SECA Core Technology Program

NETL Fuel Cell Modeling Program: Development, Validation, and Application

June 19, 2002

NETL Fuel Cell Modeling Program

- **NETL Participants:**
  - Randall Gemmen   Christopher Johnson
    Richard Pineault   William Rogers ……………………….……….**DOE**
  - Michael Prinkey   Mehrdad Shahnam…………………………… **Fluent Inc.**
  - Edward Robey   Richard Addis……………………………….. **Parsons**

- **University of Utah Participants:**
  - Anil V. Virkar
  - Yi Jiang
  - Feng Zhao

Technical Issues Addressed

- **Development of detailed CFD-based model of Solid Oxide Fuel Cell and Stack**
  - detailed modeling of fluid flow, heat transfer, electrochemistry, electrical potential fields in cell and stack
- **Couple SOFC model with FEM model for stress analysis in cell/stack**
  - output of CFD-based model used for ANSYS analysis of cell/stack stresses
- **Validate models with experimental data**
  - compare models to data from well-characterized cells and stack to validate accuracy of model predictions
- **Support use of models by SECA Industry teams**
  - provide models to Industry teams and support use of the model, correct bugs, provide model enhancements if needed

R&D Objectives and Approach

- **Development of detailed CFD-based model of Solid Oxide Fuel Cell and Stack**
  - Use commercial CFD code as underlying platform for detailed fuel cell model - FLUENT
    - FLUENT code is parallel, unstructured mesh, with well-validated models for fluid flow, heat transfer, species transport detailed modeling of fluid flow, heat transfer, electrochemistry, electrical potential fields in cell and stack
  - Model Capabilities
    - 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

R&D Objectives and Approach

- **Couple SOFC model with FEM model for stress analysis in cell/stack**
  - geometry and temperature field output from SOFC model can be input directly into ANSYS
  - Work closely with ANSYS to make the coupling process easier
    - Especially important for transient simulation of stress

R&D Objectives and Approach

- **Validate models with experimental data**
  - Compare models to data from well-characterized cells and stack to validate accuracy of model predictions
  - Data from literature
  - Data from SECA Industry Teams, and Core Technology participants
  - SOFC test facility at NETL for detailed cell and stack measurements
    - Multiple test stands for short and long-term testing
  - Collaboration with University of Utah, Department of Materials Science and Engineering
  - UU will provide anode-supported test specimens with
    - Controlled microstructure - variable anode porosity
    - Range of anode, cathode, and electrolyte thickness
  - UU to test cells and supply preliminary performance data

R&D Objectives and Approach

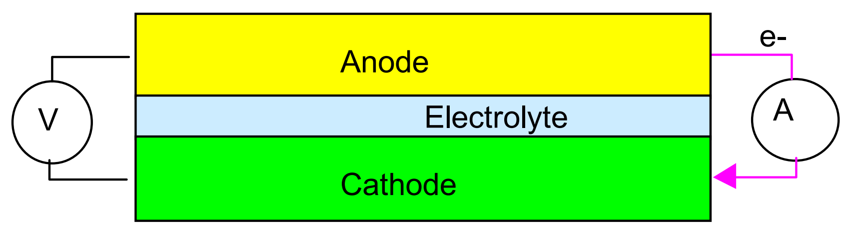
- **Support use of models by SECA Industry teams**
  - Provide models to Industry teams and support their use of the model
  - Correct bugs found during model validation and application of the models
  - Provide model enhancements if needed
  - Typical agreement in form of Memorandum of Collaboration
    - Proprietary data is protected
    - Publish collaborative work

Results

- **Development of detailed CFD-based model of Solid Oxide Fuel Cell and Stack**
  - H_2 and CO electrochemistry implemented
    - Oxidation rate of CO and H_2 is proportional to ratio of local partial pressures

$$3H_2 + 3O^{2-} \Rightarrow 3H_2O + 6e^-$$

$$CO + O^{2-} \Rightarrow CO_2 + 2e^-$$



$$2O_2 + 8e^- \Rightarrow 4O^{2-}$$

$$V_{Nernst} = E^o + \frac{R_u T}{8F} \ln\left(\frac{P_{H_2}^3 P_{CO} P_{O_2}^2}{P_{H_2O}^3 P_{CO_2} P_{tot}^2} \right)$$

Results

- **Development of detailed CFD-based model of Solid Oxide Fuel Cell and Stack**
  - The diffusion coefficient for binary gas mixtures is given by the following equation

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

  - 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:

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

  - where p is the permeation factor = porosity/tortuosity

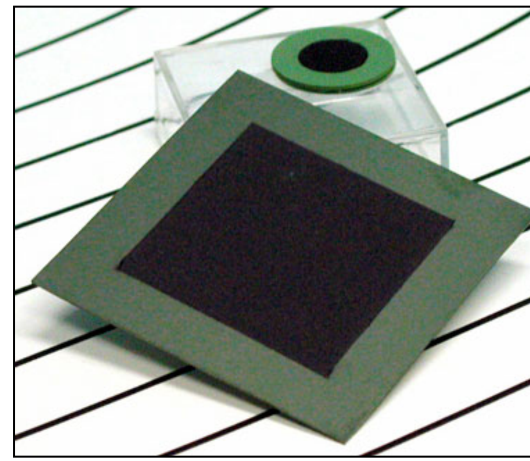
Results

- **Validate models with experimental data**
  – NETL SOFC test facility construction is 95% complete

  – Collaboration is underway with University of Utah, Department of Materials Science and Engineering - Dr. Anil Virkar and team

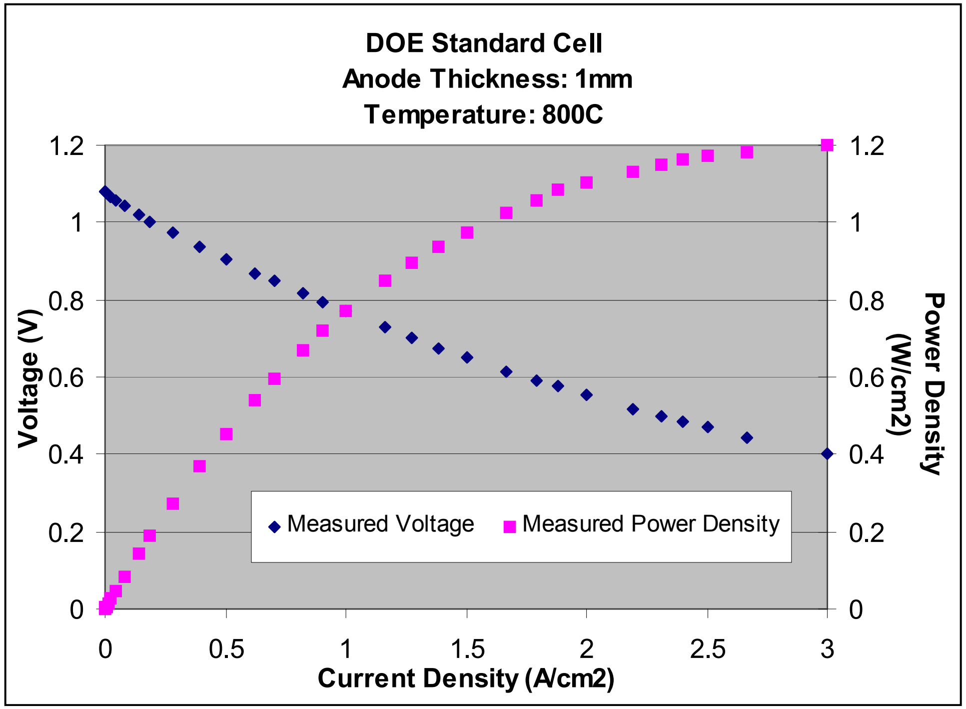
  – UU has provided anode-supported test specimens
    - "Standard" cell has been supplied
      - YSZ electrolyte, ~7-10 microns thick
      - LSM+YSZ Interlayer, ~20 microns thick
      - LSM Cathode Layer, ~50 microns thick
      - Ni + YSZ Interlayer, ~20 microns thick
      - Ni + YSZ Anode Support Layer, ~1mm thick

