Equation-Based, Object-Oriented Fuel Cell Modeling

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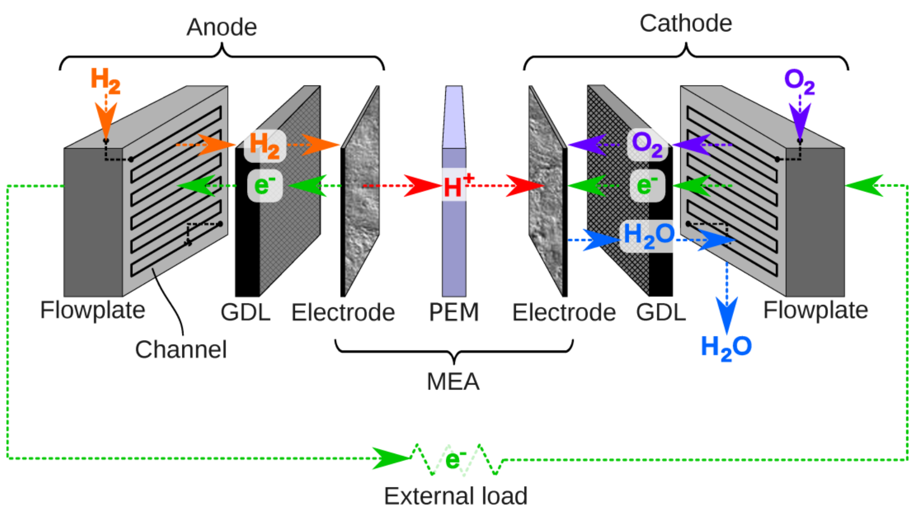
Introduction and motivation

- 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?

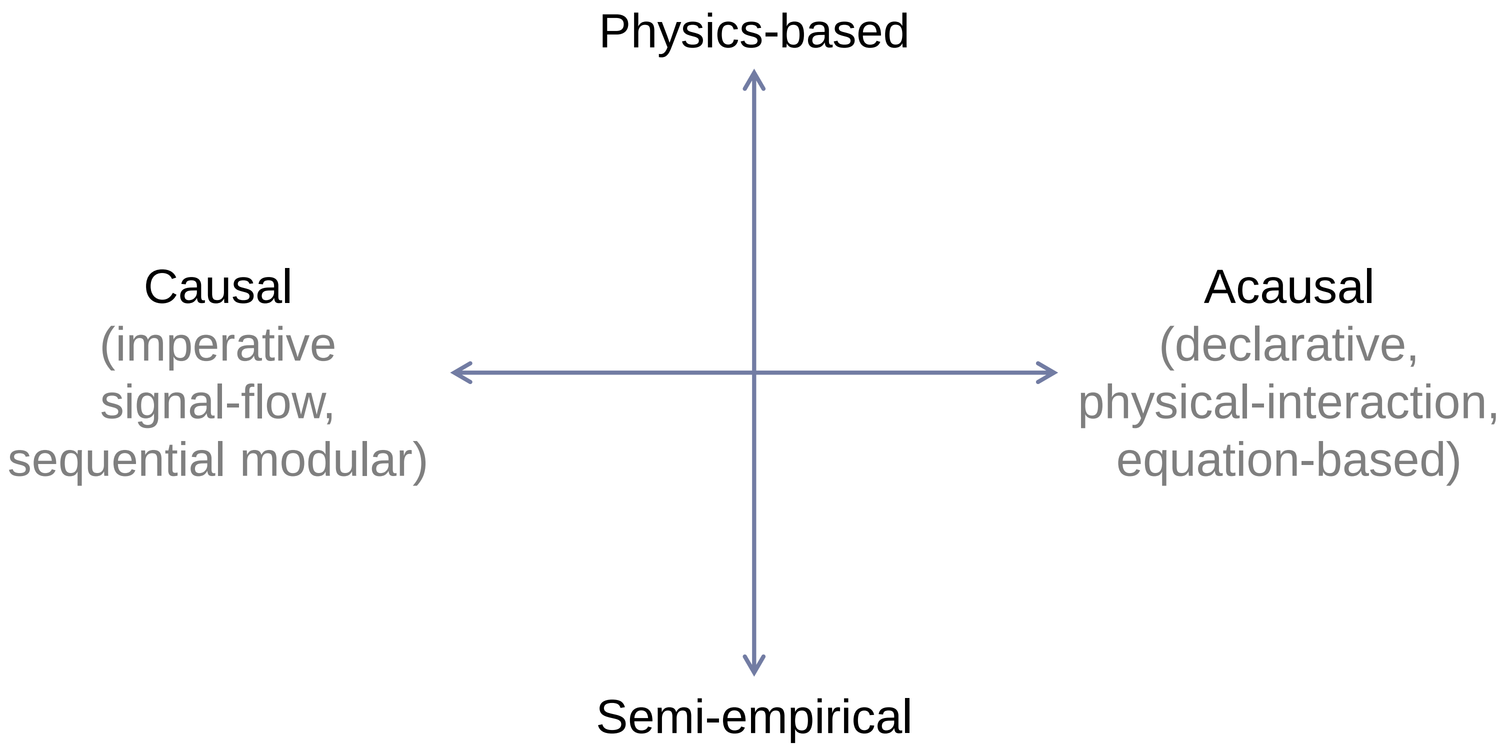
Outline

- Introduction and overview
- **Related work**
- Description of the model
- Sample results
- Contributions

Physics-based vs. semi-empirical models

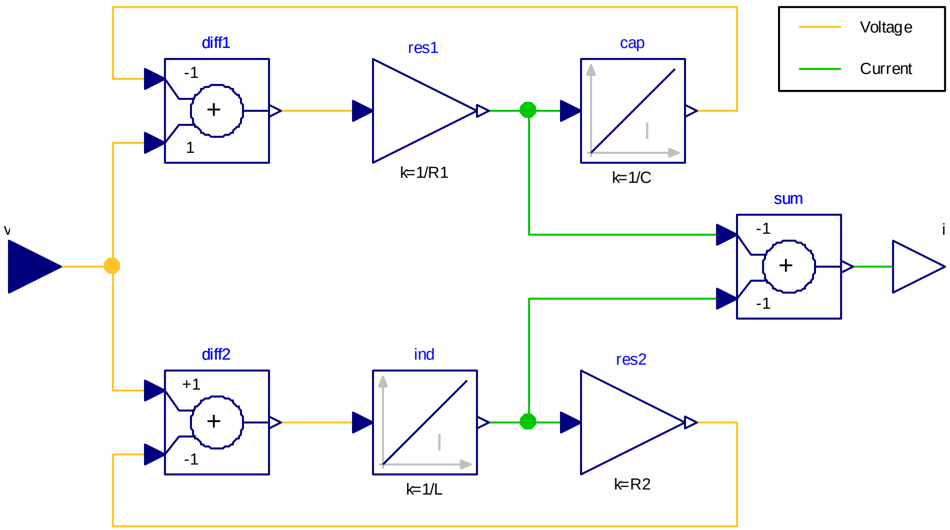
- Physics-based
  - Usually Navier-Stokes via PDEs
  - Bernardi and Verbrugge (1992) led to Kulikovsky (2003), Um and Wang (2004), and others
  - Common due to advancements in CFD
  - Still too slow for systems and controls
    - 30 min. simulation time for a quasi-3D cell model (Kim, 2010)
- Semi-empirical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

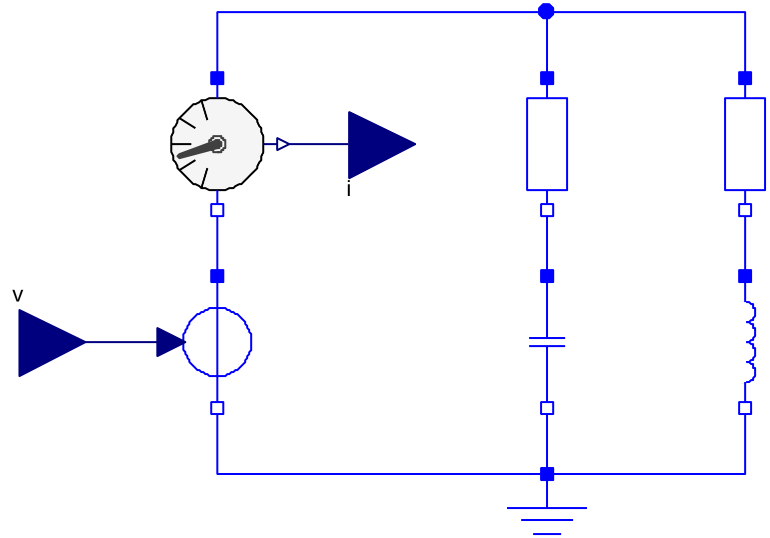
Additional classification by causality



Causal vs. Acausal

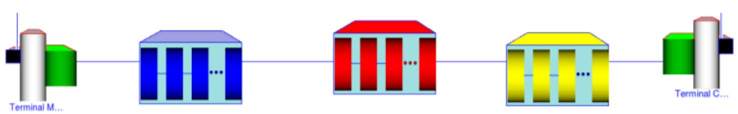
Causal	Acausal
Input/output	Efforts/flows
	
