

# Dynamic Modelling for Control of Fuel Cells

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## Abstract

Fuel-cell dynamics have been investigated with a variable-resistance board applied to a high temperature polymer fuel cell, and a particular pattern has been identified in the voltage-current density diagram. A model has been developed, using a characteristic equation to represent the external circuit as a generally nonlinear resistive load, possibly nonlinear and time-varying, rather than assuming the current density to be an independent variable. The model successfully explains the shape of the transient paths, including the different time constants observed when reversing a transient.

## Introduction

Fuel cells research has shown a rapid growth. Recently, the interest has increased also for the dynamic behaviour of fuel cells, as a topic in its own merit and as a prerequisite for control analysis and controller design. However, many models provided in the literature [1, 2, 3, 4, 5] were not intended for control studies, and in that context they are often “flawed” because they consider *current density* as an input to the system. This is unrealistic from a process-control perspective, because in reality the current is determined by the characteristics of the fuel cell and of its external load.

Currently, most PEM fuel cells are based on an electrolyte that relies on liquid water to facilitate protonic conduction, and thus an operating temperature below 100 °C unless pressurized. In polybenzimidazole (PBI)-based fuel cells, water is always produced in gaseous form (neglecting the start-up phase), and since the membrane only needs small amounts of water to function, the water management issue is minimized. Finally, high-temperature PEM fuel cells based on PBI electrolyte exhibit a high tolerance to carbon monoxide [6].

The objective of this paper is to show the development of a model using the external circuit’s characteristic as an input, and how this model is able to explain experimental results observed on a PBI fuel cell. Another objective is making the point that dynamic models for control-design purposes should make use of proper manipulated input variables, instead of using either voltage or current as an input.

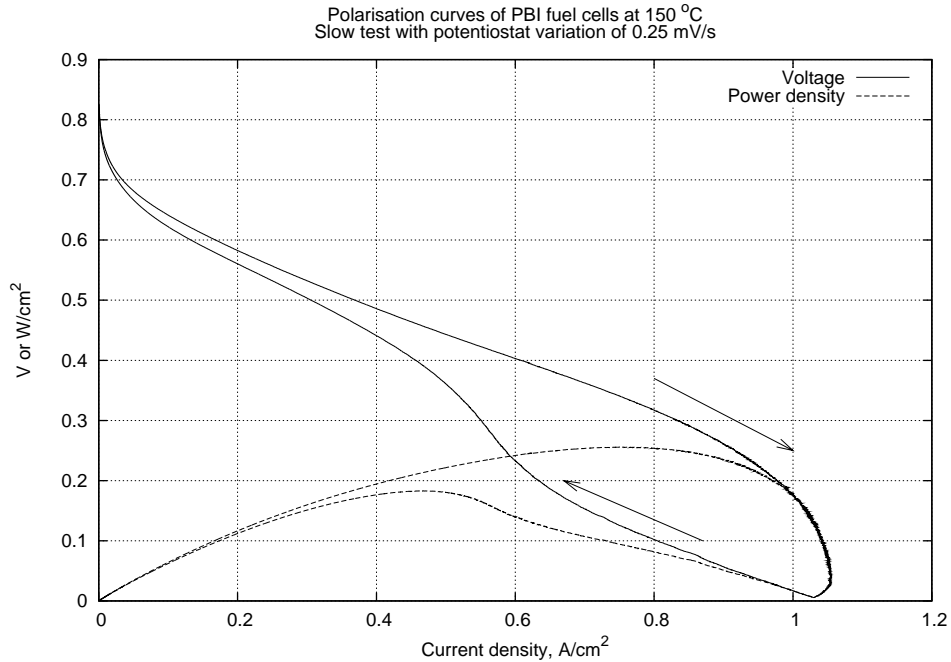


Figure 1: Polarization curve of a PBI fuel cell at 150 °C, measured with a potentiostat with voltage cycling at 0.25 mV/s. The arrows indicate the direction of the hysteresis cycle.

