Nonlinear Modelling of Fuel Cell Systems for Vehicles

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In this work a nonlinear dynamical model of a fuel cell stack is developed by means of artificial neural networks. The model presented is a black-box model, based on a set of easily measurable exogenous inputs like pressures and temperatures at the stack and is able to predict the output voltage of the fuel cell stack. The model obtained is being exploited as a component of complex control systems able to manage the energy flows between fuel cell stack, battery pack, auxiliary systems and electric engine in a zero-emission vehicle prototype.

 ${\bf Key \ words: \ nonlinear \ modelling, \ neural \ networks, \ fuel \ cell \ systems, \ automotive \ applications \ and \ applications \ applications \ application \$

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1 Introduction

More and more interest is devoted to the development of low pollution vehicles. In particular a lot of studies and implementations of fuel-cell-based vehicles are being developed. In its simplest form, a fuel-cell-based engine is fed with a stream of hydrogen, which reacts with air oxygen in a device called *fuel cell stack* [1, 2], producing electric energy which can be exploited by an electric engine.

The simplest fuel cell consists of two electrodes, separated by a polymeric membrane, in contact with an electrolyte, which is usually water. A catalyst, generally platinum, is usually placed on the interface surfaces. In a cell, the following reactions occur, for anode and cathode terminals, respectively:

$$2H_2 \longrightarrow 4H^+ + 4e^- \tag{1}$$

$$O_2 + 4e^- + 4H^+ \longrightarrow 2H_2O \tag{2}$$

It is well known that the power produced by a single fuel cell is too low to be directly supplied to an automotive system. Therefore, for effective applications, it is necessary to connect several cells in series to obtain a *stack* and surround it with auxiliary components, like pumps, valves, fuel storage systems, etc., which frequently make up a large proportion of the engineering of the whole Fuel Cell System (FCS). In particular, for automotive applications, the use of batteries in association with a fuel cell stack can reduce the overall cost of the system. This kind of configuration, called *battery hybrid* system, allows the fuel cell stack to work quite close to its maximum power at all times. When the power requirement is low, then the surplus electrical energy is stored in a rechargeable battery. On the other hand, in correspondence of peaks of power requirement, power provided by the stack is increased by energy stored in the batteries pack. In this way, the fuel cell stack has to be designed for average power requirement, leading to a less expensive system.

One of the main issues of the control activity in a hybrid FCS is the management of the power

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fluxes between the fuel cell stack, batteries pack, auxiliary systems and electric engine, according to the power requirement of the driver. The development of reliable models of fuel cell stacks is therefore of fundamental importance for both control and prediction purposes. To this aim, models must be simple enough, with good performance both in static and dynamic operational conditions, and based on simple, easily measurable inputs. So, macroscopic models able to describe the behaviour of the stack as a whole on the basis of simple exogenous inputs are strongly needed for control purposes rather than models describing the stack at cell-level based on electrochemical relationships.

In this work, a real fuel cell stack is modeled by means of artificial neural networks (ANN). Models are trained and tested with real data collected on an experimental setup. Different kinds of model are presented and results will be compared. The work is structured as follows. Next section will deal with the description of FCS systems for automotive applications. Section 3 will deal with neural-network-based modelling of the stack, by exploiting both the physical laws describing the stack, and data collected in an experimental setup. Finally, results are presented and commented in section 4, followed by our conclusions.

2 Fuel cell systems for automotive applications

A simplified scheme of a FCS for automotive applications is illustrated in Fig. 2.

As previously stated, a FCS consists of a generation system surrounded by auxiliary systems and control systems. The generation system consists of a stack of fuel cells, fed by hydrogen, which can be either stocked in a pressurised cylinder, or produced on board by a *reformer* [3]. The reformer, in its most common implementation, transforms methanol in hydrogen. Energy flux coming as output from the stack, after passing through an adequate converter, is divided



FIG. 1. A FCS for automotive applications

between the electrical engine, which provide locomotion power, and an energy storage system, which consists of a battery pack. Energy fluxes between stack, engine, and battery is regulated by a control system devoted to the conversion and storage apparatus. Other low-level controllers are devoted to the control of the stack and the reformer. Furthermore, all the controllers should be supervised by a high-level supervisor. For any control purpose, an accurate dynamical model of the stack is obviously needed.

A stack of fuel cell is an array of simple cells connected in series through bipolar plates. In each cell reactions (1) and (2) occur. As a consequence of the series connection, overall output voltage is the sum of the single cell output voltages, whereas the current remains the same in all the cells. A hydrogen stream, injected on the inlet of the stack, flows through the whole stack cells. The stack is also fed with air and water to let the reactions occur.

As a spatially extended system, the behaviour of the stack can be rigorously described by several Partial Differential Equations (PDEs). As an example, the membrane can be described by the following set of PDEs:

$$\nabla \cdot (i) = 0 \tag{3}$$

$$\nabla \cdot (N_{O_2}) = 0 \tag{4}$$

$$\nabla \cdot (N_{H_2}) = 0 \tag{5}$$

$$\nabla \cdot (V) = 0 \tag{6}$$

where *i* is the current density, N_{O_2} and N_{H_2} are the oxygen and hydrogen fluxes, respectively, and *V* is the water velocity.

Similar PDE sets describe anode and cathode gas diffusion, and anode and cathode catalyst evolution. The behaviour of the stack can be obviously modelled by solving all the PDE sets described above. Nevertheless, practical applications can hardly rely on such an approach for a twofold reason. Firstly, computational complexity would make a real time approach hard for on-board control purposes. Secondly, PDEs mentioned above manipulate physical quantities which are difficult to measure. Therefore, an alternative approach is needed.

