Object-Oriented Fuel Cell Model Library

Kevin L. Davies and Robert M. Moore
Hawaii Natural Energy Institute, University of Hawaii, Honolulu, Hawaii 96822, USA

The *PEMFCSim* library is primarily a simulation structure designed to facilitate the simulation of Polymer Electrolyte Membrane Fuel Cells. *PEMFCSim* uses methods that are physical, dynamic, and component-based. It is written in Modelica, an object-oriented, physical modeling language. The library, as currently implemented, offers one-dimensional and quasi-two dimensional fuel cell simulations and is based on existing models from the literature. The Modelica object-oriented modeling approach allows the *PEMFCSim* library simulations to use intuitive and physically representative component boundaries and connections. The discussions and examples presented in this paper are based upon an initial set of models selected from the literature, but additional assumptions and characterizations can easily be adopted within the overall simulation structure without changing other elements of the simulation. This flexibility makes the *PEMFCSim* library ideal for collaboration among researchers focusing on different aspects of fuel cell modeling and simulation.

Introduction

It is important, at the very outset, to address the issue of why yet another PEMFC (Polymer Electrolyte Membrane Fuel Cell) model is needed. At last formal count, there were approximately 300 existing models in the literature (1975-2004), and a flood of new models has continued since 2004. The answer to "why another" (insofar as this paper is concerned) is that the purpose of this paper is to introduce a proposed standard simulation structure (*PEMFCSim*) with three primary attributes: (i) it is compatible with the existing literature models, (ii) it is ideal for collaboration among researchers focusing on different research areas or different levels of detail in PEMFC modeling, and (iii) it is inherently suited for use within fuel cell system simulations.

The *PEMFCSim* library, as currently implemented, is a simulation structure including a set of component models that together simulate the operation of a PEMFC. The library uses simulation methods that are physical, dynamic, and component-based. It is not intended to replace the large number of fuel cell models that already exist in the literature. Instead, the *PEMFCSim* library offers a fuel cell modeling environment and structure which can be utilized for a wide range of applications and modeling assumptions or options concerning the many elements within a PEMFC. This permits the use of a standard model structure for any desired assumptions, equations, or level of detail for the PEMFC simulation (choosing among the many existing literature models).

The *PEMFCSim* library is written in Modelica, an object-oriented, physical modeling language (1). As a first step and to the extent possible, the library utilizes standard components from the standard *Modelica* and *Modelica_Fluid* libraries (1). As a result, the fuel cell models can interface with any other existing system components (such as

pumps, compressors, and valves) and are thus inherently suited for use within fuel cell system simulations based on Modelica or other simulation languages (e.g., Simulink).

The *PEMFCSim* library currently offers 1D (one-dimensional) and quasi-2D (two dimensional) fuel cell modeling capability. The 1D model structure represents the cell through the thickness from the cathode to the anode. The quasi-2D model structure additionally describes the primary interfaces down the length of the flow channel (i.e., the electrical connections at the endplate and the reactant media connections at the flow channel).

The object-oriented modeling approach allows the library to use intuitive and physically representative component boundaries and connections. Fuel cell components, sub-components, reactant media, and test fixtures are created as separate elements or objects that can be connected or nested. Specific implementations of objects can be modified without affecting the original object structure. For example, the length of a flow channel or even its equations can be altered for a particular cell model without affecting the original flow channel model. Since the reactant media, and the components with which it interacts, are separate objects, reactant properties can simply be referenced in the component model equations. The standard *Modelica* library inherently handles mass and energy conservation in all media, electrical, and thermal connections among components.

The discussions and examples presented in this paper are based primarily upon an initial set of models from (2-4) and other literature. In some cases, these models use different approaches to describe the same characteristic, and the library includes all of these approaches as options for that object. Additional characterizations can also be defined and the existing ones can be changed easily.

The emphasis in this introductory paper for *PEMFCSim* is placed on explaining the structure and flexibility of this simulation approach and presenting examples of its application and suitability for use in collaboration among researchers and in different areas of PEMFC research. There is no intent to provide a thorough background in the Modelica modeling language in this paper (this can be obtained from the website of the Modelica Association and Modelica texts). This is an introduction to *PEMFCSim* and a more detailed exposition of the fine details within *PEMFCSim* is in preparation for the Modelica Association website.

