SECA Core Technology Program
Modeling and Simulation Team

SOFC Model Development and Validation at NETL

October 15, 2002

National Energy Technology Laboratory

Goals and Objectives

- **SECA Program Goal**
  - The Solid State Energy Conversion Alliance (SECA) goal is to create solid oxide fuel cells (3-10 kW) that can be mass produced in modular form
  - Low cost (<$400/kW) and high efficiency SOFC systems for stationary power, transportation, and military applications.

- **Project Goals**
  - Develop validated modeling tools capable of *detailed* fuel cell and stack performance analysis
  - Apply these new tools toward development of new/novel fuel cell concepts that can achieve the SECA goals

Technical Challenges

- **Complex physics of the fuel cell**
  - electrochemical sources and sinks of species and energy
  - chemistry for methane reforming, water-gas shift, catalytic surfaces
  - porous media flow
  - complex geometry, both in the cell and in the stack

- **Numerical difficulties in coupled system**
  - “stiff” coupling between electrical field and electrochemistry

Technical Challenges - continued

- **Ensuring a productive tool given the computational requirements for modeling geometrically-complex cells and FC stacks**
  - parallel implementation is needed
  - possible use of simplified submodels for very large scale simulations

- **Accurate material properties for the model**
  - accurate thermal, electrical, mechanical, and transport properties are needed

Technical Challenges - continued

- **Validation Data**
  - Much data is proprietary
  - Detailed data is needed for validation
    - local temperature, voltage, current, species, stresses
  - Measurements are difficult to make in SOFC environment

Technical Approach

- **Use commercial CFD code as underlying platform for detailed fuel cell model**
  - FLUENT code is parallel, unstructured mesh, with well-validated models for fluid flow, heat transfer, species transport
  - Working with Fluent Software Developers and Fuel Cell Experts
  - Model will be in public domain

Technical Approach

- **NETL SOFC Model Capabilities - Existing, *Planned***
  - H_2 and CO Electrochemistry
  - Electrical field in conducting regions - current flow, ohmic heat generation
  - Contact resistance for cell/stack components
  - Species diffusion in flow channels and porous media
  - *Water-gas shift reaction*
  - *Internal reforming*
  - *Parallel Processing*
  - Single cells and cell stacks
  - Output compatible with ANSYS
  - Steady and *transient* analysis

Technical Approach - continued

- **Validate NETL SOFC Model**
  - NETL Test Facility (SOFCEL) for detailed validation data

NETL SOFC Test Stand

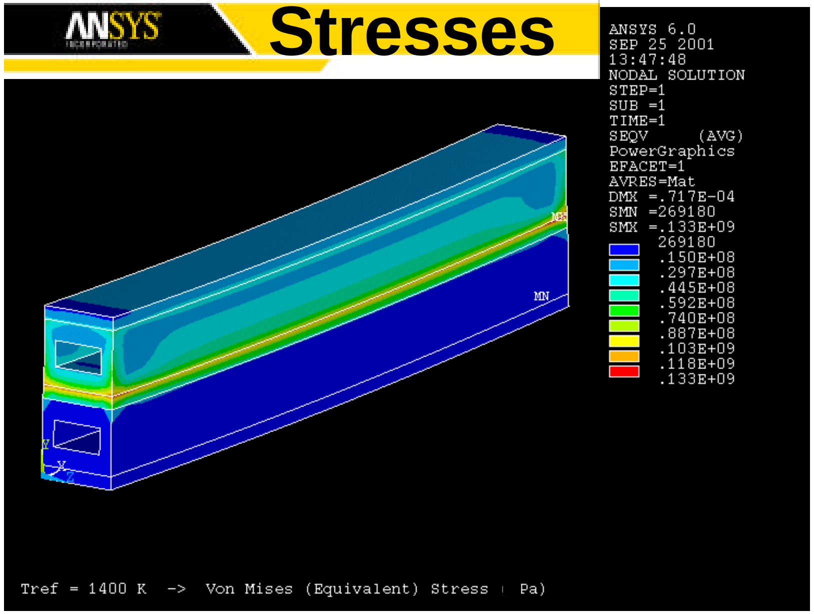
- 300 watt max

- pressure capable

- acquire test cells from partners with range of fundamental properties (component thickness, porosity, etc.)

Technical Approach - continued

- **Use temperature field from SOFC model in an FEM model to calculate thermal stresses**
  - geometry and temperature field output from SOFC model can be input directly into ANSYS
  - Work closely with ANSYS to make the coupling process easier



Stress in single SOFC cell at 1073K From NETL Model

Technical Approach - continued

- **Parallel implementation of the SOFC model for complex cell and stack simulation**
  - NETL Computation and Visualization Resources
    - 272 CPUs in 3 PC-Clusters
    - FLUENT license for NETL On-site use for all CPUs
    - 4 terabytes of RAID storage
    - Advanced visualization facilities
    - Multi-wall visualization environment for 3-D visualization
    - Access to Pittsburgh Supercomputer Center Resources

NETL PC-Clusters

Technical Approach - continued

- **Collaborate with other modeling groups and FC developers for model development and validation**
  - National Labs
  - SECA participants
  - Other developers
  - Academia

- **Publish to disseminate information and for peer review**

NETL Fuel Cell Model

Local Species Concentration
Local Temperature
Local Electrical Potential

FLUENT CFD

Species

Momentum

Energy

Electrical Potential Field

SOFC Model

Nernst Voltage

Losses at Electrolyte

Current Distribution on Electrolyte

Electrical Potential B.C.s

Species Source/Sink
Heat Fluxes
Electrical Potential B.C.s

Model Overview: Physics for Detailed Model

- **Fluid Flow, Heat Transfer, Mass Transfer**
  - Complex Flow Geometry
  - Laminar Flow
    - diffusion is important
  - Porous Media
    - flow and diffusion in porous media
- **Electrical Potential Field**
  - Coupled to Electrochemical Model
- **Electrochemical Submodel**
  - Electrolyte Submodel
  - Electrochemical Losses
  - Stack Logic

Model Overview: Species Diffusion

- **No detail today on mass, momentum, energy conservation equations and solution - "standard" FLUENT implementation**

- **The diffusion coefficient for binary gas mixtures is given by the following equation**

$$\frac{PD_{AB}}{(p_{cA}\,p_{cB})^{1/3}(T_{cA}\,T_{cB})^{5/12}\left(\frac{1}{M_A}+\frac{1}{M_B}\right)^{1/2}} = a\left(\frac{T}{\sqrt{T_{cA}\,T_{cB}}}\right)^{b} \times 1E-4$$

- **The diffusion coefficient of species *i* in the mixture is given by:**

$$D_{i,m} = \frac{1-x_i}{\sum_{j,j=i}\left(\frac{x_j}{D_{ij}}\right)}$$

- **And effective diffusion coefficient through porous media is given by:**

$$(D_{i,m})_{effective} = p \cdot D_{i,m}$$

  – where p is the permeation factor = porosity/tortuosity

Model Overview: Electrical Potential Field

- **Submodel solves for the electric potential field throughout all conductive regions**
  - porous electrodes, current collectors, interconnects)

- **Local voltage losses**

- **Distributed heat generation**
  - local ohmic heating in anode, cathode, current collectors, and interconnect regions

Model Overview: Electrical Potential Field

- **Basis for the electrical potential equation is obtained from the statement of conservation of charge for steady conditions:**

$$\nabla \cdot \underline{i} = r_i$$

  – where $\underline{i}$ is the local current density vector and r_i is the local current source
  – for the potential fields we are considering, no local sources of current will be present, so $r_i = 0$
  – current sources/sinks at the electrolyte-electrode faces are introduced through boundary conditions

- **For ohmic materials, the current density vector may be expressed in terms of the gradient of the electrical potential field:**

$$\underline{i} = -s \nabla f$$

  – where s is the conductivity of the material and f is the electrical potential

Model Overview: Electrical Potential Field

- The FLUENT capability of solving for transport of a User-Defined Scalar is used where the scalar is electrical potential f

- Ohmic heating in the conducting regions can then be calculated from the relation:

$$Q_{genC} = s \left| \nabla f \right|^2$$

- Boundary conditions are specified as fixed potential on one side and fixed flux on the other.

- This guarantees that the problem is well-posed and that the total current is conserved

Model Overview: Electrolyte Model

- **The electrolyte is always assumed thin for electrochemical modeling purposes**
  – It can be represented by a finite thickness region in the FLUENT simulation

- **The electrodes can be resolved as porous media zones to capture concentration gradients directly**
  – Fickian-based overpotential models are also included to allow the treatment of thin electrodes that are not resolved with mesh

- **Models for activation losses are also available for each electrode**
  – account for electrochemical kinetics at the electrodes

Model Overview: Electrolyte Model

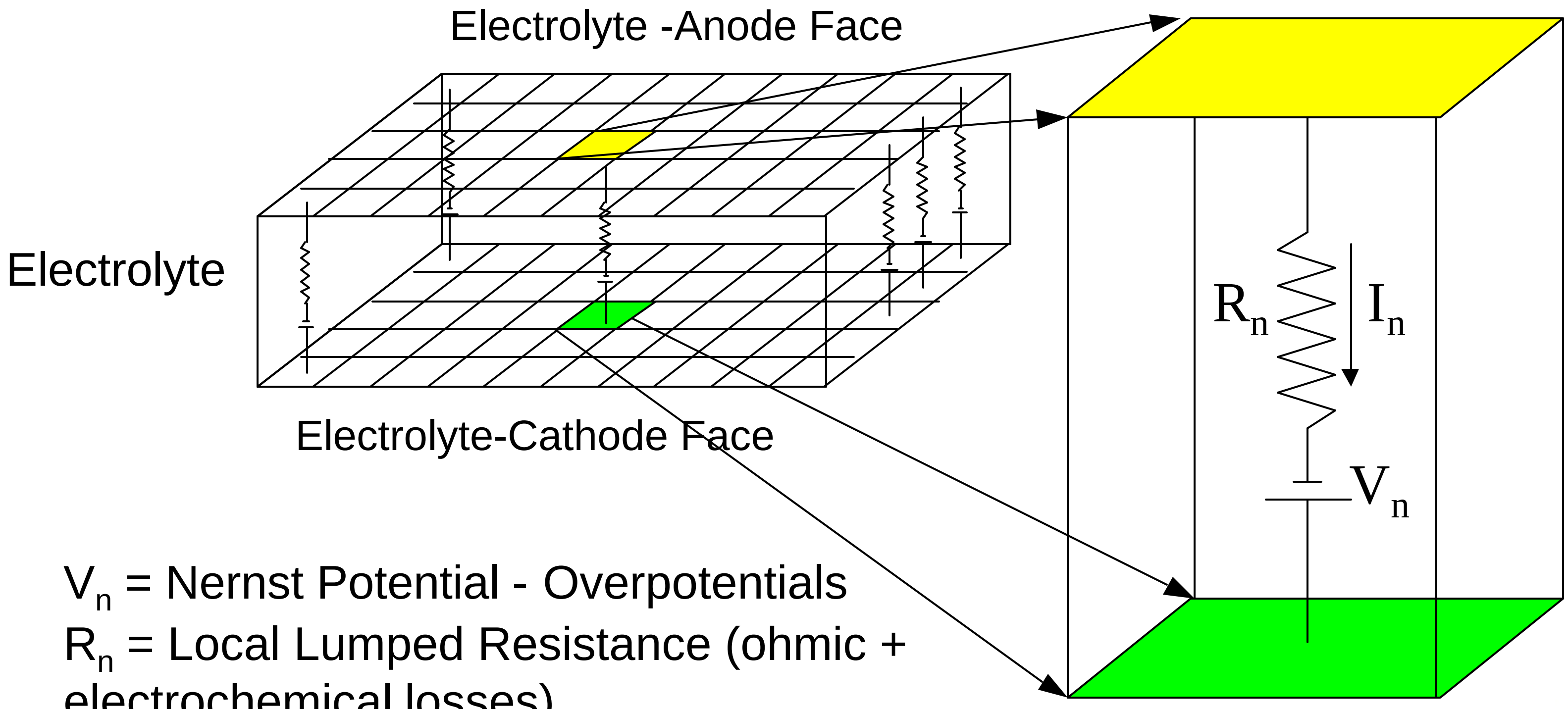
- **Anodic and cathodic faces are associated pair-wise**
  - species and temperature information give the local Nernst potential and diffusion and activation overpotentials

