A STUDY TOWARD MINIMUM SPATIAL DISCRETIZATION OF A FUEL CELL DYNAMICS MODEL

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ABSTRACT

The 24-state fuel cell water dynamics model from [1] is cast into a Dymola\textsuperscript{T M} icon-based formulation, with flexible library sub-models specific for this application. Through and across (flow and effort in bond graph terminology) variables are identified and analyzed for all relevant energy-using components. The objective is to establish the necessary model order for the fuel cell model using an energy-based measure called activity [2]. Additionally, we analyze the effect that input variation (duration, initial/final time) has on calculation and implementation of the activity. Explanation of the importance of accurate water vapor concentration gradient modeling is covered. Finally, we show that the minimum degree of discretization for each constituent within the model should be determined separately in order to generate the simplest model representation, and that the optimal discretization can be different for each species.

1 Introduction

The management of water within the fuel cell stack is critical for optimal stack performance. A balance must be struck between hydrogen and oxygen delivery, and water supply/removal. Water will condense when the reactant gases become saturated. This liquid water can accumulate in the gas channels and/or the pore space of the gas diffusion layer (GDL), and can partially coat the catalyst, reducing the power output of the fuel cell.

While computational fluid dynamics models are suitable for investigating fuel cell design issues, implementation of such complex models for real time embedded control is cumbersome. Thus, any model-based control scheme used for water management must adequately obtain implementation feasibility while still capturing the dynamic behavior of electrode flooding and two phase flow.

In this paper, we continue the work from [3] towards determination of the necessary model fidelity to accurately predict six outputs of interest: the rate of liquid water flow into the anode and cathode channels (for reactant flow blockage determination), the water vapor concentration on each side of the membrane (for humidity control), and the $O_2$ and $H_2$ concentrations on their respective sides of the membrane (for reactant starvation control).

The work of McKay et al [1] showed that spatial discretization can be used to approximate a fuel cell system described by partial differential equations. In the discrete model, the GDL of both cathode and anode sides were divided mathematically into three sections. The spatial characteristics (temperature, composition, pressure) of each section are considered to be homogeneous.

The premise for the discretization in [1] is that the inclusion...
of equations describing liquid water and gas dynamics within the GDL is necessary to predict flooding. The question we study in this paper is if this is true for all gas species and the liquid water, and if three sections is the most appropriate resolution.

While the three-section discretization has adequate prediction capability, and is not overly complex, the model still has 24 states. In order to pursue model-based control of this system, it would be beneficial to reduce the model order further to permit online parameter identification and adaptation while controlling the system in real time.

In this paper, a model order reduction methodology (MORA) developed by Stein and Louca [2], implemented in the commercially available software tool Dymola™, is utilized in an application to reduce the order of the discretized fuel cell model described in [1].

2 Nomenclature and Paper Overview

This section describes the naming conventions used in this paper. Time derivatives will be written as $d(\cdot)/dt$. Spatial derivatives through the GDL thickness in the direction normal ($y$) to the membrane are denoted as $\partial(\cdot)/\partial y$.

$A_{fc}$ is the fuel cell active area ($m^2$), $c$ is molar concentration (mol/m$^3$), $D$ is the diffusion coefficient (m$^2$/s), $D_{\text{eff}}$ is the effective diffusivity (m$^2$/s), $i$ is current density (A/cm$^2$), $I_{g}$ is the stack current (A), $M_j$ is molecular weight (kg/mol) of constituent $j$, $n$ is the molar flow rate (mol/s), $p$ is pressure (Pa), $R$ is the ideal gas constant (J/kg K), $r_e$ is the water evaporation rate (mol/m$^3$/s), $s$ is the fraction of liquid water volume to the total pore volume, $S$ is the reduced water saturation, $T$ is temperature (K), $V$ is volume ($m^3$), and $Q$ represents liquid volumetric flow rate (m$^3$/s).

The Greek letter $\alpha_w$ is the tunable diffusion parameter, $\gamma$ is used for the volumetric condensation coefficient ($s^{-1}$), $\varepsilon$ for porosity, $\rho$ for density (kg/m$^3$).

The subscript $an$ denotes variables associated with the anode, $c$ is capillary, $ca$ is cathode, $ch$ is channel, $e$ is electrode ($an$ or $ca$), $H_2$ is hydrogen, $N_2$ is nitrogen, $O_2$ is oxygen, $mb$ indicates an assignment to the cell membrane, $j$ is used as an index for fuel cell constituents, $k$ is used as an index for discretization, $l$ is liquid, $p$ is pore, $rc$ is reactions, $sat$ is saturation, and $v$ is vapor.

