PENNSTATE

Electrochemical Engine Center

Computational Fuel Cell Research and SOFC Modeling at Penn State

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URL: mtrl1.me.psu.edu

Outline

- Overview – ECEC
- Computational Modeling of PEM Fuel Cells
- SOFC Modeling & Simulation
- Fuel Cell Controls
- Summary

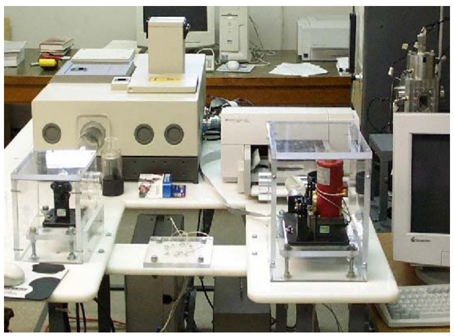
ECEC Overview

- Vision: provide fuel cell science & technology for sustainable energy future
- Mission: organize and conduct multidisciplinary research on fuel cells and advanced batteries for vehicle propulsion, distributed power generation and portable electronics
- Provide experimental & computer modeling facilities for multidisciplinary graduate education (DOE’s GATE & NSF GK-12 programs)
- Interdisciplinary team: 6-10 faculty, 5 research associates, 25 grad students, 5 undergrad assistants & 1 staff assistant
- Expertise areas: electrochemistry, materials science, multiphase transport, reactive flow, CFD modeling, experimental diagnostics, in-vehicle testing, advanced materials.
- Focus on design, modeling, fabrication, diagnostics and system integration of PEMFC, DMFC, and SOFC

ECEC Facilities (>5,000 sq ft)

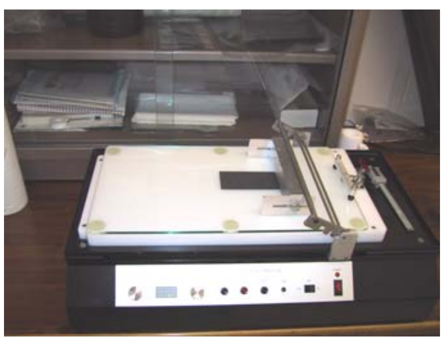
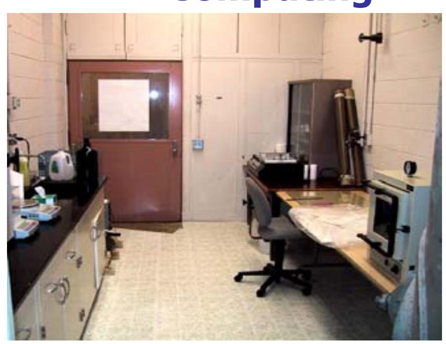


Fuel Cell/Battery Experimental Labs



Kinetics and Thermal Transport

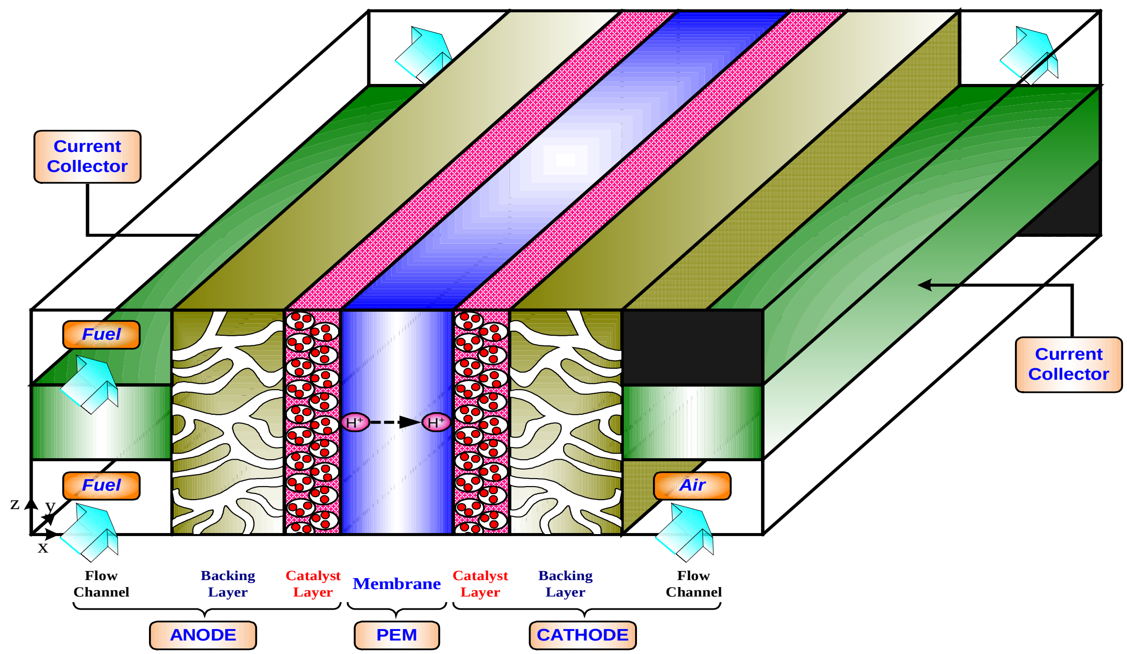
Fuel Cell/Battery Simulation and Parallel Computing


Fuel Cell Materials Research and Component Fabrication

H_2/Air PEM Fuel Cells: Modeling

- Computer simulations are increasingly part of of the discovery and design process in the competitive field of fuel cells.
- **ECEC vision**: FC Modeling must consist of four elements:
  - **- physico-chemical model development**
  - **- advanced numerical algorithms**
  - **- materials characterization (to provide accurate input parameters)**
  - **- experimental validation at detailed levels**



Physico-chemical Model Development

- Main features of ECEC models (available as in-house code, user code for STAR-CD or UDF for Fluent):

- electrochemical and transport tightly coupled

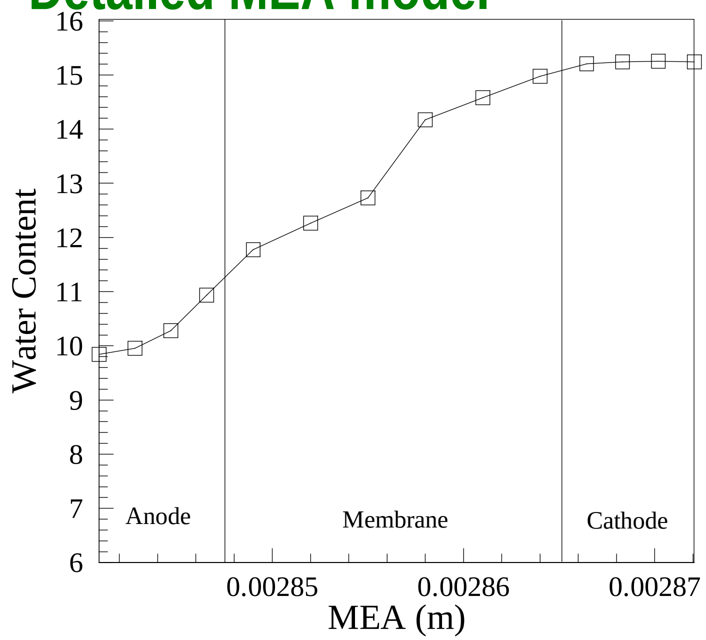
- fully resolve gas channels, GDL, catalyst layers & electrolyte

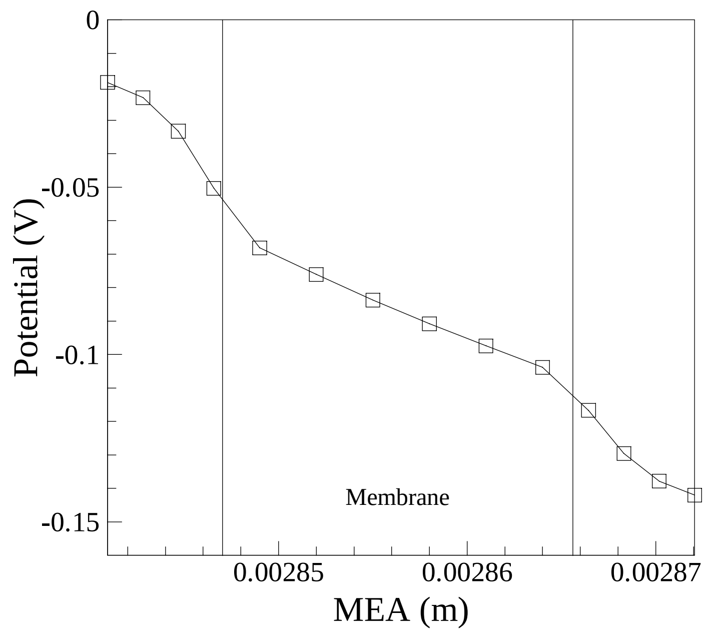
- 3-D; steady-state and transient operation

- water and proton co-transport in polymer electrolyte

- accurate modeling of liquid water transport in hydrophobic GDL (ECEC's M2 model) and water management

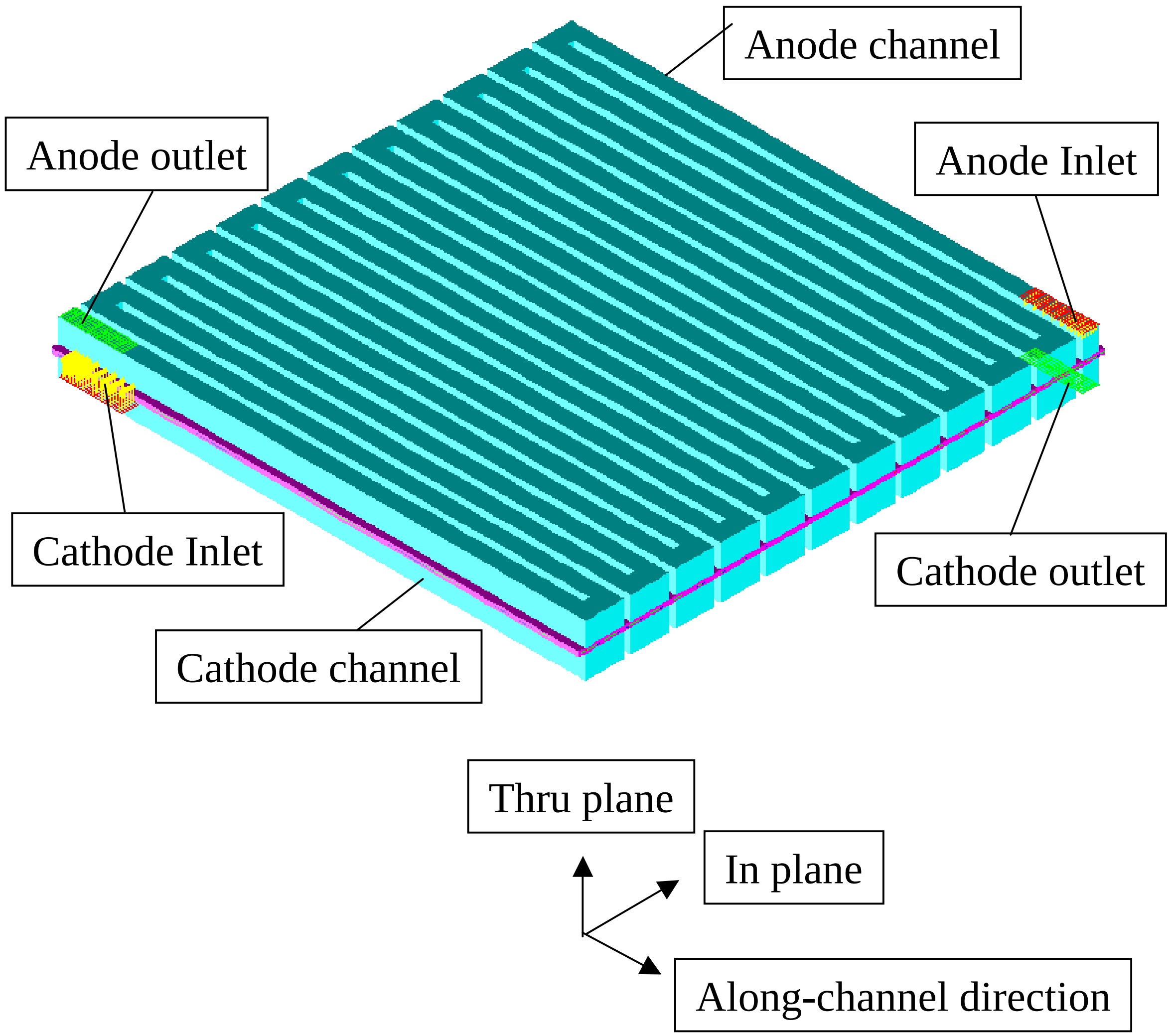
- Detailed MEA model





Size of Numerical Problem: The Mesh

- Computational Mesh:
  - Through plane direction: 6-8 grid points in each of 5 distinctive regions of MEA + 10 points in each channel = 50-60
  - Along-channel direction: 100-120 points
  - In-plane: 10 points in channel and collector shoulder = 20 grids/flow channel
- Reasonable Mesh Size: 50X100X400 (for 20-channel flowfield)= **2x10^6 gridpoints**!



Massively Parallel Computations

- ECEC has a 50-node Linux cluster (1.4GHz AMD processors) dedicated to fuel cell simulation and stack design

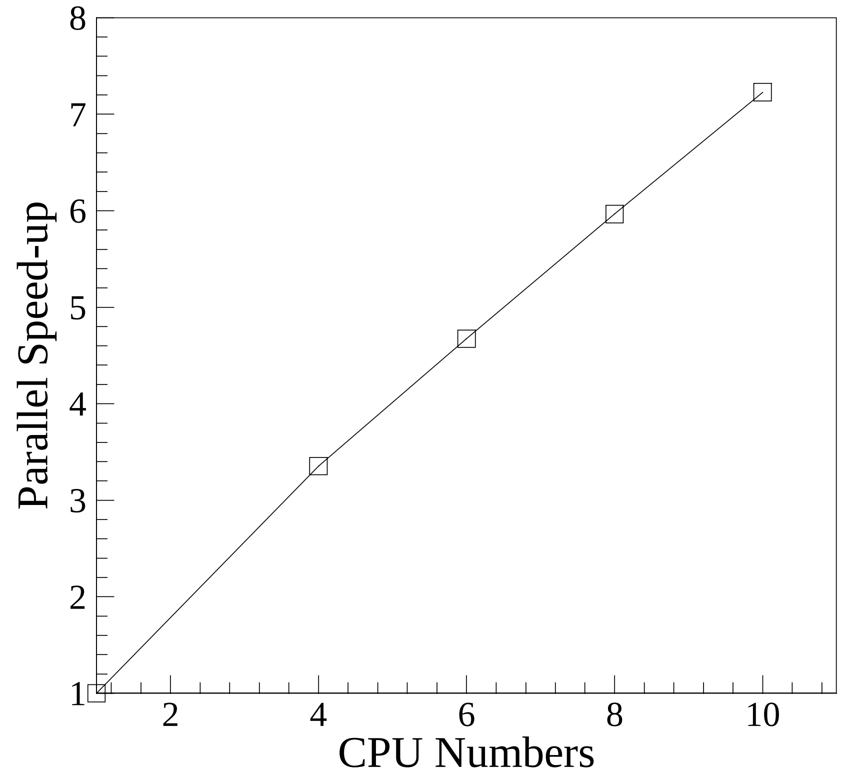
  - parallel-computing individual cells in a stack with each computer node for one cell

