ANALYSIS AND CONTROL OF FUEL CELL MODELS

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ABSTRACT

Bifurcation analysis and Multiobjective Nonlinear Model Predictive Control (MNLMPC) calculations were performed on proton exchange membrane (PEM) and solid oxide fuel cells(SOFC). The MATLAB program MATCONT was used to perform the bifurcation analysis. The optimization language PYOMO was used with the state-of-the-art global optimization solvers IPOPT and BARON for the MNLMPC calculations. The bifurcation analysis revealed the existence of limit and branch points for the PEM fuel cells. Limit points and Hopf bifurcation points were observed for the SOFC. In both cases, limit and branch points enabled the MNLMPC calculations to converge to the Utopia solution. The Hopf bifurcation points were eliminated using an activation factor involving the tanh function.

KEYWORDS

Bifurcation, optimization, control, fuel cell

1. INTRODUCTION

1.1. Background

Lehnert et al [1] modelled Gas Transport Phenomena in SOFC Anodes. Yakabe et al [2] modeled the performance of an Anode-Supported Solid Oxide Fuel Cell. Singhal et al [3] wrote a book on the design and applications of Solid oxide fuel cells. Eckl et al [4] analysed the water management in a Self-Humidifying Polymer Electrolyte Fuel Cell Stack. Kulikovsky et al [5] , investigated the origin of Voltage oscillations of a Polymer Electrolyte Fuel Cell in a Galvanostatic Regime.

Zhang et al [6] performed a bifurcation analysis of anode Potential Oscillations in PEMFCs with CO in the anode feed. Mangold et al [7] analyzed high-temperature fuel cells' current instabilities. Knights et al [8] investigated aging mechanisms and the lifetime of PEFC and DMFC. Benziger et al [9] studied the dynamic Response of PEM Fuel cells to changes in load. Katsaounis et al [10] investigated the bistability and oscillations of PEM fuel cells.

Ziegler et al [11] performed a two-phase dynamic modeling of the PEMFC. Noponen et al [12] investigated the feasibility of auto-thermally reformed natural gas on anode-supported solid oxide fuel cells. Na and Guo [13] developed an efficient and economic design of PEM fuel cell systems by multi-objective optimization while Na Guo and Diong [14] developed a nonlinear control mechanism of PEM fuel cells by exact linearization. Na and Guo [15] developed a feedback-linearization-based nonlinear control for PEM fuel cells. Huang el al [16] demonstrated the oscillation of the electric current during direct methane oxidation over Ni-Added LSCF-GDC anode of solid oxide fuel cells. Kellog et al [17] studied the effectiveness of the anode in a solid oxide fuel cell with hydrogen/oxygen mixed gases. Matsui et al [18] studied the performance deterioration of Ni/YSZ anode induced by electrochemically generated seam in solid oxide fuel cells. Talj et al [19] experimentally validated the PEM fuel-cell reduced-order model with a moto-compressor higher-order sliding-mode control. Murakami [20] demonstrated the activation of LSM Electrode related to the potential oscillation under cathodic polarization. Marina et al [21] studied the polarization-induced interfacial reactions between nickel and selenium in ni/zirconia SOFC anodes/ Wang et al [22] studied the redox of Ni/YSZ anodes and oscillatory behavior in single-chamber SOFC under methane oxidation conditions.

Lu et al [23] spontaneous oscillations of cell voltage, power density, and anode exit CO concentration in a PEM fuel cell. Yoshizumi et al [24] studied the sulfur poisoning of SOFCs. Csörgo et al [25] performed a numerical and analytical study of bifurcations in a model of electrochemical reactions in fuel cells. Rubio et al [26] performed optimal control tasks on PEM fuel cell problems while Sands and co-workers [27, 28] investigated oscillatory behavior in SOFC problems.

1.2. Motivation and Objectives

So far, all bifurcation and optimal control calculations for fuel cells have been performed disjointly. Sridhar [29] solved several problems where bifurcation analysis was conducted in conjunction with multiobjective nonlinear model predictive control(MNLMPC) calculations and demonstrated that the presence of limit points and branch points (that cause the existence of multiple steady-states) were beneficial and resulted in the MNLMPC calculations to converge to the Utopia point (the best possible solution). Sridhar[30] showed that an activation factor involving the tanh function would actually eliminate the unwanted oscillation causing Hopf bifurcation points. The main aim of this paper is to perform bifurcation analysis in conjunction with multiobjective nonlinear model predictive control(MNLMPC) calculations to 1) show that the presence of limit points and branch points result in the convergence of the MNLMPC to the Utopia solution in both PEMFC and SOFC problems and 2) show that an activation factor involving the tanh function will eliminate the Hopf bifurcations that occur in SOFC problems validating the analysis of Sridhar[29, 30]. This paper is organized as follows. First, the PEMFC and SOFC dynamic models are described. Then the details of bifurcation analysis and MNLMPC calculations are presented followed by the results, discussion, and conclusions.