- **For simple geometries, pair-wise association is not a problem. This is not necessarily true for more complicated designs. This is an area for future development**

- **The total cell current is specified as user input**

Model Overview: Electrolyte Model

- **The electrolyte is treated as a parallel resistor-voltage network for n computational cell face-pairs on either side of electrolyte**
- **Local currents, I_n through each face pair must sum to equal the specified cell current: $I_T = \Sigma_n I_n$**



V_n = Nernst Potential - Overpotentials

R_n = Local Lumped Resistance (ohmic + electrochemical losses)

Model Overview: Electrolyte Model

- **Corrections to V_{Nernst} for losses - "Overpotentials"**

$$V_n = V_{Nernst} - h_R - h_{C,Cath} - h_{C,Anode} - h_{A,Cath} - h_{A,Anode}$$

Ohmic Loss through Electrolyte: $$h_R = R \cdot i$$

Diffusion Losses through Electrodes: $$h_C = -\frac{R_u T}{nF} \ln(1 - i/i_L)$$

Chemical Kinetics of Electrode Reactions: $$i = i_o \left[\exp\left(\frac{a h_A F}{R_u T} \right) - \exp\left(\frac{(1-a) h_A F}{R_u T} \right) \right]$$

  – where R is the resistance [ohm-m²] of the electrolyte; i, local current density; i_L is the diffusion limiting current density; α is the transfer coefficient; and i_o is the exchange current density

- **These corrections are made to V_{Nernst} for each electrolyte face-pair to produce the "local" voltage across the electrolyte**

Model Overview: Electrolyte Model

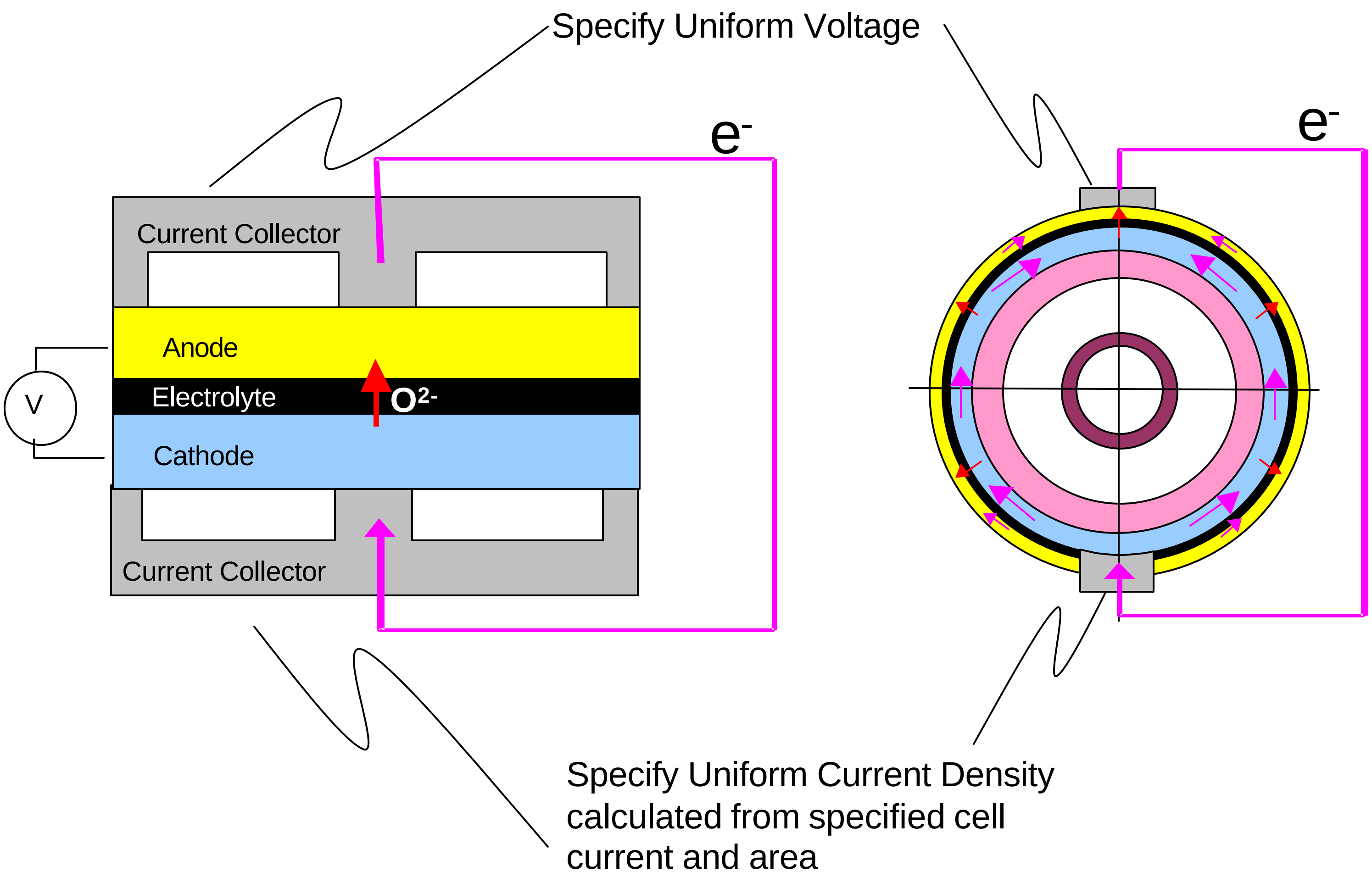
- **Using the local current information, the model applies species fluxes to the electrode-electrolyte boundaries in the FLUENT simulation**

- **Local current information is also used to account for heat generation in the electrolyte and electrodes as follows:**

$$\Delta\dot{Q}_{total}(J/s) = \Delta\dot{Q}_{rev} + \Delta\dot{Q}_{irrev} = T\Delta S \cdot \frac{I}{nF} + I^2 R_E + I h_{total}$$

- **Heat generation is calculated for each electrolyte face-pair**

Model Overview: Boundary Conditions



FY 02 Accomplishments

- **Apply Model to New Fuel Cell Geometry Concepts**
  - Study Delphi proprietary cell geometry
  - Evaluate model in tubular geometry

- **Apply model to NETL Test Facility Designs**
  - Assist in design of NETL test rig
  - Initial investigation of effect of test parameters on cell performance

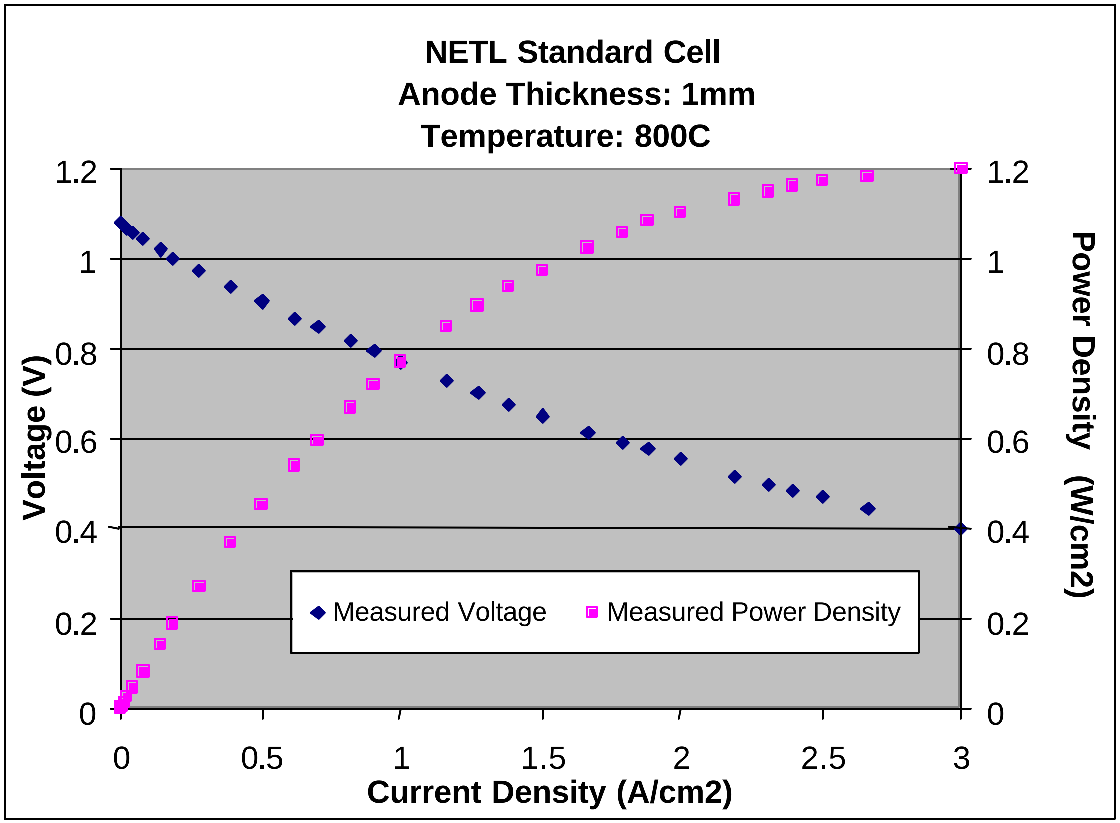
- **Preliminary Validation with University of Utah Data**

FY 02 Accomplishments

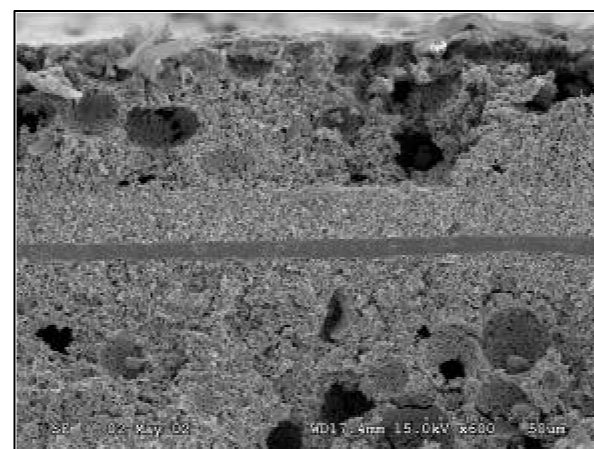
- **Compare NETL and PNNL SOFC Models**
- **Technology Transfer**
  - MOU with Siemens-Westinghouse
  - Draft MOU with GE Power Systems
- **Developed Stack model**
  - "beta" version

Validation Application: Button Cell

- **Preliminary Validation with University of Utah Data**
  - UU has tested cells and supplied representative performance data