This paper is organized to first explain the model as received and translated into Dymola™, using discrete algebraic equations to approximate partial differential equations. Next the model is linearized, and benefits and shortcomings of the linearization are discussed. Next, a variation on the MORA is applied to this case to maintain the physical meaning of the remaining states. Then an explanation of the necessity of full discretization (3 sections) for the water vapor concentration is provided. In conclusion, a proposal is made regarding a feasible degree of discretization for each constituent in the fuel cell.

3 Model Overview

On the anode side of the fuel cell, a mixture of hydrogen and water vapor flows from the channel through the GDL. A mixture of oxygen, nitrogen, and water vapor flows from the cathode channel. The species concentrations in the channels are calculated assuming the channel is homogeneous, lumped-parameter, and isothermal. The time varying channel concentrations provide one set of boundary conditions for the spatially varying reactant concentrations within the GDL. The reactant gases must diffuse through the GDL to reach the catalytic layer.

Under load, it is assumed that product water is formed as a vapor at the cathode catalyst. The combination of electro-osmotic drag and back-diffusion transport vapor through the membrane between the anode and cathode. The net molar flow of vapor through the membrane depends on the relative magnitudes of back-diffusion and drag.

Under the isothermal conditions assumed for both anode and cathode GDL for this model, once the production or transport of vapor exceeds the ability of the vapor to diffuse through the GDL to the channel, the vapor supersaturates and condenses. The condensed liquid accumulates in either or both the anode and cathode GDL until it has surpassed the immobile saturation threshold, at which point capillary flow will carry it to an area of lower capillary pressure (the GDL-channel interface). Liquid water in the GDL occupies pore space, reducing the effective area through which reactant gas can diffuse. This phenomenon is captured by the effective diffusivity, $D_{\text{eff}}$, described in [4]. The $D_{\text{eff}}$ of [4] takes into account the porosity ($\varepsilon$) of the medium as well as the presence of liquid water volume $V_{l}$ in the pore space $V_{p}$:

$$D_{\text{eff}} = D_{j} \varepsilon \left( \frac{\varepsilon - 0.11}{0.89} \right)^{0.785} \left( 1 - \frac{V_{l}}{V_{p}} \right)^{2}, \quad (1)$$

where $D_{j}$ and $\varepsilon$ have values taken from [4].

Additionally, the liquid water accumulates in the channel and forms a film that obstructs the fuel cell reaction. This obstruction ultimately reduces the active catalyst surface area, lowering the cell voltage.

A summary of the key model equations are provided below. For a complete description of the model, and more background, the reader is encouraged to see [1] and [4].

Of main interest are the concentrations of the gas species, and the volumes of liquid water, in the anode and cathode GDL. Of the four governing equations, three are partial differential equations (PDE) in space ($y$-direction perpendicular to the membrane) and time.

The non-vapor gas concentrations for the $j^{th}$ species at the $e$ electrode is

$$\frac{dc_{j,e}}{dt} = \frac{1}{V_{p}} \frac{\partial n_{j}}{\partial y}, \quad (2)$$

The water vapor concentration is determined from

$$\frac{dc_{v,e}}{dt} = \frac{1}{V_{p}} \frac{\partial n_{v,e}}{\partial y} + r_{v,e}, \quad (3)$$

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where the evaporation rate is defined as \( r_{v,e} = \gamma (c_{v,sat} - c_v) \), and the vapor saturation concentration is related to the saturation vapor pressure through \( p_{v,sat} = c_{v,sat} RT \).

The liquid water volume is given by

\[
dV_{l,e} \frac{dt}{d} = \beta_{vl} (V_{l,e}) \frac{dp_{vap,e}}{dy} - \frac{V_{l,e} M_v}{\rho_l} r_{v,e},
\]

where \( \beta_{vl} \) is a nonlinear function of the liquid water present, and other material and geometric factors such as viscosity and flow area. Capillary pressure results from surface tension of the water droplets, and is calculated as \( p_{cap} = \beta_{pc} S_{NL}(V_{l,e}) \), where \( \beta_{pc} \) is a constant that captures the geometry of the surface tension between the water and air, the porosity, and the permeability of the GDL. The nonlinear function \( S_{NL}(V_{l,e}) \) is a third-order polynomial in \( V_{l,e} \) that describes the relationship between capillary pressure and the amount of liquid water present.

