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Simulation Models of Fuel Cell Systems

Chiara Boccaletti, Gerardo Duni, Gianluca Fabbri, Ezio Santini

Abstract—The research activity aimed to analyse and model fuel cell systems for stationary applications. In particular, PEM and SOFC models have been developed and set up in the Matlab-Simulink® environment. In the paper, the steady state and dynamical operation of PEM and SOFC technologies have been analysed, and their main characteristics have been compared, e.g. the response to the air and hydrogen flow rate and pressure regulation.

Index Terms— PEM, SOFC, Fuel Cells, Distributed Power Generation, Stand Alone Power Systems, Stationary Power Generation, Modelling.

I. INTRODUCTION

IN the last years, an interest toward Fuel Cell (FC) studies has grown, as FCs are a clean and efficient source of electricity, and have a wide range of transportation and stationary applications.

FCs are electrochemical devices that convert the chemical energy of a gaseous fuel directly into electricity and are widely regarded as a potential alternative stationary power source [1]. They complement heat engines and reduce the dependence on fossil fuels and thus have significant environmental implications. For instance, SOFCs are expected to be about 50-60 % efficient in converting fuel to electricity. In cogeneration applications overall efficiencies can be as high as 85 %. Owing to their attractive characteristics, FCs are recognized as one of the most promising technologies to meet the future power generation requirements and likely to be widely used for the stationary production of electric energy.

Among the several types of fuel cells, classified by the type of electrolyte material being used, the Proton Exchange Membrane (PEM) FC and the Solid Oxide Fuel Cell (SOFC) are considered in this paper for distributed power generation applications. A general scheme of a FC system for stationary applications is shown in Fig. 1, where the FC is coupled with a steam reformer for the production of hydrogen from hydrocarbons, and directly fed with hydrogen. PEM fuel cells in integrated systems with steam-reformer, and SOFC with internal reformer can be used in co-generation units for the production of electric energy and heat; in that way following the guidelines of the Kyoto Protocol. However, an improvement of the global (fuel-to-electricity) efficiencies and of the average lifetime of the components is needed. Moreover, a substantial reduction of

the investment and maintenance costs has to be achieved, as well as an optimization of their dynamic behaviour.

Because of their complexity, the development of FC systems involves several technical problems. There are still many features to be improved, like efficiency, reliability, durability, power density and costs. To compete with existing internal combustion engines, however, fuel cell systems should operate at similar levels of performance. An efficient fuel cell system power response depends on the air and hydrogen feed, flow and pressure regulation, and heat and water management. As current is instantaneously drawn from the load source connected to the fuel cell stack, heat and water are generated, whereas oxygen is depleted. During this transient, the fuel cell stack breathing control system is required to maintain proper temperature, membrane hydration for the PEM, and partial pressure of the reactants across the electrolyte to avoid detrimental degradation of the stack voltage, and thus efficiency reduction. These critical fuel cell parameters can be controlled for a wide range of currents, and thus power, by a series of actuators such as valves, pumps, compressor motors, fan motors, humidifiers and condensers.

Model-based dynamic analysis and control design give insight into the subsystem interactions and control design limitations. They also provide guidelines for sensors selection and control coordination between subsystems. Creating a control oriented dynamic model of the overall system is an essential first step not only for understanding the system behaviour but also for the development and design of the control methodologies.

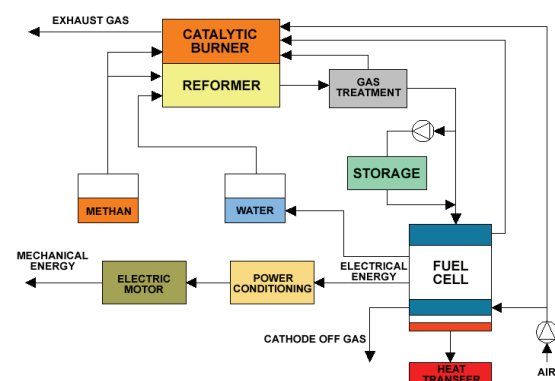


Fig. 1. General scheme of a fuel cell system for stationary applications

The major issues are the optimisation of the components, i.e. gas treatment unit, reformer, heat exchangers, blowers, valves and control systems, keeping the requirements of the particular FC into account and considering the interactions among the integrated components. An FC system for heat and power supply performs a complex process, therefore a suitable control system is required. The aim of this work was to design and implement mathematical models and a

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general controller for the whole FC system. By means of this model it is possible to develop, verify and validate the controller application, even if the actual fuel cell system is not available for testing during the development phase.

