Dynamic Behavioral Circuit Model of PEM Fuel Cell

1 Introduction

The objective of this paper is to develop a dynamical behavior of a fuel proton exchange membrane (PEM) fuel cell. Most of the literature is dedicated to characterize the fuel cell while operating in steady state [1] [2]. However, most of the applications involve the need to study the response of the fuel cell when the electrical load changes. In general, the electrical load time constants are much smaller than the ones involved in a fuel cell, mainly related to chemical processes and mechanical devices such as pumps used to drive the flow of reactants in the fuel cell. Even though there is a significant number of papers dedicated to study the dynamic behavior of a fuel cell and to develop a mathematical model [3], [4], [5], [6], few of them develop a behavioral circuit model [7], [8], [9].

In order to develop a dynamic behavioral circuit model for PEM fuel cells, this paper presents the basic equations involved in generating an electrical output in a fuel cell. Special interest is place in the equations that model the water management and the reactants flow and pressure regulation. These are differential equations and are the ones that determine the dynamic response of the fuel cell during transients. Then, these equations are used to develop an electrical circuit model of the fuel cell. Finally, the fuel cell circuit model is implemented using Dymola software package.

2 Motivation

There are several ways of simulating a system. One way is using mathematical models. Even though these models are useful for scientist they do not provide a direct indication of the process itself and sometimes they are very complicated. Another disadvantage is that a simulation takes a long time to be completed. A more suitable option for engineers is to use behavioral models. In this approach the objective is to represent the result of the physical process rather than the process itself. In addition, since the output of a fuel cell is electrical power, it is more convenient to develop an electrical circuit model. In this way, a system engineer can use the model to simulate the interaction between the fuel cell and its electrical load. Since the model is based on the

dynamic behavior of the system, it can be used to study the system in both steady state and during transients. With a steady state analysis am engineer can optimize the design of the system, while with the transient analysis, the engineer can evaluate the stability of the system in several conditions.

3 Fuel Cell Model

The objective is to model a fuel cell such as the one in Figure 1. The output voltage of the fuel cell is given by:

$$E_c = E_r - v_{act} - v_{ohm} - v_{conc} \tag{1}$$

where E_c is the fuel cell output voltage, E_r is the reverse potential for the cell, v_{act} is the activation potential, v_{ohm} is the voltage drop due to ohmic losses and v_{conc} is the concentration overvoltage.

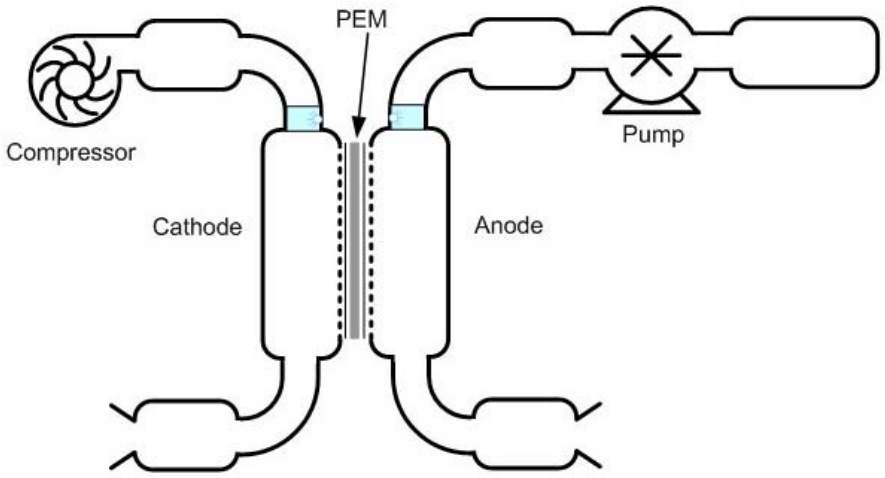

Figure 1 Fuel cell scheme.