The molar flow through the GDL is calculated from

\[
n_{j,\text{eff}} = -D_{eff} A_{j} \frac{dn_{j,e}}{dy}.
\]

Combining Eq. (5) with Eqs. (2) and (3), it can be seen that the time rate of change of the constituent concentrations is really a second-order PDE of concentration with respect to the spatial variable \( y \). For ease in discretization, these second-order PDEs are represented as cascaded pairs of first order PDEs in this application.

For application as a controls problem, it is desirable to simplify the above equations to eliminate the spatial PDE components, and focus on the ordinary differential equations (ODE) that remain. The discretization of the GDL to approximate the PDE model by a series of coupled volumes described by ODEs is reviewed in Sec. 3.1.

### 3.1 Discretization

The mass transport of gas and liquid water is divided into discrete volumes (Fig. 1). The spatial gradients are solved as difference equations, while the time derivatives are solved with standard ODE solvers.

Difference equations are used to describe the gradients for the concentrations of oxygen \((c_{O_2})\), hydrogen \((c_{H_2})\), and water vapor \((c_{v,e})\), as well as for the reduced water saturations, \( S_{ca} \) and \( S_{an} \), where \( S_e = (s_e - 0.1)/0.9 \) (with \( s = V_{l,e}/V_p \)).

As an example of a three-stage discretization of the \( O_2 \) and \( H_2 \) diffusion equations, the difference equations for the molar flow gradients of oxygen and hydrogen are:

\[
\begin{align*}
\frac{\delta n_{O_2}}{\delta y} (1) &= n_{O_2,1} - n_{O_2,2} \\
\frac{\delta n_{O_2}}{\delta y} (2) &= n_{O_2,2} - n_{O_2,3} \\
\frac{\delta n_{O_2}}{\delta y} (3) &= n_{O_2,3} - n_{O_2,4}
\end{align*}
\]

\[
\begin{align*}
\frac{\delta n_{H_2}}{\delta y} (1) &= n_{H_2,1} - n_{H_2,2} \\
\frac{\delta n_{H_2}}{\delta y} (2) &= n_{H_2,2} - n_{H_2,3} \\
\frac{\delta n_{H_2}}{\delta y} (3) &= n_{H_2,3} - n_{H_2,4}
\end{align*}
\]

where \( \delta y \) is the distance across one discrete section, and \( n_{O_2,\text{sat}} \).

Figure 1. Mass transport diagram with discretization of diffusion layer.

and \( n_{H_2,\text{sat}} \) are calculated from:

\[
n_{j,\text{sat}} = \frac{I_{sat}}{2F} \text{ with } \begin{cases} 
\xi = 1 & \text{for } j = H_2 \\
\xi = 2 & \text{for } j = O_2
\end{cases}
\]

and \( F \) is Faraday’s constant.

### 3.2 The Dymola Model

To facilitate the time-response comparison confirmation of outputs for systems with different degrees of discretization for each species present in the model, a library of subcomponents was created in Dymola. Separate subcomponent iconic models were made for water vapor, cathode-side non-vapor gases \((O_2 \text{ and } N_2)\), anode-side non-vapor gas \((H_2)\), and for the liquid water. Each subcomponent is equipped with connector pins to provide the input/output data necessary to determine it’s internal state and pass relevant information to the next discretized section.

The main reason the models are split by species is to allow the degree of discretization to be specific to each constituent, e.g. have the ability to provide three sections to describe the \( O_2 \) spatial gradient, and perhaps only two for the \( N_2 \) gradient. The icon-version of the full-order model built from the library created for this project is shown in Fig. 2. Within this model, each species within each section is represented by one icon, and it communicates with the next element in the chain (channel, sequential species icon, or membrane) and with a data bus to capture the liquid water state. The data bus icon serves a communication function between the gases and the liquid water (evaporation/condensation, liquid volume). The membrane icon contains the functions that determine net water flow between the electrodes. Since each section icon represents one state, the full-order model can be seen to have 19 states associated with the discretization (3 anode vapor, 3 cathode vapor, 3 \( O_2 \), 3 \( H_2 \), 1 \( N_2 \),

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3 anode liquid, and 3 cathode liquid), plus another 5 for the channels, which are not visible at the icon-level, and consist of vapor on each side, $O_2$, $N_2$, and $H_2$. The state that represents the gases is the concentration (mol/m$^3$), and for the liquid water the state is the volume (m$^3$).