Assignments	Equations
Algorithms	Systems of equations



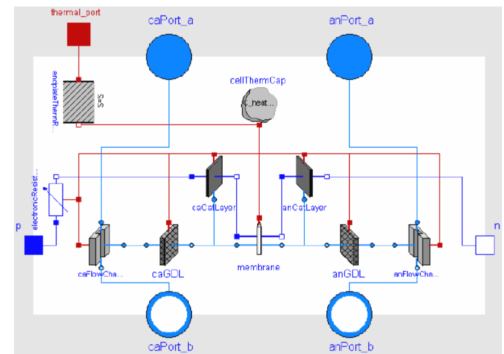


Acausal PEMFC models

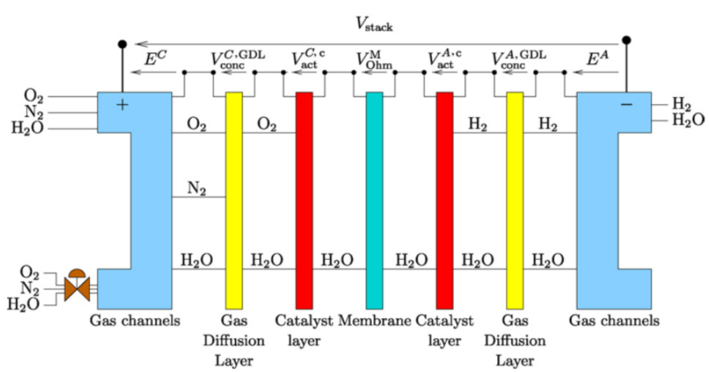
- Rubio et al. (2005 & 2010)
  - 1D
  - Isothermal
  - No external thermal or chemical connectors
  - No flow plates



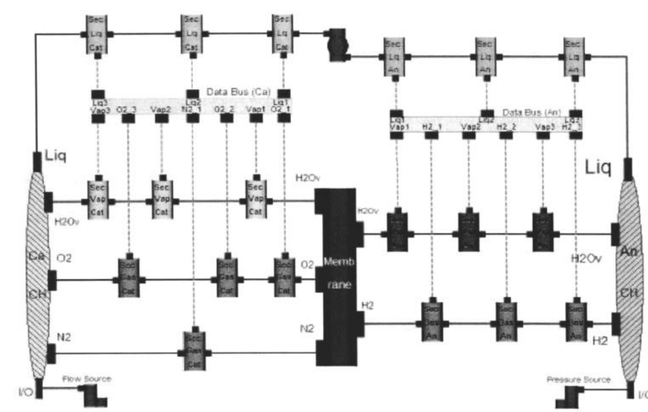
- Davies and Moore (2007)
  - Quasi-2D
  - Lumped thermal



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



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



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  - Fundamentals
  - Implementation
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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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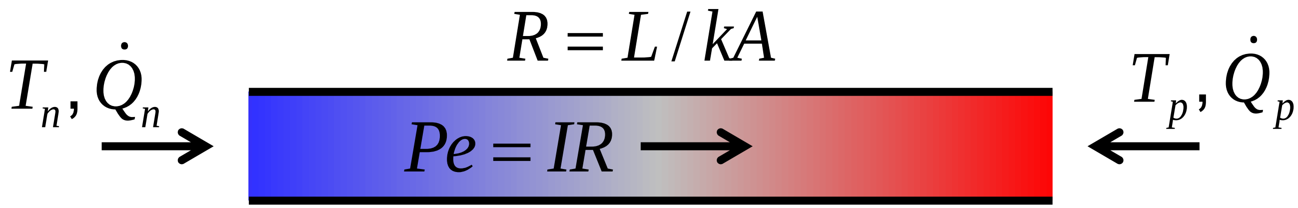
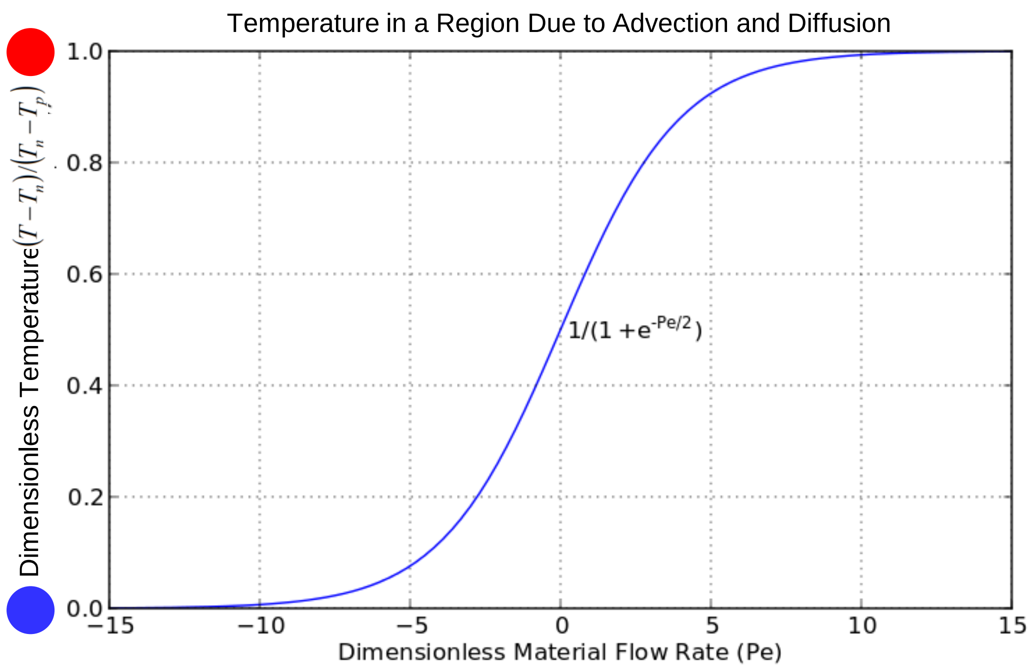
Conservation at the species level

- **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)
    - $\Rightarrow$ Exact conservation guaranteed at every boundary
  - Zero torque imposed directly on the diffusive shear forces rather than via constraint on shear strain
    - $\Rightarrow$ No nonlinear systems of equations

Upstream discretization



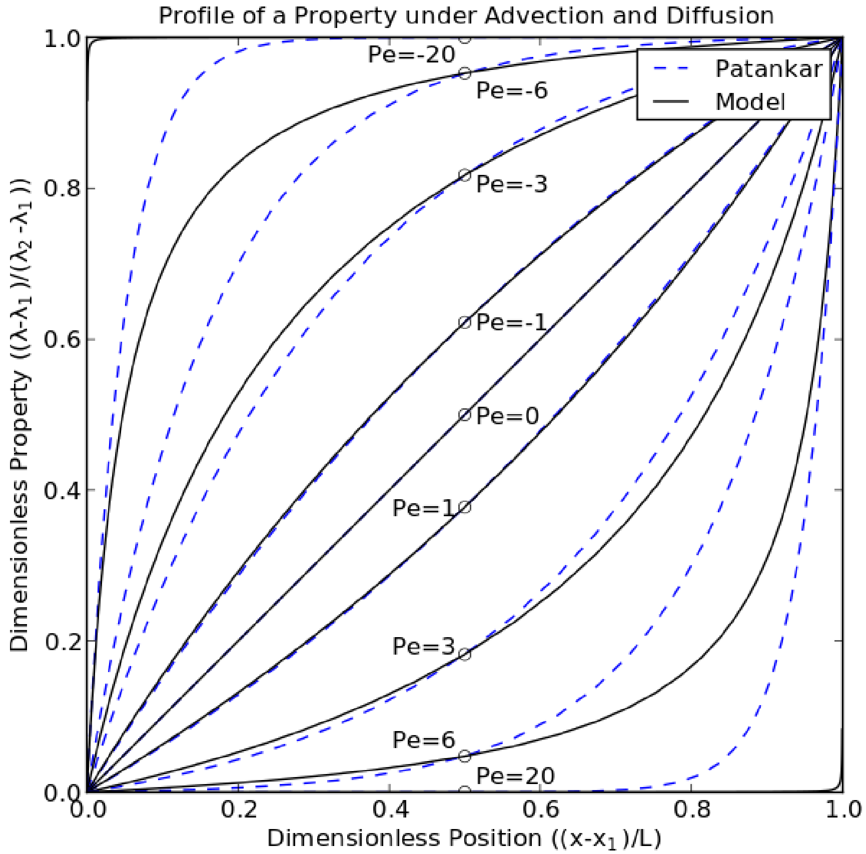
$$R\dot{Q}_i = \left(T_i - T\right)\left(1 + e^{\mp Pe/2}\right)$$



- No nonlinear systems of equations
- Also applied to material and transverse translational momentum