The reverse potential or open circuit voltage of the cell when the result of the reaction is liquid water is

$$E_r = \frac{\Delta G}{2F} + \frac{\Delta S}{2F}(T - T_0) + \frac{RT}{2F}\left(\ln(p_{H_2 a}) + \frac{1}{2}\ln(p_{O_2 c})\right) \tag{2}$$

where ΔG in kJ/mol is Gibbs energy in kJ/mol, ΔS is entropy, F is Faraday's constant (96485 C/mol), T is the fuel cell temperature in Kelvins, T_0 is the ambient temperature in

Kelvins (298.15 K), R is the molar gas constant (8.3145 kJ/mol/K), p_{H2a} is the partial pressure of Hydrogen at the cathode, and p_{O2c} is the partial pressure of Oxygen at the anode. For PEM fuel cells and using standard values for Gibbs energy and entropy, Equation (2) can be reduced to

$$E_r = 1.229 + 0.85 \cdot 10^{-3}(T - 298.15) + 4.3085 \cdot 10^{-5} T\left(\ln(p_{H_2a}) + \frac{1}{2}\ln(p_{O_2c}) \right) \quad (3)$$

The activation voltage v_{act} is given by Tafel equation:

$$v_{act} = \frac{RT}{n\beta F \log e} \log\left(\frac{i}{i_0} \right) \quad (4)$$

where i is the cell current, i_0 is the exchange current for oxygen reaction, β is the transfer coefficient (usually 0.5) and n is another coefficient that depends on the reaction. For oxygen reaction is 2. Hence,

$$v_{act} = 0.069 \log\left(\frac{i}{i_0} \right) \quad (5)$$

The voltage drop due to ohmic losses is given by the well known Ohm's law:

$$v_{ohm} = iR_{ohm} \quad (6)$$

where R_{ohm} is the electrical resistance of the cell and that can be estimated based on the dimensions and conductivity of the membrane, the two catalyst layers and the electrical contact to the output leads.

The concentration voltage v_{conc} appears as a result of the change in concentration of the reactants as they are consumed in the reaction. This voltage is [5]

$$v_{conc} = i\left(c_2 \frac{i}{i_{\max}} \right)^{c_3} \quad (7)$$

where c_2, c_3 and i_{max} are constants.

Equations (5) and (7) have some relation with Equation (6), since all of the voltage drops in these equations are functions of the circulating current. The difference is that while in Equation (6) the relationship between voltage and current is lineal, in Equations (5) and (6) the relationship is not lineal. Thus, the voltage drop v_{conc} and v_{act} can be represented in the circuit model by variable resistances that depend on the current flowing through them. Hence,

$$v_{act} = R_{act}(i)i \tag{8}$$

where,

$$R_{act}(i) = \frac{0.069}{i}\log\left(\frac{i}{i_0}\right) \tag{9}$$

and

$$v_{conc} = R_{conc}(i)i \tag{10}$$

where

$$R_{conc}(i) = \left(c_2 \frac{i}{i_{\max}}\right)^{c_3} \tag{11}$$

Equation (3) describes that the open circuit voltage is, actually, the superposition of three voltages: one that it does not depend on any other parameter, one that depends on the cell temperature, and one that depends on the cell temperature and on the partial pressures. This last voltage can also be divided in two voltages: one that is related with the cathode and the other one related with the anode. Hence,

$$E_r = E_0 + E_T(T) + E_c(p_{H2a}) + E_a(p_{O2c}) \tag{12}$$

The model, however, is still incomplete. The partial pressures of the Hydrogen and Oxygen need to still be determined so that E_r can be calculated in Equation (12). In this equation is where the dynamic nature of the model appears. From [7], and based on the Ideal Gases Law, the partial pressures in the anode and the cathode are:

$$\frac{dp_{H_2a}}{dt} = \frac{RT}{V_a}\left(Q_{H_2a} - (\rho_{H_2} U_a A)_{out} - \frac{i}{2F}\right) \tag{13}$$

$$\frac{dp_{O_2c}}{dt} = \frac{RT}{V_c}\left(Q_{O_2c} - (\rho_{O_2} U_c A)_{out} - \frac{i}{4F}\right) \tag{14}$$

where V_a and V_c are the volume of the anode and cathode, respectively, Q_{H2a} and Q_{O2c} are the flow rates of Hydrogen and Oxygen entering the anode and cathode, respectively, measured in gr.mol/sec., ρ_{H2} is the density of Hydrogen measured in gr.mol/m^3, ρ_{O2} is the density of Hydrogen measured in gr.mol/m^3, U_a is the velocity of the reactants leaving the anode and measured in m/sec, U_c is the velocity of the reactants leaving the anode and measured in m/sec, and A is the channel cross sectional area measured in m^2.

The flow rate entering the cathode and the anode is equal to the respective flow rate leaving the humidifiers. Hence,

$$Q_{H_2a} = Q_{H_2out,h} \quad \text{and} \quad Q_{O_2c} = Q_{O_2out,h} \tag{15}$$

and the dynamic equation of the behavior of the humidifiers is given by

$$\frac{dp_{H_2h}}{dt} = \frac{RT}{V_h}\left(Q_{inH_2h} - Q_{outH_2h}\right) \tag{16}$$

$$\frac{dp_{O_2h}}{dt} = \frac{RT}{V_h}\left(Q_{inO_2h} - Q_{outO_2h}\right) \tag{17}$$

where V_h is the volume of the humidifiers that are considered identical.

