

Distributed parameter PEMFC model order reduction

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ABSTRACT: *This work focuses on obtaining an order-reduced model from a nonlinear single PEMFC model, which incorporates the effects of distributed parameters that are relevant for its proper functioning and performance. The original model is an in-house MATLAB[®] code, flexible enough to manipulate the underlying model equations and apply model order reduction (MOR) techniques. The obtained order-reduced model is suitable to perform numerical simulations and design efficient controllers for the original nonlinear partial differential equations (PDE) model.*

Keywords: *PEMFC, distributed parameter modeling, model order reduction.*

1. INTRODUCTION

Distributed parameter modeling is required to accurately consider space variations, which are important regarding the performance and durability of the Proton Exchange Membrane Fuel Cells (PEMFC) [1-3]. However, the number of differential and algebraic equations (DAE) obtained from the discretization of a set of partial differential equations (PDE) is very large, and this not only slows down the numerical simulations, but also complicates the design of online model-based controllers.

The inclusion of complex DAE models within model-based control schemes requires a previous simplification. This work presents a method to simplify complex models that consists of reducing the order while preserving the relationship between certain input and output variables, applied to a nonlinear distributed parameter single PEMFC model.

2. DESCRIPTION OF THE SYSTEM

This work considers a single cell of one channel (Fig. 1) that includes all the functional parts of the PEMFC: bipolar plates, gas channels, gas diffusion layers, catalyst electrode layers, the proton exchange membrane and a cooling system. This simple model suits the detailed analysis of spatial variations. The case study selected in the work is a 0.4 m along-the-channel single cell (area $0.4 \times 10^{-3} \text{ m}^2$) with Nafion 117 membrane. The parameters of the membrane are taken from [4, 5].

A distributed parameter model was used to represent this system. Partial differential equations and algebraic constraints have been discretized by finite differences into 10 volumes (uniformly distributed) along z-direction. As a result, a set of

DAE (110 ODE and 310 algebraic equations) was obtained. This new set of model equations was implemented and numerically solved in MATLAB[®], using a DAE solver. The complete discretization process was presented in [6].

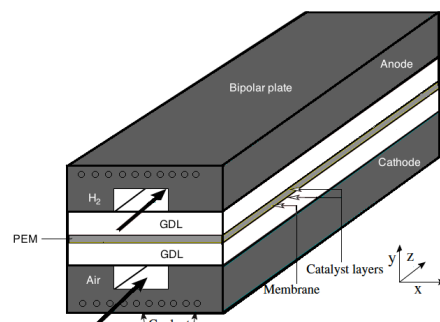


Fig. 1. Single cell distributed parameter model geometry.

3. MODEL ORDER REDUCTION

The method used to reduce the order of the case study nonlinear DAE model requires finding the underlying ODE description of the original DAE model, linearizing around an equilibrium point of interest, then computing the corresponding controllability and observability functions. The final step is finding an appropriate model realization that reveals which states of the original system can be truncated without considerably affecting the original input-output behavior [7].

3.1. Balanced truncation model order reduction

Consider the nonlinear control system, assuming that the DAE model has an underlying ODE description as stated in [7].

$$\begin{aligned}\dot{x} &= f(x) + g(x)u, \\ y &= h(x),\end{aligned}\quad (1)$$

with $x \in \mathbb{R}^N$, $u \in \mathbb{R}^M$, $y \in \mathbb{R}^P$ and $f(0) = 0$.

The controllability function $L_c(x)$ is the solution of the optimal control problem

$$L_c(x) = \inf_{u \in L^2((-\infty, 0), \mathbb{R}^M)} \frac{1}{2} \int_{-\infty}^0 \|u(t)\|^2 dt, \quad (2)$$

subject to the boundary conditions $x(-\infty) = 0$, $x(0) = x$ and the system (1). Roughly speaking, $L_c(x)$ measures the minimum 2-norm of the input signal necessary to bring the system to the state x from the origin.

