NETL SOFC Model

SECA Core Technology Workshop

May 12, 2004

Michael T. Prinkey

Fluent, Inc.

NETL SOFC Modeling Group

- **NETL Personnel**
  - William A. Rogers, Division Director, Simulation, Analysis, Computational Sciences Division
  - Randall Gemmen, Fuel Cells Research Group Leader
- **Fluent, Inc. Personnel**
  - Michael T. Prinkey, Sr. Development Engineer
  - Mehrdad Shahnam, Sr. Consulting Engineer
- **Collaboration**
  - Georgia Tech
  - Siemens Westinghouse
  - University of Utah
- **Funding provided by NETL SECA program**

NETL SOFC Modeling Effort

- Initiated in late 2000
- Robustness, geometric flexibility, and physical fidelity have improved significantly
- Current version of the model is considered ready for commercial use
- Fluent, Inc. will be adding a version of the NETL SOFC model into the FLUENT product line later this year

Software Release

- **The NETL SOFC model is available for immediate download by all SECA participants.**
- **https://lars.netl.doe.gov/sofc/sofc.zip (45 MB download)**
- **Requires FLUENT version 6.1**
- **Contains Linux and Windows versions of the module**
- **Documentation includes a comprehensive theory guide**
- **It also contains a complete tutorial and a series of example problems to illustrate problem setup for:**
  - Single cells or stacks
  - Planar or tubular geometries
  - Overview of solution procedure

SOFC Model Benefits

- Provides a predictive modeling tool for all types of solid-oxide fuel cells
- Applicable to production-scale cells and stacks
- Allows a high degree of geometric fidelity so complicated fuel cell designs can be modeled faithfully
- Tested on a wide variety of cell types and configurations
- Results compare favorably with test data
- Offers an effective design tool for fuel cell developers

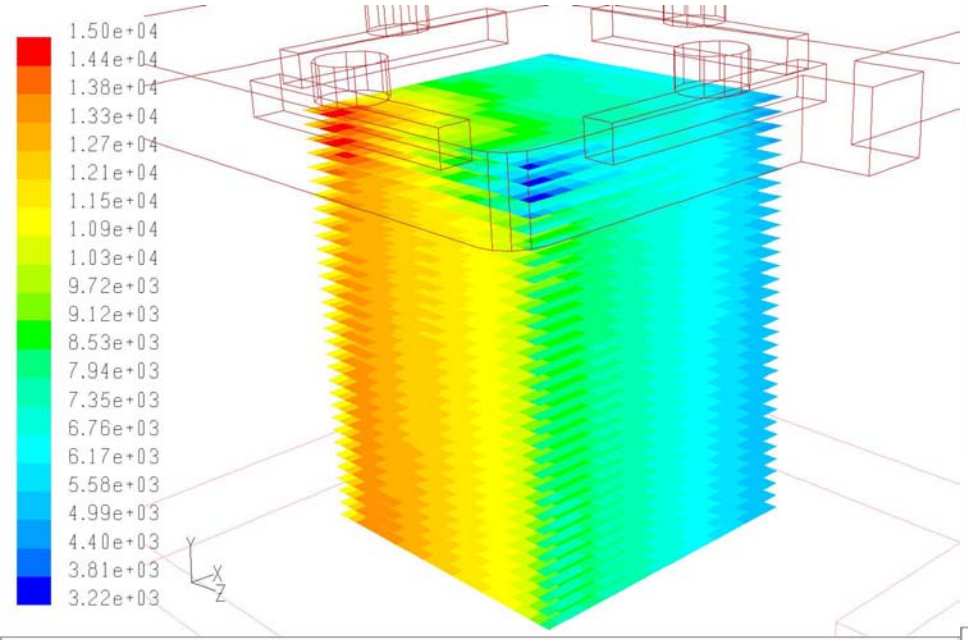
SOFC Model Capabilities

- Full coupling between flow, heat and mass transfer, electrochemisty and potential field
- Keep cell count down by not resolving the electrolyte
- H_2 and CO electrochemistry via water-gas shift
- Steam reforming of methane
- Electric field, current flow, and ohmic heat generation in all conducting regions
- Single cell or stack
- Converge to specified system current or voltage
- Steady-state and transient analysis
- Fully parallelized computing (currently beta)
- Contact resistance for cell/stack components
- Full multicomponent diffusion with tortuosity correction
- Suite of radiation models in Fluent
- Reduced radiation mechanism developed by GA Tech

Overview of Model Capabilities - I

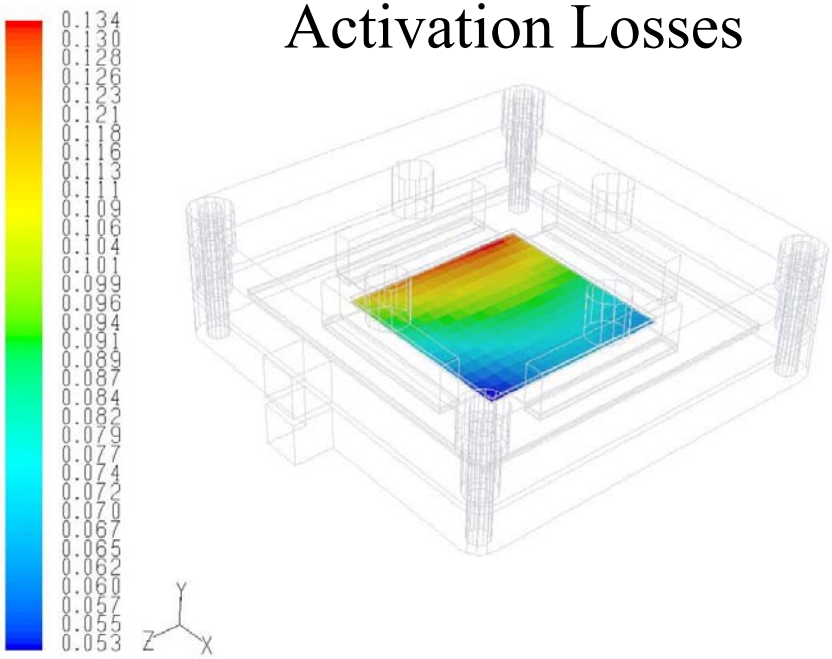
- **Quickly illustrate the type of data that the model provides**

Local Current Density



Contours of current-density-amp-per-m2
May 06, 2004
FLUENT 6.1 (3d, dp, segregated, spe4, lam)

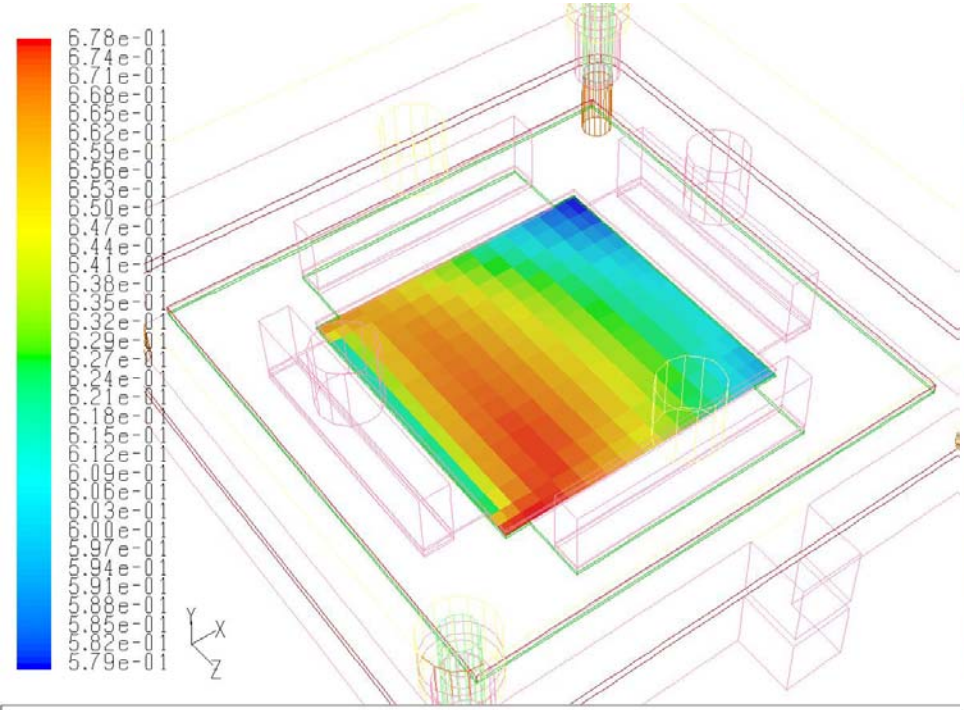
Activation Losses



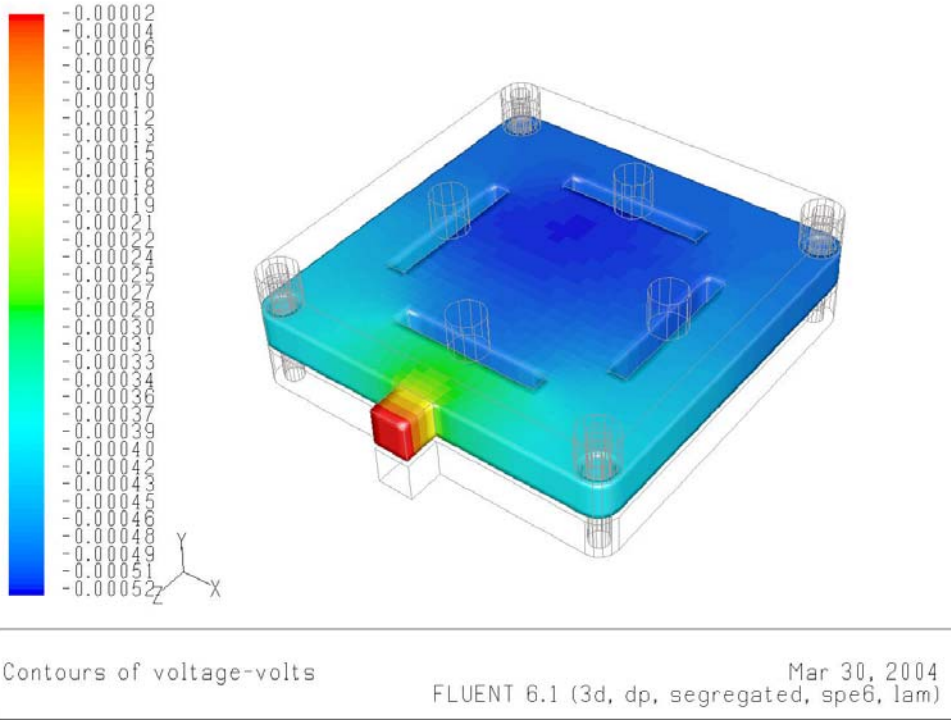
Contours of activation-overpotential-volts
Mar 30, 2004
FLUENT 6.1 (3d, dp, segregated, spe6, lam)