Profile along the transport axis

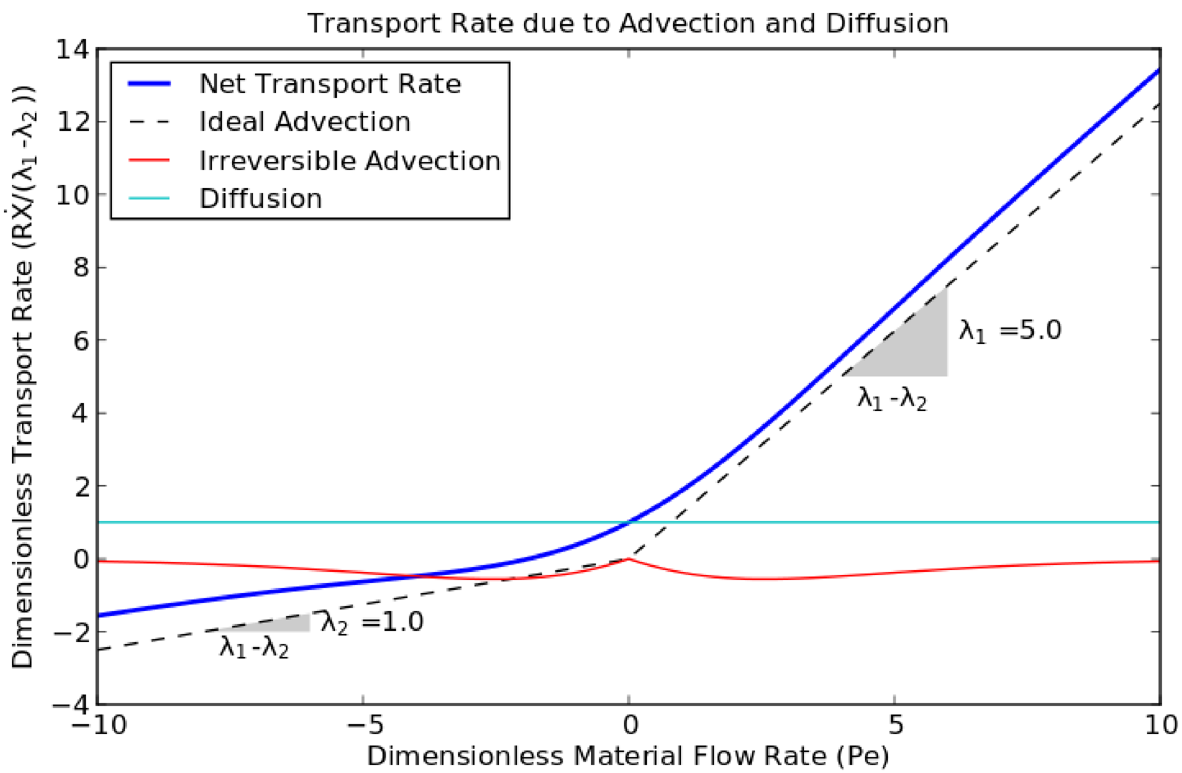
- When fluid is stagnant: central difference scheme
- As flow becomes infinite: upwind scheme



- 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:

$$\frac{\nabla \mu_i}{T} = \sum_{\substack{j=1 \\ j \neq i}}^{n_{\text{spec}}} \frac{n_i n_j}{D_{ij}} \left(\phi_j - \phi_i \right)$$

  - Nonlinear system of n_{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

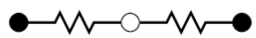
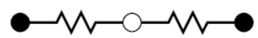
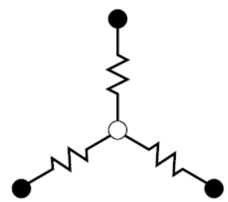
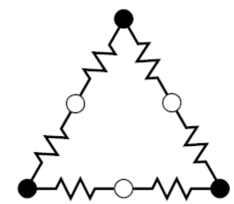
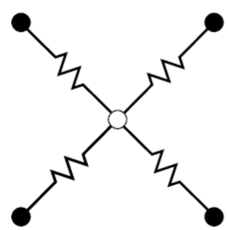
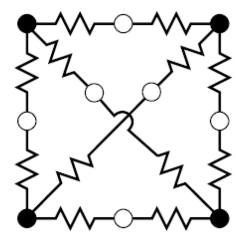
- **Problem**: How do we represent multi-component diffusion without nonlinear equations or singularities?
- **Approach**: Diffusive exchange of momentum rather than direct constraint on velocities
  - Every phase of every species *i* has a mobility with respect to each connected node *j*

$$\mu_{ij}\;\dot{m}\Phi_i = \sum_{j=1}^{n_{\text{nodes}}} N_i\left(\phi_j - \phi_i\right)$$

  - 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

Number of species	Default connection	Binary
2		
3		
4		

○ 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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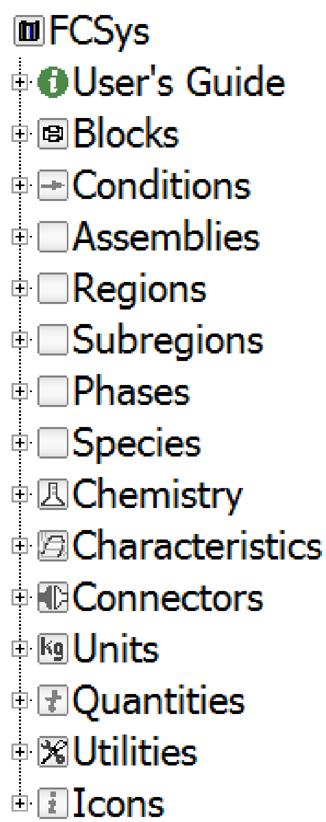
Overall goal

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

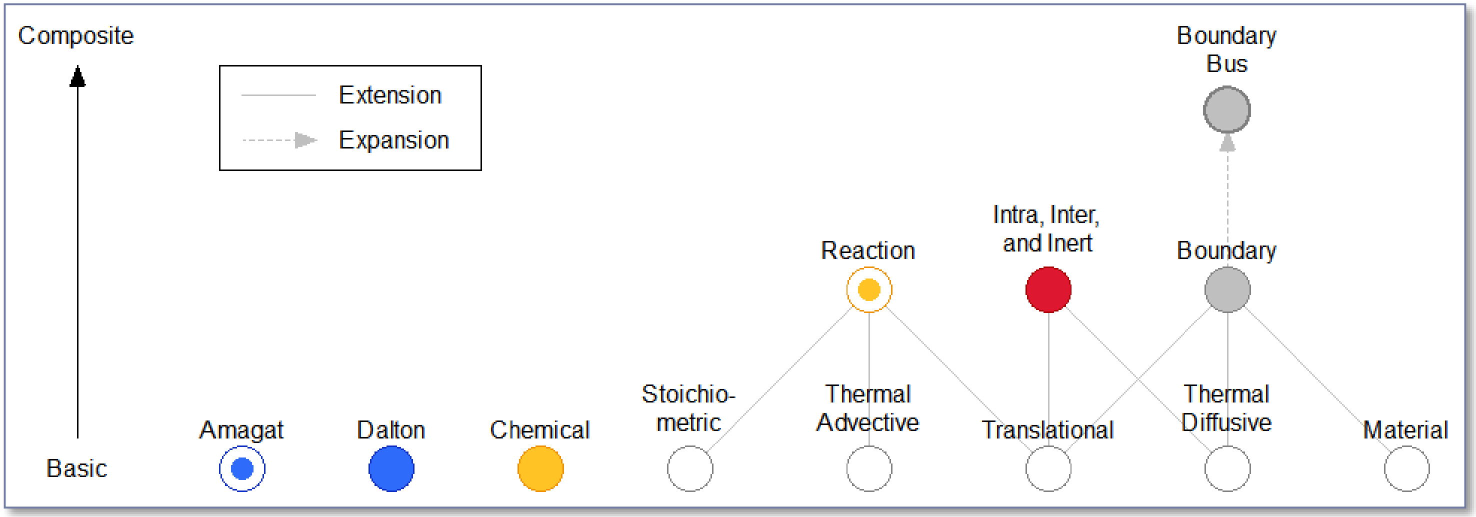
- **Problem:** How can we organize the library?
  - 196 models, 428 functions, >26,000 lines of code
  - Many levels of physical and software detail
- **Approach:** Object-oriented package hierarchy



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

Natural units

Problem:

- Faraday constant appears in model of electrical but not chemical species
  - $\Rightarrow$ Difficulty in coding a general species
- FC data is often not written in SI units
  - $\Rightarrow$ 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.: `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

