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Performance Improvement of an NMPC Problem by Search Space Reduction and Experimental Validation to a PEM Fuel Cell System

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Abstract— **The current work addresses the control issues that arise during the operation of a fuel cell system based on a novel combination of two Model Predictive Control strategies, explicit and Nonlinear MPC (NMPC). The proposed framework relies on an NMPC formulation that uses a simultaneous direct transcription dynamic optimization method that recasts the multivariable control problem into a nonlinear programming problem using a warm-start initialization method. The performance of the optimizer is improved by a search space reduction technique which is based on a piecewise affine approximation of the variable's feasible space, derived offline by a multi-parametric Quadratic Programming method. The behavior of the explicit NMPC framework is initially explored by a simulation study and subsequently it is experimentally verified through the online deployment to the fuel cell unit, demonstrating excellent response in terms of computational effort and accuracy with respect to the control objectives.**

I. Introduction

In the recent years the trend towards the development of Polymer Electrolyte Membrane (PEM) fuel cell systems is steadily increasing, as they constitute a prominent technology for zero emission electricity production and they can be applied to small stationary, mobile and portable applications. During their operation various phenomena are evolving and their behavior is affected by many variables such as temperature, partial pressures and humidity. Therefore it is necessary to be able to understand qualitatively and predict quantitatively the optimum operation of an integrated fuel cell system in order to protect its longevity and preserve its long-term performance. The control of a PEM fuel cell (FC) is a multivariable problem and a number of interesting studies can be found in the literature. Most of them focus on one operation objective or subsystem and provide a thorough simulation analysis [1,2] while others provide an insight through the experimental application of their proposed control scheme [3,4,5]. In the current work a Nonlinear Model Predictive Control (NMPC) formulation is selected to effectively handle the interrelated control objectives of a PEM fuel cell. Overall the applicability of an NMPC controller depends strongly on the computational effort caused by the online solution of a constrained finite-time optimal control problem. In this context the required time for the derivation of an optimal solution should be equal or less to the sampling time of the system. Therefore the aim of the current work is twofold. Initially a synergy that reveals the potential of exploiting the intrinsic features of two model-based control methods (explicit and nonlinear MPC) is presented. Secondly an interesting multivariable control problem that involves the optimum operation of an experimental PEM fuel cell unit is handled by the proposed synergetic framework. Based on this motivation the basis of the proposed framework is initially presented (Section II). Then the experimental FC system and the control objectives (Section III) are presented. Finally the controller is deployed online to the unit and its behavior is explored (Section IV).

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II. Proposed Synergetic Control Framework

This work presents the combination of two MPC-based strategies in a unified control framework in order to take advantage of their synergistic benefits. The first methodology is an online Nonlinear Model Predictive control (NMPC) strategy [6], which is very appealing due to its ability to handle dynamic nonlinearities of the process under consideration [10]. The second methodology is an explicit or multi-parametric Model Predictive Control (mpMPC) strategy, which can provide the optimal solution in real-time, as the solution is computed offline and can be implemented online by simple look-up functions [7].

A. Simultaneous Direct Transcription method

NMPC computes online a finite-time constrained optimization problem over a prediction horizon (T_p), using the current state of the process as the initial state. The optimization yields an optimal control sequence ($u_k..u_{k+Nc}$) over a control horizon (T_c), which is partitioned into N_c intervals and only the first control action (u_k) for the current time is applied to the system. We consider the following formulation of the NMPC problem [6]:

$$\min_u J = \sum_{j=1}^{Np} (\hat{y}_{k+j} - y_{sp,k+j})^T QR(\hat{y}_{k+j} - y_{sp,k+j}) + \sum_{l=0}^{Nc-1} \Delta u_{k+l}^T R1 \Delta u_{k+l} \quad (1)$$

$$\text{s.t.:} \quad \dot{x} = f_d\left(x,u\right), \quad y = g\left(x,u\right), \quad x(0) = x_0 \quad (2a)$$