Overview of Model Capabilities - II

Species Concentrations

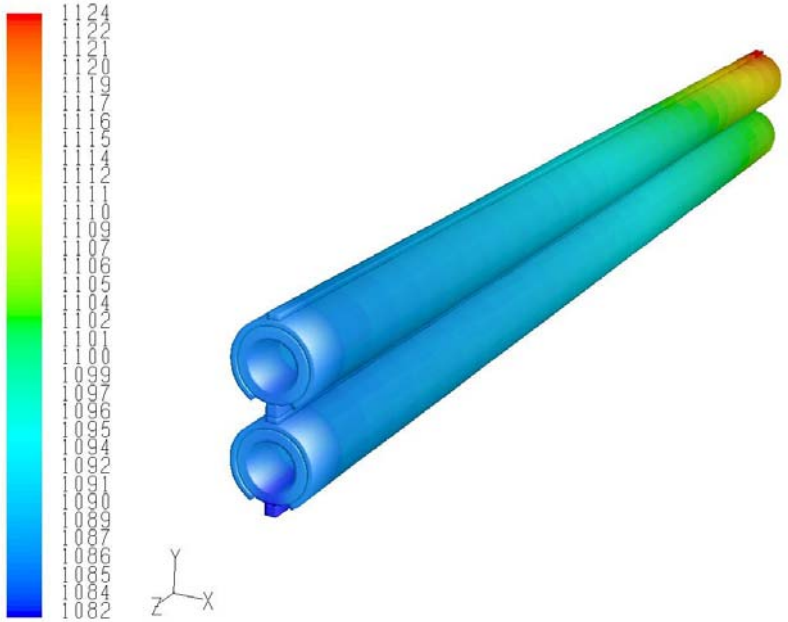


Electric Potential

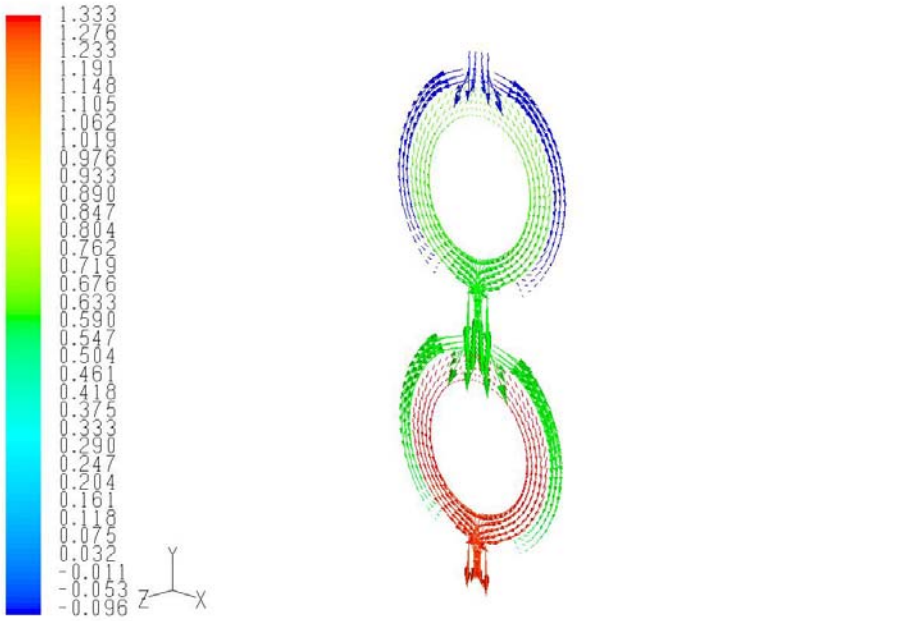


Overview of Model Capabilities - III

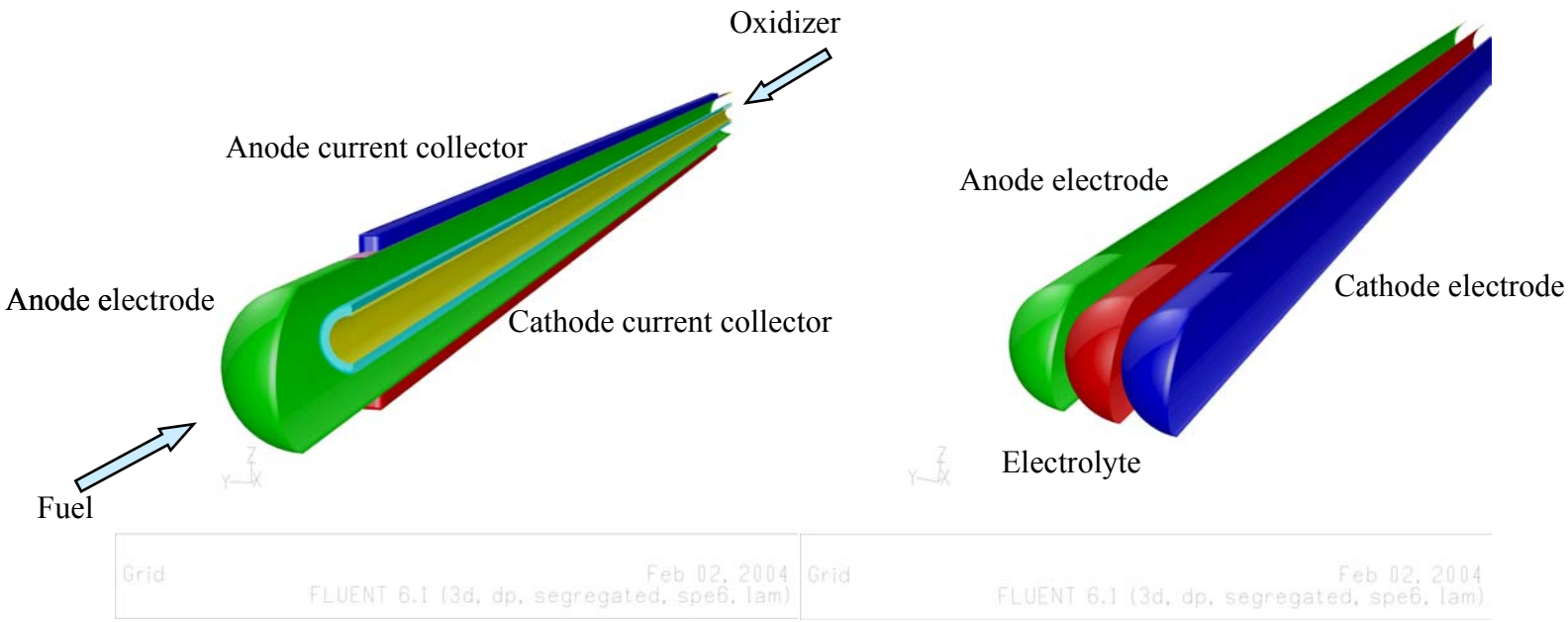
Temperature



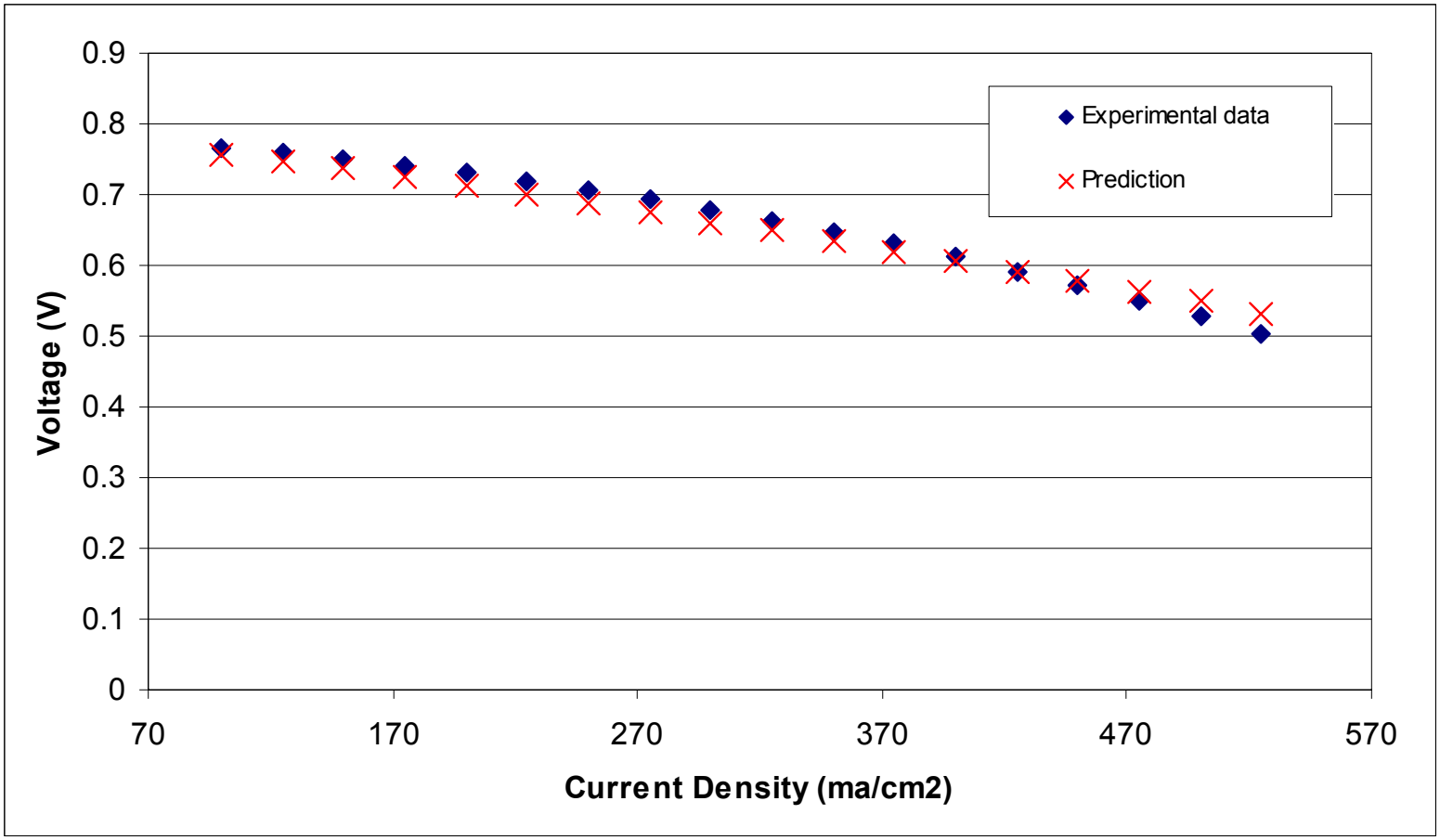
Current Density Vectors

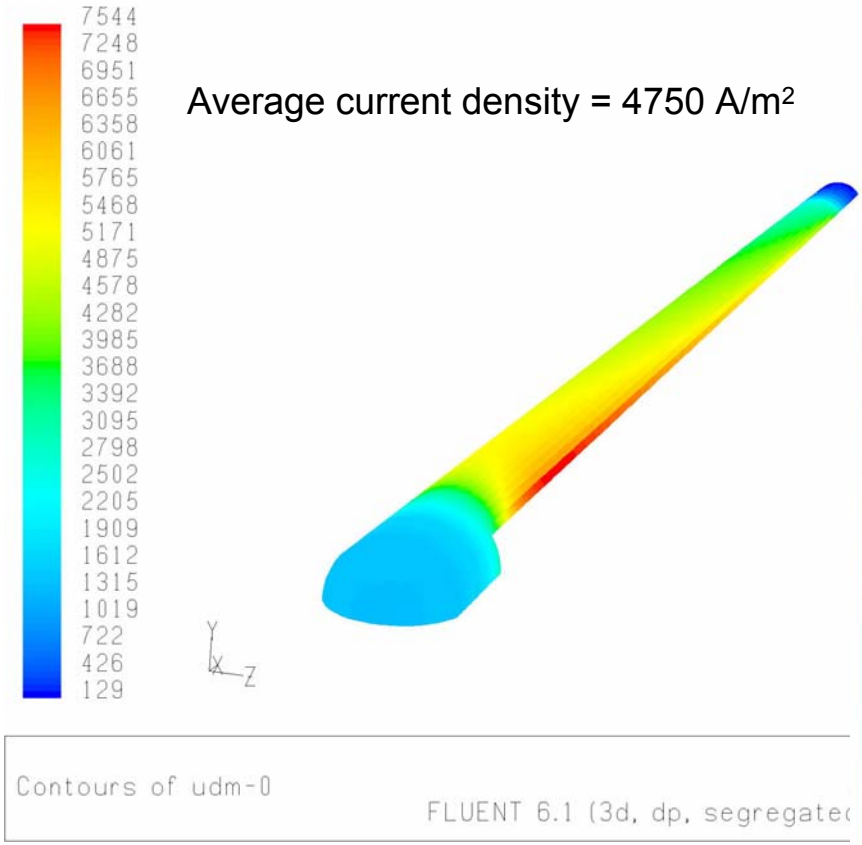


Validation Application: Siemen-Westinghouse Tubular Cell