The main idea underlying the approach is to realize a *black-box* model of the whole stack which manipulates measurable quantities and is computationally affordable. The dynamical model realised in this work include a set of inputs which has been selected by taking into account the *Nerst equation* [1], which is a static equation providing the output voltage of a single cell. Nerst equation comes in different forms. If the pressures of the reactants and products are in bar, and the water product is in the form of steam, then the equation is formalised as:

$$E = E^{0} + \frac{RT}{2F} \ln \left(\frac{P_{H_2} P_{O_2}^{\frac{1}{2}}}{P_{H_2O}} \right)$$
(7)

where:

- E^0 is the EMF at standard pressure;
- R is the 'universal' gas constant, 8.314 JK^{-1} mol⁻¹
- T is the temperature;
- $P_{H_2}, P_{O_2}, P_{H_2O}$ are the partial pressures of hydrogen, oxygen, and water steam, respectively.

The output voltage expressed by Nernst equation is subject to losses of different nature; in particular:

- Activation losses, caused by the slowness of the reaction taking place on the surface of the electrodes;
- *Fuel crossover* and *internal currents*, resulting from the waste of fuel passing through the electrolyte, and electron conduction through the electrolyte;
- *Ohmic losses* on electrodes, interconnections, and electrolyte;
- *Mass transport losses*, resulting from the change in concentration of the reactants at the surface of the electrodes as the fuel is used.



FIG. 2. Pre-processed learning data set for variable P_{H_2} .

3 Modelling the fuel cell stack

Taking into account the Nernst equation (7), a suitable set of inputs has been selected in order to build a black-box model. A first set of inputs which has been considered is the following:

- hydrogen pressure, P_{H_2} ;
- oxygen pressure, P_{O_2} ;
- water pressure, P_{H_2O} ;



FIG. 3. Pre-processed learning data set for variable P_{Air} .

• stack temperature, T.

The experimental setup perform several acquisitions, but not all the quantities mentioned above are available. Therefore, the following assumptions have been made and a new set of inputs has been built:

- hydrogen pressure P_{H_2} is directly available;
- oxygen pressure P_{O_2} is not directly available. As oxygen is provided to the stack as an air stream, air pressure in the stack P_{Air} is instead used;
- water pressure P_{H_2O} is assumed to be constant as water flows through the stack in liquid phase. Consequently, P_{H_2O} , is not considered as an input in the design of the dynamic black-box model.
- stack temperature T is not directly available; this is estimated through the temperature of the outlet stack water.

The aim of this work is to build a dynamical model able to predict the trend of the output voltage of the stack on the basis of the information cited above. It is worth to notice that all the quantities involved are easily and cheaply measurable with common acquisition systems.



FIG. 4. Pre-processed learning data set for variable T.



FIG. 5. Pre-processed learning data set for variable I.

The general form of a time-discrete nonlinear model able to predict the output voltage of the stack is the following:

$$V(k+1) = \mathbf{f}(P_{H_2}(k), \dots, P_{H_2}(k-l), P_{Air}(k), \dots, P_{Air}(k-m), T(k), \dots, T(k-n))$$
(8)



FIG. 6. Pre-processed learning data set for variablV.



FIG. 7. Modelling error.

where function \mathbf{f} is unknown and k is the discrete time index.

Nevertheless, the stack output voltage strongly depends on its load, which is the electric engine, whose characteristic change at a fast rate according to driver requirements and road condition.

The strategy adopted to obtain a reliable model is to consider the output current as a further input to the model, leading to the following



FIG. 8. Histogram of the modelling error.

equation:

$$V(k+1) = \mathbf{f}(P_{H_2}(k), \dots, P_{H_2}(k-l),$$

$$P_{Air}(k), \dots, P_{Air}(k-m), T(k), \dots, T(k-n),$$

$$I(k), \dots, I(k-o))$$
(9)

In this work, the unknown function \mathbf{f} is identified by means of Artificial Neural Networks [4], as will be described in the following. In particular, a Multi-Layer Perceptron (MLP) has been adopted.

A suitable set of experimental data has been collected in order to cover a large domain of operational conditions and build both a training and a checking data set. Data have been acquired at a sampling frequency of 10Hz and suitably filtered via a spectral analysis. In particular, air pressure needed a strong filtering action. The learning data set, consisting of about 48000 samples, in which variables have been already filtered and normalised, is reported in Figs. 3–6.

Several models with a different number of regression for each variable have been tested. An extensive trial-and-error phase has led to a model characterized by 3 regressions for each input and 30 neurons in the hidden layer. The network obtained has therefore 12 inputs, 30 hidden neu-

rons and 1 output. Figs.7–8 illustrate a comparison between actual and predicted output voltage, the prediction error performed by the model, and its histogram, respectively. The normalized MSE performed on the whole training set is $6.27 \cdot 10^{-5}$. Both the MSE and the error histogram reveal good modelling performance, and the model is computationally affordable to be implemented for real time control.

4 Conclusion

In this work a stack of fuel cells has been modelled with a black-box approach. In particular, for nonlinear modelling purposes, a Multi-Layer Perceptron has been adopted. The model obtained does not rely on a single-cell modelling, instead providing a macro-model of the whole stack. The resulting dynamic model relies on inputs which are easily measurable quantities, like reactant pressures and stack temperature. The results obtained are satisfactory, and allow to build a model suitable to be integrated on a more complex control system able to manage on board a vehicle the power fluxes between fuel cell stack, engine, and batteries.

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