Rationale and Overview

The need for a standard PEMFC simulation structure has a number of roots. Any review of the modeling literature leads quickly to three major conclusions: (i) comparisons among and between models are very difficult because many of the models address only one specific component within a PEMFC in any real detail, (ii) most models are designed to use fixed known and unknown variables (e.g., current as input and voltage as output) which makes their use in a dynamic fuel cell system model very difficult, and (iii) elements (component equations, assumptions) from different models cannot be easily exchanged or interfaced with each other to achieve a desired combination of modeling assumptions or level of detail because many different modeling platforms (languages, etc.) and modeling structures are used.

It is very desirable to have a standard PEMFC simulation structure that is compatible with the specific needs of dynamic testing, hardware-in-loop, and system simulation research (all major research activities within the Hawaii Natural Energy Institute at University of Hawaii). In addition, rather than establishing this PEMFC modeling capability by "reinventing the wheel", it is also very desirable to use a simulation structure that permits a selection of the most appropriate component descriptions, assumptions, and level of detail from within the already very rich PEMFC modeling literature. That is, depending on the intended use of the PEMFC simulation (e.g., diagnostics of static or dynamic test data, a dynamic model for use within a dynamic system and application, or diagnostics based on hardware-in-loop experiments), it is very important to have the flexibility to focus the particular simulation model on the characteristics of primary interest to the particular subject of research and to be able to select the level of detail to fit the specific need of the research. Finally, it is very desirable to have a PEMFC simulation structure that can be used for collaborative research activities with other research groups and permit the exchange of improved component descriptions on an "open software" basis.

The Modelica-based *PEMFCSim* meets all of these needs. In terms of flexibility, it is able to accommodate selectable levels of detail or fidelity for each of the 1D components or elements within the PEMFC and different characterizations can be implemented for the internal elements of the model without changes to the other (default) elements of the simulation. For example, if the research issue under investigation is PEMFC dynamics then the selection of each component characterization and level of detail can be selected for the time scales of interest (i.e., depending on whether it is the thermal, hydration, diffusion or electrical time scales that are of primary interest). In summary, *PEMFCSim* meets the varied research needs of HNEI (Hawaii Natural Energy Institute) primarily because of its basic structure: it has physically intuitive component boundaries and connections, it can be run with Modelica-based "test rigs" to explore specific PEMFC diagnostic issues, and it can be integrated with and run within HNEI's existing Simulink-based fuel cell system and fuel cell vehicle models.

This introductory paper is organized around a series of different topics. First, a high-level and very basic review of the Modelica structure and the development environment used herein is presented. Next, the specific *PEMFCSim* library fuel cell and supporting Modelica models applied in the library are discussed. The four levels of the *PEMFCSim* library are described. Then, the 1D and quasi-2D model formulations are presented and discussed, and some typical results are discussed as examples. Finally, the conclusions regarding *PEMFCSim* use and flexibility are summarized.

Modelica

Modelica is an object-oriented modeling language established and maintained by the Modelica Association (1). The Modelica association also provides open-source model software libraries with standard components, connectors, engineering units, chemical and physical media, etc., for a number of physical processes spanning most of the areas of engineering and physical science. These standard libraries, *Modelica* and *Modelica_Fluid*, have been previously tested and are freely available from the Modelica website (1).

In order to apply Modelica to a simulation, it is necessary to use a development environment. Several such development environments are available, including some that are free and open-source. For the applications and examples included in this paper the development environment chosen is a commercial software package, Dymola (5).

Modelica is an example of a "non-causal" modeling language because it is applied by joining the various standard components (or specialized components, such as those developed for *PEMFCSim*) together through the use of standard connectors that specify "through" and "across" variables at the connection (e.g., electrical current and voltage) without any assumptions as to cause and effect. This is the approach typified by electrical circuit diagrams and the use of loop and node analysis methods. In contrast, other popular simulation languages are referred to as "causal" (e.g., Simulink) and inherently assume certain of the variables are "inputs" and other are "outputs". This fundamental difference in approach is illustrated in Figure 1.