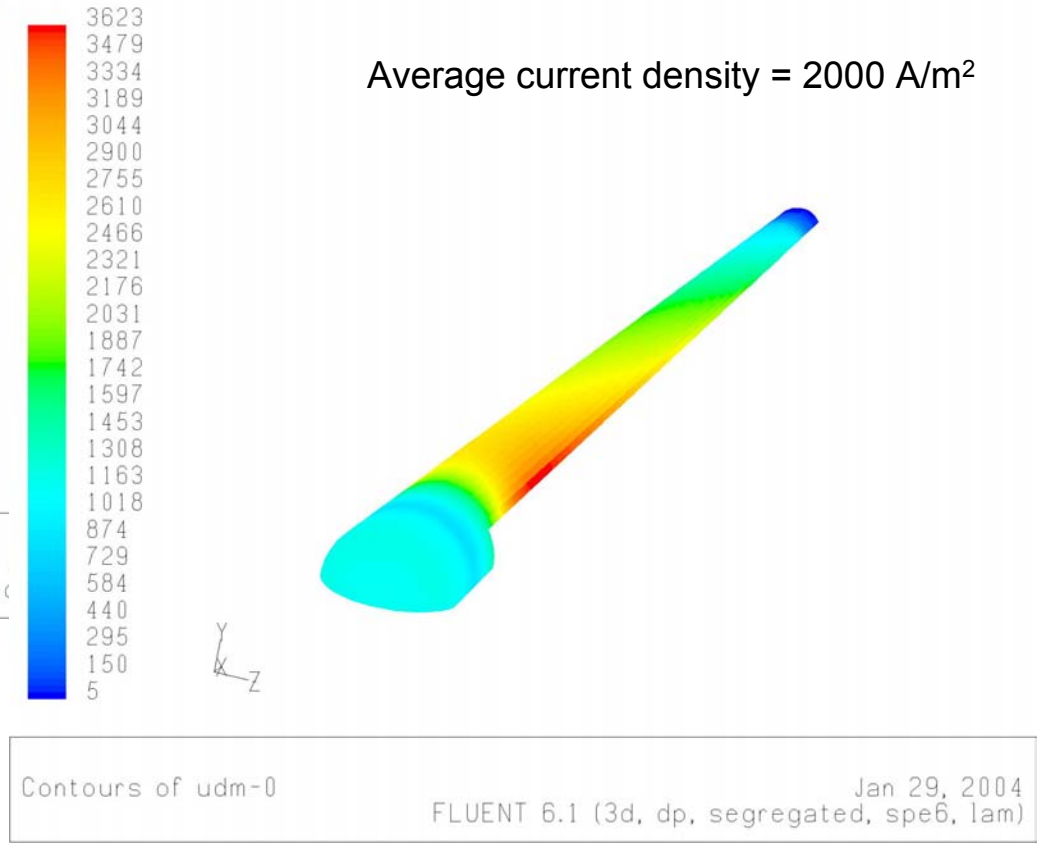


Polarization curve for the tubular fuel cell



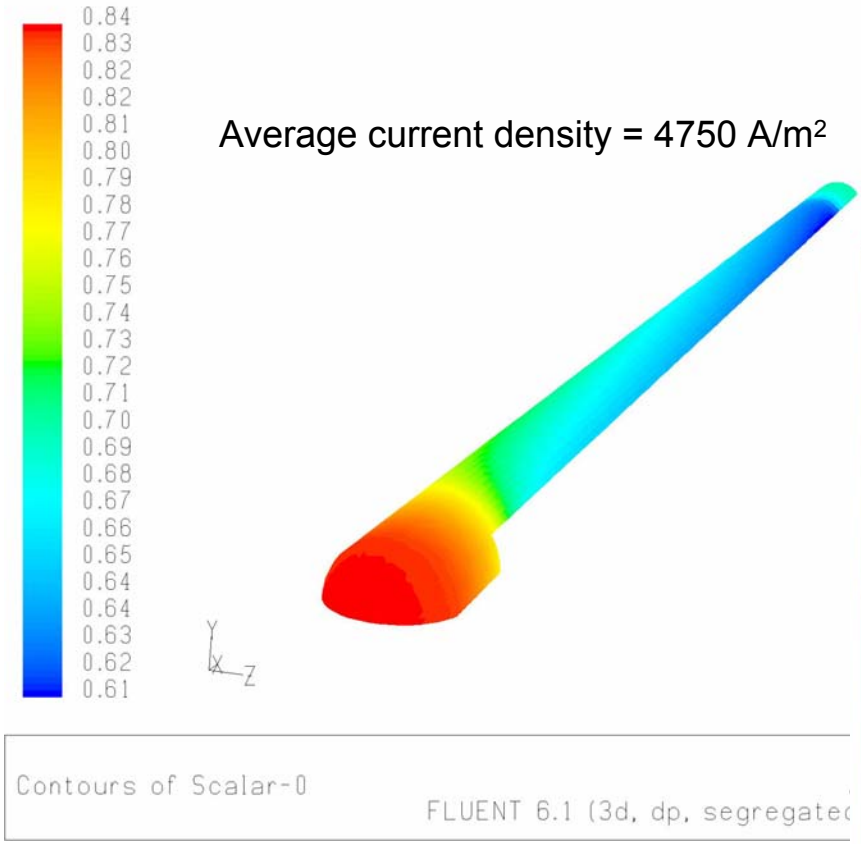


Average current density = 4750 A/m^2

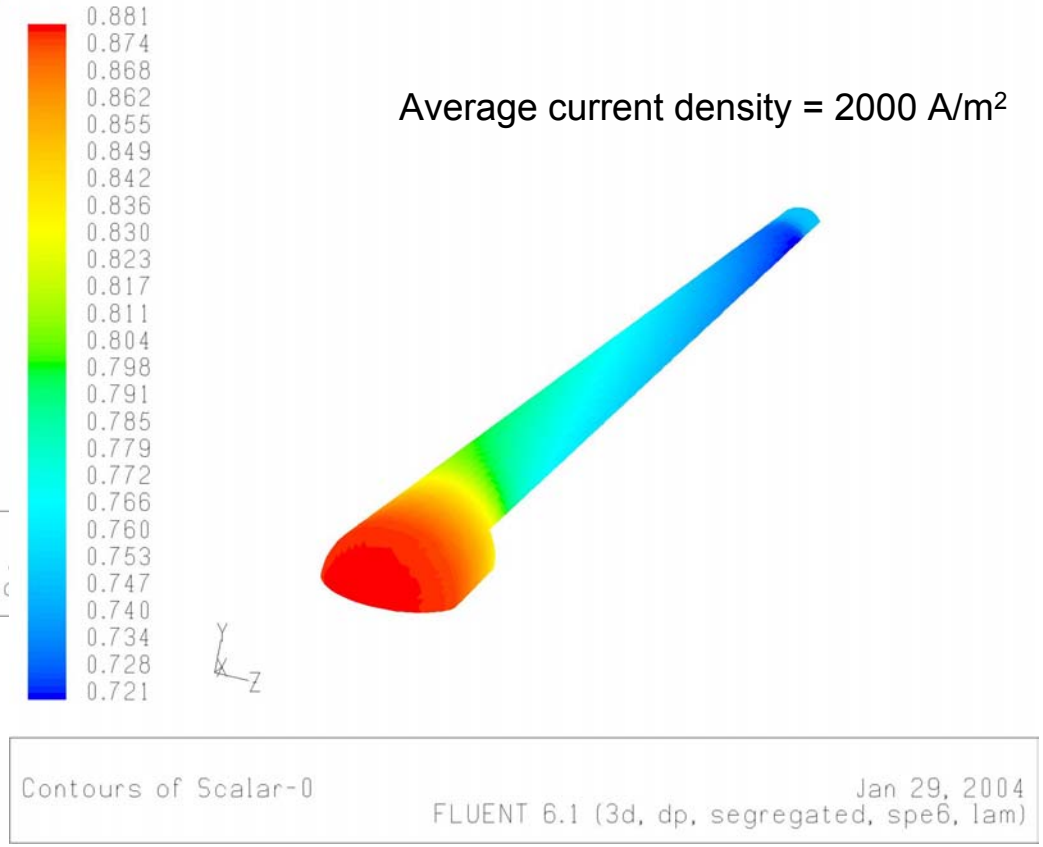


Average current density = 2000 A/m^2

Current density contours on the electrolyte surface



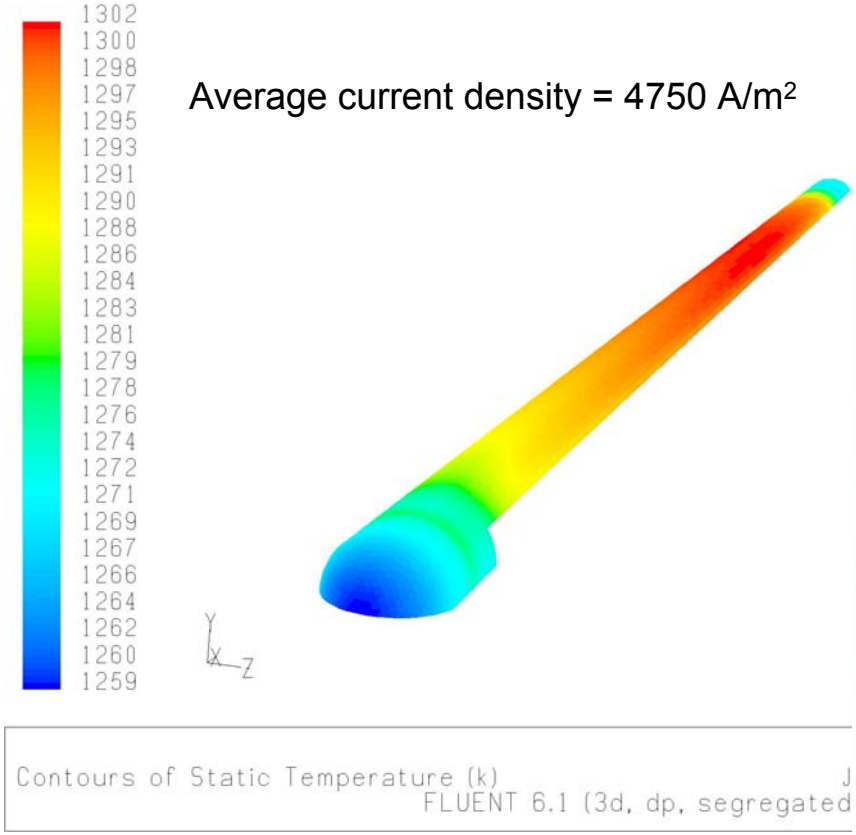
Average current density = 4750 A/m^2