### 3.3 System Inputs and Outputs

The baseline model for this research application is multiple input, multiple output (MIMO). The main operational input to the system is $I_{st}$, which also defines the airflow into the cathode at 33% utilization. The anode is pressure-controlled and dead-ended with a valve for purging. Temperature and relative humidity of the intake gas mixtures and purge frequency and duration are also inputs. For control and performance of this fuel cell water dynamics/reactant supply model, the outputs are listed in Table 1 and will be the metrics used to determine if the reduced-order model matches the full-order model with sufficient accuracy.

### 3.4 Baseline Discretized Model Verification

The 3-section discrete model [1] was verified using a 24-cell PEMFC stack capable of delivering 1.4 kW of continuous power, and a peak output of 2.5 kW. The gas is distributed from the machined graphite flow fields through double-sided, hydrophobic version 3 E-TEK Elats$^TM$ with a thickness of 0.432 mm. The catalyst-coated membrane has a surface area of approximately 300 cm$^2$. This model overcomes the simplifying assumption of isothermal conditions and makes valid predictions of the following: the cell voltage decrease due to a drop in oxygen concentration during a step up in $I_{st}$, the cell voltage response as stack temperature (cooling system temperature) varies, and the cell voltage degradation over time as liquid water builds.

The research described in this paper uses the 3-section discrete model as the baseline to investigate model order reduction. Reduced-order model verification will be obtained by state and output comparisons to the experimentally-verified full-order model from [1].

Table 1. Outputs of interest for water dynamics/reactant supply model

<table>
<thead>
<tr>
<th>Output</th>
<th>Applicability</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$ Conc at membrane</td>
<td>Prevention of $O_2$ starvation</td>
</tr>
<tr>
<td>$H_2$ Conc at membrane</td>
<td>Prevention of $H_2$ starvation</td>
</tr>
<tr>
<td>$H_2O$ Conc (Ca) at membrane</td>
<td>Humidity control of membrane</td>
</tr>
<tr>
<td>$H_2O$ Conc (An) at membrane</td>
<td>Humidity control of membrane</td>
</tr>
<tr>
<td>Liquid water in Ch (An)</td>
<td>Anode flooding control</td>
</tr>
<tr>
<td>Liquid water in Ch (Ca)</td>
<td>Cathode flooding control</td>
</tr>
</tbody>
</table>

version 3 E-TEK Elats$^TM$ with a thickness of 0.432 mm. The catalyst-coated membrane has a surface area of approximately 300 cm$^2$. This model overcomes the simplifying assumption of isothermal conditions and makes valid predictions of the following: the cell voltage decrease due to a drop in oxygen concentration during a step up in $I_{st}$, the cell voltage response as stack temperature (cooling system temperature) varies, and the cell voltage degradation over time as liquid water builds.

The research described in this paper uses the 3-section discrete model as the baseline to investigate model order reduction. Reduced-order model verification will be obtained by state and output comparisons to the experimentally-verified full-order model from [1].

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4 Model Linearization

The baseline model at the center of this research is highly nonlinear due to polynomial fits and logical switching to match experimental data (e.g. use of the Leverett J-function to describe capillary pressure). In order to gain useful insight into the system dynamics, a linearization of the 24-state model was performed. The standard state-space system:

\[ \dot{x} = Ax + Bu \]
\[ y = Cx + Du, \]

where the states \((x)\) are described in Sec. 3.2, and the inputs \((u)\) and outputs \((y)\) are explained in Sec. 3.3. The linearization was performed numerically using the linearization function within Dymola\(^{TM}\) on the full-order model (Fig. 2) coded for this research project. The linear system was then exported to Matlab\(^{TM,3}\) for analysis using the Controls System Toolbox\(^{TM,3}\). For the purpose of future comparison to experiment, the linearization point was chosen to coincide with the initial conditions for one of the experimental results in [1]: \(I_{g} = 75\text{A}, T_{st} = 323\text{K}, P_{H2} = 120\text{kPa}, O_{2}\) flow in at 300% stoichiometry.

