SECA Core Technology Program

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

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Goals and Objectives

- **Develop robust and accurate modeling tools capable of *detailed* fuel cell and stack performance analysis**

- **Develop SOFC test facility for testing of small-scale cells and stacks**
  - use well-characterized test specimens
  - produce detailed data for model validation

- **Extensive validation of SOFC models**
  - data from open literature
  - data from NETL test facility
  - data from SECA partners

- **Apply these new tools toward development of new/novel fuel cell concepts that can achieve the SECA goals**
  - support SECA developers

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

NETL SOFC Model Capabilities

- **Electrochemical SOFC submodel**
  - H_2 and CO Electrochemistry
- **Electrical field submodel to calculate electrical potential field in conducting regions**
  - Ohmic heat generation
  - Current Flow
- **Species diffusion in flow channels and in porous media in development**
- **Water-Gas Shift Reaction**
- **Parallel Code**
- **Couple model data to ANSYS FEA code**

Planned Capabilities and Validation

- **Stack Model**
- **Internal Reforming**
- **Contact Resistances**
  - current collector-electrode
  - electrode-electrolyte
  - current collector-interconnect

- **Model Validation**
  - Data from open literature
  - Data from NETL testing facilities
  - Data from SECA partners

NETL SOFC Model Overview

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

NETL SOFC Model Overview

- **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

- **Models for activation losses are also available for each electrode**
  - account for chemical kinetics

Overpotential Corrections to Nernst

$$E_{cor} = \Delta V = N - \eta_R - \eta_{CC} - \eta_{CA} - \eta_{AC} - \eta_{AA}$$

Ohmic Losses:

$$\eta_R = R \cdot i$$

Diffusion Losses:

$$\eta_C = -\frac{R_u T}{nF} \ln\left(1 - i / i_L\right)$$

Chemical Kinetics:

$$i = i_o \left[\exp\left(\frac{\alpha \eta_A F}{R_u T} \right) - \exp\left(\frac{(1-\alpha)\eta_A F}{R_u T} \right) \right]$$

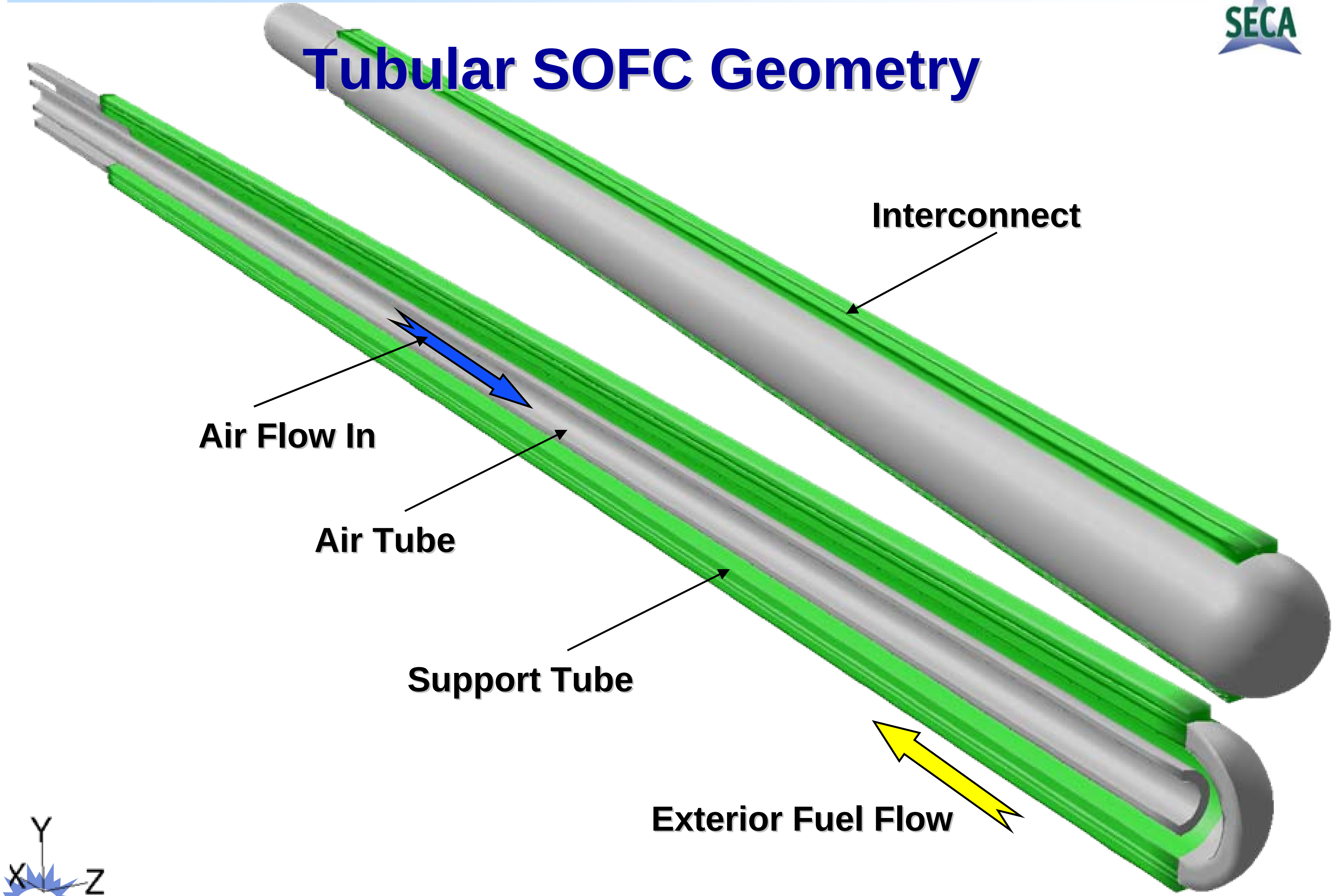
NETL SOFC Model
Non-Proprietary Examples

