SECA Core Program – Recent Development of Modeling Activities at PNNL

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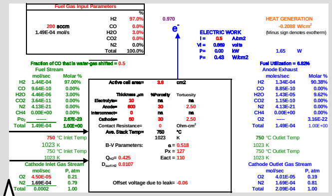
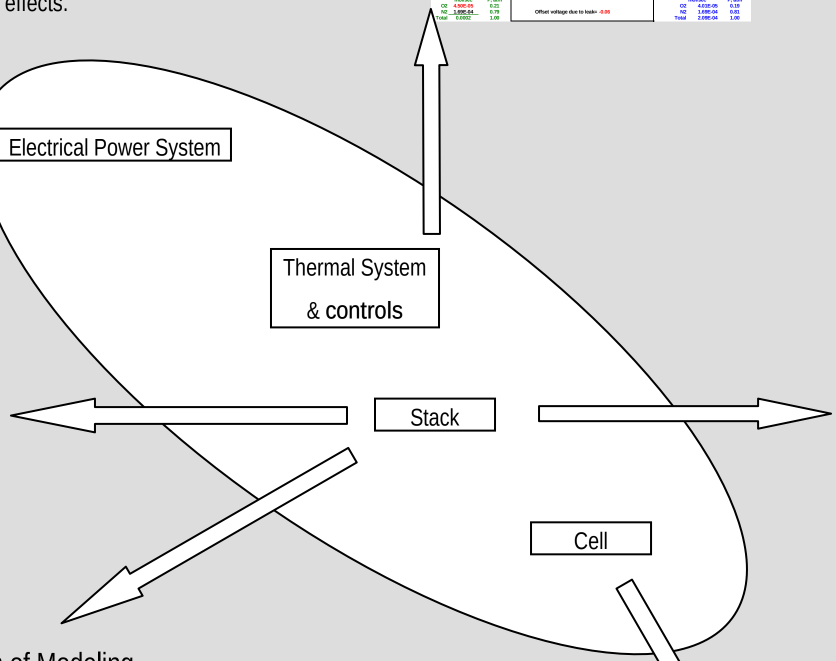
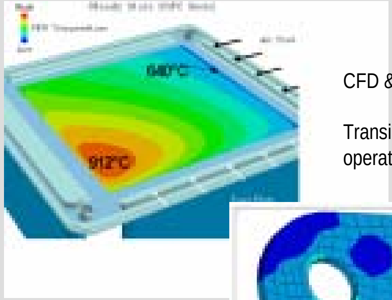
Integrated Modeling of Solid Oxide Fuel Cells

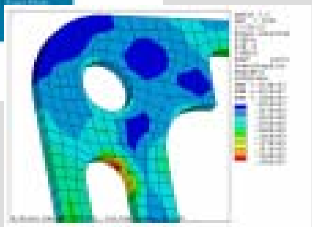
The development of modeling tools for the analysis of fuel cells is essential for the design process. These tools must include the coupling between the fluid, thermal, electrochemical,, and structural behavior. Issues peculiar to SOFC design include elevated operating temperatures, CTE mismatch, flow uniformity and start-up time. The tools being developed will address these issues. They will be used to optimize the design, predict the performance, and assess the reliability and lifetime of the cell. PNNL is taking an integrated approach to incorporate all these effects.



