward conversion between the thermofluid and electrochemical domains.

The bond graph tool strongly supported the model implementation process when evaluating different ways of representing the electrochemical losses. The resulting models were of complete integral causality, lending themselves to computationally efficient system simulations.

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