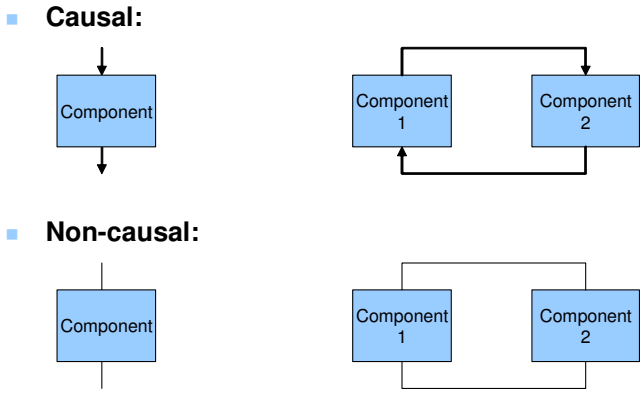

Figure 1. Causal vs. non-causal modeling

Due to the use of this non-causal formulation, the construction of higher-level Modelica models (or simulations) is very intuitive and bears a direct physical relation to the actual physical device or system that is being simulated. Examples of this are available at the Modelica website (1) and will be illustrated later for *PEMFCSim*.

The mathematical formulation of a non-causal (Modelica) modeling language vs. a causal language is basically the same as the conceptual difference between the use of explicit equations (input to output) vs. the use of implicit equations. Both forms are legitimate and they perform the same overall function, but for the explicit (causal) formulation there is an inherent assumption as to which variables are independent and which are dependant This limitation does not apply to the implicit equation formulation of Modelica, where there is no *a priori* assumption regarding cause and effect.

In summary: (i) Modelica is a multi-domain, physical, and object oriented modeling language, (ii) a model such as *PEMFCSim* is built up within Modelica using lower level objects to fully describe the system, and (iii) a wide variety of free, open source objects are available in model libraries from the Modelica Association. Thus, Modelica is ideally suited to PEMFC simulation, particularly for dynamic and system applications.

Structure of the *PEMFCSim* Library

The *PEMFCSim* library includes the basic structure of the PEMFC model. This structure is best understood in terms of four levels of organization. The first two of these levels deal with modeling components that are used within the 1D (and quasi-2D) fuel cell models, and the second two levels are the 1D and quasi-2D models.

Level 1, the lowest level, consists of Fundamental Components such as media models, control volumes, and so forth, analogous to the standard components in *Modelica* and *Modelica_Fluid*.

The next highest level, Level 2, contains the Fuel Cell Components that have been specifically developed for the fuel cell application. For example, this includes components for the GDL (gas diffusion layer), the PEM (polymer electrolyte membrane), the flow channel, the cathode catalyst layer, and the anode catalyst layer.

Within Level 1 there are two Media Models, representing the cathode and anode reactant streams. For the cathode the media is a mixture of water, oxygen, and nitrogen (H_2O, O_2, N_2) and for the anode it is a mixture of water, carbon monoxide, and hydrogen (H_2O, CO, H_2). These media models are independent of the physical component models within Levels 1 and 2. They permit a free choice of state variables and include equations for saturation pressure, density, Enthalpy, Entropy, and Gibbs Free Energy of the species present in the cathode and anode reactant streams.

The first of the two fuel cell modeling levels, Level 3, is the model for the 1D Fuel Cell. This is constructed by connecting components from Levels 1 and 2. The second of the fuel cell modeling levels, Level 4, is the Quasi-2D Fuel Cell model. This is constructed by selecting the number of 1D Fuel Cell models needed to represent the distributed nature of a real PEMFC. The number of 1D cells needed depends on the conditions under which the cell is operated as well as the application of the PEMFC simulation. The quasi-2D model structure describes the effect of the distributed nature of the PEMFC down the length of the flow channel (i.e., the electrical connections at the endplate and the reactant media connections at the flow channel).

The 1D Fuel Cell Model

The 1D Fuel Cell model, as currently implemented in the *PEMFCSim* library, is presented schematically in Figure 2. Within Figure 2 the components from Levels 1 and 2 of the *PEMFCSim* library are interconnected to simulate the various processes occurring within the PEMFC.