Modeling Validation

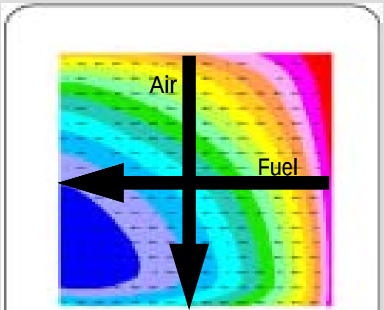






CFD & FEA Models

Transient & Steady state operating conditions

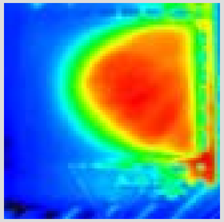


H_2 concentration

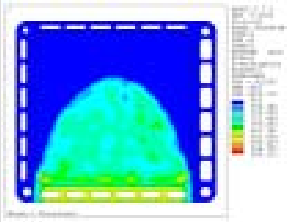
Continuum Electrochemistry Results

Experimental Validation of Modeling

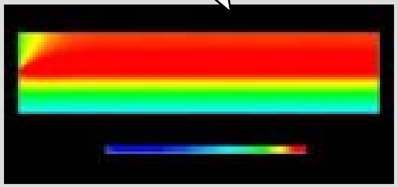
Rapid (<30 sec.) heating of ceramic PEN to 700°C with 20 KW infrared heaters. Temperature profile controlled with parabolic shaped mask

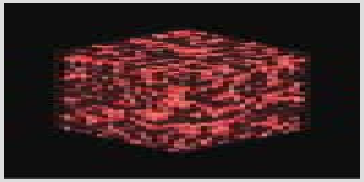


Infrared image of temperature profile



Finite element modeling of test





Microstructural electrochemistry modeling shows the hydrogen concentration as the fuel traverses the length of the cell and diffuses through the electrodes.

Outline

- Quick Updates on SECA supercomputer, software tools and training
- Experimental validation case for the thermo-fluid-electrochemical modeling of planar SOFC stacks.
- Coupled thermal, electrochemistry and flow simulation for full geometry planar SOFCs by finite element analysis.
- Thermal-mechanical stress analysis of compressive seals in SOFC stacks.
- SOFC system modeling and controls.

Solid-State Energy Conversion Alliance (SECA)
Modeling and Simulation Training Session

August 28th and 29th

AGENDA

Day 1:

STAR-CD basics & fuel cell modeling (adapco)
MARC basics
MARC fuel cell modeling
FLUENT basics & fuel cell modeling

Reception

Day 2:

EC Spreadsheet Model User Training
EC in CFD code (using STAR-CD as example)
Matlab / System Models User Training
EC in FE code (using MARC as example)
Feed back / Comments

Training Participants

Georgia Institute of Technology

FuelCell Energy

MSRI

Cummins Power Generation

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General Electric Company

New SECA Computational Resource

- Objectives:
  - Provide SECA Industrial Teams access to a high-performance computer for numerical analysis of Fuel Cell designs using commercial software with PNNL developed Fuel Cell sub-models
  - Provide platform for continued sub-model development and testing
- Time Line:
  - Arrived Friday September 26th
  - Operational within 2 weeks

Computer Information

- Silicon Graphics Inc
  - 3700 Altix Server
  - Linux based
  - 24 Intel “Madison” CPUs
  - Expandable to 64 CPUs in current chassis
  - 64 GBytes RAM - Shared Memory - also greatly expandable
  - Binary compatibility with PNNL 128 CPU SGI computer

Offsite Access for SECA Industrial Team Members

- All offsite non-PNNL users will need to be hosted by a PNNL staff member
- Host will complete a Computer Access Request Form and Smartcart Request
- Offsite computers must have a Hardware Firewall (PNNL staff use Linksys), or a software Firewall (Hardware Firewall is preferred)
- Access is via:
  - VPN software for PC or Macintosh Platforms (provided by PNNL)
  - ssh (secure shell) for Unix/Linux
  - Users connect into PNNL using Smartcard (transient passwords in sync with PNNL base station)

PNNL 128 CPU SGI Computer

Commercial Software Tools

Steve MacDonald, the president of the CD adapco Group, has agreed with Dr. Moe Khaleel of PNNL to develop an expert system module for solid oxide fuel cell simulation. The **es-sofc** module will use as it's basic engine the PNNL electro chemical simulation subroutines in combination with STAR-CD.
The first release will occur in January,2004.