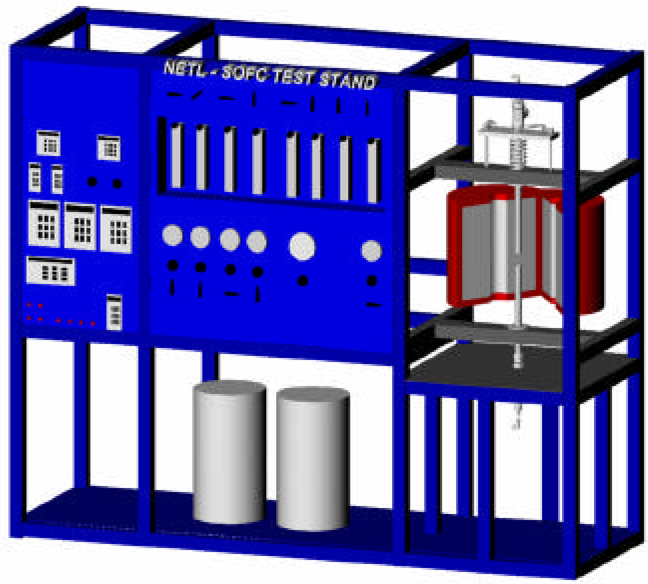


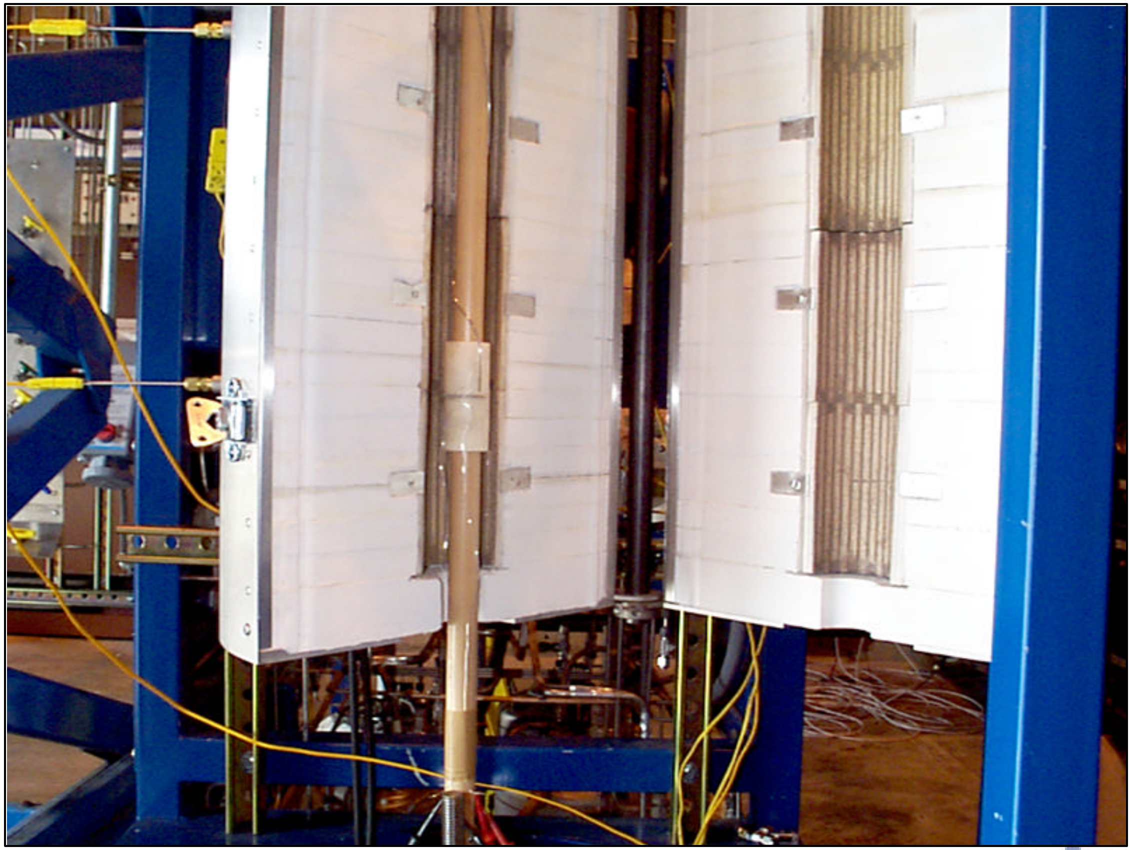
SEM of NETL Standard Button Cell



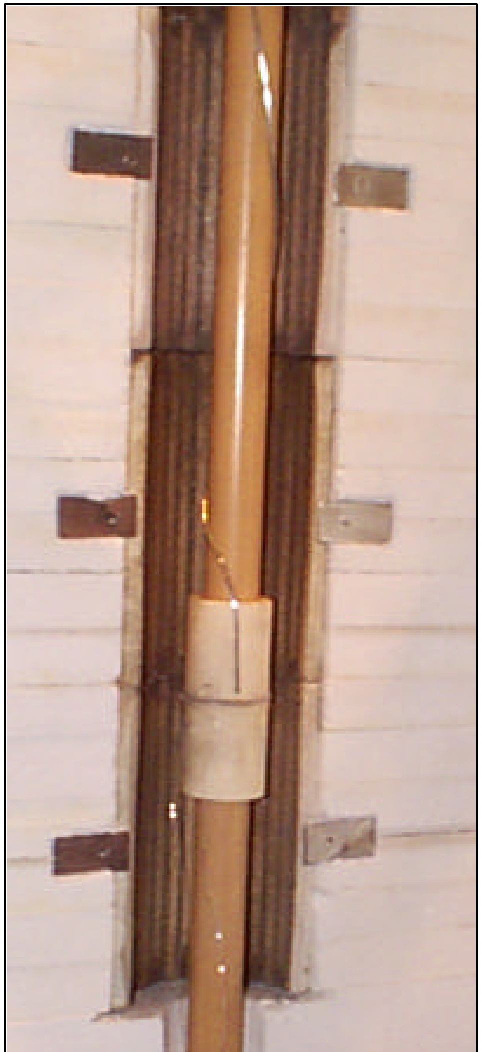
Validation Application: Button Cell

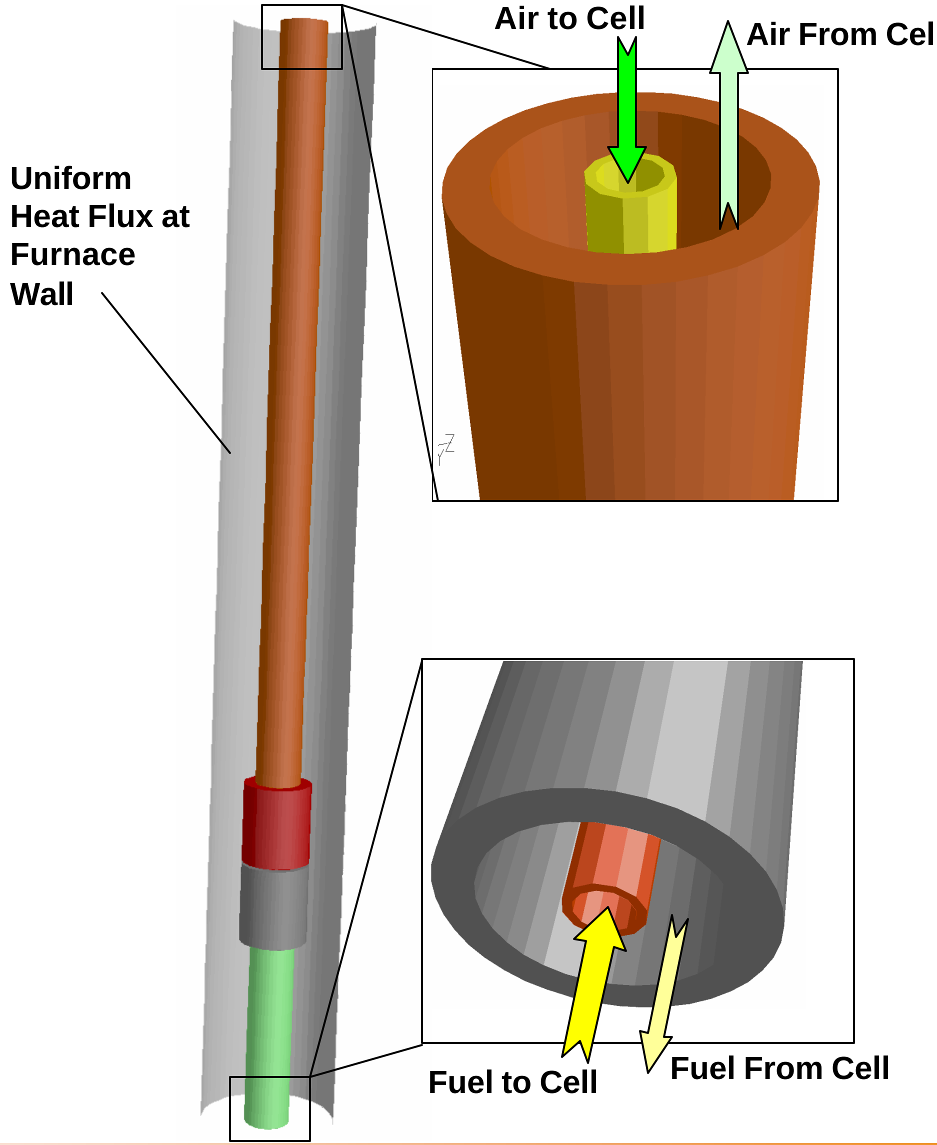
- **Validate models with experimental data**
  – Preliminary Model Validation using University of Utah Data
  – Simulate button cell performance in NETL test rig - compare to U of U data





