Solid Oxide Fuel Cell Modeling with FLUENT

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The Right Answer in CFD

NETL SOFC Fuel Cell Modeling Team

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- SOFC Modeling effort with FLUENT started in 1999.
- SOFC Model has undergone three major revisions since that time
  - Including more physics
  - Increase robustness and geometric flexibility

Fuel Cell Technologies

- Fuel cells are categorized by the electrolyte type they use. Major fuel cell technologies are:
  - Polymer Electrolyte Membrane Fuel Cells (PEMFC)
  - Alkaline Fuel Cells (AFC)
  - Phosphoric Acid Fuel Cells (PAFC)
  - Molten Carbonate Fuel Cells (MCFC)
  - Solid Oxide Fuel Cells (SOFC)

Fuel Cell Technologies

- Of the five major fuel cell types, fuel cells modeled with FLUENT are
  - Polymer Electrolyte Membrane Fuel Cells (PEMFC)
  - Alkaline Fuel Cells (AFC)
  - Phosphoric Acid Fuel Cells (PAFC)
  - Molten Carbonate Fuel Cells (MCFC)
  - Solid Oxide Fuel Cells (SOFC)

Summary of the “1-D” PEMFC Model

- MEA layer is treated a reaction layer and ion transport is not modeled.
- Current density is computed based on the local Nernst potential, activation losses, and MEA resistivity.
- Source terms are computed for the mass, species, and energy equations based on the current density.
- Since the MEA layer is not resolved, fewer computational cells are required than other approaches.
- This reduced MEA model requires more experimental correlations and submodels.

Summary of the “3-D” PEMFC Model

- The catalyst layers and the membrane (MEA) are fully resolved for accurate modeling of electrochemical reactions, water formation and transport
- Two electro potential fields (for electrons and ions) are solved which play a role in determining the local current density
- Water transport, contact resistance, joule heating, reaction heating, phase-change, transient effects, etc. included
- Fully-implicit numerical treatment; fully parallel
- User-friendly setup: GUI input
- Friendly environment for users to implement their own models via User-Defined Functions (UDF) and User-Defined Scalars (UDS)

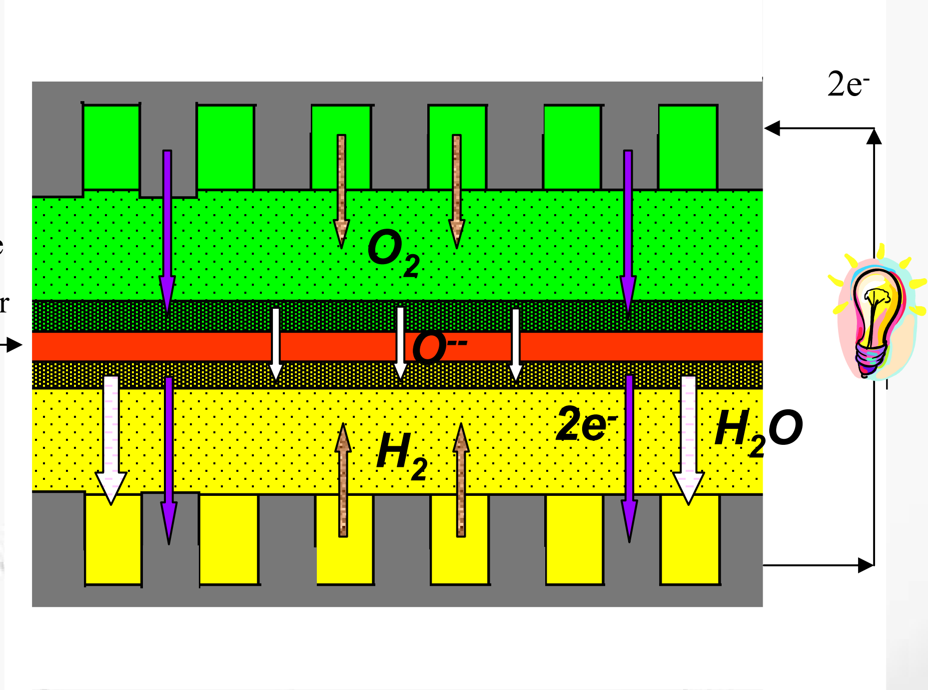
Other Fuel Cell Activities

- SOFC and PEM Reformer modeling
  - Uses FLUENT’s stiff chemistry solver
  - Includes ISAT to significantly (x100) increase the speed of chemistry computations
- Vision21 Integration of Aspen/PLUS and FLUENT
  - Allows flowsheet-type analyses with CFD-level detail as needed
  - Currently using the SOFC model in FLUENT as a component

SOFC

- Solid Oxide Fuel Cell (SOFC)
  - *Electrolyte:* solid zirconium oxide with ytrria
  - *Operating Temperature:* 600 – 1000 ^{o}C
  - *Application:* large electrical power generation
  - *Advantages:* inexpensive catalyst, higher efficiency, internal reforming, better match with small gas turbines
  - *Disadvantages:* high temperature enhances breakdown of cell components, gas sealing difficult

SOFC



Cathode
- Current collector
- Flow channel
- Cathode electrode
- Cathode interlayer