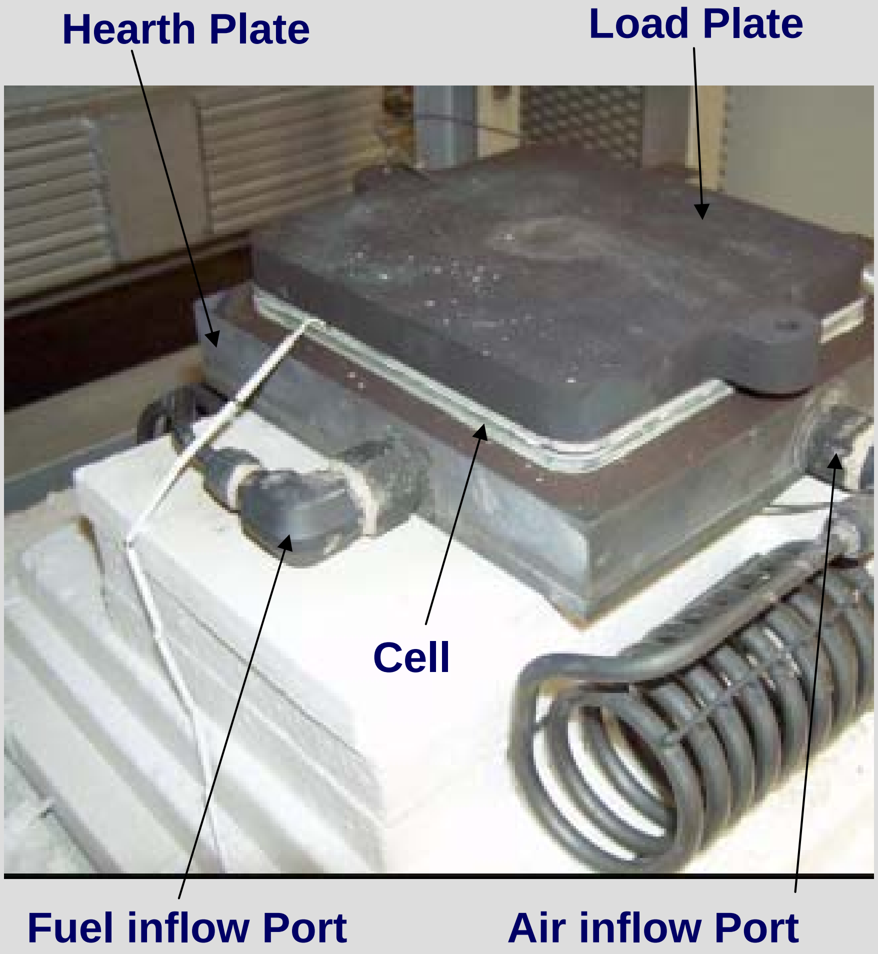
Reza Sadeghi, VP for software development at MSC, has agreed to develop within the MARC code solid oxide fuel cell simulation (flow, electrochemical, thermal and stress) with a user interface. The module will use as it's basic engine the PNNL electro chemical simulation subroutines in combination.
The first release will occur in January,2004.

Lewis Collins, Fluent, and PNNL signed a joint development agreement to work on the development of solid oxide fuel cell simulation. The agreement was signed August 2003.

Experimental validation case for the thermo-fluid-electrochemical modeling of planar SOFC stacks

Experimental Setup - Hardware

- Typical One-cell, cross-flow stack
  - 110 cm^2 active cell area
  - Stack rested upon 3.1 cm thick hearth plate and insulating material
  - Air and fuel inflow and outflow lines enter and exit the hearth plate sides via metal tubing.
  - Atop the stack was a 1.5 cm thick load plate
  - The assembly was enclosed in an electric resistance heated oven to control stack temperature.
- Fuel and air inflow and outflow temperatures were measured using thermo-couples located mid-manifold, within the hearth plate, near the gas ports.