    - Cells with range of anode thickness have been supplied
      - Anode thicknesses of 0.5mm, 1mm, 1.5mm, 2.5mm
      - Other specifications same as standard cell

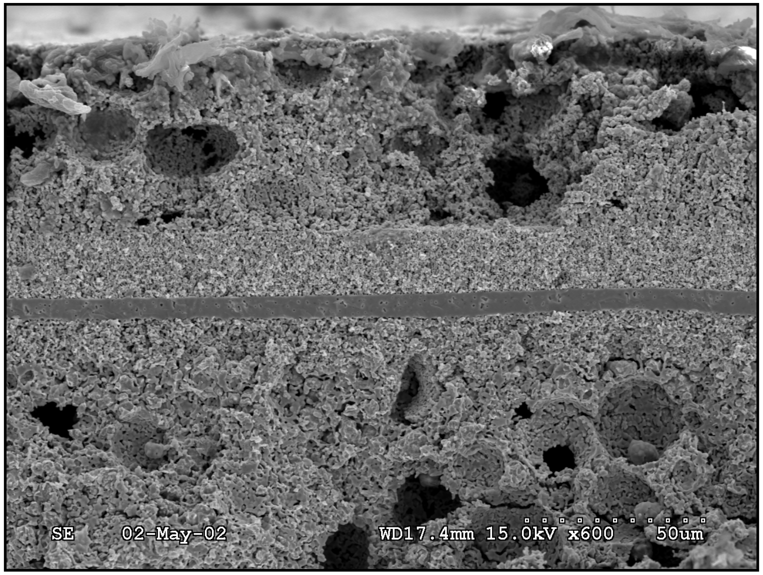


Results

- **Validate models with experimental data**
  - UU has tested cells and supplied representative performance data