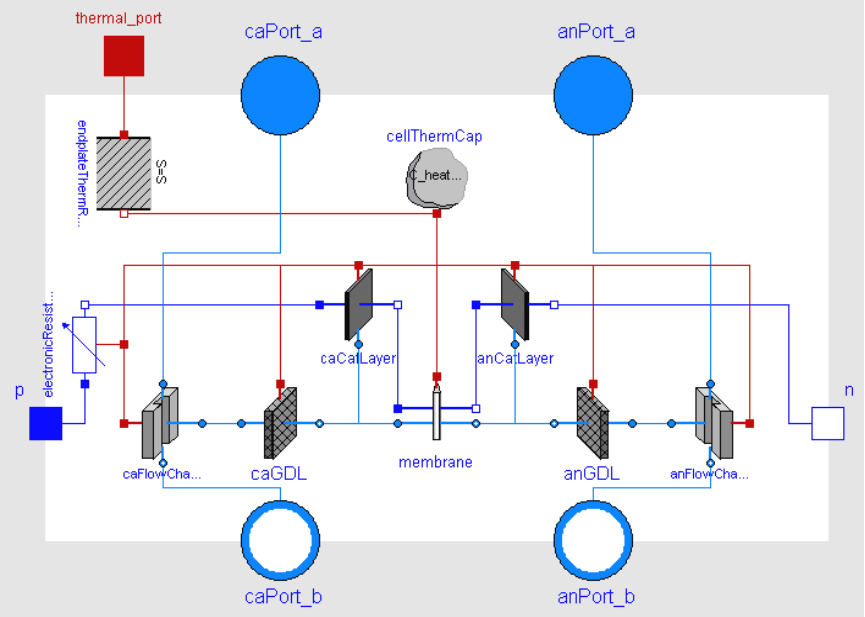

Figure 2. Model Schematic of 1D Fuel Cell Model

This schematic illustrates the physical nature of the Modelica modeling process. As can be seen in Figure 2, there are external connections for the thermal (thermal_port), reactant input and output (caPort_a, caPort_b, anPort_a, and anPort_b), and electrical ("p" and "n") processes and variables. These connectors can be used to interface the 1D Fuel Cell model into an external system or, as will be discussed later, can be used to connect the 1D Fuel Cell model into a quasi-2D model.

The physical structure of the 1D Fuel Cell, as currently implemented in the *PEMFCSim* library, is presented schematically in Figure 3. It is a seven layer structure for the PEMFC representing the direction through the cell thickness from the cathode to the anode.

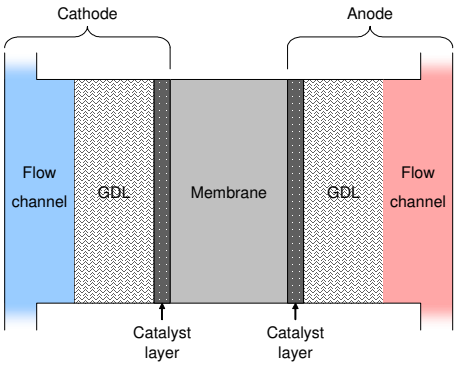

Figure 3. Physical Structure of 1D Fuel Cell

The seven layers in Figure 3 correspond to the actual physical layers through the fuel cell thickness and, as can be seen, are also directly equivalent to the model components that appear in the model schematic of the 1D Fuel Cell (Figure 2). Not only can the descriptions of any one of the physical layers within the component models of Figure 2 be independently changed, but an additional physical layer (e.g., a micro-porous layer

between the cathode GDL and Catalyst Layer) can also be added to the model schematic without affecting the other components.

Each of the model components in Figure 2 are described in Level 2 of the *PEMFCSim* library using the Modelica software language. For example, the membrane is described in terms of water content, water flow by electro-osmotic drag, water flow by diffusion, the protonic current and the voltage drop across the layer. An illustration of the level of detail that is available within the 1D model is presented in Figure 4, which shows the membrane hydration level across the thickness of the membrane for a particular set of simulation conditions (the conditions corresponding to Fig. 4 of Ref. (2)).