Electrolyte

Anode
- Anode interlayer
- Anode electrode
- Flow channel
- Current collector

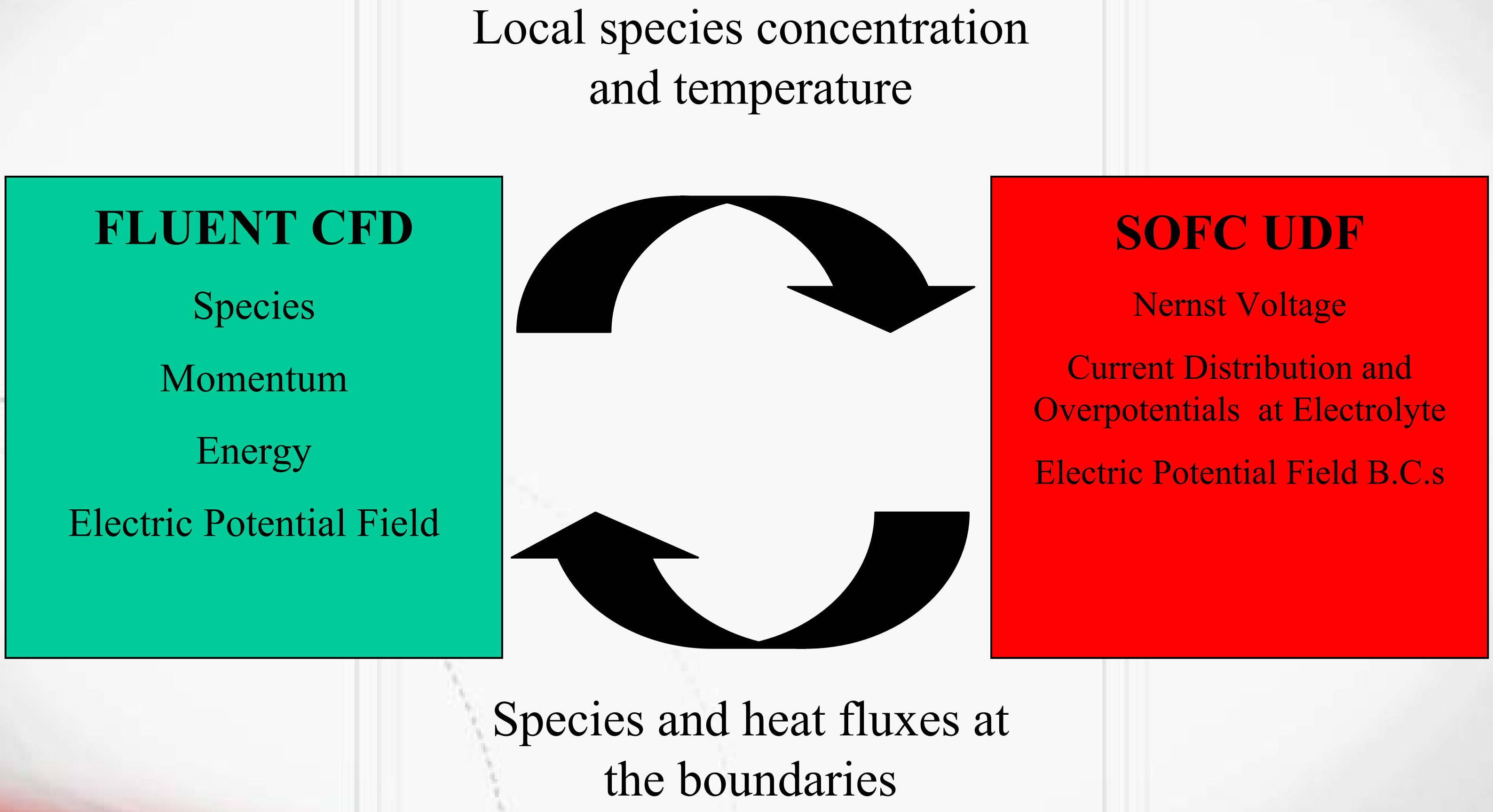
Fuel Cell Modeling

- SOFC modeling requires modeling of:
  - Fluid flow, heat transfer, and mass transfer in porous media (anode and cathode)
  - Electrochemical reactions
  - Transport of current and potential field in porous media and solid conducting regions

SOFC Modeling

- FLUENT handles all aspects of the hydrodynamics, species transport and heat transfer in the flow channels and the porous electrodes (anode and cathode).
- A User Defined Function (UDF) is used to model
  - electrochemical reactions
  - potential field in the electrically conducting zones
- The model is parallelized and shows identical scaling to normal Parallel FLUENT. The fuel cell model is only a small computation
- Includes treatment for CO/H2 electrochemistry
- The model has been tested for stack configurations
- The model has also been used in a transient CFD simulation (with the electrochemistry assumed quasi-steady

SOFC Modeling



Local species concentration and temperature

FLUENT CFD

Species

Momentum

Energy

Electric Potential Field

SOFC UDF

Nernst Voltage

Current Distribution and Overpotentials at Electrolyte

Electric Potential Field B.C.s

Species and heat fluxes at the boundaries

SOFC Models

- ***Electrochemical Model:*** predicts local current density, voltage distributions.

- ***Electric Potential Field Model:*** predicts current and voltage in porous and solid conducting regions along with contact resistance.

SOFC Models

- **Electrochemical Model**
- Electric Potential Field Model

Electrochemical Model

- The general electrochemical reaction is*

$$\sum_{j}^{N} a_j A_j \Leftrightarrow n e^{-}$$

a_j stochiometric coefficient of species *i*

A_j chemical species

n number of electrons

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* J.S. Newman, "Electrochemical Systems", Prentice Hall, Englewood Cliffs, New Jersy, 1973.

Electrochemical Model

- The rate of Consumption or destruction of the species is

$$S = -\frac{a\, i}{n\, F} \quad \text{(g-mole/sec)}$$

S source or sink of species

a stochiometric coefficient

i current

n number of electrons per mole of fuel

F Faraday constant

Electrochemical Model

- Electrochemical reduction of oxygen at the cathode:

$$1/2O_2 + 2e^- \Leftrightarrow O^{2-} \qquad (SOFC)$$

- Electrochemical oxidation of hydrogen at the anode:

$$H_2 + O^{2-} \Leftrightarrow H_2O + 2e^- \qquad (SOFC)$$

Electrochemical Model

- By convention*, the current density is positive when it flows from the electrode into the solution (electrolyte)

- The current densities are positive at the anodes

- The current densities are negative at the cathode

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* J.S. Newman, “Electrochemical Systems”, Prentice Hall, Englewood Cliffs, New Jersy, 1973.

Electrochemical Model

- In SOFC at the anode electrode:

$$H_2 + O^{--} \Leftrightarrow H_2O + 2e^- \qquad or \qquad H_2 + O^{--} - H_2O \Leftrightarrow 2e^-$$

$$S_{H_2} = -\frac{i}{2F}$$

g-mole/s of H_2 is consumed

$$S_{H_2O} = -\frac{(-1)\,i}{2F} = \frac{i}{2F}$$

g-mole/s of H_2O is produced

$$S_{O^{--}} = -\frac{i}{2F}$$

g-mole/s of O^{--} is consumed

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Electrochemical Model

- In SOFC at the cathode electrode:

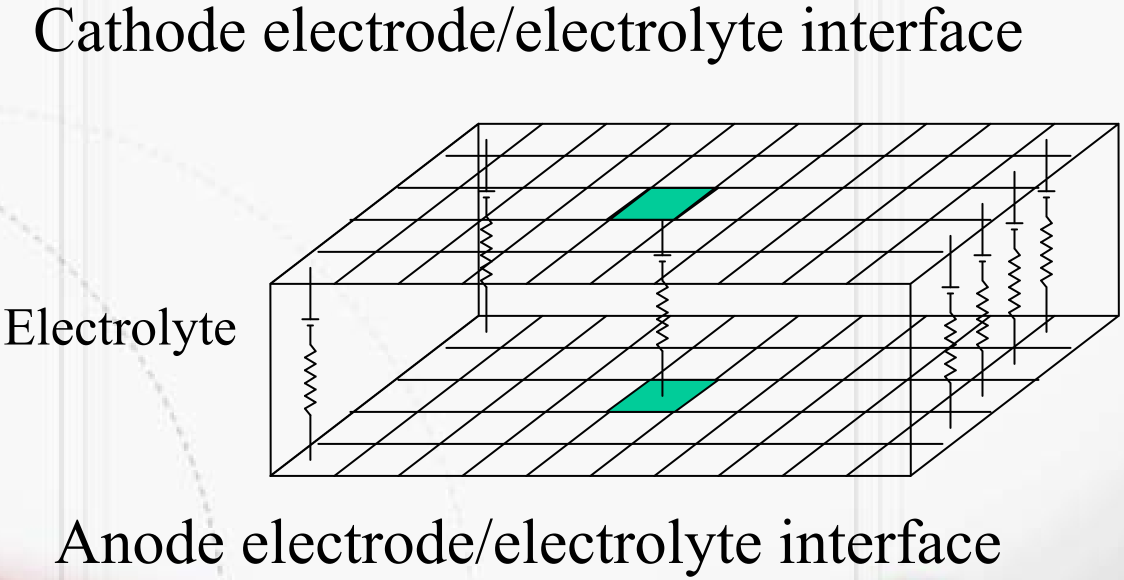
$$\frac{1}{2}O_2 + 2e^- \Leftrightarrow O^{--} \qquad or \qquad -\frac{1}{2}O_2 + O^{--} \Leftrightarrow 2e^-$$