II. PEM vs SOFC

This study offers a way to compare PEM and SOFC behaviours and to foresee the response of an integrated FC system to the air and hydrogen flow rate and pressure regulation. Fuel cells have been lately receiving a lot of attention due to their potential in becoming a new energy source with a large range of applications. The benefits of energy production from fuel cells are the high efficiency and their environmentally friendly by-products. In FCs a chemical reaction takes place to convert hydrogen and oxygen into water, releasing electrons (current) in the process. In other words, the hydrogen fuel is burnt in a simple reaction to produce water and an electric current.

A typical fuel cell consists of two electrodes (anode and cathode) where the reactions take place. The electrodes are also the mediums that the current flows between. Sandwiched between the electrodes is an electrolyte material which the ions flow through to keep the reactions continuous. There are several types of fuel cells being studied at present. These include alkaline, proton exchange membrane, phosphoric acid, molten carbonate, and solid oxide. They differ in electrode and electrolyte materials, chemical reactions, catalysts, and operating temperatures and pressures. Fuel cells can be incorporated with other components to create high efficiency industrial power plants. These power plants usually consist of a pump or blower to circulate the working fluids through the fuel cell, a reformer to convert the fuel into hydrogen, pressure regulators, and power conditioners. Typically, the fuel cell takes up a small percentage of the overall size of a fuel cell power plant. Most fuel cells do not use straight hydrogen as fuel. Therefore, they must incorporate a reformer to convert the fuel being used into hydrogen. Fuels that can be reformed are methane, ammonia, methanol, ethanol, and gasoline. The fuel storage is a major issue in fuel cell power plant design.

PEM fuel cells operate at low temperatures (less than 100 degrees Celsius), making them temperature-compatible with many of today's automotive systems and also allowing faster startups. However, due to a relatively small temperature gradient to the ambient atmosphere, the produced waste heat is low-grade and requires large heat exchangers.

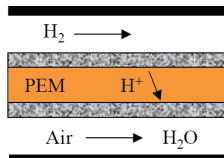
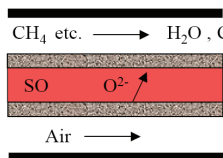
SOFCs operate at extremely high temperatures - of the order of 700 to 1000 degrees Celsius. As a result, they can tolerate relatively impure fuels, such as those obtained from the gasification of coal. Waste heat is high-grade, allowing smaller heat exchangers and the possibility for co-generation to produce additional power.

The power densities of both PEM and SOFC systems are of the order of some 500 mW/cm² under typical operating conditions. The peak power densities under idealized conditions have been reported to be greater than 1000 mW/cm². The reformer system for SOFCs is less complex than PEM reformers. This is because SOFC can use carbon monoxide along with hydrogen as fuel. In addition, SOFCs show a high tolerance to fuel impurities such as natural gas.

Also, the operating temperature of the reformer and the stack are compatible in SOFC systems, whereas in PEM systems the stack operating temperature is about 80–100 °C and that of the reformer is about 900–1000 °C. The water management is not a concern in SOFC because the electrolyte is solid-state and does not require hydration. The by-product is steam rather than liquid water, which has to be drained away in PEM systems. SOFCs do not need precious metal catalysts. The relatively simple design (because of the solid electrolyte and fuel versatility), combined with the significant time required to reach the operating temperature and to respond to changes in electricity demand, make SOFCs suitable for large to very large stationary power applications. The startup time for the SOFC is of the order of 20 to 30 minutes, whereas the PEM system could be started in less than a minute. Hence, SOFCs are not suitable for automotive applications. Moreover, the startup time is not a major issue in stationary power generation units. In the following Table I some of the main features and differences of the two types of cells are shown.

TABLE I. Main differences between PEM and SOFC.

