An efficient multi-objective model predictive control framework of a PEM fuel cell

Ziogou Chrisovalantou[1], Simira Papadopoulou[1,3], Panos Seferlis[1,2] , Spyros Voutetakis[1]

[1]*Chemical Process Engineering Research Institute (C.P.E.R.I.), CEntre for Research and Technology Hellas (CE.R.T.H.), P.O. Box 60361, 57001 Thermi-Thessaloniki, Greece (Tel: +30-2310-498 317; e-mail:ziochr@cperi.certh.gr, paris@cperi.certh.gr)*

[2]*Department of Mechanical Engineering, Aristotle University of Thessaloniki, P.O. Box 484, 54124 Thessaloniki, Greece (Tel: +30-2310-498 169; e-mail:seferlis@cperi.certh.gr)*

[3]*Department of Automation, Alexander Technological Educational Institute of Thessaloniki, P.O. Box 14561, 54101 Thessaloniki, Greece (Tel: +30-2310-498 319; e-mail:shmira@teithe.gr)*

Abstract: Fuel cell systems can produce clean energy and have attracted the interest of both industrial and basic research in the recent years. They are part of a promising benign and environmentally friendly technology and they can be used both in mobile and stationary applications. A dynamic model was constructed and validated using experimental data based on a specific application, consisting of a high temperature PEM Fuel Cell (FC) working at a constant pressure and a Power Conversion Device that controls the current drawn from the FC. An integrated framework that consists of an online maximum power point prediction algorithm and a non-linear model based control scheme is presented. The proposed framework aims to maintain the fuel cell close to the optimum power point and the corresponding oxygen excess ratio level. Simulation studies show that the proposed control framework results in improved performance regarding the efficient and safe fuel cell operation under varying operating conditions.

Keywords: fuel cell control, model predictive control, power management

1. INTRODUCTION

Fuel cells are electrochemical devices that convert the chemical energy of a fuel directly into electricity and are under intensive development by several manufacturers. They are categorized according to the type of electrolyte used, operating conditions or fuel. The Polymer Electrolyte Membrane or Proton Exchange Membrane fuel cells (PEMFC) are currently considered by many to be in a relative more developed stage for ground vehicle applications and portable devices. PEMFC's have high power density, solid electrolyte, long cell and stack life, as well as low corrosion. Lately PEM fuel cells working at higher temperatures of up to 200°C have appeared such as those that use phosphoric acid doped polybenzimidazole (PBI) membrane, which is considered one of the most successful membrane systems so far [Jensen, 2007]. The benefits of operation at elevated temperature are mainly the tolerance to carbon monoxide concentration at the hydrogen feed, commonly present when operating with reformate streams, that can be increased by many orders of magnitude compared to that of a common PEM and also the water management which is a lesser issue, since the water is in vapor state. Additionally, the PBI membranes are conductive at very low relative humidity and consequently no moisture management is needed. Moreover, the high working temperature eliminates the possibility of water condensation in pores or channels of the fuel cell. Due to the higher temperature difference to the surroundings thermal management can be satisfactorily performed by a smaller cooling system [Jensen, 2007]. However, due to material limitations, the power of the fuel cell cannot be arbitrary used without prior consideration on the internal effects such as the provision for fuel and oxidant supply, temperature gradients, condition of the membrane (humidity) and so forth. The choice of the operating region leads to different characteristics for the unit regarding its profitability, effectiveness and safety. The dynamic response of a fuel cell is affected when the power demand fluctuates or when the fuel cell does not operate at its optimal steady-state design point [Golbert, 2007]. An optimization algorithm is used to search off-line for the optimum excess oxygen ratio level and the corresponding near maximum power. The primary objective of this paper is to demonstrate that model-based predictive control (MPC) is a suitable approach for efficient and safe fuel cell operation. The paper is organized as follows: Section 2 gives an overview of the dynamic fuel cell mathematical model. In section 3, the model validation procedure is presented. Section 4 presents the model-based predictive control structure along with the conventional control that is present for the pressures of the anode and the cathode compartments of the FC. Section 5 discusses the maximum power targeting algorithm The simulated results of the proposed MPC framework are presented and discussed in section 6.