$$e_k = (y_{pred} - y_{meas})_k \quad (2b)$$

$$\hat{y}_{k+j} = y_{pred,k+j} + e_k \quad (2c)$$

where *u,y,x* are the manipulated, the controlled and the state variables, $y_{pred}, y_{meas}, y_{sp}$ are the predicted, the measured variables and the desired set-points and *QR, R1* are the output tracking and the input move weighing matrices. The minimization of functional *J* (eq. 1) is also subject to constraints of *u, x* and *y*. In the current work a direct optimization simultaneous method is selected for the implementation of the NMPC problem (1) using an augmented Lagrangian solver [8]. The nonlinear dynamic model is discretized using a direct transcription method based on orthogonal collocation on finite elements (OCFE) [9] which is selected due to its numerical properties. The input, state and output variable profiles are approximated with a family of Lagrange polynomials (NE). Within each finite element these profiles are discretized around collocation points (N_{cop}) based on Legendre polynomials:

$$x(t) \approx \sum_{j=0}^{Ncop} x^{i,j} \Omega_j(t), \;\; i = 1..NE\,,\; j = 0..N_{cop}\,, t \in [t_i, t_{i+1}] \quad (3)$$

$$\Omega_j(t) = \prod_{k=0,k\neq j}^{Ncop} \frac{(t - t_{i,k})}{(t_{i,j} - t_{i,k})} \quad (4)$$

where t is the scalar independent dimension defined in the fixed domain $[0, t_f]$, $x^{i,j}$ is the value of the state vector at collocation point *j* of the i^{th} finite element and Ω is the basis function. After this discretization the problem is expressed as a large-scale but sparse NLP problem [9]:

$$\min_{x^{i,j}, z^{i,j}, u^i} \sum_{i=1}^{NE} \sum_{j=1}^{Ncop} w_{i,j} \phi\left(x^{i,j}, z^{i,j}, u^i\right), \; i = 1..NE, \; j = 1..N_{cop} \quad (5)$$

$$\text{s.t.}: \sum_{k=0}^{Ncop} \dot{\Omega}_k(\tau_{i,j}) x^{i,k} = h_i f_d\left(u^i, x^{i,j}, z^{i,j}\right) \quad (6a)$$

$$0 = f_a\left(u^i, x^{i,j}, z^{i,j}\right) \quad (6b)$$

$$x^{1,0} = x_0, \quad x(t_f) = \sum_{j=0}^{Ncop} x^{NE,j} \Omega_j(1) \quad (6c)$$

$$x^{i,0} = \sum_{j=0}^{Ncop} x^{i-1,j} \Omega_j(1), \;\; \mathrm{i} = 2..NE \quad (6d)$$

$$x_l \le x^{i,j} \le x_u, z_l \le z^{i,j} \le z_u, u_l \le u^i \le u_u \quad (6e)$$

where ϕ is the objective function and f_d, f_a are the differential and the algebraic equations and h_i is the length of each element. To enforce zero-order continuity of the state variables at the element boundaries, connecting equations are used (6d). It is important that the NLP problem (5) is solved within the period defined by the sampling time of the system to avoid delays and deterioration of the control performance [10].

A. *Offline PWA function calculation (mpQP problem)*

Explicit or multi-parametric MPC (mpMPC) is a multi-parametric programming technique that can compute off-line the control law for a given optimization problem using a piecewise affine (PWA) approximation defined over a polyhedral partition of the feasible variable space. The optimization problem is solved off-line and the control law is obtained as a function of the parameters of the process and the regions in the state/output space where these parameters are valid [7]. The mpMPC approach involves the use of a discrete-time constrained state space linear time-invariant system. Considering that, the MPC problem (1) can be recast as a multi-parametric Quadratic Problem (mpQP) which can be solved with multi-parametric programming techniques [7] and involves a systematic exploration of the parameter space (ϑ). The resulting map consists of a set of convex non-overlapping polyhedra, critical regions (*CR)*, which are bounded by a unique set of active constraints while the corresponding control law is piecewise linear in the form:

$$A_{CR,i}\vartheta \le b_{CR,i} \Rightarrow u = C_{CR,i}\vartheta + d_{CR,i} \quad i = 1,2,\ldots N_{CR} \quad (8)$$

where N_{CR} is the number of critical regions, $A_{CR}, b_{CR}, C_{CR}, d_{CR}$ are constants defining each region CR, i and the derived optimal control action within.

