

## Order Reduction of a Distributed Parameter PEM Fuel Cell Anode Gas Channel Model

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### 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. A method to simplify complex models consists of reducing the order while preserving the relationship between certain input and output variables, determined from the control objectives. These Model Order Reduction (MOR) techniques have been extended to DAE systems [4].

This work focuses on obtaining an order reduced model, from a PEMFC anode gas channel PDE model, which incorporates the effects of distributed parameters that are relevant for the proper functioning and performance of PEMFC. The original model is an in-house MATLAB® code, flexible enough to manipulate the underlying model equations and apply MOR techniques. The obtained order-reduced model is suitable to perform numerical simulations and design efficient controllers for the original nonlinear PDE model.

### 2. DESCRIPTION OF THE SYSTEM

The case study is the anode gas channel of a single PEM fuel cell (Fig. 1). The length of the channel is 0.4 m. A 10-segment grid has been considered to study spatial variations of hydrogen and water concentrations, flow velocity, channel pressure and temperature. The inputs to the system are hydrogen and water inlet flows, and the selected outputs for future control purposes are concentrations of each species at the end of the channel. All variables are indicated in Fig. 1.

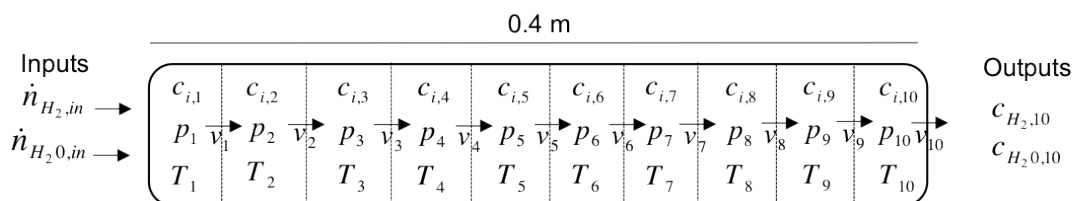


Figure 1: Single PEMFC anode gas channel

### 3. ANODE GAS CHANNEL MODEL EQUATIONS

In the following equations,  $k$  denotes segment number ( $k = 1 \dots MZ$ ,  $MZ = 10$  in this case) and  $i$  refers to gas components ( $i = H_2, H_2O$ ). The total number of states is 30, which is the number of differential equations, and there are 30 algebraic variables and corresponding relations. The complete discretization process was presented in [5], which led to the following discretized equations. The general mass conservation equation for component  $i$  and segment  $k$  is:

$$\frac{dc_{i,k}}{dt} = -\frac{v_k c_{i,k} - v_{k-1} c_{i,k-1}}{\Delta z} - \frac{\dot{n}_{i,k}}{\delta}, \quad (1)$$

where  $\Delta z$  is the segment size,  $\delta$  is the channel height and  $\dot{n}_{i,k}$  is the flow rate of component  $i$  from segment  $k$  to the Membrane Electrode Assembly (MEA). The  $\dot{n}_{i,k}$  values are set from a current density profile assumed. The boundary condition remains an algebraic equation as follows

$$v_0(t) c_{i,0}(t) = \dot{n}_{i,in} \quad (2)$$

This algebraic equation is used to calculate concentrations in the first segment of the gas channel. Calculation of flow velocity, using forward differencing is:

$$v_k = -K \frac{p_{k+1} - p_k}{\Delta z} \quad (3)$$

considering a boundary condition for the end segment

$$v_{MZ} = -K \frac{p^{amb} - p_{MZ}}{\Delta z} \quad (4)$$

where  $p^{amb}$  is the ambient pressure. The ideal gas law gives the pressure in the gas channel

$$p_k = RT_k \sum_i c_{i,k} \quad (5)$$

Accumulation of internal energy  $\rho u$  in the gas channel is

$$\begin{aligned} \frac{d(\rho u)}{dt} = & -\frac{1}{\Delta z} \left( \sum_i v_k c_{i,k} h_{i,k}(T_k) - \sum_i v_{k-1} c_{i,k-1} h_{i,k-1}(T_{k-1}) \right) \\ & + \lambda \frac{T_{k+1} - 2T_k + T_{k-1}}{\Delta z^2} + \frac{\alpha_1}{\delta} (T_k^S - T_k) - \sum_i \frac{\dot{n}_{i,k}}{\delta} h_{i,k}(T_k) \end{aligned} \quad (6)$$

where  $h$  is gas enthalpy,  $\lambda$  is the heat conductivity coefficient and  $\alpha_1$  is the heat transfer coefficient.