2. MODELING AND ANALYSIS

The application is consisting of a high temperature PEM Fuel Cell working at a constant pressure and a Power Conversion Device capable of controlling the current drawn from the FC. In order to define a model based control strategy it is important to have an accurate model that reflects the transient dynamics and fuel cell system behavior and in the same time fast in execution in order to be useful for a real-time application. The mathematical model equations that describe the operation of the fuel cell consists of the voltage-current characteristics and a relationship for the consumption of the reactants as a function of the current drawn from the fuel cell. The main purpose of the detailed model is to describe the dynamic behavior in a way that the fundamental operating parameters current and pressure are established as manipulated variables and temperature as disturbance and power and excess oxygen ratio as controlled variable.

2.1 General

The main components of a PEM fuel cell are three - an anode, typically featuring platinum-containing catalyst, a thin, solid polymeric layer which acts as electrolyte, and a cathode, also coated with platinum [Mann, 2000]. In the PEM fuel cell the only reaction that takes place is the production of water from hydrogen and oxygen. In order to accurately describe the fuel cell behavior the mass balance and the equations that affect the voltage calculation are analyzed in the following section. The development of the fuel cell model is based on some assumptions. The gases are ideal and uniformly distributed inside anode and cathode. The stack is fed with hydrogen and air. The temperature is constant and uniform for each experiment. The gas channels along the electrodes have a fixed volume with small lengths, so that it is only necessary to define one single pressure value in their interior.

2.2 Electrochemistry and Voltage Calculation

Typical characteristics of FC are normally given in the form of polarization curve, which is a plot of cell voltage versus cell current density. To determine the voltage-current relationship of the cell, the cell voltage has to be defined as the difference between an ideal, Nernst voltage and a number of voltage losses and it is described in the current section. The main losses are categorized as activation, ohmic and concentration losses. The activation losses are caused by the slowness of the reactions taking place on the surface of the electrodes. A portion of the voltage generated is lost in driving the chemical reaction that transfers the electrons to or from the electrodes. The activation losses are described by the Tafel equation, which can be calculated as [Mann, 2000]:

$$\Delta V_{act} = \xi_1 + \xi_2 T + \xi_3 T \ln(C_{O_2}) + \xi_4 T \ln(i) \qquad (1)$$

where ξ(i = 1–4) are parametric coefficients for each cell model. The term C_{O_2} is the concentration of oxygen on the electrolyte membrane at the gas/liquid interface (mol/cm^3), which can be expressed as [Zhong, 2008]:

$$C_{O2} = \frac{p_{O2}}{5.08 \cdot 10^6 e^{\left(\frac{-498}{T}\right)}} \qquad (2)$$

The ohmic losses are caused by the resistance to the flow of electrons through the material of the electrodes and the various interconnections, as well as by the resistance to the flow of protons through the electrolyte. The ohmic losses are given by:

$$\Delta V_{ohm} = R_{mem} \cdot i \qquad (3)$$

The ohmic resistance is described by:

$$R_{mem} = \frac{r_m \cdot mem_{thick}}{A} \qquad (4)$$

where r_m is membrane resistivity (Ωcm) to proton conductivity, mem_{thick} is the membrane thickness (cm) and A is the active cell area (cm^2). Membrane resistivity depends strongly on membrane humidity and temperature, and can be described by an empirical expression given by Mann et. al. [Mann, 2000]. Finally the mass transport or concentration losses result from the change in concentration of the reactants at the surface of the electrodes as the fuel is used [Larminie J., 2003]:

$$\Delta V_{conc} = me^{ni} \qquad (5)$$

where m and n are constants that can be estimated to give better fit to measured results. Thus, the actual voltage will be less due to the aforementioned losses that occur because of the various electrochemical phenomena. The Nernst voltage or open circuit voltage falls as the current supplied by the stack increases. The reversible thermodynamic potential is calculated using the Nerst equation and can be expressed as:

$$E = E^0 + \frac{RT}{2F} \ln\left[\frac{P_{H2} P_{O2}^{\frac{1}{2}}}{P_{H2O}}\right] \qquad (6)$$

where F is the Faraday's constant (C/kmol) and p_i are the partial pressures (atm) (with i=H_2, O_2, H_2O). The equation that combines the above irreversibilities expresses the actual cell voltage:

$$V_{cell} = E - V_{act} - V_{ohm} - V_{conc} \qquad (7)$$

The above equation is able to predict the voltage output of PEM fuel cells of various configurations. Depending on the amount of current drawn the fuel cell produces the output voltage according to (7). The electric power delivered by the system equals the product of the stack voltage V_{cell} and the current drawn I:

$$P = I \cdot V_{cell} \qquad (8)$$

2.3 Mass Balance Equations

The model equations consist of the standard material balance of each component. Every individual gas follows the ideal gas equation. Therefore mass is described through partial pressures of each gas in the material balances:

$$\frac{d}{dt}p_g = \frac{R \cdot T}{V}\left[q_g^{in} - q_g^{out} - q_g^{r}\right] \quad (9)$$

where R is the universal gas constant (J (kmol K)$^{-1}$)), T is the temperature (K), V is the anode or cathode volume (1). For each gas q_g^{in} is the input flow, q_g^{out} is the output flow and q_g^{r} is the consumption or production due to the reaction. The same expression is used for oxygen, hydrogen and the produced water by replacing the term g with the corresponding gas. The amount of hydrogen consumed due to reaction is calculated as:

$$q_{H2}^{r} = \frac{I}{2F} \quad (10)$$

and for the oxygen :

$$q_{O2}^{r} = \frac{1}{2}\frac{I}{2F} \quad (11)$$

while the water production can be described by :

$$q_{H2O}^{r} = -\frac{I}{2F} \quad (12)$$

The water production rate is the same as the hydrogen's reaction rate, since water is produces as hydrogen is consumed. The oxygen reaction rate is the half of that of the hydrogen due to the stoichiometry of the reaction. As the load draws current, the reactants become depleted in the fuel cell and partial pressure of oxygen and hydrogen drop accordingly. A common practice to protect the fuel cell from reactants starvation is to supply it with excessive amounts of hydrogen and oxygen.

2.4 Oxygen Excess Ratio

There are two phenomena that can deteriorate or even destroy the fuel cell, flooding and oxygen starvation. Flooding is related to temperature and humidity, which are assumed constant and stable in the developed model since it is a high temperature FC where flooding is rather avoidable. The second one, the oxygen starvation, when it occurs the operation of the FC must be stopped in order to prevent fuel cell malfunction. The lack of oxygen is a complicated phenomenon that occurs when oxygen falls below a critical level at any location within the cathode. This phenomenon entails a rapid decrease in cell voltage, which in severe cases can cause a hot spot, or even burn-through on the surface of a membrane. To prevent this catastrophic event, the system must either remove the current from the stack or trigger a shut-down procedure. For all these reasons in a PEM fuel cell it is considered important to control the amount of available oxygen in the cathode. The air flow needs to be controlled rapidly and efficiently to avoid oxygen starvation and extend the life of the stack [Pukrushpan, 2004]. Although the oxygen concentration is not homogenous throughout the cathode, the control can be achieved by defining a parameter that indicates the oxygen level status in the cathode, named excess oxygen ratio level λ_{O2}. The excess ratio level is an unmeasured but observable variable that can be expressed as the inlet flow q_{O2}^{in} to the rate of oxygen consumption q_{O2}^{r} :

$$\lambda_{O2} = \frac{q_{O2}^{in}}{q_{O2}^{r}} \quad (13)$$

As can be observed by (11) and (13) the oxygen excess ratio level depends on the current drawn from the cell. This relationship can cause an abrupt and momentarily drop of the λ_{O2}, while it is related to the fuel consumption High values of λ_{O2}, and thus higher partial oxygen pressure improves the overall power. Low values of λ_{O2} indicate low oxygen concentration that could lead to oxygen starvation. Moreover, the temperature within the fuel cell may rapidly increase when oxygen concentration is too low. Therefore, the oxygen should be replenished quickly as it is depleted in the cathode [Vahidi, 2006].