2. FUEL CELL MODELS

We use the model of the PEM fuel cell dynamics described by Rubio et al. [26]. The model equations are

$$\begin{aligned}
\frac{dxd1}{dt} &= \frac{RT}{V_a}\left(-\frac{u_1}{P_{OP}}+\frac{2K_rA_Cu_3}{P_{OP}}\right)xd1+\frac{RTu_1}{V_a}-\frac{RT}{V_a}(2K_rA_Cu_3) \\
\frac{dxd2}{dt} &= \frac{RT}{V_c}\left(-\frac{u_2}{P_{OP}}+\frac{K_rA_Cu_3}{P_{OP}}\right)xd2+\frac{RTu_2}{V_c}-\frac{RT}{V_c}(K_rA_Cu_3) \qquad (1) \\
\frac{dxd3}{dt} &= \frac{RT}{V_c}\left(-\frac{u_2}{P_{OP}}-\frac{2K_rA_Cu_3}{P_{OP}}\right)xd3+\frac{RT}{V_c}(2K_rA_Cu_3)
\end{aligned}$$

The parameter values are

$V_a = 6.495;\ A_C = 136.7;\ R = 8.314;\ T = 353;\ N = 35;$

$P_{OP} = 1.01; E_0 = 1.3;\ F = 96485;\ u_1 = 0.2; u_2 = 0.3$

$(xd1, xd2, xd3)$ are the partial pressures of hydrogen, oxygen, and water.

R is the gas constant, F *the* Faraday's constant ; P_{OP} the operating pressure, N the number of cells in the stack. $K_r = N / 4F; V_A, V_C$ are the anode and cathode volumes. u_1, u_2, u_3 are the input Hydrogen, input oxygen and current density. For the bifurcation analysis $u_1 = 0.2; u_2 = 0.3$ and u_3 is the bifurcation parameter. For the MNLMPC u_1, u_2, u_3 are taken as the control variables.

The SOFC model described by Sands [28] is considered. The model equations are

$$\frac{da}{dt} = D_a(a_0 - a) - (\frac{2ab^2}{2a+1})$$
$$\frac{db}{dt} = -D_b b + (\frac{8ab^2}{2a+1}) - 2b^2 \quad (2)$$

D_a, D_b are the dimensionless diffusion coefficients. a is the non-dimensional concentration of methane, and b is the nondimensional concentration of hydrogen, and a_0 (4.02) is the non-dimensional concentration of methane in the fuel stream. For the bifurcation analysis D_a is 2 while D_b is the bifurcation parameter. For the MNLMPC calculations D_a, D_b are the control parameters.

3. Bifurcation Analysis

The MATLAB program MATCONT . (Dhooge Govearts, Kuznetsov, Mestrom and Riet,)[31]. is to locate limit points, branch points, and Hopf bifurcation points. Limit and Branch points cause multiple steady-states while Hopf bifurcation points result in limit cycles/oscillatory behavior. For a set of OD

$$\dot{x} = f(x, \beta) \quad (3)$$

$x \in R^n$.

Let the matrix A be defined as

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} & \frac{\partial f_1}{\partial x_4} & \cdots\cdots & \frac{\partial f_1}{\partial x_n} & \frac{\partial f_1}{\partial \beta} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} & \frac{\partial f_2}{\partial x_4} & \cdots\cdots & \frac{\partial f_2}{\partial x_n} & \frac{\partial f_2}{\partial \beta} \\ \cdots & & & & & & \\ \cdots & & & & & & \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \frac{\partial f_n}{\partial x_3} & \frac{\partial f_n}{\partial x_4} & \cdots\cdots & \frac{\partial f_n}{\partial x_n} & \frac{\partial f_n}{\partial \beta} \end{bmatrix} \quad (4)$$

β would be the bifurcation parameter. A can be written as

$A=[B| \quad \partial f / \partial \beta]$ (5)

The tangent-vector at any point x; ($v=[v_1,v_2,v_3,v_4,....v_{n+1}]$) satisfies

$$Av=0 \qquad (6)$$

B is singular at both limit and branch points.. The n+1 th component of the tangent vector v_{n+1} = 0 at a limit point (LP) and for a branch point (BP) the matrix $\begin{bmatrix} A \\ v^T \end{bmatrix}$ must be singular. At a Hopf bifurcation point,

$$\det(2 f_x(x,\beta) @ I_n) = 0 \qquad (7)$$

@ indicates the bialternate product while I_n is the n-square identity matrix. Hopf bifurcations result in unwanted limit cycles (which in turn cause problems for optimization and control) and should be eliminated.