Equations (13), (14), (16) and (17) are dynamic equations. Electrically, they can be represented as a resistance and capacitance circuit where the pressure represents the capacitor voltage, the ratio RT/V_h represents the capacitance and the flow rates represent currents [7]. In equations (16) and (17) the flow rates entering the humidifier act as a current source whose output depends on the speed of the compressor (in the case of the Oxygen) or the pump (in the case of the Hydrogen) that control the flow of reactants into the cell. The equation that describes the pump or the compressor is also dynamic ones

$$T_c = J_c \frac{d\omega_c}{dt} = T_{mc} - K_c\omega_c^2 \tag{18}$$

and

$$T_p = J_p \frac{d\omega_p}{dt} = T_{mp} - K_p\omega_p^2 \tag{19}$$

where T_c and T_p is the net torque in the compressor and the pump, respectively, J_c and J_p is the moment of inertia of the compressor and pump, T_{mc} and T_{mp} is the torque of the motor driving the compressor and the pump, respectively, ω_c and ω_p are the angular speeds of the compressor and pump, respectively and K_c and K_p are constants.

The angular speed of the pump or the compressor is related with the flow rate as described in the following equations:

$$Q_{inH_2h} = \rho_{H_2} A U_c = \rho_{H_2} A r_p \omega_p \tag{20}$$

and

$$Q_{inO_2h} = \rho_{O_2} A U_a = \rho_{O_2} A r_c \omega_c \tag{21}$$

where r_p and r_c are the radius of the rotating part of the pump and the compressor, respectively. As a result of Equations (18) – (21), any command trying to achieve a change in the flow rate will not achieve the goal immediately because the inertia of the pump and compressor will introduce a transient evolution lasting a time depending on J until the desired steady state level is reached.

4 Circuit Simulations

Although the previous section serves to describe the behavior of a fuel cell in great detail, from a simulation perspective is not practical. Figure 2 shows the complete simulation physical model of just the fuel cell stack, without including the pump and compressor models. It clearly shows the complexity of the model. The effect of this complexity is very slow and impractical simulations. Since the objective of this paper is to provide with a behavioral model than it can represent the dynamic behavior of the fuel cell system in a quick and simple way, then the physical system shown in Figure 2 needs to be simplified.

To simplify the model we can first assume that there are no leaks in between the pump or compressor and the output of the humidifier and that the same flow that exist the pump or the compressor enters the anode or cathode. That is, $QH_2a = Q_{inH_2h}$ and $Q_{O_2c} = Qi_{nO_2h}$. We can further assume that all the Hydrogen that enters the anode and all the Oxygen that enters the cathode reacts, leaving no Hydrogen or Oxygen leaving through the exhausts. Thus, Equations (13) through (17) are reduced to:

$$\frac{dp_{H_2a}}{dt} = \frac{RT}{V_a}\left(Q_{inH_2h} - (\rho_{H_2} U_a A)_{out} - \frac{i}{2F}\right) \tag{22}$$

$$\frac{dp_{O_2c}}{dt} = \frac{RT}{V_c}\left(Q_{inO_2h} - (\rho_{O_2} U_c A)_{out} - \frac{i}{4F}\right) \tag{23}$$

But the behavior of the system can be further simplified by realizing that the time constants of the pump and compressor, are much larger than the time constant of the cathode and anode. While the time constant of the first two is dominated by J and it is in the order of seconds, the time constant of the last two is in the order of nanoseconds. Hence, the transient behavior is heavily dominated by the dynamic behavior of the pump and the compressor and Equations (22) and (23) can be replaced by

$$\frac{dp_{H_2a}}{dt} = \frac{1}{\tau}\left(p_{H_2a} - p_0\right) \tag{24}$$

$$\frac{dp_{O_2c}}{dt} = \frac{1}{\tau}\left(p_{O_2c} - p_0\right) \tag{25}$$

where τ is the pump and compressor time constant. These are the basic dynamic equations that govern the behavior of the fuel cell.