B. *Search Space Reduction*

The main barrier for the applicability of NMPC is its computational demands caused by the online solution of the optimization problem at every iteration. A number of very promising works appear in the literature that approach this issue including the use of a warm-start homotopy path method [11], a PWA approximation for warm-starting [12], and advanced preprocessing [9]. Our primary objective focuses on the same issue, the reduction of the computational effort for the solution of the NLP problem between successive iterations. This is achieved by the use of a warm-start initialization procedure of the NLP solver that takes advantage of the information gained from the previous iteration at each interval and can significantly decrease the number of iterations towards the optimum point [13]. Furthermore a Search Space Reduction (SSR) technique of the feasible space is used which constitutes the main idea of the proposed framework. The SSR technique defines the region in a variable's feasible space that includes the optimum solution for a given objective function. The proposed synergy reduces the search space to a smaller subset around a suggested solution provided by a PWA approximation of the system's feasible space. Thus, the NLP solver has a reduced variable space to explore. Based on the fact that the special treatment of the bounds can lead to substantial computational savings [14] we aim at the adjustment of the search space through the modification of the bounds at every iteration. In this context an mpMPC controller is used prior to the solution of the NLP problem. Although the mpMPC controller is designed based on a linearized approximation of the nonlinear model, it can provide an initial estimate of the region where the optimum solution of the NLP problem lies. This suggested solution (u_{mp}) is transformed into upper and lower bounds ($bu_{act,low}, bu_{act,up}$) augmented by a deviation term (e_{bu}):

$$e_{bu} = \frac{bu_{f,up} - bu_{f,low}}{by_{f,up} - by_{f,low}} e_{y,\max} \tag{9}$$

where $bu_{f,up}, bu_{f,low}$ are the feasible upper and lower bounds of variable u, while $by_{f,up}, by_{f,low}$ are the respective bounds for variable y. The term $e_{y,\max}$ is the maximum model mismatch between the linearized and the nonlinear model and it is determined by an offline simulation study that involves the whole operating range of y. The modification of the bounds is performed at every iteration and as a consequence the search space of u is reduced:

$$bu_{act,low} = \begin{cases} u_{mp} - e_{bu} & ,(u_{mp} - e_{bu}) \geq bu_{f,low} \\ bu_{f,low} & ,(u_{mp} - e_{bu}) < bu_{f,low} \end{cases} \tag{10}$$

$$bu_{act,up} = \begin{cases} u_{mp} + e_{bu} & ,(u_{mp} + e_{bu}) \leq bu_{f,up} \\ bu_{f,up} & ,(u_{mp} + e_{bu}) > bu_{f,up} \end{cases}$$

where $bu_{act,low}, bu_{act,up}$ are the active bounds for u. Therefore the optimizer has a set of updated bounds for the respective manipulated variable u. Apart from the bounds modification the rest of the NLP problem formulation remains the same [15]. The proposed strategy at sampling interval k is summarized in Algorithm 1.

Algorithm 1 SSR based on PWA and NLP problem

Input: Warm-start solution (x_k, u_k, y_k, Hessian H), measured variables (y_k^{meas}), parameters (p_k), set-points ($y_{sp,k}$)

Output: Vector of manipulated variables u_{k+1}

1: Calculate error e_k and $\hat{y}_k$

2: Locate CR_i for parameter vector ϑ_k and obtain u_{mp}

3: Calculate $bu_{act,low}, bu_{act,up}$

4: Modify bounds $u_l = bu_{act,low}, u_u = bu_{act,up}$

5: Solve NLP problem (5)

6: Obtain u_{k+1}^1 from $u_{k+1} = [u_{k+1}^1, \ldots, u_{k+1}^{NE}]$

Based on the above analysis the explicit solution can direct the warm-start procedure for the solution of the NLP problem and thus improve its performance. The proposed method is used subsequently to control a PEMFC system.

III. PEM Fuel Cell System

A PEM fuel cell system has four distinct, yet interacting, subsystems which are related to the power production, the gas supply, the temperature and the water management. Each subsystem has its own control objective [1] and a number of sensors and actuators are used to monitor the system's behavior. In our work a small-scale fully automated fuel cell unit was used which was designed and constructed at CPERI/CERTH [5]. The variables that constitute the Input Output (I/O) field of the unit are acquired by a Supervisory control and Data Acquisition (SCADA) system. The PEM fuel cell is by Electrochem®, the power is drawn from the fuel cell through a DC load, and the air and the hydrogen are supplied from pressurized cylinders. Hydrators and heated lines are used to provide the proper humidity of the inlet gases. The temperature is maintained by an air cooling subsystem and an electrical resistance. The fuel cell unit is modeled by an experimentally validated semi-empirical nonlinear dynamic model [16] that takes into account the mass balances of the gases, an energy balance and electrochemical equations and it is used at the core of the proposed control scheme.