The linearization provides an understanding of the time constants associated with the system. For this model, the time constants all relate to filling dynamics for either gases or liquid water. The time constants for the original system of 24th order are listed in Table 2. The most significant information to be gathered

<table>
<thead>
<tr>
<th>Time Constants ((\tau_{f})) [sec]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1x10^{-4}</td>
</tr>
<tr>
<td>2.9x10^{-4}</td>
</tr>
<tr>
<td>1.2x10^{-3}</td>
</tr>
<tr>
<td>1.5x10^{-3}</td>
</tr>
<tr>
<td>2.5x10^{-3}</td>
</tr>
<tr>
<td>2.8x10^{-3}</td>
</tr>
</tbody>
</table>

from this table is the separating line that can be drawn between fast and slow modes of this system. An analysis of the eigenvectors for the 24 modes reveals that the slowest six modes are precisely and exclusively related to the filling dynamics of the six discretized sections of the GDL related to liquid water. This insight will have significant impact on the model order reduction process through selection of the time window for activity measurement.

5 Model Order Reduction Algorithm Application

As explained in detail in [2], the Model Order Reduction Algorithm is a method that seeks to simplify complex models by creating a metric named activity to determine the energetic contribution of every element of a model. Starting from the concept of \(Power = P = \text{effort \cdot flow}\), the activity is defined:

\[ activity_j = \int_0^T \| P_j(t) \| dt = \int_0^T | e_j - f_j | \cdot dt, \]

where the \textit{effort} and \textit{flow} variables for this application, (derived in [3]), are concentration \((\text{mol} / \text{m}^3)\) and molar flow rate \((\text{mol} / \text{sec})\) for the gas constituents, and capillary pressure, \(p_c\) (Pa) and volumetric flow rate \((\text{m}^3 / \text{sec})\) for the liquid states, respectively.

As can be seen from Eq. (9), it is necessary to assign a time duration for the activity calculation. This is a critical aspect of the method, as results will vary depending upon this time window. This issue is studied in more depth in Section 5.1.

Once the activity of an element is determined, it is normalized by an Activity Index \((AI)\) to determine whether the element has significant contribution to the overall energy of the system. The definition of the Activity Index \((AI)\) is:

\[ AI_j = \frac{\text{Activity}_j}{\sum_{m}^{m} \text{Activity}_m} \times 100\%, \]

where \(m\) is the total number of energetic (energy-utilizing) elements in the model.

As a function of the sum total of all the individual element activities, the \(AI\) provides a means to compare elements from any part of the model.

An important aspect of the MORA is that it reduces model complexity while maintaining the physical meaning of the variables and parameters. It is also applicable to nonlinear systems, which, due to the nonlinear nature of this model, makes it attractive for use here.

5.1 Activity Analysis and Results

To reiterate, activity results are strongly dependent upon the duration of the simulation and the inputs to the system. For this analysis, an attempt was made to systematically determine the influence on the activity for appropriate durations and inputs. Inputs considered were a step change in \(I_{st}\), a purge event, and a ramp input temperature increase. A logical choice for activity measurement duration would involve system time constants, but as shown in Sec. 4, there is a wide range of time constants for the states of this system. Activity calculations were performed for all the possible combinations of input mentioned above, and a range of durations that were tied to mode speeds of the system. The results were then normalized into percentages of the total activity \((AI)\). Review of the results showed that using the longer time constant of the system gave a disadvantage to the concentration states, that reach equilibrium quickly, as their net flow goes to zero early in the time window. At the opposite extreme, using the time constant of the fastest mode as the duration undervalues the slow modes.

From Sec. 4 it was found that it is possible to separate the modes into a fast group associated with gas concentration states, and a slow mode group associated with the liquid water volume states. To address the full potential of each group of states, an activity calculation was made for each group using a representative time window. The results of the activity simulations using

\(^{3}\text{Trademark of the MathWorks}\)
durations of 0.002 sec for the fast mode group and 30 sec for the slow mode group are listed in Table 3.