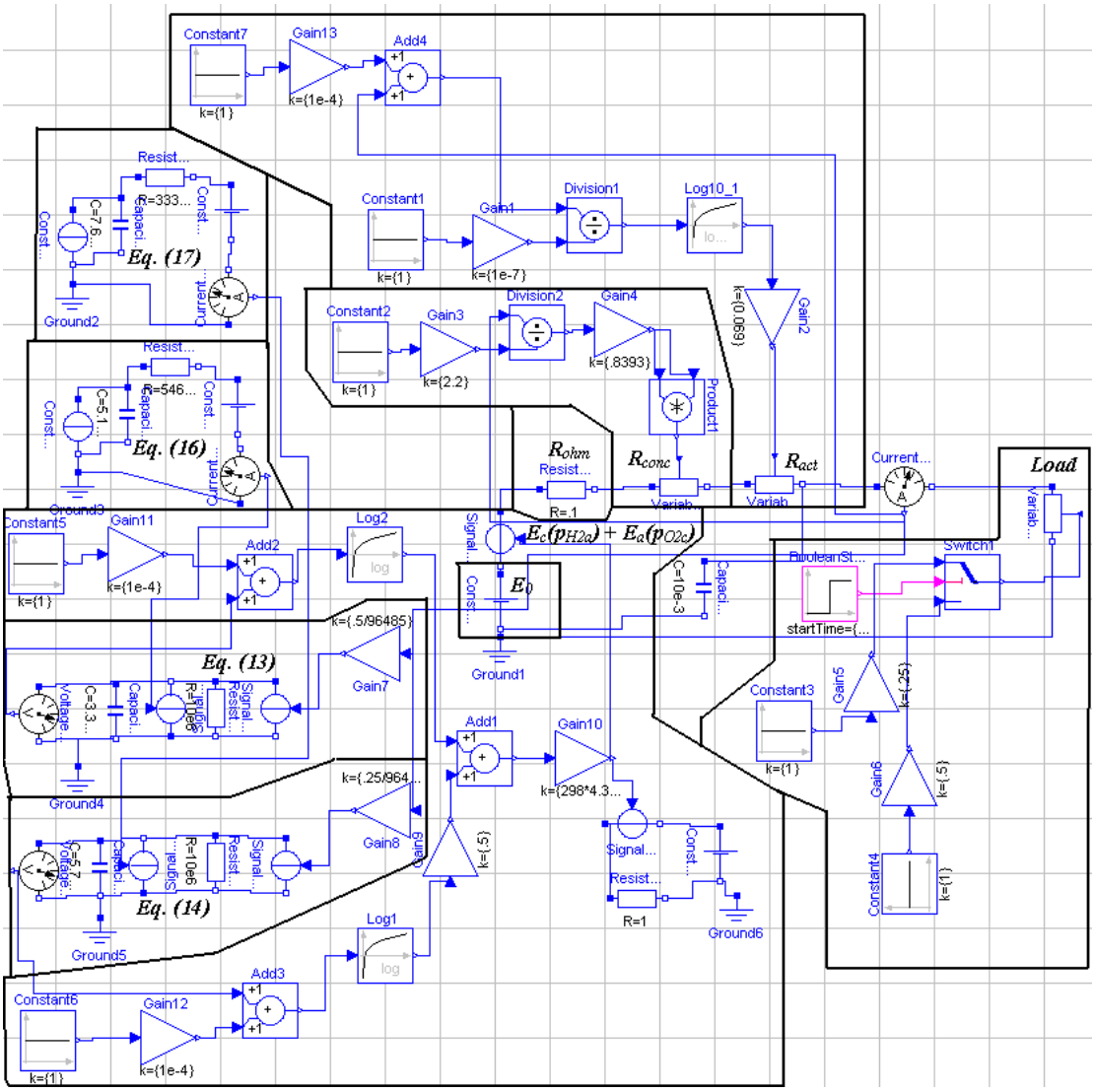

Figure 2 Complete fuel cell physical model

Having obtained the desired behavioral model we can simulate the fuel cell in a typical application to verify this model. Typically, the fuel cell is used in applications

where the fuel cell is considered to be an ideal voltage source. To achieve this behavior the pump and compressor are controlled so that the output of the fuel cell has a constant voltage regardless of the load. By controlling the partial pressured, the third term of Equation (3) can be adjusted to achieve the voltage target. If we assume that the fuel cell operates at ambient temperature the second term of Equation (3) vanishes. I will also assume that the fuel cell has an area of 1 cm^2. Other parameters necessary to model the fuel cell can be obtained from [5]. These are:

$i_0 = 1\ 10^{-5}$ A cm^{-2}

$c_2 = 0.8393$

$c_3 = 2$

$i_{max} = 2.2$ A cm^{-2}

$p_0 = 1$ atm

Figure 3 shows the new simulation model as implemented with Dymola. The feedback loop on the output voltage generates a control signal equal to *ln(p)* that modifies a variable voltage source that represents the last term of Equation (3). To compensate for the dynamics of the control loop, a R-L circuit is introduced in the path of the control signal so that the final time constant is approximately 1 second.