- Tube Geometry
- Crossflow - Monolith
- Single - Channel Monolith

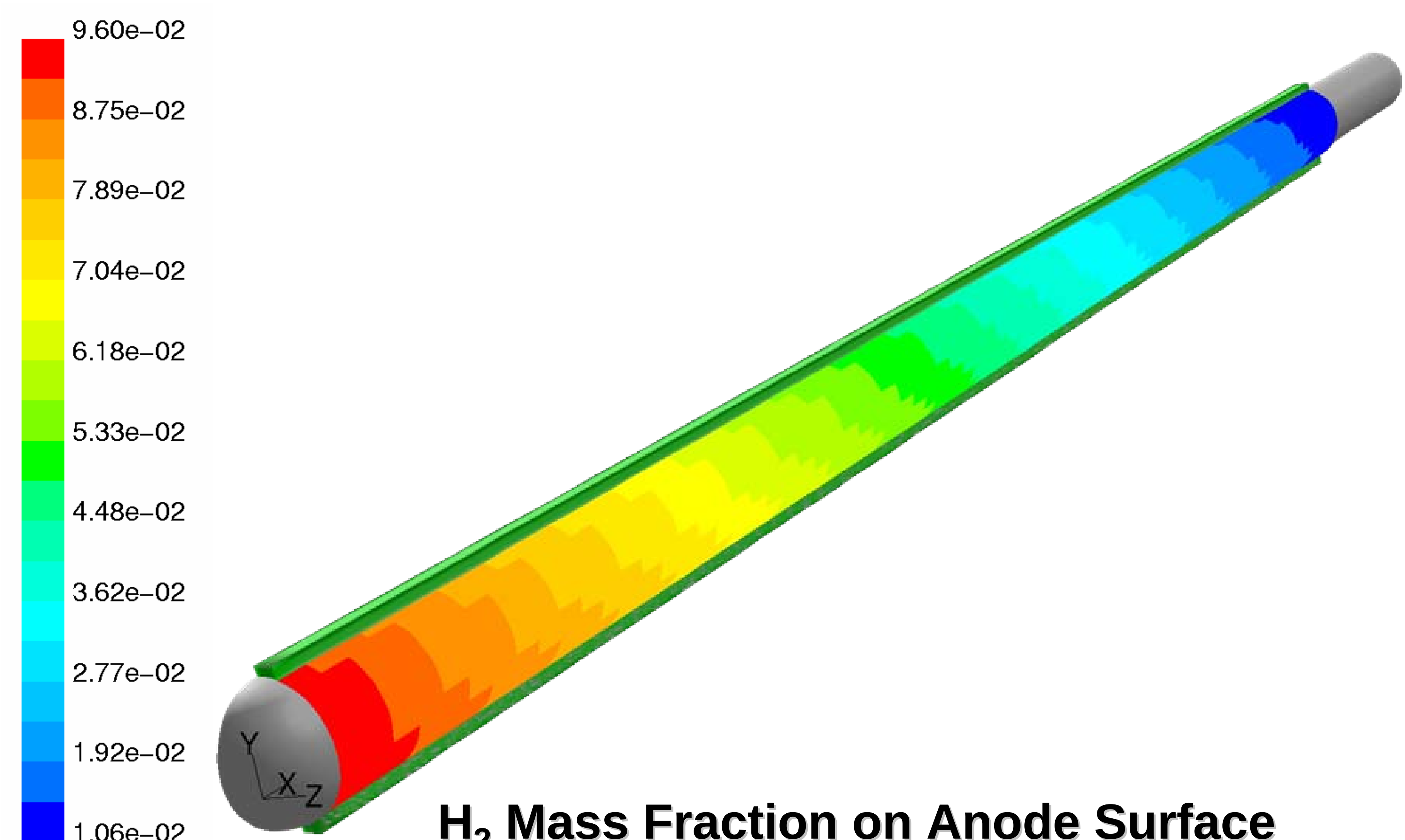
Tubular Cell Example

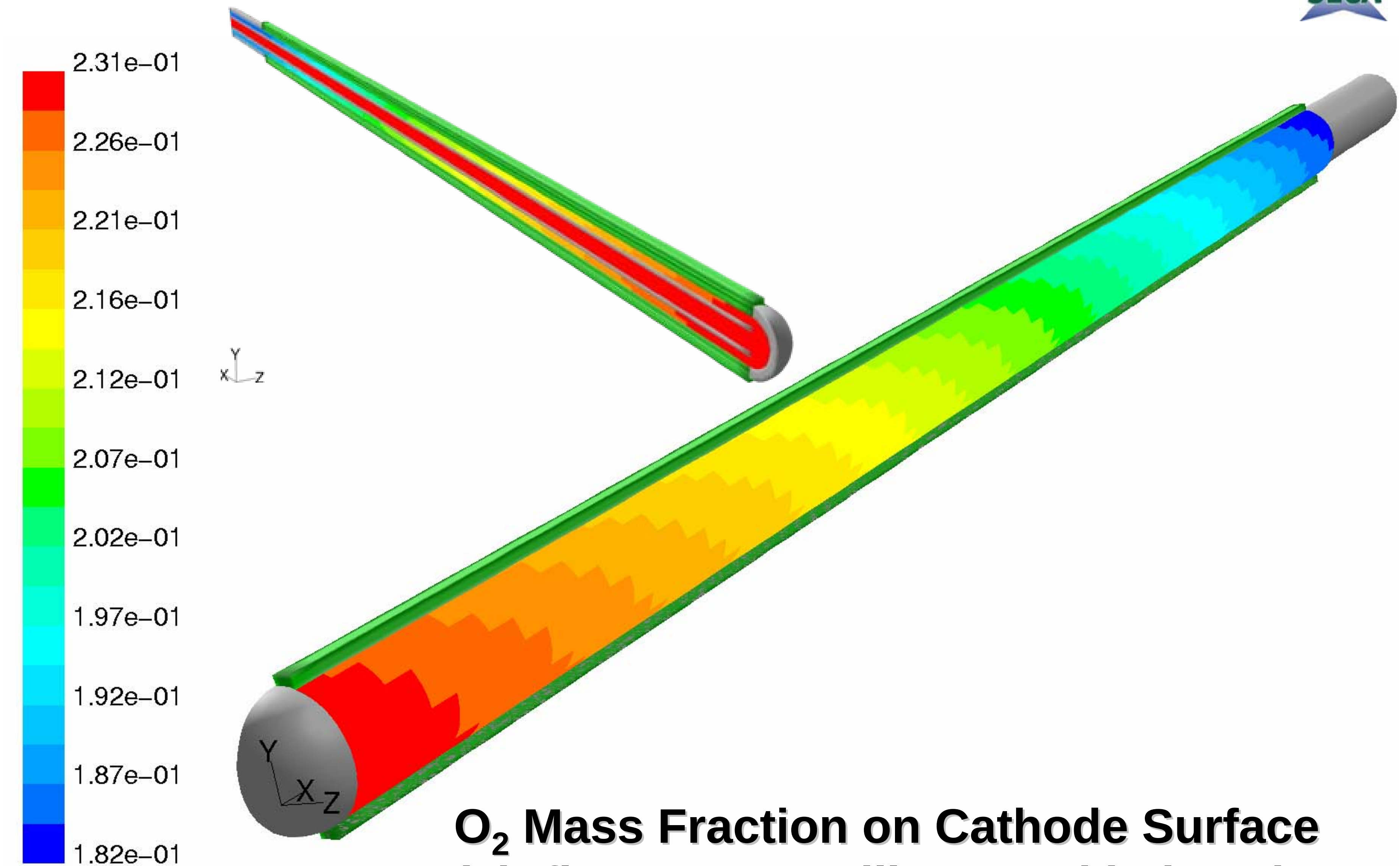
- Current Density = 1850 A/m^2
- 11 Amp
- Support Tube Geometry
- Fuel - 55.7% vol. H_2 , 10.8% vol. CO, 5.8%vol. CO_2 and 27.7% vol. H_2O (80% util.)
- Oxidizer - Air (25% util.)