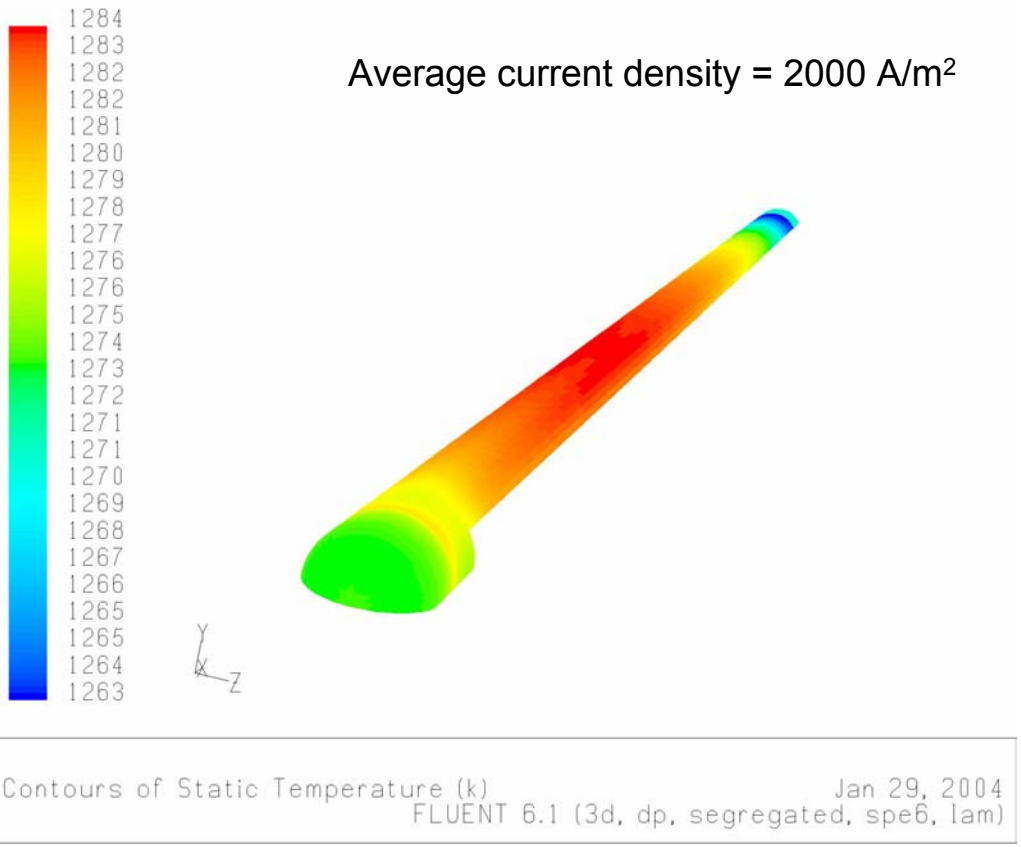
Average current density = 2000 A/m^2

Voltage contours on the electrolyte surface

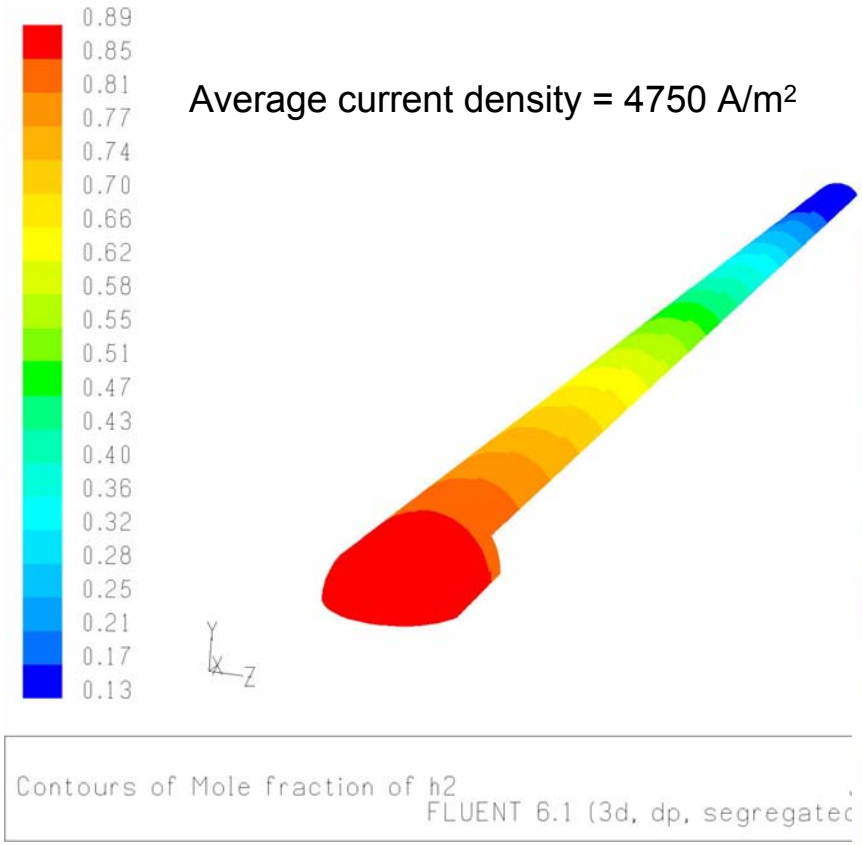
Average current density = 4750 A/m^2



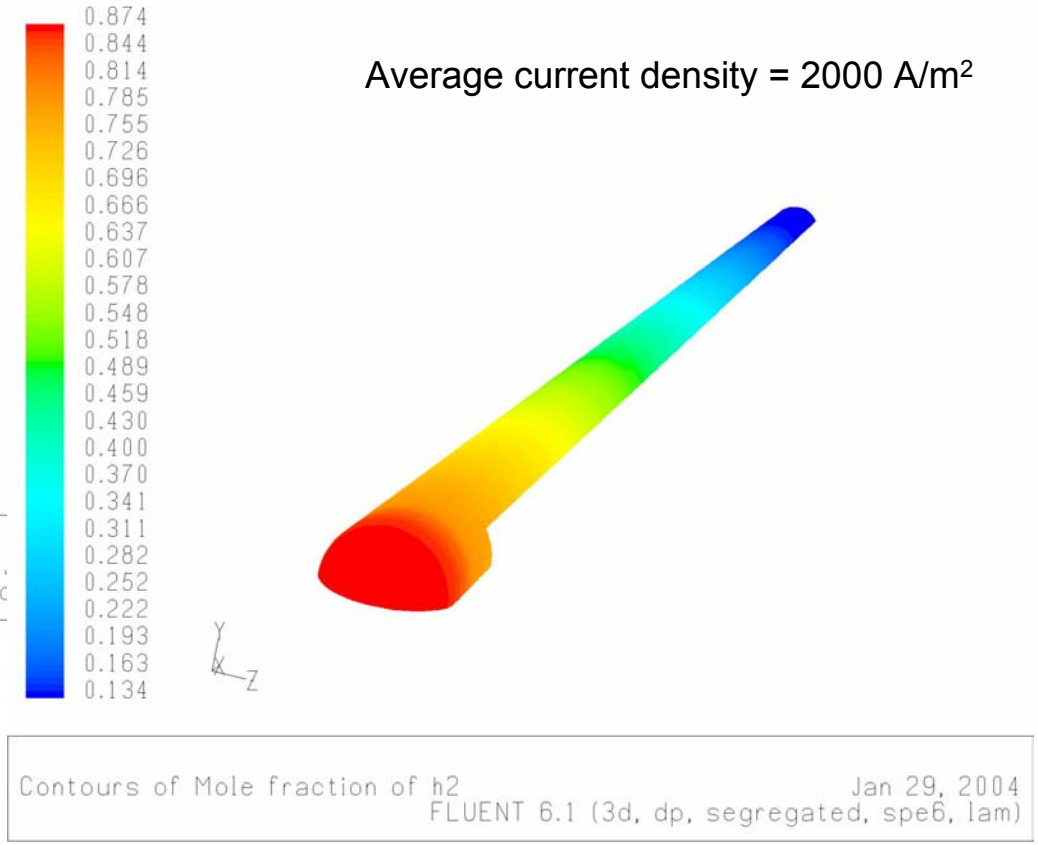
Average current density = 2000 A/m^2



Temperature contours on the electrolyte surface



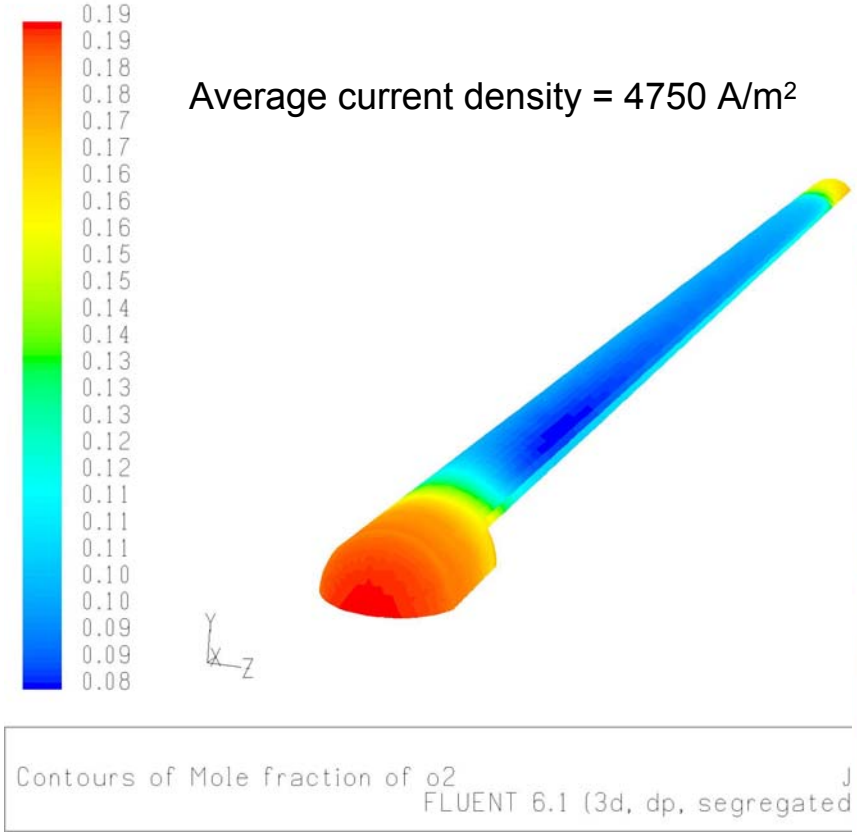
Average current density = 4750 A/m^2