$$S_{O_2} = -\frac{(-0.5)(-i)}{2F} = -\frac{i}{4F}$$ g-mole/s of O_2 is consumed

$$S_{O^{--}} = -\frac{(-i)}{2F} = \frac{i}{2F}$$ g-mole/s of O^{--} is produced

Electrochemical Model

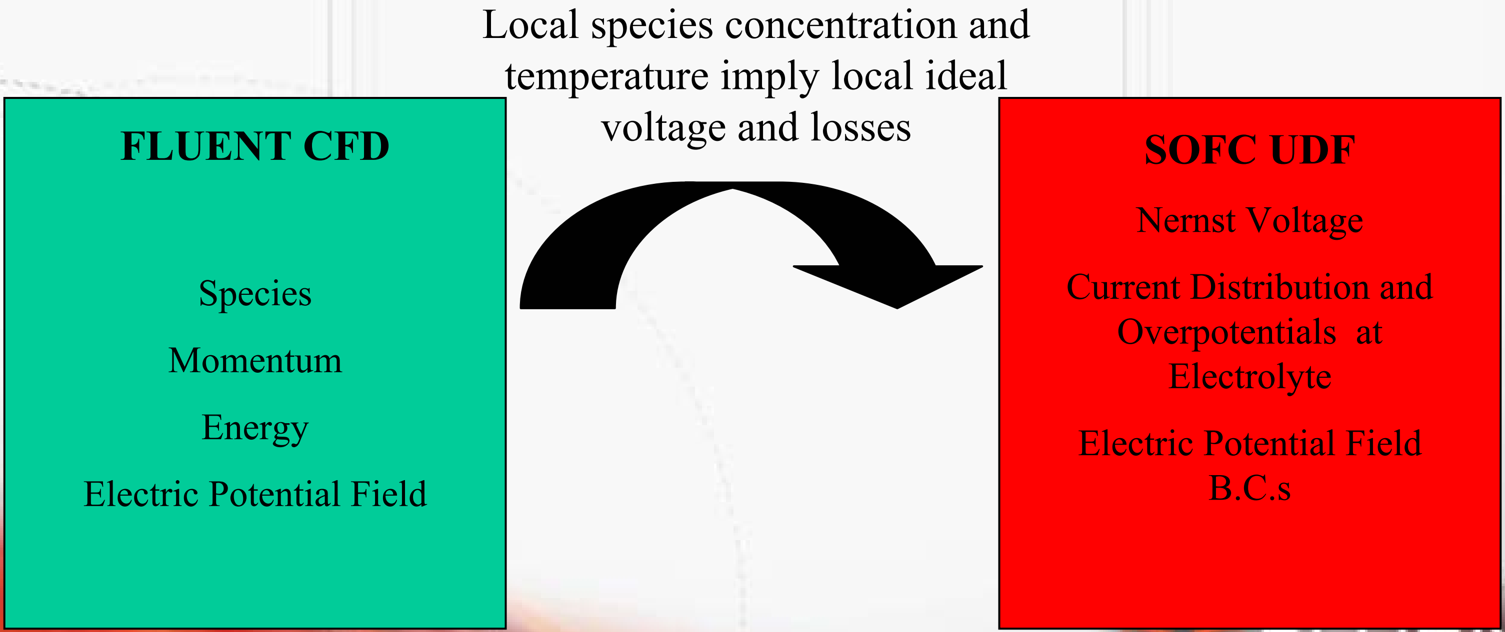
- Assumptions:
  - Due to geometrical considerations, ionic flow across the electrolyte is assumed to be one dimensional.



Electrochemical Model

- Ideal cell potential is calculated by Nernst equation

$$E_{ideal} = -\frac{\Delta G}{nF} = E^{o} + \frac{R\,T}{2F}\ln\left(\frac{p_{H_2}p_{O_2}^{1/2}}{p_{H_2O}}\right)$$



Local species concentration and temperature imply local ideal voltage and losses

FLUENT CFD

Species

Momentum

Energy

Electric Potential Field

SOFC UDF

Nernst Voltage

Current Distribution and Overpotentials at Electrolyte

Electric Potential Field B.C.s

Electrochemical Model

- The terminal cell potential is:

$$E_{actual} = E_{ideal} - \eta_{ohmic} - \eta_{act,a} - \eta_{act,c}$$

where η_{ohmic}, $\eta_{act,\ a}$, and $\eta_{act,\ c}$ represent losses due to ohmic overpotential, activation overpotential at the anode, and activation overpotential at the cathode respectively

Polarization Losses

- Ohmic polarization:
  - Ionic losses through the electrolyte
  - Electrical resistance in the conducting porous electrodes and current collectors
  - Electrical resistance at the interface of the current collectors and the electrodes or the electrodes and the electrolyte (contact resistance)

$$\eta_{ohmic} = i \cdot R$$

Polarization Losses

- Activation polarization:
  - Potential losses due to slowness of electrochemical reactions at the anode and the cathode electrodes

$$i = i_o \left[\exp\left(\frac{\alpha_a \eta_{act} F}{R\,T} \right) - \exp\left(- \frac{\alpha_c \eta_{act} F}{R\,T} \right) \right]$$

Butler-Volmer

where

$$i_0 = a\ i_{0,ref}\ (Y_j)^\gamma$$

a:ratio of active area to membrane geometrical area

$i_{0,ref}$: exchange current density at reference condition

Y_j : mole fraction

γ :concentration exponent

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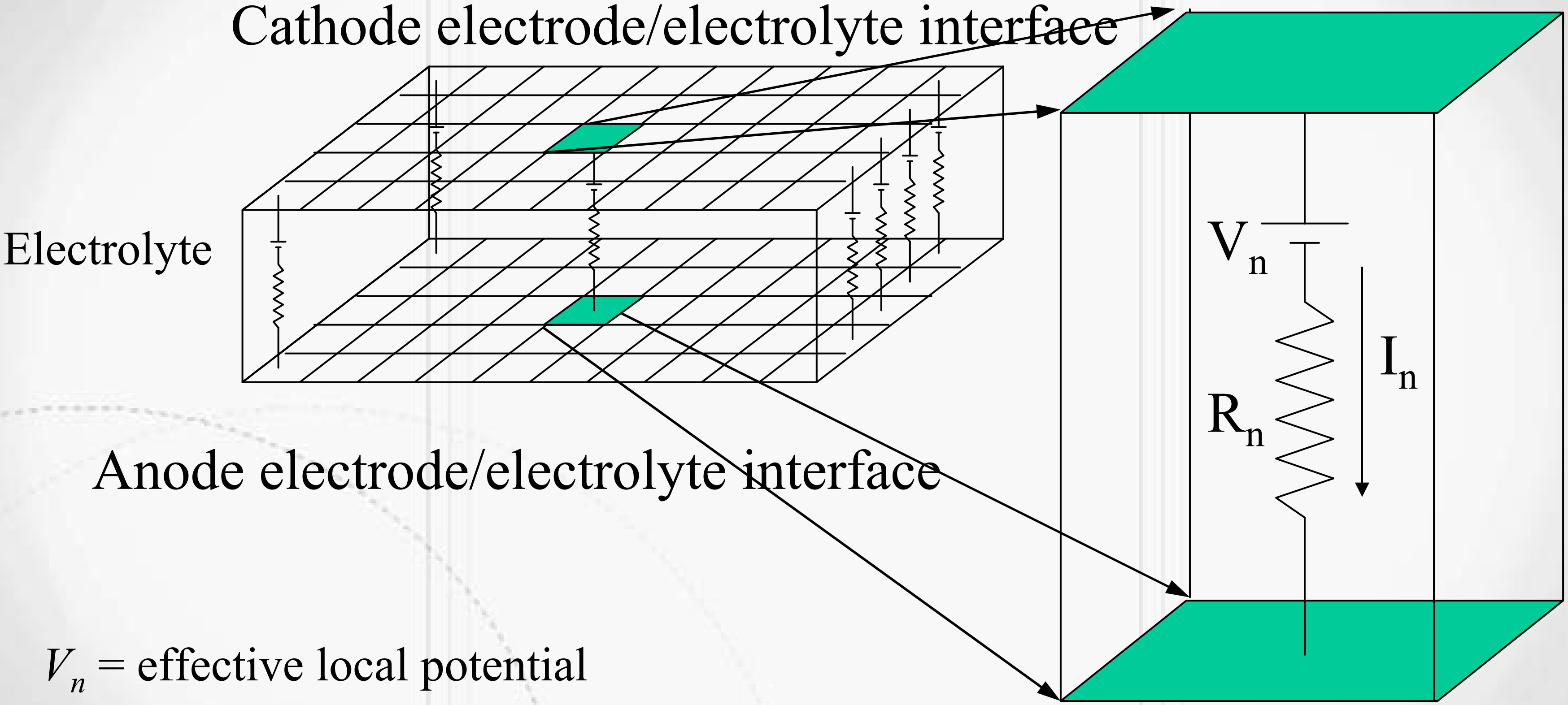
Electrochemical Cell Values