3. PARAMETER IDENTIFICATION

The dynamic process model described in the previous section is validated using experimental data from a high temperature PEMFC. Nonlinear regression techniques are used to estimate the model parameters. The selected estimated parameters are the following: the parametric coefficient in activation losses (ξ_1) and the parameters in concentration losses (m, n). The characteristic cell voltage and the applied current density were measured through an on-line supervisory control and data acquisition system. Experiments were performed at the single cell system at constant temperatures between 170°C to 200°C. The activation area of the cell is 25cm2. The estimated values of the parameters are presented in Table 1.

Table 1 Estimated parameters

Parameter	Estimated value
ξ_1	-1.771
m	7.04E-05 V
n	9.44 E-03 cm^2 mA

Fig 1 compare the model predictions with the experimental data for various operating temperature levels for the polarization curves Fig 1 reveal that model predictions are in good agreement with the experimental data. As can be observed in the experimental results, a temperature increase raises cell voltage and consequently the fuel cell power output.

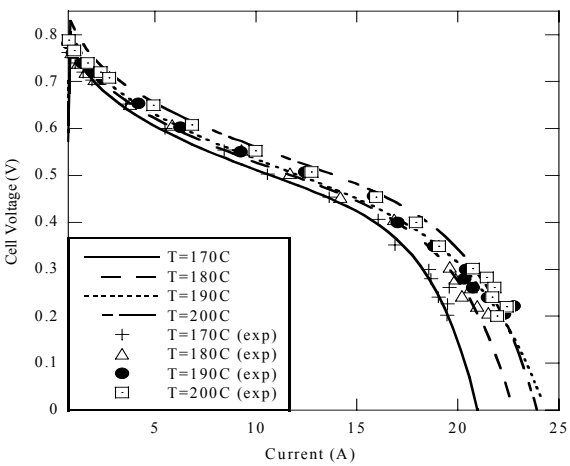

Fig. 1 Model predicted and experimental polarization curves

4. MAXIMUM POWER TARGETING

The power of the fuel cell depends nonlinearly on the applied current. As it is observed from the power curve there exists a unique operating point for each set of operating conditions, where the delivered power reaches a maximum power point (MPP). The operation of the system beyond MPP is not safe and should be avoided. The purpose of the control strategy is to deliver a near optimum power and at the same time to choose the proper operating region to ensure high fuel cell efficiency and avoid oxygen starvation. Thus a MPP tracking algorithm is developed that calculates the highest possible power as operating conditions vary. Fuel cell operation at the MPP is not very beneficial because the corresponding fuel efficiency is at best 50%. [Zhong, 2008]. As illustrated in Fig. 2 there exists an area where the power is near its MPP and the corresponding oxygen excess ratio level guarantees a safe and efficient fuel cell operation. The calculation of the MPP from process measurements is not possible as it depends on numerous factors that change during operation (e.g., relative humidity, gas mole fractions) and furthermore the entire power curve needs to be inferred to identify its maximum. Therefore, the fuel cell mathematical model is used in order to determine a desired trajectory towards the near MPP.

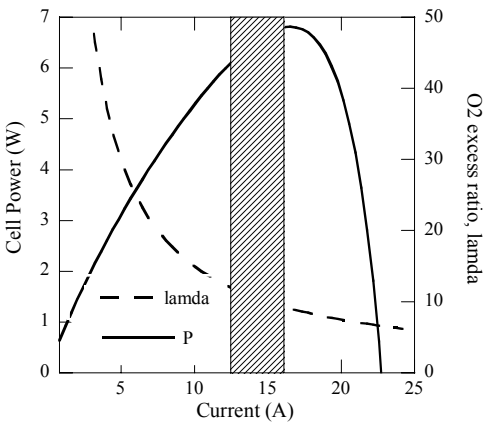

Fig. 2 Power curve and λ_{O2} (lamda) trajectory. Desired area of operation is shadowed.