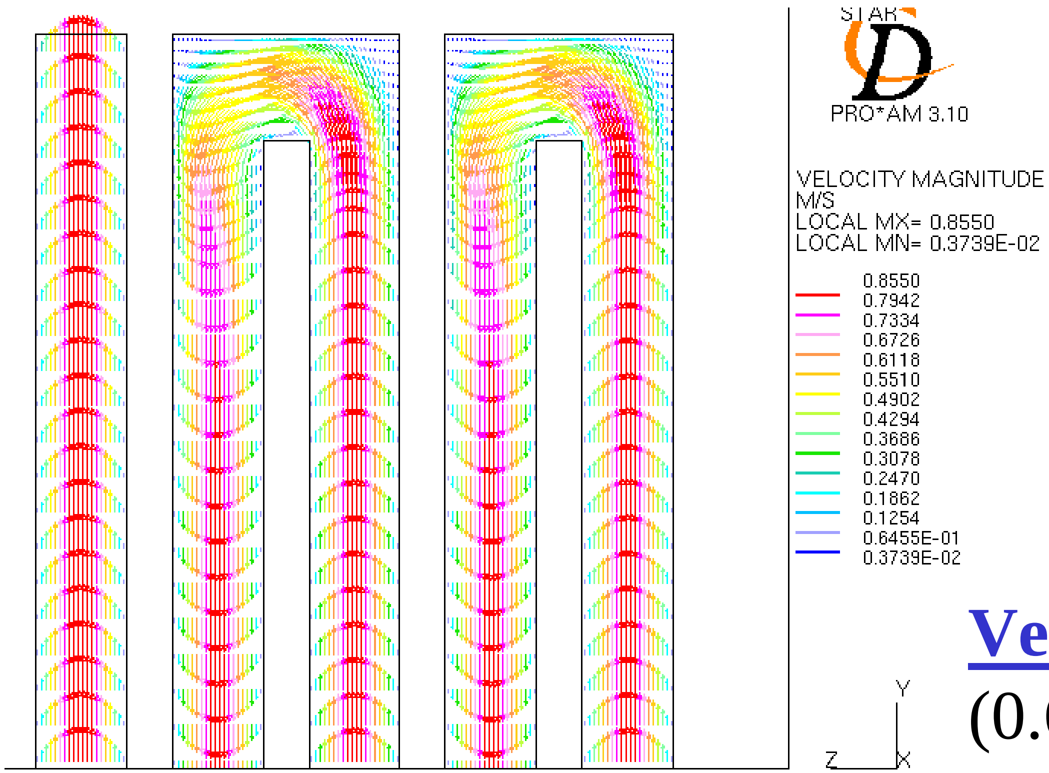
  - domain decomposition for large-scale simulation

- PSU clusters: Lion-XL (160 2.4GHz P4 processors), Lion-XE (256 1GHz P3 processors)

Massively Parallel Computations

- Parallel computing performance
  - >7x speed-up with every 10 nodes
  - roughly 300 iterations
  - <1.5 hours for 1M comp. cell problem with 10 nodes





Velocity Field

(0.66 V, 0.96 A/cm^2)

Ex: Large-Scale Cell Simulation

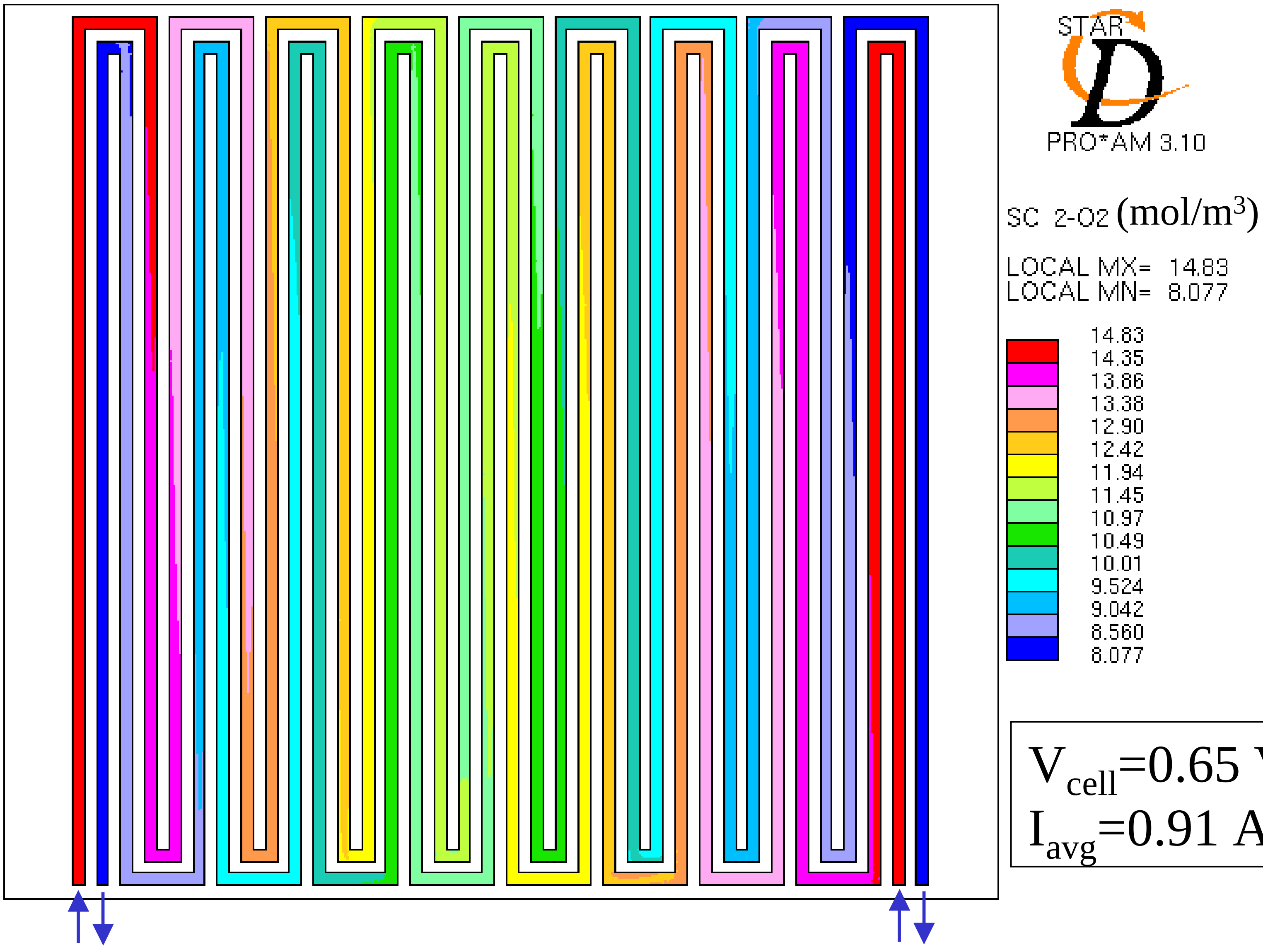
36-channel, double-pass serpentine fuel cell

Cell Specifications:

- Anode: 2 passes are co-flow
- Cathode: 2 passes are counter-flow
- Membrane: N112
- A/C Stoich: 3/2 @ 1 A/cm^2
- A/C Pressure: 2.1 bars
- T_{cell}: 80^{o}C; V_{cell}=0.65 V
- A/C RH: 100%/5%

Computational details: 2.56 M cell mesh, 300 iterations for convergence, **5 hours** on ECEC Linux cluster using 9 processors.

Macro View: O_2 Distribution



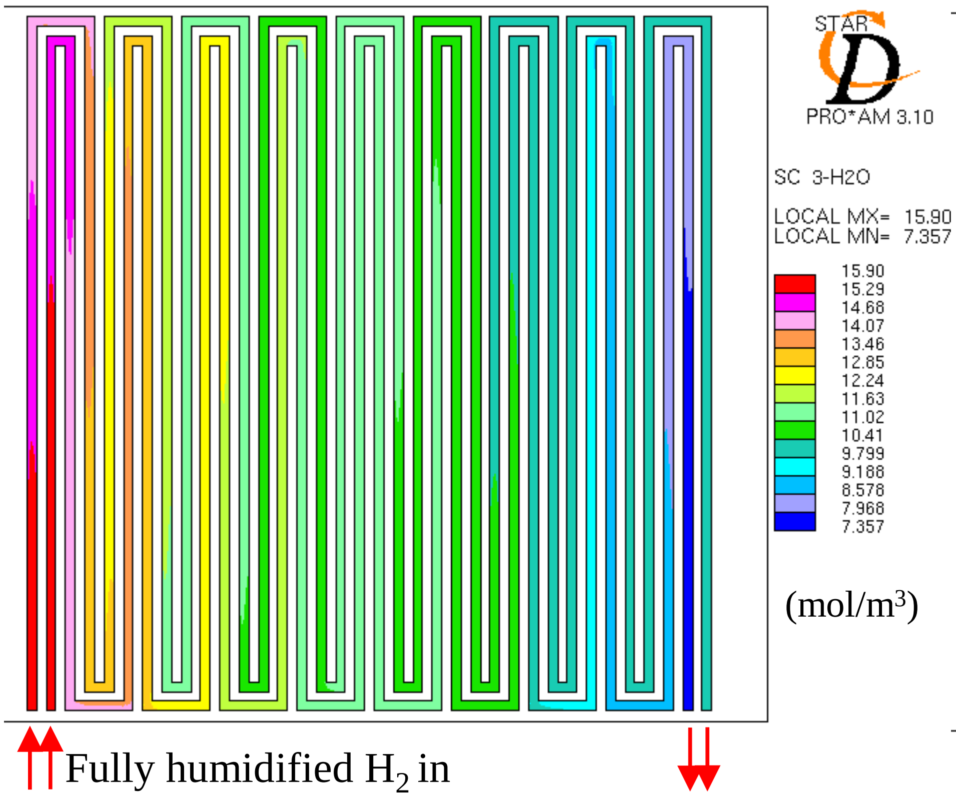
V_{cell}=0.65 V
I_{avg}=0.91 A/cm^2

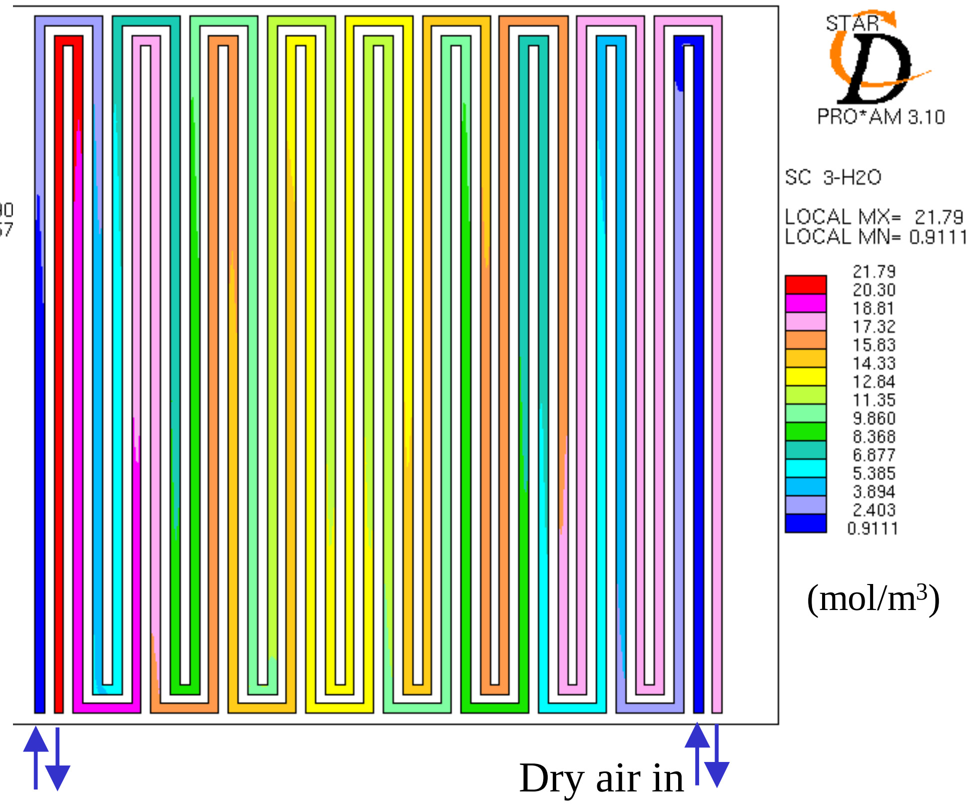
O_2 distribution in the cathode gas channels

Macro View: H_2O Distribution

V_{cell}=0.65 V; I_{avg}=0.91 A/cm^2

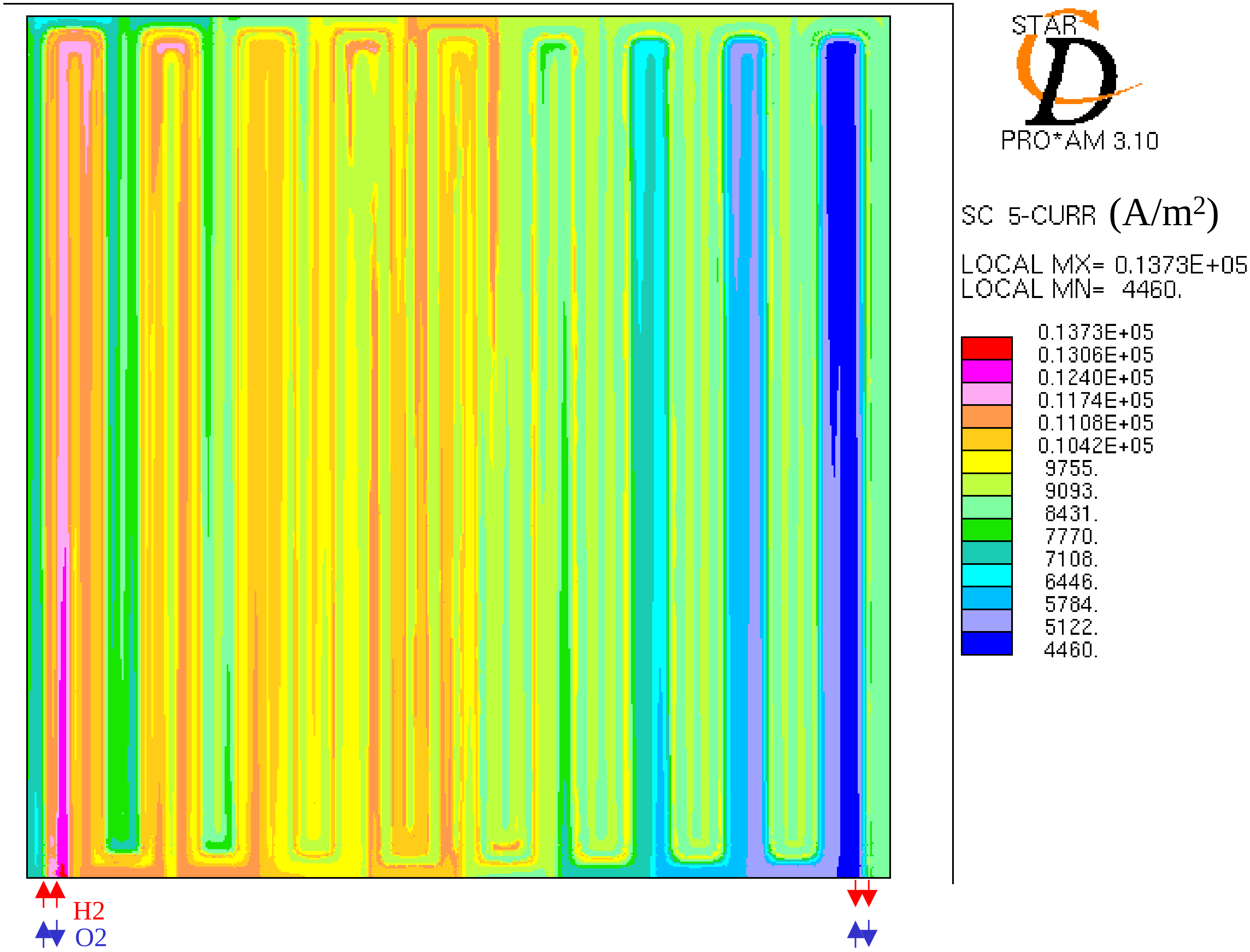
- Anode gas channels
- Cathode gas channels