As shown in [8], L_c obeys the Hamilton-Jacobi-Bellman PDE

$$\partial_x L_c f + \frac{1}{2} \partial_x L_c g g^T \partial_x^T L_c = 0, \quad (3)$$

in a domain $U_c \subset \mathbb{R}^M$ containing the origin, where the vector field $-(f + g g^T \partial_x^T L_c)$ is asymptotically stable.

The observability function $L_o(x)$ is the 2-norm of the output signal obtained when the system is relaxed from the state x

$$L_o(x) = \frac{1}{2} \int_0^\infty \|y(t)\|^2 dt = \frac{1}{2} \int_0^\infty \|y(t)\|^2 dt, \quad (4)$$

with $x(0) = x$ and subject to (1) with $u = 0$, that is, $\dot{x} = f(x)$. It obeys the Lyapunov PDE

$$\partial_x L_o f + \frac{1}{2} h^T h = 0, \quad L_o(0) = 0 \quad (5)$$

in a domain $U_o \subset \mathbb{R}^N$ where $f(x)$ is asymptotically stable.

For linear control systems,

$$\begin{aligned}\dot{x} &= Ax + Bu, \\ y &= Cx,\end{aligned}\quad (6)$$

assumed to be observable, controllable and Hurwitz, both $L_c(x)$ and $L_o(x)$ are quadratic functions

$$L_c(x) = \frac{1}{2} x^T W_c^{-1} x, \quad (7)$$

$$L_o(x) = \frac{1}{2} x^T W_o x, \quad (8)$$

where $W_c > 0$ and $W_o > 0$, the controllability and observability Gramians, are the solutions to the matrix Lyapunov equations

$$\begin{aligned}AW_c + W_c A^T + BB^T &= 0 \\ A^T W_o + W_o A + C^T C &= 0\end{aligned}\quad (9)$$

and are explicitly given by

$$\begin{aligned}W_c &= \int_0^\infty e^{At} BB^T e^{A^T t} dt \\ W_o &= \int_0^\infty e^{A^T t} C^T C e^{At} dt\end{aligned}, \quad (10)$$

although the direct numerical solution of (12) is computationally preferred.

As shown by Moore [9], the matrix W_c provides information about the states that are easy to control (in the sense that signals u of small norm can be used to reach x), while W_o allows finding the states that are easily observable (in the sense that they produce outputs of large norm). From the point of view of the input-output map given by (6), it is desirable to select the states that score well on both counts, and this leads to the concept of balanced realization, for which $W_c = W_o$.

The balanced realization is obtained by means of a linear transformation $x = Tz$, with T computed as follows:

1. Solve the Lyapunov equations (9), with solutions $W_c > 0$, $W_o > 0$.
2. Perform Cholesky factorizations of the Gramians

$$W_c = XX^T, \quad W_o = YY^T, \quad (11)$$

with $X > 0$ and $Y > 0$.

3. Compute the SVD of $Y^T X$

$$Y^T X = U \Sigma V^T, \quad (12)$$

with U and V orthogonal and

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_N), \quad (13)$$

with $\sigma_1 > \sigma_2 > \dots > \sigma_N > 0$.

The σ_i are the Hankel singular values, and their squares $\tau_i = \sigma_i^2$ are often referred to as the squared singular values of the system.

4. The balancing transformation is given then by

$$T = X V \Sigma^{-1/2}, \quad \text{with } T^{-1} = \Sigma^{-1/2} U^T Y^T. \quad (14)$$

5. The balanced realization is given by the linear system

$$\tilde{A} = T^{-1} A T, \quad \tilde{B} = T^{-1} B, \quad \tilde{C} = C T, \quad (15)$$

and in the new coordinates

$$\begin{aligned}\tilde{W}_c &= T^{-1}W_cT^{-T} = \Sigma, \\ \tilde{W}_o &= T^TW_oT = \Sigma.\end{aligned}\quad (16)$$

Notice that, in the balanced realization,

$$\begin{aligned}\tilde{L}_c(z) &= \frac{1}{2} \sum_{i=1}^N \frac{z_i^2}{\sigma_i} = \frac{1}{2} z^T \Sigma^{-1}, \\ \tilde{L}_o(z) &= \frac{1}{2} \sum_{i=1}^N \sigma_i z_i^2 = \frac{1}{2} z^T \Sigma z,\end{aligned}\quad (17)$$

to assure that the state with only nonzero coordinate z_i is both easier to control and easier to observe than the state corresponding to z_{i+1} for $i = 1, 2, \dots, N-1$.