4. Multiobjective Nonlinear Model Predictive Control (MNLMPC)

The MNLMPC strategy first proposed by Flores Tlacuahuaz [32]is used. For the ODE set given by

$$\frac{dx}{dt}=F(x,u) \qquad (8)$$

$$h(x,u)\le 0 \quad x^L \le x \le x^U; \quad u^L \le u \le u^U$$

let $\sum_{t_{i=0}}^{t_i=t_f} p_j(t_i)$ (j=12..n); be the variables that need to be minimized/maximized simultaneously, t_f is the final time value, and n is the total number of variables that have to be optimized simultaneously. First, the dynamic optimization problems that independently minimize/maximize each variable $\sum_{t_{i=0}}^{t_i=t_f} p_j(t_i)$ are solved individually. The minimization/maximization of each $\sum_{t_{i=0}}^{t_i=t_f} p_j(t_i)$ will lead to the values p_j^* . Then the optimization problem that will be solved is

$$\min\left(\sum_{j=1}^{n}\left(\sum_{t_{i=0}}^{t_i=t_f} p_j(t_i)-p_j^*\right)\right)^2$$

$$\textit{subject to } \frac{dx}{dt}=F(x,u); \quad h(x,u)\le 0 \qquad (9)$$

$$x^L \le x \le x^U; \quad u^L \le u \le u^U$$

This will provide the control values for various times. The first obtained control value is implemented and the rest are ignored. The procedure is repeated until the implemented and the first obtained control values are the same or if the Utopia point ($\sum_{t_{i=0}}^{t_i=t_f} p_j(t_i) = p_j^*$; for all j) is achieved. The optimization package in Python, Pyomo (Hart et al[33]), where the differential equations are automatically converted to algebraic equations will be used. The resulting optimization problem was solved using IPOPT (Wächter And Biegler)[34]. The obtained solution is confirmed as a global solution with BARON (Tawarmalani, M. and N. V. Sahinidis)[35].

5. COMBINATION OF BIFURCATION ANALYSIS AND MNLMPC

A recently published article by Sridhar[29] demonstrated that when MNLMPC calculations converged to the Utopis solution on problems that exhibited Limit and Branch points. This was done by incorporating the singularity condition (because of the limit and branch points) on the co-state equation for the optimal control problem. Details can be found in Sridhar[29].

The tanh activation function where a control value u is replaced by $(u \tanh u/\varepsilon)$ is commonly used in optimal control problems to eliminate spikes in the optimal control profile. Hopf bifurcation points cause oscillatory behavior. Oscillations are similar to spikes and the results demonstrate that the tanh factor also eliminates the Hopf bifurcation by preventing the occurrence of oscillations. Sridhar [30] explained with several examples how the activation factor involving the tanh function successfully eliminates the limit cycle causing Hopf bifurcation points.

6. RESULTS AND DISCUSSION

The bifurcation analysis of the PEM fuel cell showed the existence of branch and limit points both of which cause multiple steady-states. Two limit points for $[xd1, xd2, xd3, u3]$ values of (0.990000 1.010000 0.404000 8.066465) and (1.020080 1.010000 0.404000 8.066465) were found. Additionally a branch point whose $[xd1, xd2, xd3, u3]$ values were (1.010000 1.010000 0.404000 8.066465) was located. This branch point produces two branches. The bifurcation diagram is shown in Fig. 1.

For the MNLMPC calculation involving the PEM fuel cell, the square of difference between $\sum_{t_{i=0}}^{t_i=t_f} (xd1)(t_i)$ and the set point $2+0.5\sin(\pi t_i)$; $(\sum_{t_{i=0}}^{t_i=t_f} (xd1)(t_i) - (2+0.5\sin(\pi t_i)))^2$ was minimized this resulted in a value of zero. Similarly $(\sum_{t_{i=0}}^{t_i=t_f} (xd2)(t_i) - (2+0.5\sin(\pi t_i)))^2$ and $(\sum_{t_{i=0}}^{t_i=t_f} (xd3)(t_i) - (2+0.5\sin(\pi t_i)))^2$ was minimized individually and both results on a value of zero. The overall optimal control problem involved the minimization of

$$(\sum_{t_{i=0}}^{t_i=t_f} (xd1)(t_i) - (2+0.5\sin(\pi t_i)))^2 + (\sum_{t_{i=0}}^{t_i=t_f} (xd2)(t_i) - (2+0.5\sin(\pi t_i)))^2 + (\sum_{t_{i=0}}^{t_i=t_f} (xd3)(t_i) - (2+0.5\sin(\pi t_i)))^2$$