Numerous methods have been proposed for maximum power tracking such as the perturbation and observe, adaptive extremum seeking algorithm, artificial intelligence methods and model-based methods to name a few [Zhong 2008, Krstic, 2000]. The current approach utilizes the developed non-linear dynamic model to determine off-line the near optimum region of operation and calculate the corresponding oxygen concentration level at the specific operating point usually defined as a function of temperature and pressure. The higher oxygen excess ratio level leads to a safer operation. The resulting strategy aims to an operation where a compromise between the maximum achievable power output and the optimal oxygen excess ratio is sought.

5. MODEL PREDICTIVE CONTROL FRAMEWORK

A Model Predictive Control (MPC) framework is formulated for the satisfaction of the control objectives described in the previous section. The fuel cell system presents a number of control challenges, the most significant of which is the nonlinearity in the area of the maximum power. Also an important control objective is the effective regulation of the oxygen concentration in the cathode. Furthermore, it is of interest to ensure safe operation during transients and sudden load changes. MPC is able to satisfy multiple control objectives under the presence of changes in process characteristics. Another important feature is its ability to deal with constraints. When a fuel cell operates near the MPP and consequently close to its operation limits constraints violations are critical in the achieved control performance.

5.1 Anode and Cathode Pressure Control

To regulate the anode and the cathode pressure a fast proportional-integral (PI) controller is implemented as used in the real system. The conventional PI controllers are used independently of the MPC scheme, which assumes that the anode and cathode pressure is held at a constant level as the dynamics of the PI control system are relatively fast. In the performed experiments it is assumed that the cathode and anode pressure is at 2 barg. These secondary loops are tightly controlled and assumed not to interact with the main control objectives of the system.

5.2 Model Predictive Control

Model predictive control (MPC) is part of a family of optimization-based control methods, which are based on on-line optimization of future control moves. Also MPC is based on the fact that past and present control actions affect the future response of the system. Using a process model, the optimizer predicts the effect of past inputs on future outputs. The deviation of the model prediction from the actual response is recorded and considered as the error of the process model, as shown in the block diagram of the MPC framework. The calculated error defines a bias term that is used to correct future predictions and it is constant for the entire prediction horizon. The block diagram describing the MPC scheme and the near optimum power targeting scheme is illustrated in Fig. 3.

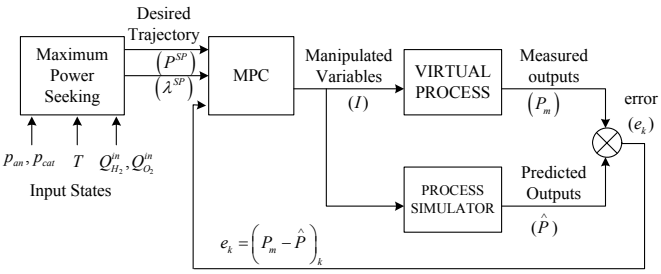

Fig. 3 Block diagram of the MPC control framework

The control structure utilizes two instances of the aforementioned dynamic model; the one corresponds to the Virtual Process (VP) and the second one to the Process Simulator (PS) or Model, and they are concurrently executed. Successive iterations between the optimizer, that evaluates the optimum value for the manipulated variable, and the model, that calculate the response of the process to the imposed control action are performed. The mathematical representation of the MPC algorithm is as follows:

$$\min_{k+j-1} J = \sum_{j=1}^{Np} \left\| \hat{P}_{k+j} - P_{k+j}^{SP} \right\|_{w_P}^2 + \left\| \hat{\lambda}_{k+j} - \lambda_{k+j}^{SP} \right\|_{w_\lambda}^2 \quad (14)$$