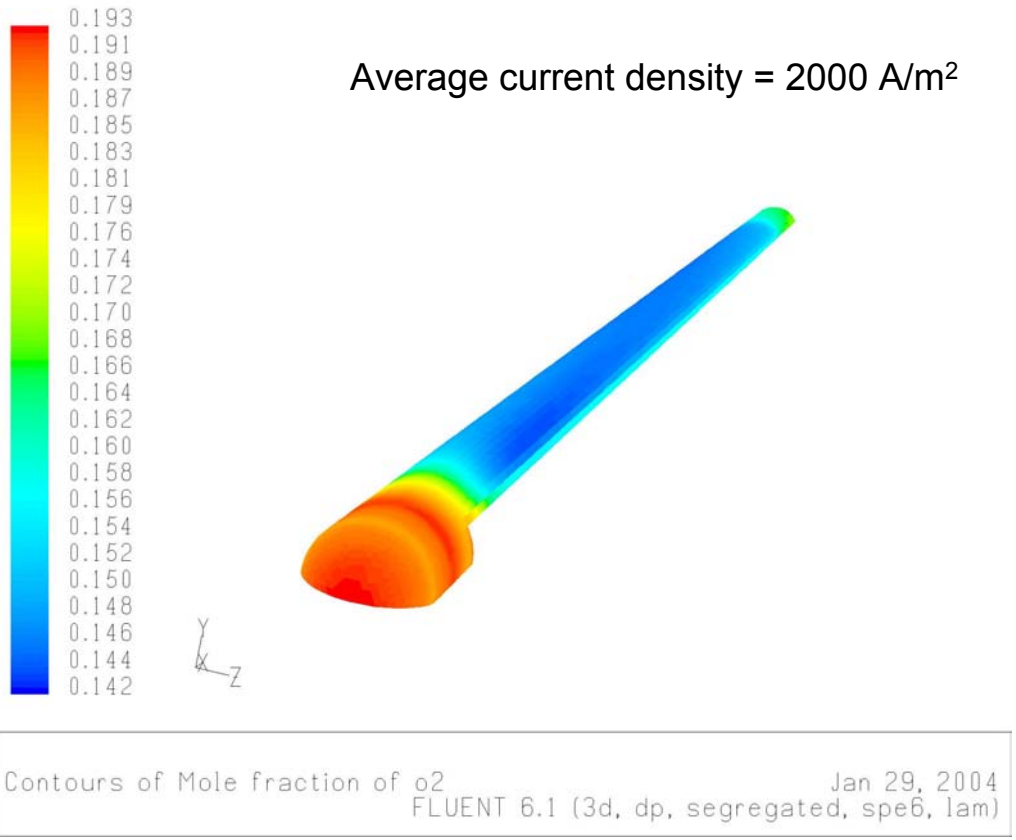
Average current density = 2000 A/m^2

H_2 mole fraction contours on the electrolyte surface

Average current density = 4750 A/m^2

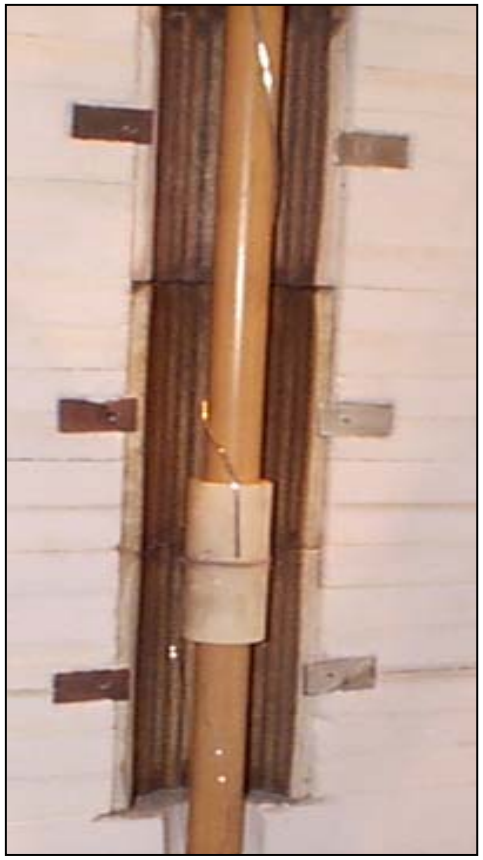


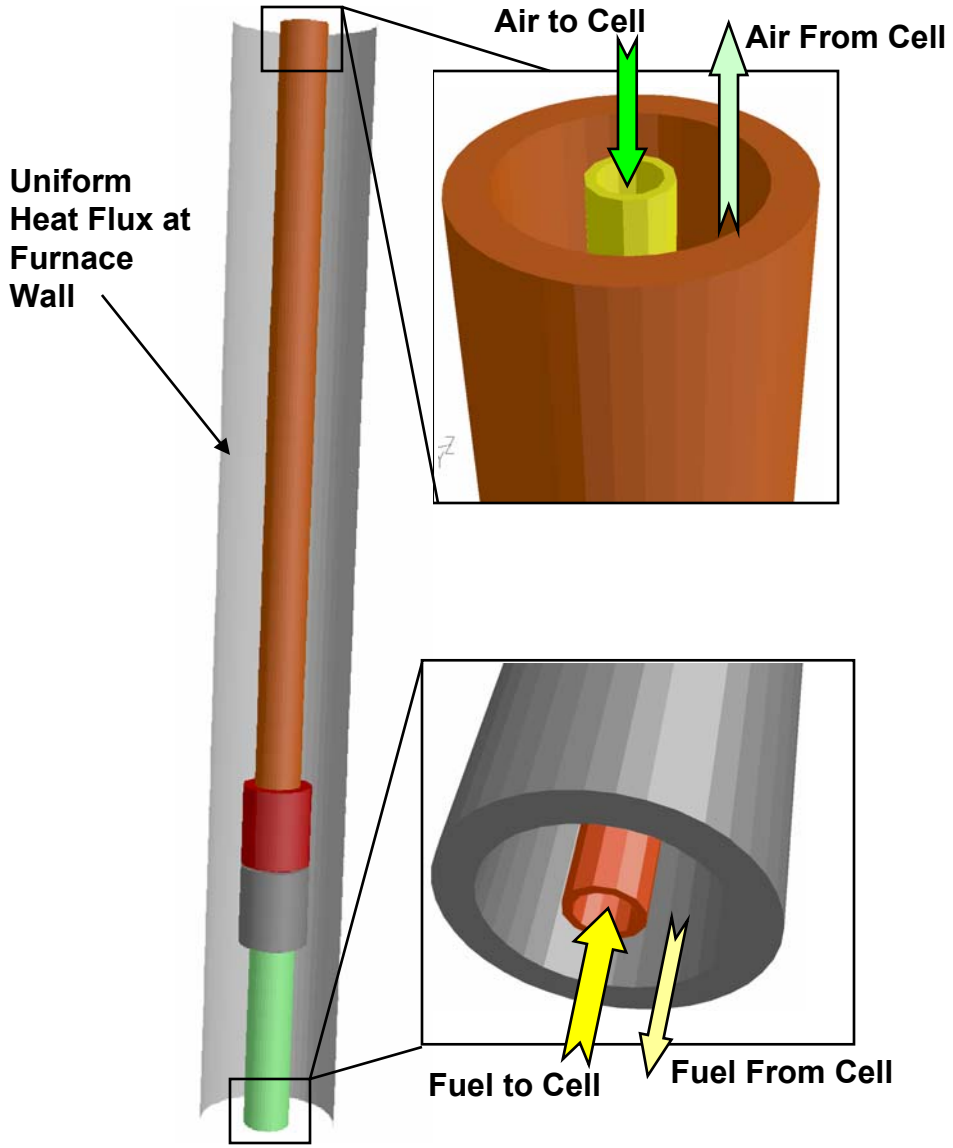
Average current density = 2000 A/m^2



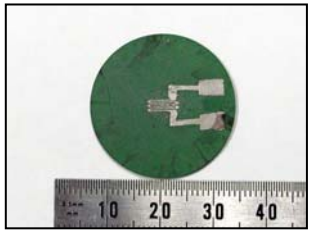
O_2 mole fraction contours on the electrolyte surface