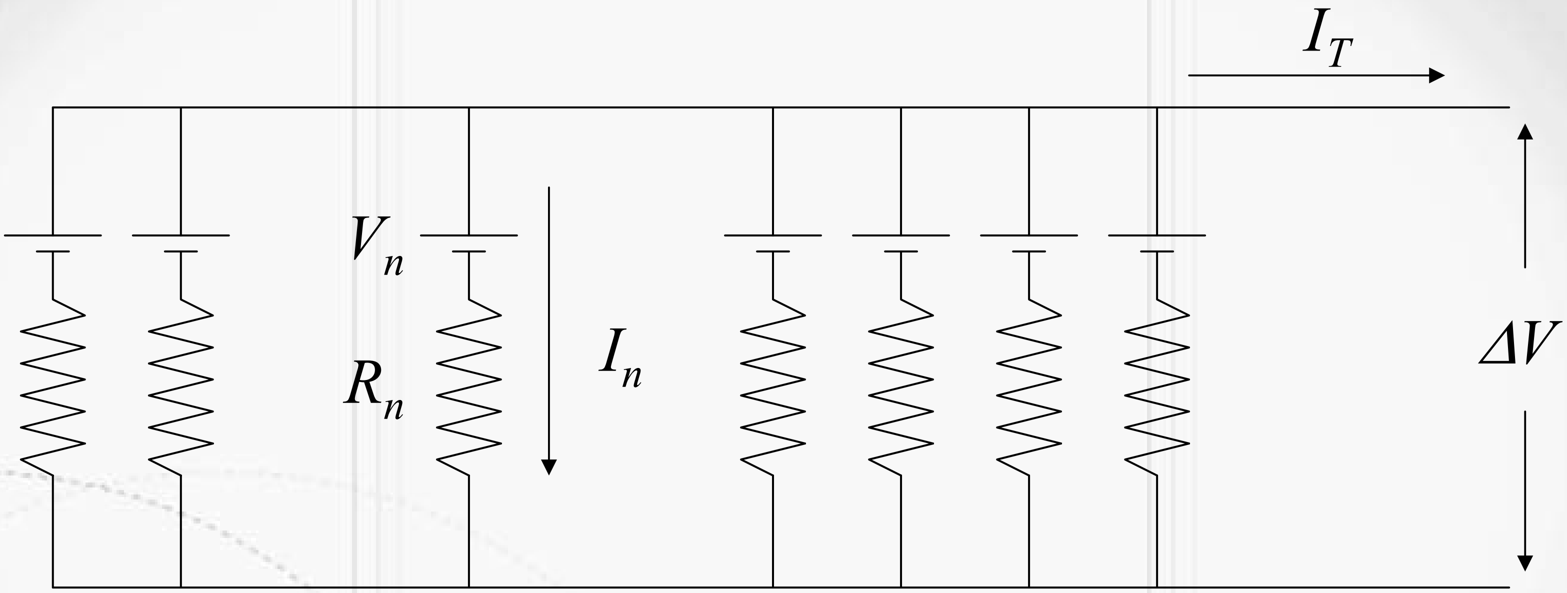


V_n = effective local potential

R_n = effective local resistance

I_n = local current

Electrochemical Model



$\Delta V_n = V_n - I_n R_n$ for each face (n)

$I_T = \Sigma_n I_n$

I_T is the total system current specified as a user input

Species Fluxes

- The species production or destruction term in the species equation is:

$$\frac{i}{nF} M$$

- Using the local current information, the fuel cell model applies species fluxes to the electrode boundaries in the FLUENT simulation.

Fuel Cell Models

- Electrochemical Model
- **Electric Potential Field Model**

Electric Potential Field Model

- Electric potential field model provides:
  - Ohmic losses in the electrically conducting materials (current collectors and electrodes)
  - Contact resistance at appropriate interfaces
  - Ohmic heating through conducting materials as the result of ohmic losses

Electric Potential Field Model

- Electric potential field throughout all conductive regions is calculated by charge conservation

$$\nabla \cdot \underline{i} = 0$$

since

$$\underline{i} = -\sigma \nabla \phi$$

then

$$\nabla \bullet (\sigma \nabla \phi) = 0$$

σ is the electric conductivity

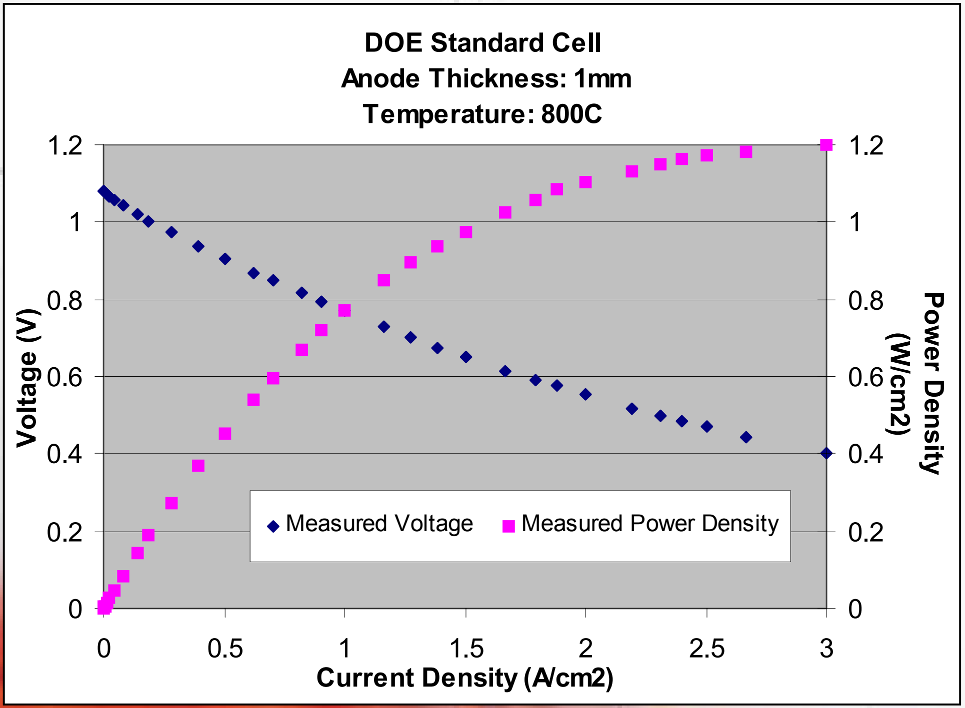
ϕ is the electric potential field

Electric Potential Field Model

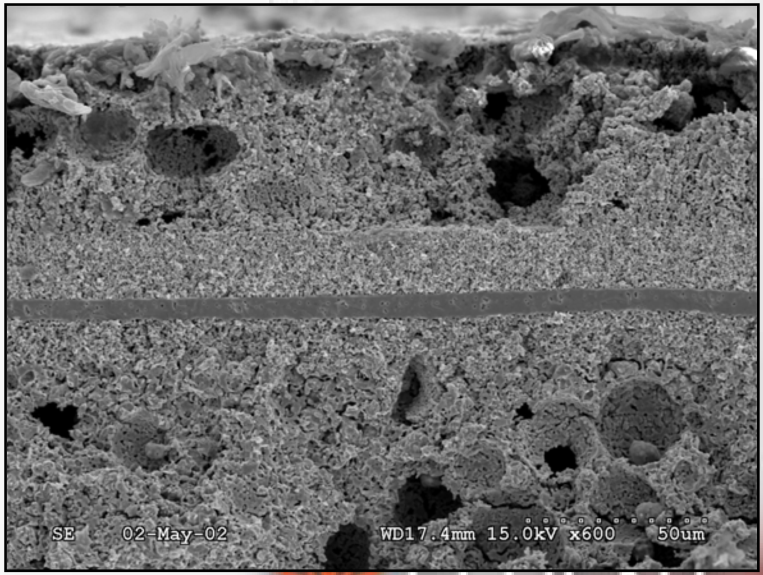
- Changes in electrical potential at the a surface due to contact resistance or electrochemistry is included
- Local current distribution in the conducting regions is used to obtain the ohmic heating (I^2R).
- As more complexity is introduced into the fuel cell geometry, the coupling of the electric field and electrochemistry becomes very important.
  - Tubular cells
  - planar-type cells with small area current collectors

