Equation-Based, Object-Oriented Fuel Cell Modeling

Kevin Davies
HiSERF
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Introduction and motivation

- Many uses of models in FC research and development:
  - To evaluate hypotheses of physical behavior
  - To run tests quickly and cheaply
  - To take virtual measurements
  - To design hardware and controls
  - For model-based control and model-in-the-loop

- Unfortunately,
  - Specialized models are needed for these tasks
  - Model development is labor intensive
  - Source code is not widely shared
Research gap

- PEMFC models are limited by:
  - Range of operating conditions
  - Reusability under different:
    - Boundary conditions
    - Physical configurations
  - Fidelity:
    - Dynamics
    - Spatial resolution
    - Dimensionality
    - Phases
    - Physical domains
    - Second-order phenomena
  - Computational performance
Overview of research

Vision: An open-source PEMFC model library suitable for many applications

1. **Fidelity and flexibility:** How can we model all the relevant physical phenomena of FCs to support the analysis and design of PEMFC systems, inclusive of hardware and controls?

2. **Model architecture:** How can the equations be structured so that they can be symbolically manipulated to improve computational speed and to allow linearization for control design?

3. **Performance:** Which combinations of accuracy and speed can be achieved by adjusting fidelity?
Outline

- Introduction and overview
- Related work
- Description of the model
- Sample results
- Contributions
Physics-based vs. semi-empirical models

- **Physics-based**
  - Usually Navier-Stokes via PDEs
  - Bernardi and Verbrugge (1992) led to Kulikovsky (2003), Um and Wang (2004), and others
  - Common due to advancements in CFD
  - Still too slow for systems and controls
    - 30 min. simulation time for a quasi-3D cell model (Kim, 2010)

- **Semi-empirical**
  - Usually causal ODE or DAE
  - Beginning from Springer et al. (1991)
  - Fast simulation, suitable for dynamics
  - Limited insight into physical behavior
  - Not well-suited for design
Additional classification by causality

- **Physics-based**
- **Acausal** (declarative, physical-interaction, equation-based)
- **Semi-empirical**
- **Causal** (imperative signal-flow, sequential modular)
Causal vs. Acausal

Input/output

Assignments

Algorithms

Efforts/flows

Equations

Systems of equations

\[ \begin{align*}
\text{Voltage} & = v \\
\text{Current} & = i \\
\text{Inductor} & = \frac{1}{L} \\
\text{Resistor} & = \frac{1}{R_1} \\
\text{Capacitor} & = \frac{1}{C} \\
\text{Resistor 2} & = R_2 \\
\end{align*} \]
Acausal PEMFC models

- Rubio et al. (2005 & 2010)
  - 1D
  - Isothermal
  - No external thermal or chemical connectors
  - No flow plates

- Davies and Moore (2007)
  - Quasi-2D
  - Lumped thermal

- Blunier and Miraoui (2008)
  - Quasi-2D
  - Isobaric along channels
  - Isothermal

- McCain et al. (2008)
  - 1D
  - Partitioned by species
Outline

- Introduction and research overview
- Related work
- **Description of the model**
  - Desired features
  - Fundamentals
  - Implementation
- Sample results
- Contributions
Ideally, what would a FC model cover?

Goal: To support FC research and development

- Dynamics
- Spatial distributions
- Multiple dimensions
- Multiple phases
- Heat generation
- Thermal conduction and convection
- Fluid dynamics
- Multi-component diffusion
- Electro-osmotic drag
- Ohmic losses
- Electrode kinetics
- Effects of material characteristics
Key architectural choices

- Physics-based
  - Detail about why certain behavior is observed
- Modular
  - Flexible cell architecture
  - Combinations of various species, phases, and regions
  - Object-oriented
- Reconfigurable
  - Flexible boundary conditions and assumptions (spatial resolution, dimensionality, included species, etc.)
  - Acausal or equation-based

Equation-based, object-oriented (EOO)
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Conservation at the species level

- **Problem**: How do we formulate exact conservation equations for each region, regardless of the size, when species are included in dynamically-varying amounts?