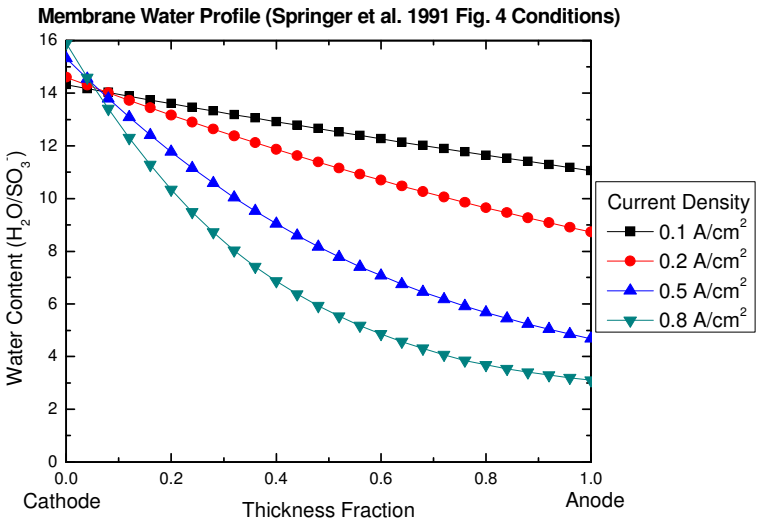

Figure 4. Hydration through membrane thickness

This result is obtained by segmenting the thickness of the membrane layer within the membrane component model. Although this level of detail can be useful in, for example, carrying out detailed diagnostics based on PEMFC static testing results it is unlikely to be used for system simulation research. In this latter case a less detailed level of description is likely to be used to simulate the membrane component.

There are a number of options currently implemented for describing the variables and modeling parameters associated with the physical processes in each of the layers in Figure 3, or the analogous components in Figure 2. *PEMFCSim* library permits a selection of the physical process representation for each of the layers (component models) of the 1D model from a menu, as well as a selection of the level of detail employed. The options available for selecting the physical process representation is shown in Table I.

TABLE I. Selectable Model Options

Component	**Characteristic**	**Option**
1D Fuel Cell	Open Circuit Voltage	Constant
		Thermodynamic
Flow Channel	Media Concentrations	Outlet concentrations
		Average mass concentrations of total mixture
		Average mole concentrations of total mixture
		Average mole concentrations of gas mixture

	Wall Friction	No Friction
		Laminar regime
		Quadratic regime
		Laminar and quadratic regime
		Whole regime
Gas Diffusion Layer	Pressure-Diffusivity Products	Constant
		Temperature dependent
Cathode Catalyst Layer	O_2 Partial Pressure	Direct
		Backing layer limited
	Overpotential	LANL empirical
		Tafel
		Butler-Volmer
	Tafel Slope	Constant
		Temperature dependent
Membrane	Temperature Dependent	Constant
		Current density dependent
		Water content dependent
	Diffusion	Constant
		Water content dependent polynomial
		Water content dependent table

This is another illustration of the flexibility of the Modelica simulation structure. As noted earlier, this flexibility is particularly important in a PEMFC model that is intended for use in a variety of applications (e.g., the particular viewpoints required for PEMFC static or dynamic testing, hardware-in-loop experimentation, or system simulation research). Since the purpose of this paper is an introduction to the *PEMFCSim* library, the details of the component models will not be discussed here in further detail. A more detailed exposition of the details within the *PEMFCSim* library is currently in preparation for publication.

The fuel cell V-I curves shown in Figure 5 are the typical results of a 1D fuel cell simulation using the *PEMFCSim* library.

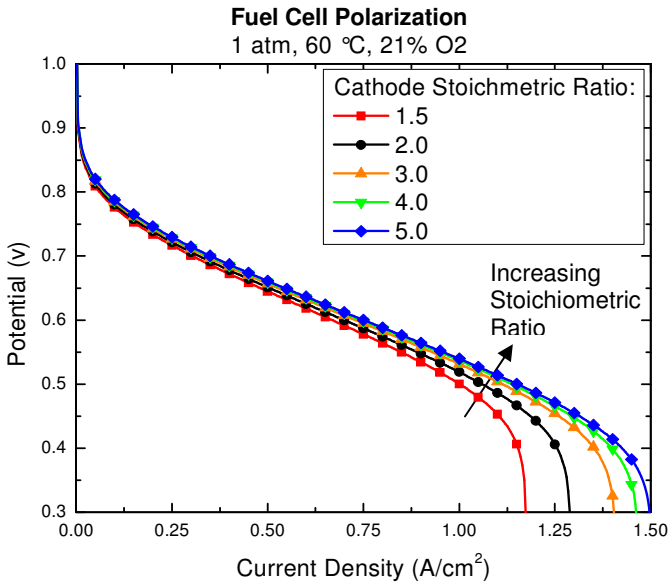

Figure 5. Modeled effects of cathode flow air stoichiometry

This figure illustrates the effect of the mass transport limitations that occur in the cell thickness direction, primarily due to the binary diffusion of oxygen, nitrogen and water

vapor through the cathode GDL and the porosity of this layer. The effects of other cell operating conditions (e.g., pressure or temperature) or parameters of the 1D layers (e.g., porosity or dimensions) can also be evaluated using the 1D model.