SOFC Model Validation (courtesy of DOE/NETL)

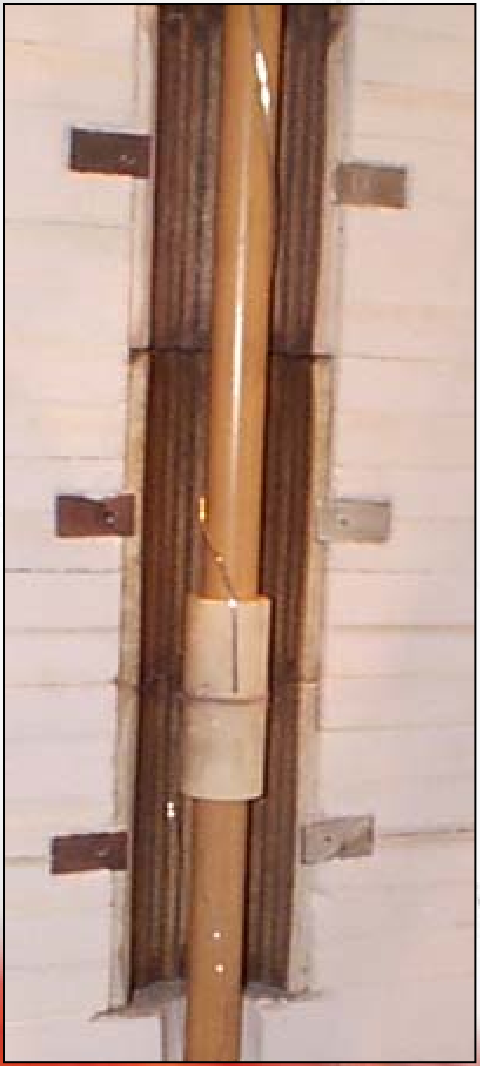
- Validate models with experimental data
  - University of Utah has tested cells and supplied representative performance data