## Methods

Experiments were carried out on a PBI fuel cell, previously assembled in the laboratory of the Department of Materials Technology of NTNU, to determine the transient response of the cell to a variable load.

The load itself was assembled as a variable-resistance board, with two resistances in parallel; in series with one of these resistances, a switch could be opened and closed manually.

The PBI fuel cell was kept at a constant temperature of 150 °C by an external electric heater. The fuel cell ran on industrial-grade hydrogen and oxygen at atmospheric pressure. Oxygen enters the cell directly, whereas hydrogen bubbles through a 37.5%  $\text{H}_3\text{PO}_4$  solution, in order to make up for any loss of phosphoric acid in the cell's membrane. The oxygen flow, which was found to have a significant effect on the performance of the system, was kept at 3.71  $\text{cm}^3/\text{s}$ . Hydrogen flow was usually at 5.78  $\text{cm}^3/\text{s}$ , but it was found to have none or negligible effect on the cell's performance.

A polarization curve for the cell was measured as well. Because of the slow heat dynamics, the measurement took several hours.

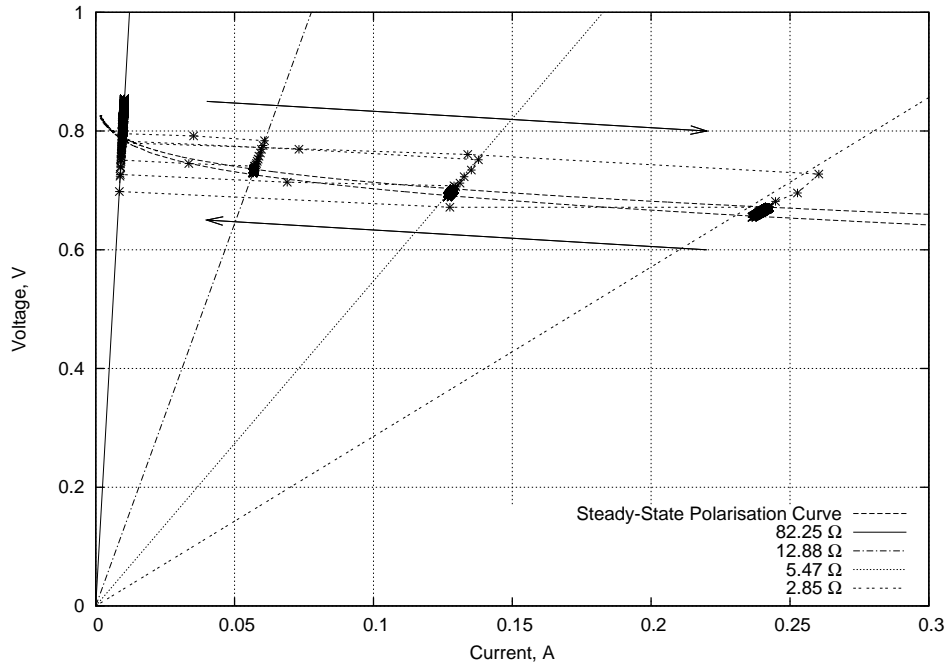


Figure 2: Operating points' path in the  $V$ - $I$  diagram after step changes in the external circuit's resistance, starting from  $82.25\ \Omega$  and switching back. The arrows indicate the path in the  $I$ - $V$  plan.

## Results

The polarization curve obtained at the conditions described in the previous section is shown in figure 1; the plot highlights a clear hysteresis when cycling between open voltage and short-circuit.

The results obtained switching from an initial resistance to a smaller one and back is shown in figure 2. It can be seen how the operating point moves from a resistance's characteristic to the other along parallel lines. As a reference, the steady-state characteristic is plotted as well; however, given the hysteresis cycle that was experienced, this reference is not completely precise. Results were influenced by the sensitivity to temperature changes of the fuel cell. It was also noted that just changing the oxygen flow rate would start a significant transient.