Subject to :

$$e_{k+j-1} = \left(y^{meas} - y^{pred} \right)_{k+j-1}, \; y_k = P_k \quad (15)$$

$$\hat{y}_{k+j} = y_{k+1}^{pred} + e_{k+j-1} \quad (16)$$

$$N_c = (T_c - T_k) / \Delta t_c \quad (17)$$

$$N_p = (T_p - T_k) / \Delta t_p \quad (18)$$

Where vectors $\hat{P}_k^{SP}$ and $\hat{\lambda}_k^{SP}$ denotes the desired response trajectories. The difference e_k between the measured variables y^{meas} and their predicted values y^{pred} at time instance k is assumed to persist constant for the entire number of time intervals N_p of the prediction time horizon T_p. While T_c denotes the control horizon reached through N_c time intervals. Also this minimization is subject to constraints on the manipulated and controlled variables:

$$I_{\min} \le I_{k+j-1} \le I_{\max} \quad (19)$$

$$\lambda_{O_2,\min} \le \lambda_{O_2} \le \lambda_{O_2,\max} \quad (20)$$

Eq (19) imposes a constraint to the input variables that corresponds to their physical limits. Eq (20) imposes a constraint on lamda to avoid starvation. Tuning parameters of the algorithm are the weight factors in the objective function (w_p, w_λ) and the length of the prediction and control horizon. The selection of the appropriate prediction horizon is mainly dictated by the time scale characteristics of the system. The computational time to reach a solution of the nonlinear dynamic program may affect the duration of the control interval.

6. SIMULATION RESULTS

The performance of the proposed MPC framework is evaluated through a number of simulated examples for a high temperature PEMFC. In all cases, unless otherwise stated, the system operates at constant temperature ($T_{sim} = T_{process} = 180^\circ C$) and constant cathode pressure ($p_{an} = p_{cat} = 2$barg). The influence of the controller tuning parameters on the closed-loop performance of the MPC is investigated. The main parameters are the control and the prediction horizons and the weighting factors of the power and oxygen concentration terms. Both prediction and control horizons were chosen equal to 15 seconds while the intervals of the control actions were chosen equal to 5 seconds. The length between two consecutive control actions (Δt_c) was selected according to the required computational time of the optimization problem.

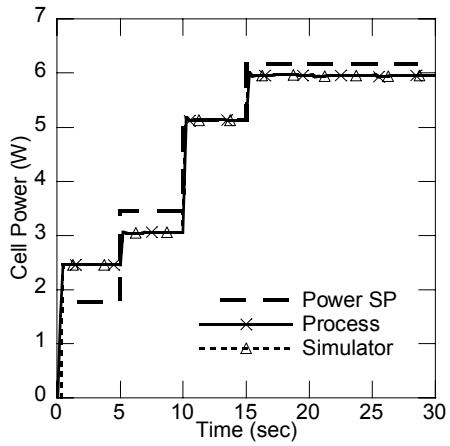

Fig. 4 Power response with unequal weights $w_p = 0.8,\ w_\lambda = 0.2$

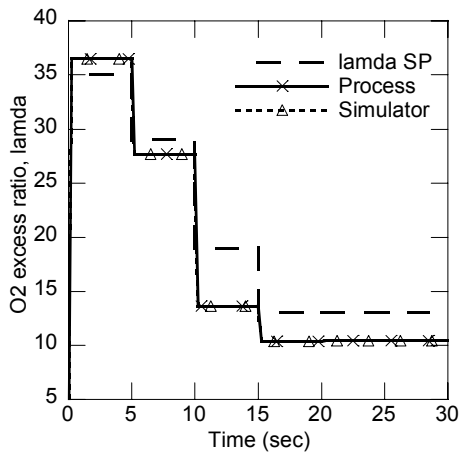

Fig. 5 Oxygen excess ratio level with unequal weights $w_p = 0.8,\ w_\lambda = 0.2$

Fig 4-7 show the sensitivity of the MPC performance on the weighting factors in the objective function. In the first case (Fig 4-5) more importance is given on the tracking of the power output while in the second case (Fig 6-7) an equal importance to both control objectives is imposed. In both

cases the desired setpoints were followed satisfactorily. However, in the first case excess O_2 is quite low which may cause difficulties in the fuel cell operation (i.e. oxygen starvation). The power output offset is small in the first case where a larger weight is used for the power output difference term. A better compromise is achieved in the second case with the excess oxygen closer to the desired level.