A. Operation and control objectives

The performance and longevity of the PEMFC are strongly influenced by the operating conditions therefore it is important to control each subsystem. The main control objective is to deliver the demanded power while operating at a safe region and concurrently minimize the fuel consumption at stable temperature conditions. These objectives are accomplished by the configuration of Fig. 1.

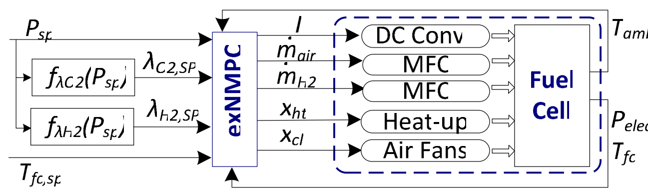

Figure 1. Control configuration and information flow

The power demand (P_{SP}) is achieved by a proper current (I) determination which is applied to the FC by the converter (DC load) connected to the system. The safe operation is maintained by manipulating the air and hydrogen flows ($\dot{m}_{air}, \dot{m}_{H2}$) in order to achieve certain set points of the excess ratios ($\lambda_{O2}, \lambda_{H2}$) and avoid starvation. The excess ratios are expressed as the ratios of the input flow of each gas to the consumed quantities due to reaction [1,3]. Furthermore an important issue is to minimize the air and fuel consumption; therefore the control scheme adjusts online the excess ratio set-points ($\lambda_{O2,SP}, \lambda_{H2,SP}$). This adjustment is based on a function ($f_{\lambda i}(P_{SP}), i \in (O_2, H_2)$) derived by the experimental evaluation of the excess ratios for different power demands at various current levels [5]. The updated set-points are then applied in a feedforward manner to the controller. Finally the operating temperature ($T_{fc,SP}$) is controlled by two mutually exclusive subsystems, one for the heat-up (x_{ht}) and another for the cooling (x_{cl}).

As the fuel cell system operates over time, the produced voltage might deviate from its nominal. When the system starts-up a temporary deviation may occur caused by the fact that the membrane might not be fully hydrated. For longer periods of time, (e.g. few months) a permanent deviation from the initial behavior is observed due to the degradation in the membrane. Driven by these practical issues it is important to rely on a control scheme able to compensate such an offset in the system's behavior.

B. Problem formulation

The NLP problem is formulated based on the dynamic nonlinear model [15] and it is solved using a reduced gradient-based solver [8] that executes a sequence of major and minor iterations until the optimum solution is found. At the major iterations a linearly constrained NLP subproblem issolved, whereas in the minor iterations the reduced gradient method is applied. According to the control objectives ($y_{SP} = [P_{SP}, T_{fc,SP}, \lambda_{O2,SP}, \lambda_{H2,SP}]$), there are five manipulated variables ($u = [I, \dot{m}_{air,in}, \dot{m}_{H2,in}, x_{ht}, x_{cl}]$) and four controlled variables ($y = [P_{SP}, T_{fc}, \lambda_{O2}, \lambda_{H2}]$). Three of the manipulated variables (I, x_{ht}, x_{cl}) are selected to have varying bounds during the operation of the system, that mainly affect two of the controlled variables (P_{SP}, T_{fc}). These variables are selected due to their influence on the PEMFC system. Based on the SSR technique analyzed in Section II.C a PWA function for each controlled variable is required. Prior to the solution of the mpQP problem two linear discrete state space models are derived by a model identification procedure. The first model (ss_P) approximates the behavior of power, has one input (*I*), one output variable (*P*) and two states ($x_{P,1}, x_{P,2}$). The second model (ss_{Tfc}) approximates the temperature and has two input variables (x_{ht}, x_{cl}), one output (T_{fc}), one disturbance (T_{amb}) and two states ($x_{Tfc,1}, x_{Tfc,2}$). For each linear model (ss_P, ss_{Tfc}) an mpQP problem is formulated in order to derive a PWA function. The first mpQP problem involves one optimization variable (*I*) and five parameters $\vartheta_P = [x_{P,1}\ x_{P,2}\ I\ P\ P_{sp}]$ and the resulting optimal map consists of $N_{CR,P} = 57$ critical regions, whereas the second involves six parameters $\vartheta_{Tfc} = [x_{Tfc,1}\ x_{Tfc,2}\ T_{amb}\ T_{fc}\ T_{fc,sp}]$ and the resulting space, is partitioned into $N_{CR,Tfc} = 23$ critical regions. Based on these critical regions ($N_{CR,P}, N_{CR,Tfc}$) the bounds of I, x_{ht}, x_{cl} are adjusted accordingly while the bounds of the other two variables ($\dot{m}_{air}, \dot{m}_{H2}$) are fixed at their feasible bounds. The nonlinear dynamic model of the PEMFC is discretized at 10 finite elements (NE) having 4 collocation points (N_{cop}) each, resulting to 441 variables and 381 equations. The Jacobian matrix was calculated analytically and has 3375 non-zero elements (density: 2.009%). The prediction (T_p) and control (T_c) horizons are 5sec and 500ms.