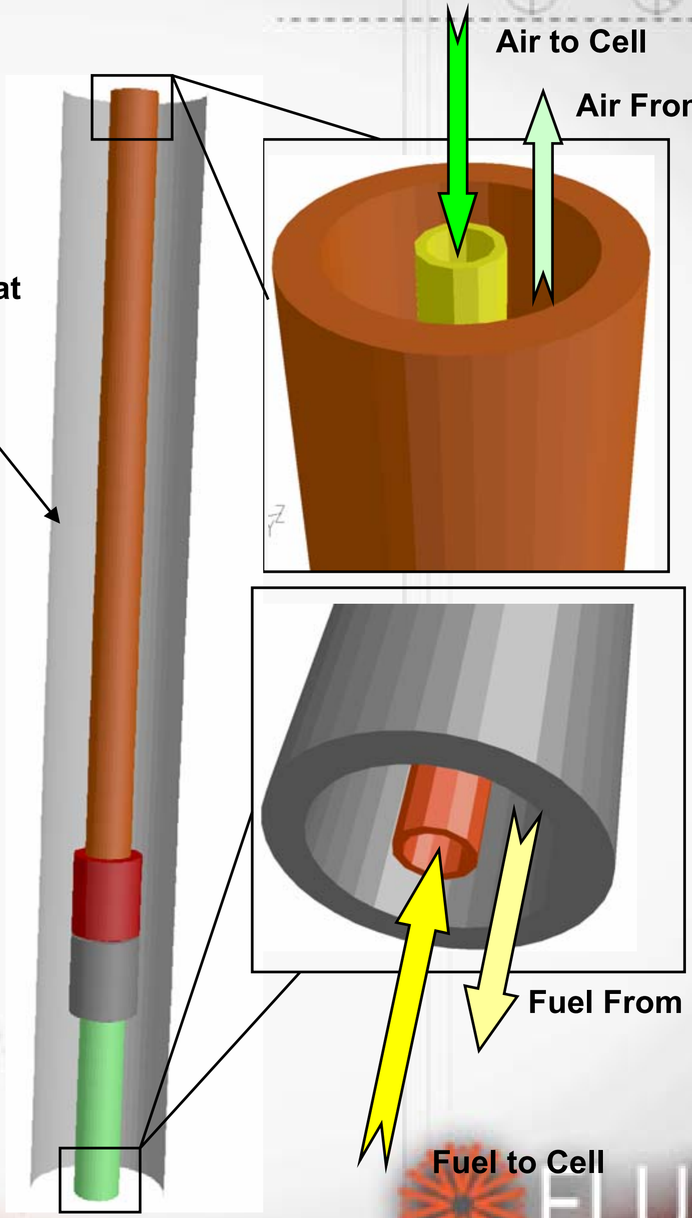


SEM of Standard Button Cell



Courtesy of DOE/NETL





Uniform Heat Flux at Furnace Wall

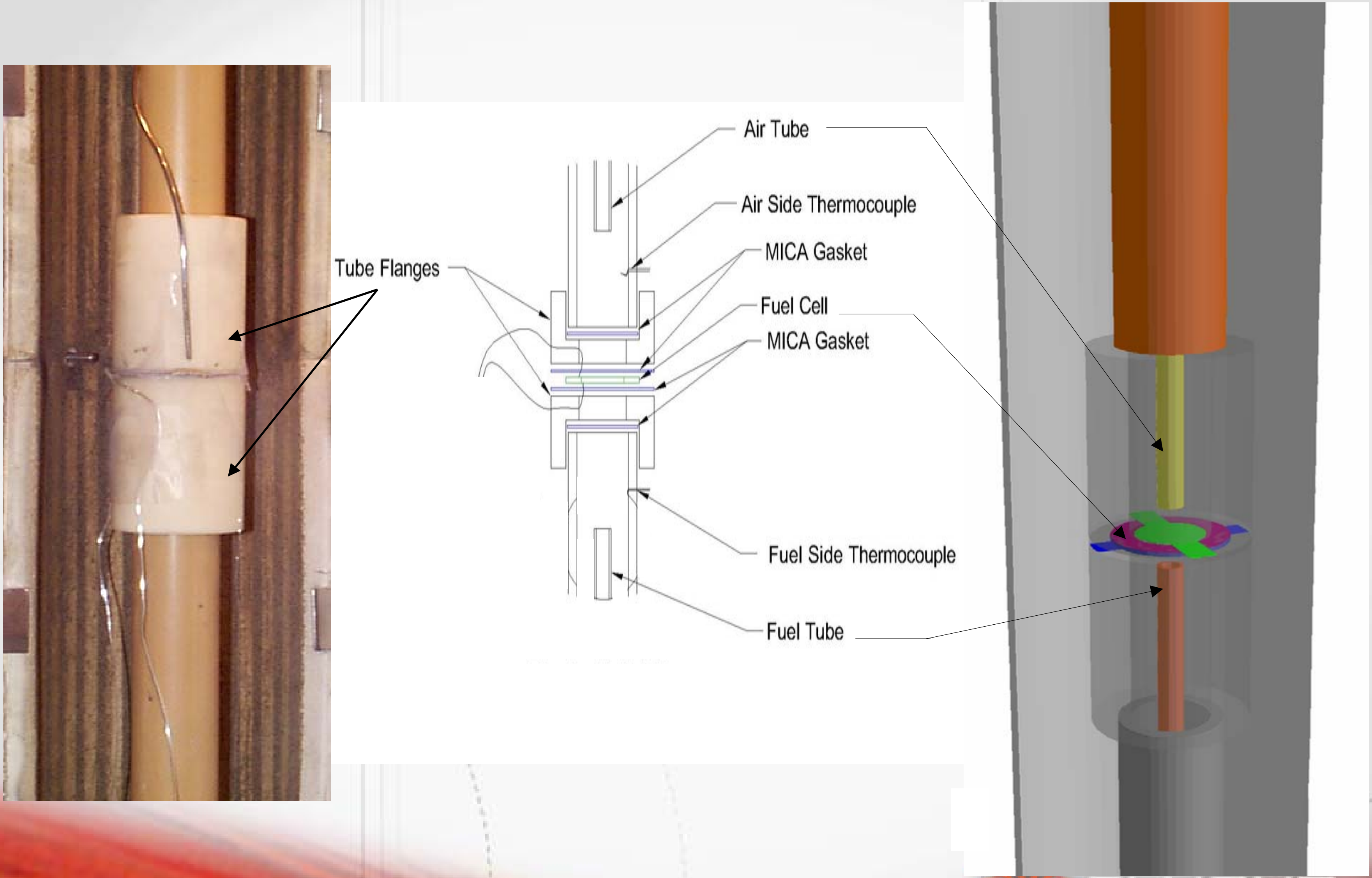
Air to Cell

Air From Cell

Fuel From Cell

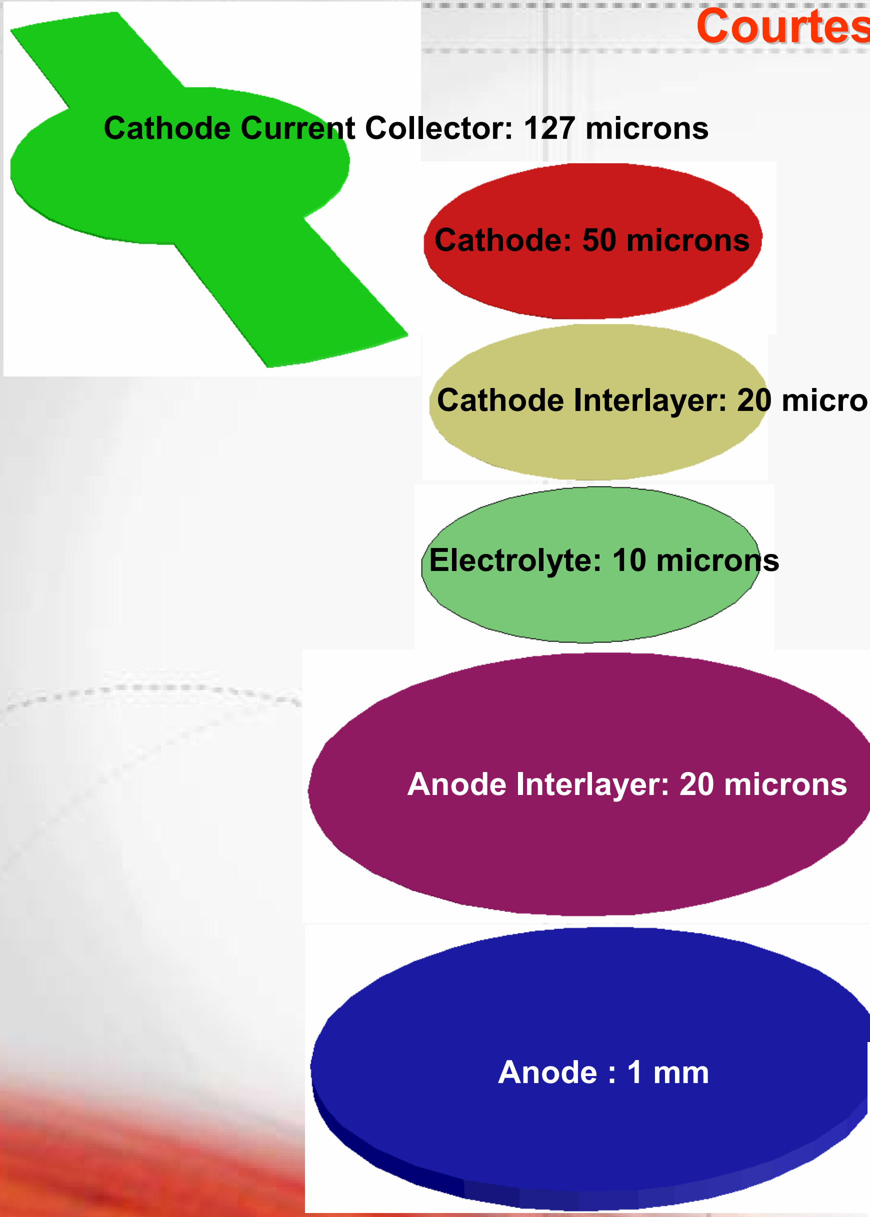
Fuel to Cell

Courtesy of DOE/NETL



Courtesy of DOE/NETL

Detail of Modeled Cell



Cathode Current Collector: 127 microns

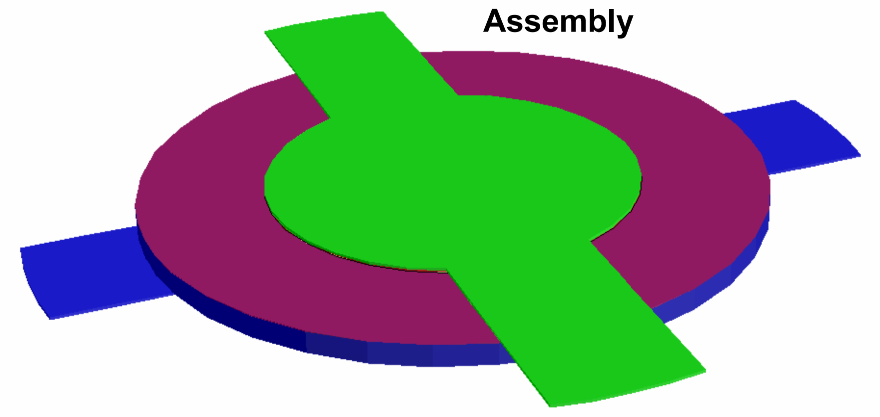
Cathode: 50 microns

Cathode Interlayer: 20 microns