This too resulted in a value of zero demonstrating that the MNLMPC calculations converged to the Utopia point confirming the analysis of Sridhar(2024a)[29] that the presence of limit and branch points would enable the MNLMPC calculations to converge to the Utopia solution. The obtained MNLMPC control values were $[u_1, u_2, u_3]$ =[2.48265, 0.22162, 2.62675]. Figs 2 and 3 show the $[xd1, xd2, xd3]$ and the $[u_1, u_2, u_3]$ profiles. The $[u_1, u_2, u_3]$ profiles exhibit a lot of noise (Fig. 3) This was remedied using the Savitzky-Golay Filter. The Savitzky-Golay filter, is a digital filter widely used for data smoothing and differentiation. The Savitzky-Golay filter maintains the integrity of the original signal preserving the shape and features of the signal. The smoothed-out version of this profile is shown in Fig. 4.

The bifurcation analysis of the SOFC problem revealed a limit point and a Hopf bifurcation point at $[a, b, D_b]$ values of (1.917695 2.302363 2.700133) and (1.657202 2.480196 2.660935). This bifurcation diagram is shown in Fig. 5. The limit cycle caused by this Hopf bifurcation point is shown in Fig. 6. When the bifurcation parameter D_b was modified to $D_b \tanh(D_b)/2$ the Hopf bifurcation point disappears but the limit point (1.917689 2.302367 5.400486) remains (Fig. 7). This confirms the validity of the analysis of Sridhar (2024b)[30] where it was demonstrated that the use of an activation factor involving the tanh function would eliminate the unwanted oscillation causing Hopf bifurcations. For the MNLMPC calculations in the SOFC problem $(a-a_0)^2$ and b^2 were individually minimized. Each minimization resulted in a value of 0. The overall optimal control problem involved the minimization of $(a-a_0)^2 + b^2$ which too resulted in a value of 0 demonstrating that the MNLMPC calculations converged to the Utopia solution confirming the analysis of Sridhar[29] that the presence of limit and branch points would enable the MNLMPC calculations to converge to the Utopia solution. The MNLMPC values of $[D_a, D_b]$ were [2.4390551865805263 2.852301784765789].The [a,b] and the $[D_a, D_b]$ profiles are shown in figures 8 and 9.

These results demonstrate that limit points branch points and Hopf bifurcation points occur in fuel cell problems. The limit and branch points enable the MNLMPC calculations to converge to the Utopia point, confirming the analysis of Sridhar[29] . The Hopf bifurcation points that cause unwanted limt cycles can be eliminated by using an activation factor involving the tanh function confirming the analysis of Sridhar[30].

7. Conclusions and Future work

Rigorous bifurcation analysis and multiobjective nonlinear model predictive control calculations were performed on simple PEM and SOFC fuel cell models. Even these exhibit a high degree of nonlinearity by exhibiting limit points branch points and Hopf bifurcation points. The limit and branch points are actually beneficial as they enable the multiobjective nonlinear model predictive control calculations to converge to the Utopia solution. The Hopf bifurcation points can be eliminated by using an activation factor involving the tanh function. The future work will involve similar work on more complex fuel cell models.

Availability of data and material

All data used is presented in the paper

Competing interest

The author, Dr. Lakshmi N Sridhar has no conflict of interest.

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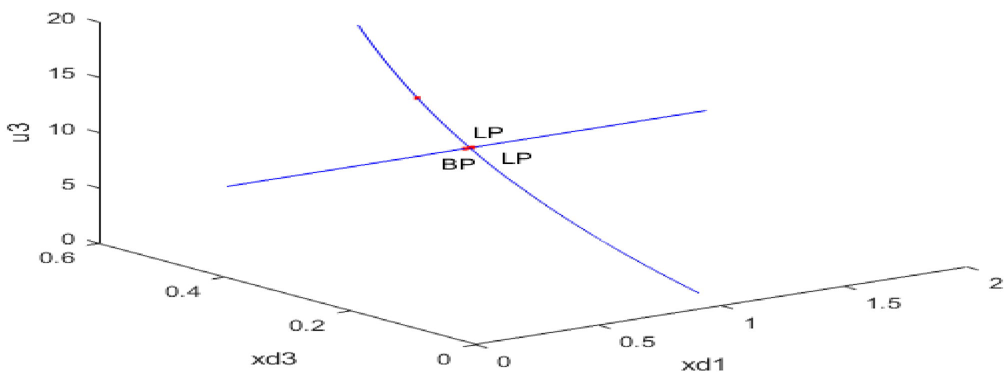