<i>PEM vs. SOFC</i>	
<i>PEM</i>	<i>SOFC</i>
<i>Polymer electrolyte membrane</i>	<i>Solid Oxide</i>
<i>Polymer electrolyte</i>	<i>Ceramic electrolyte</i>
<i>Proton-conduction</i>	<i>Oxide-ion conduction</i>
<i>Low T (~100 °C)</i>	<i>High T (~700 °C)</i>
<i>Requires H₂ fuel</i>	<i>Can use hydrocarbon fuel</i>
<i>CO is a poison</i>	<i>CO is a fuel</i>
<i>No reforming</i>	<i>Can use reforming</i>
<i>Precious-metal catalysts</i>	<i>Inexpensive catalysts</i>
<i>Requires cooling</i>	<i>Requires heating</i>
<i>Antifreeze required</i>	<i>No antifreeze</i>
<i>Small devices, "mature"</i>	<i>Larger, "5 yrs behind"</i>

In this paper modular dynamic models of the main components of a fuel cell system will be given. The proposed mathematical models were built in the Matlab-Simulink[®] environment. In Fig. 2 the main elements of the system are shown. These are:

1. Fuel cell stack voltage model
2. Heat Exchanger model
3. Hydration model
4. Anode and Cathode flow model
5. Compressor model
6. Supply and return manifolds

In the following paragraphs the model of the fuel cell stack voltage will be described together with the control system. For the description of the other components see [2]-[4]. Two configurations will be then developed and simulated using Matlab-Simulink[®] software and basic controls will be applied to study the behaviour of PEM and SOFC systems.

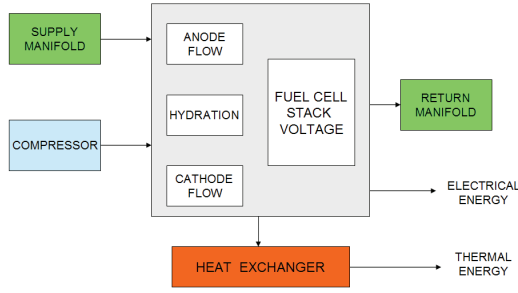


Fig. 2. Main elements of the proposed model.

III. FUEL CELL MODEL

The FC model takes a model developed for dynamic power simulation of FCs available in the literature [5] as a starting point. The assumptions for the model are as follows:

- The gases are ideal
- The fuel cell is fed with hydrogen and air
- The electrode channels are small enough that the pressure drop across them is negligible
- The ratio of pressures between the inside and outside of the electrode channels is large enough to assume choked flow
- The fuel cell temperature is stable
- The Nerst equation applies
- The losses are as follows: Ohmic, Activation, Mass Transport.

The model development begins with the flow equation for choked flow:

$$\frac{\dot{m}_{fc}}{P_u} = K\sqrt{M} \quad (1)$$

where:

- \dot{m}_{fc} : mass flow rate
- K : valve constant
- P_u : upstream pressure (inside the electrode channels)
- M : fluid molar mass
- $\dot{m}_{fc,H_2,reacted}$: amount of hydrogen that reacts with the oxygen ions
- $\dot{m}_{fc,H_2,in}$: amount of hydrogen entering the anode

A utilization factor (U_f) is defined as the ratio of the amount of hydrogen that reacts with the oxygen to the amount of hydrogen entering the anode.

$$U_f = \frac{\dot{m}_{fc,H_2,reacted}}{\dot{m}_{fc,H_2,in}} \quad (2)$$

By considering that the molar flow of any gas through the valve is proportional to its partial pressure, the following equations are derived

$$\frac{q_{H_2}}{p_{H_2}} = \frac{K_{an}}{\sqrt{M_{H_2}}} = K_{H_2}, \quad \frac{q_{H_2O}}{p_{H_2O}} = \frac{K_{an}}{\sqrt{M_{H_2O}}} = K_{H_2O} \quad (3)$$

where

q_{H_2} , q_{H_2O} : molar flow rates of hydrogen and water, respectively

p_{H_2} , p_{H_2O} : partial pressures of hydrogen and water, respectively

K_{an} : valve constant of the anode

K_{H_2} , K_{H_2O} : valve molar constants for hydrogen and water, respectively

By substituting equations (2) and (3), equation (1) can be written as

$$\frac{\dot{m}_{fc}}{p_{an}} = K_{an} \left[(1 - U_f) \sqrt{M_{H_2}} + U_f \sqrt{M_{H_2O}} \right] \quad (4)$$

being p_{an} the pressure inside the anode channel.