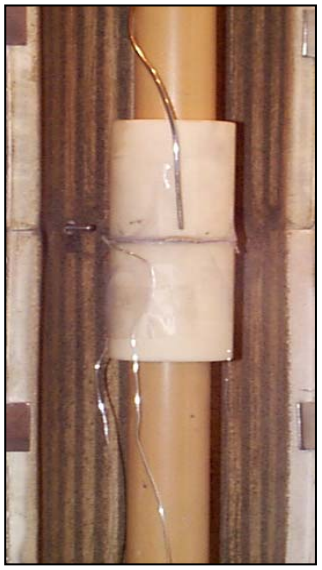
Validation Application: Button Cell

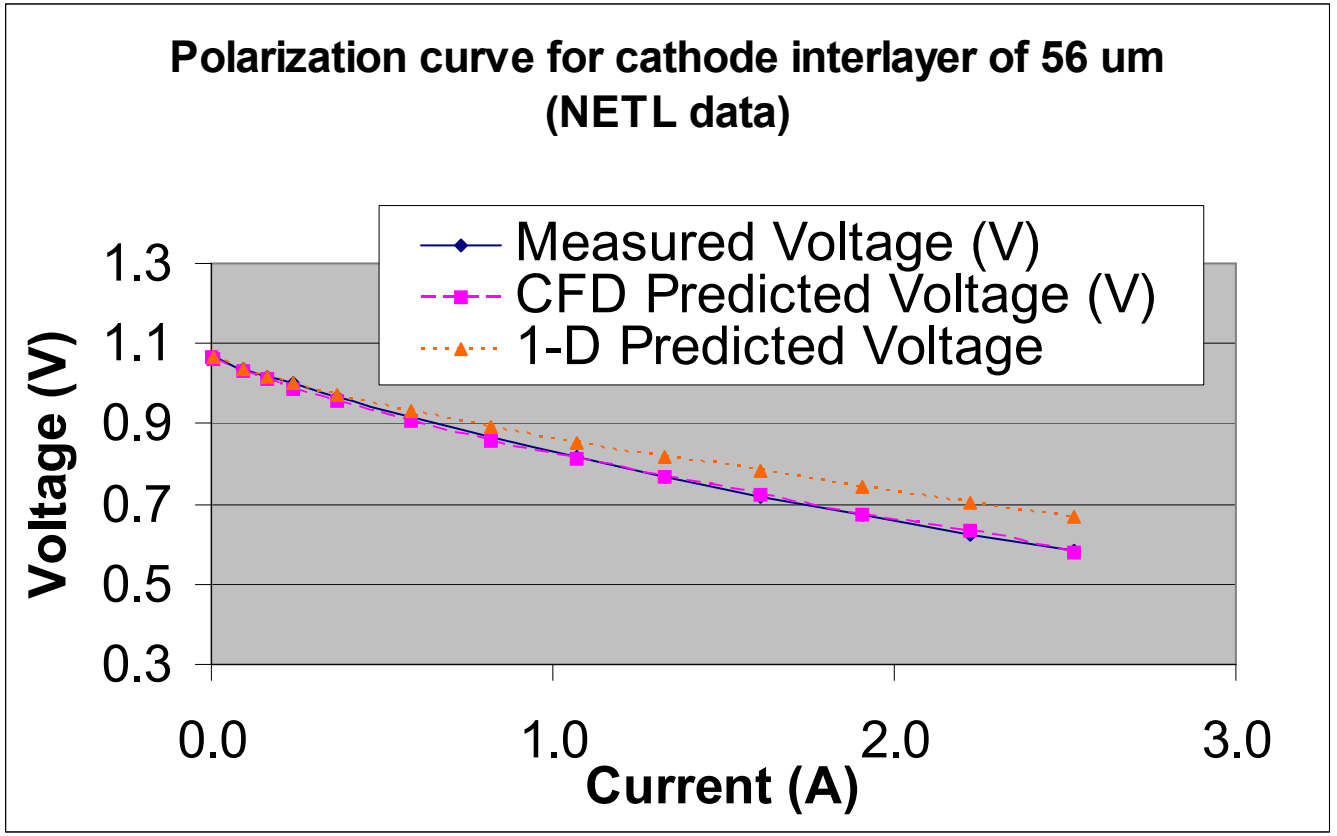




Validation Application: Button Cell

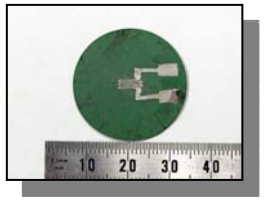


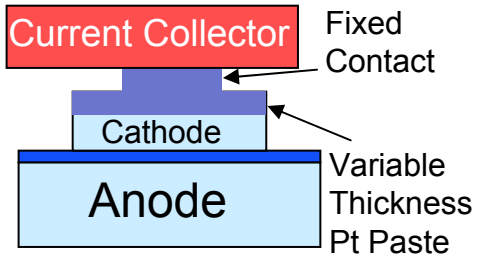




2.14 cm^2 active area; 859 deg. C
Io=0.12 A/cm^2
Contact Resistance=0.19ohm-cm^2

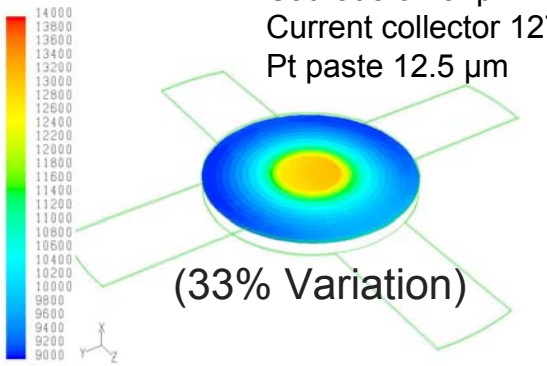
Fuel Cell Modeling
--Sensitivity Study--





(gas diffusion in Pt paste ignored)

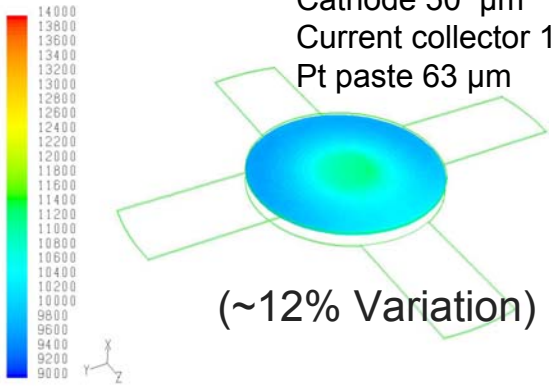
Cathode 37.5 μm
Current collector 127 μm
Pt paste 12.5 μm



(33% Variation)

Current Density in Electrolyte (A/m2)

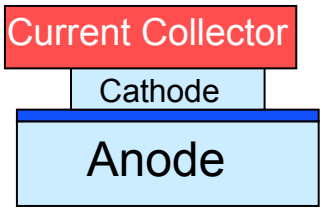
Cathode 50 μm
Current collector 127 μm
Pt paste 63 μm



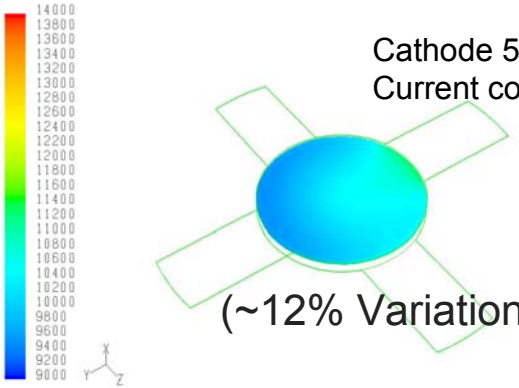
(~12% Variation)

Current Density in Electrolyte (A/m2)

Full Collector
Contact to
Cathode



Cathode 50 μm
Current collector 127 μm



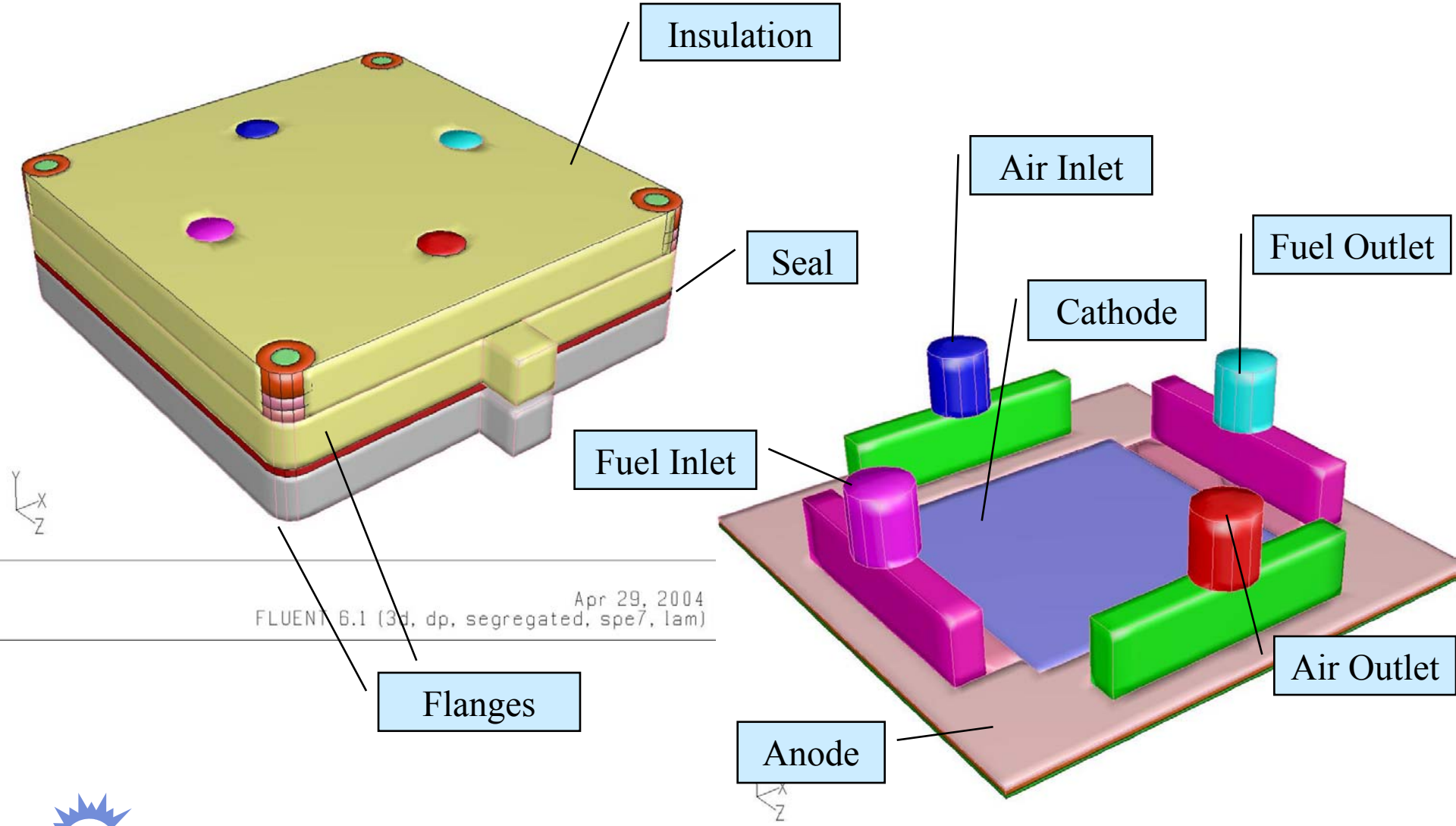
(~12% Variation)

Current Density in Electrolyte (A/m2)