Tubular SOFC Geometry

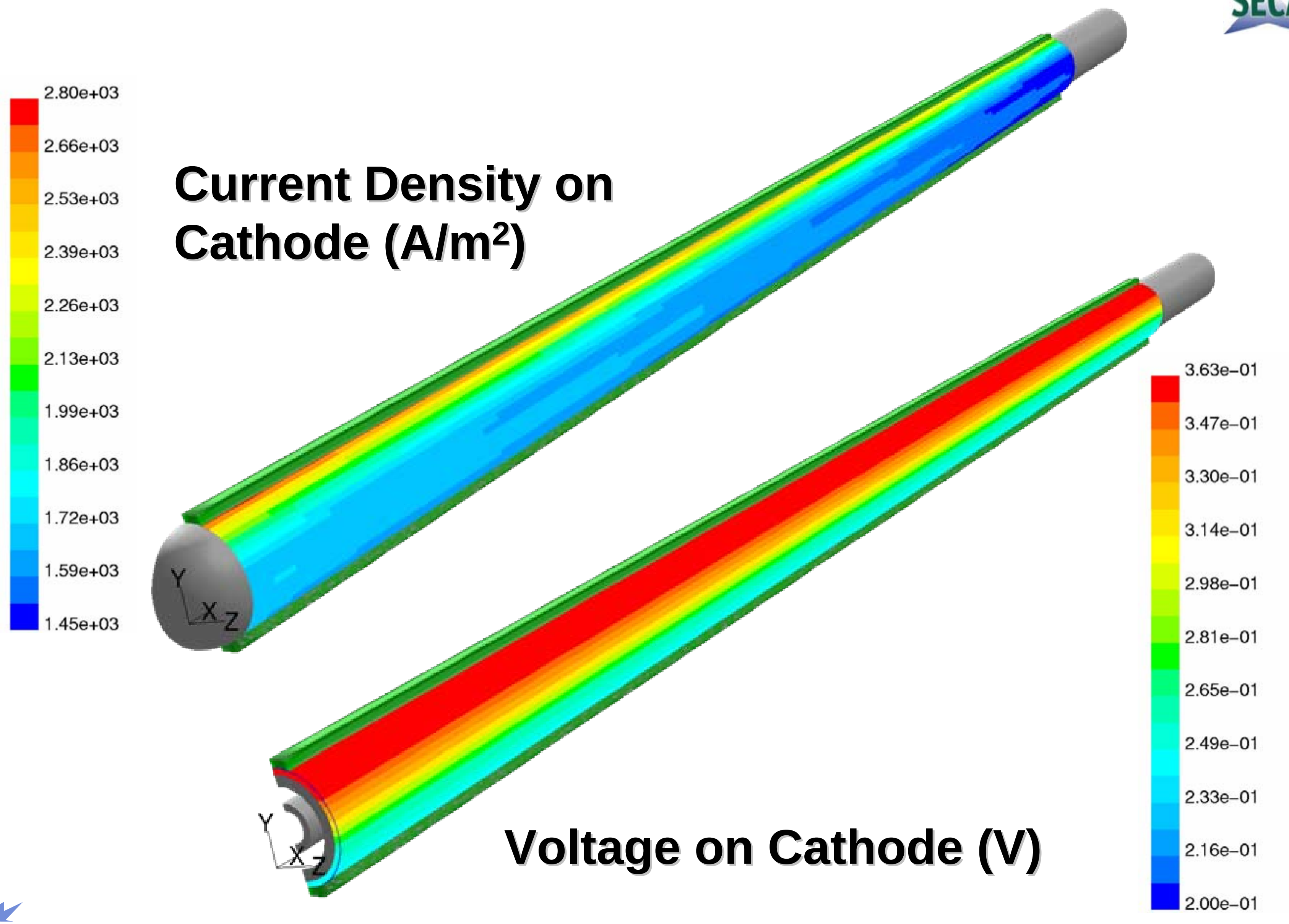


H_2 Mass Fraction on Anode Surface



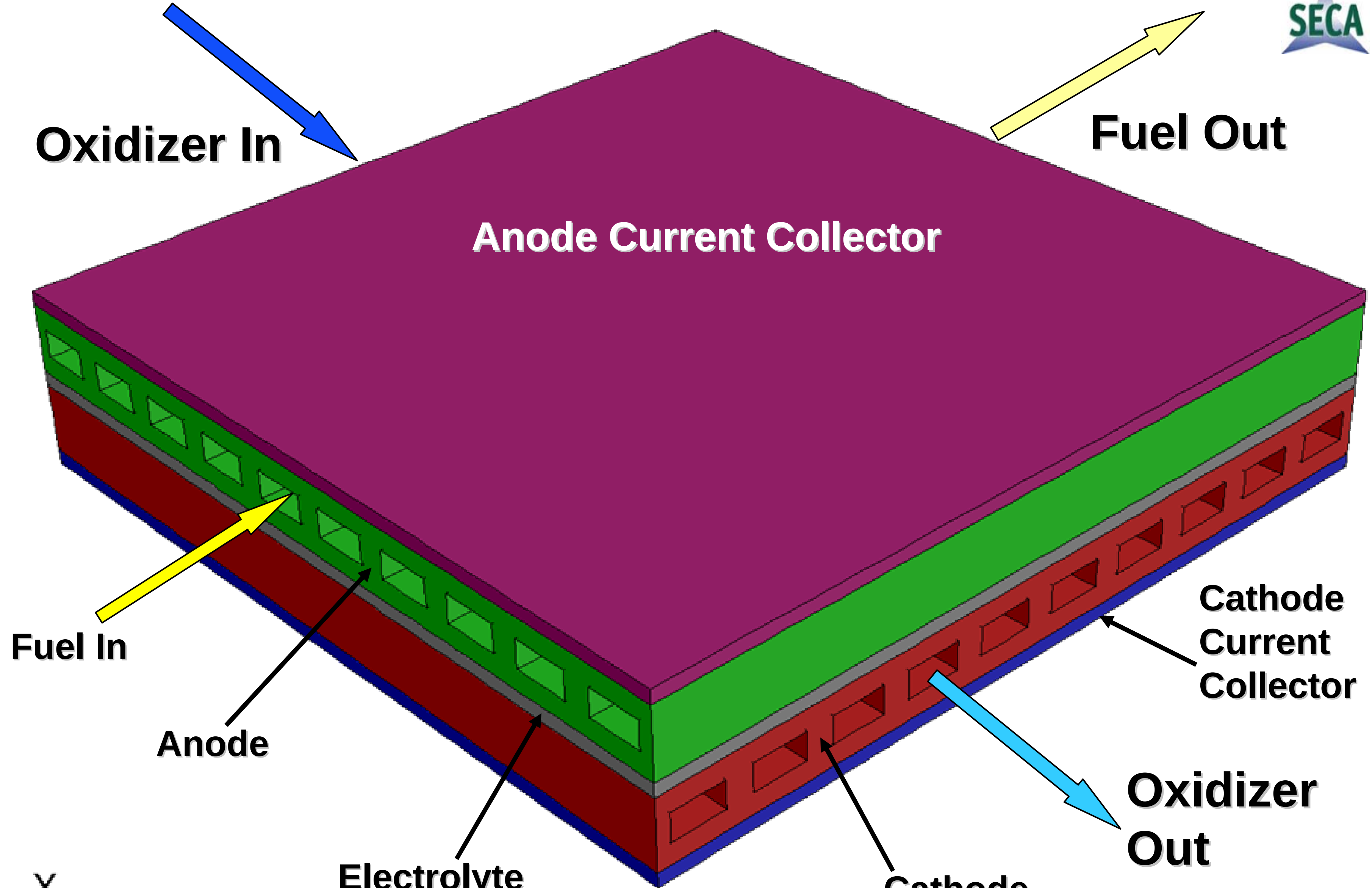


O_2 Mass Fraction on Cathode Surface (air flow passage illustrated in inset)

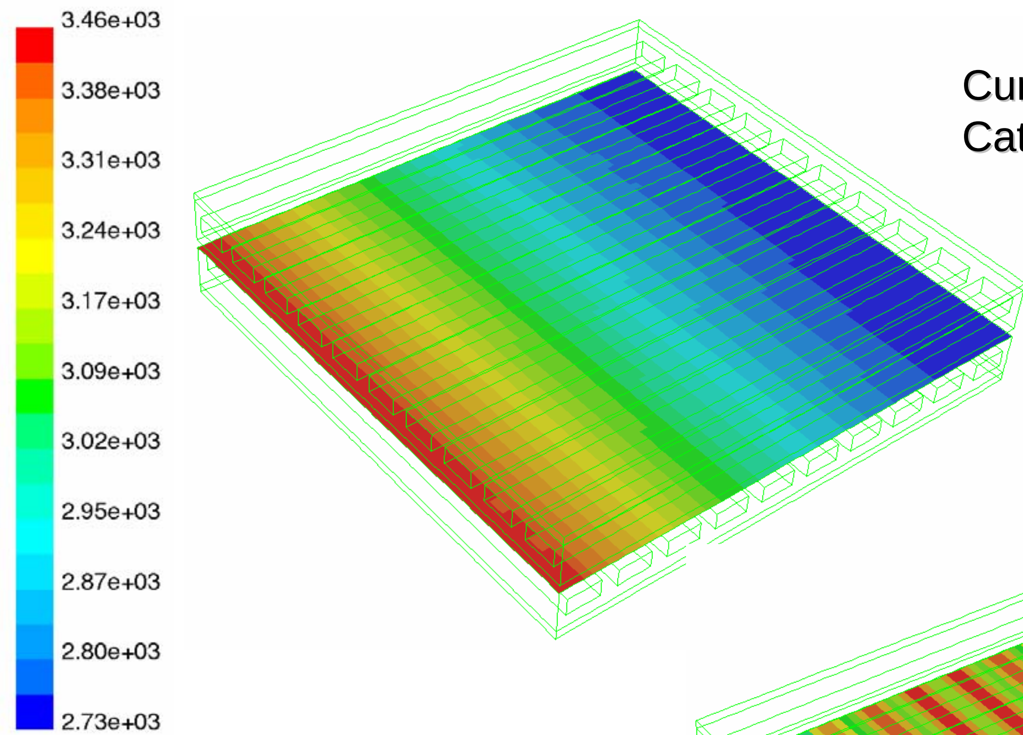

Current Density on Cathode (A/m²)
2.80e+03
2.66e+03
2.53e+03
2.39e+03
2.26e+03
2.13e+03
1.99e+03
1.86e+03
1.72e+03
1.59e+03
1.45e+03
Y
X
Z
Voltage on Cathode (V)
3.63e−01
3.47e−01
3.30e−01
3.14e−01
2.98e−01
2.81e−01
2.65e−01
2.49e−01
2.33e−01
2.16e−01
2.00e−01

Cross-Flow Monolith Geometry

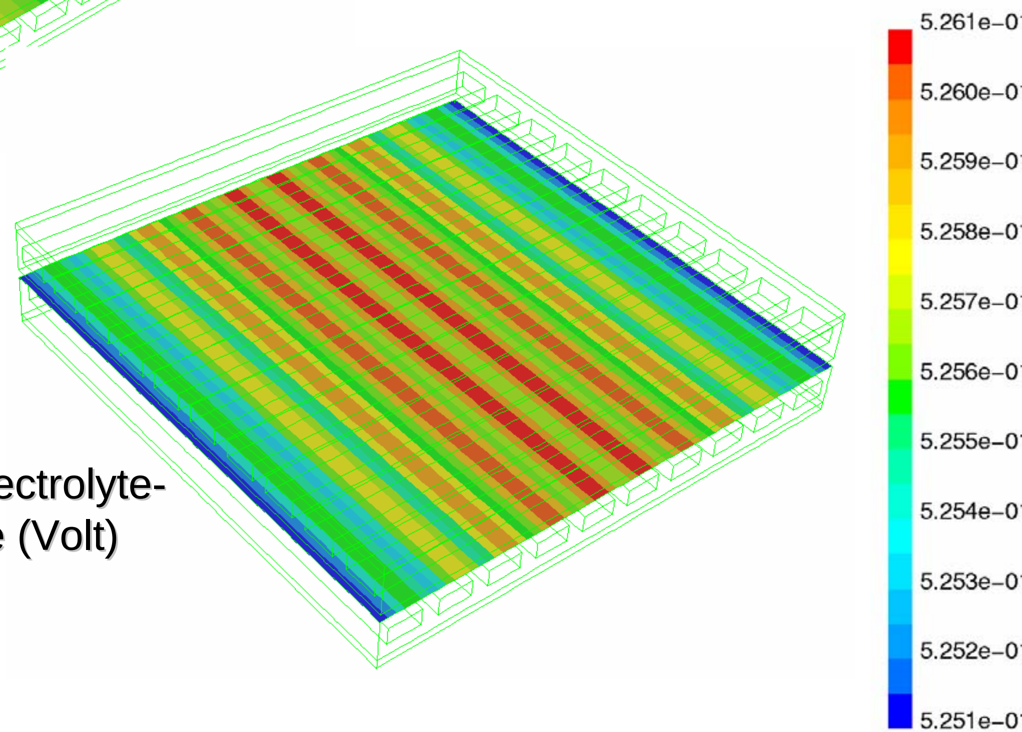
- Current Density = 3000 A/m^2
- 2.7 amp
- 30 cm x 30 cm
- Fuel - 97% vol. H_2 and 3% vol. H_2O (80% util.)
- Oxidizer - Air (30% util.)