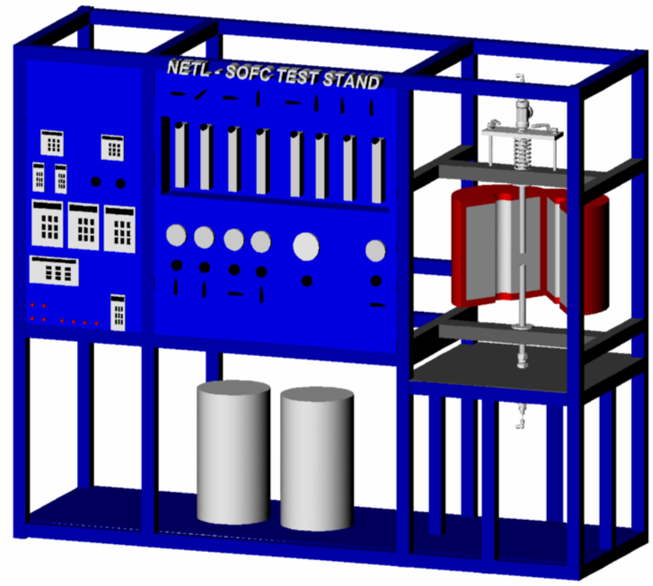


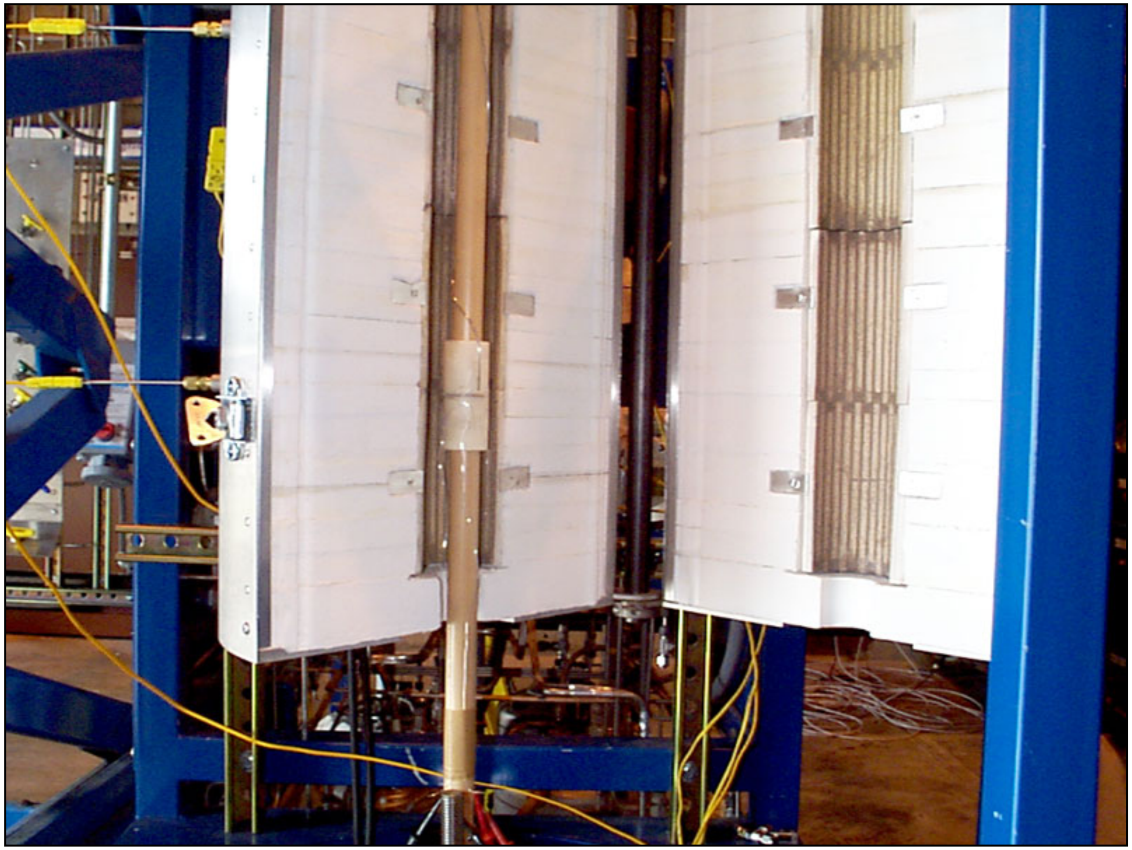
SEM of Standard Button Cell



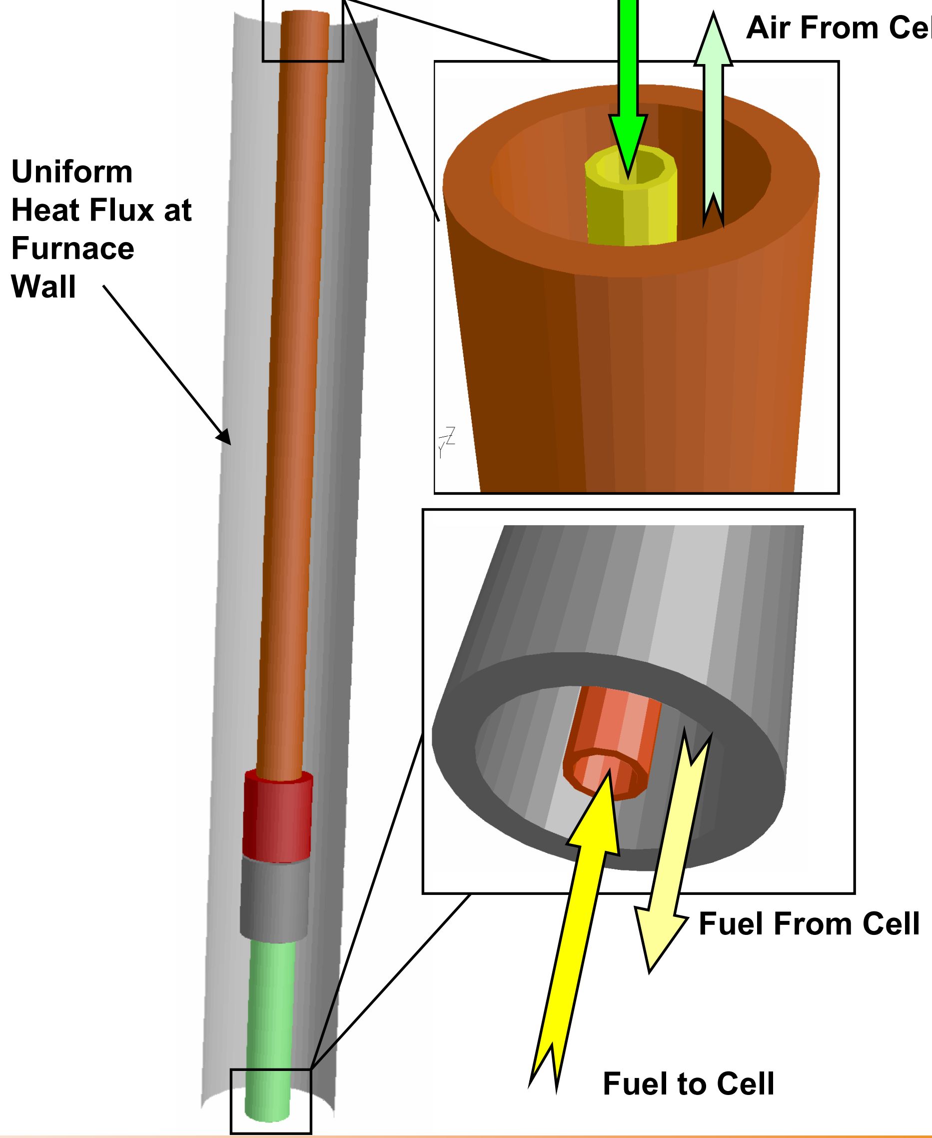
Results

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



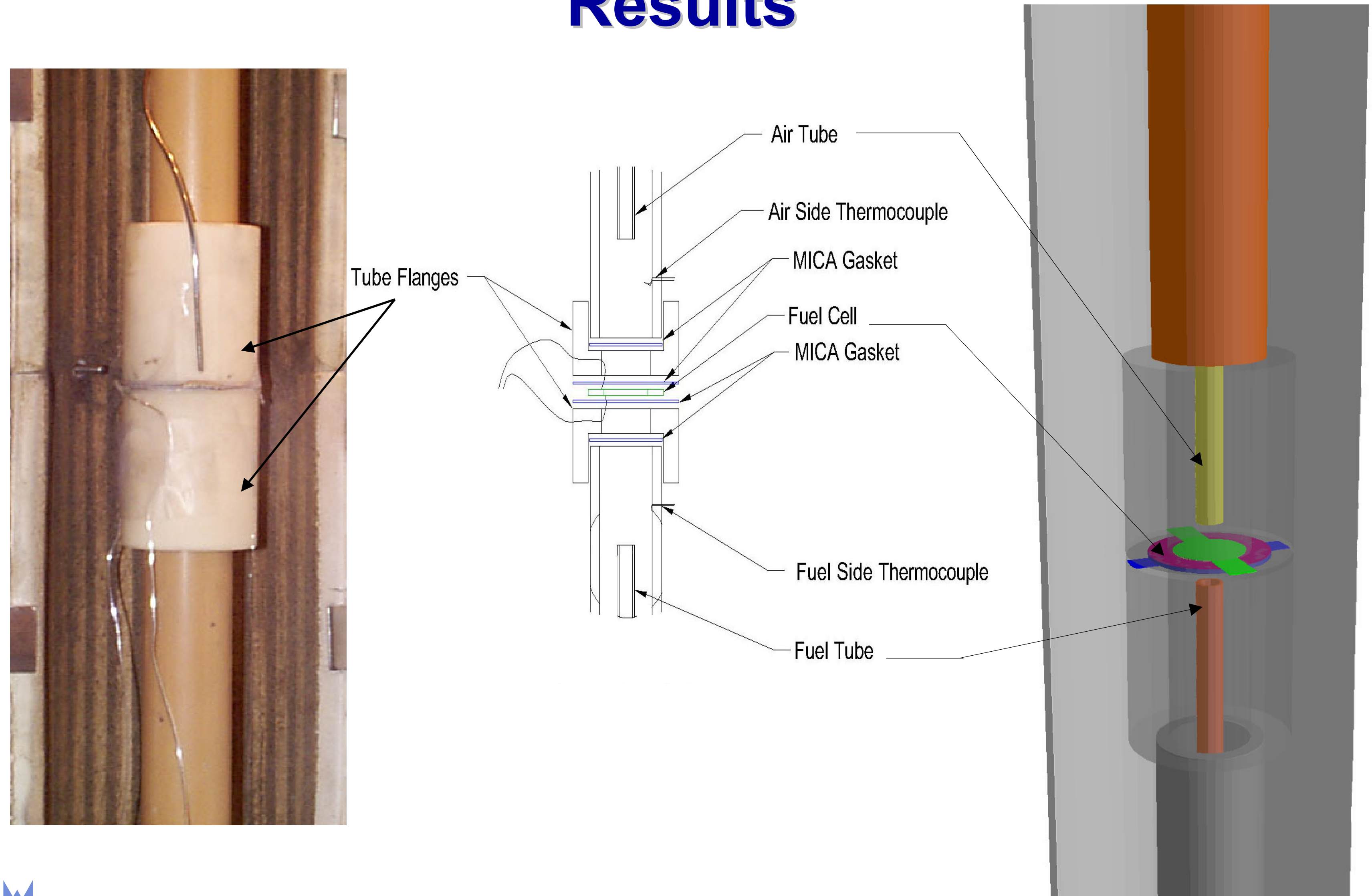


Results



Air to Cell
Air From Cell
Uniform Heat Flux at Furnace Wall
Fuel From Cell
Fuel to Cell