Fig. 1 bifurcation diagram for PEM fuel cell problem

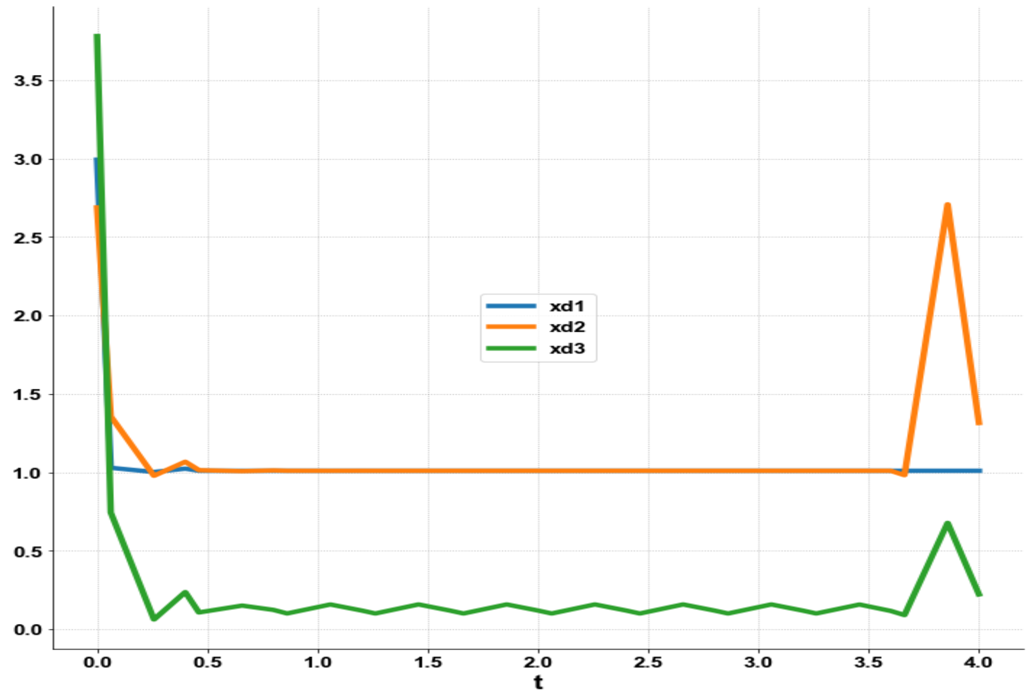

Fig. 2 xd1 xd2 xd3 profiles for MNLMPC involving PEM fuel cell

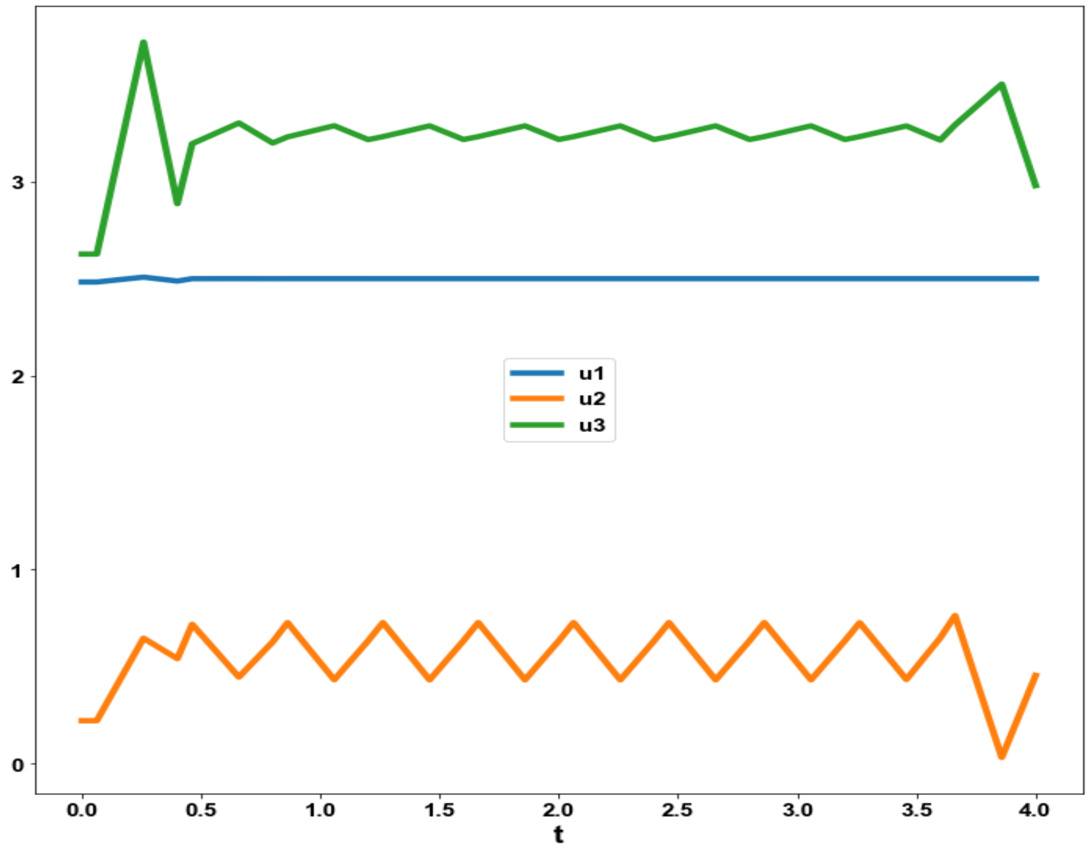