Concept Planar Fuel Cell

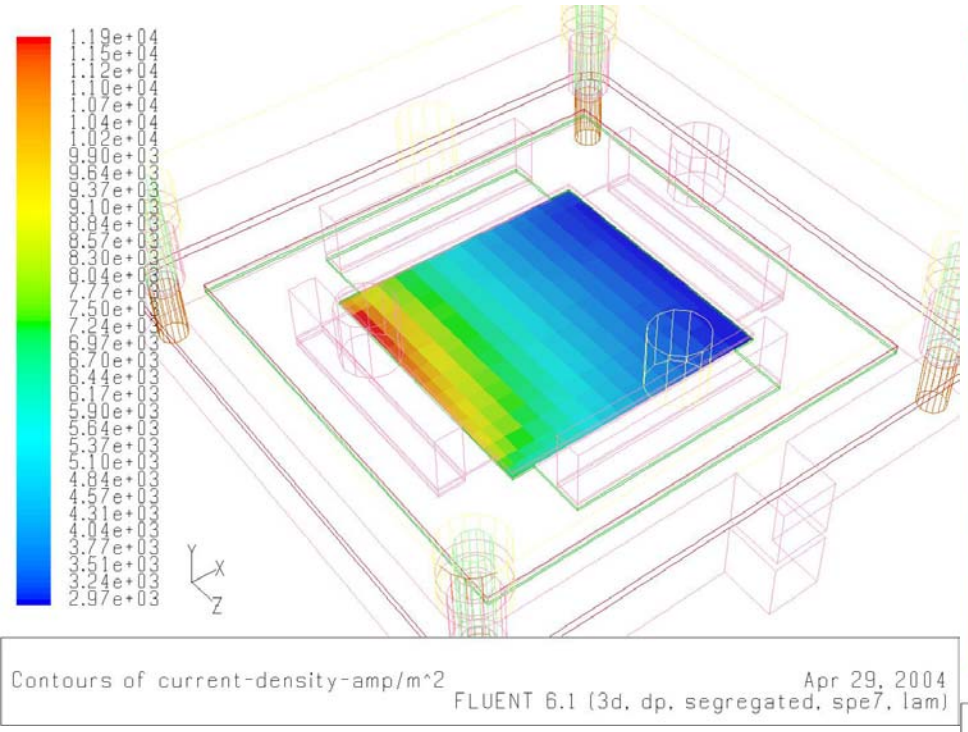
- **Realistic geometric complexity**
- **Anode supported**
- **Includes manifolds, interconnects, current collectors, top and bottom flanges with current taps, insulation, and seals**
- **Completely resolves both electrodes and porous current collectors.**
- **Approximately 67,000 computational cells. Requires ~10 minutes to converge (0.1 mV tolerance) on a 2.8 GHz Pentium4.**
- **Fuel cell configuration is "modular" so that it can be stacked.**
- **Two separate cases:**
  - CO/H_2 electrochemistry via water-gas shift reaction
  - CH_4 internal steam reformation and water-gas shift

SECA Concept Cell - Assembly

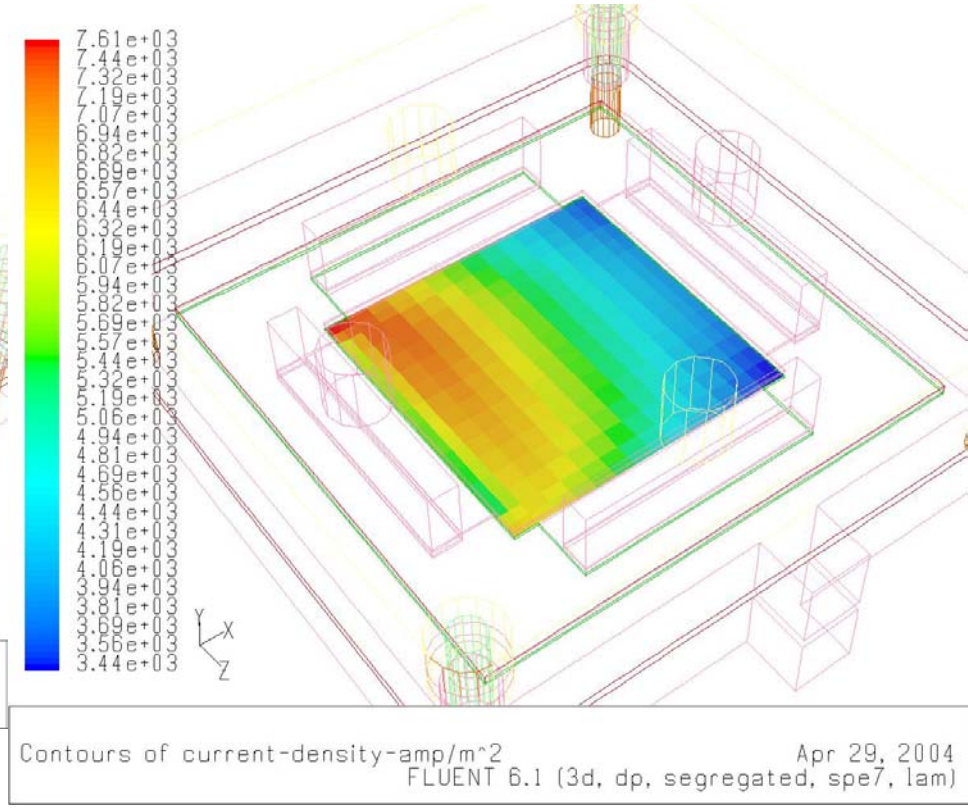


SECA Concept Cell – Current Density H_2/CO and $H_2/CO/CH_4$

Water-Gas Shift

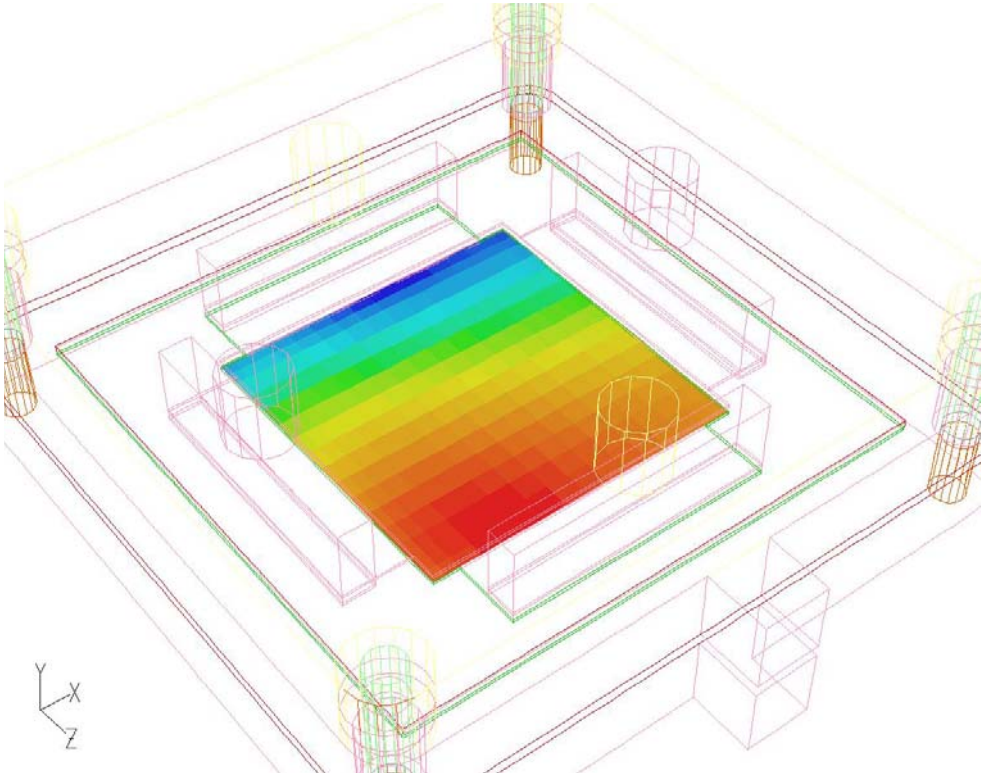


Methane steam reformation plus Water-Gas Shift

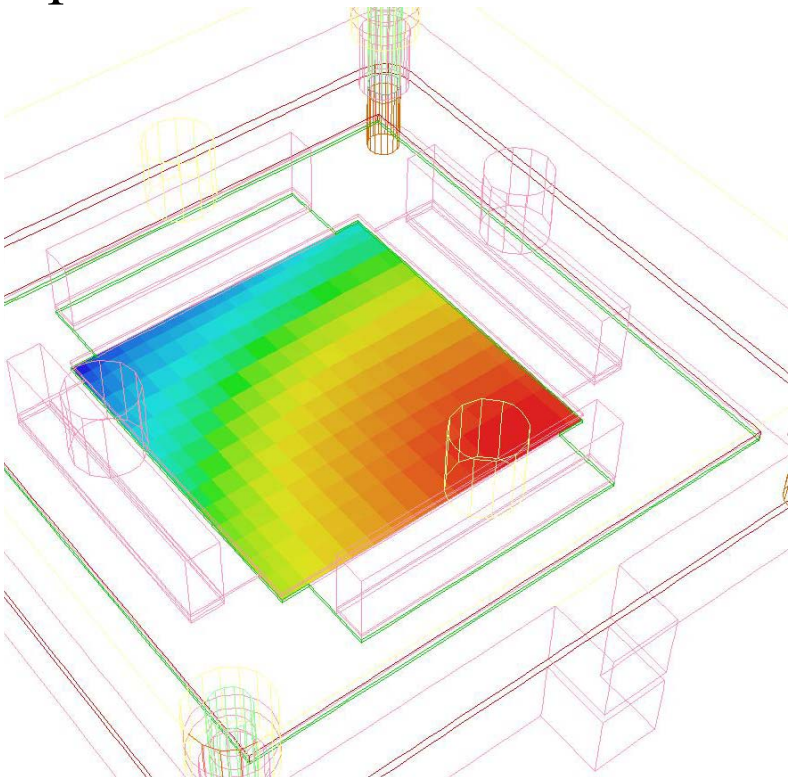


SECA Concept Cell – Anode Temperature H_2/CO and $H_2/CO/CH_4$

Water-Gas Shift



Methane steam reformation plus Water-Gas Shift

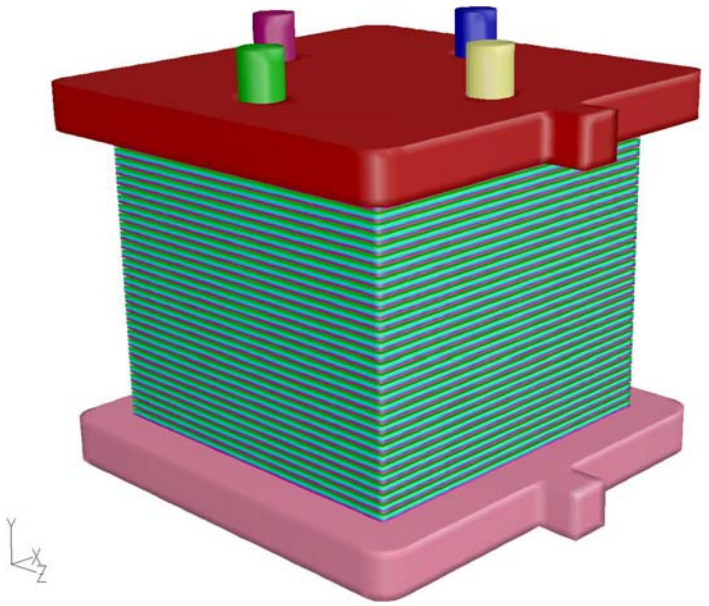


Concept Planar Stack

- **32 fuel cells of the previous design stacked, using the same manifolds and flanges.**
- **Approximately 900,000 computational cells, solution time was ~6 hours on an single 2.8 GHz Intel Pentium4 with 2 GBs of RAM.**
- **Model details:**
  - Running only on hydrogen, though other fuels and reforming chemistry can be added
  - Total system current 20 A
  - Includes metal interconnects
  - 20% Oxygen utilization,