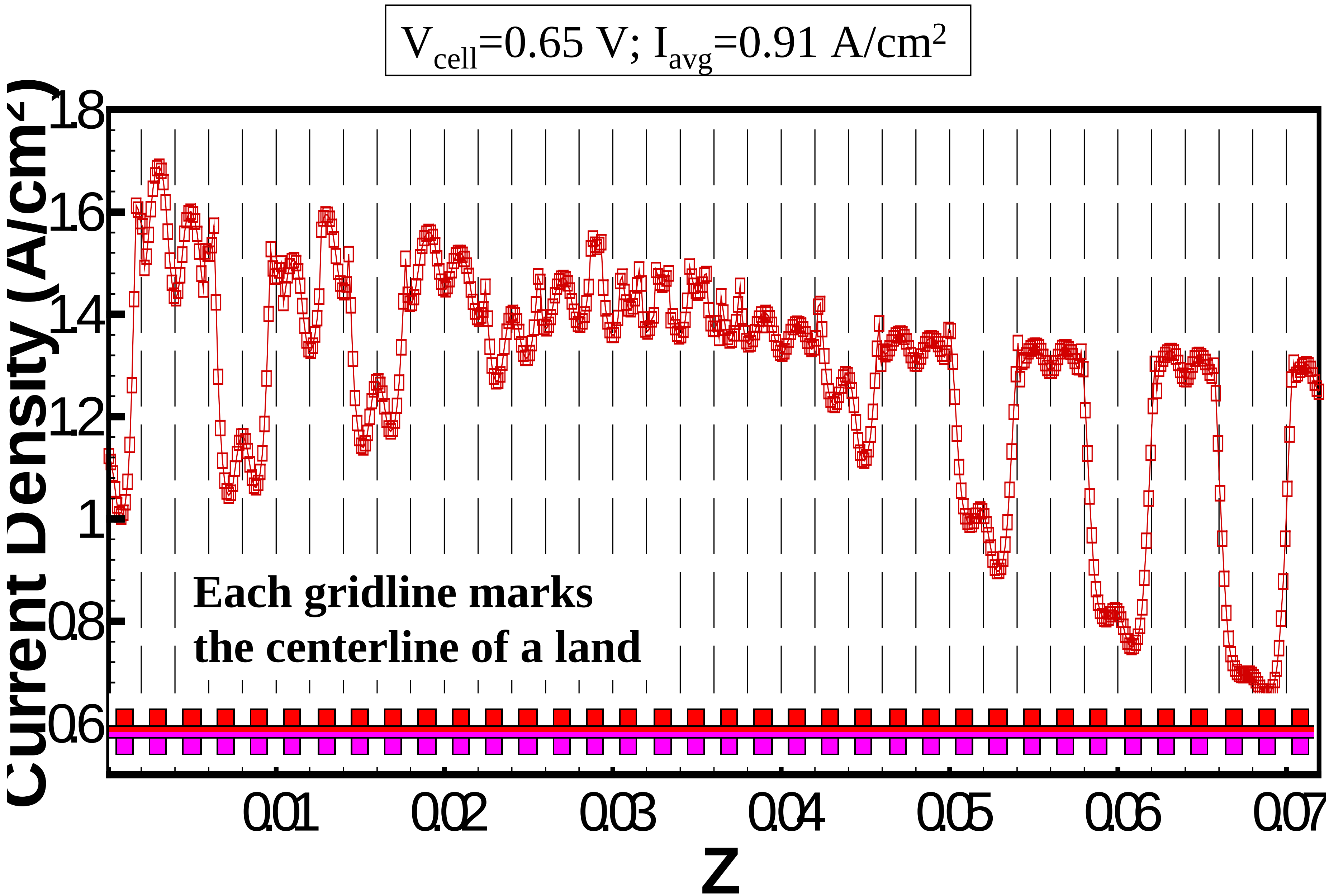


Macro View: Current Distribution

$V_{cell}=0.65$ V; $I_{avg}=0.91$ A/cm^2

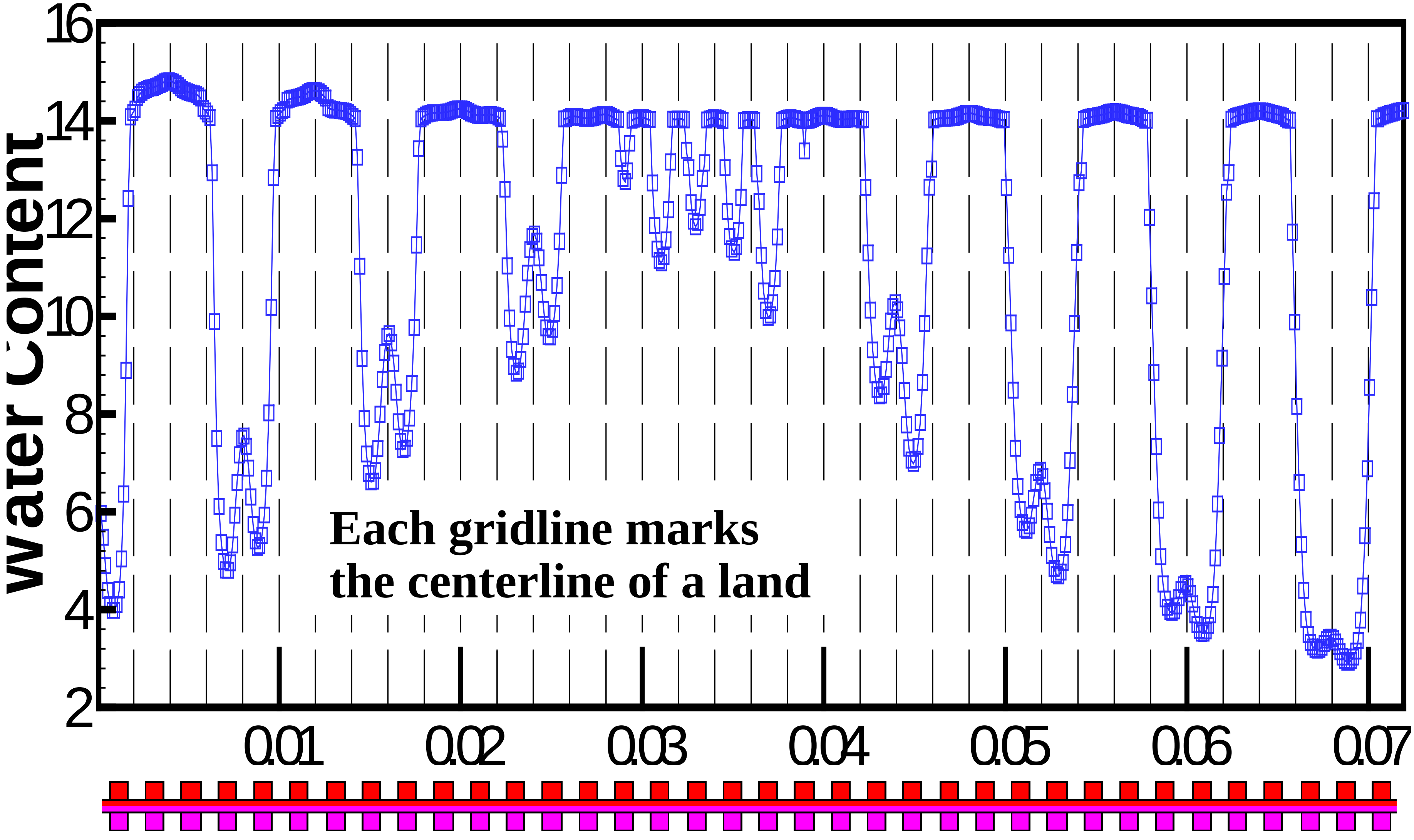


Micro View: Current Density Profile



Micro View: Water Content Profile

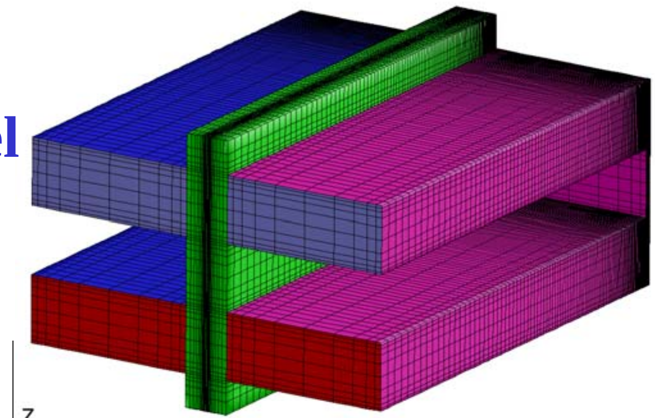
Water content @ cathode/GDL interface in the middle section of gas channels (V_{cell}=0.65 V; I_{avg}=0.91 A/cm^2)



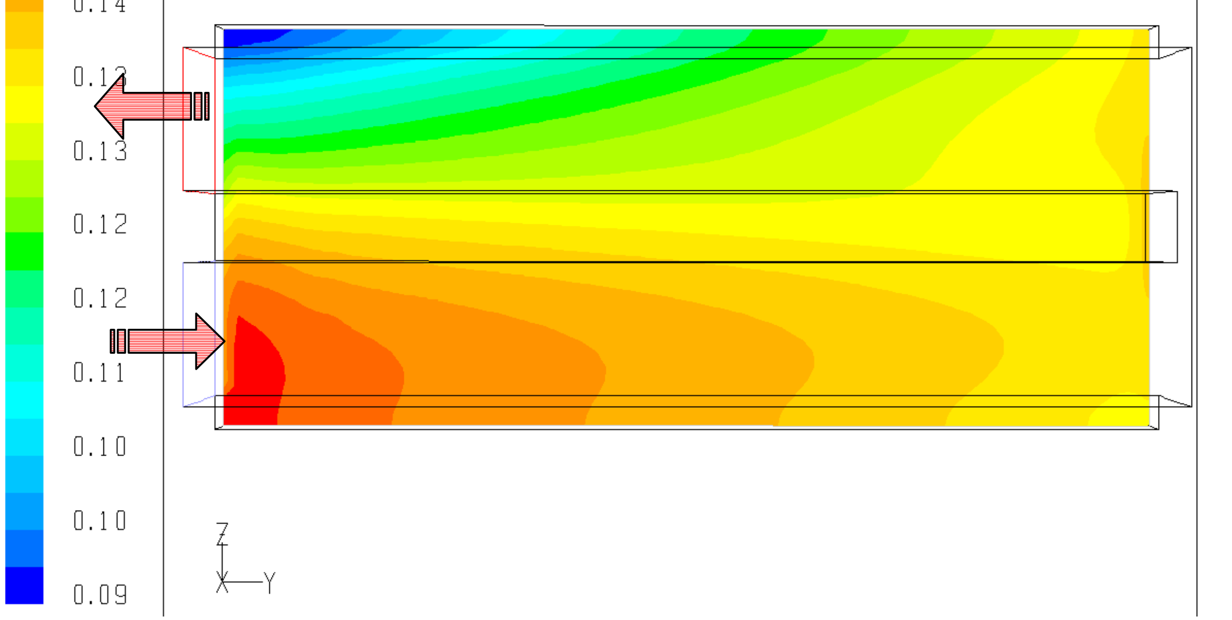
Flooding Prediction by M2 Model

- Fully 3-D, two-phase, whole cell modeling and flooding prediction as function of the GDL wetting properties are available.

2-channel serpentine fuel cell

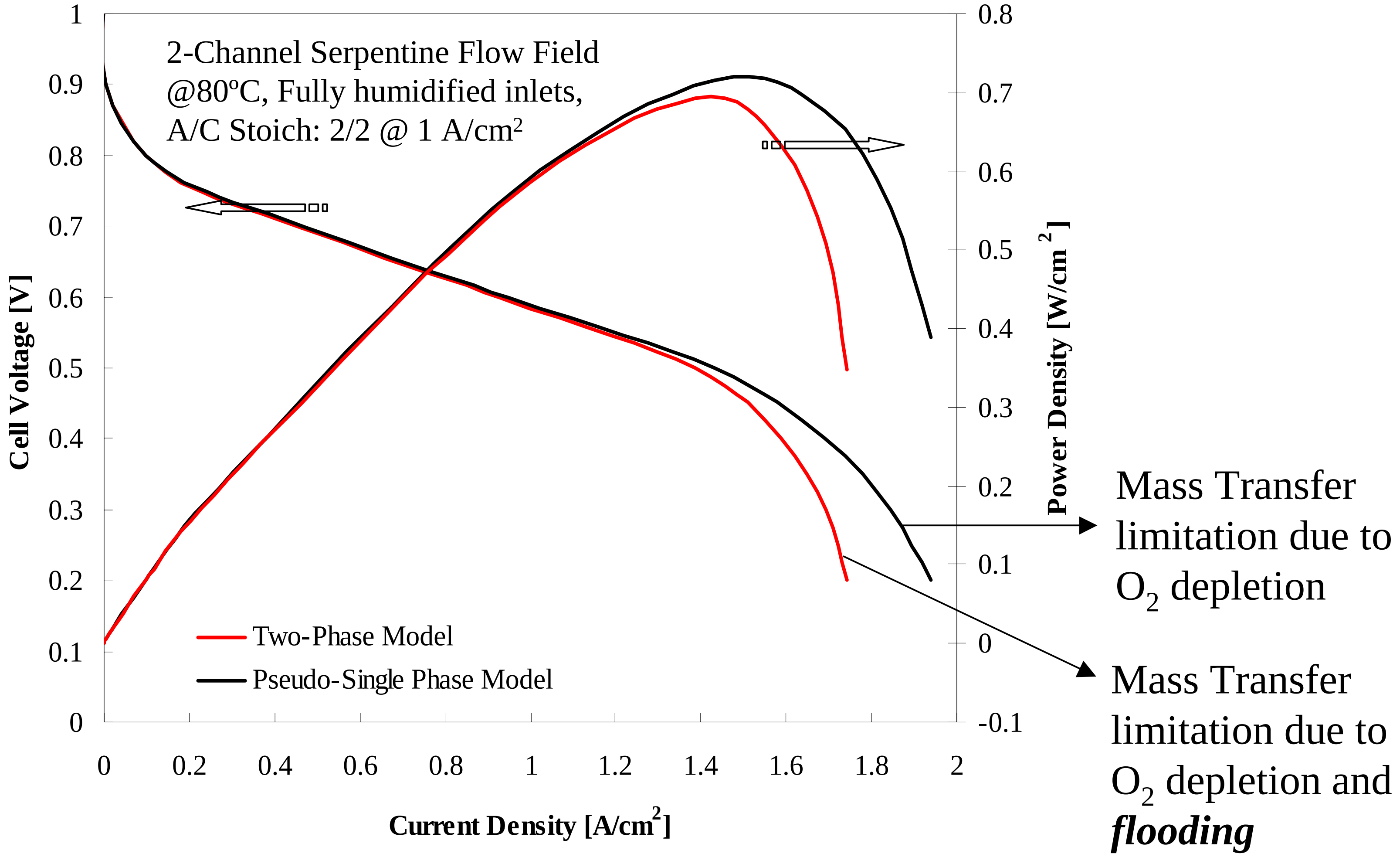


Liquid Saturation Distribution at Cathode/GDL Interface (A/C RH: 100%/100%; Stoich: 2/2 @ 1A/cm^2, V_{cell}=0.4V, I_{avg}=1.59 A/cm^2, GDL CA=105^o)



1. Flooding occurs near the inlet of fully humidified cathode where current density is highest.
2. Liquid water does not transport transversely in plane, thus flooding is a localized phenomenon.