The Quasi-2D Modelica Fuel Cell Model

The quasi-2D model structure describes the effect of the distributed nature of the PEMFC down the length of the flow channel due to the electrical connections at the endplate, the reactant media connections at the flow channel, and the thermal connections to the temperature control system. The quasi-2D fuel cell mode is constructed by interconnecting multiple 1D fuel cell models to represent the distributed nature of a real PEMFC. The number of 1D cells needed depends on the conditions under which the cell is operated as well as the intended application of the PEMFC simulation.

Implementation of the quasi-2D fuel cell model is a straightforward interconnection of 1D fuel cell models (Figure 2) using the connectors illustrated. The electrical interconnection is accomplished by making all of the electrical "p" and "n" connectors common electrical nodes of the quasi-2D model. The "down the channel" effects of the reactant flows are simulated by connecting the cathode flow channel segments (caPort_a and caPort_b of Figure 1) of the multiple 1D models in series (i.e., caPort_b of first 1D model to caPort_a of second 1D model, and so forth). Although it will not be discussed further here, the distributed effects of the cell cooling system can also be included through the thermal connector (thermal_port) of the 1D cell model.

The quasi-2D fuel cell model can be used to evaluate the "down the channel" effects that are characteristic of the distributed nature of a real PEMFC. For example, Figure 6 illustrates the effect of the diminishing oxygen content of the cathode reactant flow for a fuel cell that is modeled by connecting ten 1D fuel cell models.

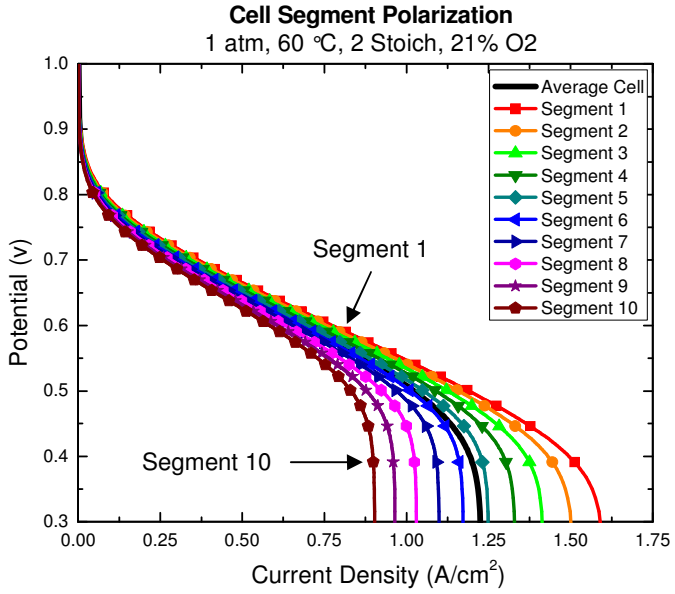

Figure 6. Modeled effects for quasi-2D fuel cell

The overall fuel cell V-I curve for the distributed cell is shown by the heavy black curve in Figure 6, whereas each of the ten 1D fuel cell segments have a dramatically different V-I relationship due to the varying oxygen content of the reactant flow stream.

An extreme version of this "down the channel" effect is provided in Figure 7.