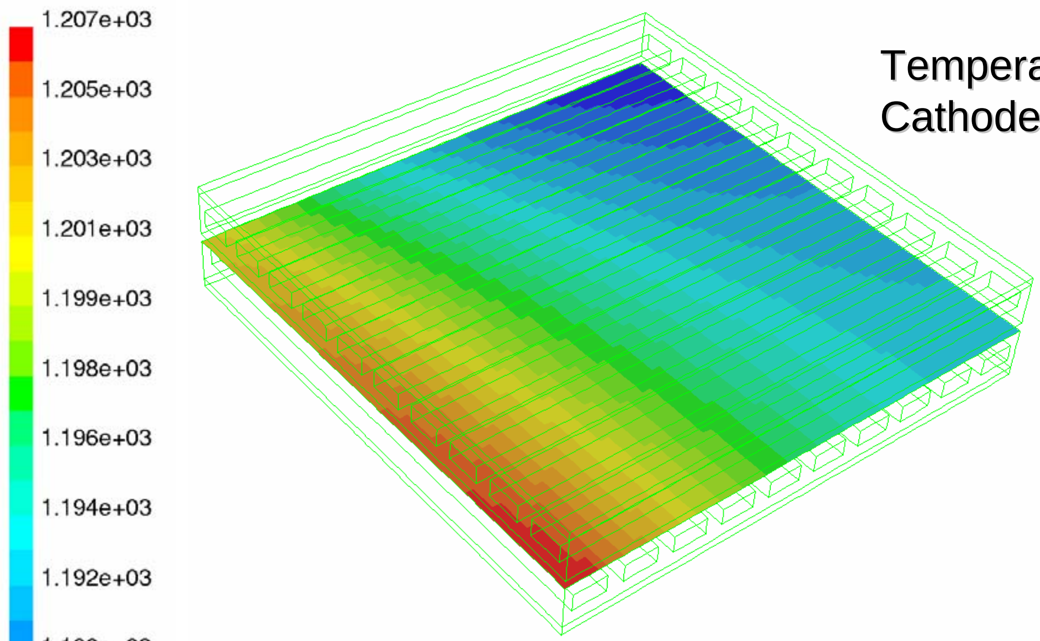

Oxidizer In
Fuel Out
Anode Current Collector
Fuel In
Anode
Electrolyte
Cathode
Cathode
Current
Collector
Oxidizer
Out
X

Current Density on Electrolyte-Cathode Face (amp/m^2)

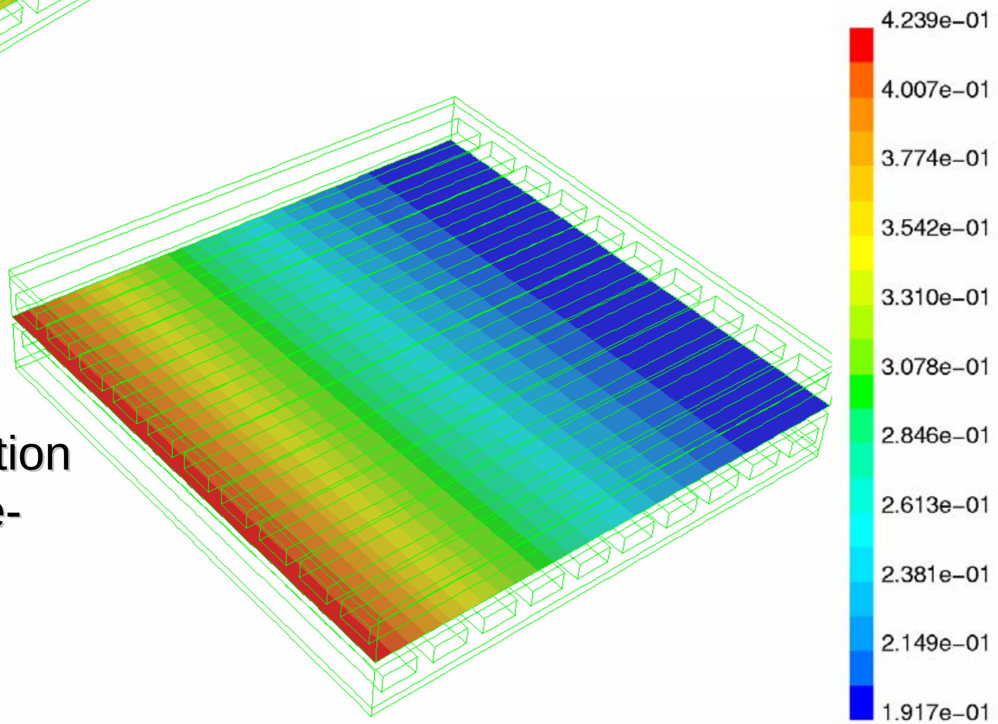


Voltage on Electrolyte-Cathode Face (Volt)





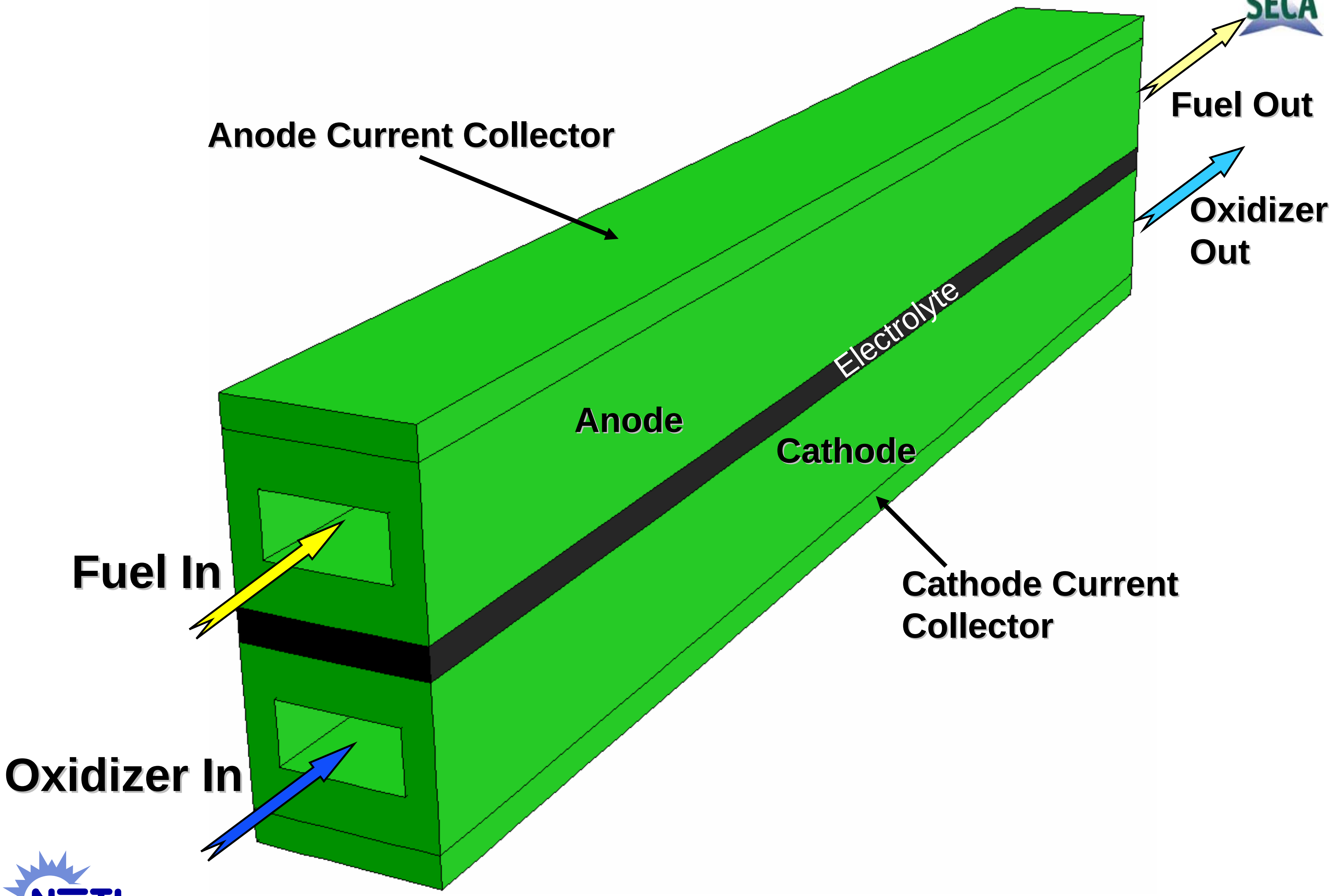
Temperature on Electrolyte-Cathode Face (K)