Validation Application: Button Cell





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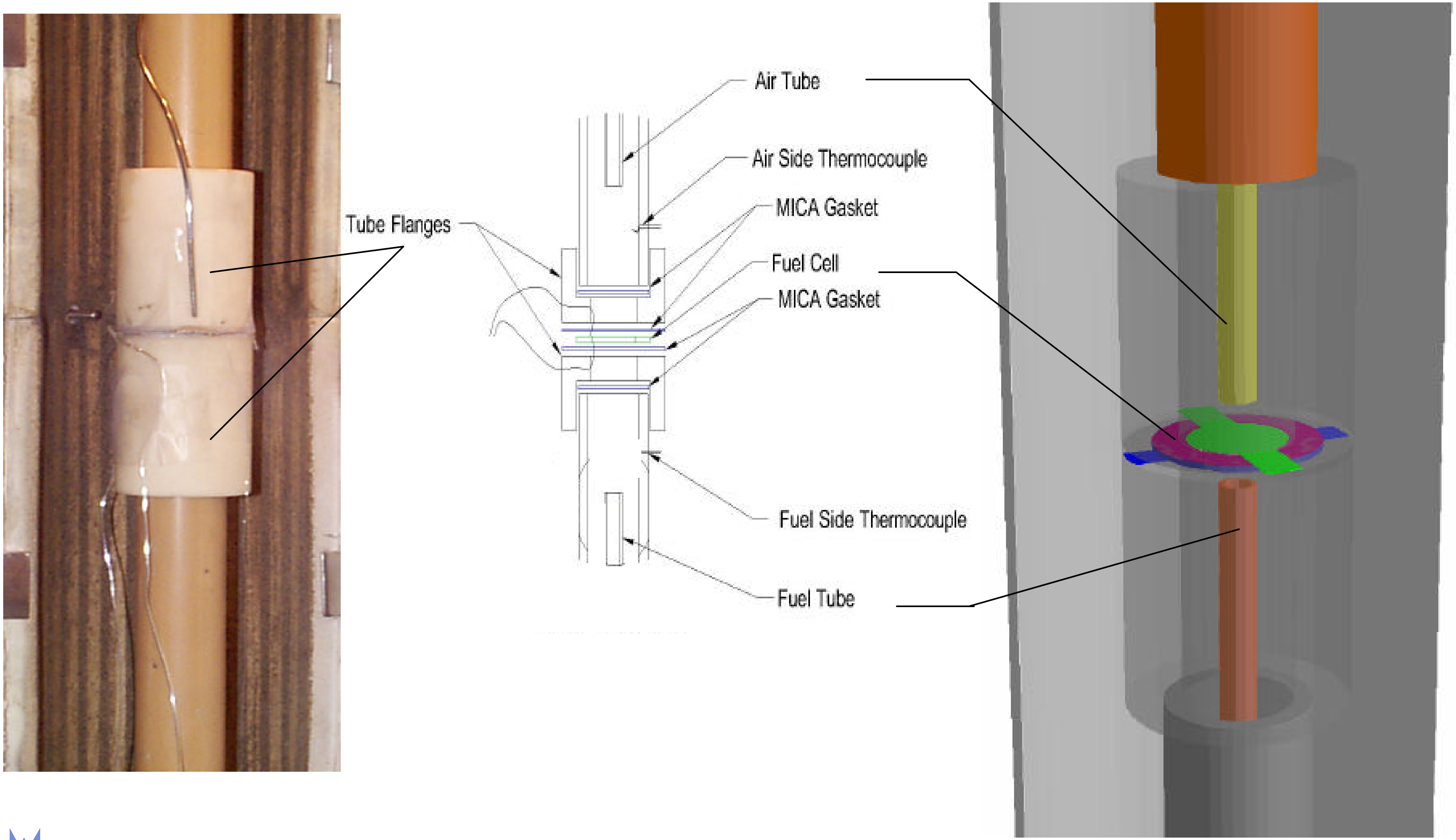

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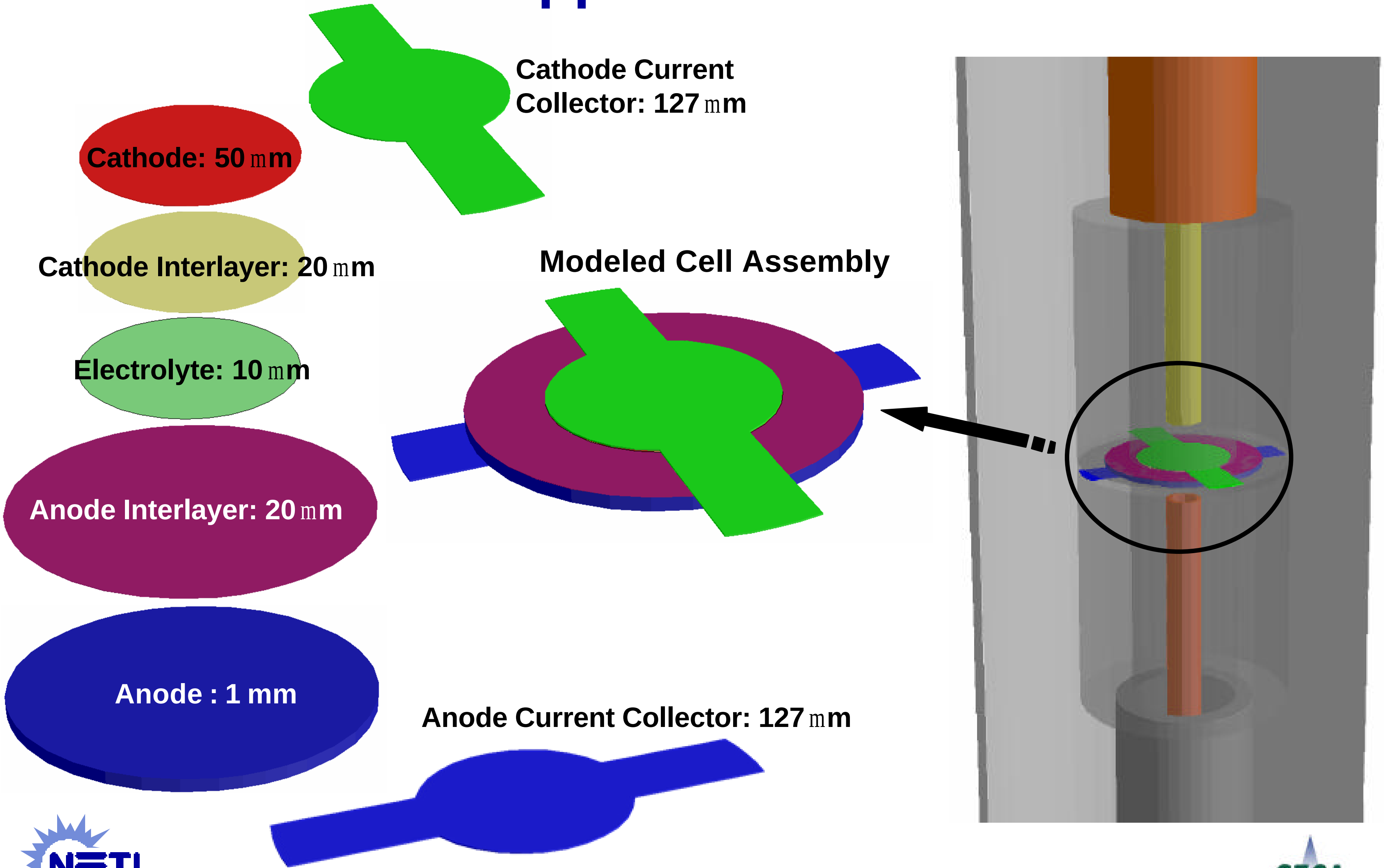