SECA Concept Stack - Assembly

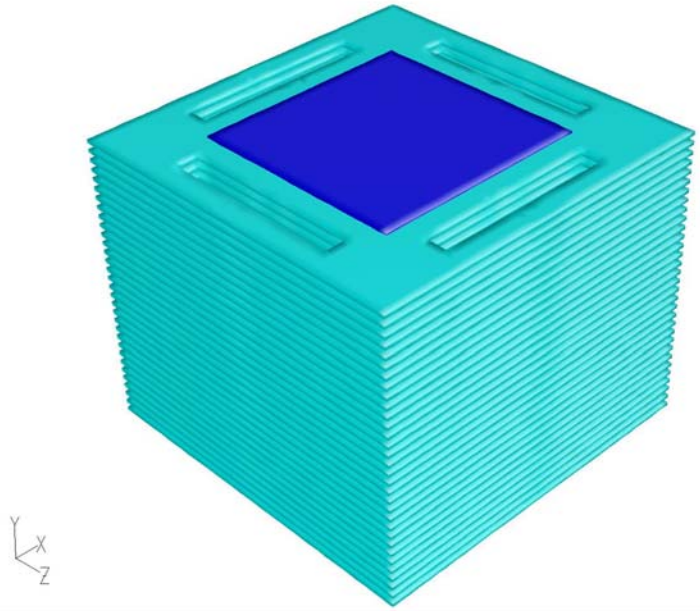
Full Assembly minus Insulation



Grid

May 06, 2004
FLUENT 6.1 (3d, dp, segregated, spe4, lam)

Fuel Cells

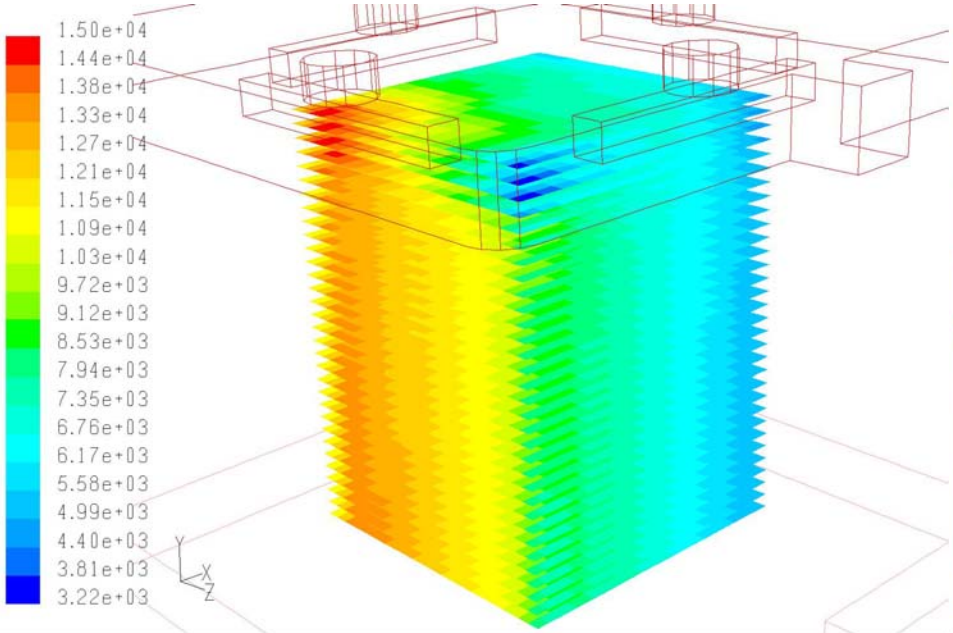


Grid

May 06, 2004
FLUENT 6.1 (3d, dp, segregated, spe4, lam)

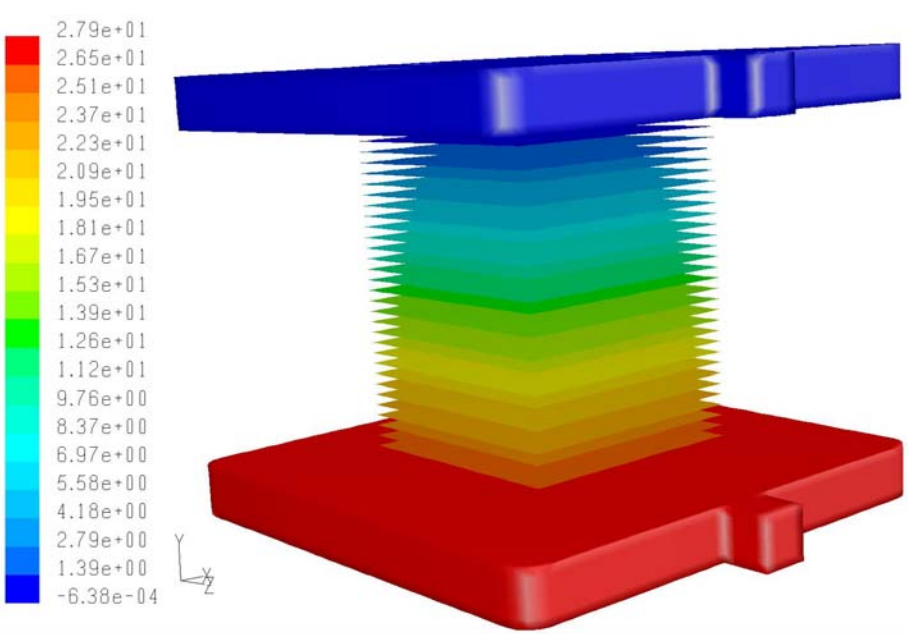
SECA Concept Stack
Current Density and Potential Field

Current Density



Contours of current-density-amp-per-m2
May 06, 2004
FLUENT 6.1 (3d, dp, segregated, spe4, lam)

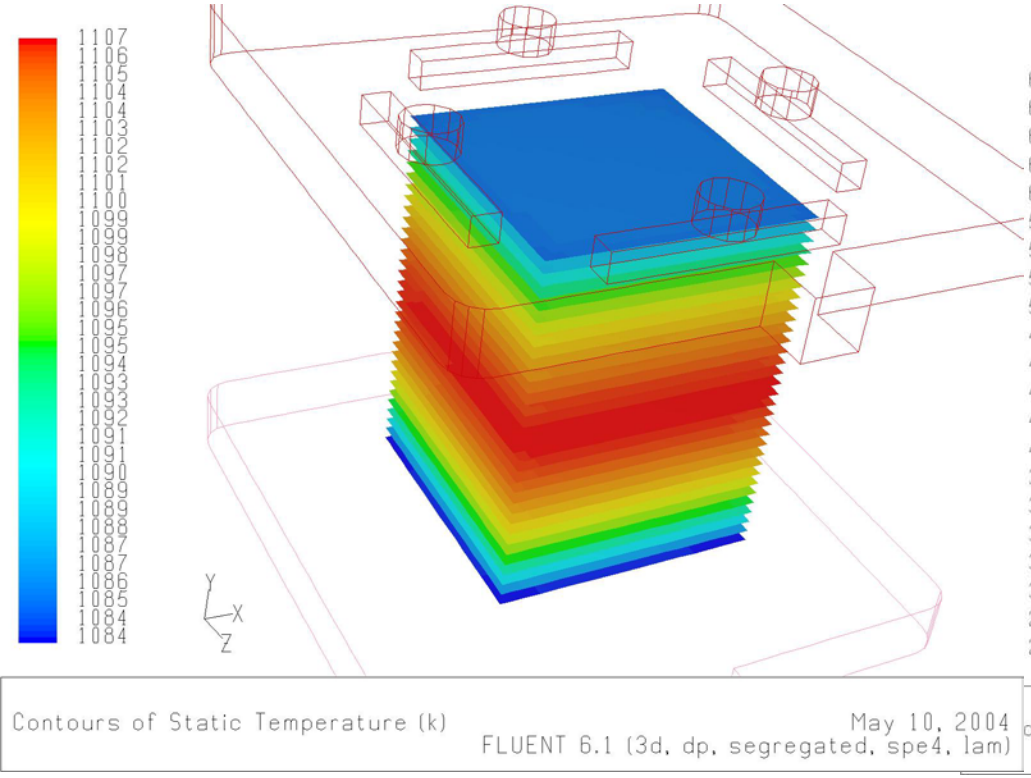
Electrical Potential



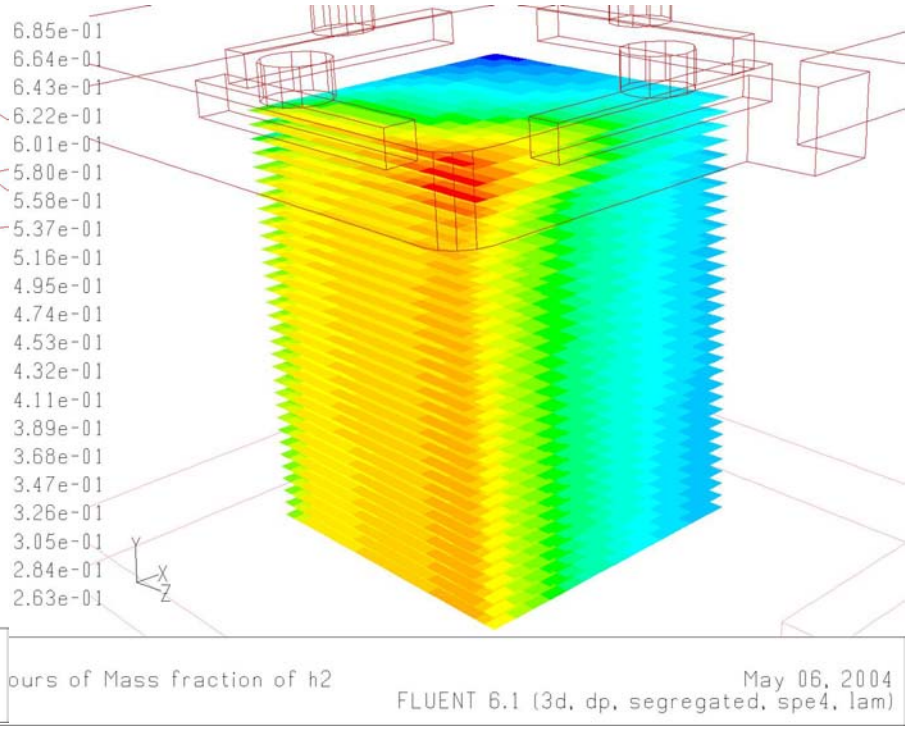
Contours of electric-potential-v
May 06, 2004
FLUENT 6.1 (3d, dp, segregated, spe4, lam)

SECA Concept Stack
Temperature and H_2 Concentration

Anode Temperature



Anode H_2 Mass Fraction



Summary

- The NETL-Fluent SOFC model provides an accurate thermal-fluid representation of SOFC systems, making it an effective design tool for SECA developers.
- Local electrochemical reactions coupling the electric field and the mass, species, and energy transport.
- Electric field solution in all porous and solid cell components, including ohmic heating in the bulk material.
- Ability to use H_2, CO, or CH_4 as fuel via shift and reforming reactions.
- Inclusion of tortuosity for porous regions
- Ability to treat an arbitrary number of electrochemical cells arrayed as a stack.
- Significant geometric flexibility for treating planar, tubular, and other nonstandard SOFC configurations.