<table>
<thead>
<tr>
<th>Element(Ca)</th>
<th>Diff sec1</th>
<th>Diff sec2</th>
<th>Diff sec3</th>
</tr>
</thead>
<tbody>
<tr>
<td>O_2 Diff sec1</td>
<td>0.71</td>
<td>6.28</td>
<td>H_2 Diff sec1</td>
</tr>
<tr>
<td>O_2 Diff sec2</td>
<td>0.64</td>
<td>6.22</td>
<td>H_2 Diff sec2</td>
</tr>
<tr>
<td>O_2 Diff sec3</td>
<td>0.63</td>
<td>6.08</td>
<td>H_2 Diff sec3</td>
</tr>
</tbody>
</table>

Table 3. Activities split by fast and slow modes

In a typical activity analysis, it is common to compare activity magnitudes, and conclude that either an element is negligible and can be eliminated, or that its dynamics are fast enough to justify assignment of instantaneous equilibrium. A common threshold for such considerations is $< 0.1\%$. As can be seen from the data in Table 3, using such a threshold would yield different results for the different calculation time windows, and necessary elements might be removed if the wrong duration is used. Further, the small activities of the vapor elements imply that they are relatively inconsequential to the system. As the point of the model is to predict liquid water dynamics, and it can be shown that vapor concentration prediction accuracy is important, removal of these elements is not appropriate for this case.

A key point to remember is that the goal of this reduction is to determine the minimal level of discretization. Therefore, this application will use the activity to determine how many sections are required. With this view, comparing the activity levels, it can be seen that the elements of some species have small variation in activity from section to section. It is hypothesized that small variation in diffusion activity implies over-discretization.

We look at the definition of activity for a diffusion element to explain why similar diffusion activity implies associated state reduction feasibility. As described in [3], the diffusion of the gas species through the liquid water-filled GDL pores and the resistance to liquid water flow in the GDL can be modeled as resistance elements, and therefore have the power ($P$) through them determined by the concentration across multiplied by the flow through, or $P = (c_j(k) - c_j(k+1))n_j(k)$.

Some elements in the model see ranges of activity variation on the order of 100, therefore, the threshold for being considered to have small variation is set at less than one order of magnitude for potential discretization reduction. Following this interpretation, the species listed in Table 4 have potential for reduction (based on small variation ($< 10$) between the minimum and maximum values of the resistance-type elements associated with the species - gas diffusion and liquid flow).

While it is clear that the diffusion elements for $O_2$ and $H_2$ are very similar, it is unclear if the degree of variation for the liquid water flows can be judged similar or not, as the difference in minimum and maximum activity values are just barely within the single order of magnitude threshold. It should be noted that the data from the two durations under investigation (0.002 sec and 30 sec) imply that for minimum discretization using diffusion activity, the results are similar between the fast and slow mode analyses.

Figure 3. $O_2$ and $H_2$ distributions in the GDL are linear, implying single section discretization sufficiency.

For the non-vapor gases $O_2$ and $H_2$, once equilibrium in the section is reached, the flow into a section equals the flow out. Since the concentrations reach equilibrium very fast (Sec. 4), the flow through each section is nearly equivalent. It is only variations in concentration that separate the diffusion activities. Therefore, similar activity results in the diffusion elements imply a linear distribution of concentration in the GDL, which indicates single section sufficiency.

<table>
<thead>
<tr>
<th>Element(Ca)</th>
<th>Diff sec1</th>
<th>Diff sec2</th>
<th>Diff sec3</th>
</tr>
</thead>
<tbody>
<tr>
<td>H_2O Diff sec1</td>
<td>0.110</td>
<td>0.807</td>
<td>H_2O Diff sec1</td>
</tr>
<tr>
<td>H_2O Diff sec2</td>
<td>0.008</td>
<td>0.063</td>
<td>H_2O Diff sec2</td>
</tr>
<tr>
<td>H_2O Diff sec3</td>
<td>0.001</td>
<td>0.006</td>
<td>H_2O Diff sec3</td>
</tr>
</tbody>
</table>

Table 4. Candidate elements for reduction based upon similar Activities

<table>
<thead>
<tr>
<th>Fast Mode Element</th>
<th>Slow Mode Element</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$ Diff</td>
<td>$O_2$ Diff</td>
</tr>
<tr>
<td>$H_2$ Diff</td>
<td>$H_2$ Diff</td>
</tr>
<tr>
<td>Liq flow (Ca)</td>
<td>Liq flow (Ca)</td>
</tr>
<tr>
<td>Liq flow (An)</td>
<td>Liq flow (An)</td>
</tr>
</tbody>
</table>
the membrane transport parameter $\alpha$ vapor concentration gradient in the GDL will be nonlinear, and $H$ and $H$ desired outputs. A 3-section model to a 1-section model is not significant for our ter volume. It is true that an assumption of a linear distribution none of the outputs of interest are highly sensitive to liquid wa-

ducing discretization, the results of a sensitivity study show that the influence of the nonlinear liquid water volume gradient must be active during the expected range of operation of the model are active.