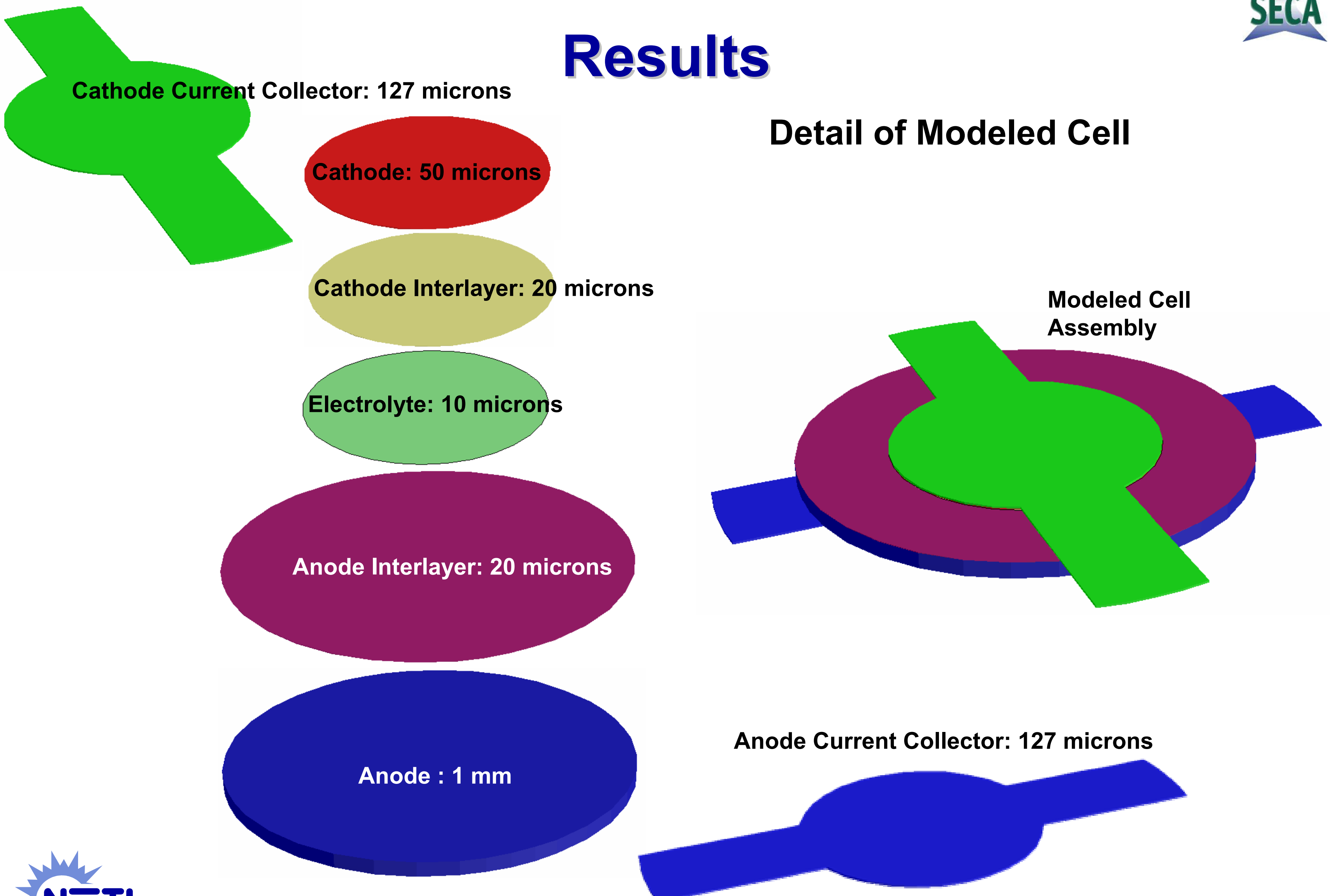
Results



Tube Flanges
Air Tube
Air Side Thermocouple
MICA Gasket
Fuel Cell
MICA Gasket
Fuel Side Thermocouple
Fuel Tube