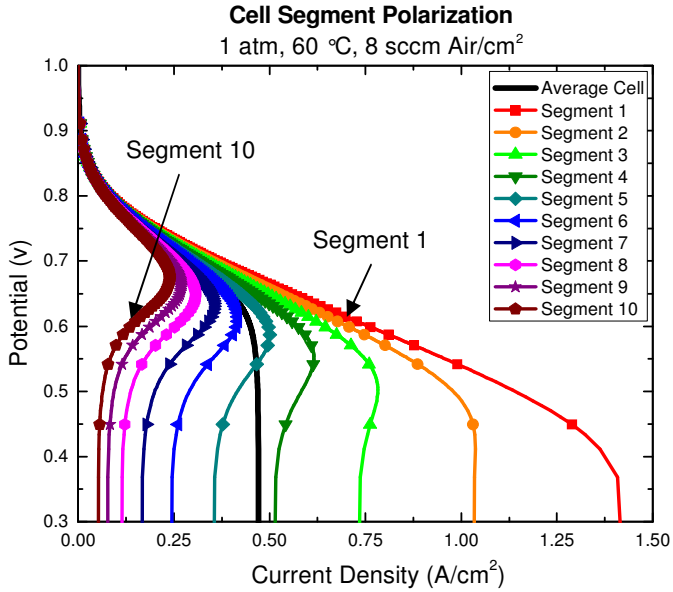

Figure 7. "Oxygen starvation" in quasi-2D fuel cell

In this figure, the simulation variable for the cathode air flow has been chosen to lead to "oxygen starvation" in the downstream fuel cell segments. Although the overall fuel cell V-I curve (heavy black line) appears rather normal, the far downstream cell segments show evidence of severe "oxygen starvation".

In addition to simulating the distributed nature of a real PEMFC for different fuel cell operating conditions, the quasi-2D model offers the opportunity to simulate the effects of realistic non-uniform properties in a PEMFC. For example, non-uniformities in any of the cell layer properties (e.g., porosity, thickness, resistance, and catalyst loading) can be incorporated into the model by varying these parameters over the different 1D models incorporated in the quasi-2D model.

The non-causal nature of the *PEMFCSim* library allows variables that are typically simulation inputs to be utilized as outputs and vice versa. For example, an operating condition such as anode humidification, which is typically an input, can be defined as an output. Correspondingly, dynamic fuel cell properties, such as membrane hydration, can be defined as inputs. The directionality is defined at the top level of the simulation without affecting any of the underlying fuel cell model equations. This capability is useful, for instance, to determine the humidification necessary to maintain a known membrane hydration level which is necessary to prevent membrane degradation.

As an example, the model is operated under two conditions. First, as a baseline, the dew point of the anode feed is fixed at the cell temperature of 80 °C (i.e., 100% humidification). In the second scenario, the membrane hydration at the anode surface

(typically the driest side) is fixed at 14 H_2O/SO_3^-, and the dew point of the anode feed is adjusted as required.

Figure 8 shows the membrane hydration at the anode and cathode surfaces of the membrane. In the baseline scenario, the hydration drops at higher current densities, but in the second scenario, the desired hydration is maintained.