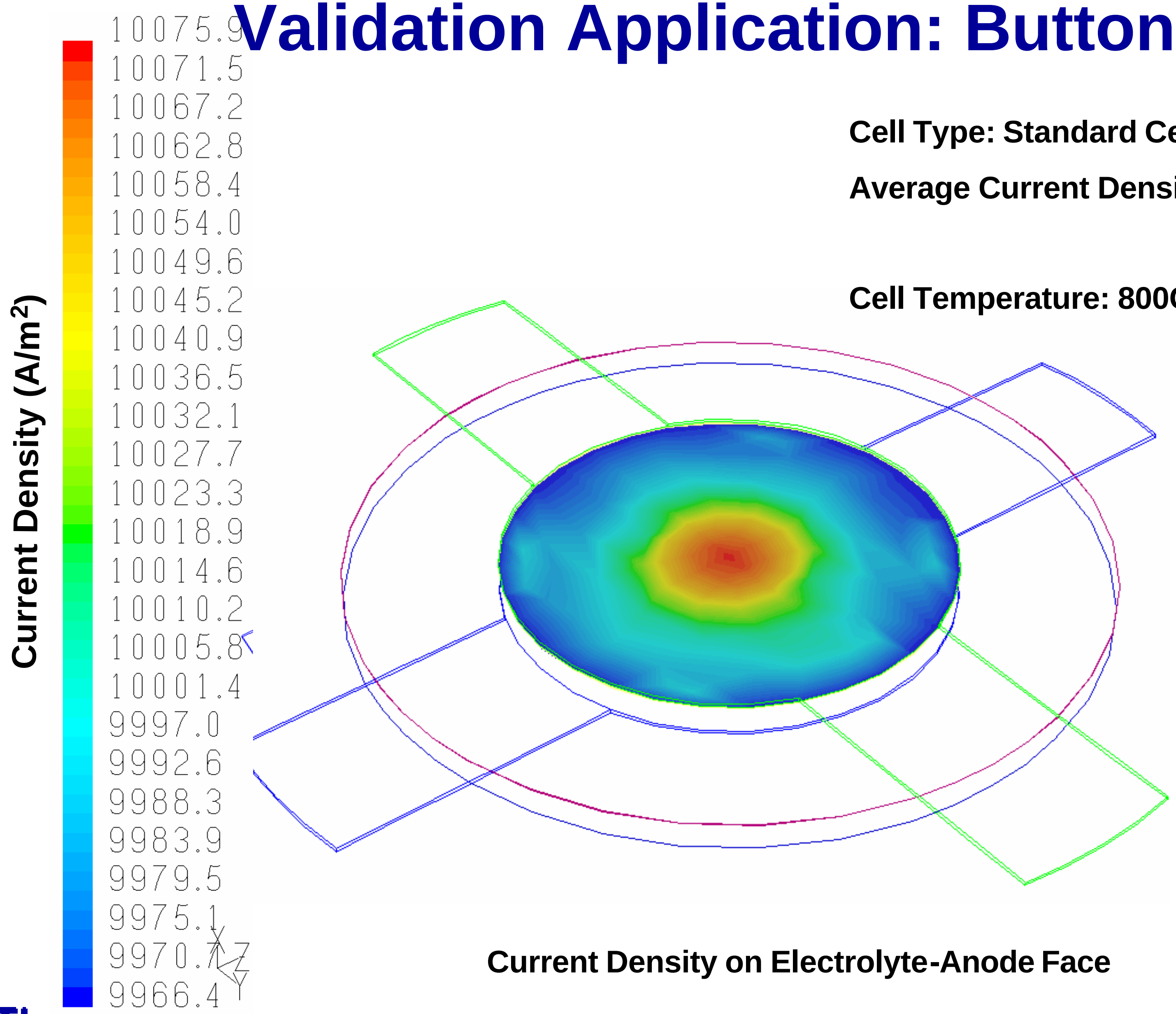
Validation Application: Button Cell

Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

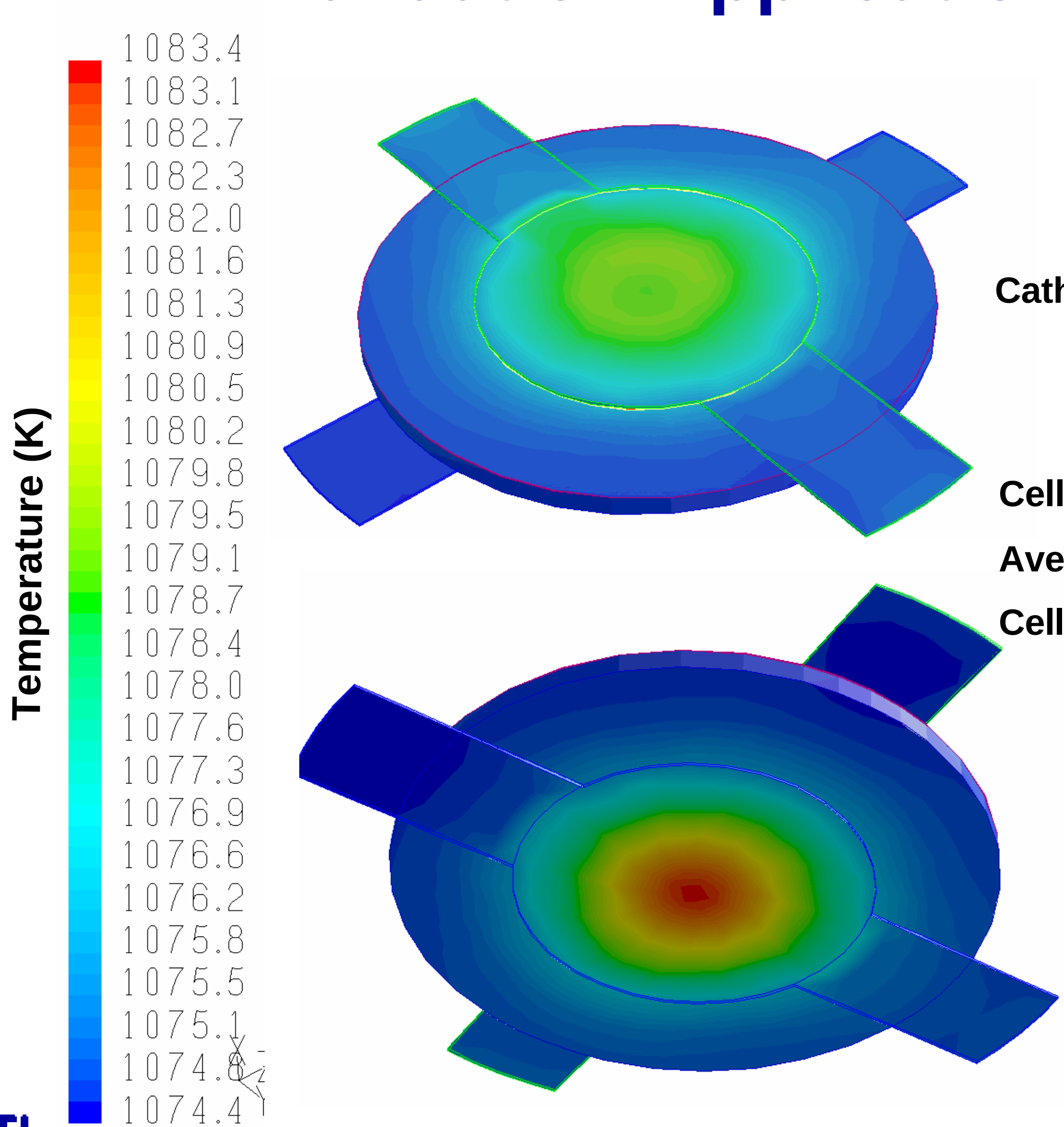
10,000A/m2

Cell Temperature: 800C / 1073K



Current Density on Electrolyte-Anode Face

Validation Application: Button Cell



Cathode Side Temperature

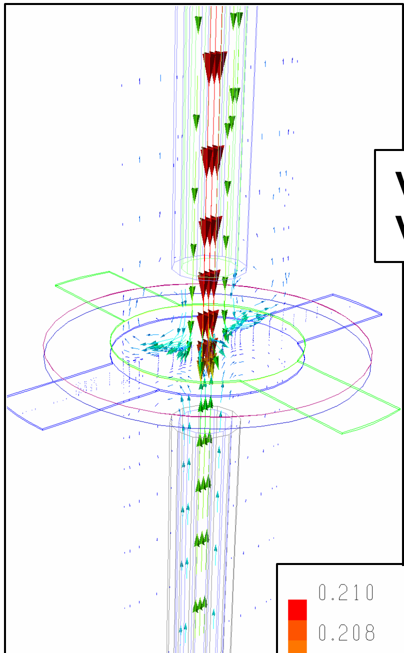
Cell Type: Standard Cell, 1mm Anode

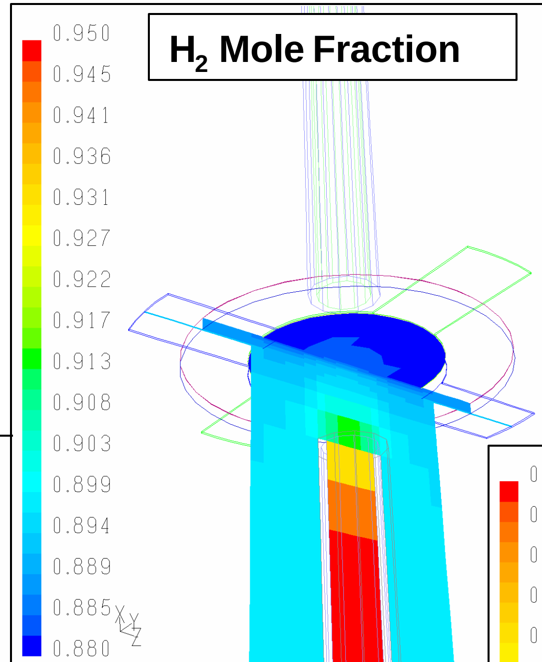
Average Current Density: 1A/cm2

Cell Temperature: 800C / 1073K

Anode Side Temperature

Validation Application: Button Cell

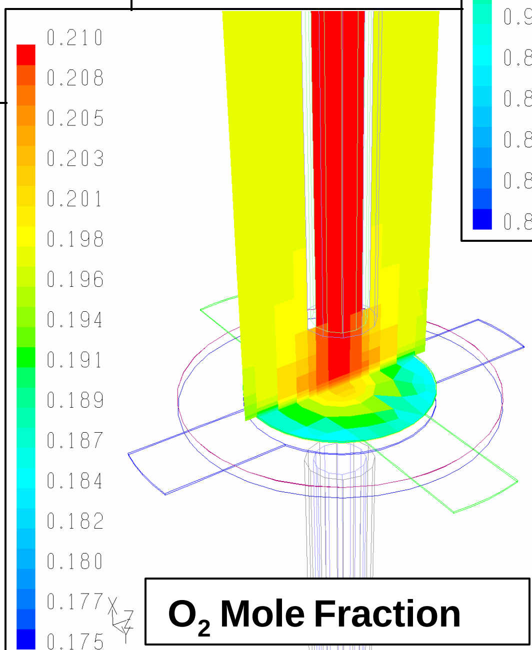


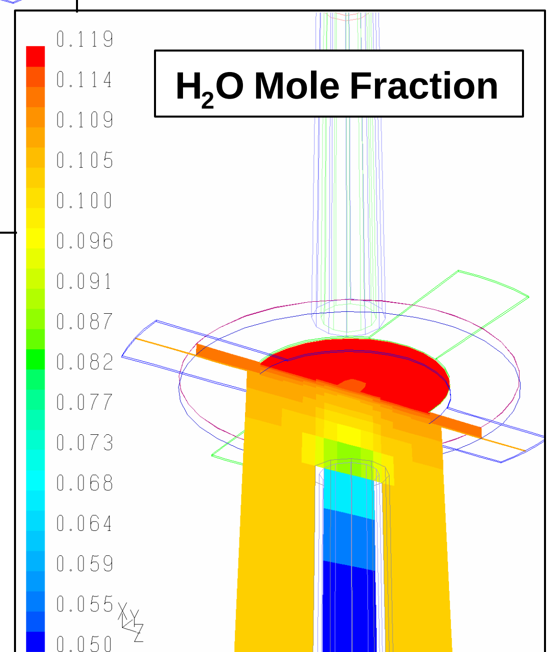


Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

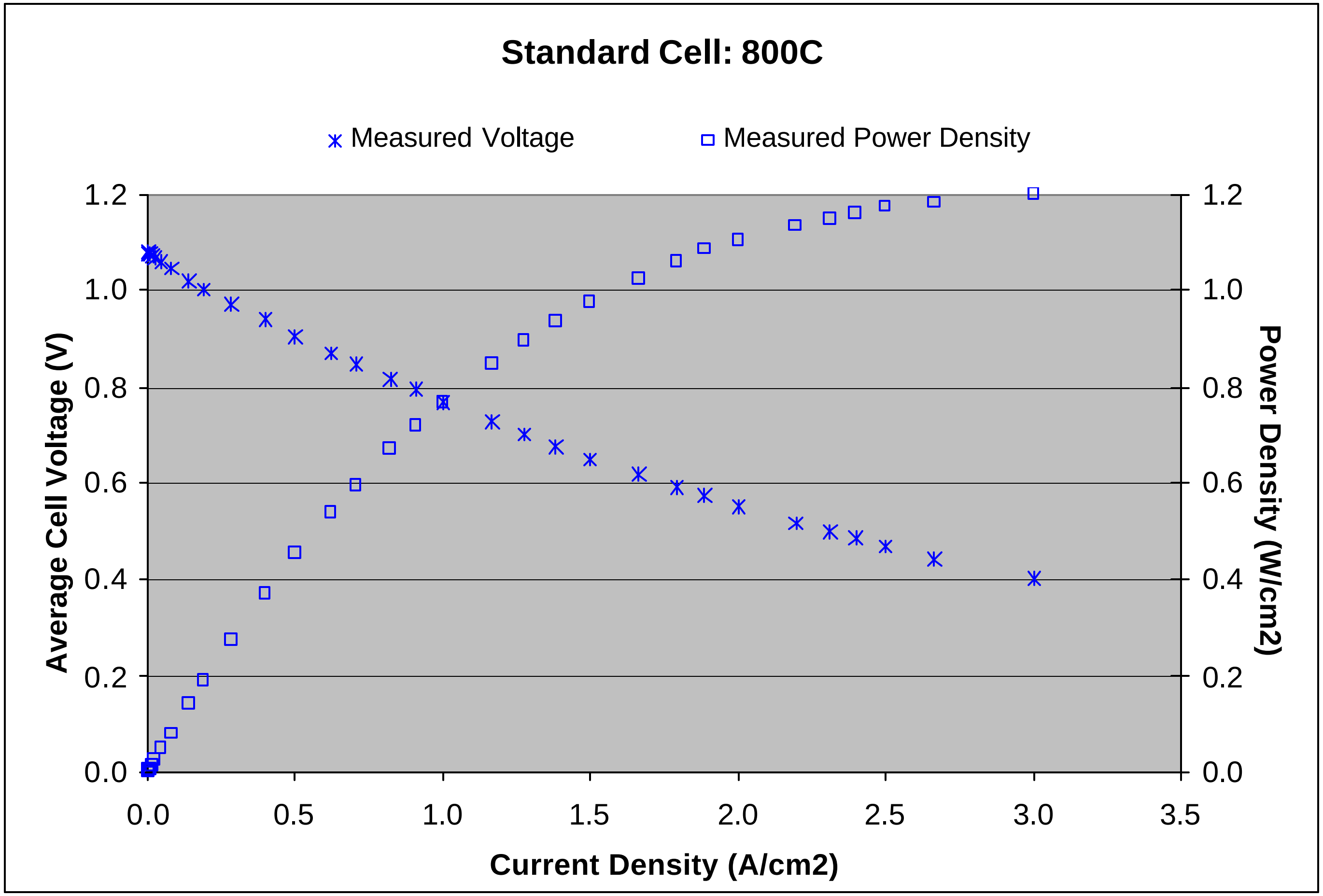
Cell Temperature: 800C / 1073K



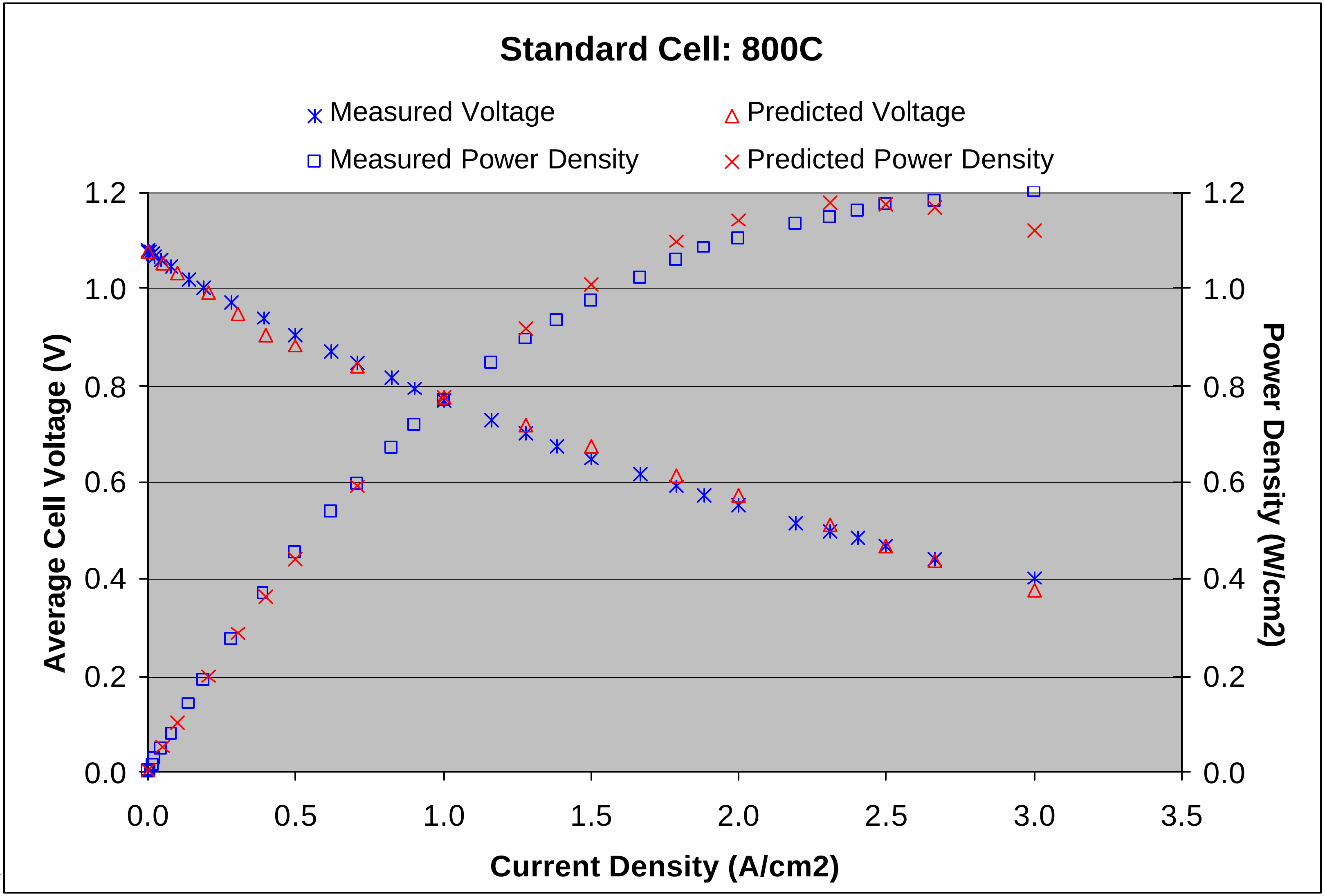


Validation Application: Button Cell

- **Validate models with experimental data**
- **Data from tests by Virkar et al., May 2002**



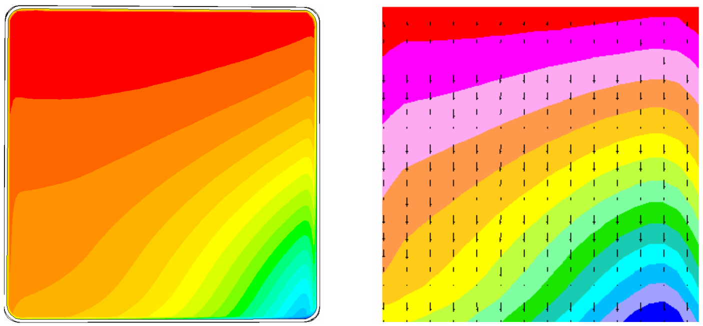
Validation Application: Button Cell



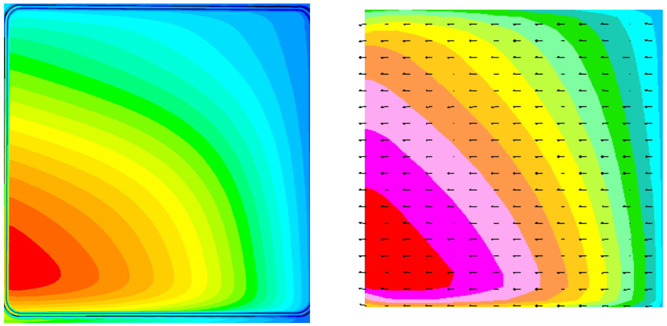
Compare NETL and PNNL Models

- **Comparison of NETL SOFC model with PNNL SOFC model was performed**
  - Proprietary cell geometry was used for comparison
  - Qualitative agreement was good between the models
  - Models give consistent predictions for planar geometry