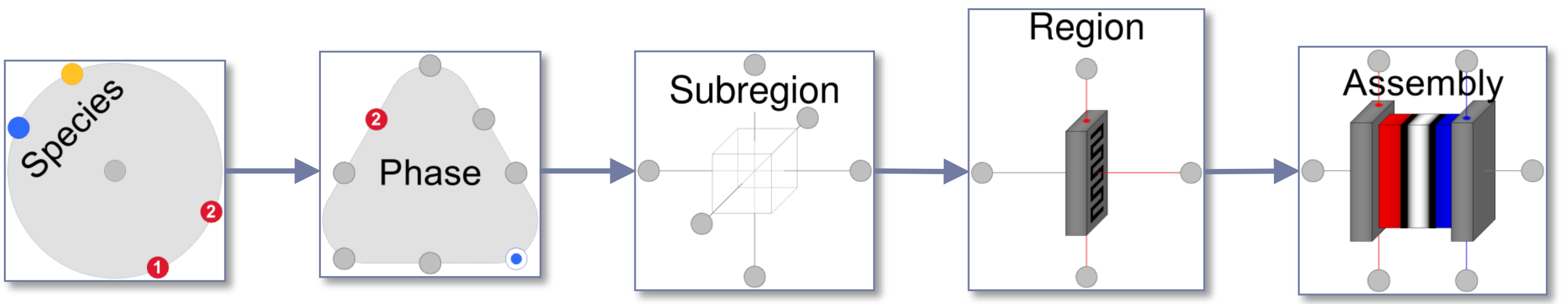
Adjustable fidelity

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

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

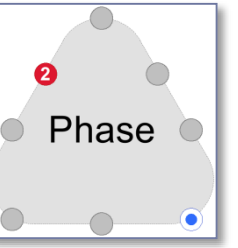
- **Problem**: How can we implement all of the models systematically and without excessive redundancy?
  - 8 species, 2 fluid phases, 2 solid phases, 7 layers
- **Approach**: Inheritance and instantiation



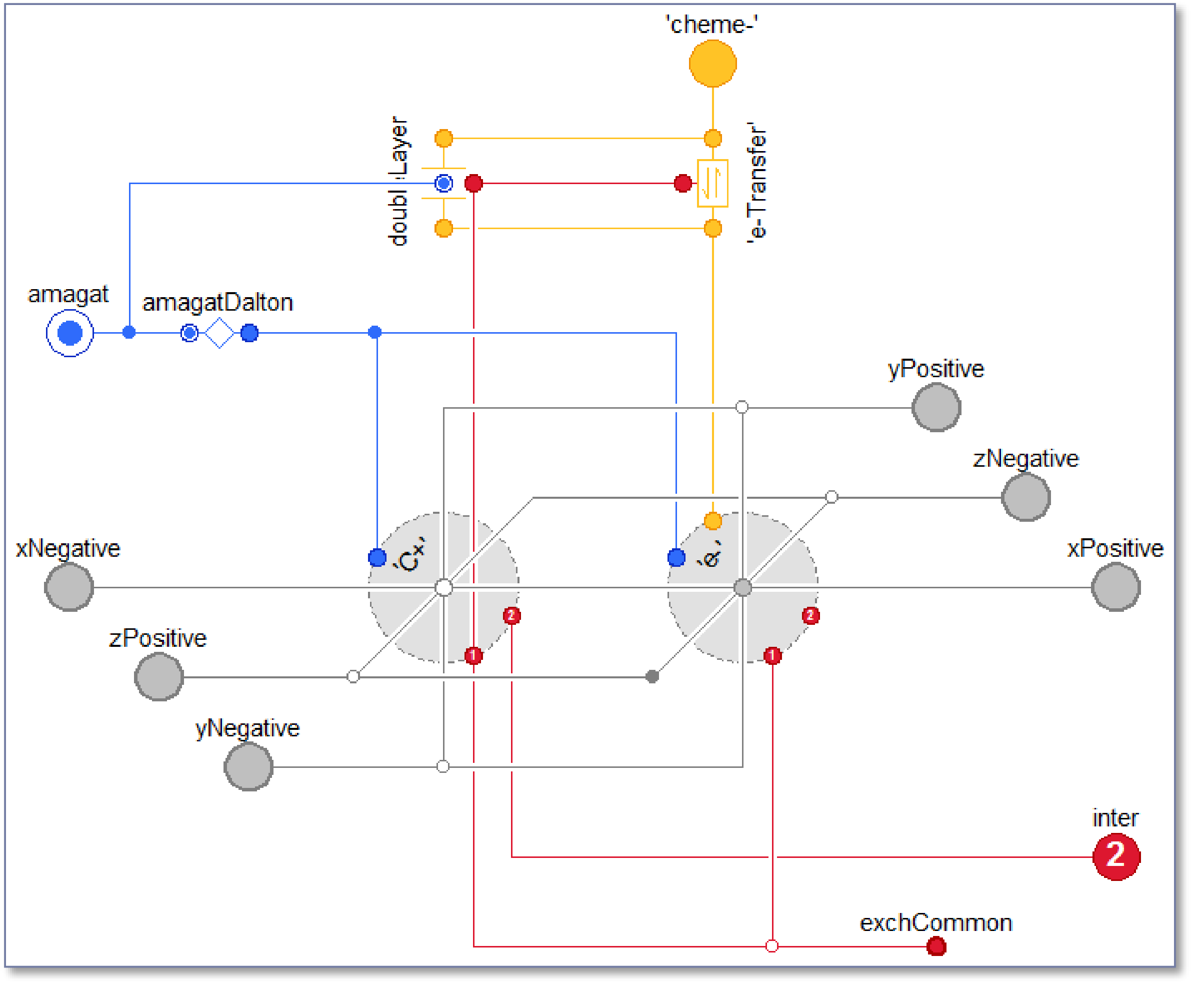
  - 1 base model for all species
  - Species conditionally included
  - Material characteristics in a replaceable package

Phase model

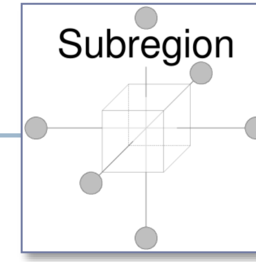
- Contains interconnected species models



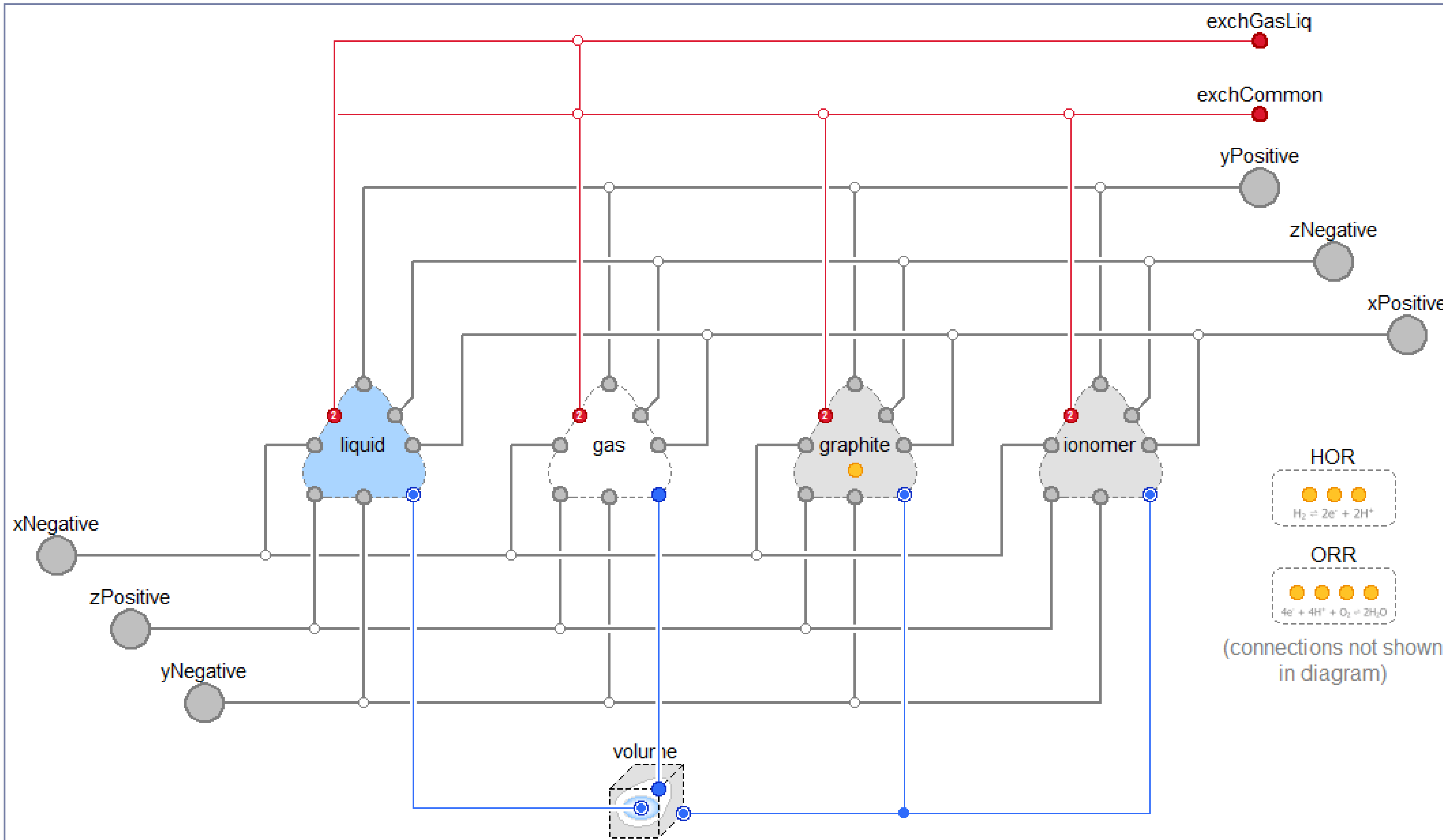
Graphite:



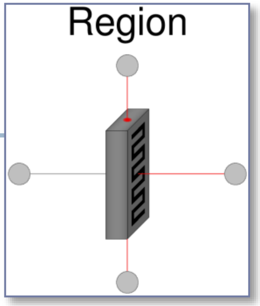
Subregion model



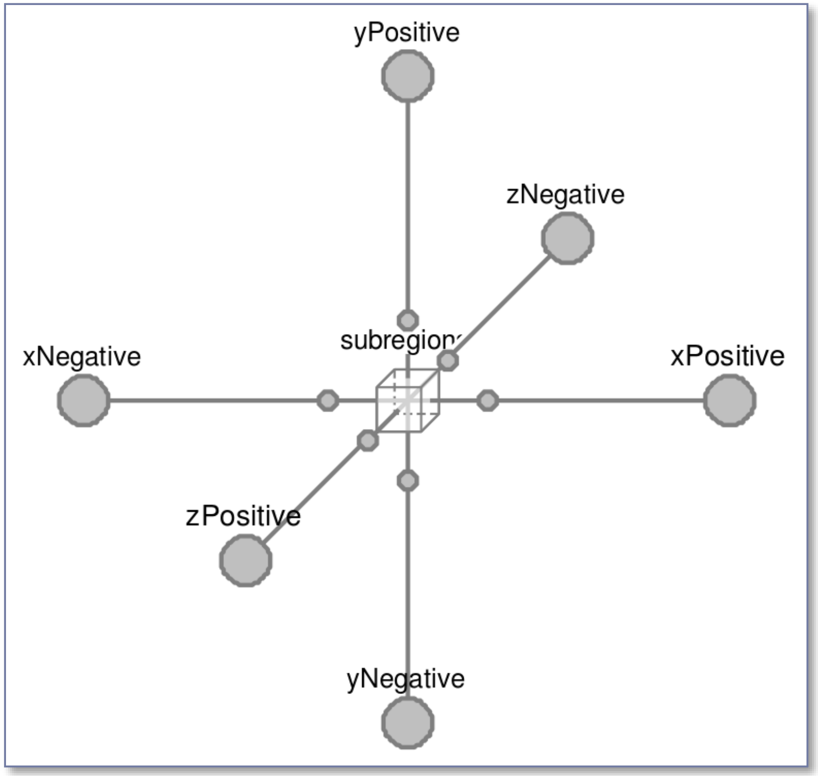
- Lowest level of spatial resolution

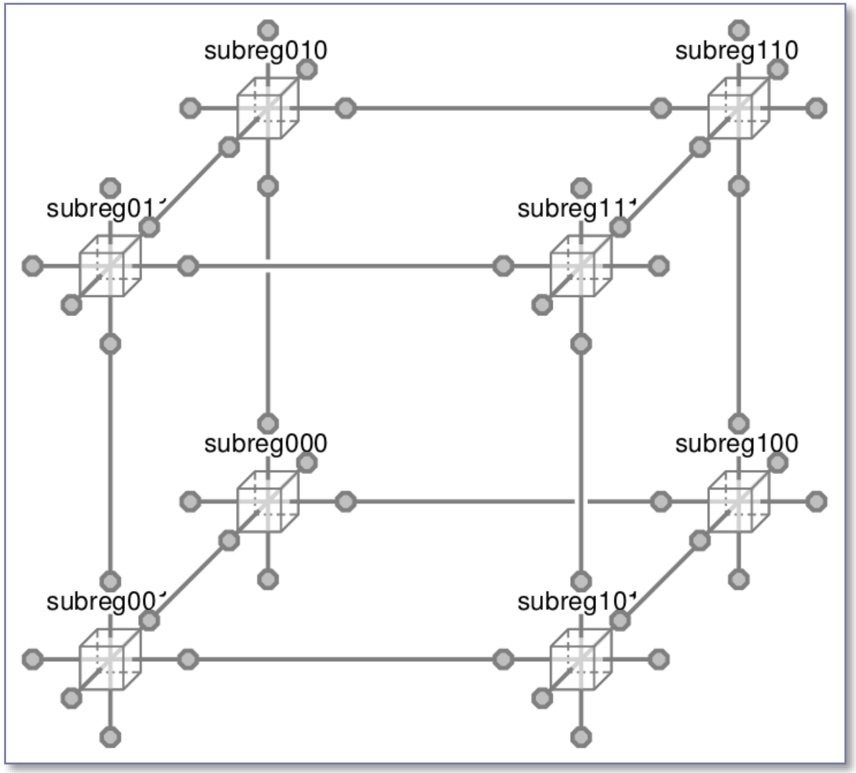


Region model

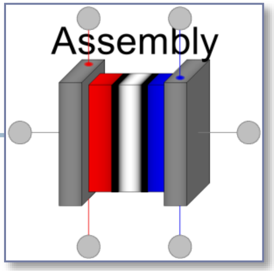


- Represents layers of cell
- 3D, rectilinear array of subregions

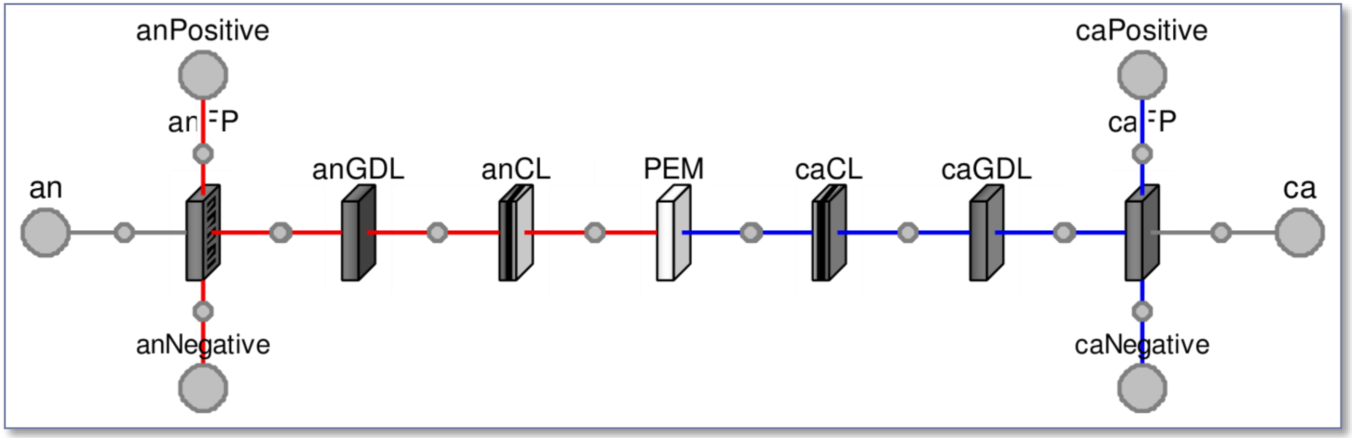


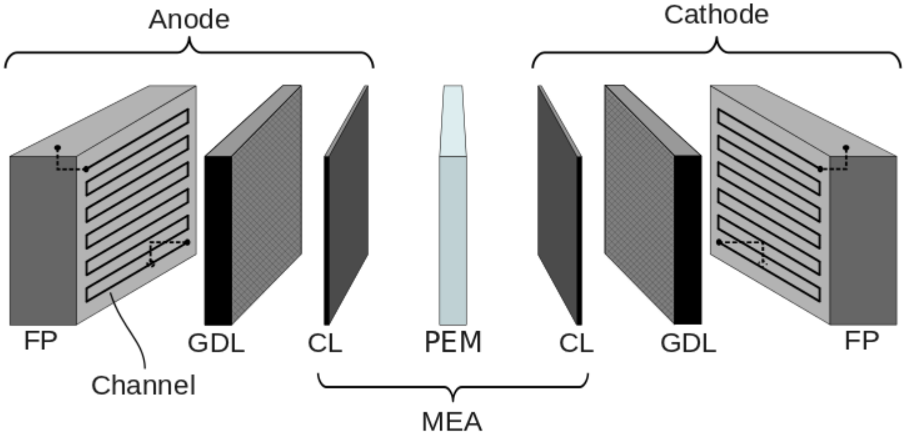


Cell model



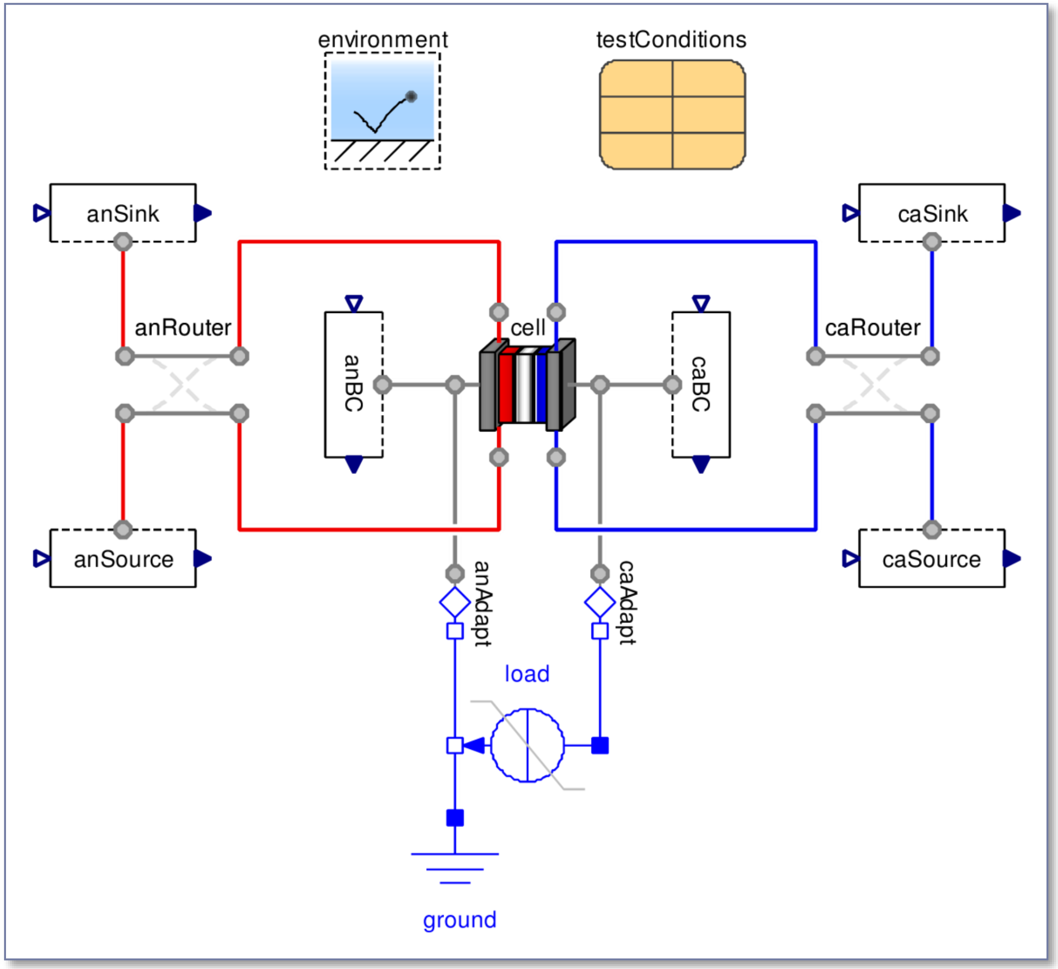
- Single-cell PEMFC
- Up to 3 dimensions, but quasi-2D by default





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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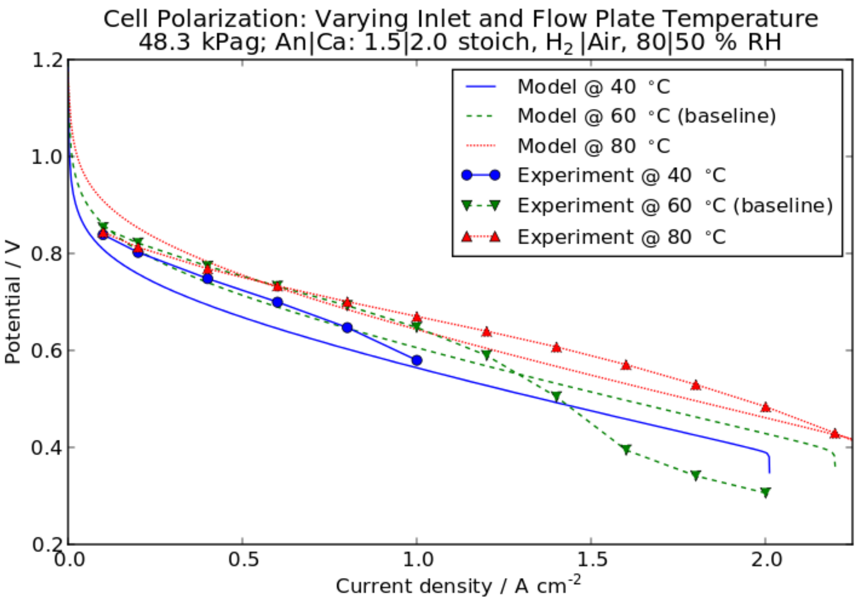
- Description of the model
- **Sample results**
- Contributions

Modeling and simulation statistics

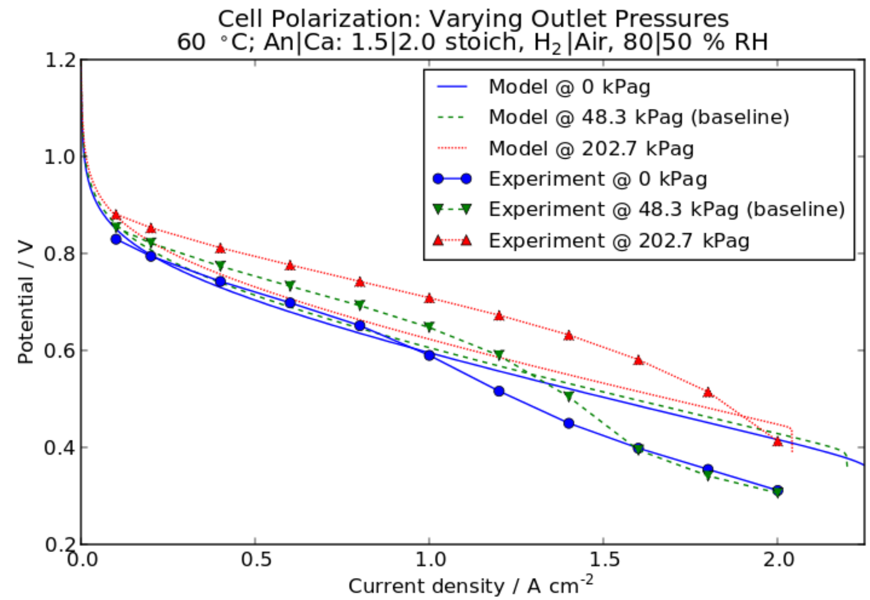
- Test stand with a single cell (1 segment down the channel) has:
  - 6887 variables (2749 time-varying)
  - 55 states
  - No nonlinear systems of equations
- And takes:
  - ~23 s to translate
  - ~1.6 s to simulate a polarization curve (10 hrs of represented time)