- **Approach**: Conservation equations for material, momentum, and energy of each species individually, with explicit contributions of advection and diffusion
  - Advection is direct rather than via PDE (material derivative)
    - Exact conservation guaranteed at every boundary
  - Zero torque imposed directly on the diffusive shear forces rather than via constraint on shear strain
    - No nonlinear systems of equations
Upstream discretization

\[ T_n, \dot{Q}_n \quad \rightarrow \quad R = \frac{L}{kA} \quad \rightarrow \quad Pe = IR \quad \rightarrow \quad T_p, \dot{Q}_p \]

\[ R\dot{Q}_i = (T_i - T) \left( 1 + e^{\mp Pe/2} \right) \]

- No nonlinear systems of equations
- Also applied to material and transverse translational momentum
Profile along the transport axis

- When fluid is stagnant: central difference scheme
- As flow becomes infinite: upwind scheme

- Same as Patankar (1980) at midplane and at $Pe = 0$
- No singularity at $Pe = 0$
- Patankar solution was derived under assumption of zero net flow
Coupled advection and diffusion

- Advection and diffusion are additive.
- Rate of diffusion is independent of advection, but the property at the boundary depends on advection.
- Diffusion is important during flow reversal ($Pe \approx 0$).
Stefan-Maxwell diffusion

**Background:** Many FC models use Stefan-Maxwell equations for binary diffusion:

\[
\frac{\nabla \mu_i}{T} = \frac{n_{\text{spec}}}{\sum_{j=1}^{n_{\text{spec}}} n_i n_j} \left( \phi_j - \phi_i \right)
\]

- Nonlinear system of \( n_{\text{spec}} \) equations
- Singular as written
  - One equation (arbitrary choice!) is replaced with a bulk mass transport equation, or
  - A term is added to each equation to consider drag with the solid (singular as Knudsen diffusion becomes negligible!) (Weber & Newman, 2005)
Generalized Stefan-Maxwell diffusion framework

- **Problem**: How do we represent multi-component diffusion without nonlinear equations or singularities?
- **Approach**: Diffusive exchange of momentum rather than direct constraint on velocities
  - Every phase of every species \( i \) has a mobility with respect to each connected node \( j \)
  
  \[
  \mu_{ij} \dot{m} \Phi_i = \sum_{j=1}^{n_{\text{nodes}}} N_i (\phi_j - \phi_i)
  \]
  - This force is included in momentum balance
  - Describes electrical resistance and electro-osmotic drag
  - Also appropriate for thermal exchange (with change of variables)
### Diffusive exchange

- Nodes are added among species as needed

<table>
<thead>
<tr>
<th>Number of species</th>
<th>Default connection</th>
<th>Binary</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>![Diagram for 2 species]</td>
<td>![Diagram for 2 species]</td>
</tr>
<tr>
<td>3</td>
<td>![Diagram for 3 species]</td>
<td>![Diagram for 3 species]</td>
</tr>
<tr>
<td>4</td>
<td>![Diagram for 4 species]</td>
<td>![Diagram for 4 species]</td>
</tr>
</tbody>
</table>

○ Node  
● Species
Advective exchange

- In the case of reactions and phase change, translational momentum and energy are exchanged via advection.
- Intensive properties are those of the source.
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Overall goal

An open-source PEMFC model library suitable for many applications

1. Descriptive
2. Modular
3. Reconfigurable
4. Quick to simulate
Structure of the model library

- **Problem**: How can we organize the library?
  - 196 models, 428 functions, >26,000 lines of code
  - Many levels of physical and software detail
- **Approach**: Object-oriented package hierarchy

- FCSys
- 📜 User's Guide
- 🎨 Blocks
- ☑ Conditions
- ☑ Assemblies
- ☑ Regions
- ☑ Subregions
- ☑ Phases
- ☑ Species
- ☑ Chemistry
- ☑ Characteristics
- ☑ Connectors
- 🎨 Units
- 📜 Quantities
- ☑ Utilities
- 🎨 Icons
Physical interactions

- **Problem:** How can we best manage all the interactions among models?
  - Up to 50 variables involved in a single layer interface

- **Approach:** Hierarchy of acausal connectors
Novel application of efforts and flows

- Efforts and flows are usually power conjugates
- But also well-suited to:
  - Dalton’s law of additive pressures
    - Effort volume, flow pressure
  - Amagat’s law of additive volumes
    - Effort pressure, flow volume
- Another pair of opposites:
  - Chemical diffusion of a species
    - Effort potential, flow current
  - Reaction equilibrium
    - Effort reaction rate, flow stoichiometrically-weighted potentials
Problem:

- Faraday constant appears in model of electrical but not chemical species
  - Difficulty in coding a general species
- FC data is often not written in SI units
  - Entry is tedious and error-prone

Approach:

- Quantities written as the product of a number and a unit
- Units derived from universal physical constants
  - E.g.: \texttt{constant Q.Length m=10973731.568539*rad/R_{inf} "meter"};
  - Rydberg constant
- Those constants can be given any value
- Gas and Faraday constants normalized to 1 and eliminated from model
Adjustable fidelity

- **Problem**: How can we create detailed models and simple, fast-simulating models from the same library?