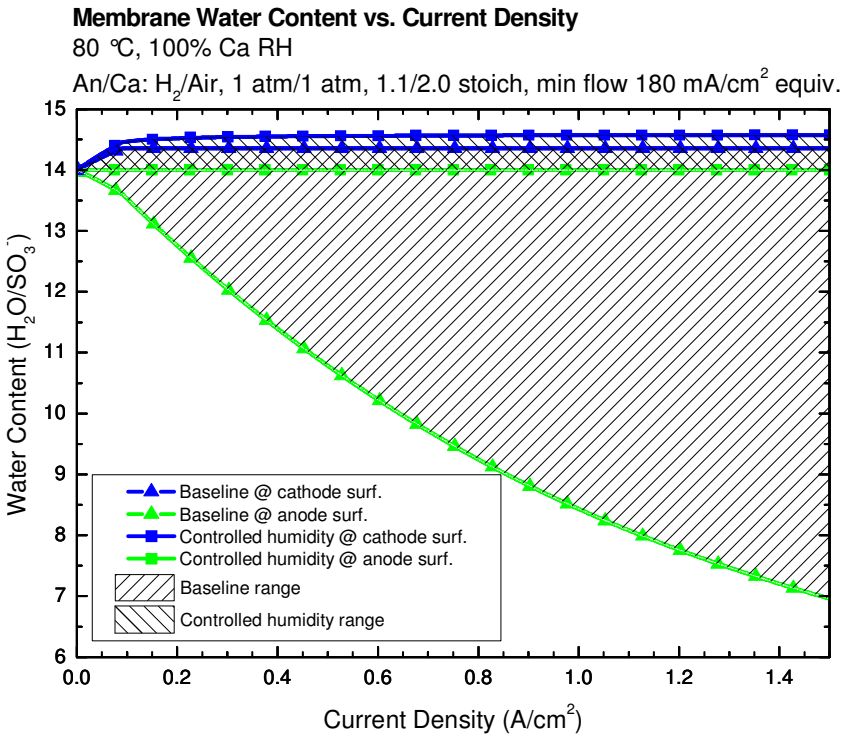

Figure 8. Membrane water content vs. current density

Figure 9 shows the anode feed dew point for the two scenarios. As expected, the dew point must be increased to maintain the required membrane hydration.

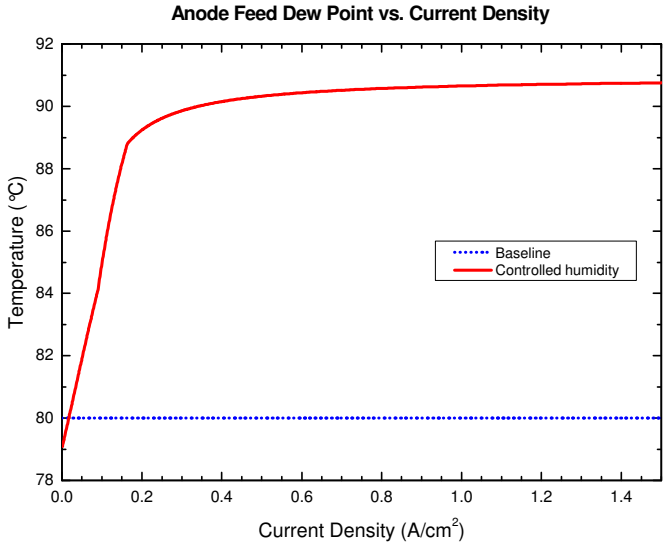

Figure 9. Anode feed dew point vs. current density

Finally, the model structure in the *PEMFCSim* library is inherently suited for dynamic application simulations. The 1D and quasi-2D models can be used to evaluate the dynamic behavior of PEMFCs due to membrane hydration, flow channel convection, layer diffusion, and electrochemical double-layer effects. Although the limited length and introductory nature of this paper does not allow the development of this topic herein, the structure of the Modelica model lends itself to dynamic simulations.

Summary

This paper has introduced a proposed standard simulation structure (*PEMFCSim* library) with three primary attributes: (i) it is compatible with the existing literature models and can incorporate any selected elements of existing models, (ii) it is ideal for collaboration among researchers focusing on different research areas or different levels of detail in PEMFC modeling, and (iii) it is inherently suited for use within fuel cell system simulations.

The *PEMFCSim* library is based on Modelica, an object-oriented, physical modeling language (1). To the extent possible, the library utilizes standard components from the *Modelica* and *Modelica_Fluid* libraries which are freely available from the Modelica Association and have been previously tested. The basic purpose of this paper has been to introduce the basic structure of the *PEMFCSim* library, the flexibility of the Modelica modeling language, and the suitability of *PEMFCSim* for use as a standard simulation approach to support PEMFC static and dynamic testing, hardware-in-loop evaluation, and system simulation research.

In order to facilitate the presentation and explanation of the utility of the *PEMFCSim* library, examples have been presented of the effects and simulation results for membrane hydration, stoichiometry of the cathode air flow, and "down the flow channel" changes in oxygen reactant including the extreme case of "oxygen starvation".

Acknowledgments

The research reported in this paper was funded by the Office of Naval Research under Grant N00014-06-1-0086.

References

1. Modelica Association, *Modelica - A Unified Object-Oriented Language for Physical Systems Modeling, ver 2.2.1*, http://www.modelica.org/, Linköping, Sweden (2005).
2. T. E. Springer, T. A. Zawodzinski and S. Gottesfeld, *J. Electrochem. Soc.*, **138**, 2334 (1991).
3. A. Z. Weber and J. Newman, *Chem. Reviews*, **104**, 4679 (2004).
4. M. Ceraolo, C. Miulli and A. Pozio, *J. Power Sources*, **113**, 131 (2003).
5. Dynasim AB, *Dymola - Dynamic Modeling Laboratory* Lund, Sweden (2007).