Looking carefully at figure 2, it is clear that in the descent to steady-state some transients are faster than others; this can be seen by the number of markers on the trajectory in the  $V$ - $I$  plane. It appears that the electrochemical transient to  $12.88\ \Omega$  is slower than the one to  $5.47\ \Omega$ , which is in turn slower than the one to  $2.85\ \Omega$ .

There is therefore an indication that the electrochemical transient can have *different time constants* depending on both the start and the end point. This behavior could be related to the one observed in a Master's thesis written at NTNU [7], where the same proportional controller performed too aggressively in some operating ranges, and too mildly in others.

## Modeling

The model is fundamentally based on a simple differential equation, the charge balance of a capacitor (3). The model neglects the anodic overvoltage and concentrates instead on the cathodic one, since it is normally much more important. Butler-Volmer's equation (1) is implemented with an iterative loop to find the value of the overvoltage, using Tafel's approximation as an initial value for the iterative algorithm. The dynamics of cathode gas diffusion were investigated to find whether they needed to be considered in this model, and were found to be fast enough to be assumed instantaneous. A scheme of the model is provided in figure 3.

A preliminary analysis was run to establish the influence of diffusion transients on the response of fuel cells. The results indicated diffusion transients in the order of  $10^{-2}$  s, which is faster than the bandwidth of interest; the model will therefore assume that diffusion transients settle instantaneously, and also that all partial-pressure profiles are linear from bulk to reaction site.

The model neglects any overvoltages on the anode, and considers the cathode's only. The model includes a steady-state part, which is later encapsulated in the complete dynamic model. At steady-state, the reaction current density  $i_r$  is the same as the circuit current density  $i$ ;  $i_r$  represents the reaction rate resulting from Butler-Volmer's equation, and  $i$  the actual current flowing in the external circuit divided by the cell's area.

The activation overvoltage  $\eta$  can be calculated for a given current, according to the Butler-Volmer equation:

$$i_r = i_0 \left( e^{\alpha \frac{nF}{RT} \eta} - e^{-(1-\alpha) \frac{nF}{RT} \eta} \right) \quad (1)$$

The reversible potential  $E^{rev}$  can be found with well-known thermodynamic data, and the ohmic loss is  $r_{cell} i$ . The cell voltage is then found as:

$$V = E^{rev} - \eta - r_{cell} i \quad (2)$$

During transients the reaction current density  $i_r$  is different from the current density, which we calculate dividing the current in the circuit by the fuel cell's area. Looking at the following differential equation [1], it is obvious to see that the difference  $i - i_r$  is actually the driving force of the transient behaviour of the activation overvoltage:

$$\dot{\eta} = \frac{i - i_r}{C} \quad (3)$$

This is the only differential equation that we will be considering in order to compute

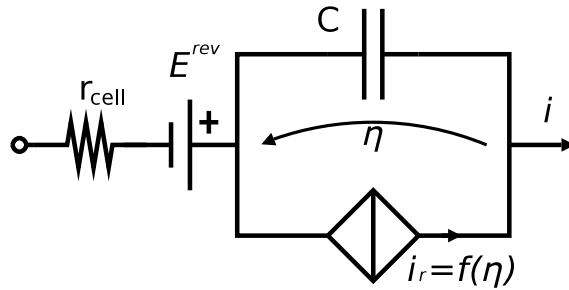


Figure 3: Diagram of the fuel-cell model.

the transient of the fuel cell. The cell's load in the model is generally allowed to vary with time, and is described by a function in the form  $I = f(V, t)$ .

The model can be expressed in an electrical-circuit diagram, as shown in figure 3. There, one can see the internal resistance  $r_{cell}$ , the reversible potential  $E^{rev}$ , the capacitor  $C$  and its voltage  $\eta$ . The bipole in parallel with the capacitor is a nonlinear voltage-controlled current generator, that enforces the Butler-Volmer law, and imposes a current  $i_r$  as a function of  $\eta$  (and many other parameters). This last bipole is often also modelled as a nonlinear resistance [8], or a linearized value in an area of interest. Incidentally, the ideal generator  $E^{rev}$  and the resistance  $r_{cell}$  in series with it can be viewed as a Thevenin equivalent circuit.