Results

Detail of Modeled Cell



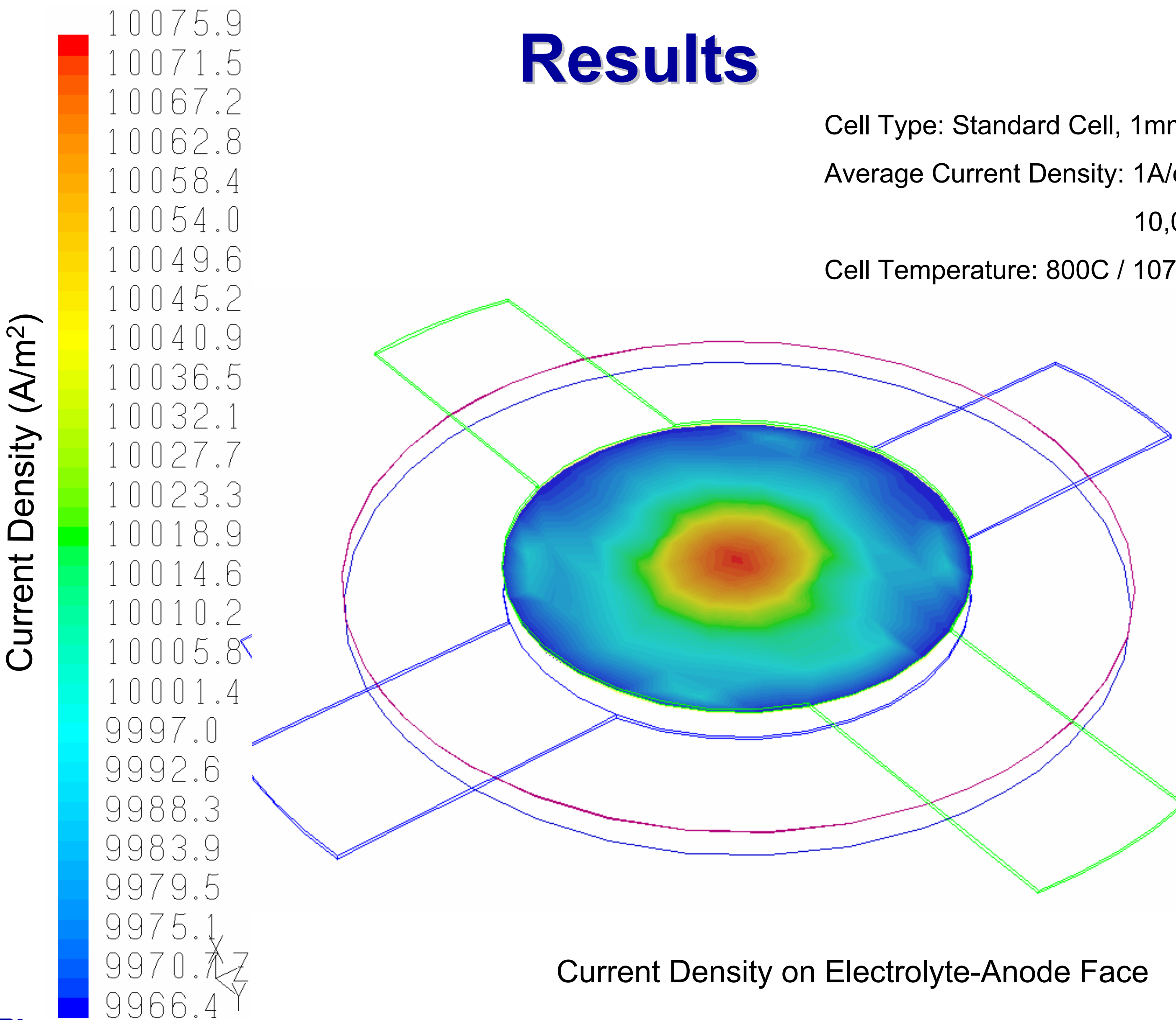
Results

Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

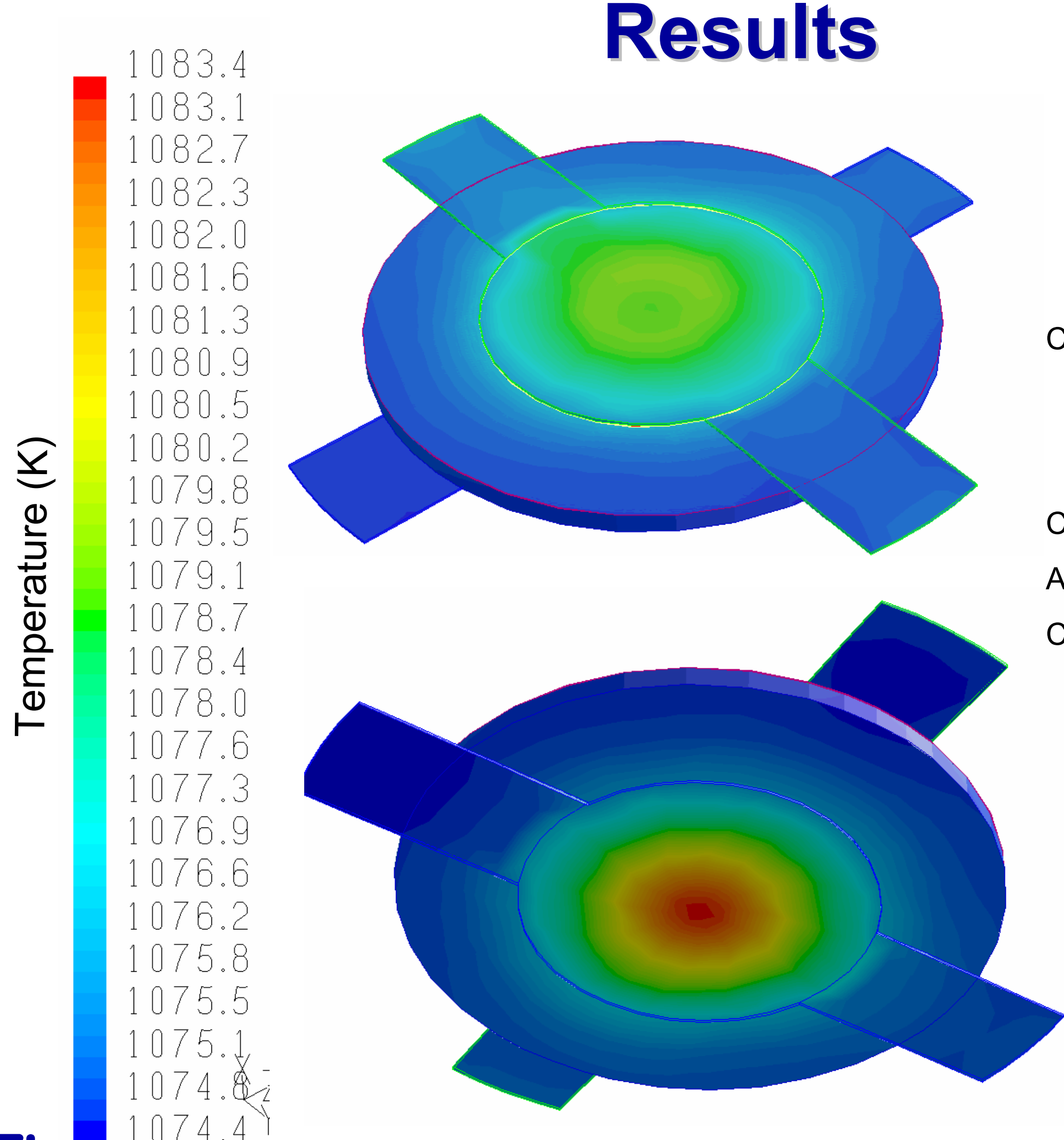
10,000A/m2

Cell Temperature: 800C / 1073K



Current Density on Electrolyte-Anode Face

Results



Cathode Side Temperature

Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

Cell Temperature: 800C / 1073K

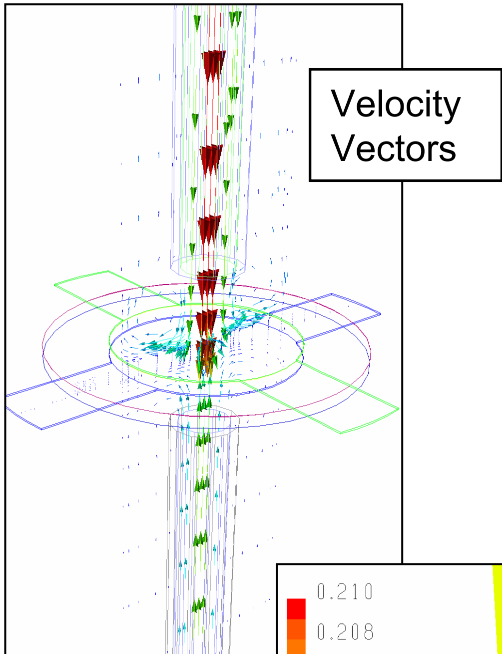
Anode Side Temperature

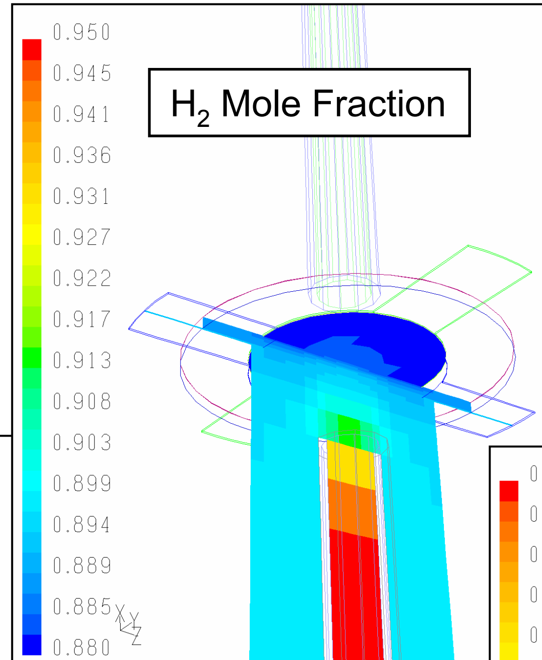
Results

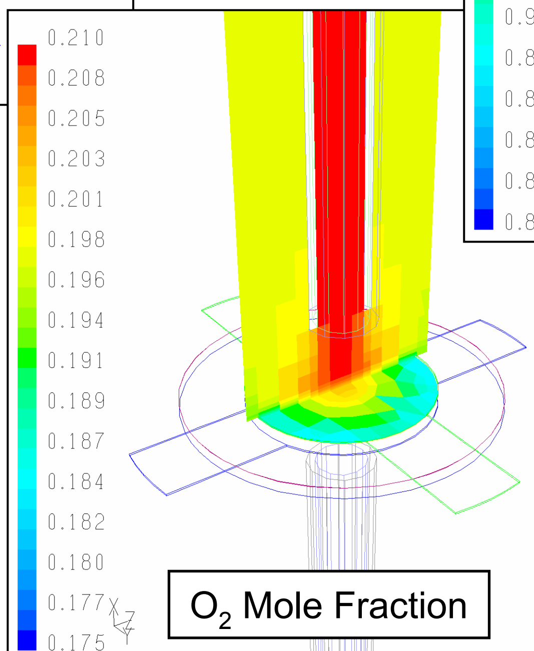
Cell Type: Standard Cell, 1mm Anode

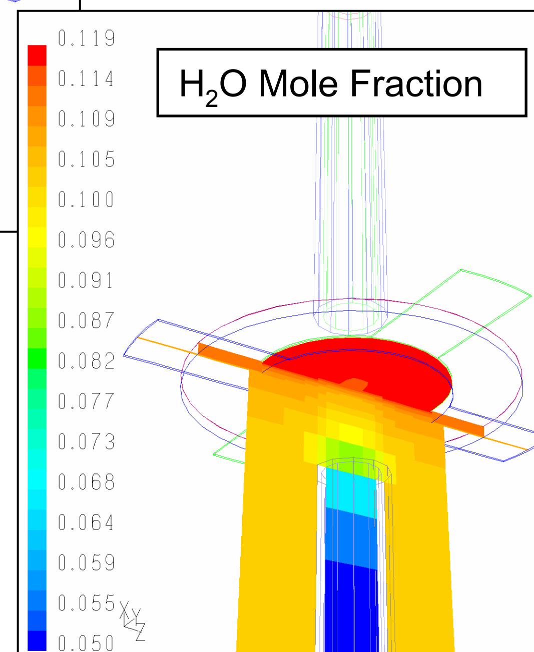
Average Current Density: 1A/cm2

Cell Temperature: 800C / 1073K



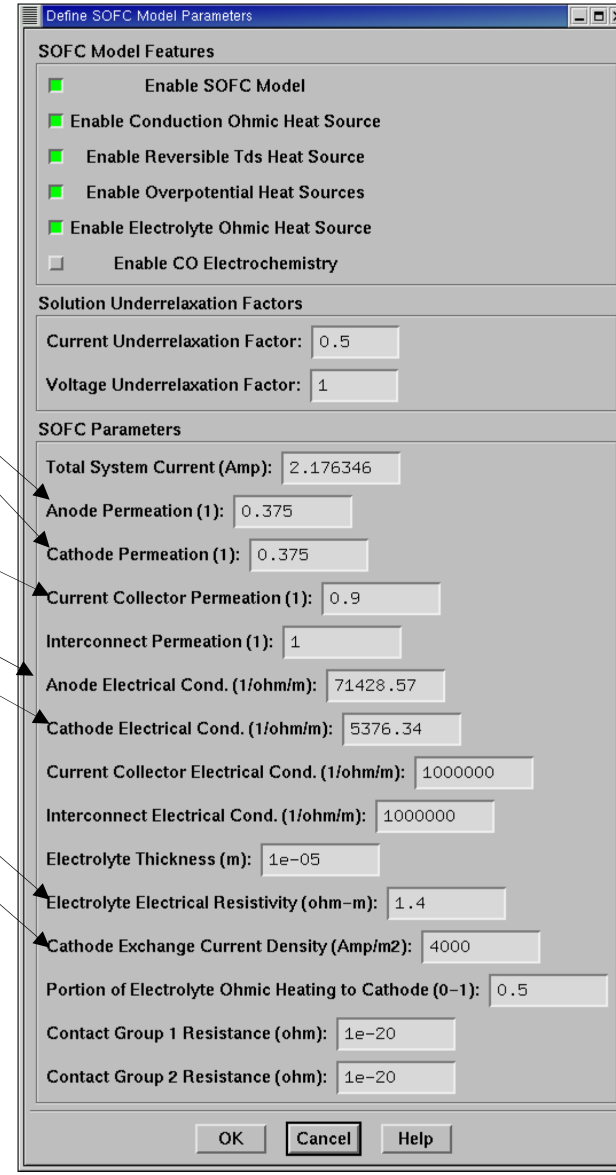






Results

- **Validate models with experimental data**
  - Generate VI curve with SOFC model, compare to UU data
  - Unknown cell physical parameters required for model