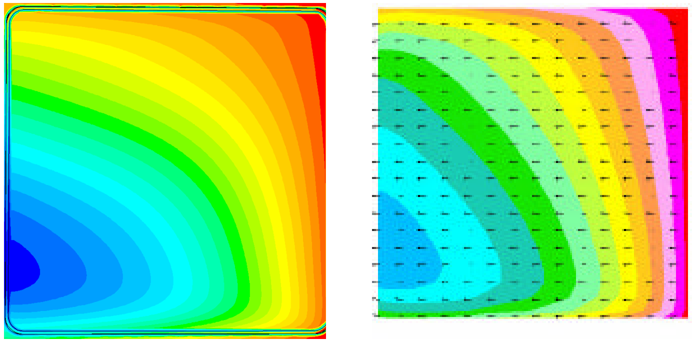
Compare NETL and PNNL Models



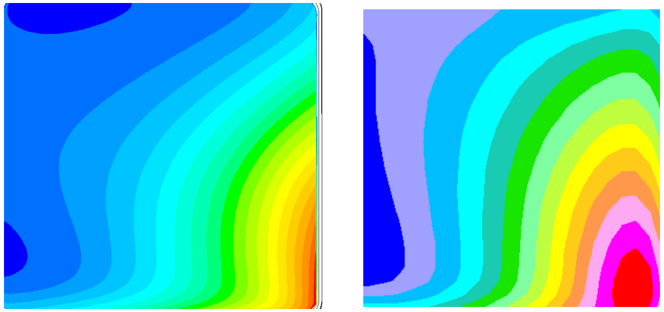
O_2 Concentration at electrolyte face



H_2O Concentration at electrolyte face



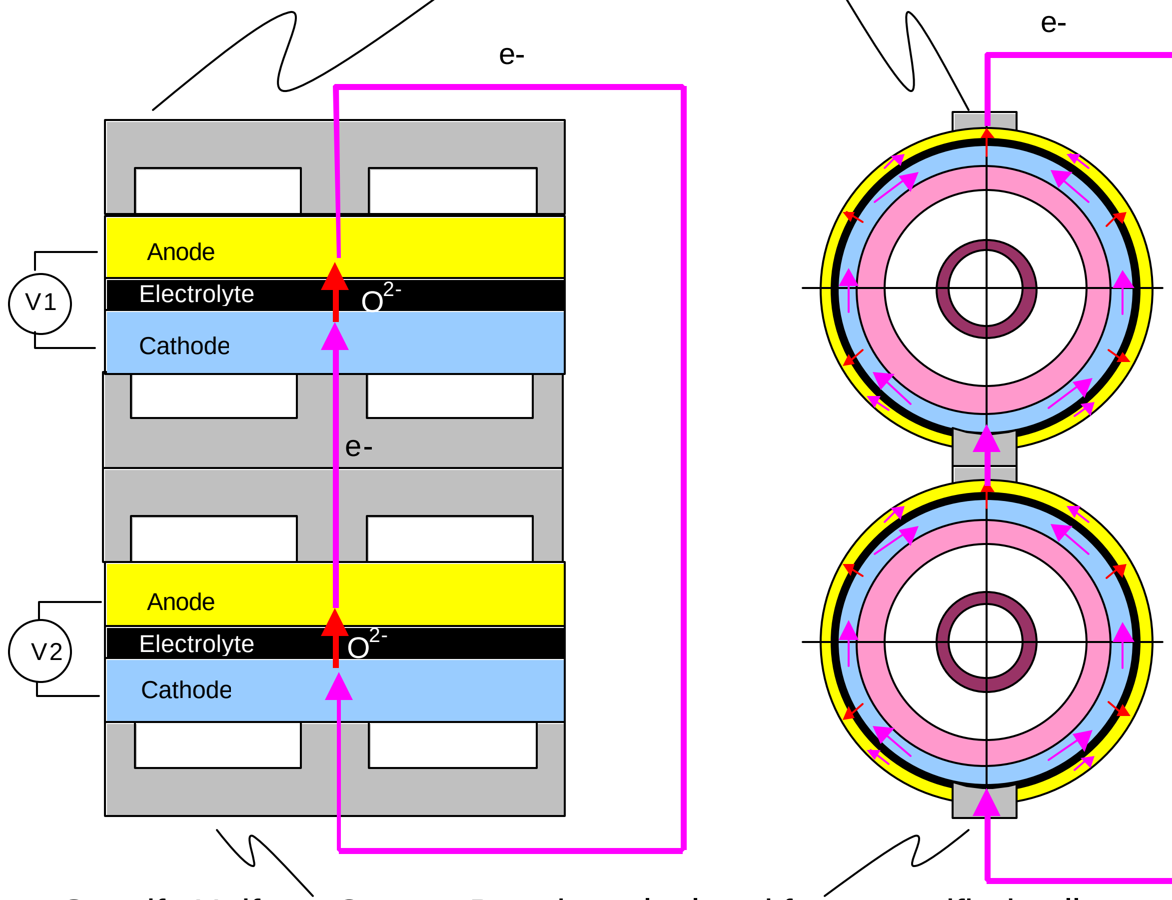
H_2 Concentration at electrolyte face



Current Density at electrolyte face

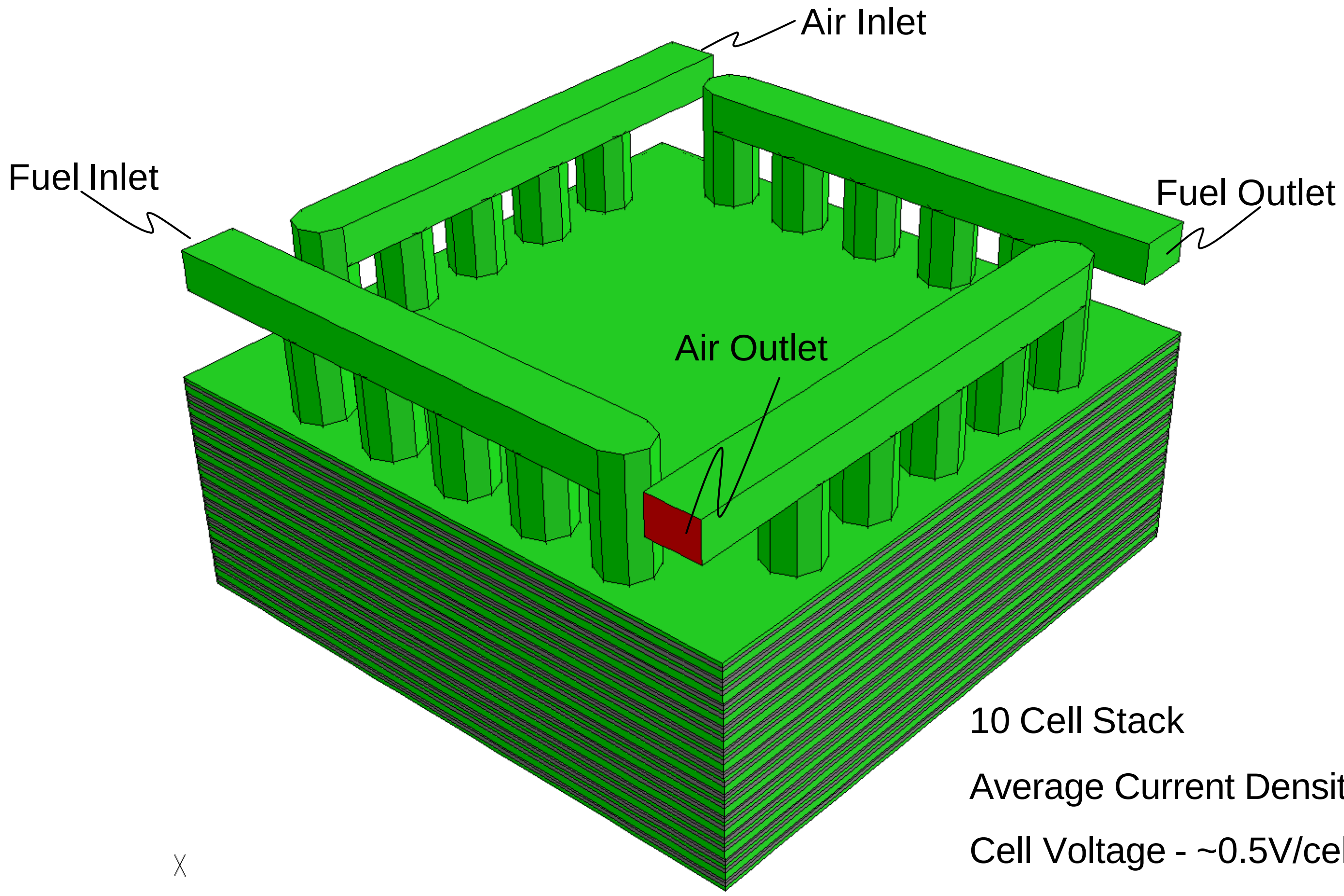
Model Overview: Extend to Stack

Specify Uniform Voltage



Specify Uniform Current Density calculated from specified cell current and area

Model Overview: Extend to Stack



10 Cell Stack

Average Current Density - 5000 A/m^2 (0.5A/cm^2)