- **Approach**:
  1. **Index reduction**
     - States combined automatically when directly coupled, e.g.:
     - Zero thermal resistance among species $\Rightarrow$ same temperature for all
  2. **Modularity**
     - Some layers can be combined
  3. **Options to**:
     - Vary spatial resolution and dimensionality
     - Apply assumptions—ideal gas, incompressible flow, etc.
Object-oriented features

- **Problem**: How can we implement all of the models systematically and without excessive redundancy?
  - 8 species, 2 fluid phases, 2 solid phases, 7 layers

- **Approach**: Inheritance and instantiation
  - 1 base model for all species
  - Species conditionally included
  - Material characteristics in a replaceable package
Phase model

- Contains interconnected species models

Graphite:
Subregion model

- Lowest level of spatial resolution
Region model

- Represents layers of cell
- 3D, rectilinear array of subregions
Cell model

- Single-cell PEMFC
- Up to 3 dimensions, but quasi-2D by default
Test stand model

- Applies boundary conditions to evaluate cell performance

  - BCs are replaceable:
    - Current or potential
    - Heat flow rate or temperature
    - Air or pure O$_2$

  - And adjustable:
    - Flow rates
    - Humidities
    - Outlet pressure
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Test stand with a single cell (1 segment down the channel) has:

- 6887 variables (2749 time-varying)
- 55 states
- No nonlinear systems of equations

And takes:

- ~23 s to translate
- ~1.6 s to simulate a polarization curve (10 hrs of represented time)
Polarization curves under varying conditions

**Temperature**

Cell Polarization: Varying Inlet and Flow Plate Temperature
48.3 kPag; An|Ca: 1.5|2.0 stoich, H₂|Air, 80|50 % RH

- Model @ 40 °C
- Model @ 60 °C (baseline)
- Model @ 80 °C
- Experiment @ 40 °C
- Experiment @ 60 °C (baseline)
- Experiment @ 80 °C

**Pressure**

Cell Polarization: Varying Outlet Pressures
60 °C; An|Ca: 1.5|2.0 stoich, H₂|Air, 80|50 % RH

- Model @ 0 kPag
- Model @ 48.3 kPag (baseline)
- Model @ 202.7 kPag
- Experiment @ 0 kPag
- Experiment @ 48.3 kPag (baseline)
- Experiment @ 202.7 kPag

- Trends are qualitatively correct, but significant quantitative differences; may be due to
  - H₂ cross over
  - Transport behavior of the liquid
Energy balance

- ORR activation dominates the loss

Energy Balance
Baseline Conditions @ 1.5 A/cm²

Key:
- Thermal cond.
- Fluid
- Electrical

Anode
Cathode

PEMFC

- \( \text{H}_2 \text{O}_2 \) ca 28.8W
- \( \text{H}_2 \text{O}_1 \) ca 76.0W
- \( \text{O}_2 \) ca 0.2W
- \( \text{N}_2 \) ca 0.0W
- ca 54.3W

- \( \text{H}_2 \) an 0.4W
- \( \text{H}_2 \text{O}_1 \) an 11.2W
- \( \text{H}_2 \text{O}_2 \) an 9.5W
- an 14.3W

38.6W
Distributed temperature

- Temperatures up to ~5.5 K higher within cell due to heat generation (hottest in cathode CL)
Oxygen partial pressure

- Roll-off at concentration limit

**O$_2$ Pressure from the Inlet to the ORR**

**Baseline Conditions**

- Inlet
- caFP
- caFP-caGDL interface
- caGDL
- caGDL-caCL interface
- caCL/ORR

**Pressure / kPa**

**Current density / A cm$^{-2}$**
Segmented cell

- Liquid not included
- 31,990 variables (12,711 time-varying)
- Simulates in ~11 s
Sinusoidal electrical load

- 0.3 Hz
- Amplitude of 140 mA/cm²
- Offset of 80 mA/cm²
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Contributions

- First acausal, physics-based FC model
- Highly modular, reconfigurable, and descriptive
- Possible extensions to other fluidic or electrochemical devices
- Novel equations which are consistent with fundamental transport theory

Available online
- Google “FCSys”
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## References