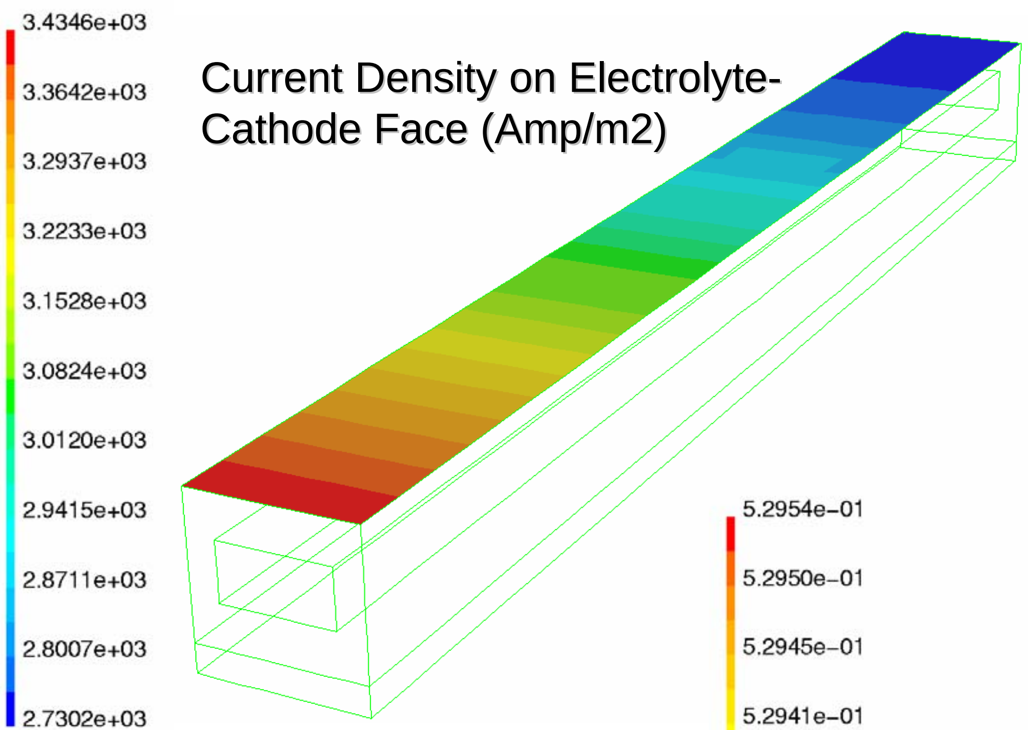


H_2 Mole Fraction on Electrolyte-Anode Face

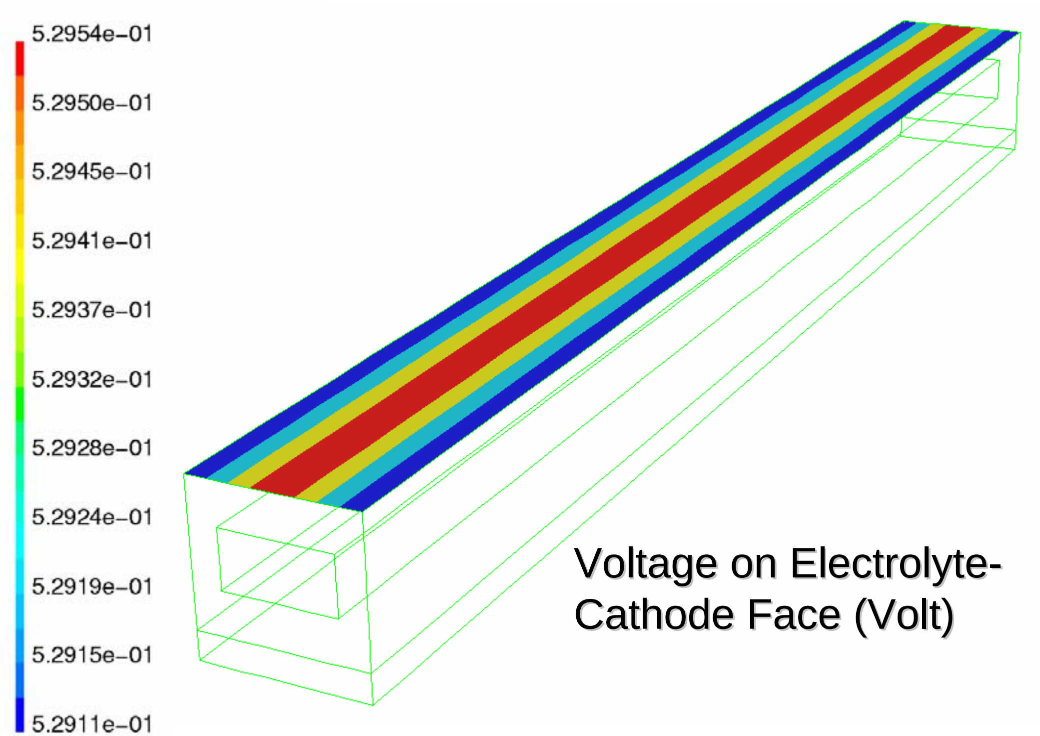
Co-Flow Monolith Channel

- Current Density = 3000 A/m^2
- 0.27 amp
- 30 cm x 3mm
- Fuel - 97% vol. H_2 and 3% vol. H_2O (80% util.)
- Oxidizer - Air (30% util.)
- *Couple with ANSYS*

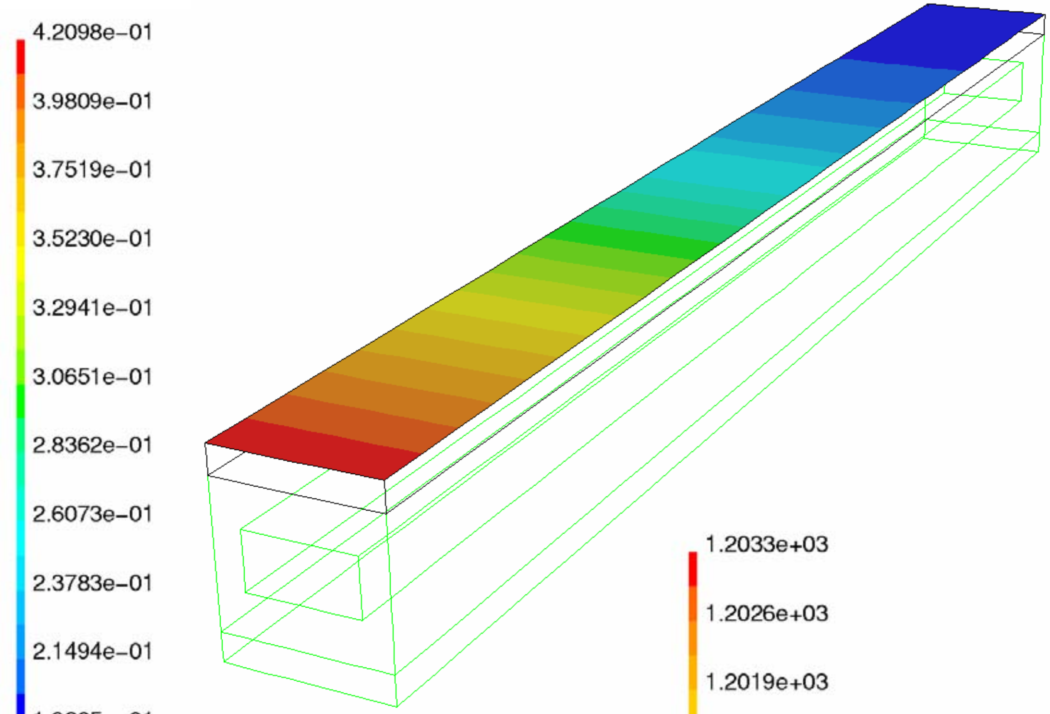

Anode Current Collector
Fuel Out
Oxidizer Out
Electrolyte
Anode
Cathode
Fuel In
Cathode Current Collector
Oxidizer In



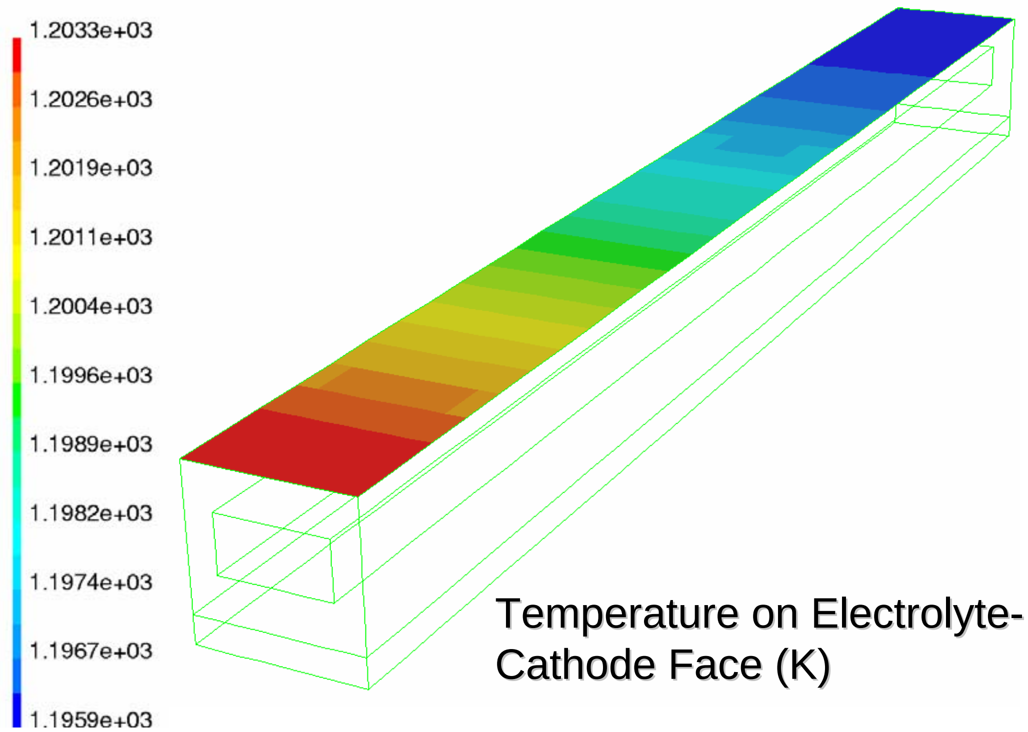
Current Density on Electrolyte-Cathode Face (Amp/m2)



Voltage on Electrolyte-Cathode Face (Volt)