IV. Analysis of Simulation and Online Experiments

The behavior of the proposed framework is illustrated through two case studies. The first case explores the effect that the SSR technique has to the solution of the NLP problem whereas in the second case the exNMPC is deployed to the experimental unit and its response is presented.

A. Case study 1 - Simulation Results

The fist case involves a scenario with few step changes of the power demand while the fuel cell temperature is maintained at a specific level (65°C). The response of the proposed exNMPC is compared to an NMPC controller using the same nonlinear dynamic model (Section II.B) and the same optimization method (Section II.A). The difference between them is that in the exNMPC the bounds of the selected variables are adjusted based on the proposed SSR technique. The simulation duration is 40sec.

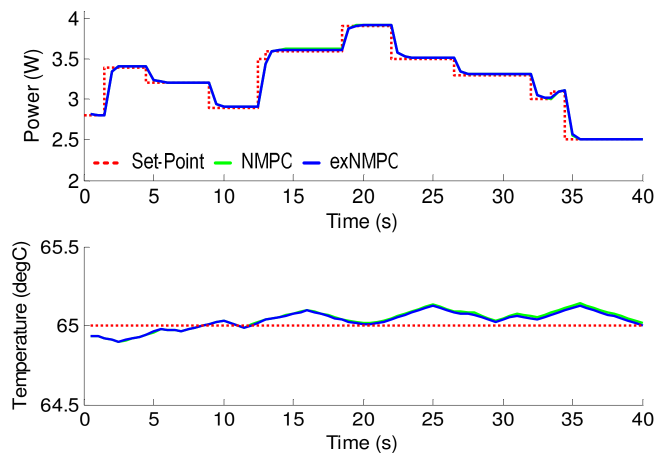

Figure 2. a) Power demand profile and produced power by exNMPC and NMPC. B) Fuel cell temperature.

Fig. 2. illustrates that the power demand is delivered upon request by both controllers (NMPC, exNMPC). Furthermore the temperature is controlled at the desired set-point with a negligible error (±0.3°C).

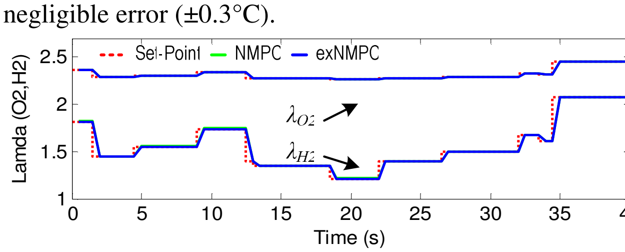

Figure 3. Oxygen and hydrogen excess ratio profiles.

Fig. 3 illustrates the respective oxygen and hydrogen excess ratio profiles that are adjusted according to the power demand. The fuel cell operates at a safe region since the excess ratios of the gases are kept above the minimum ($\lambda_{O2}, \lambda_{H2} > 1$). Figs 2 and 3 show that both controllers (NMPC and exNMPC) have similar behavior in terms of accuracy. Subsequently the importance of the proposed SSR technique and its effect to the solution of the NLP problem regarding the computational requirements is presented. The aforementioned simulation scenario is tested with four different methods regarding the initialization of the optimization problem. First a cold start optimization is performed (M1), followed by a test where the cold start is complemented by the SSR technique (M2). The next two tests are performed with a warm start initialization method, with (M4) and without (M3) the SSR technique. Figs 2 and 3 present the results from M3 and M4, namely the NMPC and the exNMPC controllers and Table 1 presents the performance metrics of these four methods.