Polarization curves under varying conditions

<u>Temperature</u>



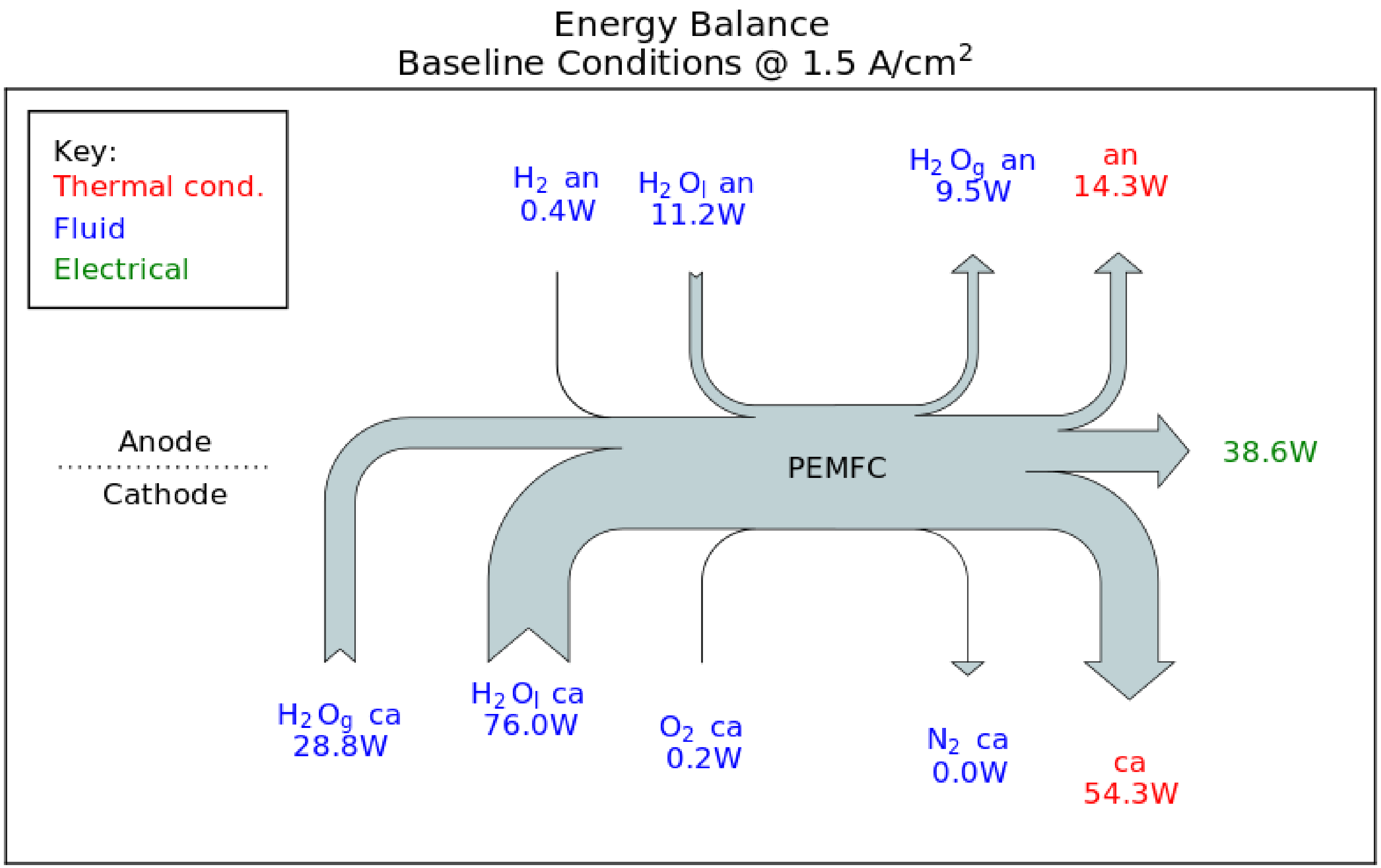
<u>Pressure</u>



- Trends are qualitatively correct, but significant quantitative differences; may be due to
  - H_2 cross over
  - Transport behavior of the liquid