Experimental Setup – Test Conditions

Inputs:

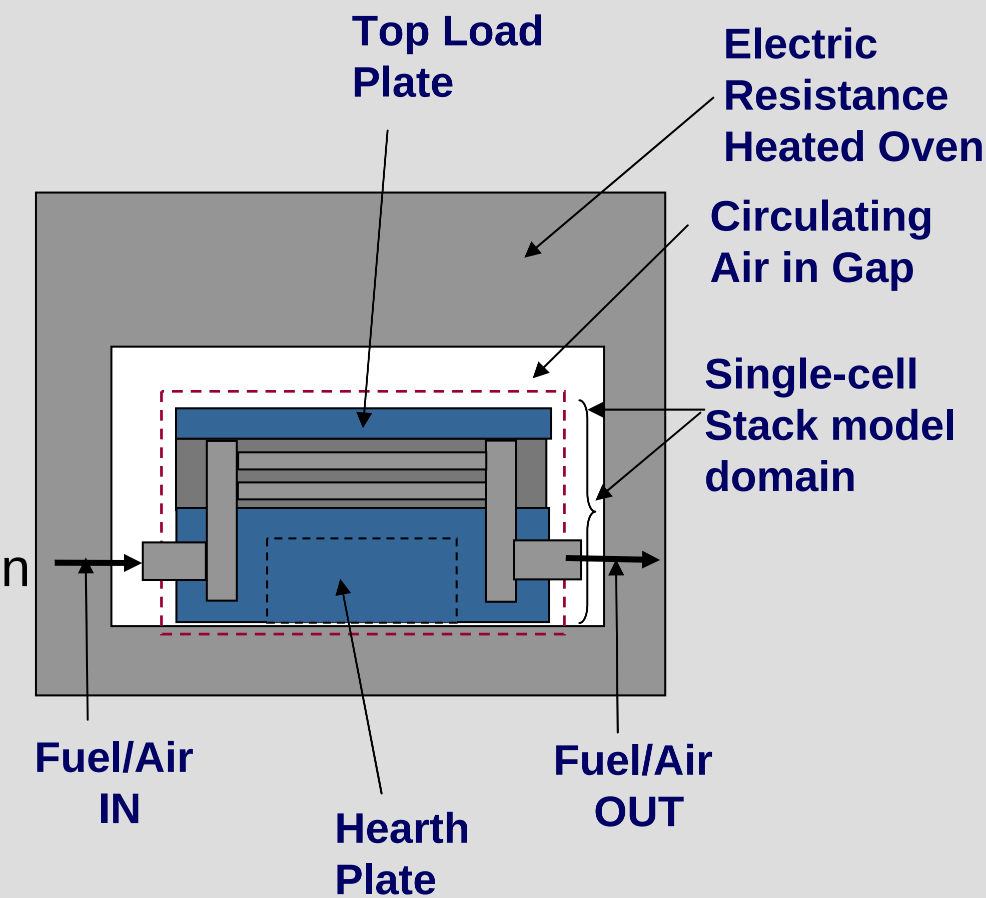
- Fuel: 2 slpm H_2 + 2 slpm N_2
- Air: 6 slpm
- Cell Voltage: 0.7
- Target operating temperature: 750 C
  - Controlled by the oven temperature and monitoring of the gas inflow and outflow temperatures

Outputs:

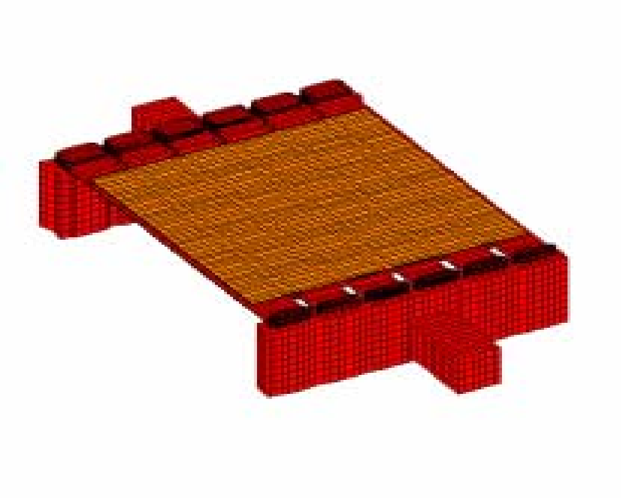
- Quantities for comparison with prediction:
  - ***Power = 40 Watts (57 Amps @ 0.7 Volts), [20% fuel utilization]***
  - ***Measured gas stream temperatures***