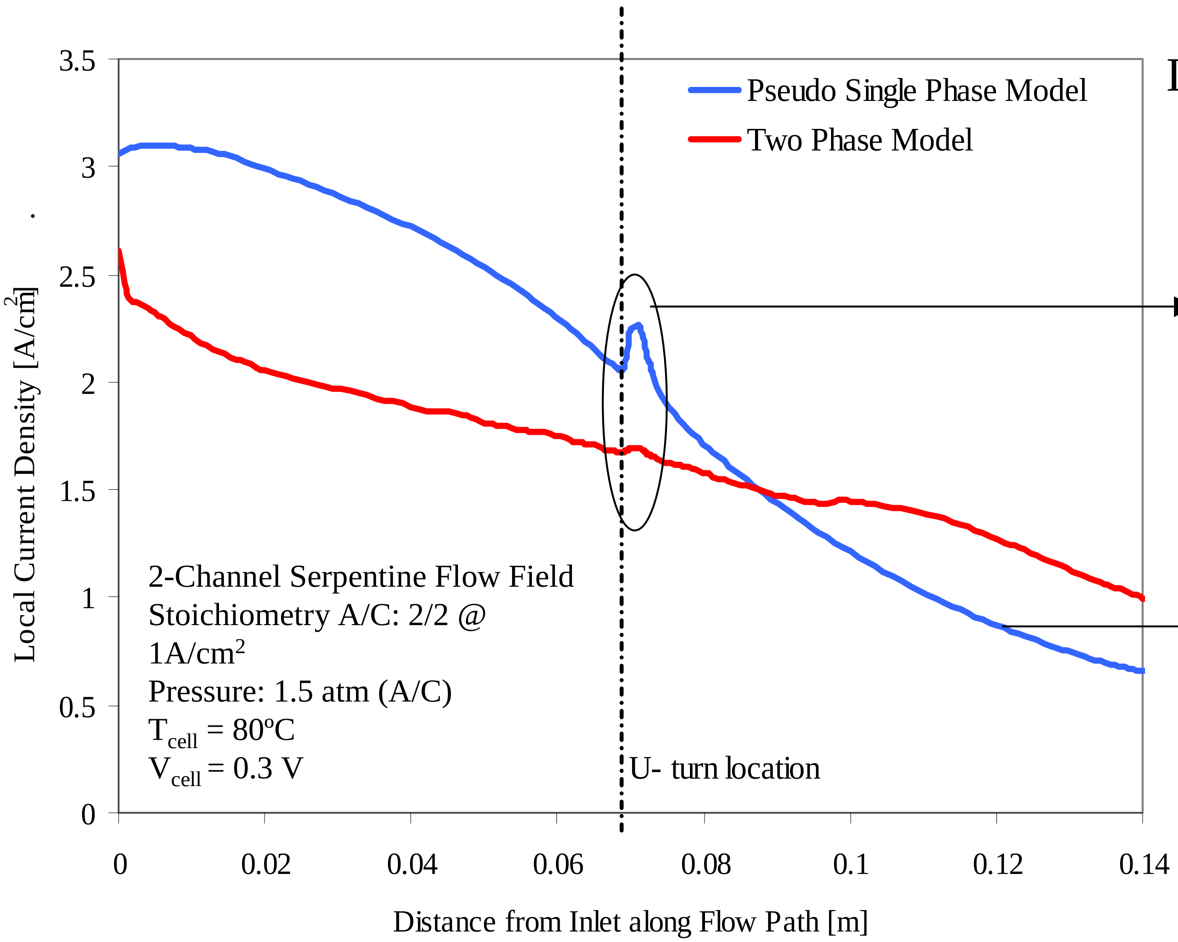
Flooding Prediction by M2 Model



Source: Pasaogullari & Wang, ECS Paris Mtg, April 2003.

Flooding Prediction by M2 Model

Current Distributions w/ and w/o Flooding



I_{avg} = 1.84 A/cm^2 (single phase)

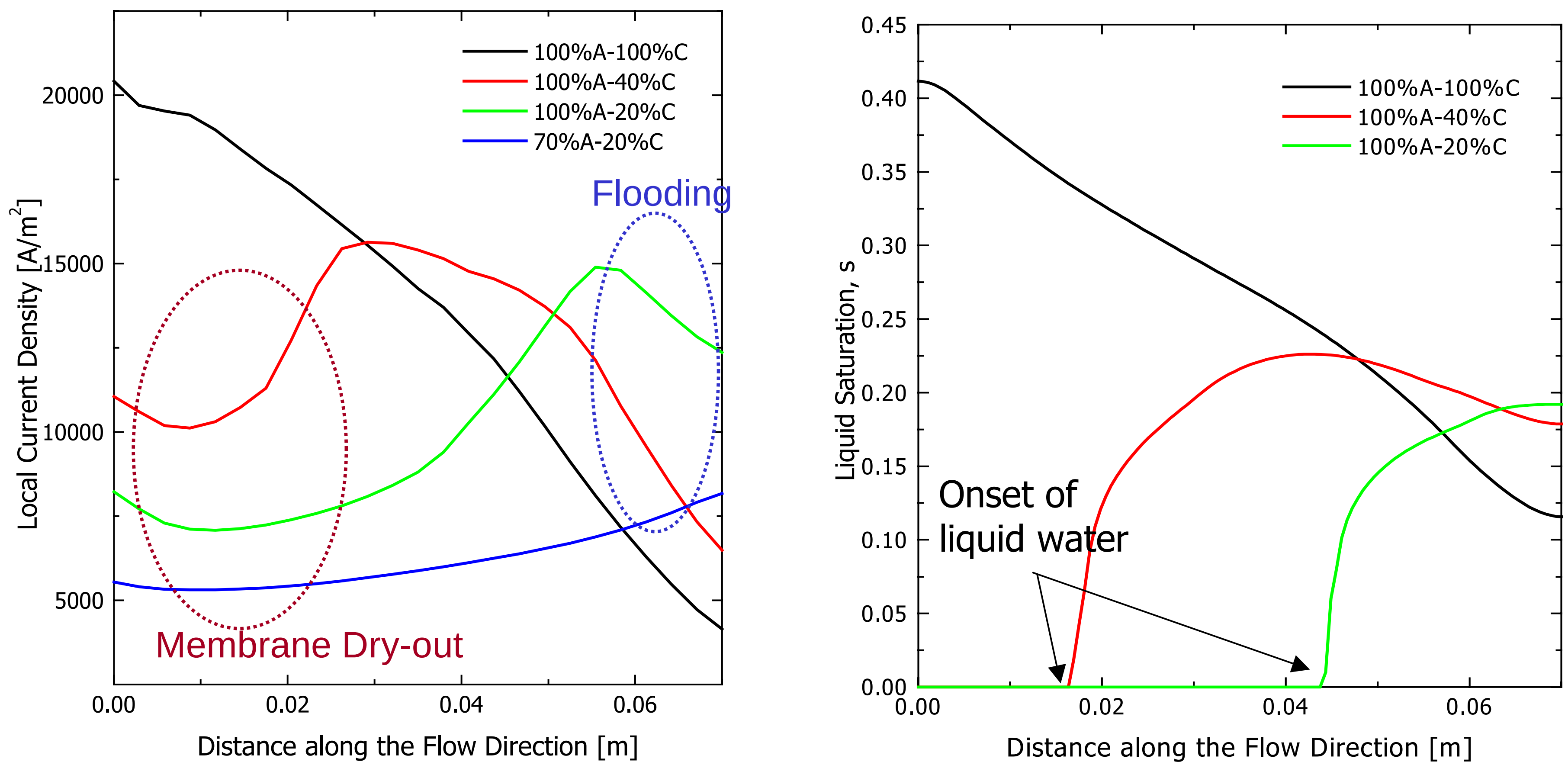
1.69 A/cm^2 (two-phase)

Increased mass transfer due to mixing effect at the U-turn region

Higher mass transfer resistance due to higher depletion of oxygen at the inlet region

Source: Pasaogullari & Wang, ECS Paris Mtg, April 2003.

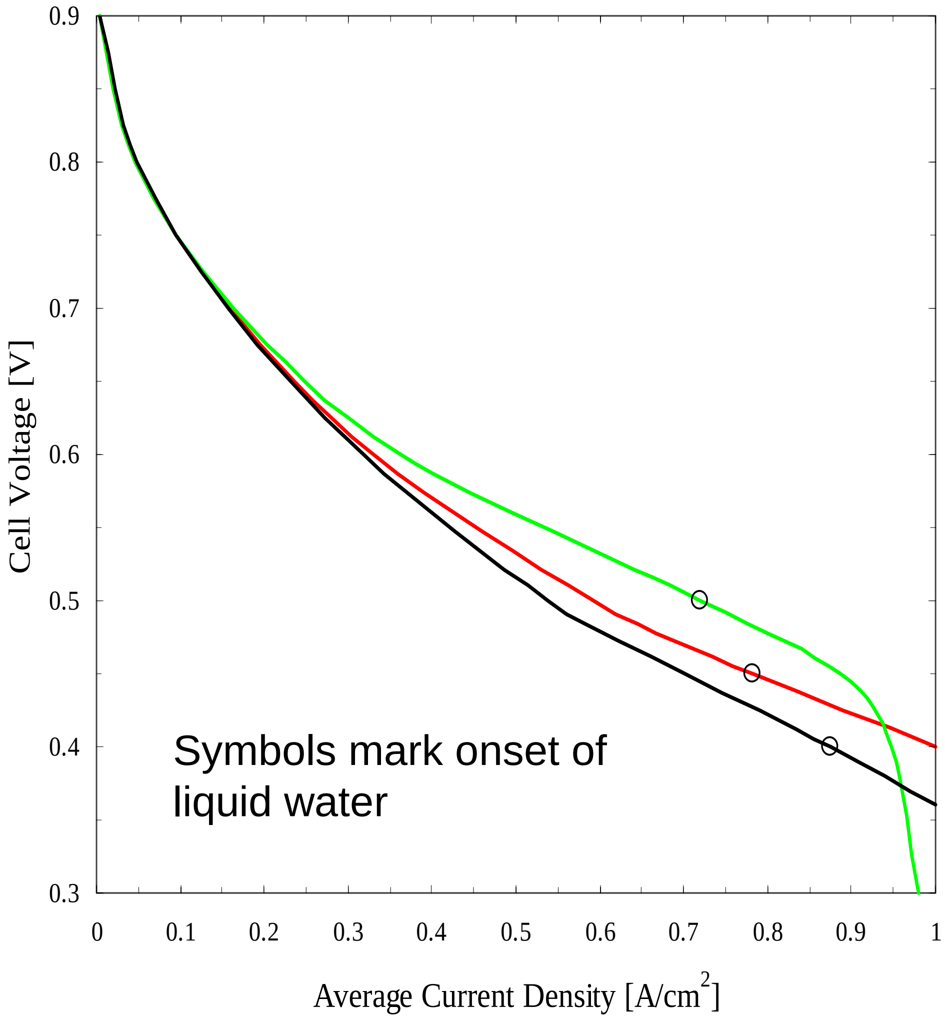
Effect of Inlet Humidity



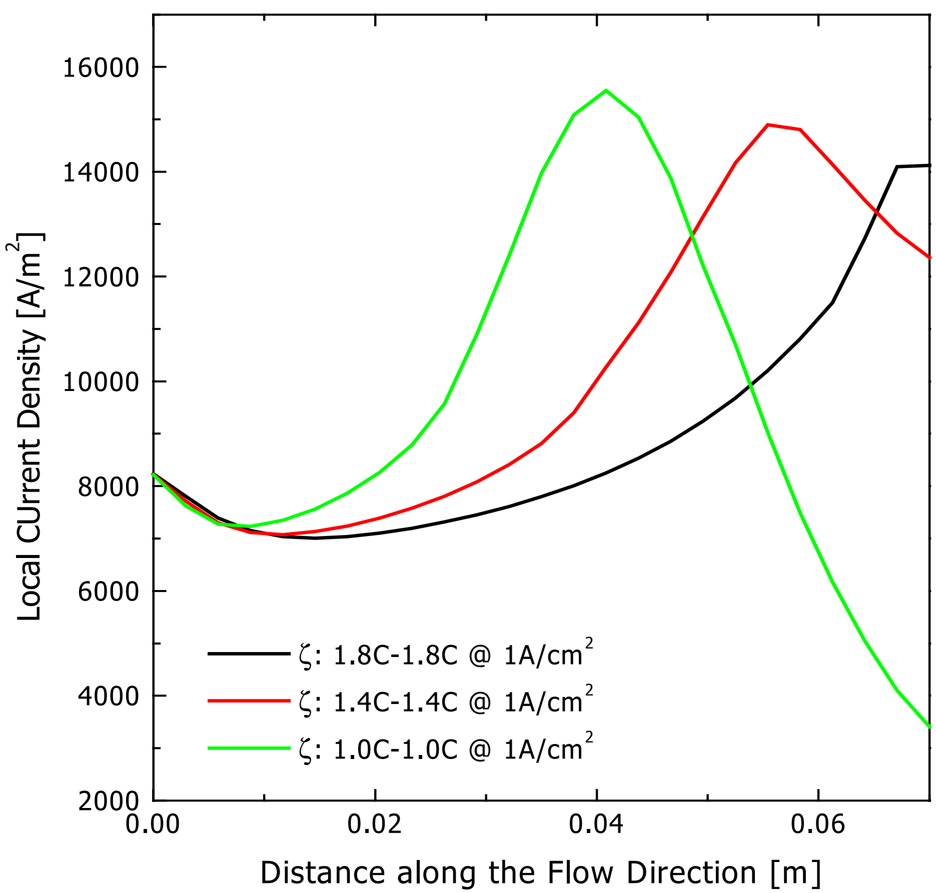
Note that M2 model can predict single-phase region in low-humidity operation, location of the onset of liquid water (unknown *a priori*), and two-phase region all together in one problem.