TABLE I
OPTIMIZATION TIME, ITERATION AND FUNCTION CALLS

Method	Max opt time (s)	Avg time (ms)	Total minor Iters	Max minor Iters	Max Fun. calls
M1:Cold	3.93	1086	23594	1639	3443
M2:Cold+ SSR	2.30	861	20370	1063	2101
M3:Warm	0.863	413	5038	346	762
M4:Warm+SSR	0.48	207	1851	124	368

The maximum and the average optimization time are decreased when the search space is adjusted (M2) even though a cold start initialization is performed. But the maximum optimization time is beyond the system sampling time specifications. Therefore it is not practical to use cold start initialization methods (M1, M2). On the other hand, the warm start initialization (M3, M4) of the optimizer shows superior performance compared to the cold start. We observe an improvement of the average optimization time in M4 method which is affected by the iterations that the optimizer performs in order to find the optimum values for the decision variables. The total number of iterations is decreased by 64% when the search space is adjusted (M4).

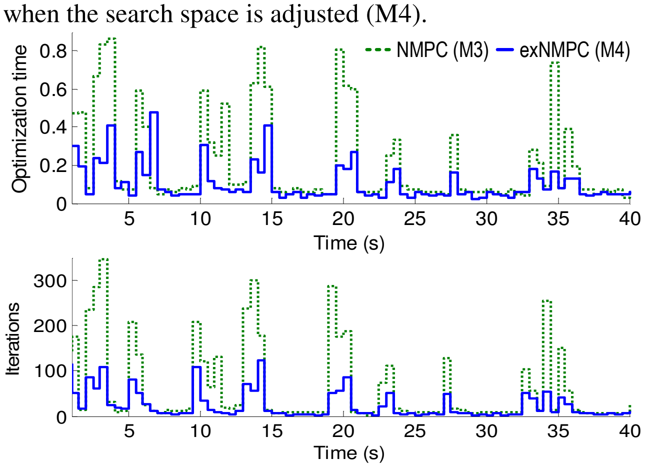

Figure 4. a) Optimization time per interval and b) Iterations per interval for methods M3 (NMPC) and M4 (exNMPC)

In steady state both methods (M3, M4) have similar behavior with optimization time 40ms to 60ms. After a step change M4 method requires less effort concerning the number of iterations to minimize the objective function as it searches in a reduced space (Fig. 4). Method M3 requires a greater number of iterations and performs much more function calls. Fig. 5 depicts the exploration of the search space for the optimum value of I during one sampling interval after a power step change ($t = 19\sec, P_{sp} = 3.9W$).

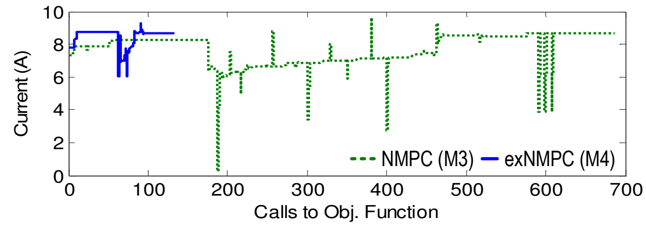

Figure 5. Function evaluation during one sampling interval after a power step change.

In M3 method, I changes between 0.3A and 9.9A and the optimizer performs 685 function calls, while in M4, I deviates between 6.2A and 9.1A and only 132 function calls are performed. Both methods results to the same optimum value (M3: 8.689A, M4: 8.683A) but M3 requires 811ms while M4 requires only 201ms. By this illustrative example the effect of the SSR is clearly shown.

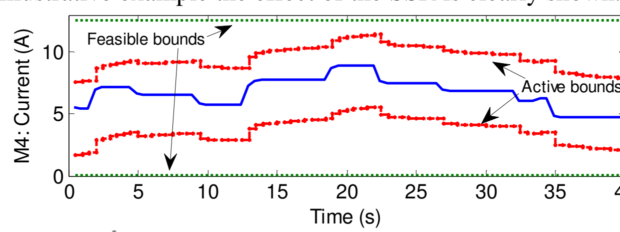

Figure 6. Feasible and active upper and lower bounds and optimum values for I (use of exNMPC, method:M4)

Fig. 6 presents the upper and lower bounds of I, along with the optimum I profile for method M4. Both methods result to the selection of the same optimum current value with a maximum difference of 11mA. From the aforementioned analysis it is obvious that method M4 outperforms the others, for the given problem. Besides the improved optimization time the accuracy of the solution remains the same between M3 and M4. Thus, it is selected to be applied online to the system.