The corresponding boundary equations are  $T_{MZ+1} = T_0 = T^{amb} = 298.15$  K. Temperature in the gas channel is given by the thermodynamic relation

$$(\rho u)_k + p_k = \sum_i c_{i,k} h_{i,k}(T_k) \quad (7)$$

#### 4. MODEL ORDER REDUCTION

The method used to reduce the order of the case study nonlinear DAE model requires linearizing the original DAE model 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 [6]. Consider a nonlinear DAE model, as the one presented in the previous section

$$\begin{aligned} F_1(\dot{x}_1, x_1, x_2, u) &= 0 \\ F_2(x_1, x_2, u) &= 0 \\ y - h(x_1, x_2, u) &= 0 \end{aligned} \quad (8)$$

where  $x_1 \in \mathbb{R}^d$  is the state vector,  $x_2 \in \mathbb{R}^a$  are algebraic variables,  $u \in \mathbb{R}^r$  are the control inputs, and  $y \in \mathbb{R}^q$  are the outputs. Assuming that this DAE model has an underlying ODE description,

$$\begin{aligned} \dot{x}_1 &= \mathcal{L}(x_1, x_2, u) \\ x_2 &= \mathcal{R}(x_1, u) \end{aligned} \quad (9)$$

it follows that

$$\begin{aligned} \dot{x}_1 &= \mathcal{L}(x_1, \mathcal{R}(x_1, u), u) \\ y &= h(x_1, \mathcal{R}(x_1, u), u) \end{aligned} \quad (10)$$

#### 4.1 COMPUTATION OF THE CONTROLLABILITY FUNCTION

The controllability function  $L_c(x_{1,0})$  measures the minimal amount of energy in the control signal  $u$ , required to reach a specific state  $x$ . It is defined as the solution to the optimal control problem [4]:

$$\begin{aligned} L_c(x_{1,0}) &= \min_{u(\cdot)} Jc \\ \text{s.t.} \quad & \dot{x}_1 = L(x_1, x_2, u) \\ & x_2 = R(x_1, u) \\ & x_1(0) = x_{1,0} \in \Omega_x \\ & 0 = \lim_{t \rightarrow -\infty} x_1(t) \end{aligned} \quad (11)$$

where  $Jc$  is a measure of the control signal energy

$$J_c = \frac{1}{2} \int_{-\infty}^0 u(t)^T u(t) dt \quad (12)$$

Due to the original model complexity, a local solution of the controllability function is computed, valid in a neighborhood of a specific equilibrium point. The result expressed as a convergent power series expansion up to some desired order is

$$L_c(x_1) = \frac{1}{2} x_1^T G_c x_1 + L_{ch}(x_1) \quad (13)$$

where  $G_c$  is a positive definite matrix, which is the inverse of the controllability Gramian, and  $L_{ch}(x_1)$  contains terms of order three or higher. In this case study,  $L_{ch}(x_1) = 0$ . Therefore, the controllability function is approximated by a quadratic form that corresponds to a linear approximation of the original nonlinear model around a desired equilibrium point (section 4.3). The  $G_c$  matrix is derived

from solving the Lyapunov equation

$$G_c A + A^T G_c + G_c B B^T G_c = 0 \quad (14)$$

where  $A$  and  $B$  are the resulting state and input matrices of the previously linearized DAE system.

#### 4.2 COMPUTATION OF THE OBSERVABILITY FUNCTION

The observability function measures the energy in the output signal for certain initial state conditions. It is defined as

$$\begin{aligned} L_o(x_1(0)) &= \frac{1}{2} \int_0^\infty y(t)^T y(t) dt \\ x_1(0) &= x_{1,0} \in \Omega_x \\ u(t) &= 0, \quad 0 \leq t < \infty \end{aligned} \quad (15)$$

Considering a DAE model in the form of (8), the goal is to find  $L_o(x_1)$  as a convergent power series on some neighborhood of  $x_1 = 0$ , up to a desired order

$$L_o(x_1) = \frac{1}{2} x_1^T G_o x_1 + L_{oh}(x_1) \quad (16)$$

where  $G_o$  is the observability Gramian (positive definite matrix) computed by solving the following Lyapunov equation

$$G_o A + A^T G_o + C^T C = 0 \quad (17)$$

and  $A$  and  $C$  are the resulting state and output matrices of the linearized DAE system. The observability function is approximated by a quadratic form as well, which corresponds to a linear approximation of the original nonlinear model.