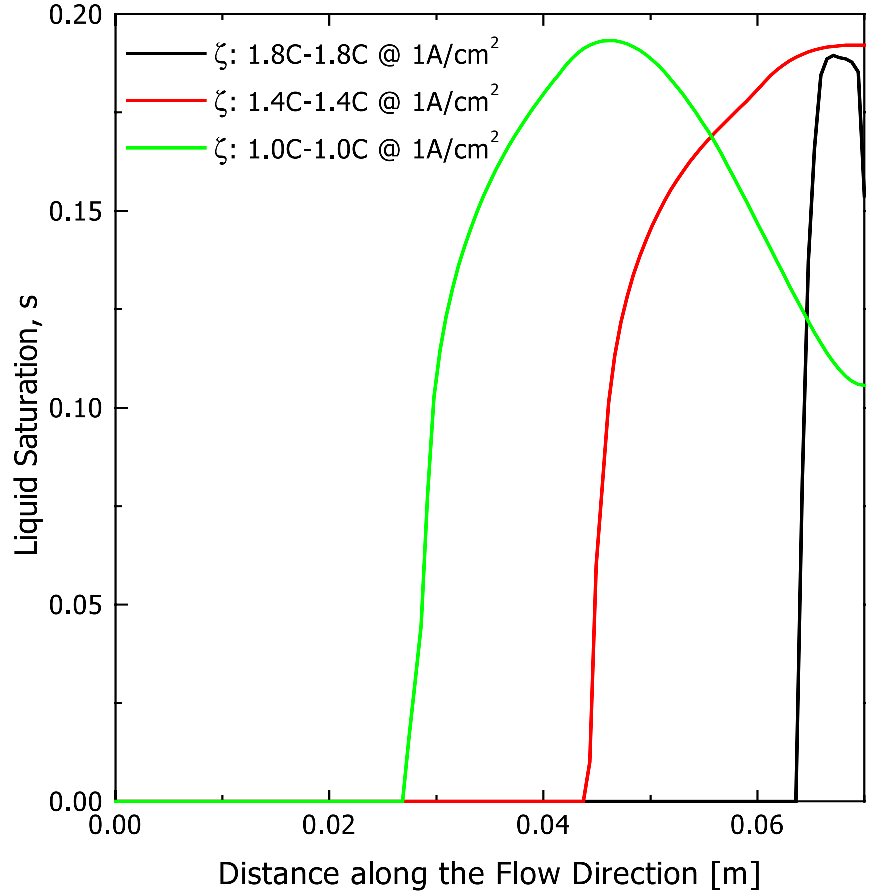
Effect of Stoichiometry

- Same test cell as humidity case.
  - Inlet Relative Humidity:
    - 20% Cathode
    - 100% Anode
  - Test Case Stoichiometry @ 1A/cm^2:
    - 1.0/1.0 A/C
    - 1.4/1.4 A/C
    - 1.8/1.8 A/C



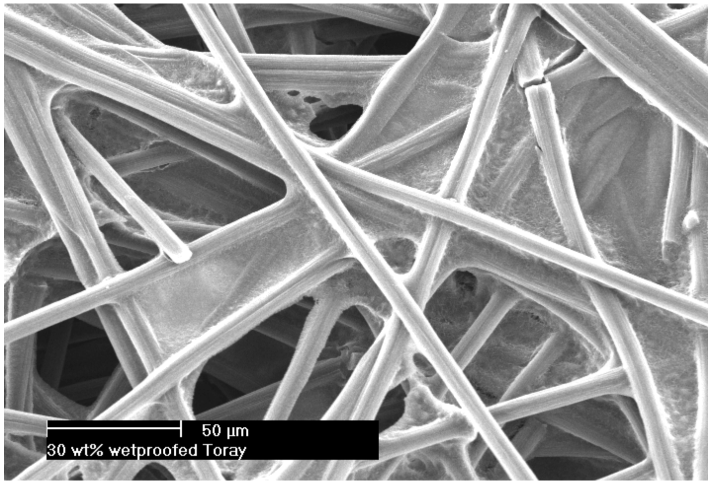
Effect of Stoichiometry





Materials Characterization

- Materials properties are required on
  - **Membranes**
  - **Membrane-electrode assembly (MEA) properties including electrokinetic data for catalyst layers**
  - **Gas diffusion layers (GDL)**
  - **Bipolar plates**
  - **Chemical reactants and products.**

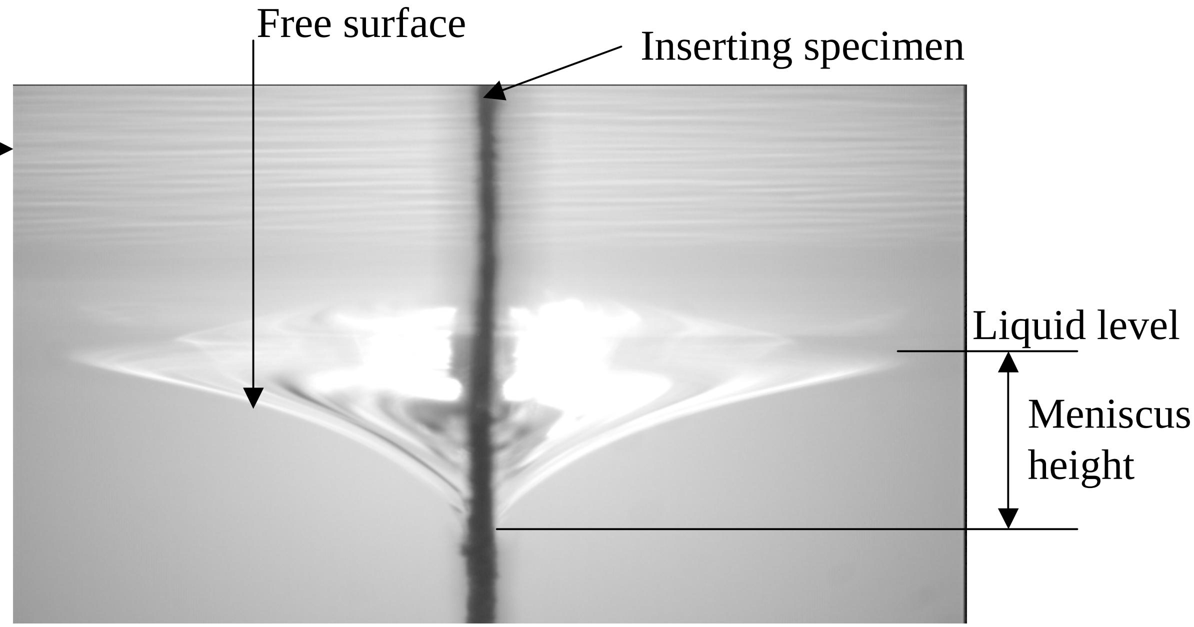


SEM of Toray carbon paper

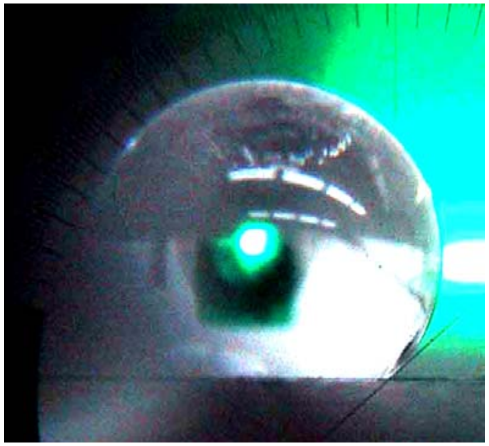
SEM of carbon cloth

Materials Characterization

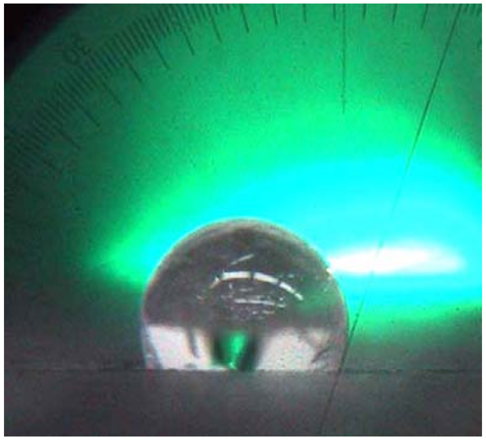
Contact angle measurement



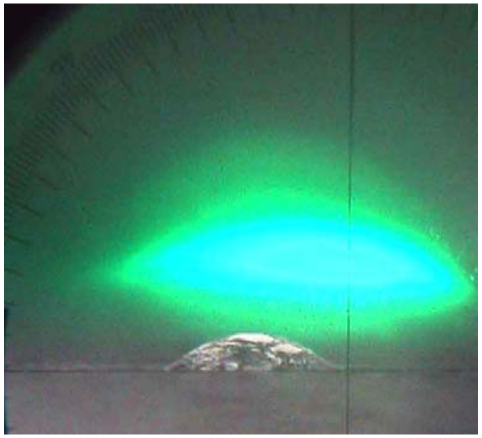
Water drops on GDL surface at 70 ºC



Highly hydrophobic GDL

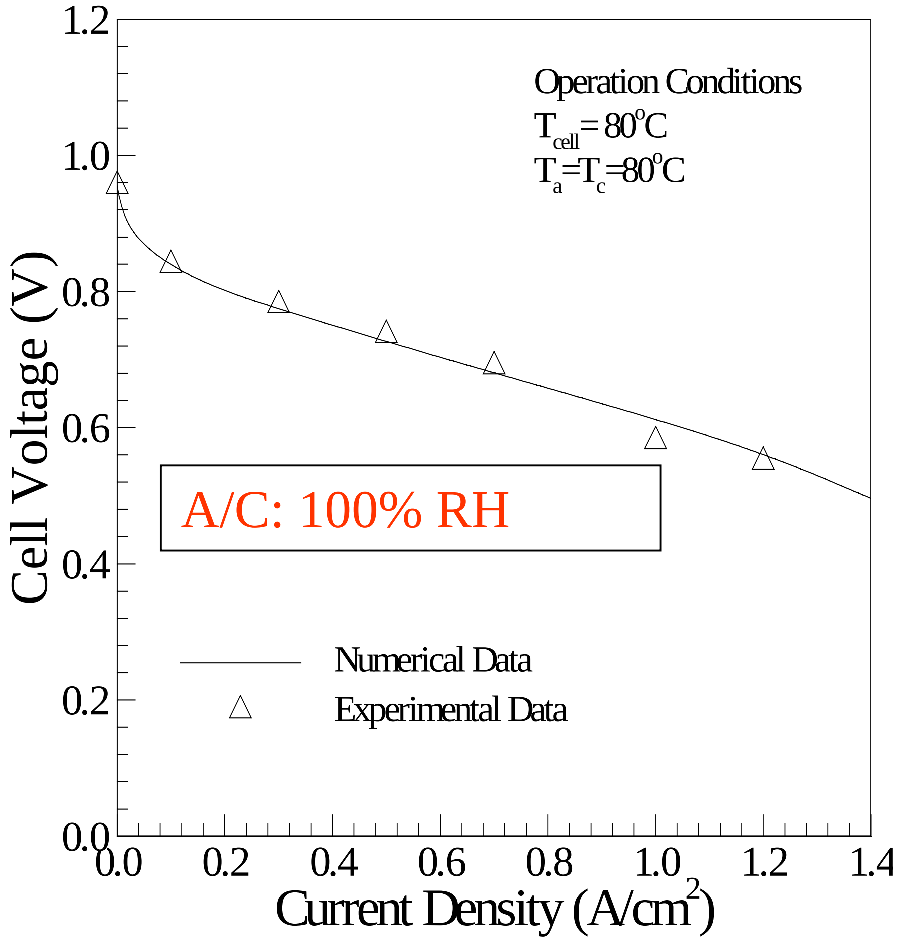


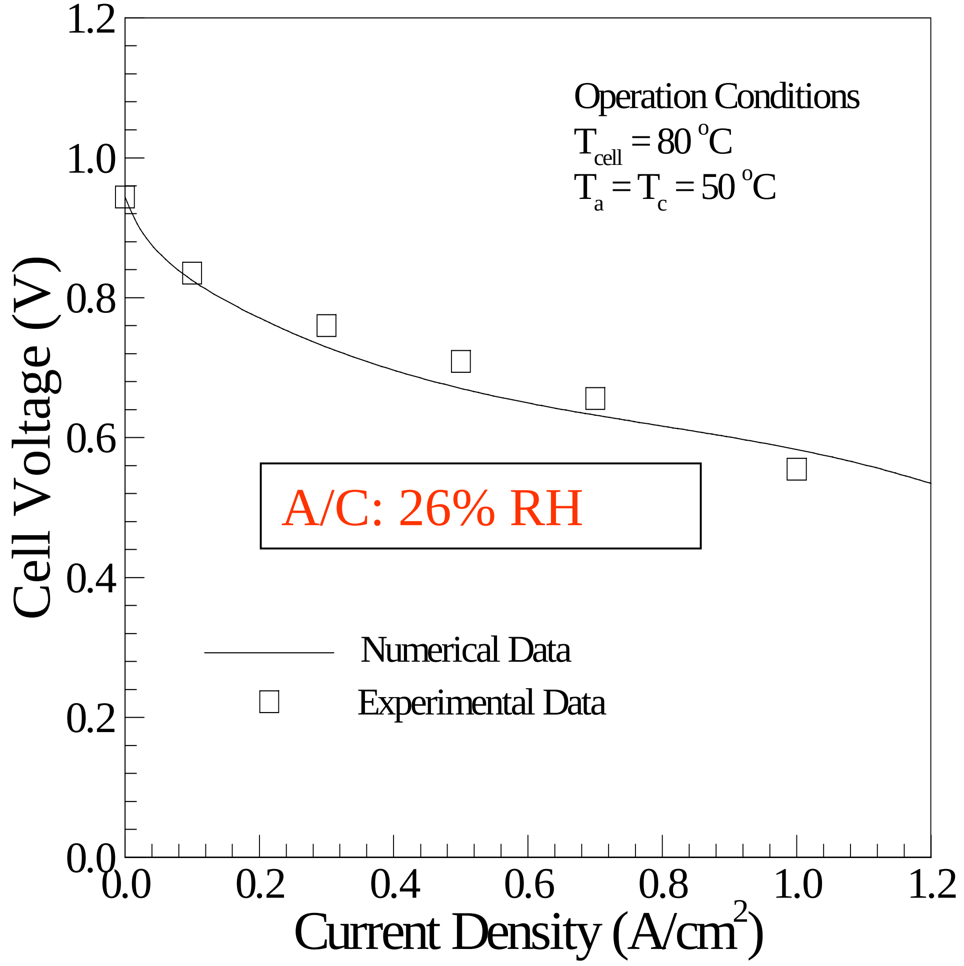
Hydrophobic GDL



Hydrophilic GDL

Experimental Validation

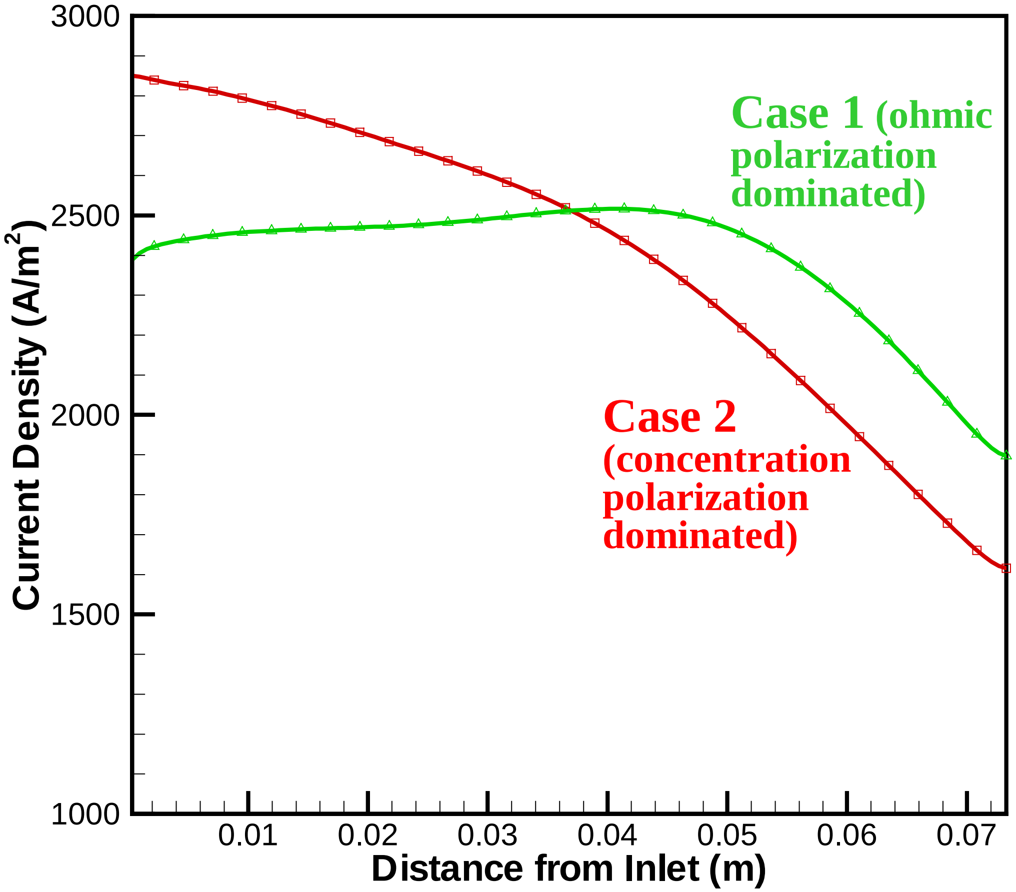




Is Pol Curve Sufficient for Model Validation?