The ideal gas law will be used to find the partial pressures of the gases flowing through the electrodes. This formula will be applied to all the gases. Only the expression for hydrogen is derived here

$$p_{H_2} V_{an} = n_{H_2} RT \quad (5)$$

where

T : temperature

V_{an} : volume of the anode channel

n_{H_2} : moles of hydrogen in the channel

R : ideal gas constant

By isolating the pressure and taking the first time derivative, one has

$$\frac{dp_{H_2}}{dt} = \frac{RTq_{H_2}}{V_{an}} \quad (6)$$

The hydrogen flow can be subdivided into three parts, therefore equation (6) can be rewritten as follows

$$\frac{dp_{H_2}}{dt} = \frac{RT}{V_{an}} (q_{H_2}^{in} - q_{H_2}^{out} - q_{H_2}^r) \quad (7)$$

where

$q_{H_2}^{in}$: molar flow rate of hydrogen into the channel

$q_{H_2}^{out}$: molar flow rate of hydrogen out of the channel

$q_{H_2}^r$: molar flow rate of hydrogen reacting in the channel

According to the electrochemical relationships, the amount of hydrogen that reacts can be calculated by

$$q_{H_2}^r = \frac{N_0 I}{2F} = 2K_r I \quad (8)$$

where

N_0 : number of cells in the stack series

F : Faraday's constant

I : stack current

K_r : modeling constant

By substituting equations (8) and (3) into equation (6), applying the Laplace transform, and isolating the partial pressure term, the following equation can be derived

$$p_{H_2} = \frac{1/K_{H_2}}{1 + \tau_{H_2}s} (q_{H_2}^{in} - 2K_r I) \quad (9)$$

where

τ_{H_2} : the system pole associated with the hydrogen flow.

The stack output voltage is described by the Nerst equation [6]. The $-rI$ term is the ohmic loss. This is the loss due to the resistance of the electrodes and to the resistance of the flow of O_2 ions through the electrolyte. It yields

$$V = N_0 \left[E_0 + \frac{RT}{2F} \left(\ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right) \right] - rI \quad (9)$$

where:

V: fuel cell output voltage

E_0 : open cell voltage (based on the Gibbs free energy)

R: ohmic losses of the stack

The activation loss is caused by the sluggishness of the reactions at the electrode surfaces. A portion of the voltage is lost in driving the chemical reaction that moves the electrons to the electrodes. A way to account for these losses is to use the Tafel equation [7]. This equation was derived by physical experimentation on various electrochemical reactions. It provides a relationship between the overvoltage at the surface of an electrode and the natural logarithm of the current density and can be used to calculate the activation voltage loss for the fuel cell [5]

$$\Delta V_{act} = -A \ln(i) \quad (11)$$

where

ΔV_{act} : activation voltage loss

A : slope of Tafel line (constant specific for SOFC)

i : current density (current/electrode area)

Mass transport losses are due to the difference in concentration of the fuel as it passes through the electrode. The concentration will be high when the fuel and air enter the electrodes, but as they travel through, they get used up in the reaction. This concentration affects the partial pressure of the reactants and has an effect on the voltage that portion of the electrode can produce. Unfortunately this loss cannot be calculated analytically with enough accuracy. Therefore, experimental results are used to estimate the loss. Following equation (12) has been developed on an experimental basis and is accepted as a good approximation of the mass transport losses [7].

$$\Delta V_{trans} = m \cdot e^{ni} \quad (12)$$

where

ΔV_{trans} : voltage loss due to mass transfer and concentration loss

m, n: constants derived from experiments (specific to SOFC and PEM)

Combining all the losses into equation (10), an equation for the overall voltage of a single FC can be obtained. In an actual FC power plant, multiple cells would be combined in series to provide the necessary voltage and current demand. The total stack voltage is

$$V = N_0 \left[E_0 + \frac{RT}{2F} \left(\ln \frac{p_{H_2} p_{O_2}^{0.5}}{p_{H_2O}} \right) \right] - rI - A \ln(i) + m e^{(ni)} \quad (13)$$

The total power generated by the FC (P_{FC}) is:

$$P_{FC} = N_0 V I \quad (14)$$

The complete FC Simulink scheme is shown in Fig. 3.