    - Anode and Cathode Permeation (porosity/tortuosity)
    - Current Collector Permeation
    - Anode Electrical Conductivity
    - Cathode Electrical Conductivity
    - Electrolyte Resistivity
    - Cathode Exchange Current Density



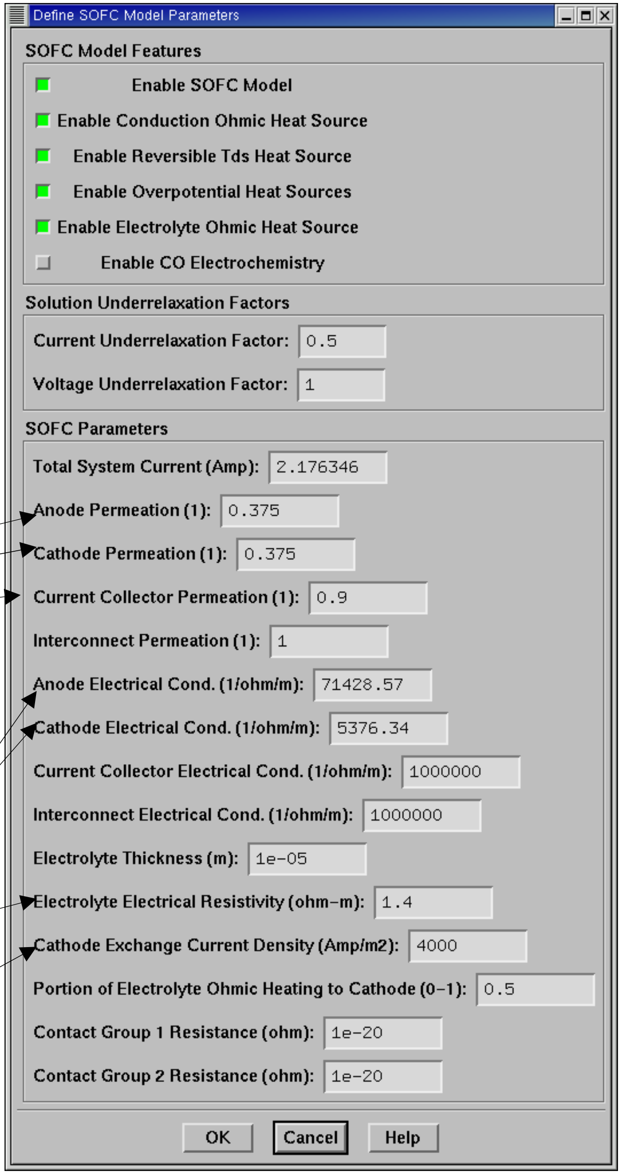
  - Most of these values will be measured for the test cells for model validation
  - ***This is "preliminary" validation effort - this data has just become available from U. of Utah***

Results

- **Validate models with experimental data**
  - Generate VI curve with SOFC model, compare to UU data
  - Unknown cell physical parameters required for model
    - Anode and Cathode Permeation (porosity/tortuosity)
    - Current Collector Permeation
    - Anode Electrical Conductivity
    - Cathode Electrical Conductivity
    - Electrolyte Resistivity
    - Cathode Exchange Current Density

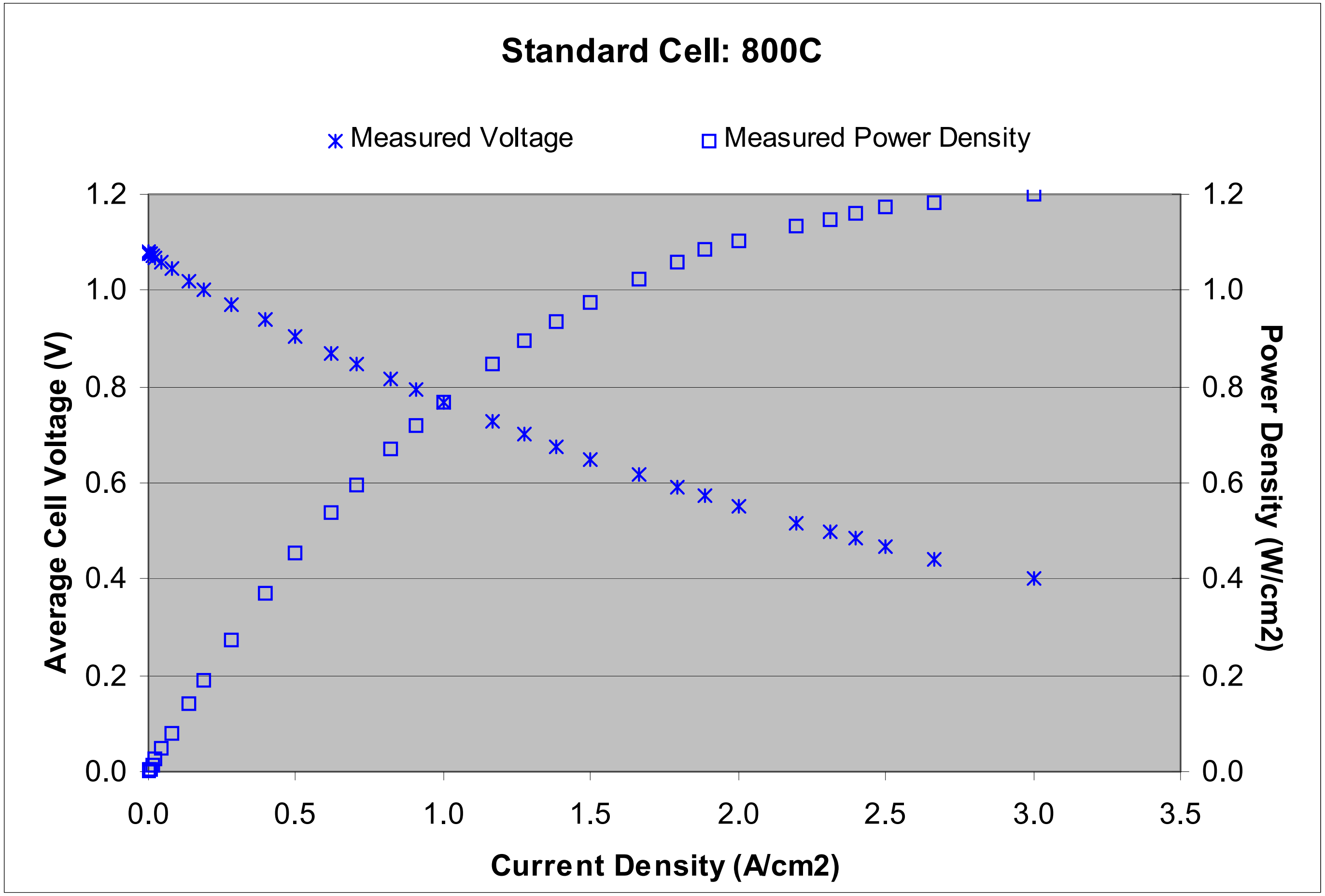
For this preliminary effort:

- Assume permeation values
  - Excess fuel and oxidizer in the experiments, little effect of permeation observed in model predictions
- Use values for anode/cathode conductivity from literature
- Set electrolyte resistivity to match measured voltage at highest current density data point on VI curve
- Assume Cathode Exchange Current Density



Results

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



Results

- Validate models with experimental data
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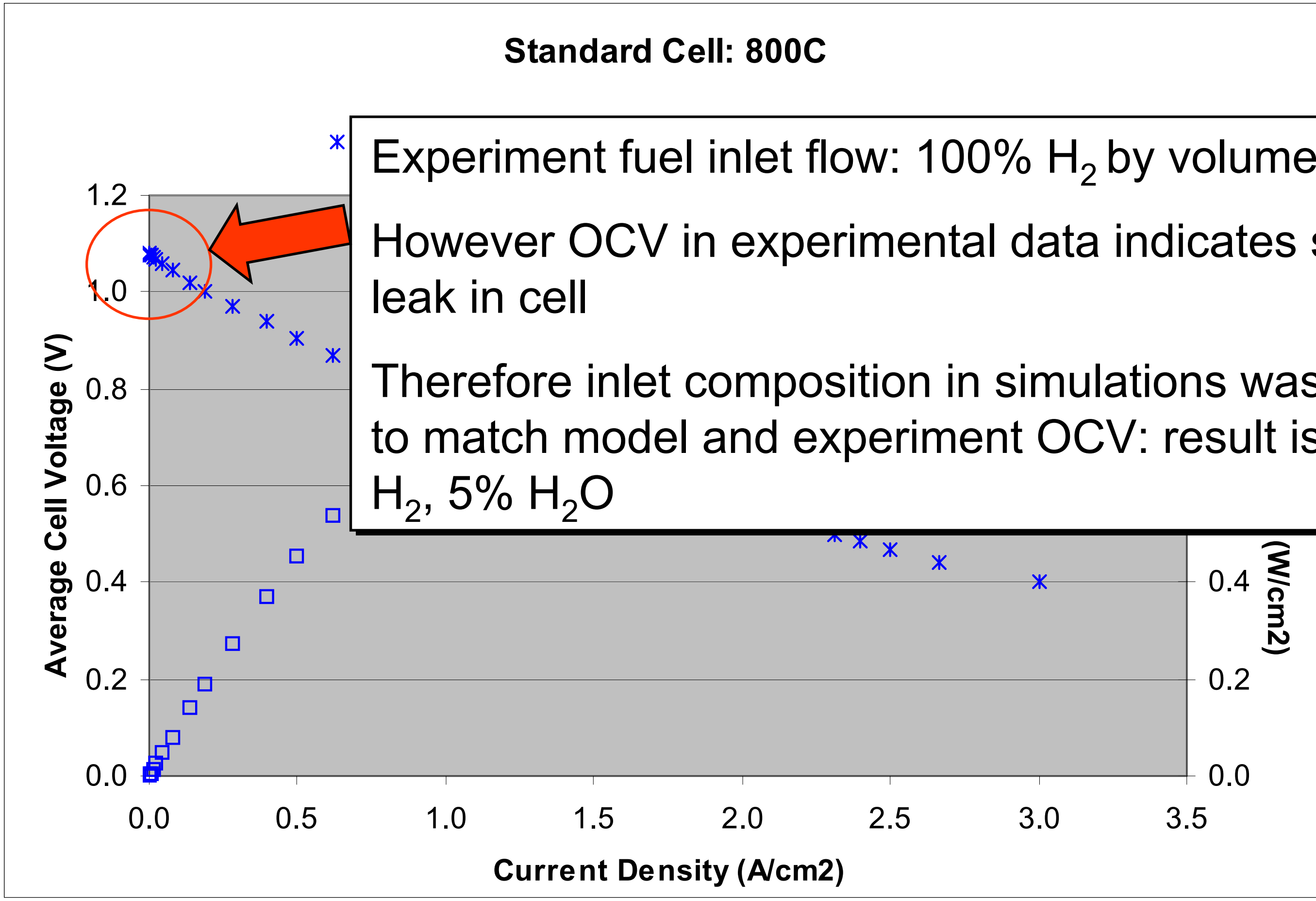