- Consider a single-channel, 7 cm long fuel cell with Gore 18 μm membrane and operated at 80°C and A/C stoich of 3/2 and RH of 42%/dry.

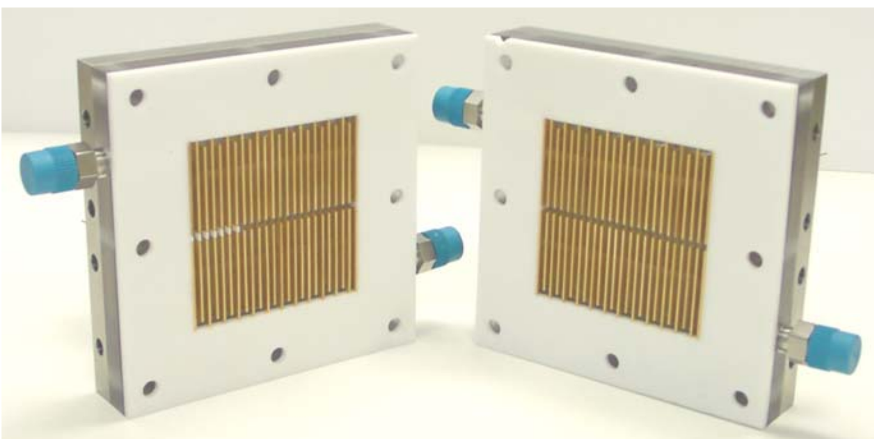
	Case 1 (ohmic polarization dominated)	Case 2 (concentration polarization dominated)
Catalyst layer ionic resistance	included	neglected
Product of specific active area and ORR exchange current density, aj_o (A/m^3)	2.53×10^4	1.95×10^4
I_{avg} @ 0.75V, A/cm^2	0.24	0.24



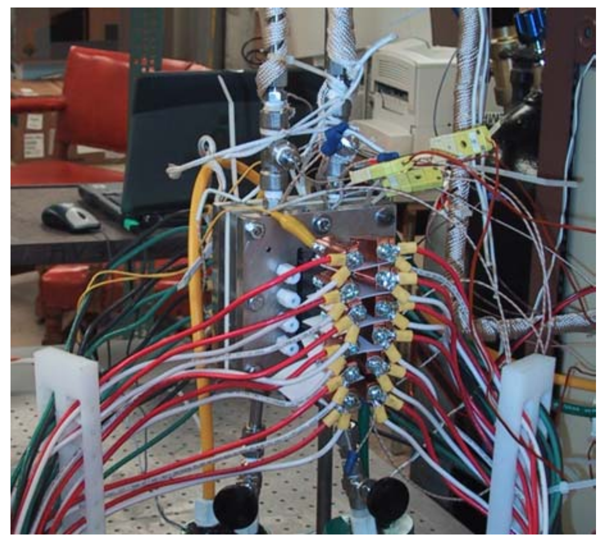
- Obviously the average I-V curve is largely insufficient for validation of detailed fuel cell models. Experimental validation at the distribution level (current, species and temperature) is required!

Detailed Diagnostics

- ECEC has extensive MEA fabrication and fuel cell test facilities for experimental diagnostics and model validation.
- These data include not only I-V curves but also detailed distributions of current, species, and temperature as well as visualization of two-phase flow and flooding.
- ECEC has developed unique capabilities for current, concentration and (membrane) temperature mapping.

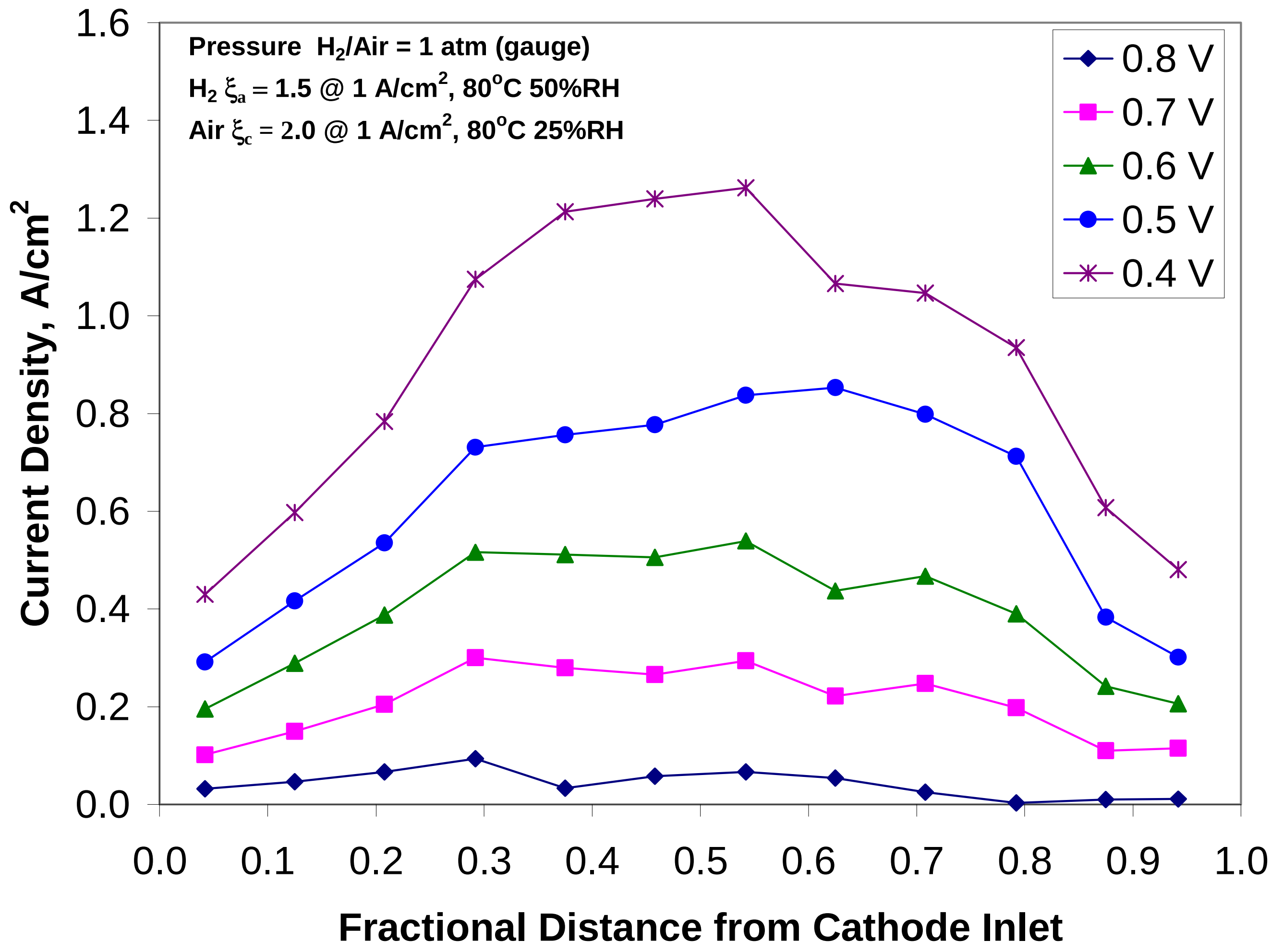


Segmented flow plates w/ 48 separate current collection ribs for current density distribution measurement by a multi-channel potentiostat

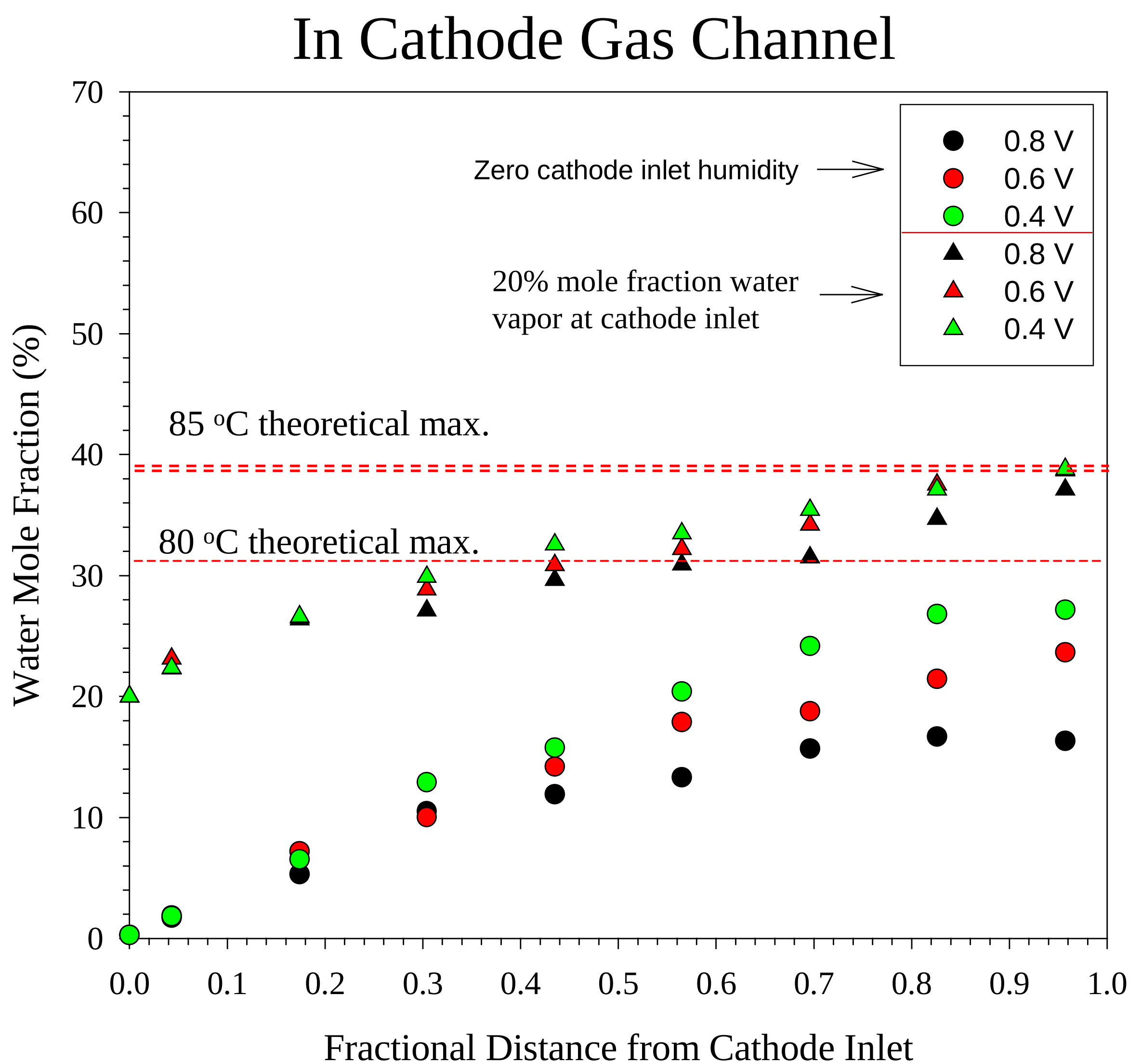


a 50cm^2 cell in testing for current and concentration mapping

Measured Current Distributions



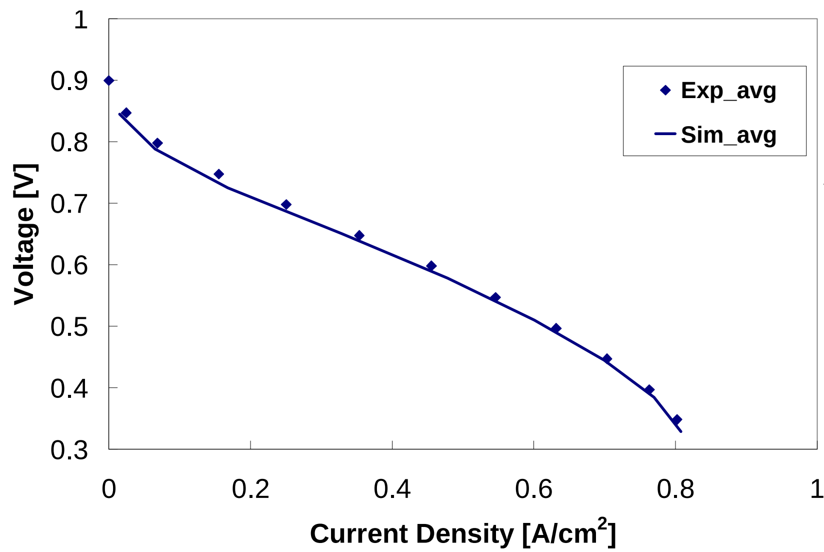
Measured Water Distributions



Pressure A/C = 1.5 atm	100% RH @ 90°C H_2 Anode
ξ_c = 2.0 @ 1 A/cm^2	ξ_a = 1.5 @ 1 A/cm^2

Validation by Current Distribution Data

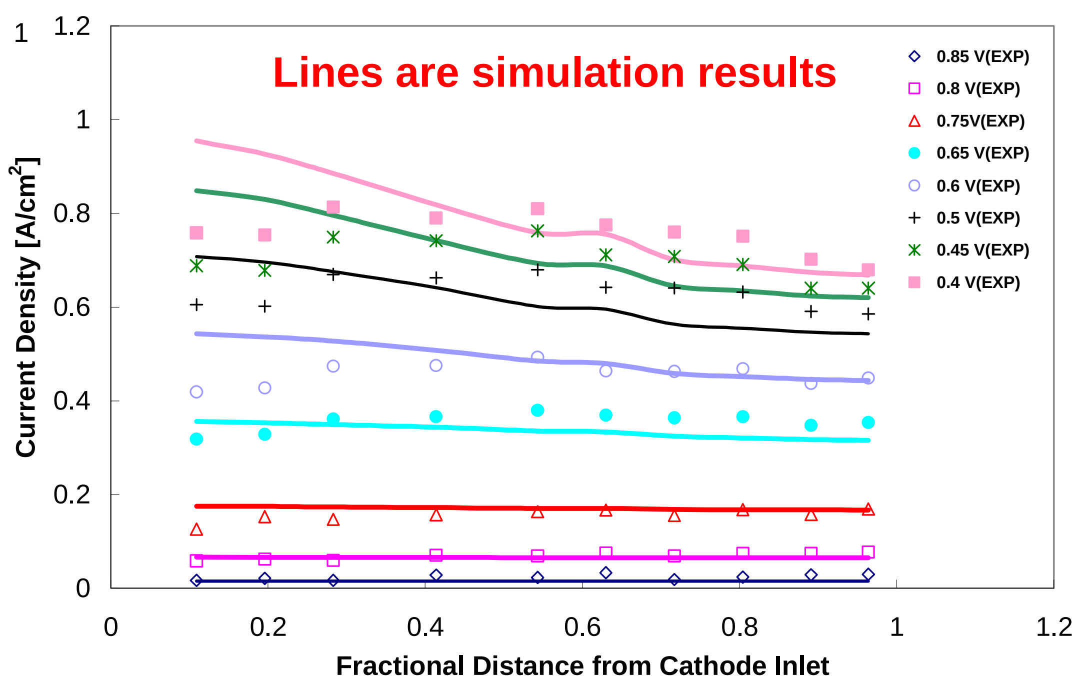
Comparison of average polarization curves for 3.0 @ 0.75 A/cm² cathode stoichiometry



Comparison of average current density can be excellent!