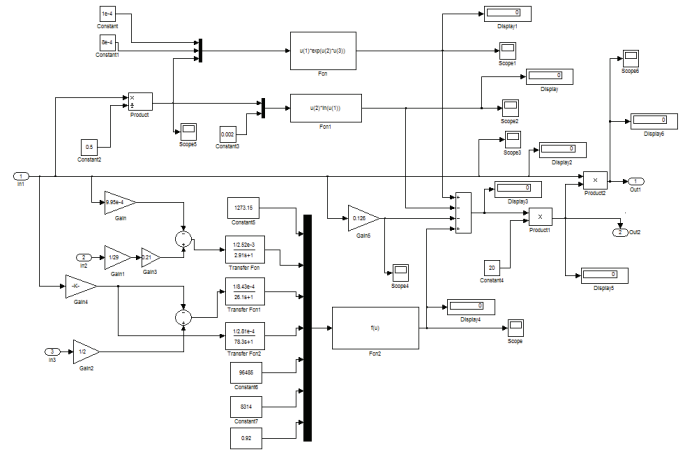


Fig. 3. Fuel cell Simulink scheme.

IV. HYDROGEN VALVE CONTROL

In the system considered in this study, hydrogen is supplied by a high-pressure tank and the flow rate is controlled by a valve. The inlet hydrogen flow is assumed to have 100% relative humidity. Due to the high-pressured storage, the hydrogen flow rate can be adjusted quickly. The goal of the hydrogen flow control is to minimize the pressure difference between anode and cathode. Using simple proportional control based on the pressure difference, the pressure in the anode (p_{an}) can quickly follow the changes in the cathode pressure. It is assumed that the hydrogen flow rate can be directly controlled by a fast valve based on the feedback of the pressure difference. The controller is in the form

$$W_{an,in} = K_1 (K_2 p_{sm} - p_{an}) \quad (15)$$

where $K_1=2.1$ (Kh/s/kPa) is the proportional gain and $K_2=0.94$ takes a nominal pressure drop between the supply manifold (subscript sm) and the cathode into account. By applying the hydrogen valve proportional control, the dynamics of the FC system are governed mainly by the air supply system dynamics. The two variables considered for the control performance are the concentration of the oxygen in the cathode and the FC system power. For certain stack currents, the stack voltage increases with increasing air flow rate to the stack because the cathode oxygen partial pressure increases. The excess amount of air flow provided to the stack is normally indicated by oxygen excess ratio λ_{O_2} ,

defined as the ratio of supplied oxygen to oxygen used up in the cathode, that is

$$\lambda_{O_2} = \frac{W_{O_2, in}}{W_{O_2, react}} \quad (16)$$

A high oxygen excess ratio, and therefore a high oxygen partial pressure, improves the FC power. The highest power is achieved at an oxygen excess ratio between 2 and 2.4, depending on the stack ratio.

V. SIMULATION OF A 75 kW PEM SYSTEM

First, the model has been used to simulate the behaviour of a direct-H₂ 75 kW PEM system. Owing to the low operating temperature, the dynamics of the stack temperature are considered to be relatively slow and as a result the stack temperature is a set-point to the reactant systems. A series of step changes in stack current is applied as input (Fig. 4). Various compressor motor input voltages give different levels of oxygen excess ratios.

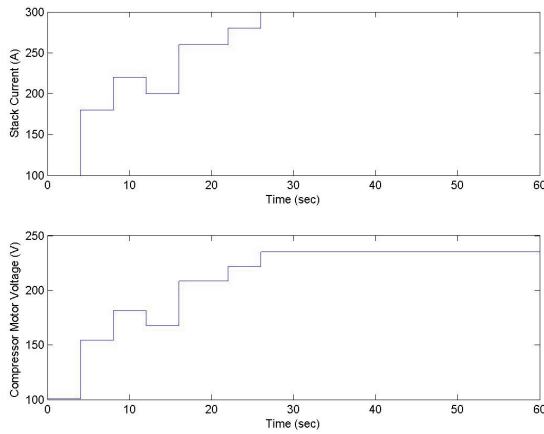


Fig. 4. Stack current (top) and compressor voltage vs time.