The actual integration of equation 3 is not very simple, since  $i_r$  is a function of many parameters, and also of  $\eta$  itself, through the Butler-Volmer equation (1). An iterative loop is therefore necessary to calculate  $i_r$  at all integration steps, and this is the major computational cost of the simulation.

## Model Results and Insights

The cause of the sudden iso- $\eta$  “kick” in the dynamic path diagram, as can be seen in the simulation in figure 4 and in experimental results in figure 2, is caused by the simple fact that the operating point *must* always lie on the load's characteristic, when the load is purely resistive. It is possible to determine to *which coordinates* on the load's characteristic the operating point will jump, considering that the activation overvoltage  $\eta$  varies *continuously* with time; when a step change in the outer load happens at time  $t_0$ ,  $\eta$  will therefore be the same for times  $t_0^+$  and  $t_0^-$ .

Using the load characteristic as the model's input has allowed to simulate real laboratory results, and has given the possibility of simulating the implementation of MOSFETs as manipulated variables in control of fuel cells.

Looking at figure 4, it is clear that the drawn part of the polarization curve is closer to

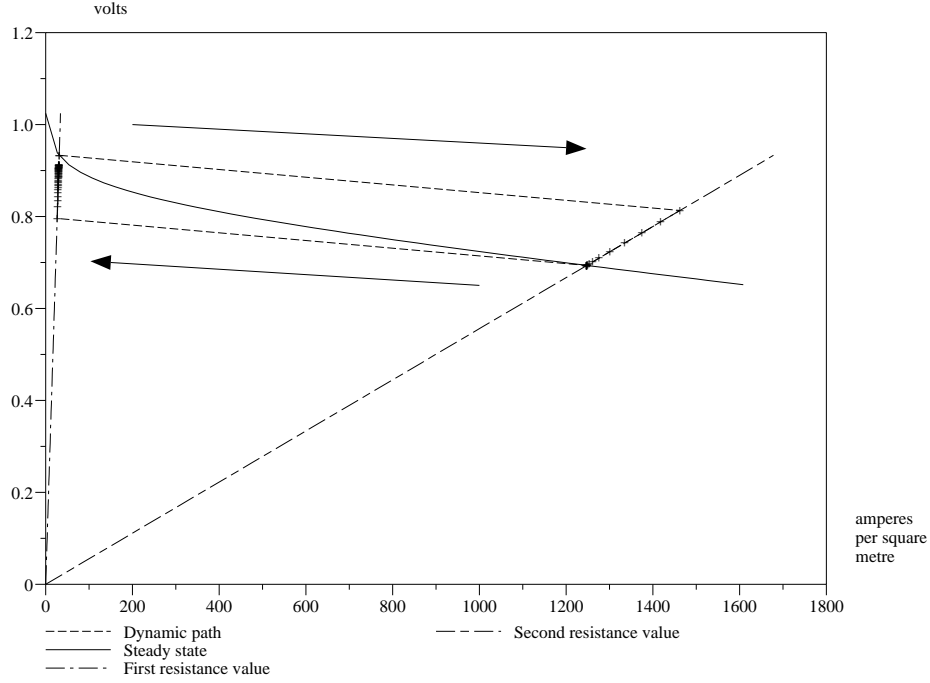


Figure 4: A typical output of the model: a simulation of a transient from a steady-state operating point to a new value of the external resistance, and back. Assumed temperature is 150 °C. The markers are spaced by 0.01 s.

the characteristic of the higher resistance, when distance is measured along the  $i$  axis. Since  $\dot{\eta}$  is proportional to the distance between the intersections of the instantaneous characteristic with the polarization curve and the external resistance along the  $i$  axis, i.e.  $i - i_r$ , it follows that the transient to the lower resistance will be faster than the one coming back, because of the higher values of  $i - i_r$  along that path; this is confirmed by the experimental measurement shown in figure 2.