To reduce the order of the model already in balanced realization, if, for a given r , $1 \leq r \leq N$, there is a major gap between two singular values, i.e. $\sigma_r \gg \sigma_{r+1}$, then it is only necessary to keep the states corresponding to the coordinates z_1, z_2, \dots, z_r , from the point of view of the map between u and y . This is known as balanced realization model order reduction. A further linear transformation can put the system into input normal form

$$\begin{aligned}\tilde{L}_c(z) &= \frac{1}{2} \sum_{i=1}^N z_i^2 = \frac{1}{2} z^T z, \\ \tilde{L}_o(z) &= \frac{1}{2} \sum_{i=1}^N \sigma_i^2 z_i^2 = \frac{1}{2} z^T \Sigma^2 z,\end{aligned}\quad (18)$$

for which the same comments apply (now all the states are equally easy to control, and the differences have been loaded completely on the observability function).

As shown in [10], \mathcal{H}_∞ -norm lower and upper error bounds of the balanced truncation method are given by

$$\sigma_{r+1} \leq \|G(s) - G_r(s)\|_{\mathcal{H}_\infty} \leq 2 \sum_{i=r+1}^n \sigma_i \quad (19)$$

From these inequalities it follows that, in order to get the smallest error for the truncated system, one should, in any case, disregard the states associated with the smallest Hankel singular values.

3.2. Model Order reduction of the discretized PEM fuel cell model

The original model was discretized using 10 volumes (Fig. 2), which led to a 110-state nonlinear DAE model. The selected inputs are gas species inlet flows, inlet temperatures and total cell voltage (8 inputs). The outputs correspond to the complete membrane current density profile along z -direction (10 outputs). Each output corresponds to current density in one volume along the z -direction. The chosen operating condition is cell current 1.98 A and voltage 0.7 V. These inputs and outputs allow a complete state controllable and observable model.

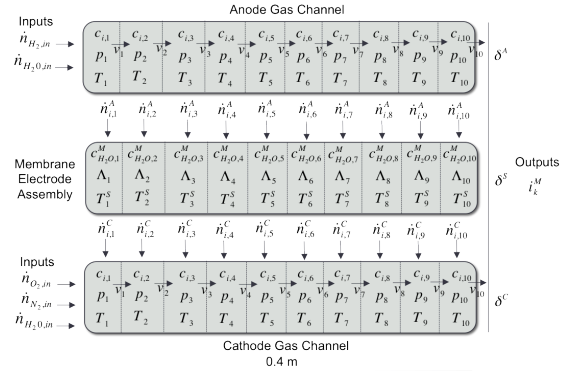


Fig. 2. Single cell distributed parameter model domain, discretization and variables.

Applying the order reduction process to this 110-state model results in the following Hankel Singular values plot, which indicates that, approximately, a 10-state model should be good enough to preserve the input-output behavior of the original model.

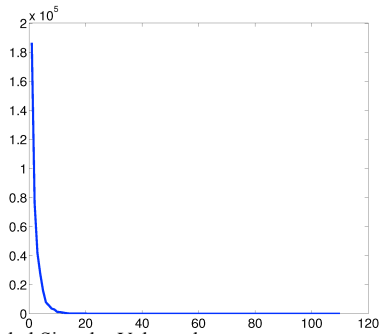


Fig. 3. Hankel Singular Values plot.

4. RESULTS AND DISCUSSION

In order to test the reduced-model behavior, step input-output responses from the original model and reduced models of different orders were simulated and compared. Time responses of important variables to a voltage step change at time 3 s are shown. In order to analyze other important model internal variables, these are also selected as outputs.