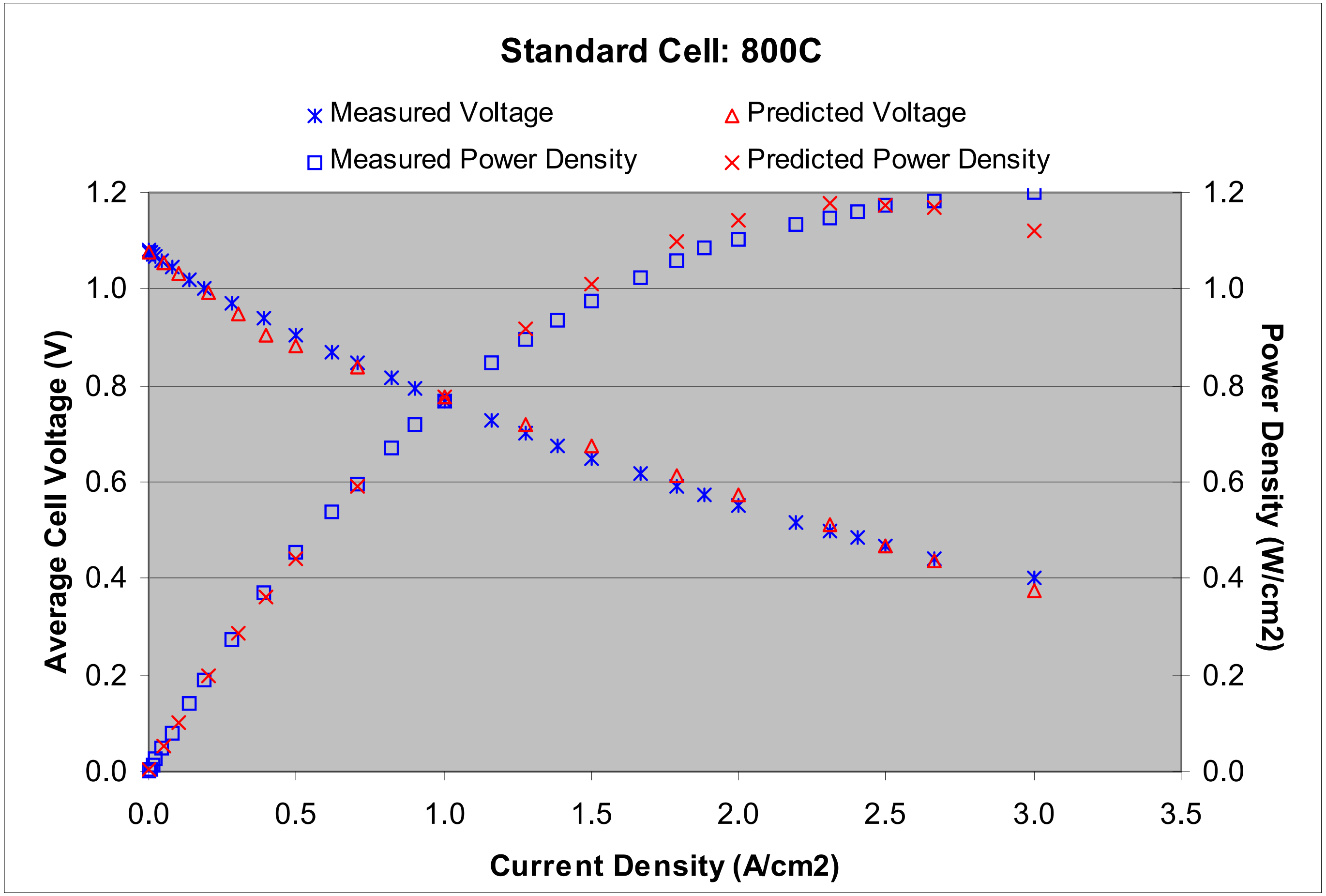
Experiment fuel inlet flow: 100% H_2 by volume

However OCV in experimental data indicates slight leak in cell

Therefore inlet composition in simulations was set to match model and experiment OCV: result is 95% H_2, 5% H_2O

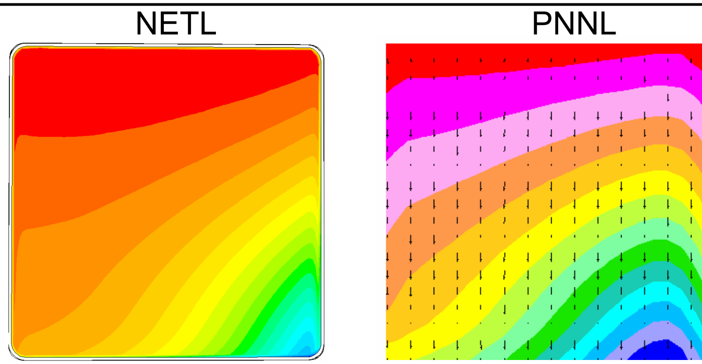
Results

- **Validate models with experimental data**
- **Comparison of Data and Simulation - Standard Cell**

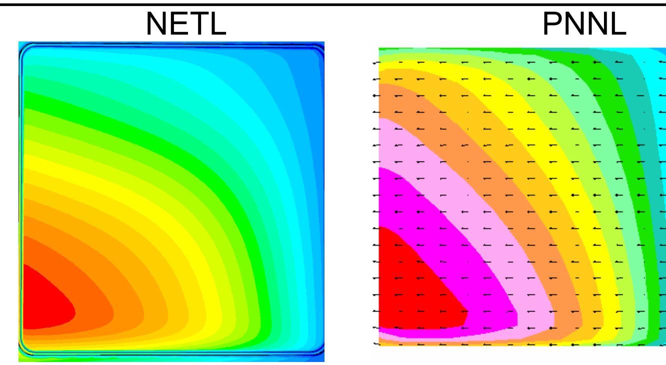


Results

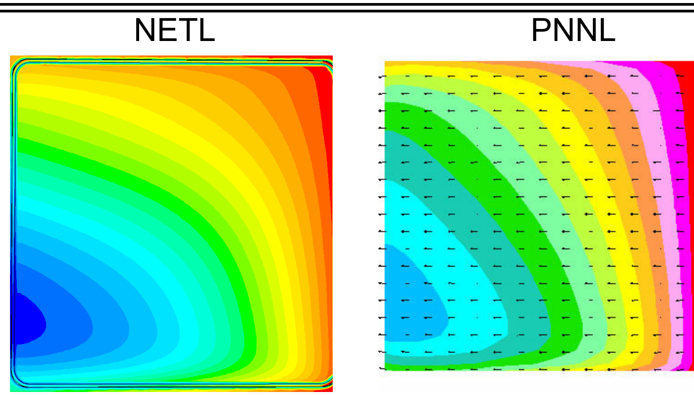
- **Validate models with experimental data**
  - Comparison of NETL SOFC model with PNNL SOFC model was performed
  - Proprietary cell geometry was used for comparison
  - Qualitative agreement was good between the models



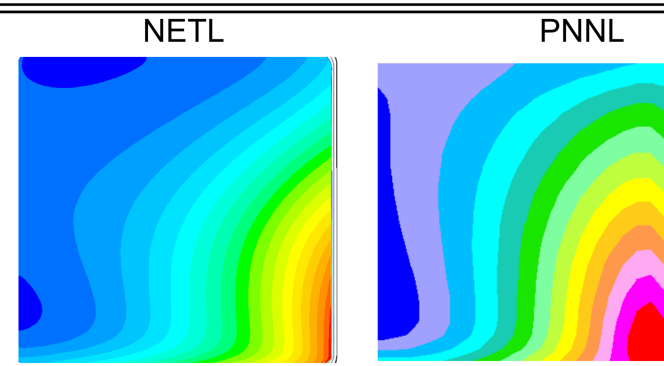
O_2 Concentration at electrolyte face



H_2O Concentration at electrolyte face



H_2 Concentration at electrolyte face



Current Density at electrolyte face

Results

- **Support use of models by SECA Industry teams**
  - ***Memorandum of Collaboration*** has been signed between Siemens Westinghouse Power Corporation and NETL
    - Signed 5/29/02
  - Collaboration to improve SOFC modeling and provide SWPC with a validated model to assist in SECA development activities
  - NETL SOFC model validation with SWPC tube data
    - demanding application for electrical field model
    - excellent configuration to validate all model capabilities
  - NETL SOFC model customization for SWPC applications
  - Provide NETL SOFC model to SWPC and support its use

Applicability to SOFC Commercialization

- **Accurate and detailed models will be useful for cell and stack design**
  - accurate modeling capability will be cost effective tool for industrial teams
  - value of CFD-based models has been proven in aerospace, automobile, HVAC, and chemical process industries
- **Industrial Teams have already exhibited interest in helping to validate and use these models in their development programs**
- **CFD companies are interested in model commercialization and long-term user support**
- **Evolving technology**
  - Better computer hardware
  - More accurate models
  - Faster models

Activities for Next 6-12 Months

- **Contact Resistances - more accurate electrical field (3 month)**
  - current collector-electrode
  - electrode-electrolyte
  - current collector-interconnect
- **Extend Single Cell Model to Stack Model (6 month)**
  - Parallel implementation for speed
- **Transient Capability (6 month)**
- **Implement Internal Reforming Model (6 month)**
- **Continue Model Validation Activities (ongoing)**
  - NETL SOFC facility
  - University of Utah collaboration
  - Siemens Westinghouse Power Corporation Collaboration