5.2 Effect of Operating Point and Input on Results

To confirm that this activity-based model order reduction method is robust to input and operation point variation, several scenarios were investigated. Ramp, low-frequency, and high-frequency $I_{el}$ inputs were checked, along with operating points with low current density and no flooding conditions. For all cases except the no flooding case, the results of the model order reduction were unchanged. Without flooding, there will be no liquid water flow across the section boundary, resulting in zero flow for the purposes of activity calculation. This is a special aspect of this model (which has conditional statements that modify the model structure), and illustrates a key aspect of activity-based analysis: The activity calculation must be performed for conditions such that all elements that can be active during the expected range of operation of the model are active.

6 Further Reduction Considering Fast Dynamics

A common step in reduction of model order complexity is accomplished by noting that the ODEs associated with fast dynamics can be well-approximated by assuming they reach equilibrium instantaneously.

From the analysis of the eigenvectors of the linearized system, it is possible to determine that the fastest time constant of this system is associated with the $H_2$ concentration in the anode channel (Sec. 4). Assigning instant equilibrium for this state, comparison of the full-order vs. reduced order model outputs for $H_2$ at the membrane shows that the influence of this reduction is minimal. To confirm that $H_2$ tracking is robust through all feasible inputs to the system, this result was also confirmed through a purge event with minimal deviation.

Application of the same method for $O_2$ channel concentration does not realize the same success. The upper plot of Fig. 6 shows that the result of $O_2$ concentration tracking at the membrane becomes out of phase if $c_{O_2, ch}$ is assumed to change to equilibrium values instantaneously, causing over 25% error. This is likely unacceptable since $O_2$ starvation is potentially damaging to the PEM.

The $N_2$ dynamics, as an inert component in the cathode side mixture also having fast dynamics, seems like an obvious choice for reduction to an algebraic equation. However, a major conclusion from this research is that the dynamics of the $N_2$ in the channel are essential for accurate modeling of $O_2$ at the membrane. The lower plot of Fig. 6 shows what happens to the tracking of $O_2$ if the dynamics of $N_2$ in the channel are neglected. This occurs because the response of the pressure within the cathode channel is strongly influenced by $N_2$ concentration dynamics.

The conclusion is that the only channel gas dynamics that of the water vapor concentration gradient is critical to prediction of channel flooding. Therefore, section reduction for water vapor is not pursued.
The $O_2$ concentration at the membrane is strongly influenced by dynamics of both $O_2$ and $N_2$ in the cathode channel, suggesting those ODEs cannot be reduced to algebraic equations.

can be made instantaneous for state reduction is the concentration element $c_{H_2, ch}$ in the anode channel if accurate $O_2$ modeling at the membrane is required.

Considering the activity analysis of Sec. 5.1, the fast dynamics study of this section, and the outputs of interest, the model shown in Fig. 7 is proposed as an acceptable order-reduced model for the fuel cell water dynamics model of [1] that also can be used to model $O_2$ and $H_2$ starvation and humidity near the membrane. In the reduction from Fig. 2 to Fig. 7, the liquid water discretization for both electrodes has been reduced to one, as have the discretizations for $H_2$ and $O_2$. The $N_2$ section has been absorbed into the channel Nitrogen dynamics. The vapor sections were left at three for reasons explained in Sec. 5.1.

7 Conclusions

We have successfully reduced the model order of a 24-state system to 14 states while maintaining the physical meanings of the states. The applicability to reduction in discretization through use of activity variation in diffusion elements was shown. We learned about the importance of keeping the spatial distribution of water vapor concentration in the GDL. It also became clear that dynamic modeling of $N_2$ in the channel is critical for modeling $O_2$ concentration at the membrane.

8 Future Work

Determination of a methodology for choosing the membrane water transport parameter $\alpha_w$ remains, and a sensitivity study relating $\alpha_w$, vapor concentration, and liquid water volume rate of change will be investigated for the purpose of $\alpha_w$ identification. Consolidation and further theoretical justification for the model order reduction methodology used in this research needs more work. Finally, further model order reduction is still possible.

REFERENCES


Figure 7. Dymola reduced-order model Icon version with 14 states