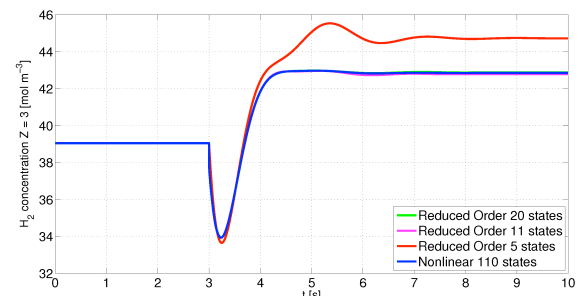


Fig. 4. Time variation of hydrogen concentration at volume 3.

Fig. 4 and Fig. 5 show the comparison of three different order-reduced models with the original

nonlinear full order model. The studied variables are hydrogen concentration at volume 3 and anode water at volume 5 (see Fig. 2). Notice that the 20-state model is already a perfect approximation of the nonlinear model.

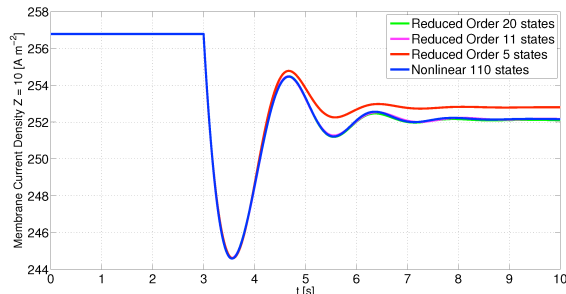


Fig. 5. Time variation of membrane current density at volume 10.

The 11-state model is almost as good as the 20-state model. Using fewer states (5-state model) results in not very good approximations, which is why the chosen order-reduced model has 11 states (as predicted by the Hankel Singular Values plot). Fig. 6 and 7 show the same results for membrane current density, oxygen concentration and solid part (MEA) temperature.

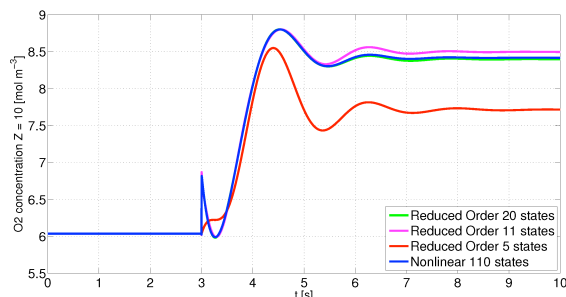


Fig. 6. Time variation of oxygen concentration at volume 10.

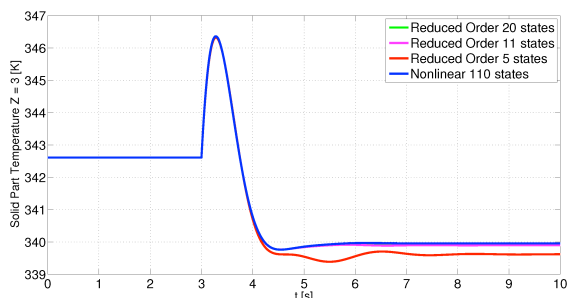


Fig. 7. Time variation of solid part temperature at volume 3.

5. CONCLUSIONS

Promising results have been found by applying an order reduction technique to a complex distributed parameter model of a PEM Fuel Cell model. The methodology consists of finding the controllability and observability functions of the

original nonlinear model, computing a change of coordinates to obtain a balanced realization that reveals the important states, and truncating less important states to approximate the original model. For the analyzed case study, a quadratic form of the controllability and observability functions has been used. Results have shown that reducing the order of the distributed parameter model from 110 states down to 11 states gives a very good approximation. An interesting next step is to study the range of operating conditions (around the equilibrium) for which the reduced model is valid. Currently, this order-reduced model is being applied to design model-based controllers for PEM Fuel Cells.

Acknowledgements

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