B. Case study 2 - Online Implementation

The exNMPC framework is deployed online to the fuel cell unit using a custom made OPC-based interface that was developed for the communication between the optimizer and the SCADA system. An experimental scenario is presented involving two step changes in temperature and various changes in power demand. The duration of the scenario is 19min and the sampling time is 500ms. The scope of the controller is to concurrently fulfill the four objectives ($y_{SP} = [P_{SP}, T_{fc,SP}, \lambda_{O2,SP}, \lambda_{H2,SP}]$) within the predefined time constraints of the system. Fig. 7 illustrates the fuel cell temperature and the desired profile. The temperature drops from 55°C to 48°C and then it rises to 61°C. When the set-point is reached the system settles to the desired value with a negligible deviation of ±0.1°C after a few oscillations. The maximum overshoot and undershoot is 0.6°C and -0.9°C.

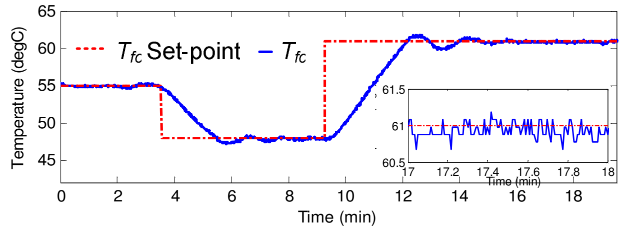

Figure 7. Step changes of the fuel cell temperature and zoom in at steady state for one minute

A number of power demand changes were also applied to the system (Fig. 8) and we observe that the exNMPC framework exhibits good response to frequent and abrupt changes of the power demand. Finally the mean squared error (MSE) and some performance metrics are presented in Table 2.

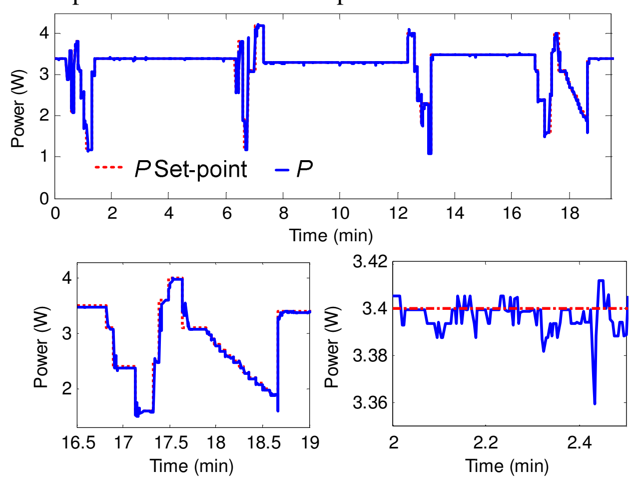

Figure 8. Power response a) during the experimental scenario (19min), b) zoom-in at a few step changes (2.5min), c) steady state behavior (30sec)

TABLE 2
PERFORMANCE OF THE ONLINE EXNMPC FRAMEWORK

MSE from set-point		Performance metrics	
Power	12mW	Max. opt. time	307ms
Temperature	0.1°C	Average opt. time	197ms
λ_{O2}	1.4×10^{-3}	Max. Iterations	162
λ_{H2}	7.2×10^{-4}	Max. func. calls	425

The MSE shows that the exNMPC can accurately fulfill the objective for power delivery (P_{SP}) in a safe operating region while minimizing the gas consumption ($\lambda_{O2,SP}, \lambda_{H2,SP}$) and concurrently provide a stable environment with respect to the temperature ($T_{fc,SP}$) condition. From the performance metrics of Table 2 it is evident that the computational constraints are satisfied and the results from the simulation study are verified by the online application of the controller to the fuel cell unit. Hence, the optimum operation of the fuel cell is achieved at varying operating conditions and rapid power changes.

V. CONCLUSIONS

In this work a new approach that reduces the computational requirements of an NLP solver which is used in an NMPC formulation is presented. A warm-start method is complemented by an SSR technique, relying on a PWA function that sets the basis for the improved behavior of the optimizer. The importance of this synergy is illustrated by a challenging multivariable nonlinear control problem with measured and unmeasured variables that involves concurrently four operation objectives for a PEM fuel cell system. The response of the proposed framework is initially presented through a simulation study that focuses on the influence of the SSR to the solution of the NLP problem. Afterwards the exNMPC is deployed to the experimental fuel cell and it is validated online. The performance of the exNMPC controller shows promising behavior in terms of computational demands and at the same time it guarantees that the PEMFC system operates at an optimum manner.

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