Fig. 3 u1 u2 u3 profiles for MNLMPC involving PEM fuel cell (no filter was used)

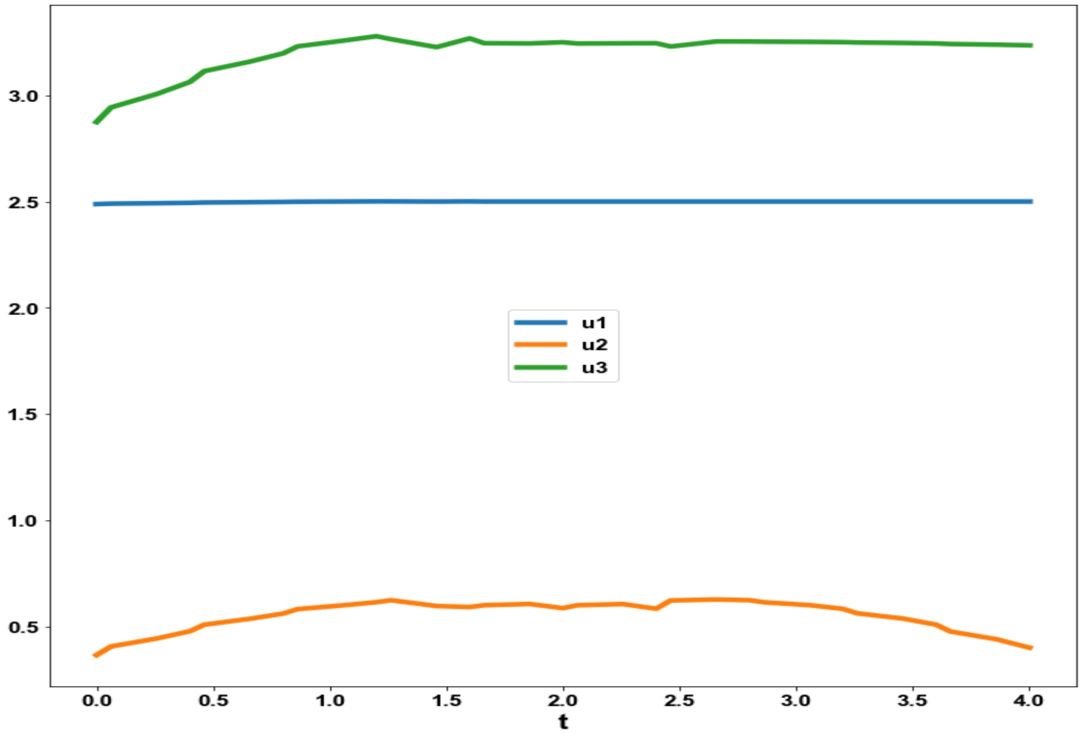

Fig. 4 u1 u2 u3 profiles for MNLMPC involving PEM fuel cell (Savitzky Golay Filter was used)