Figure 4 shows the simulation results. As expected, when the load is changed after 5 seconds of operation, the current and the output power take approximately half a second to reach the new steady state value. The voltage also shows an interesting behavior: when the load changes the output voltage drops immediately to approximately half its desired value (0.25 V). This sudden drop is also observed in the output power.

5 Conclusions

With this paper I have achieved the objective of developing a dynamic behavioral model of a fuel cell. The model that I developed takes as a starting point some physical models previously developed by other authors [5] [7] and then I simplify them to achieve a simple and practical model. In this way the model that I have proposed is a valuable tool for engineering design and analysis.

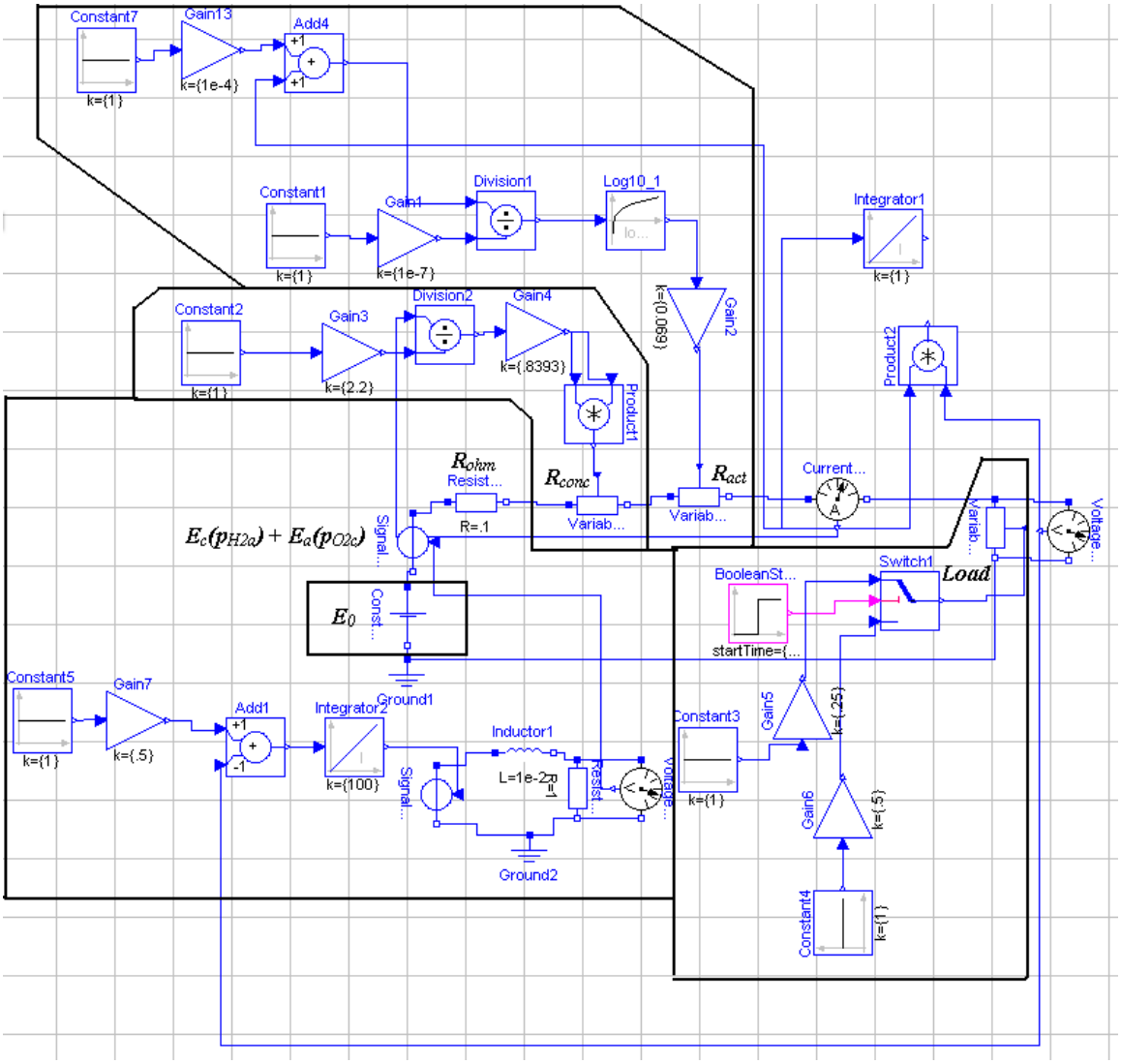

Figure 3 Fuel cell dynamic behavioral model