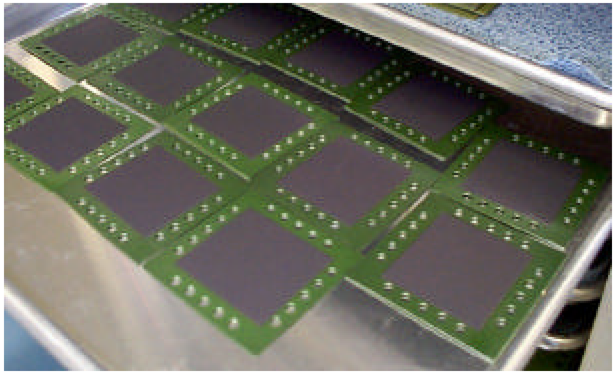
Cell Voltage - ~0.5V/cell

H2 Utilization - 80%

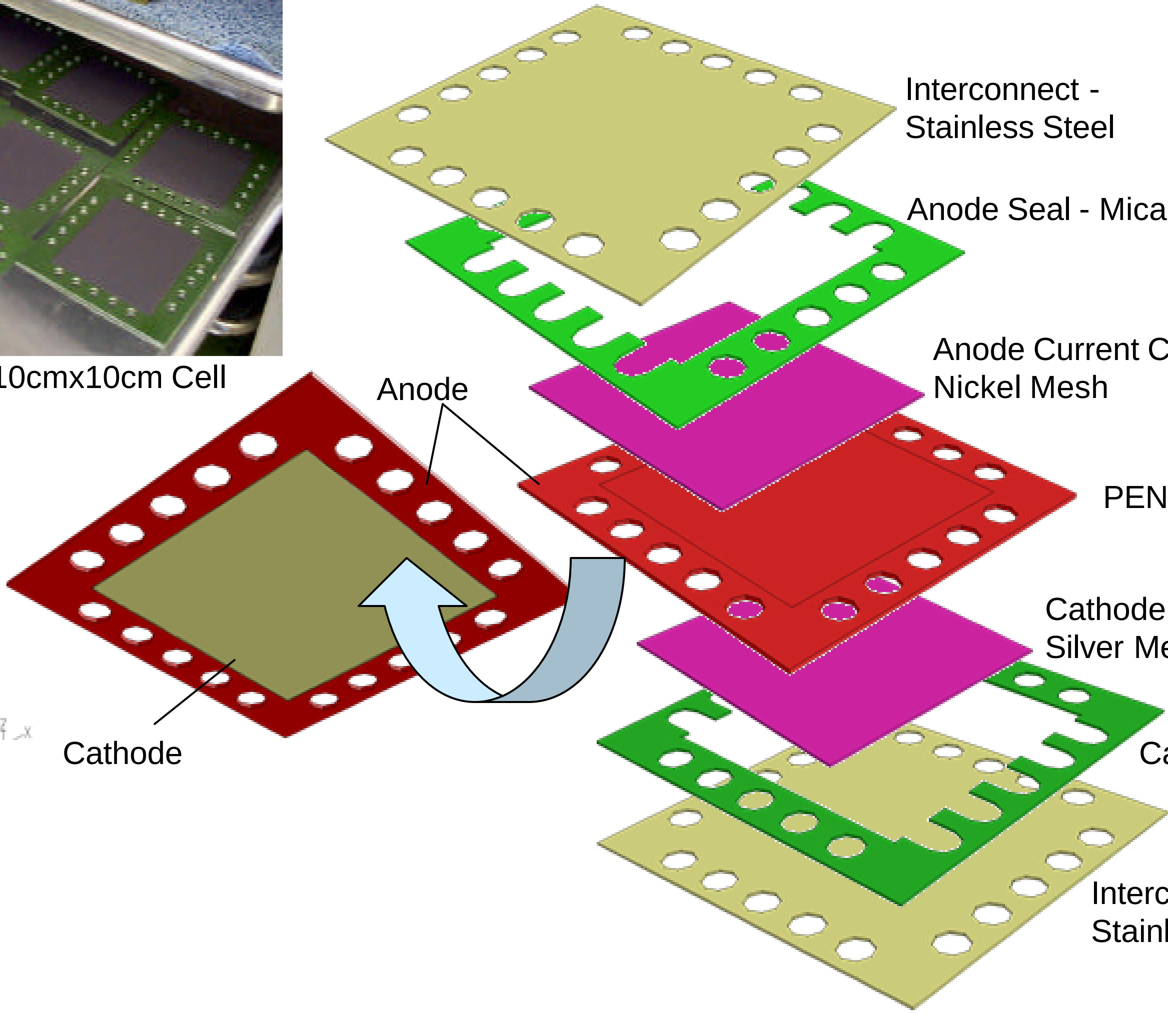
O2 Utilization - 20%

80 W stack

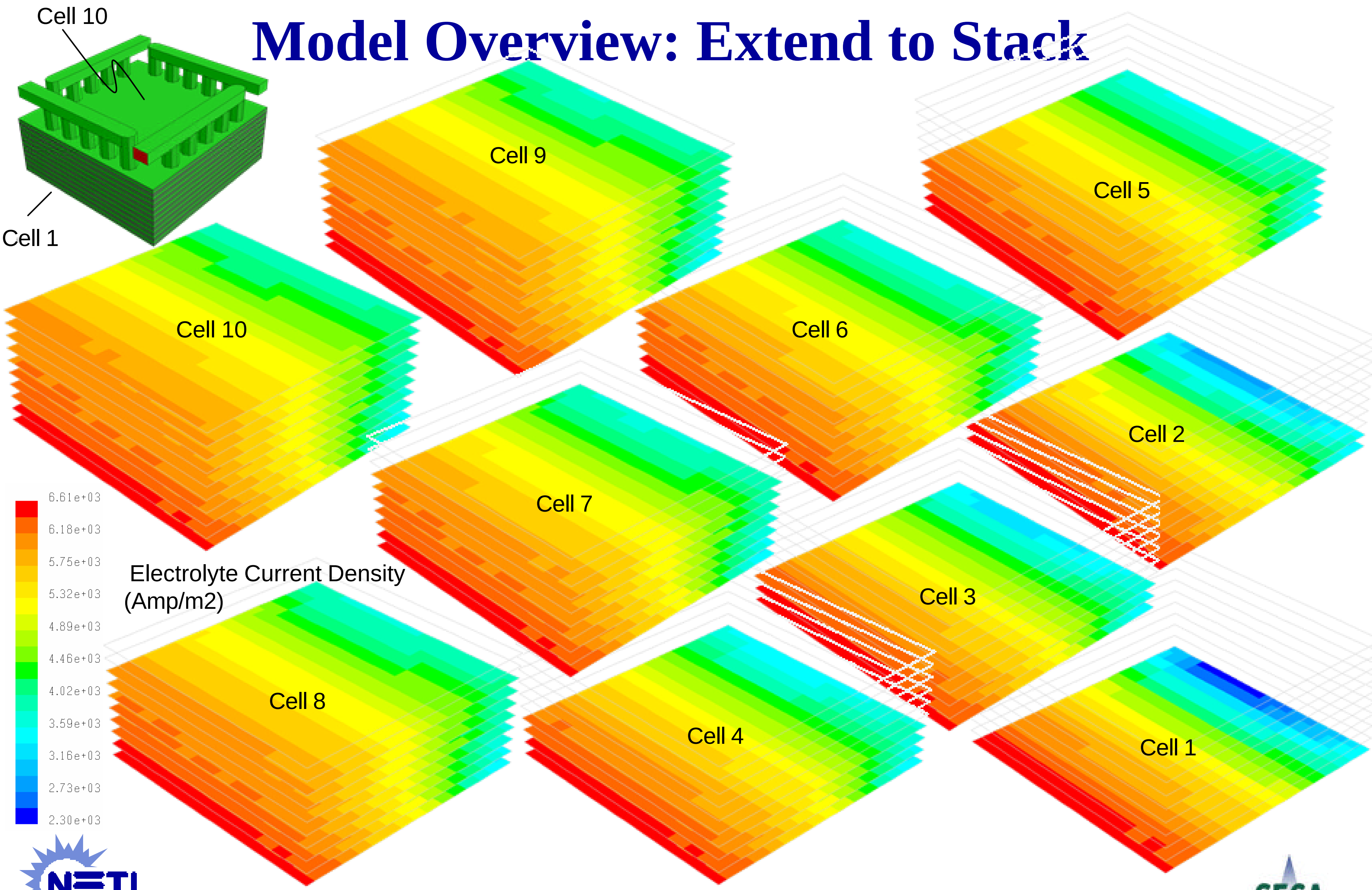
Model Overview: Extend to Stack



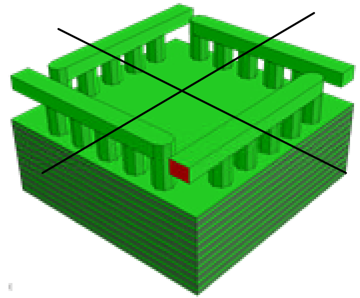
Cell based on U of U 10cmx10cm Cell

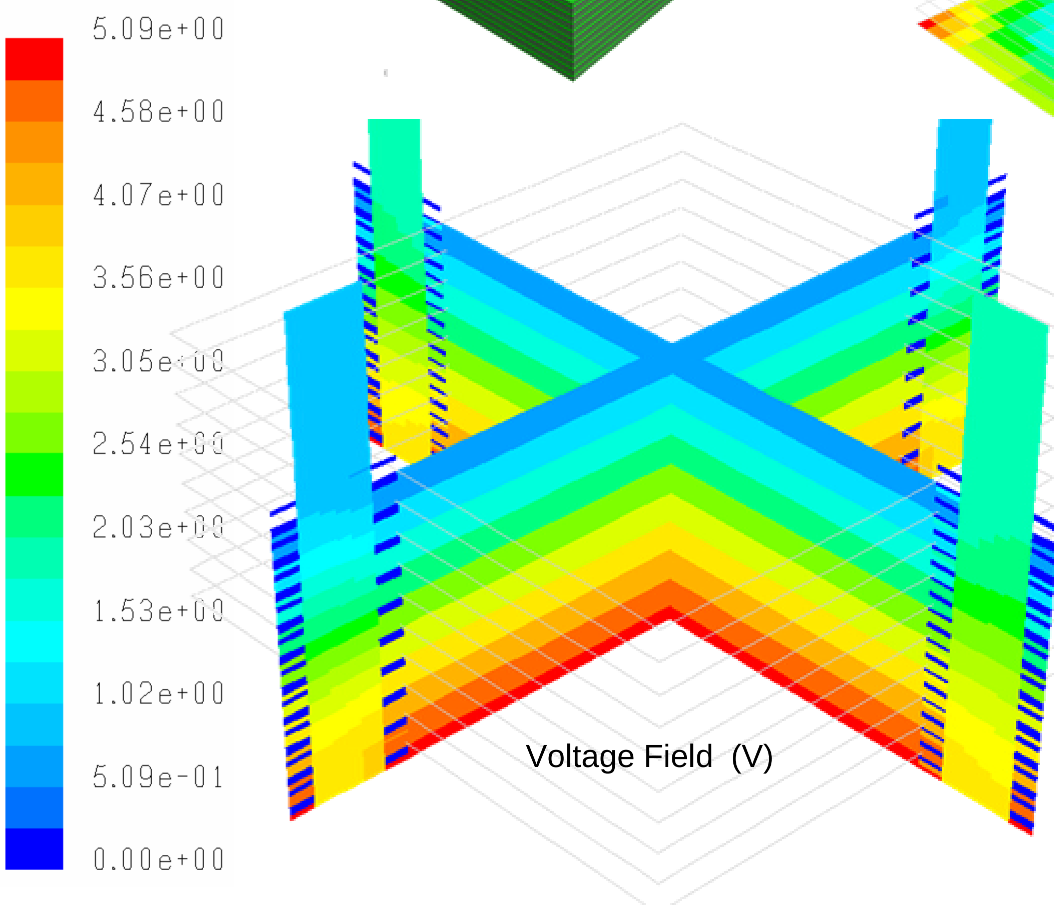


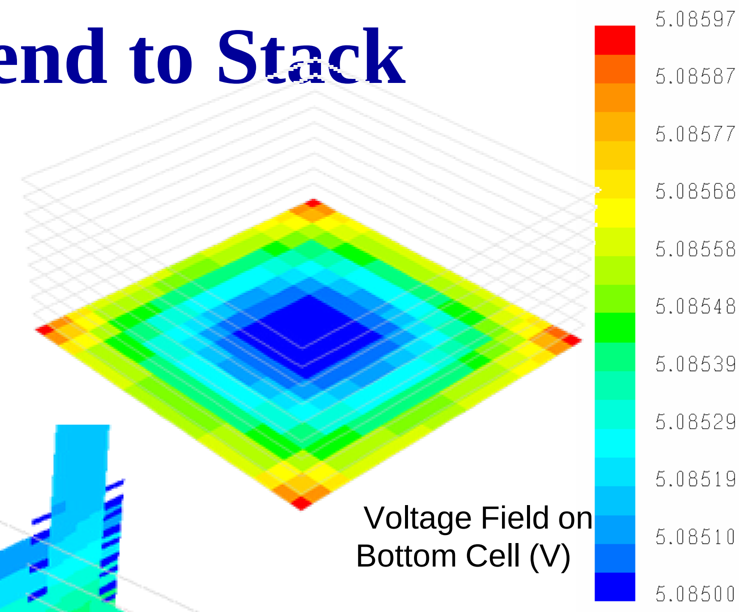
Model Overview: Extend to Stack



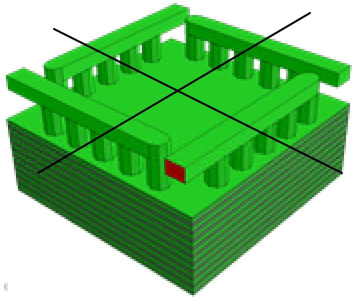
Model Overview: Extend to Stack

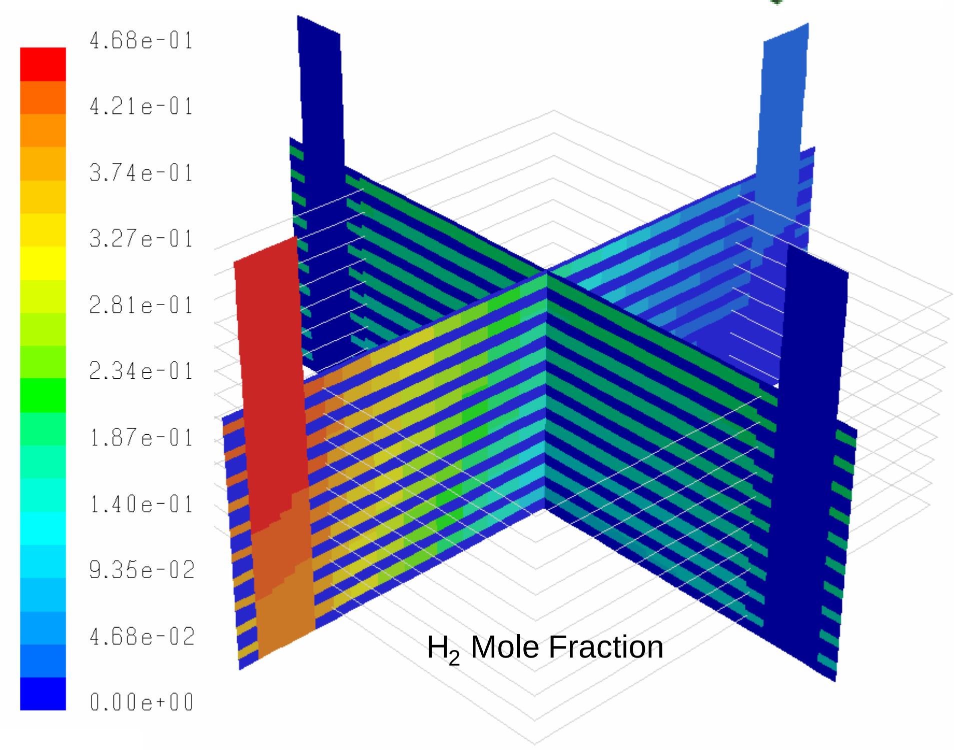


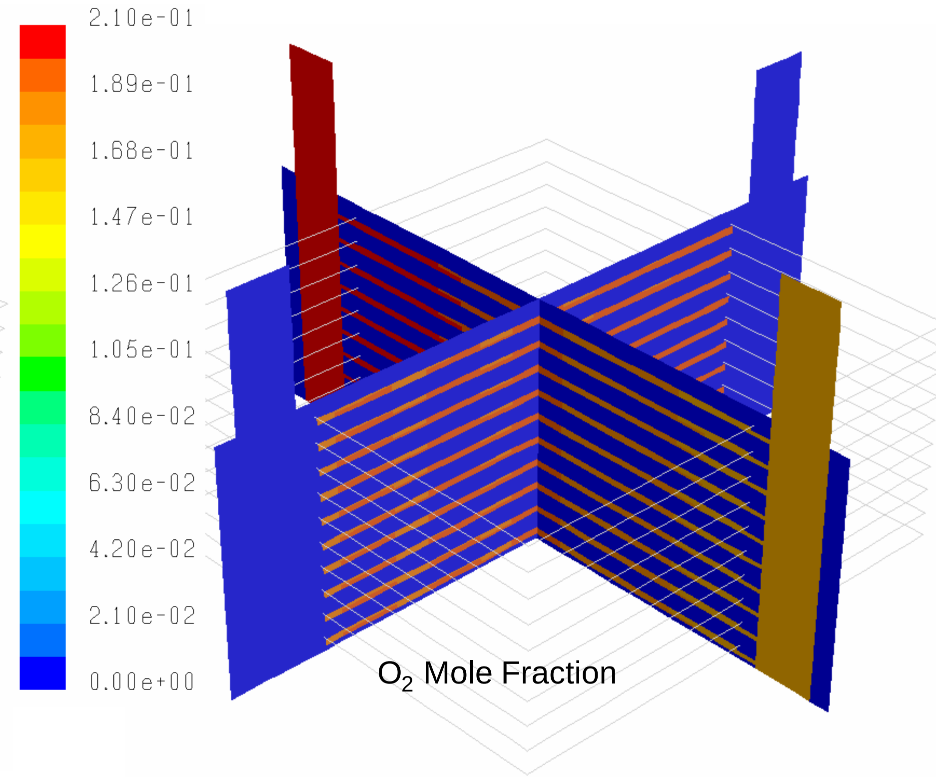




Model Overview: Extend to Stack







Collaborations

- **Collaborations to date**
  - PNNL
    - Comparison of SOFC models
    - Core Technology Plans for Simulation and Modeling
  - Delphi
    - Application of NETL Model to SECA cell geometry
  - University of Utah
    - U of U supplying data and test cells for model validation
  - National Research Council Canada
    - Discussion for potential collaboration on modeling and visualization

FY 03 Work Plans

- **NETL SOFCEL Test Facility**
  - Facility Startup, Shakedown
  - Button Cell Tests
    - Vary anode, electrolyte, cathode thickness
    - Vary Anode Porosity
    - Measure Sensitivity of data to experimental parameters
  - 10cm x 10cm Cell Testing

FY 03 Work Plans

- **Model Development Activities**
  - Complete Parallel Version of the NETL Model
  - Add Internal Methane Reforming Chemistry
  - Add Water-Gas Shift
  - Complete Implementation of Stack Model
  - Implement Transient Capability

FY 03 Work Plans

- **Model Validation Activities**
  - Data from NETL Testing and Validation Facility
    - Button cell data
    - 10cm x 10cm cell data
    - Validation data over range of geometry, compositions, operating conditions
  - Data from University of Utah
  - Data from SECA developers
    - Planar data
    - Tube data

FY 03 Work Plans

- **Apply the Model - collaborate with SECA development team members**
  - Siemens-Westinghouse Power Corporation
  - GE Power Systems

- **Link NETL SOFC Model with ANSYS**
  - validation
  - application

FY 03 Work Plans

- **Work with PNNL, ORNL under Core Technology Program**
  - model development
  - material properties
  - technology transfer to SECA developers
  - SECA Core Technology

- **Publish**