During a positive current step the oxygen excess ratio drops, as shown in Fig. 5, due to the depletion of oxygen. This causes in turn a significant drop in the stack voltage. The same figure shows the effect of operating at a higher λ_{O_2} than the optimum value (2÷2.4).

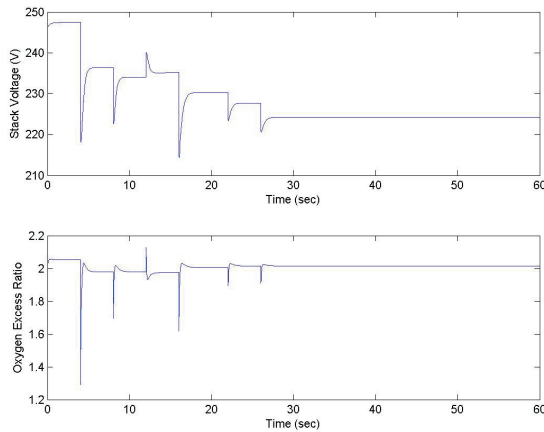


Fig. 5. Stack voltage (top) and oxygen excess ratio vs time.

Fig.6 shows the stack power with a simulation time of 60 seconds and a stack temperature of 80°C.

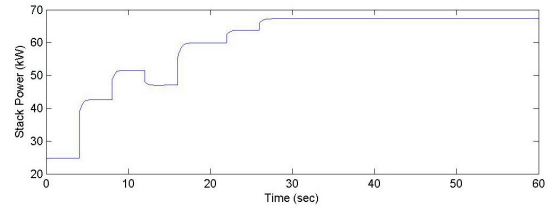


Fig. 6. Stack power @ 80 °C.

The results show that the model is capable of catching the effects of transient oxygen and hydrogen partial pressure on the fuel cell system and predicting a transient behaviour which is in good agreement with similar test reported in the literature.

VI. SIMULATION OF A 200 kW SOFC SYSTEM

Then, the model has been used to simulate and predict the behaviour of a 200 kW SOFC system. The model has been validated by means of an experimental prototype built by an Italian research company. Fig. 7 shows a picture of a prototype stack.

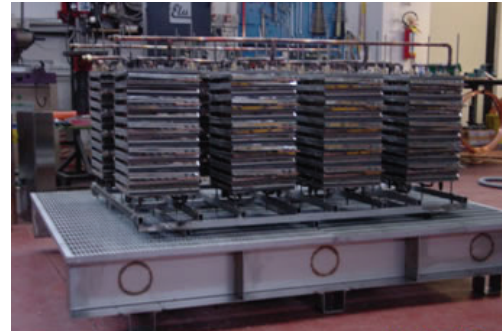


Fig. 7. SOFC prototype.

The model was run using parameters given by the company and summarized in Table II. Figures 8 and 9 show the voltage and power outputs of the model, respectively. The initial transients are due to the start-up of the model, the initial conditions of the transfer functions being zero. It can be seen that the fuel cell produces approximately 200 kW of power with a 300 A current demand at steady state. 20 fuel cells connected in series are modeled.

TABLE II. SOFC Simulation Parameters.

Symbol	Quantity
K_r	9.95 e-4
FC Temp	1273.15 K
Kmol/Kg air	1/29
Kmol/Kg H ₂	1/2
No	20
K_{H_2}	8.43e-4 kmol(atm s)
K_{H_2O}	281e-4 kmol(atm s)
K_{O_2}	2.52e-3 kmol(atm s)
τ_{H_2}	26.1 s
τ_{H_2O}	78.3 s
τ_{O_2}	2.91 s
r	0.126 ohm

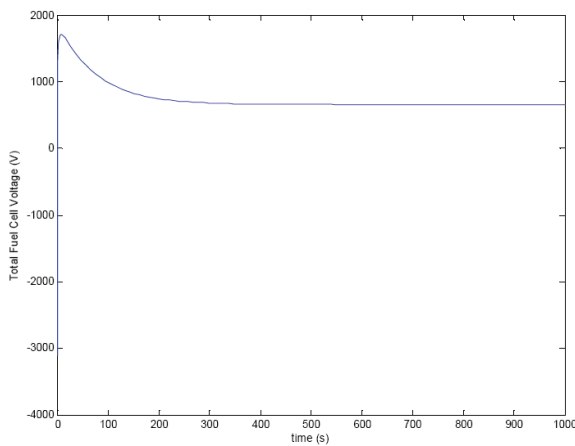


Fig. 8. Total FC output voltage.