Even though the model is simpler than the one proposed by other authors, my model represents the dynamic behavior of a PEM fuel cell accurately. The simulation shows that the output current of the fuel cell varies slowly when the load changes, with a time constant in the order of a second. The simulation also shows the typical sudden voltage drop when the load increases that it is also well documented in literature [5]. This behavior creates a significant engineering problem in system where a fast dynamic response and a regulated constant voltage is needed, such as in automobiles traction and in stationary applications to power telecommunications and data centers. The solution to this problem is to add batteries or some other energy storage device (ultracapacitors or

fly-wheels) at the fuel cell output. However, these energy storage devices are expensive and bulky so better solutions to this problem are still being sought and constitutes a very important research field in electrical engineering.

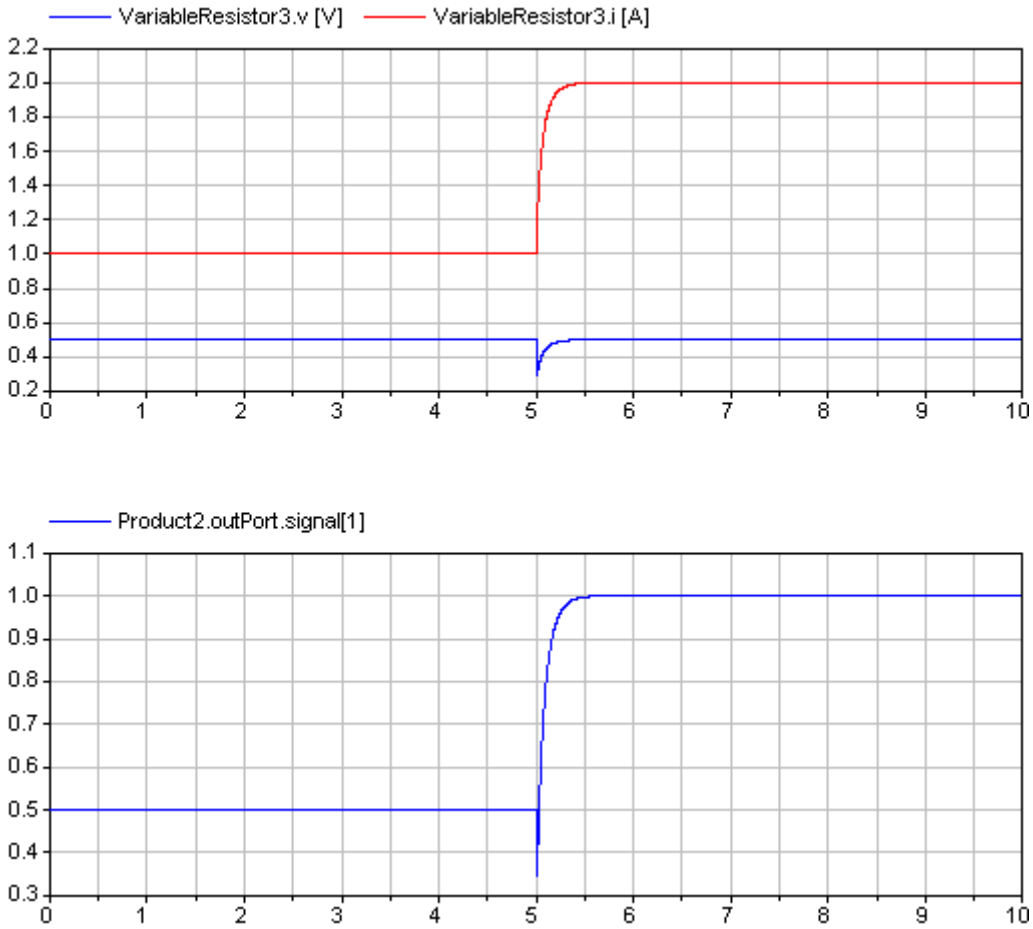

Figure 4. Simulation results. **Top Red**: Current. **Top Blue**: Voltage. **Bottom**: output power

6 References

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