An analytic expression for the time constants has been found. Assuming that  $C$  and  $r_{cell}$  are constant, and that functions  $\Psi(i)$  (the external load's characteristic) and  $\eta(i_r, \dots)$  are given, the time “constant”  $\tau$  depends essentially on  $i$  and  $i_r$ :

$$\tau(i, i_r) = \frac{C}{\left(r_{cell} + \frac{d\Psi}{di} \Big|_i\right)^{-1} + \left(\frac{d\eta}{di_r} \Big|_{i_r}\right)^{-1}} \quad (4)$$

Considering the basic expression of the voltage of a fuel cell (2), and looking at figure 4, it is evident that the instantaneous characteristic at a given steady-state point stays at higher voltages than the polarization curve when moving to higher values of current density, and, conversely, at lower voltages for lower values of current density. Under these assumptions, a

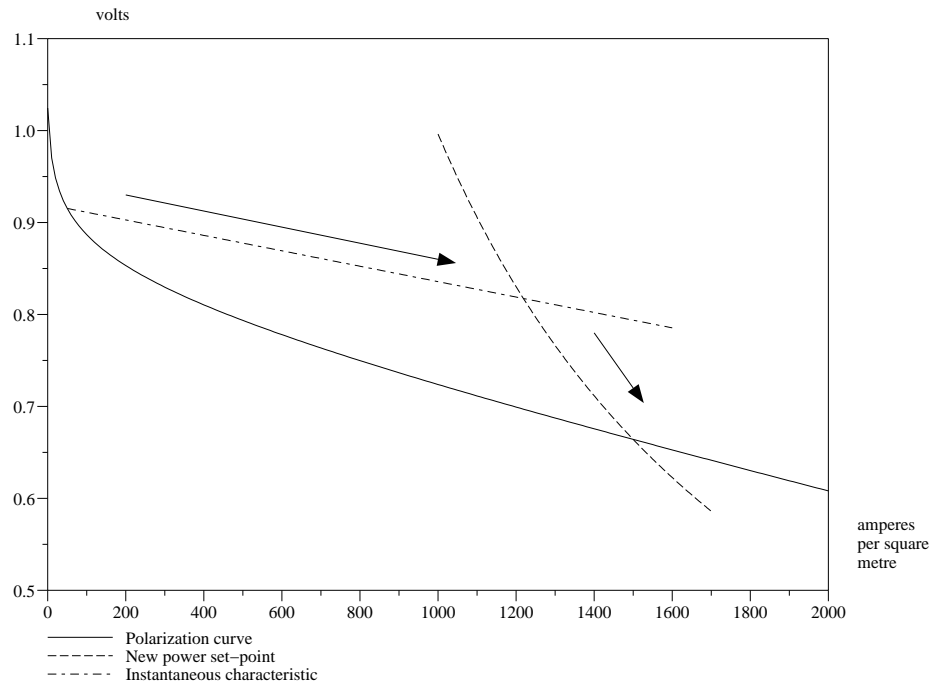


Figure 5: A perfect response to a step in the set-point for power might be obtained moving the operating point to the intersection of the iso- $\eta$  curve with the iso-power curve, and following the iso-power curve until steady-state is achieved.

perfect step change in power output can be obtained if the controller manages to steer the fuel cells as shown in figure 5.

## Conclusion

A pattern was identified in transient tests of PBI fuel cells when changing the resistance of the load. A dynamic model based on the Butler-Volmer equation has been developed: its novelty is the use of a function, the external load characteristic, as input, rather than the more common approach of using current or voltage. This new approach allowed to explain the observed transient paths in a simple way, identifying the activation overvoltage  $\eta$  as a state of the fuel cell. The model was also able to simulate the different dynamics observed when switching back and forth between two external resistances. A simple formula to estimate the time constants of the dynamics has been developed, which allows to predict an approximate value for the transient's time constant  $\tau$  for an operating point. Finally, it was shown how a step in the set-point for power output can in theory be perfectly matched by the power output of the fuel cell, if proper control could be applied, under quite general assumptions on operating conditions.

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