But, the comparison of current distribution is far from satisfactory

Simulated and measured current density distributions along the cathode path for 3.0 @ 0.75 A/cm² cathode stoichiometry



Solid Oxide Fuel Cells

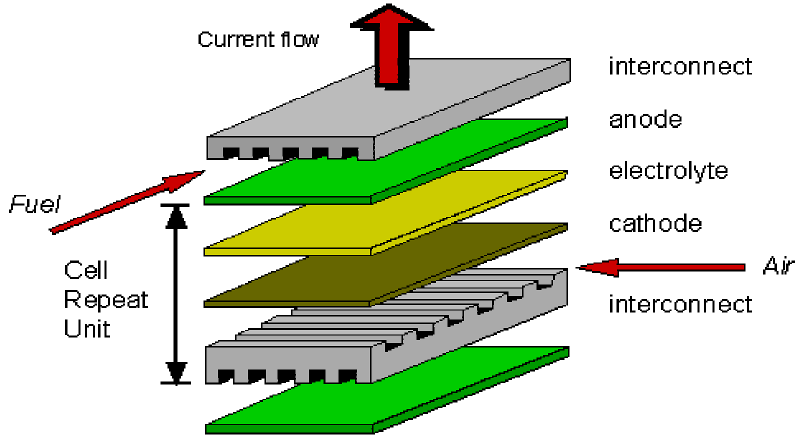
- **Electrode Reactions**

  Oxidation of fuel at anode

  $$H_2 + O^{2-} \rightarrow H_2O + 2e^-$$

  Reduction of oxidant at cathode

  $$\frac{1}{2}O_2 + 2e^- \rightarrow O^{2-}$$



- **Cell Materials**

  Anode:

  Nickel / Yttria – Stabilized Zirconia Cermet

  Cathode:

  LSM Layer: $La_{1-x}Sr_xMnO_3$

  Electrolyte:

  YSZ: Y_2O_3 doped ZrO_2 material

SOFC Modeling

- SOFC modeling is simpler than PEMFC as there is no complex water transport and distribution issue
- It is a problem very similar to chemically reactive flows except that there is charge transport thru electrolyte and active layers.
- New numerical issues are: (1) nonlinear source terms described by Tafel kinetics; (2) multiple anodic reactions (e.g. H_2+CO oxidation); (3) solution of two potential equations (electronic and ionic); and (4) implementation of constant total current as a boundary condition instead of a constant cell voltage;
- ECEC has developed a unified framework for SOFC and PEMFC modeling, with the former requiring no elaborative treatment of water transport.

SOFC Model Equations

	Conservation Equation	Source Terms			
		Flow Channels	Porous Electrodes	Active Electrodes	Electrolyte
Mass	$\frac{\partial(\varepsilon\rho)}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0$			$\vec{u} = 0$	$\vec{u} = 0$
Momentum	$\frac{1}{\varepsilon}\left[\frac{\partial\rho\vec{u}}{\partial t} + \frac{1}{\varepsilon}\nabla\cdot(\rho\vec{u}\vec{u})\right] = -\nabla p + \nabla\cdot\tau + S_u$		$S_u = -\frac{\mu}{K}\vec{u}$		
Species	$\frac{\partial(\varepsilon c_k)}{\partial t} + \nabla\cdot(\vec{u}\, c_k) = \nabla\cdot(D_k^{eff}\nabla c_k) + S_k$			$S_k = -\frac{s_k j}{nF}$	
Charge	$\nabla\cdot(\kappa^{eff}\nabla\Phi) + S_\Phi = 0$			$S_\Phi = j$	
Heat	$\frac{\partial(\varepsilon\rho c_P T)}{\partial t} + \nabla\cdot(\rho c_P \vec{u}\, T) = \nabla\cdot(k^{eff}\nabla T) + S_T$			$S_T = j\left(\eta + T\frac{dU_0}{dT}\right) + \frac{i^2}{\kappa^{eff}}$	$S_T = \frac{i^2}{\kappa^{eff}}$

Electrochemical Reaction:

$$\sum_k s_k M_k^z = n e^-$$

where

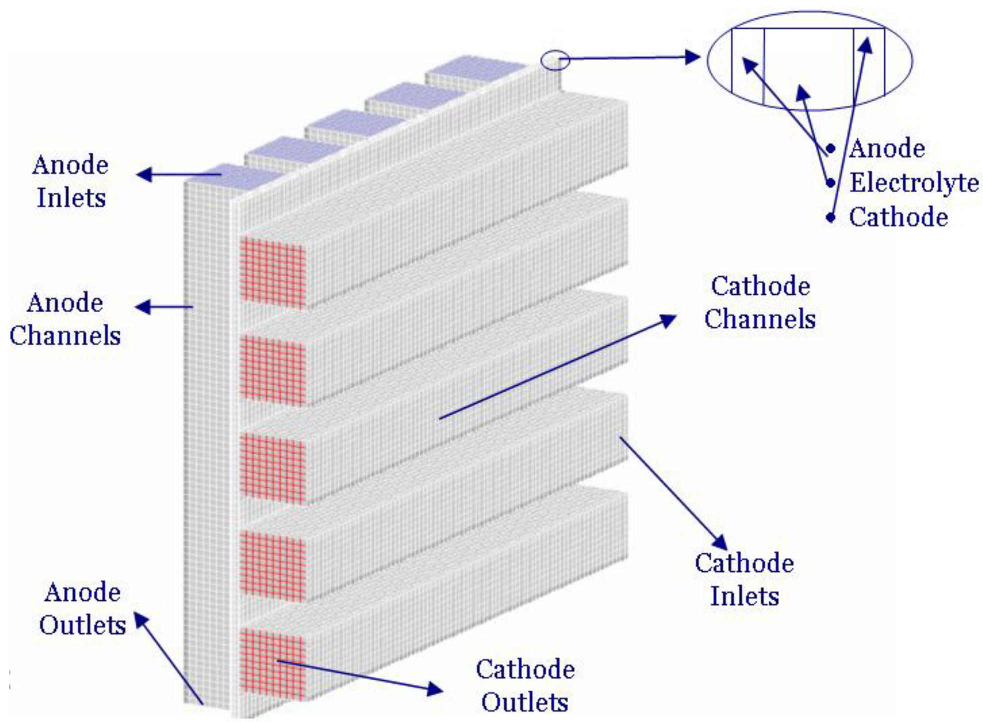
$M_k \equiv$ chemical formula of species k
$s_k \equiv$ stoichiometry coefficient
$n \equiv$ number of electrons transferred

Source: Pasaogullari & Wang, SOFC Symposium VIII, April 2003.

Electrolyte-Supported SOFC

– Cell Dimensions (2.5 cm^2)
  - Cell Length: 16 mm
  - Anode Channel: 2x2 mm^2
  - Anode Electrode Thickness: 50 μm
  - Cathode Electrode Thickness: 50 μm
  - Cathode Channel: 2x2 mm^2
  - Electrolyte: 180 μm

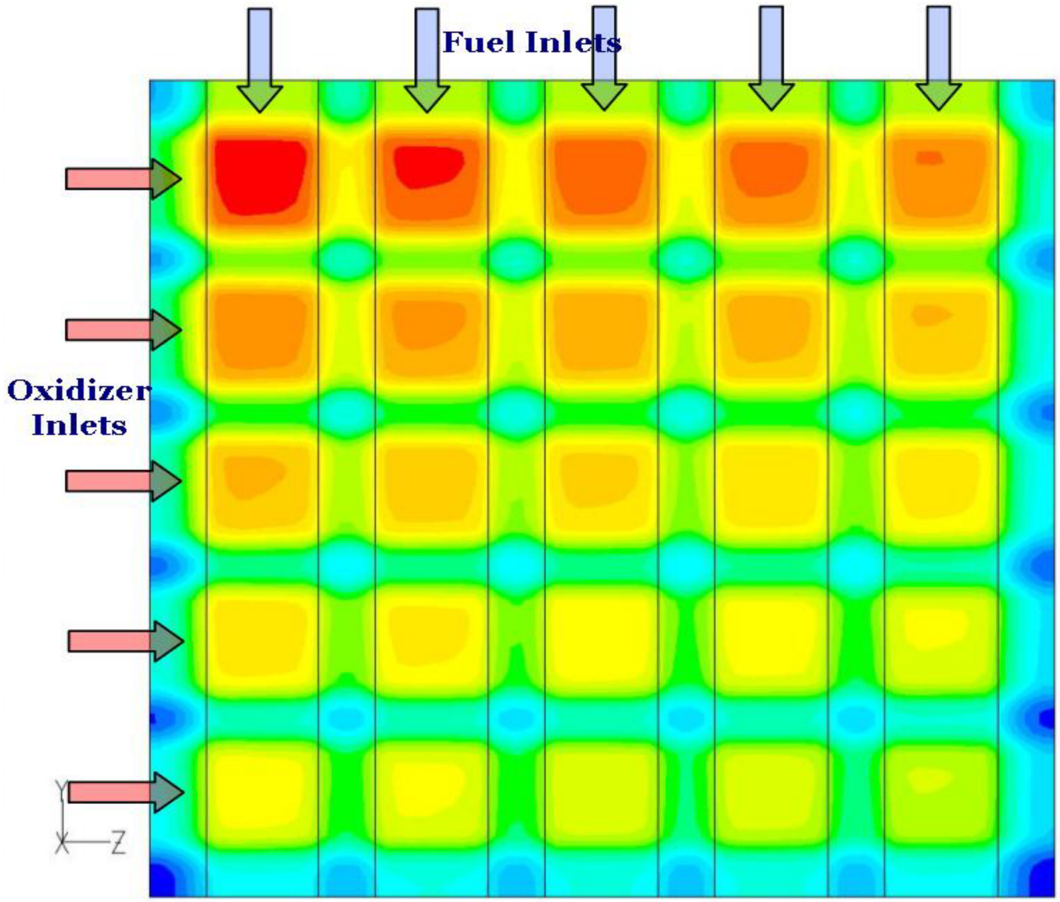
– Operating Conditions
  - Operating Temperature: 1000°C
  - Anode Stoichiometry: 1.5
  - Cathode Stoichiometry: 2.0



Cross Flow SOFC Configuration

Electrolyte-Supported SOFC

- **Electrochemical, flow, transport and thermal coupled modeling in 3-dimensions**

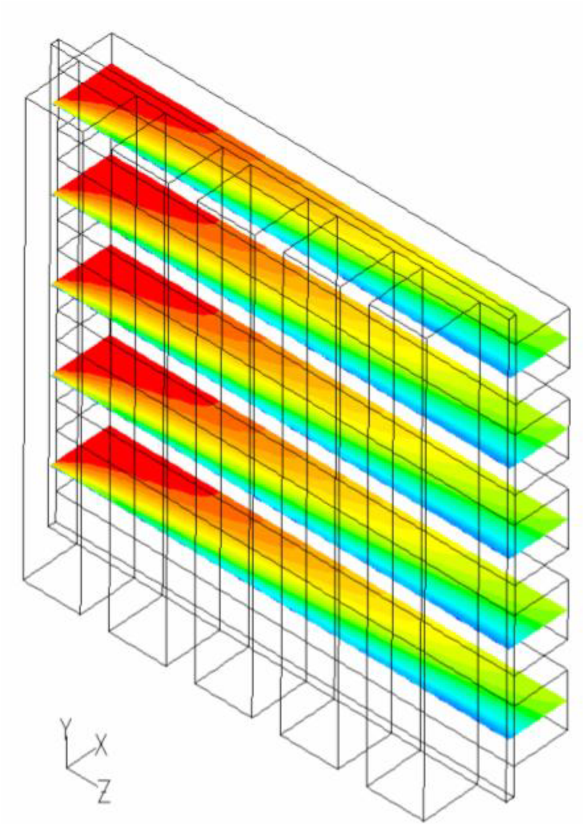


Current Distribution

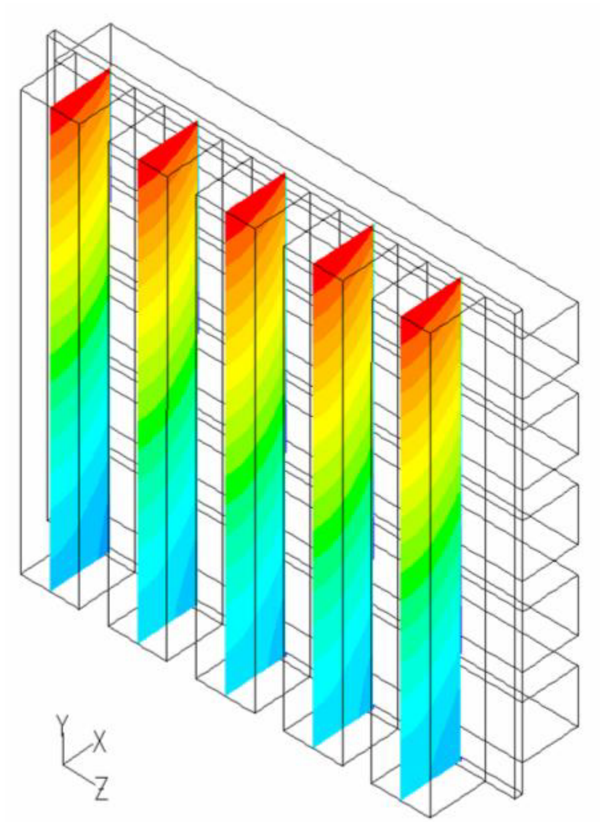
Thermal effect is insignificant here due to small cell size