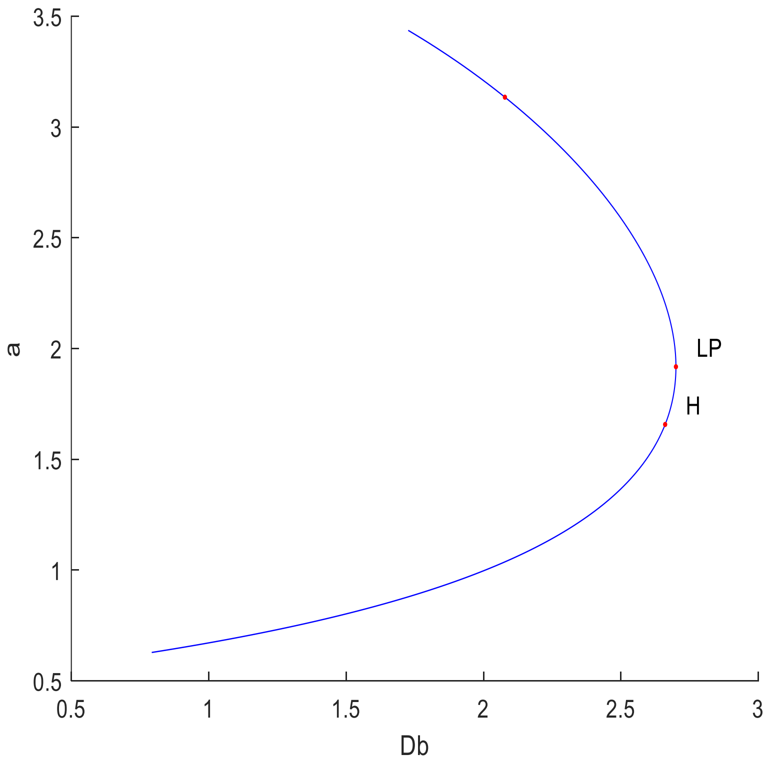

Fig. 5 Bifurcation diagram for SOFC

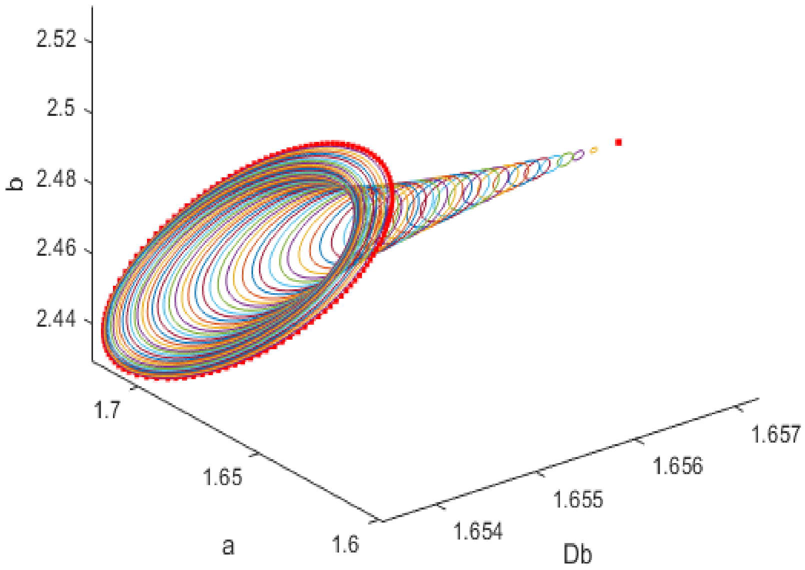

Fig. 6 Limit cycle produced by Hopf bifurcation in SOFC

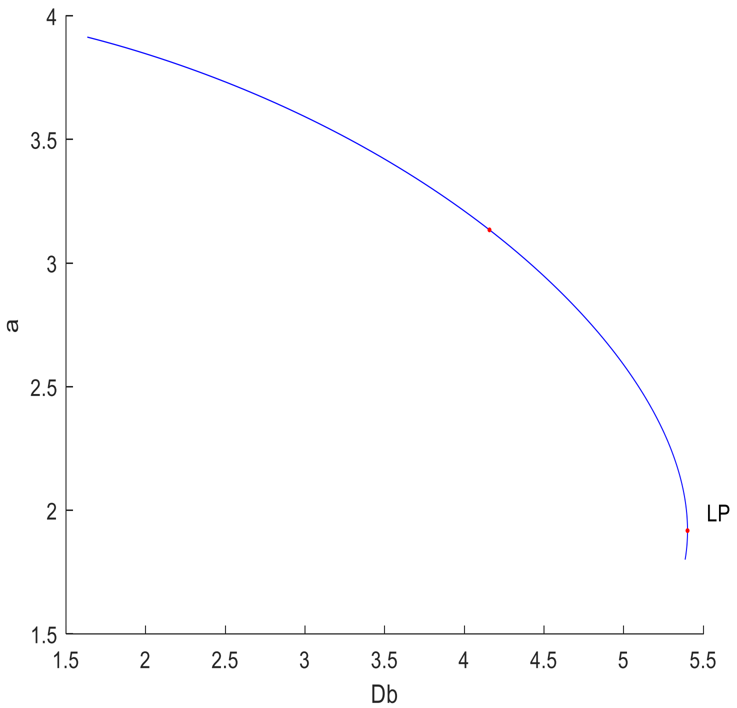

Fig. 7 Hopf bifurcation point eliminated when D_b was modified to $D_b \tanh(D_b)/2$