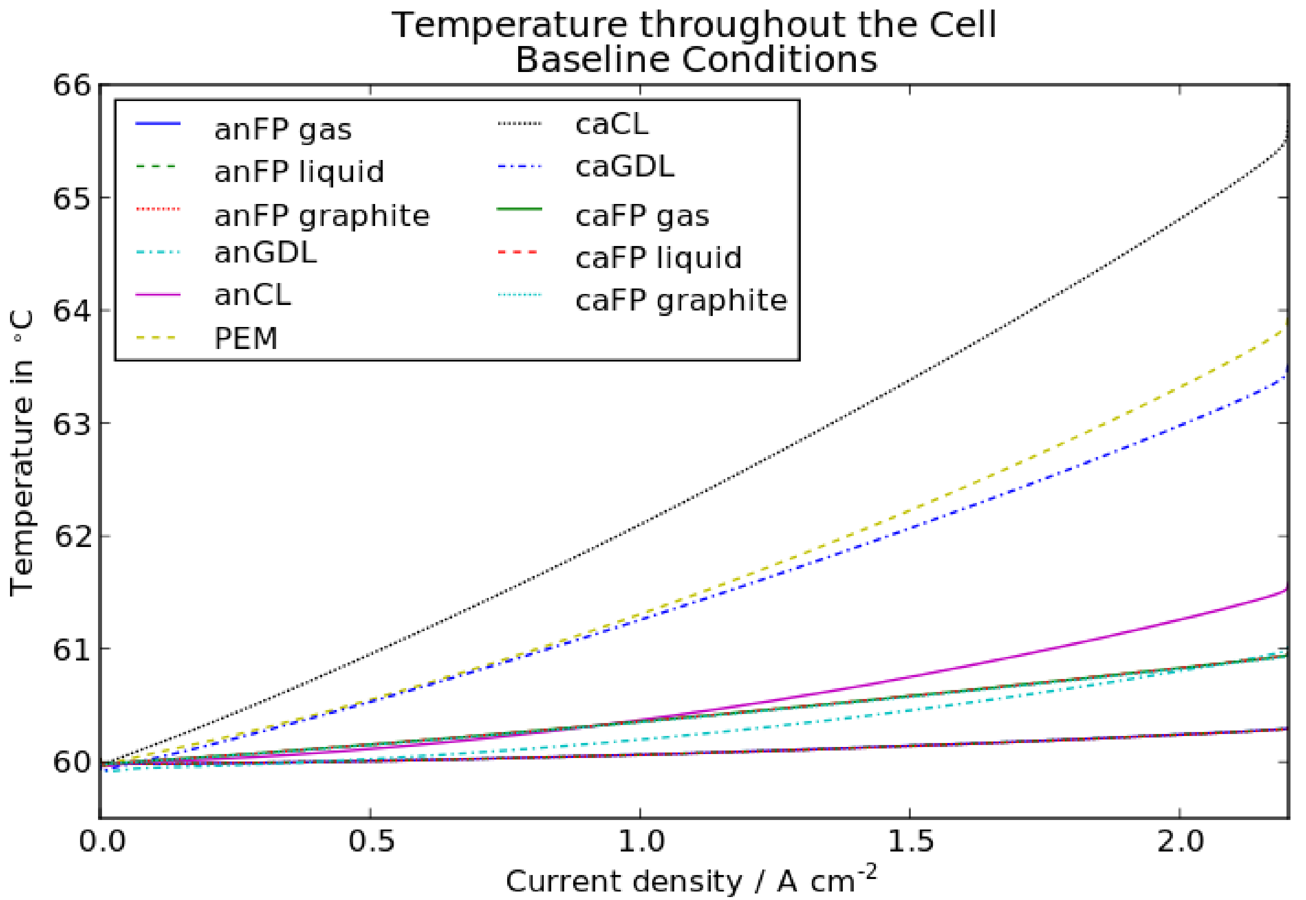
Energy balance

- ORR activation dominates the loss



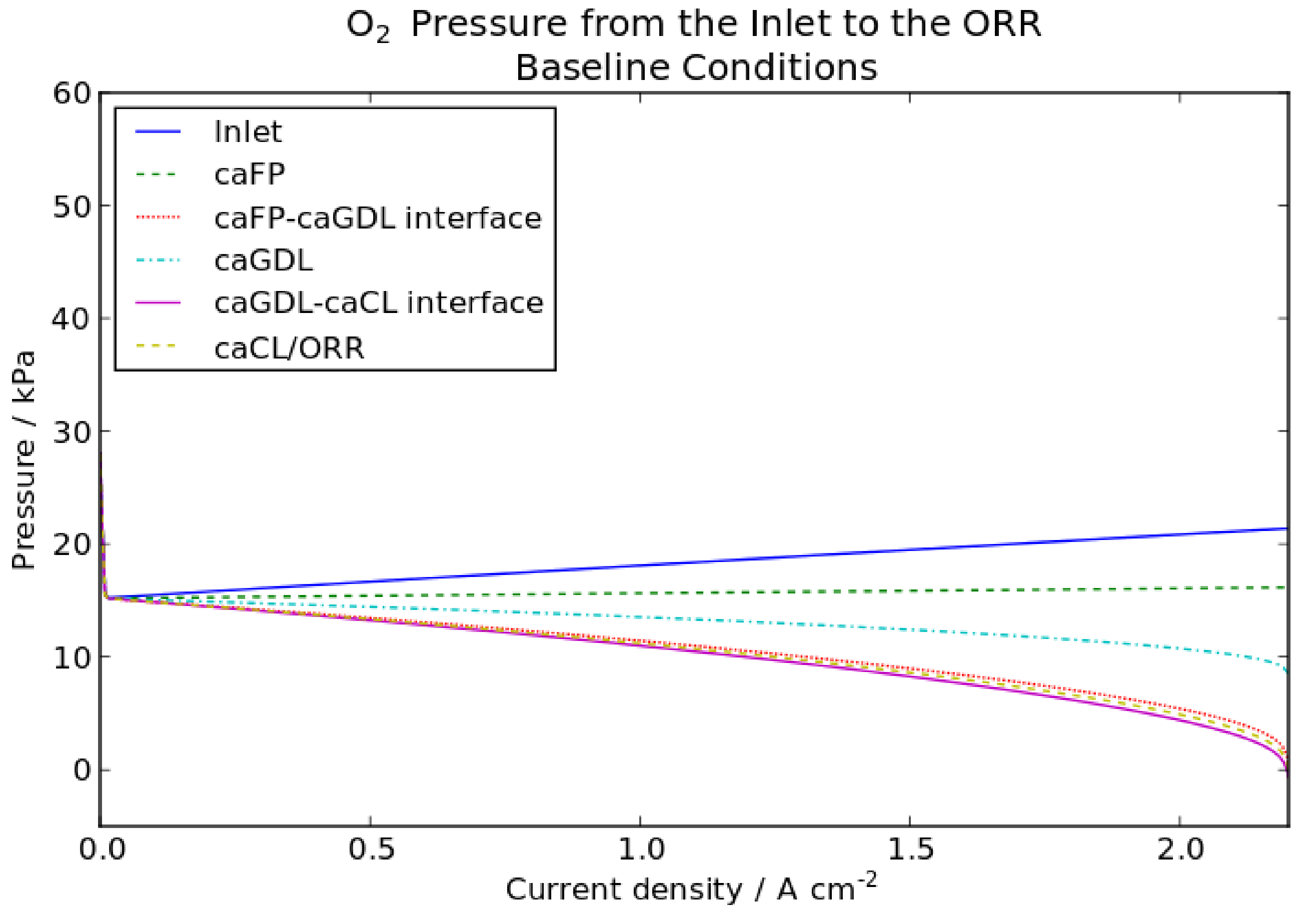
Distributed temperature

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



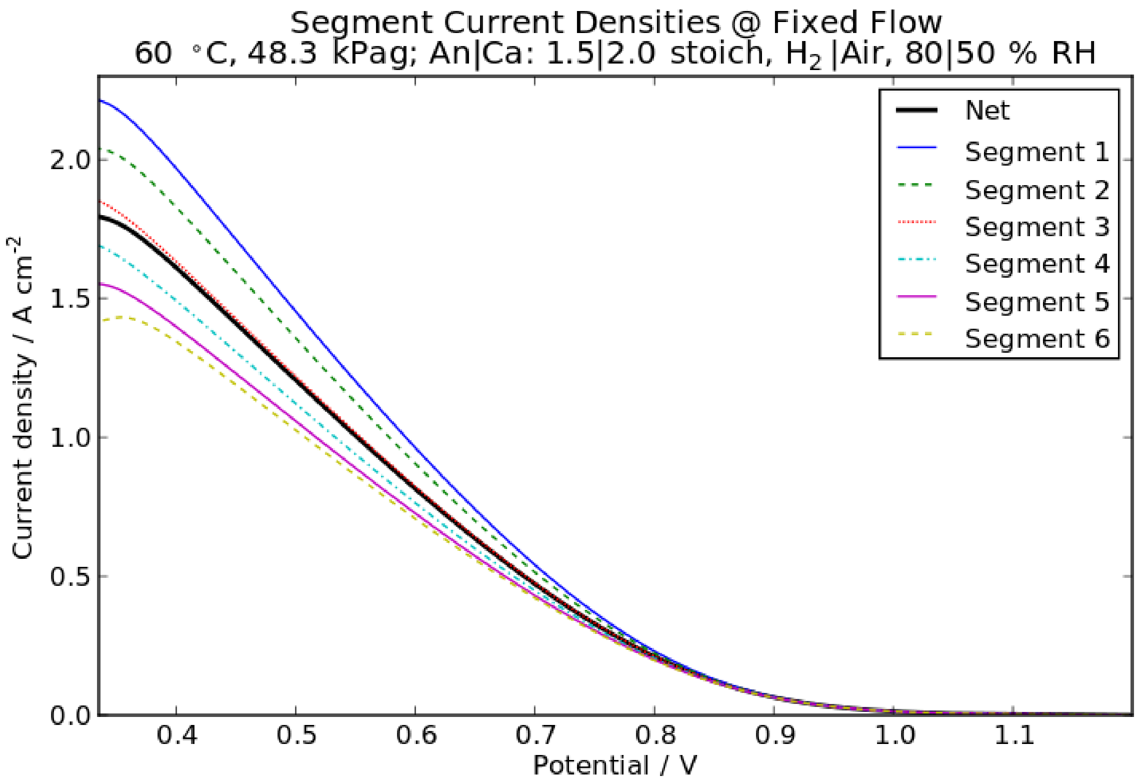
Oxygen partial pressure

- Roll-off at concentration limit



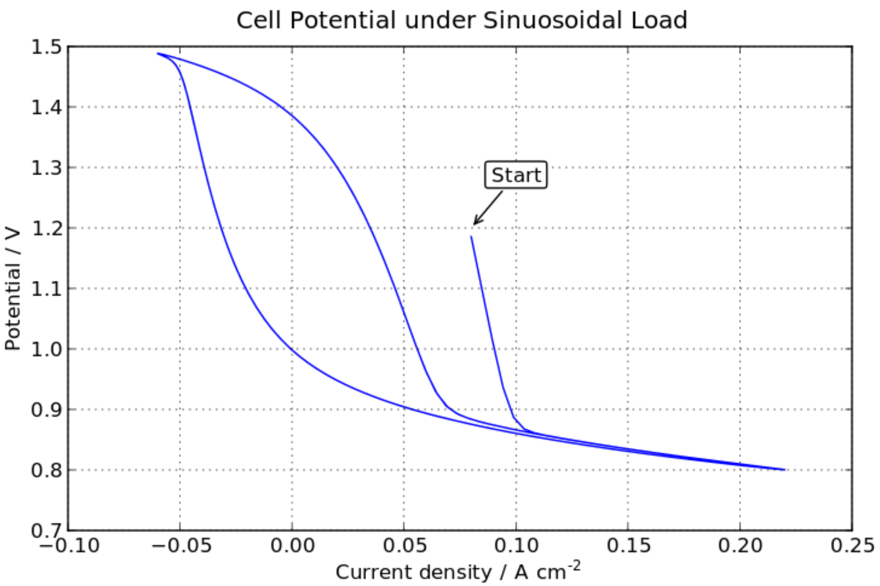
Segmented cell

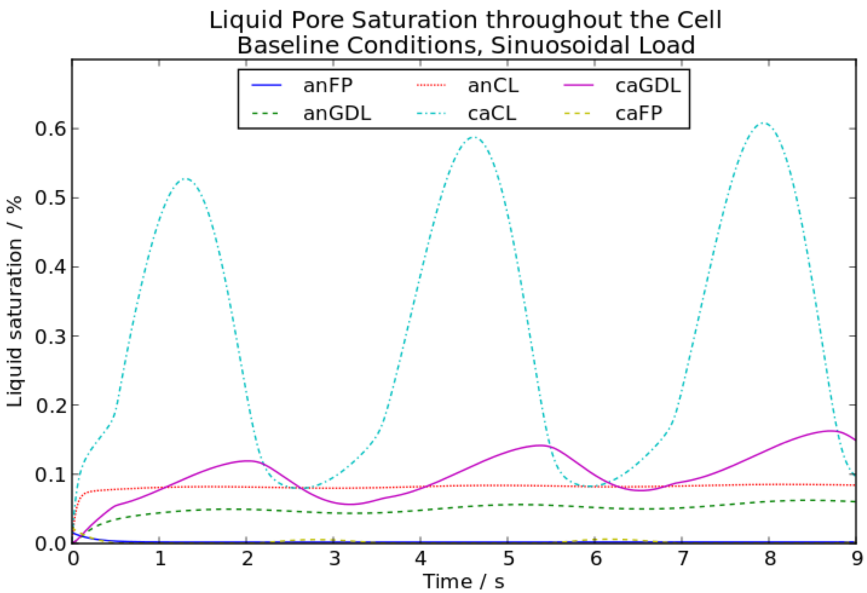