Electrolyte-Supported SOFC

- **3-D reactant concentration contours**



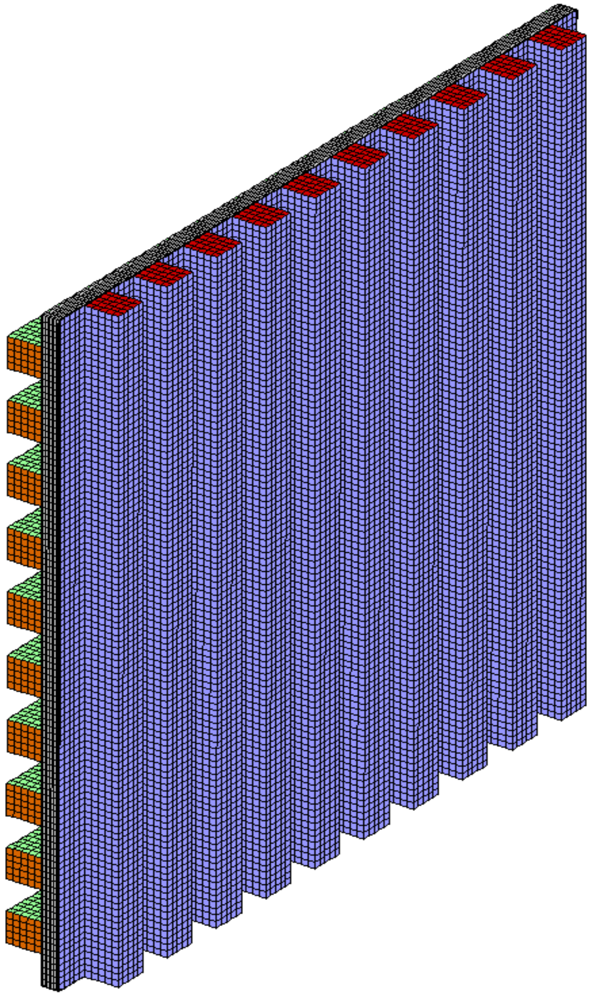
O_2 Concentration in Cathode of SOFC



H_2 Concentration in Anode of SOFC

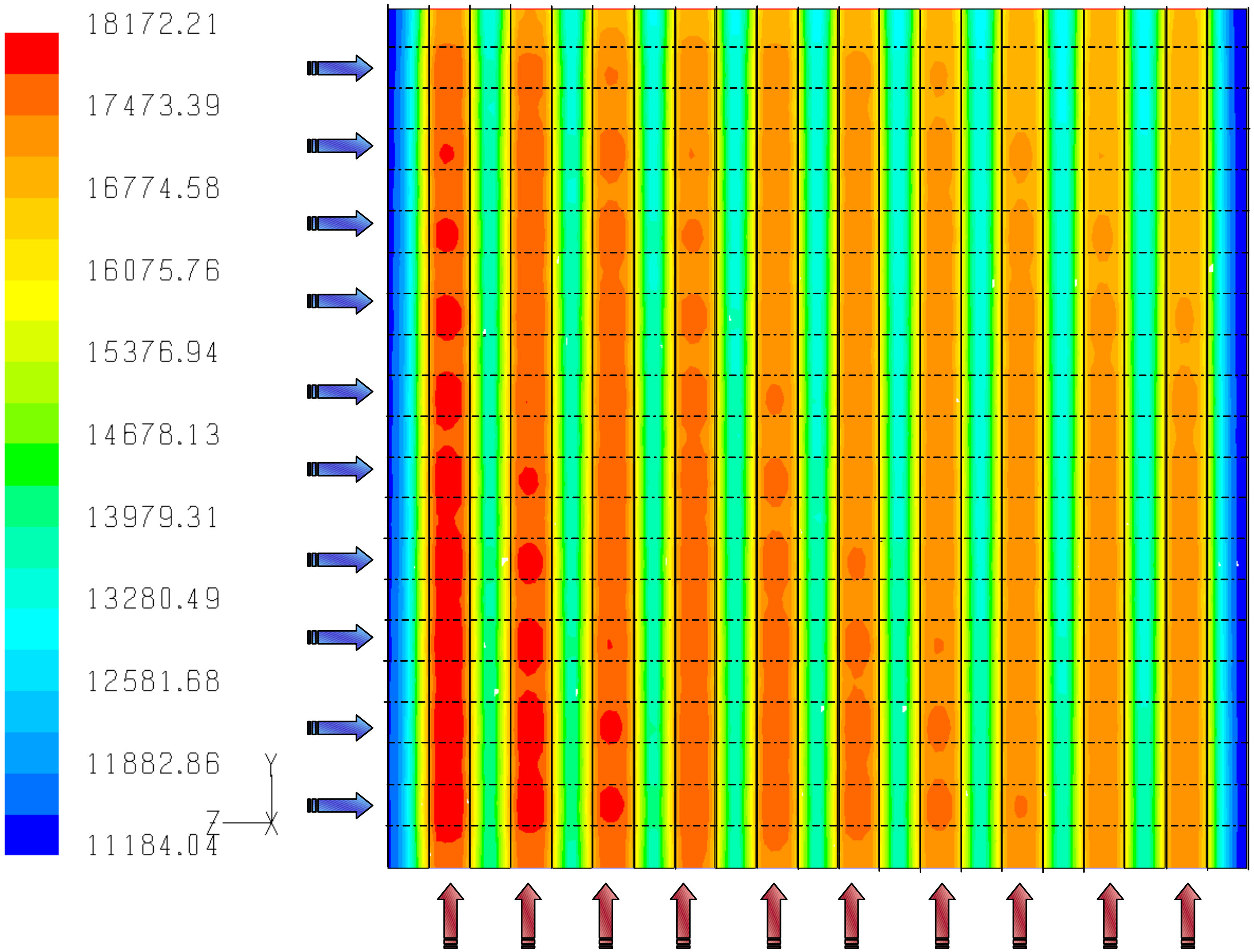
Anode-Supported SOFC

- Geometry
  - 10-Channel Cross-Flow
  - Anode Electrode: 1mm
  - Cathode Electrode: 50 μm
  - Electrolyte: 10 μm
- Operating Conditions
  - 2 atm Anode/Cathode Inlet Pressure
  - Operating Temperature: 800ºC
  - Anode/Cathode Stoichiometry: 2/2 @ 2 A/cm^2



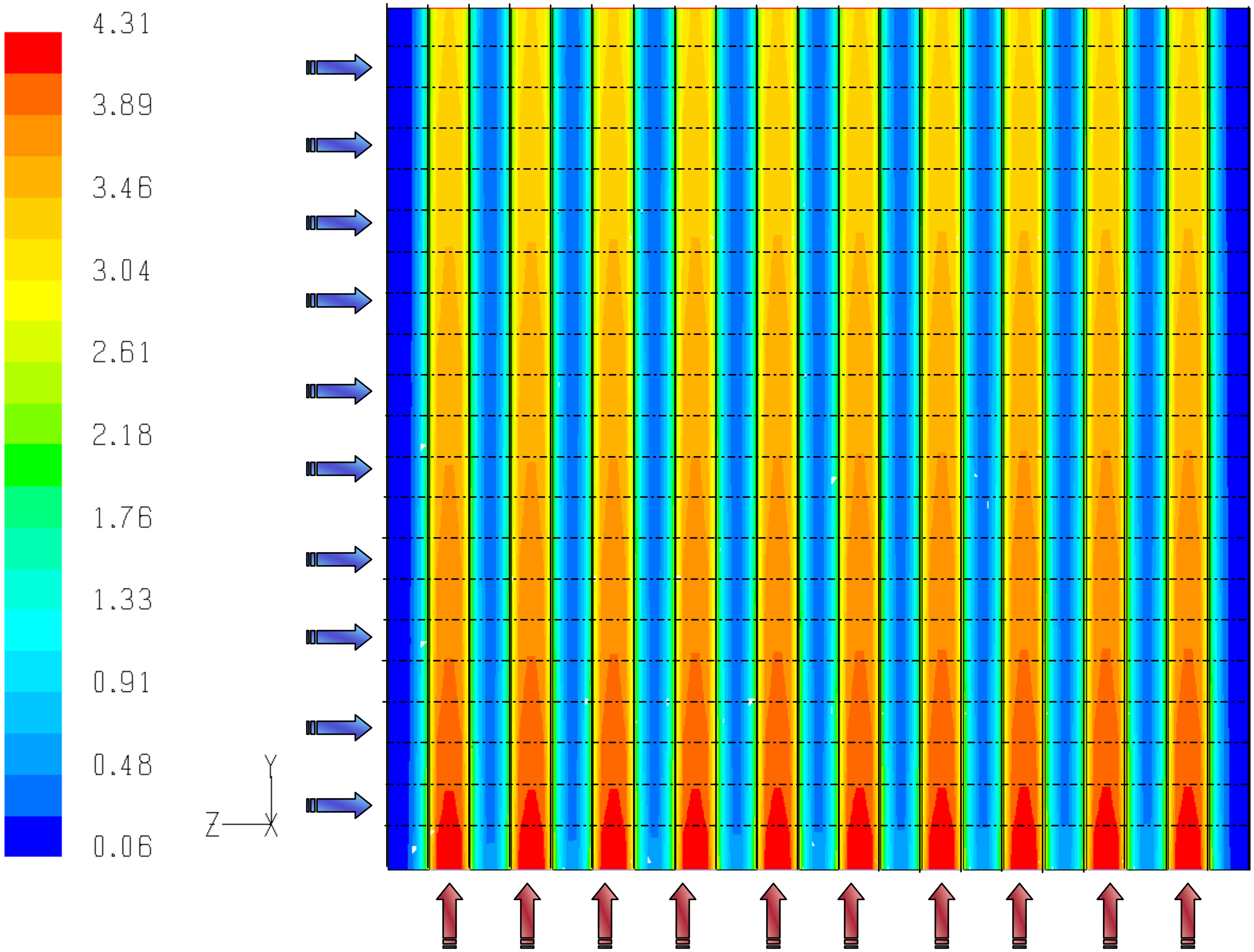
Anode-Supported SOFC

Local Current Density (A/m²) @ 0.7V; I_{avg}=1.5 A/cm²



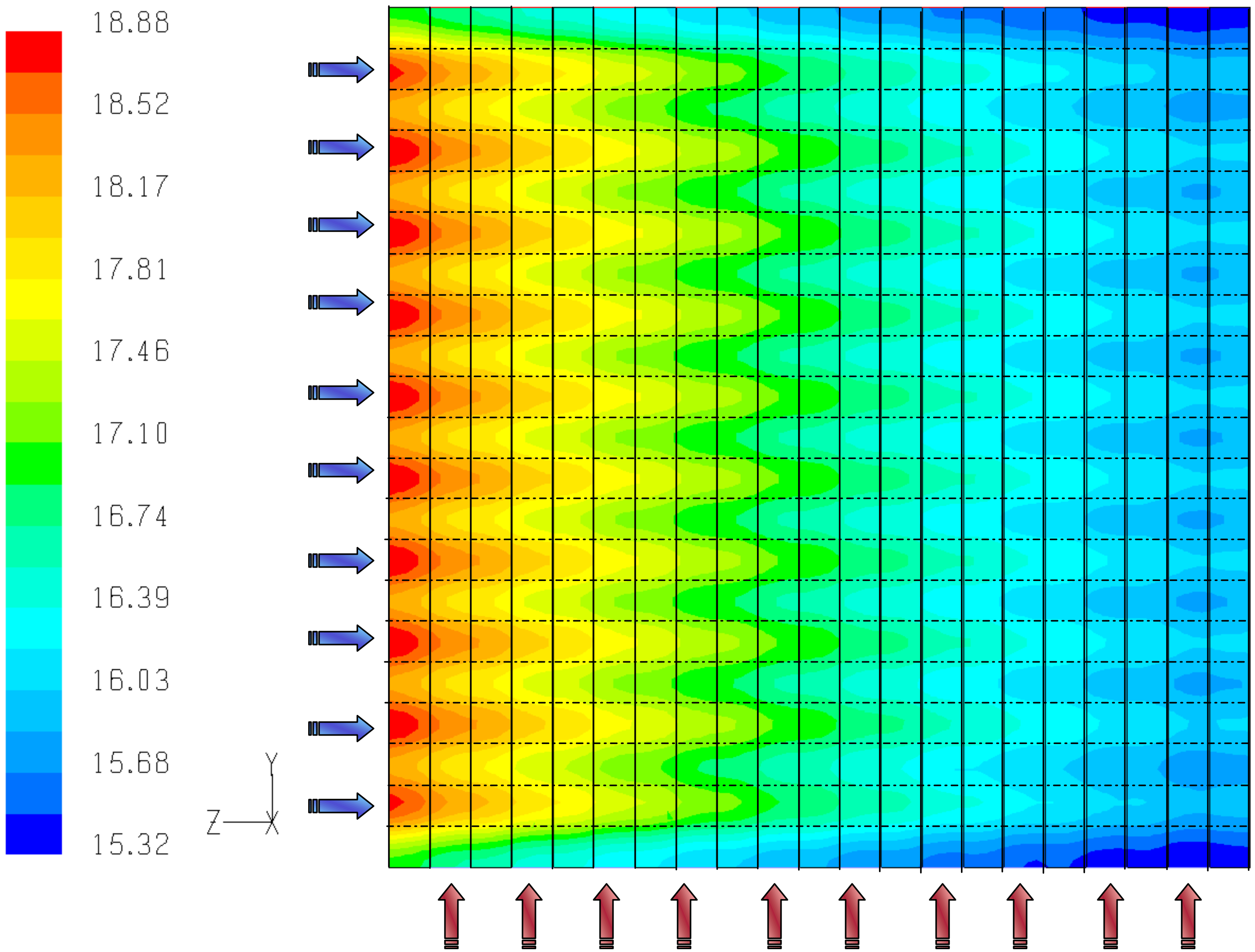
Anode-Supported SOFC

O_2 Concentration (mol/m^3) at Cathode-Interlayer Interface

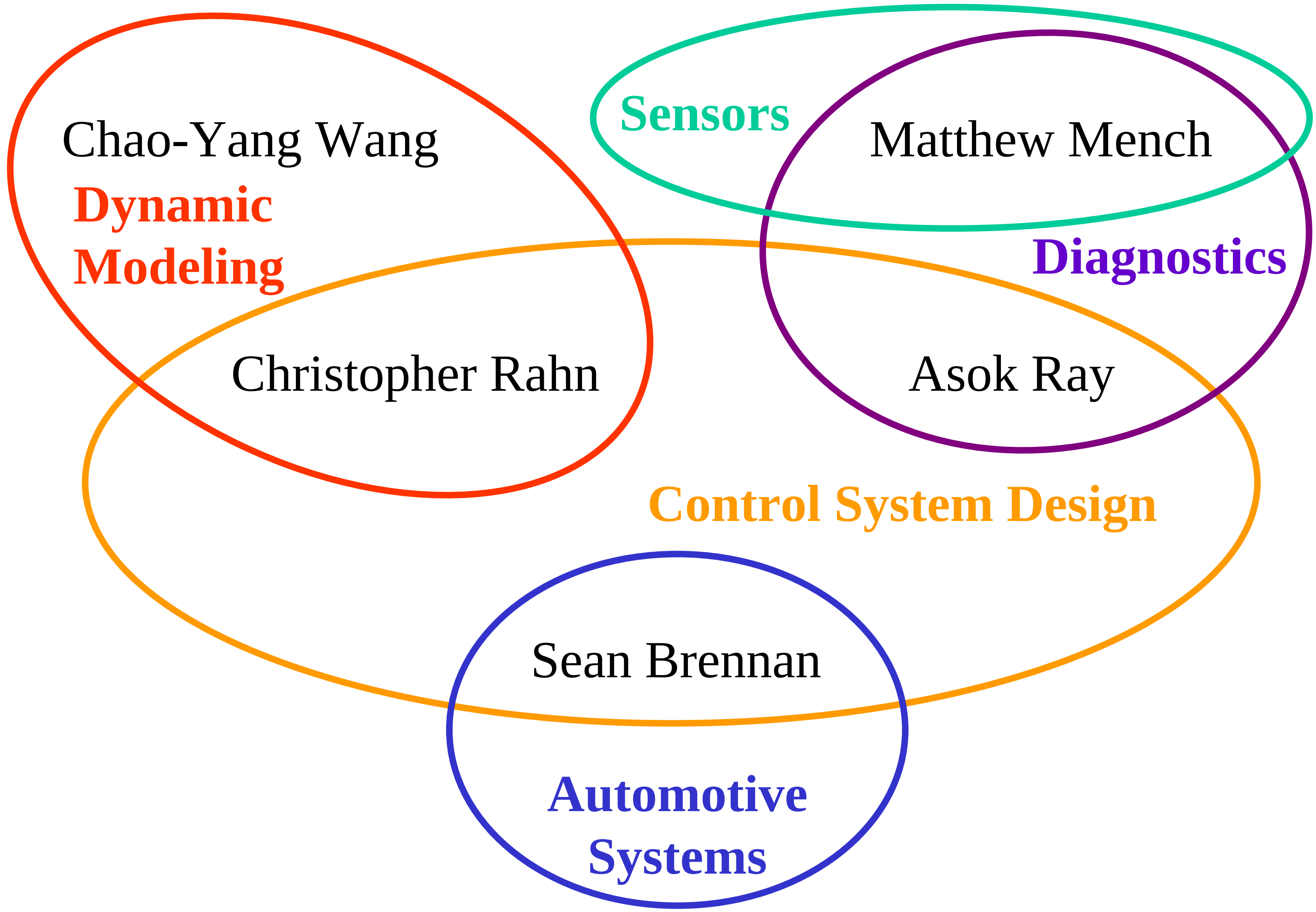


Anode-Supported SOFC

H_2 Concentration (mol/m^3) at Anode-Interlayer Interface



ECEC Fuel Cell Controls Group



Summary

- Multidisciplinary computational fuel cell research encompasses: (1) physicochemical model development, (2) numerical algorithm development, (3) materials characterization, and (4) model validation at detailed levels.
- PEMFC model is mature for use in product design and optimization. Considerable capabilities are available: fully coupled electrochemical/ flow modeling, 3-D, water and heat management, cathode flooding, CO poisoning, cold start, etc.
- ECEC also has developed an electrochemical-transport coupled model for SOFC in commercial CFD packages.
- Fuel cell control strategies are studied and integrated at early stages to enable design for high performance, design for robust controls, or design for high reliability.

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