#### 4.3 COMPUTATION OF AN APPROPRIATE COORDINATE CHANGE

Once the controllability and observability functions are computed up to order two in this case study

$$L_c(x_1) = \frac{1}{2} x_1^T G_c x_1 \quad (18)$$

$$L_o(x_1) = \frac{1}{2} x_1^T G_o x_1 \quad (19)$$

a linear change of coordinates is used to simultaneously diagonalize  $G_c^{-1}$  and  $G_o$  as

$$\Sigma = G_c^{-1} = G_o = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n), \quad (20)$$

where  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n > 0$  [4]. These  $\sigma_i$  values ( $i = 1, \dots, n$ ) are denoted Hankel singular values and  $\sigma_1$  is the Hankel norm of the system. A representation where the two Gramians are equal and diagonal is called balanced. A small  $\sigma_i$  means the amount of control energy required to reach the state  $z = (0, \dots, 0, z_i, 0, \dots, 0)$  is large, while the output energy generated by the same state is small ( $z$

being the new set of states). Computing this balanced realization requires performing Cholesky factorizations of the Gramians:

$$G_c = XX^T, \quad G_o = YY^T, \quad (21)$$

$X > 0$  and  $Y > 0$ . Then, the singular value decomposition (SVD) of  $Y^T X$  is computed

$$Y^T X = U \Sigma V^T \quad (22)$$

where  $U$  and  $V$  are orthogonal. Finally

$$\Sigma = \text{diag}(\sigma_1, \sigma_2, \dots, \sigma_n) \quad (23)$$

The balancing transformation is given by

$$T = XV \Sigma^{-1/2}, \quad \text{with } T^{-1} = \Sigma^{-1/2} U^T Y^T \quad (24)$$

The balanced realization is given by the linear system

$$\tilde{A} = T^{-1} A T, \quad \tilde{B} = T^{-1} B, \quad \tilde{C} = C T \quad (25)$$

and

$$\Sigma = \tilde{G}_c^{-1} = \tilde{G}_o \quad (26)$$

#### 4.4 TRUNCATION

The reduced model is obtained finding a major gap between two Hankel singular values, *i.e.*, if  $\sigma_k \gg \sigma_{k+1}$  for some  $k$ . The last  $z_{k+1}$  to  $z_n$  states of the balanced realization are left out without considerably affecting the input-output behavior, compared to the original system [4]. Recalling the original DAE model of (10), the balanced realization can be expressed as

$$\begin{aligned} \dot{z} &= \hat{L}(z_a, z_b, u) \\ y &= \hat{h}(z_a, z_b, u) \end{aligned} \quad (27)$$

where  $z = (z_a, z_b)$  is the new set of states divided into two subsets determined by the Hankel singular values. The reduced order model would be

$$\begin{aligned} \dot{z}_a &= \hat{L}(z_a, 0, u) \\ y &= \hat{h}(z_a, 0, u) \end{aligned} \quad (28)$$

## 5. SIMULATION RESULTS

In order to test the reduced-model behavior, step and sinusoidal input-output responses from the original model, linearized model (full order) and reduced model were simulated and compared. Fig. 2 (a) shows the response of output 1 (hydrogen concentration at the end of the channel) to unitary step changes (both inputs) at time 1. Fig. 2 (b) shows the response of output 2 (water concentration at the end of the channel) to unitary step changes (both inputs) at time 1. Fig. 2 (a) shows the

response of both outputs to a sinusoidal input type at the hydrogen inlet flow. Fig. 2 (d) is the plot of Hankel singular values, which is important in order to decide how many states will be left out to reduce the order of the original model. This figure shows that approximately 5 states out of 30 are necessary.