- Liquid not included
- 31,990 variables (12,711 time-varying)
- Simulates in ~11 s



Sinusoidal electrical load

- 0.3 Hz
- Amplitude of 140 mA/cm^2
- Offset of 80 mA/cm^2





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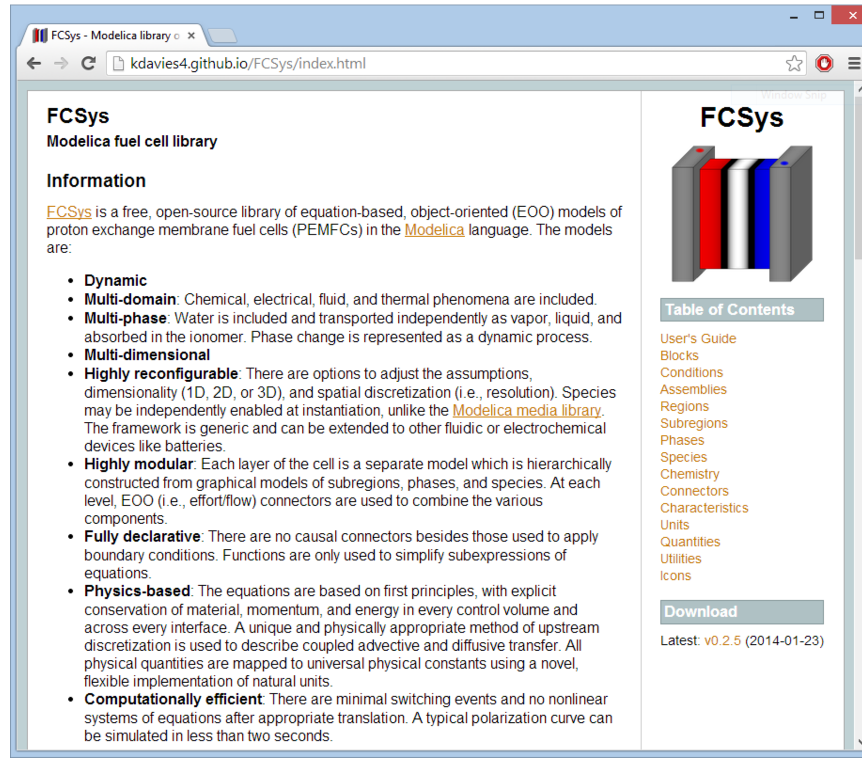
Contributions

- 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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