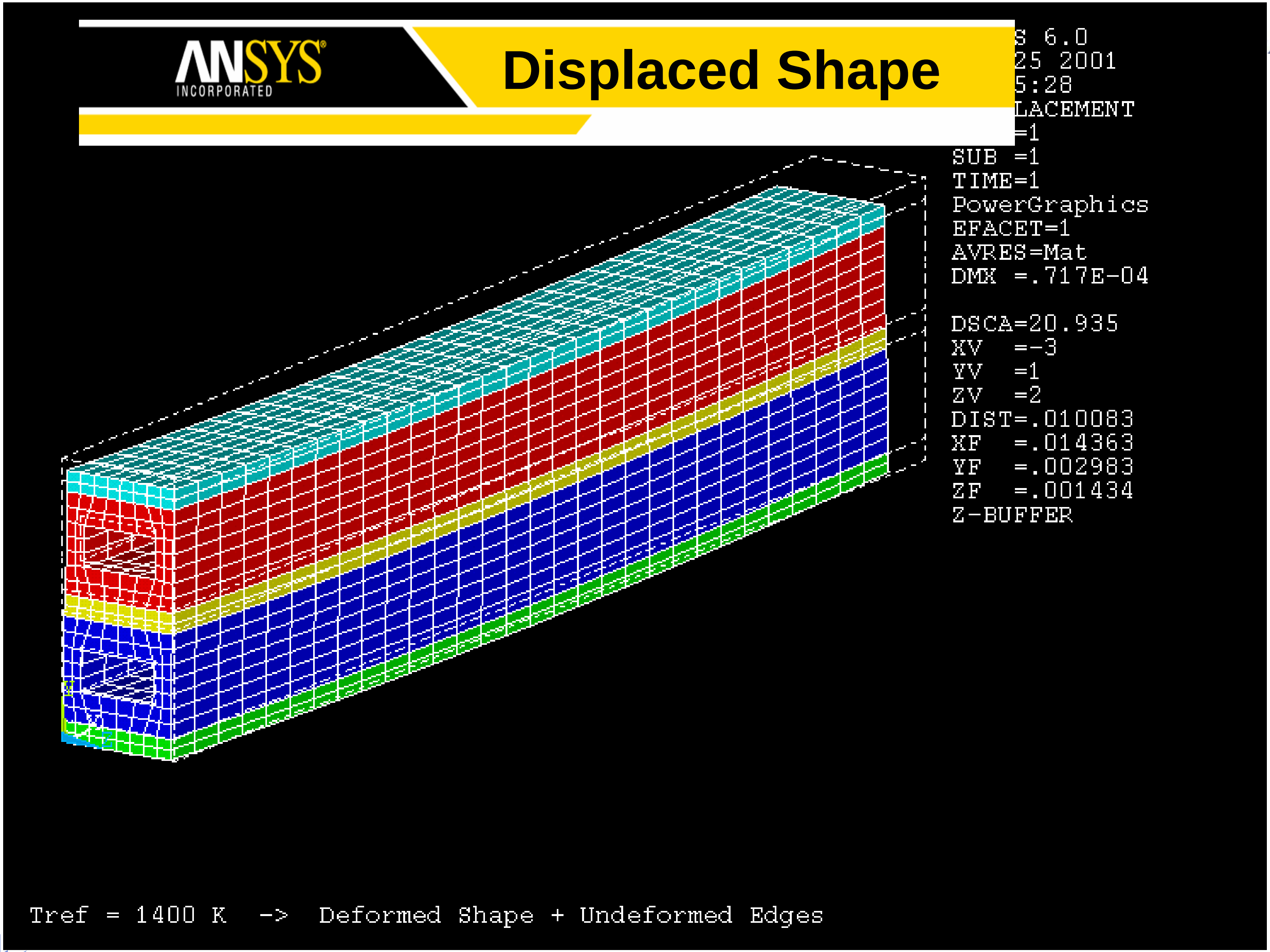


H_2 Mole Fraction on Electrolyte-Anode Face

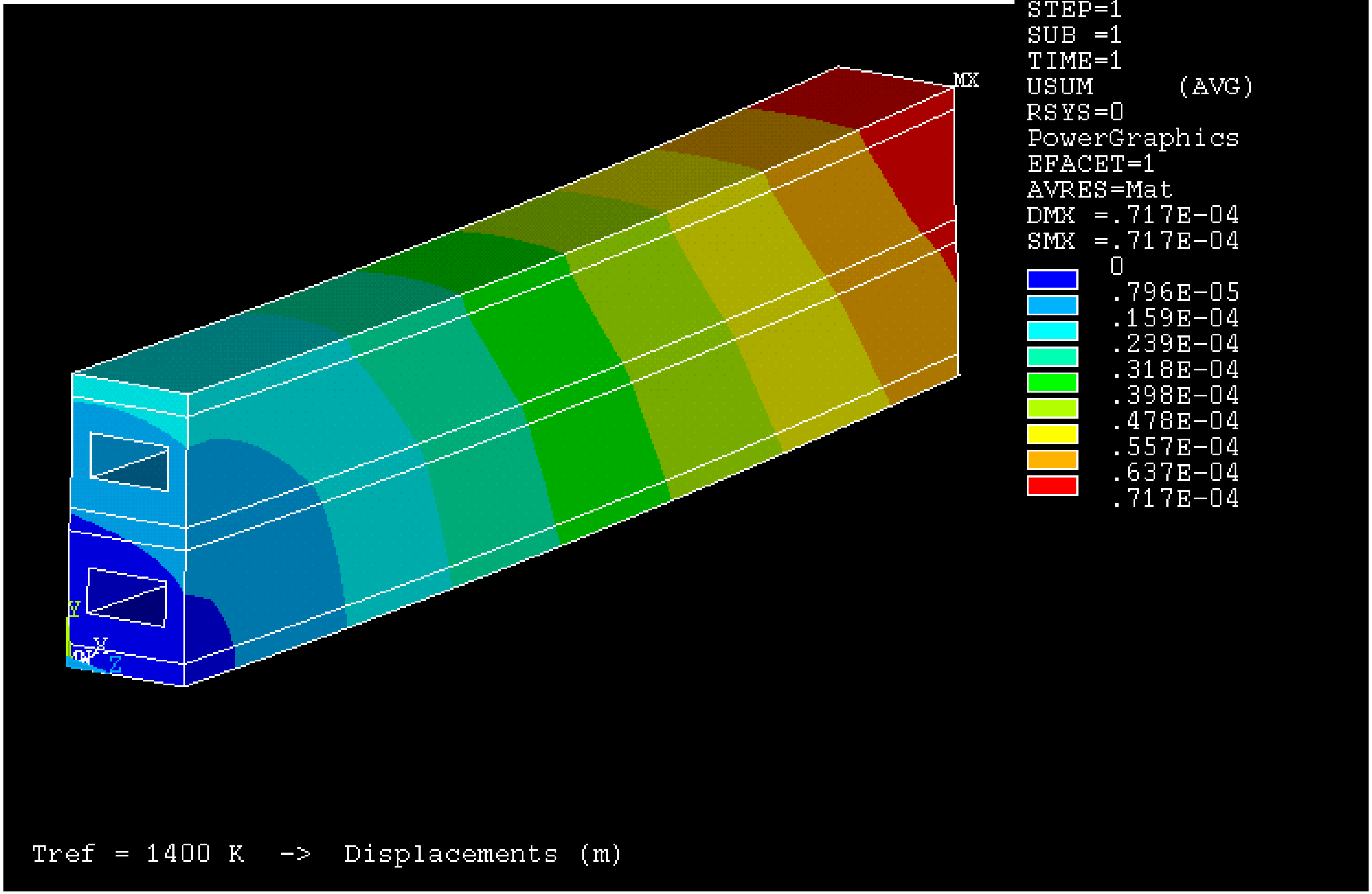


Temperature on Electrolyte-Cathode Face (K)