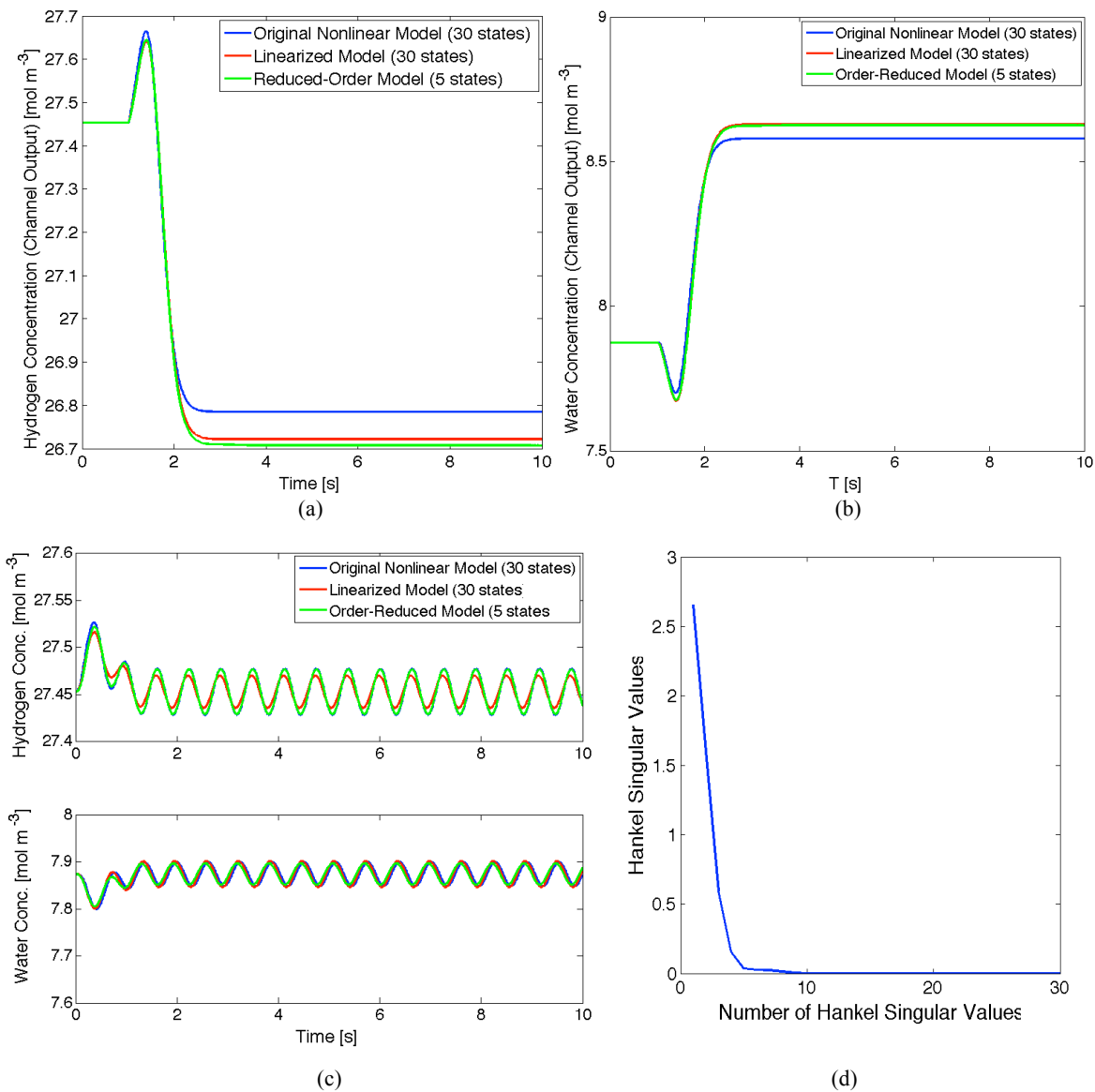


Figure 2: (a) Step change at time  $t = 1$ s (Hydrogen Output) (b) Step change at time  $t = 1$ s (Water Output) (c) Sinusoidal input (both outputs) (d) Hankel Singular Values

## 6. CONCLUSIONS AND ONGOING RESEARCH

Promising results have been found by applying an order reduction technique to a complex distributed parameter model of a PEM Fuel Cell Anode Gas Channel. 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 30 states down to 5 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. In this moment, this model reduction technique is being applied to reduce an entire single PEMFC distributed parameter 1+1D model of approximately 100 states. The goal is to obtain an order-reduced model appropriate to design model-based controllers for PEM Fuel Cells.

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