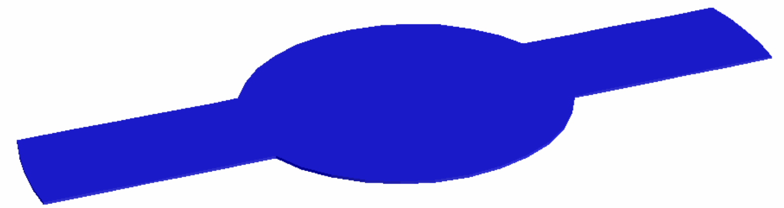
Electrolyte: 10 microns

Anode Interlayer: 20 microns

Anode : 1 mm

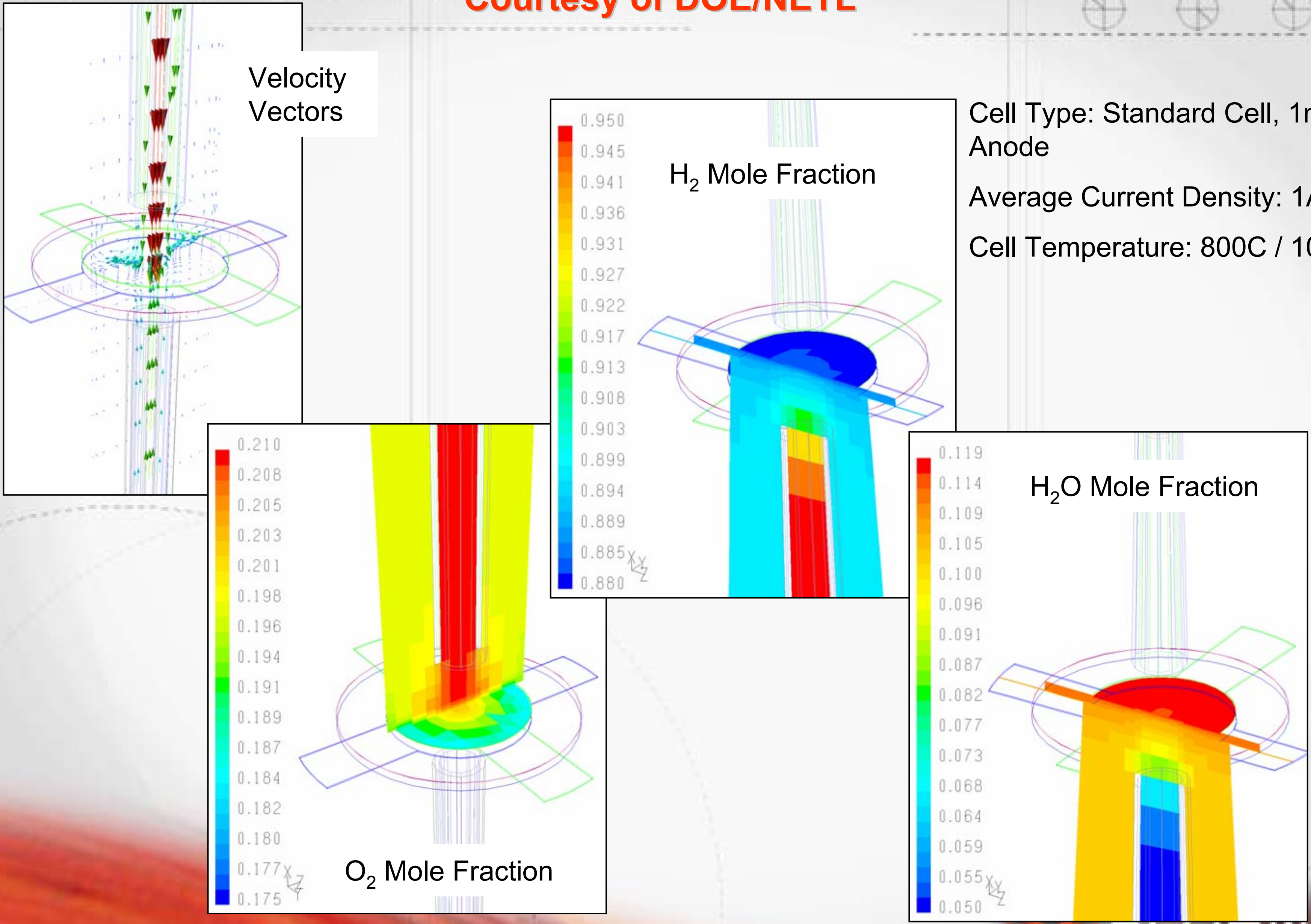


Modeled Cell Assembly



Anode Current Collector: 127 microns

Courtesy of DOE/NETL



Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

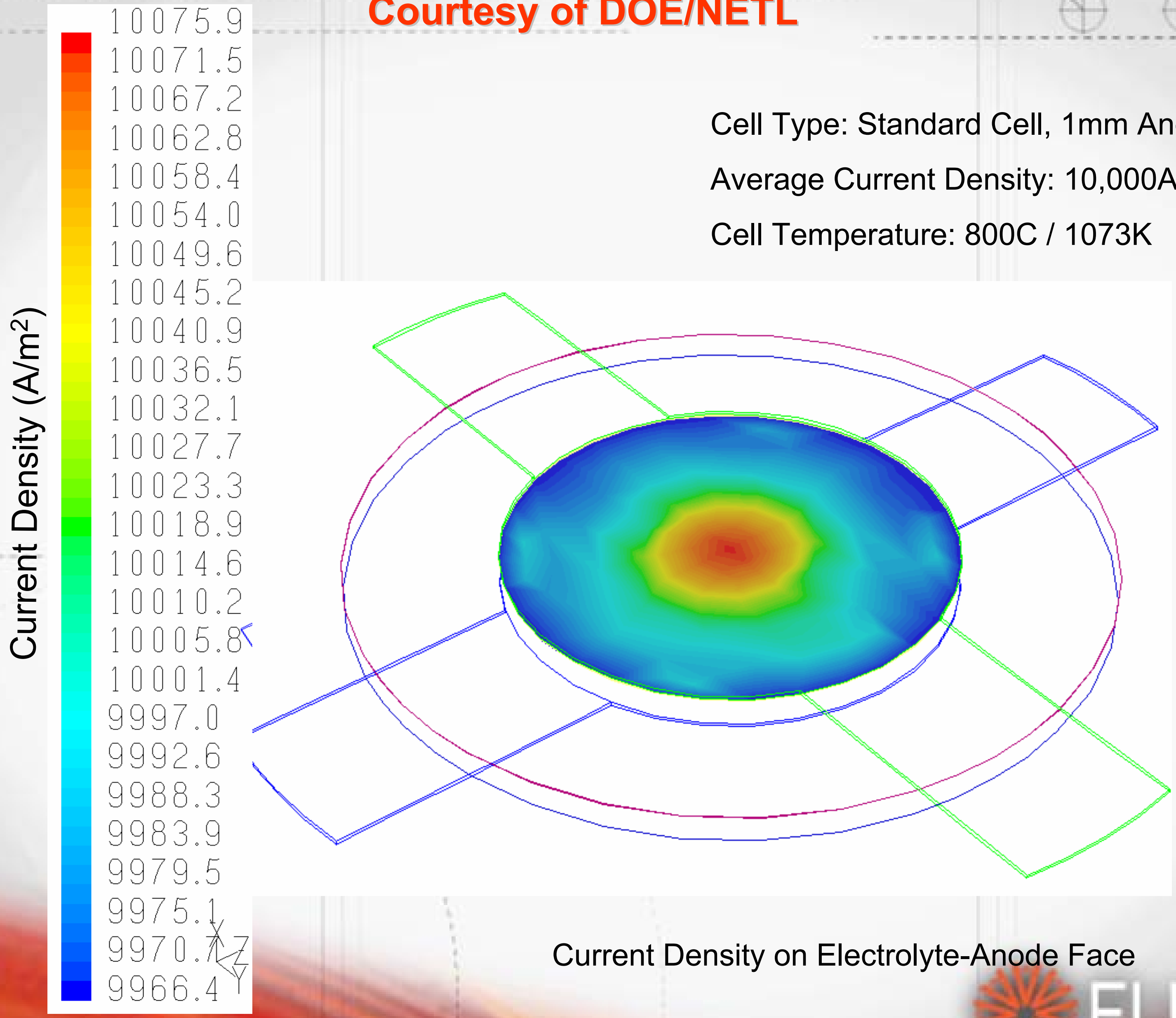
Cell Temperature: 800C / 1073K

Courtesy of DOE/NETL

Cell Type: Standard Cell, 1mm Anode

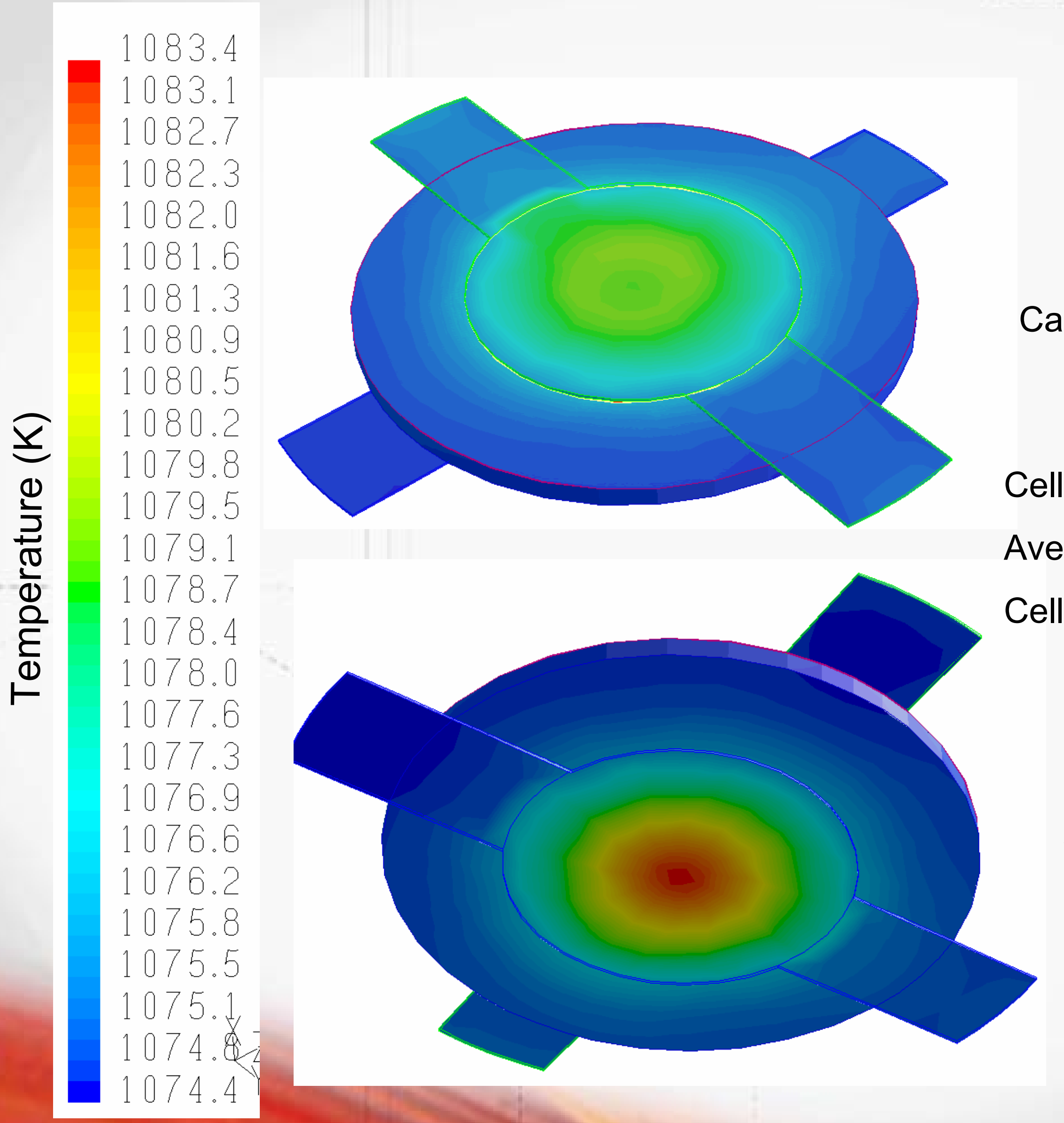
Average Current Density: 10,000A/m2