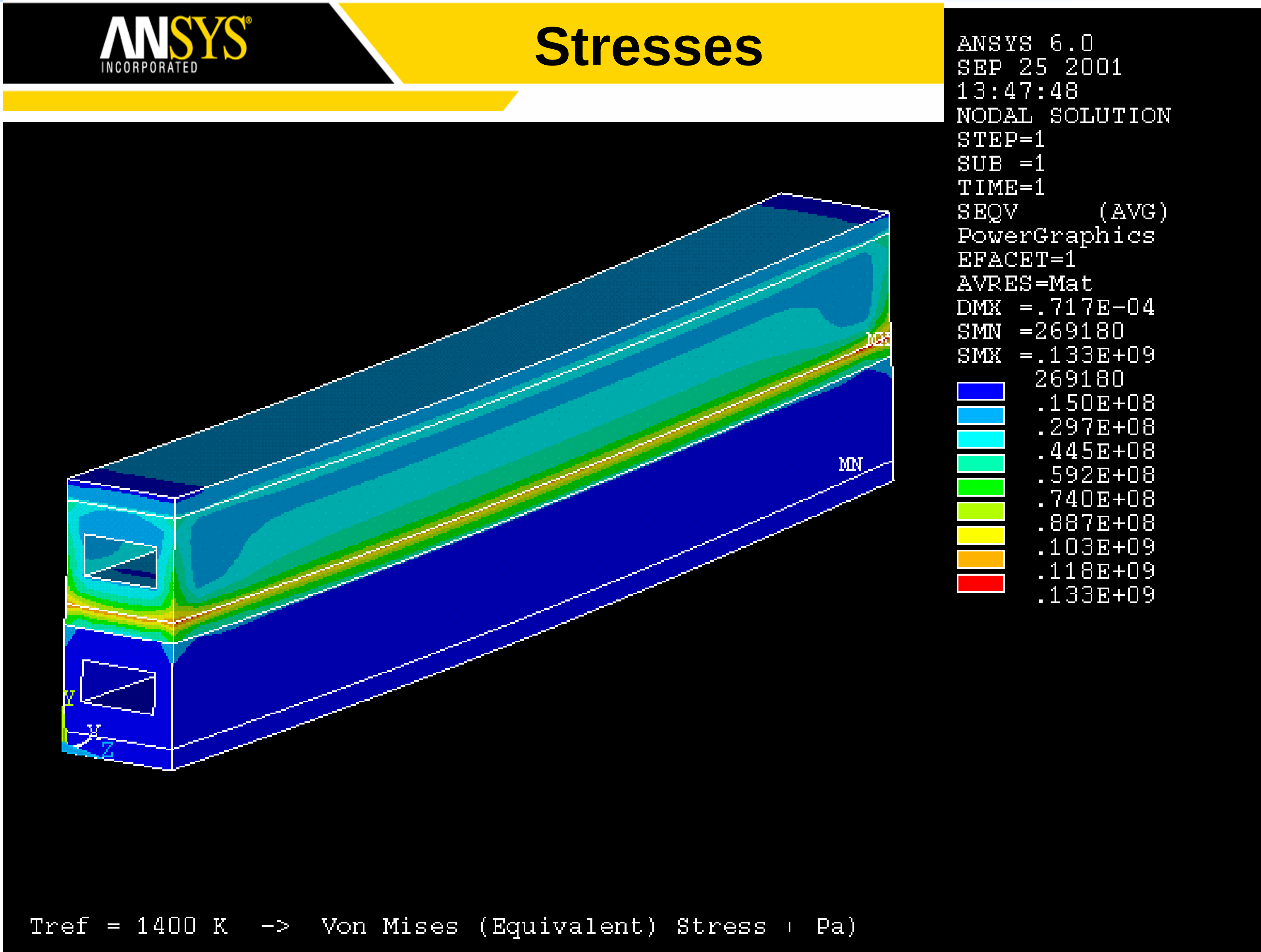
Displaced Shape



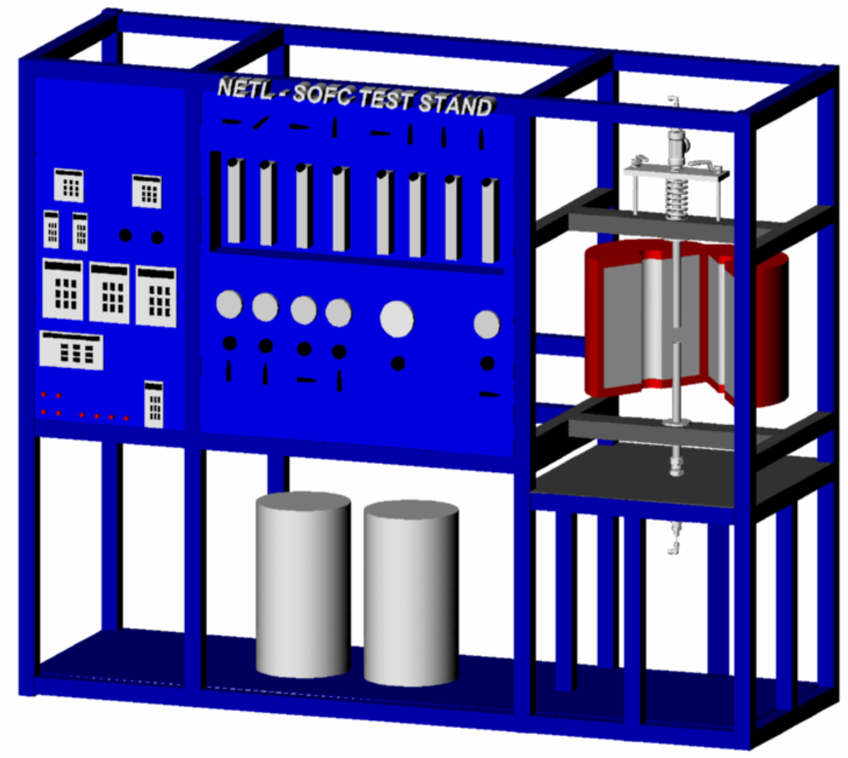
Displacement

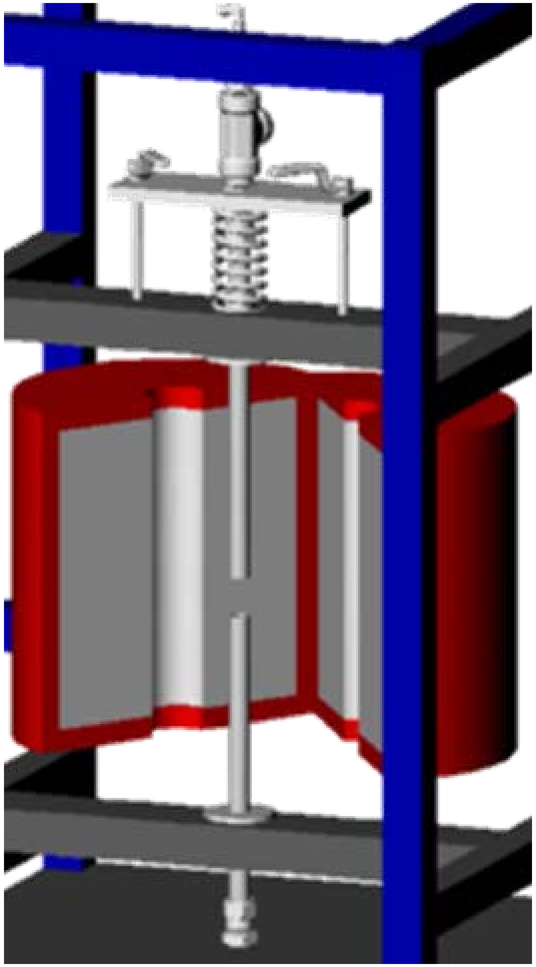


Stresses


ANSYS 6.0
SEP 25 2001
13:47:48
NODAL SOLUTION
STEP=1
SUB =1
TIME=1
SEQV (AVG)
PowerGraphics
EFACET=1
AVRES=Mat
DMX =.717E-04
SMN =269180
SMX =.133E+09
269180
.150E+08
.297E+08
.445E+08
.592E+08
.740E+08
.887E+08
.103E+09
.118E+09
.133E+09
MX
MN
Y
X
Z
Tref = 1400 K -> Von Mises (Equivalent) Stress (Pa)

SOFC Cell and Small Stack Testing for Model Validation



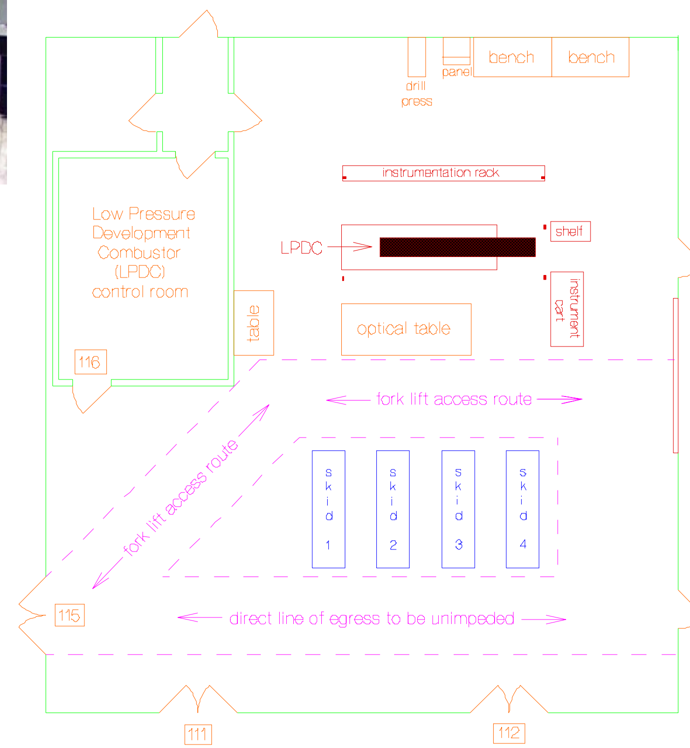


Technical Approach

- **Collaborate with cell/stack developers that can provide ‘generic-customized’ test specimens**
- **Partner with labs capable of property analysis**
  - Single & composite material analysis
  - Porous media characterization
  - Post test analysis (ensure consistent and proper operation of specimens under test)
- **Work closely with model developers to ensure data relevancy for model validation purposes**
- **Redundant testing**