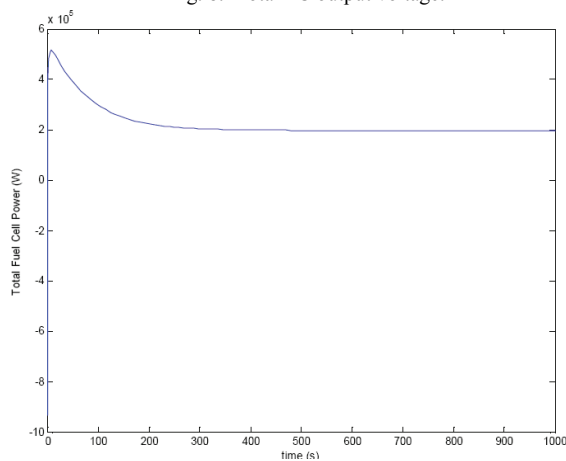


Fig. 9. Total FC power output.

A second simulation was run using a linear current ramp starting at 10 A with a slope of 1. Figure 10 shows the voltage response of the FC. Initially, the voltage is low until the current reaches a relatively high level. This is due to the transfer functions initial conditions of zero. The voltage reaches a peak just past 400 s after which it starts to drop. This is typical of FCs and has to do with the irreversibilities when the current reaches a certain level.

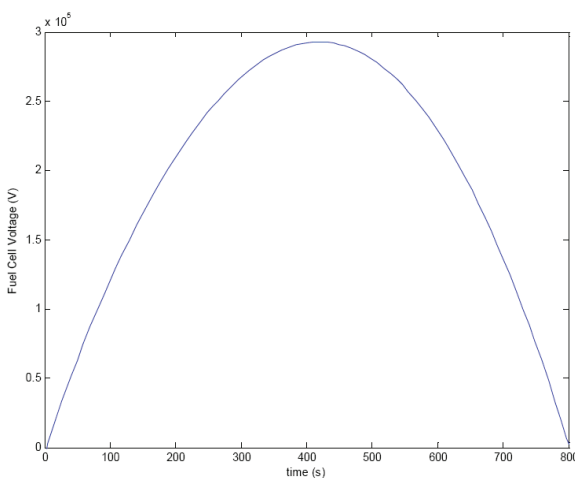


Fig. 10. Voltage response to a current ramp.

VII. CONCLUSIONS

The realized models can be used as a tool for the design optimization of fuel cells, cell stacks and fuel cell power systems. If the models are implemented into an integrated

framework, the synergies among multiple technologies may also be predicted. Using the models described in paragraph III, various simulations have been performed to find the optimal operation and control strategies of a PEM fuel cell plant and of a SOFC system in order to analyse the systems behaviour. Numerical results are provided. 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 obtainable from a single power source. The resulting system exhibits a synergism in which the combination of different technologies has far greater efficiency than the one that could be provided by each system operating alone. For instance, combining a fuel cell with a gas turbine increases the overall cycle efficiency while reducing per kilowatt emissions. In addition, the research activity is also going on to combine fuel cells with wind power and solar power generation for back-up power generation and energy storage. Getting higher efficiencies combined with low emissions, hybrid systems are likely to be the choice for the next generation of advanced power generation systems [8].

A hydrogen generation and distribution infrastructure based on renewable energy from wind, water, solar energy and fuel processor will help to reduce our dependency on fossil fuels. Thus, as a future development of the present work, it could be very useful to set up a flexible tool to model and simulate energy systems using H_2 as energy carrier and to simplify the task of evaluating design solutions for stand-alone and distributed generation applications. Such a tool would allow us to account for variations in energy source availability and to evaluate the technical feasibility of a large number of hybrid technology options such as

- SOFC - Gas turbine systems
- SOFC – Thermal-photovoltaic systems
- PEM FC - Solar power hybrid systems
- PEM FC - Wind power systems

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