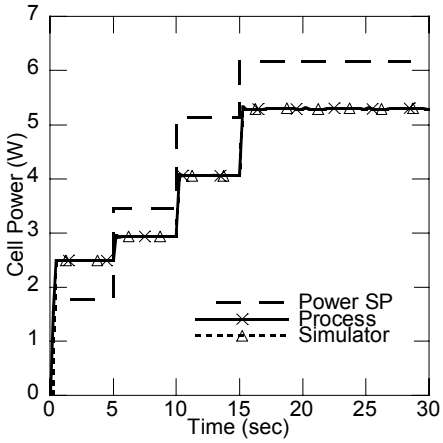

Fig. 6 Power response with equal weights $w_p = 0.5,\ w_\lambda = 0.5$

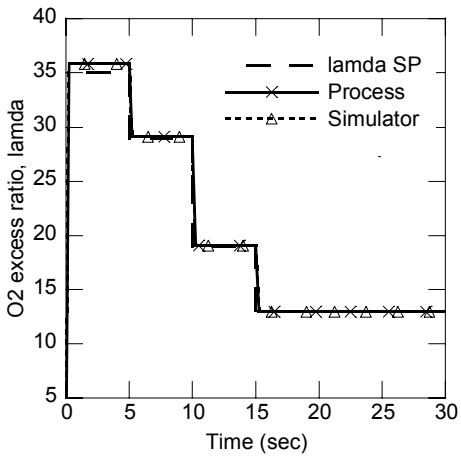

Fig. 7 Oxygen excess ratio level with equal weights $w_p = 0.5,\ w_\lambda = 0.5$

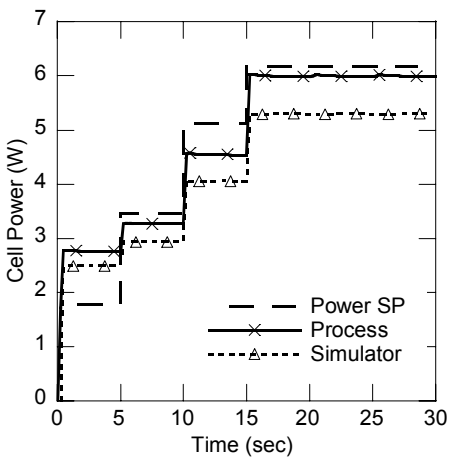

Fig. 8 Power response with altered process temperature

In another case study (Fig 8), significant mismatch in the fuel cell temperature between the Virtual Process and Process Model ($T_{sim} = 180^\circ C$, $T_{process} = 140^\circ C$) is deliberately introduced in order to asses the robustness of the proposed strategy to a significant disturbance. Fig. 8 illustrates the ability of the nonlinear MPC scheme to compensate for the temperature variation and successfully satisfy the control objective by close tracking of the desired power output level. The application of the constrained MPC framework allowed for an accurate targeting of the desired oxygen concentration and was able to give a near maximum power.

7. CONCLUSIONS

In this work a dynamic model for a high temperature PEM fuel cell stack based on single cell was developed and an advanced constrained predictive control framework was implemented. Having tested and verified some selected operational parameters a reliable MPC scheme was resulted. The MPC framework that combines two contradictive operational objectives, can safely lead to an operation that maximizes the power of a given size FC. The proposed MPC will be implemented and verified in the experimental fuel cell system. In order to improve the overall efficiency and safe operation, the controller would further include mathematical models for the auxiliary subsystems.

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