Cell Temperature: 800C / 1073K



Current Density on Electrolyte-Anode Face

Courtesy of DOE/NETL



Cathode Side Temperature

Cell Type: Standard Cell, 1mm Anode

Average Current Density: 1A/cm2

Cell Temperature: 800C / 1073K

Anode Side Temperature

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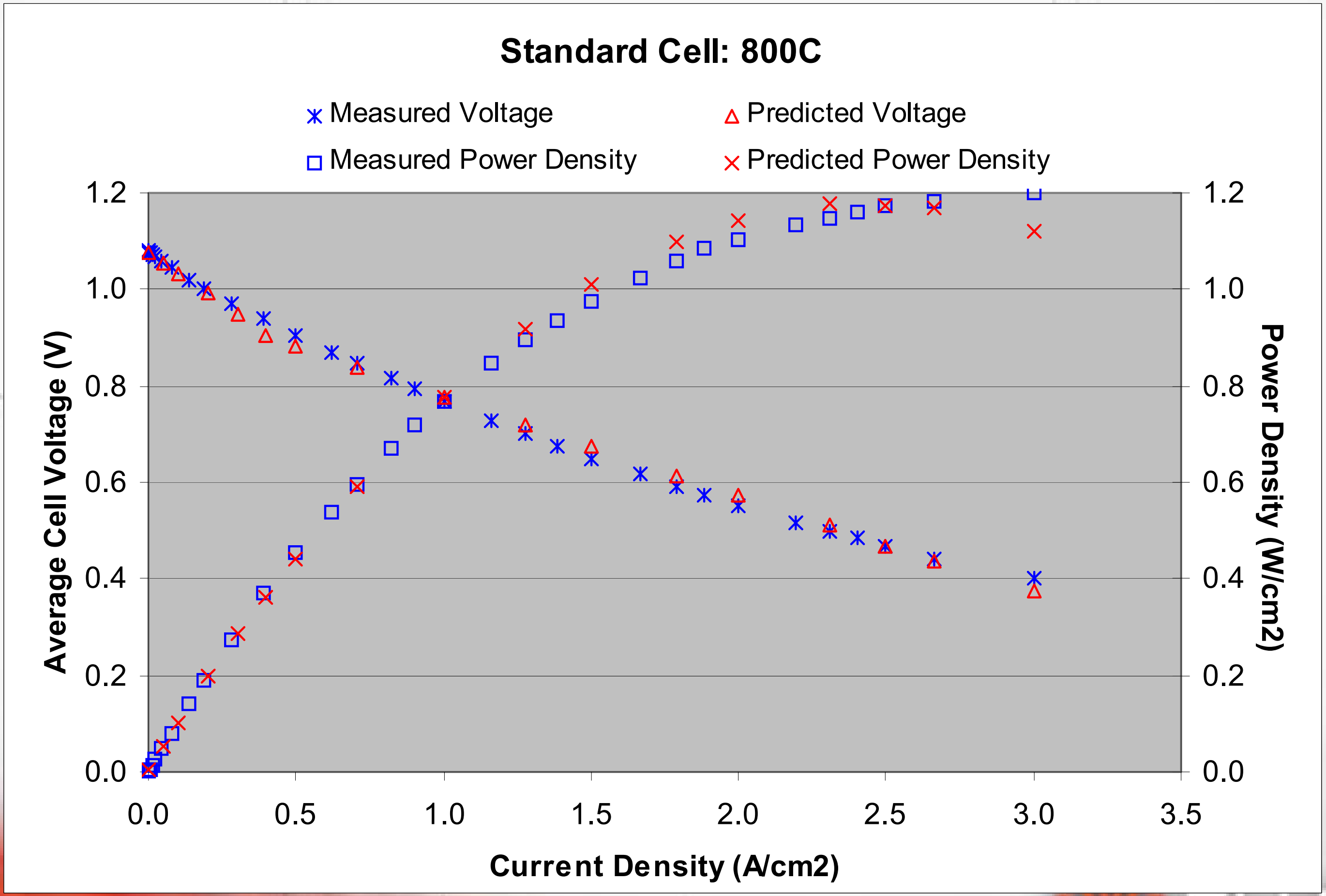
Courtesy of DOE/NETL

Polarization Curve

Experimental data of Virkar et al., May 2002



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