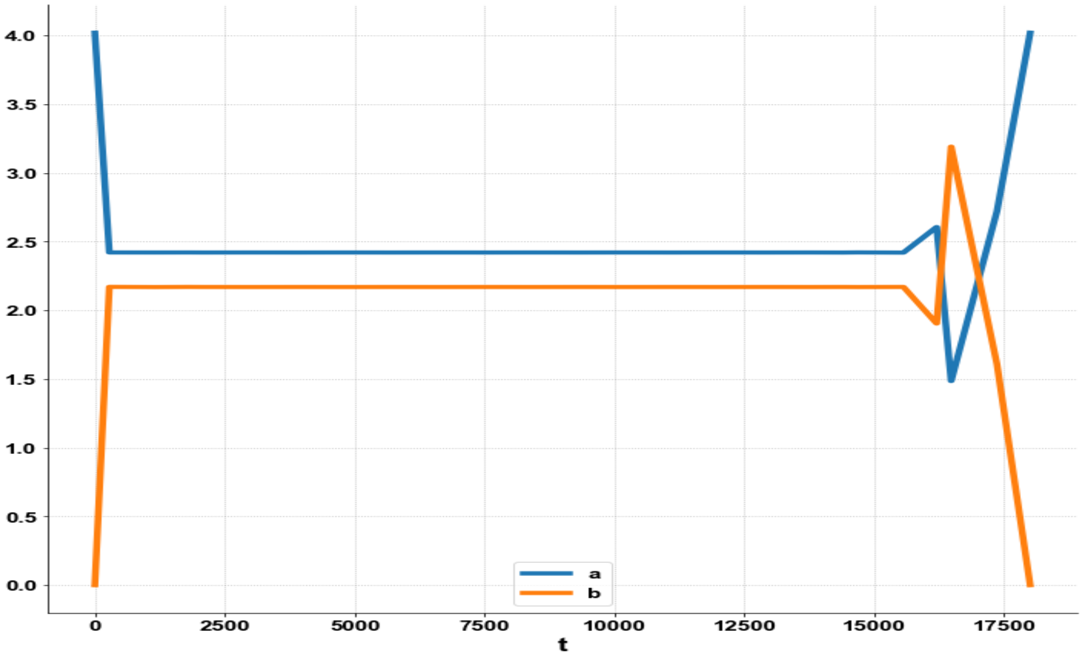

Fig. 8 [a,b] profiles for MNLMPC calculations of SOFC

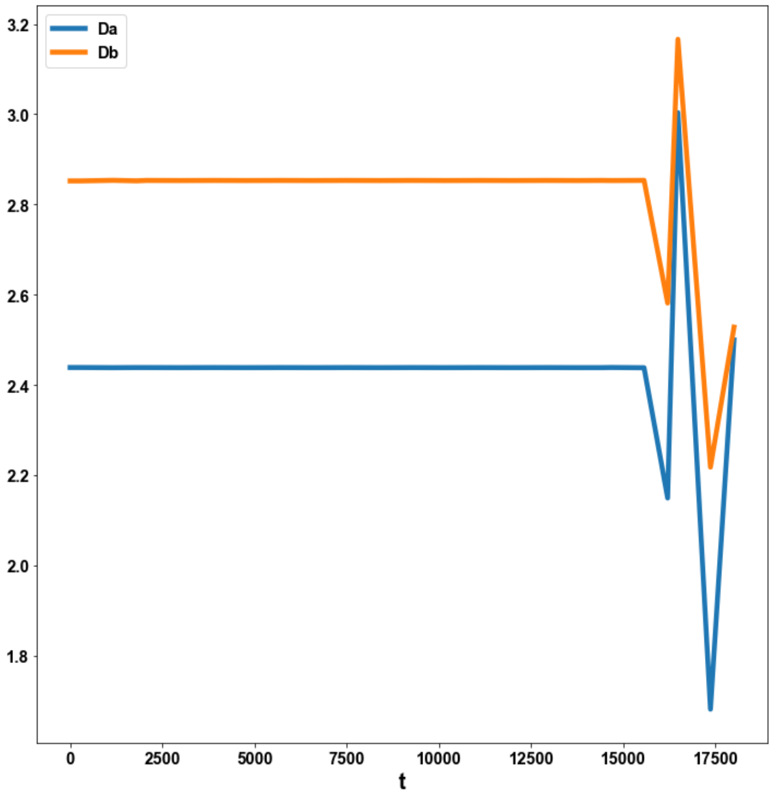

Fig. 9 $[D_a, D_b]$ MNLMPC of SOFC problem