Test Facility

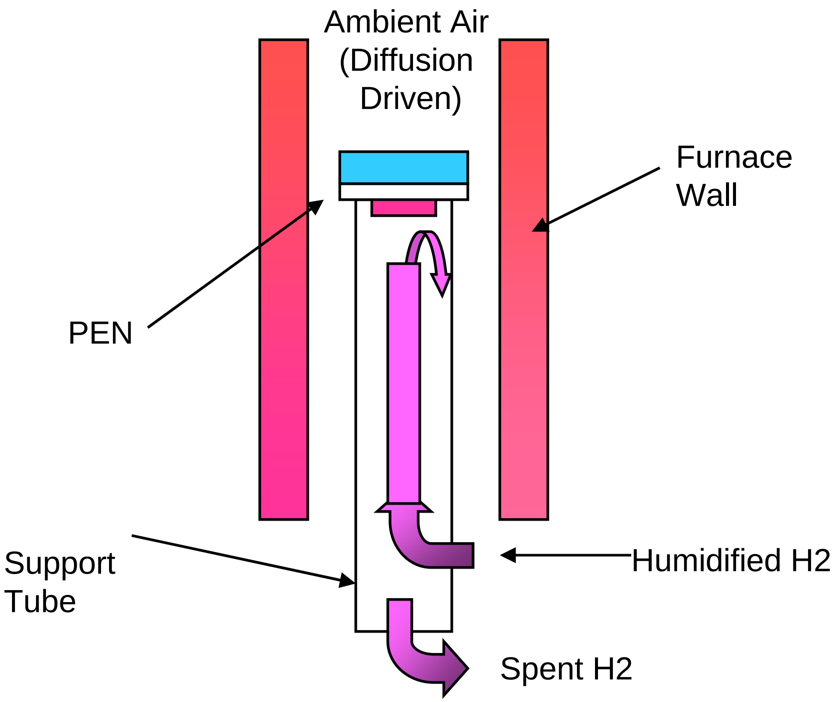
- **Four SOFC test stands are being installed**

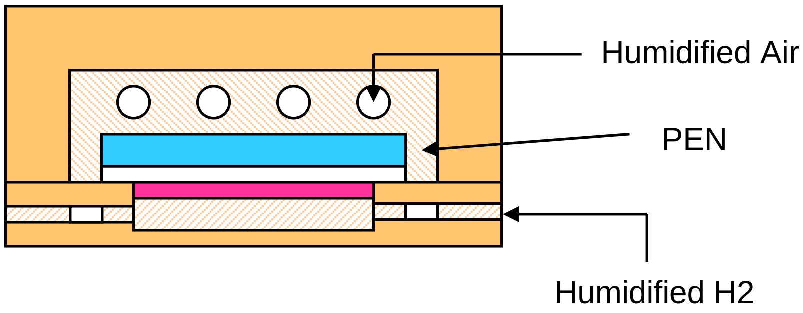


SOFCEL plotplan for B4 area 115

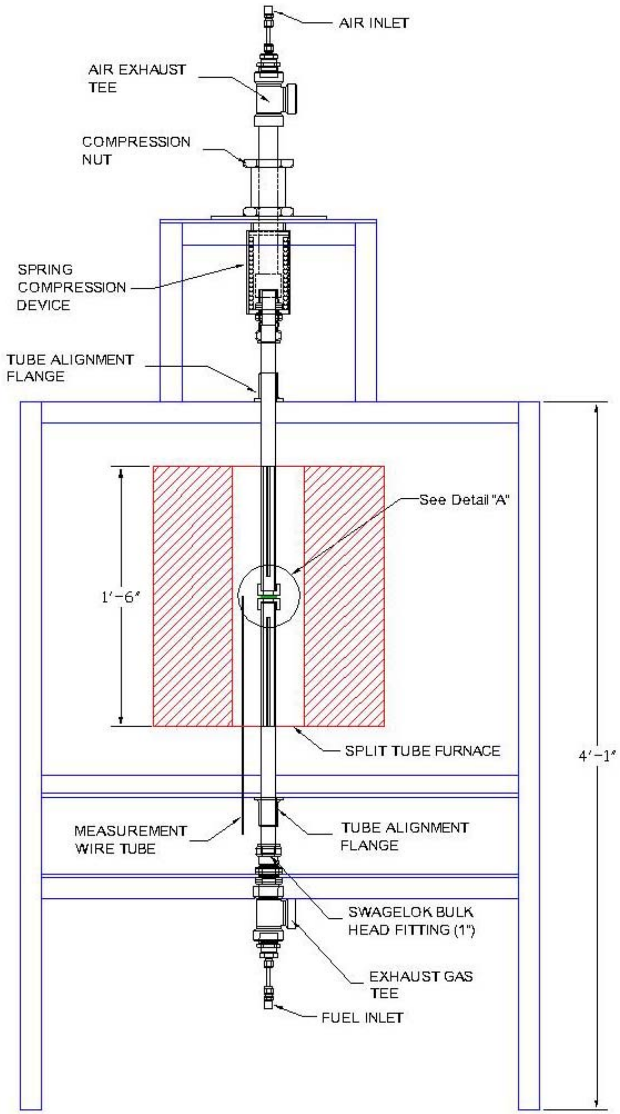
Specimen Test Fixtures

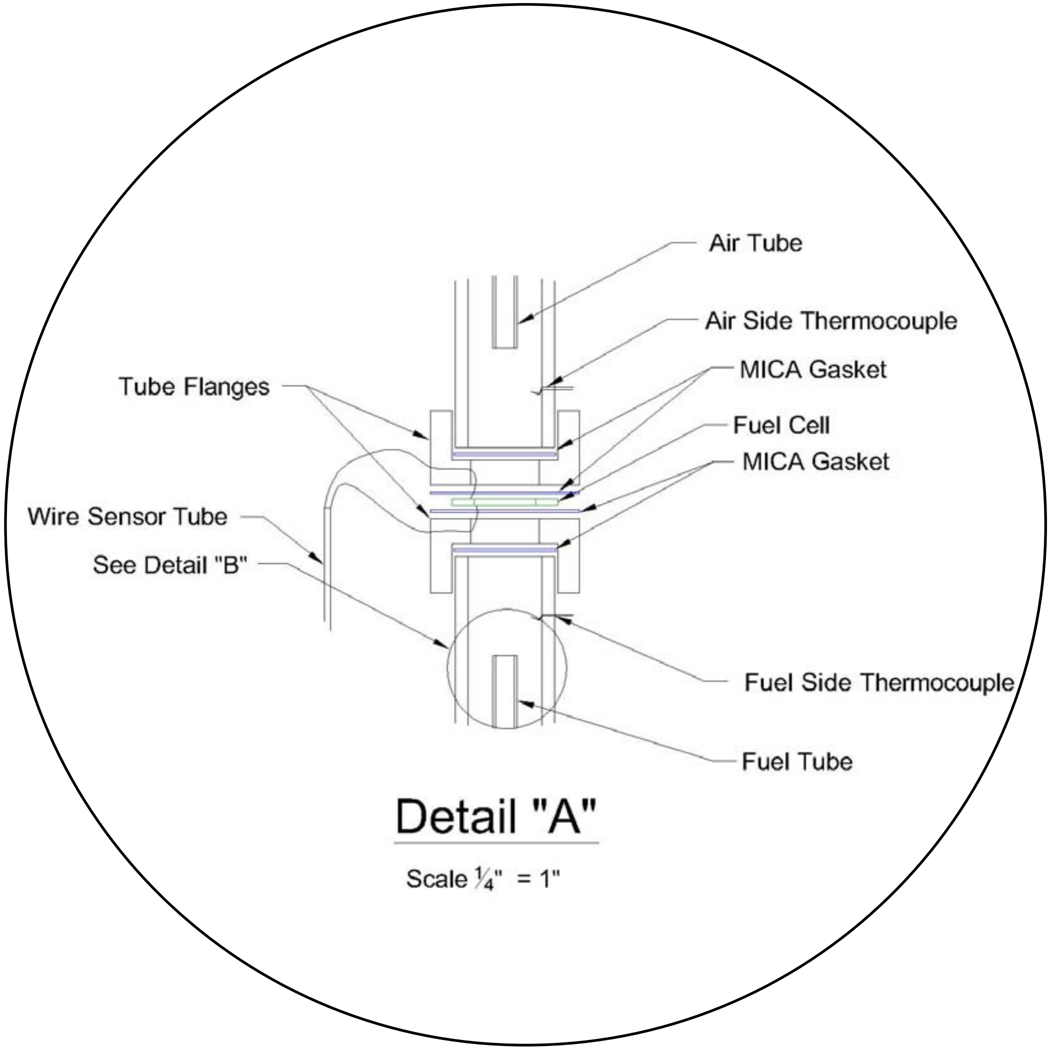
- **Model validation using different flow conditions:**
  - Stagnant environment
  - Convective environment





Specimen Test Fixtures





Resources, Partnerships, Collaborations

- **NETL Computing Clusters**
  - 300 CPU + system all with FLUENT License
- **Collaboration with Pittsburgh Supercomputer Center**
  - CPU time and consulting
- **Simulating Proprietary Geometry for SECA Developer**
- **Discussions with leading SOFC developers**
  - Support NETL testing for model validation
- **Collaboration with ANSYS and Mallet Technologies**
  - "Multiphysics" models - use CFD data in FEM code for stress analysis

Resources, Partnerships, Collaborations

- **NETL/Fluent Incorporated CRADA for fuel cell model development and validation (11/14/01)**

- **Fluent plans to offer commercial versions of SOFC and PEMFC models in 2nd Quarter 2002**

Resources, Partnerships, Collaborations

- **SECA Prototype Test Facility**
  - Periodically assess progress in meeting SECA Fuel Cell Program Goals
  - Independently test each prototype system at NETL under well controlled and monitored conditions
  - Report technical performance to SECA managers

Resources, Partnerships, Collaborations

- **Experience with PEMFC testing**
  - PEMFC test facility at NETL
  - Provide data for validation of PEMFC model (NETL/Fluent CRADA)

Other Collaborations

- PNNL doing material property analyses and compilations
- PNNL working with ORNL to examine lifetime issues
- LBL performing novel low cost cell designs (non-anode supported technology)
- ANL performing cathode optimization and property analyses