Single-Cell Full Stack Model

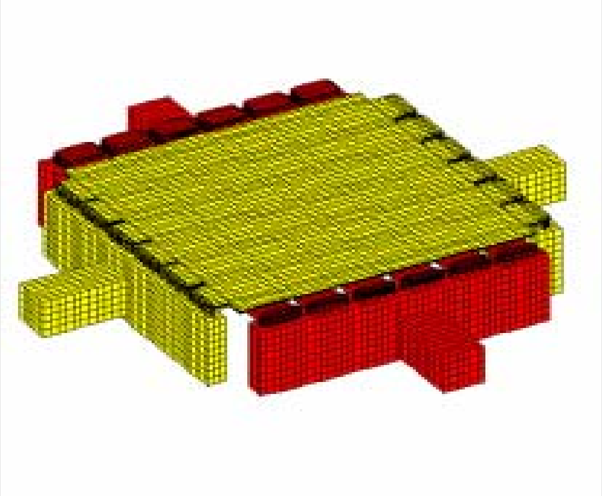
- Model domain is the full, 1-cell stack geometry with some simplifications
  - Undersized hearth plate
  - Rectangular gas ports
- Convection and Gap Radiation heat transfer to/from perimeter walls of model are incorporated into wall boundary conditions.
- Assumed 25 degree C temperature decrease from oven walls to stack walls for the radiation.
- Constant Inflow boundary flow rates with variable temperature to control to desired operating temperature (760 C average on cell active area)



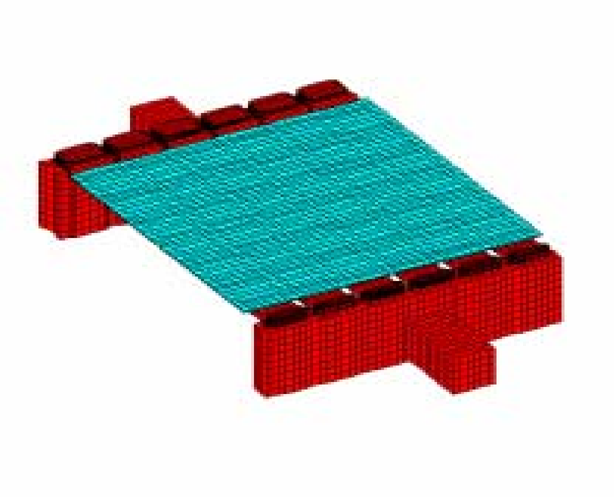
Cathode Air Elements Only



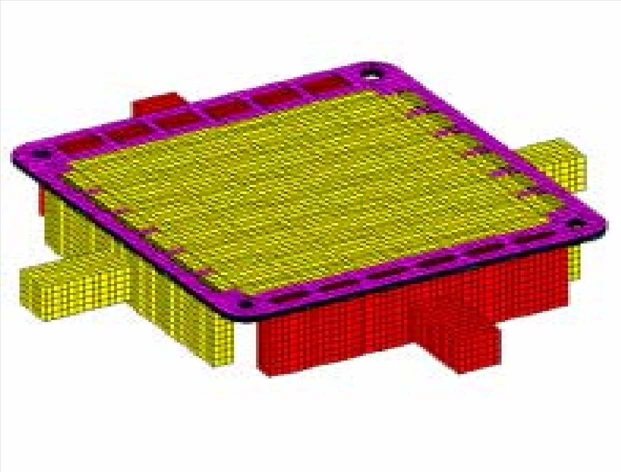
Cathode Air, PEN, & Fuel Elements



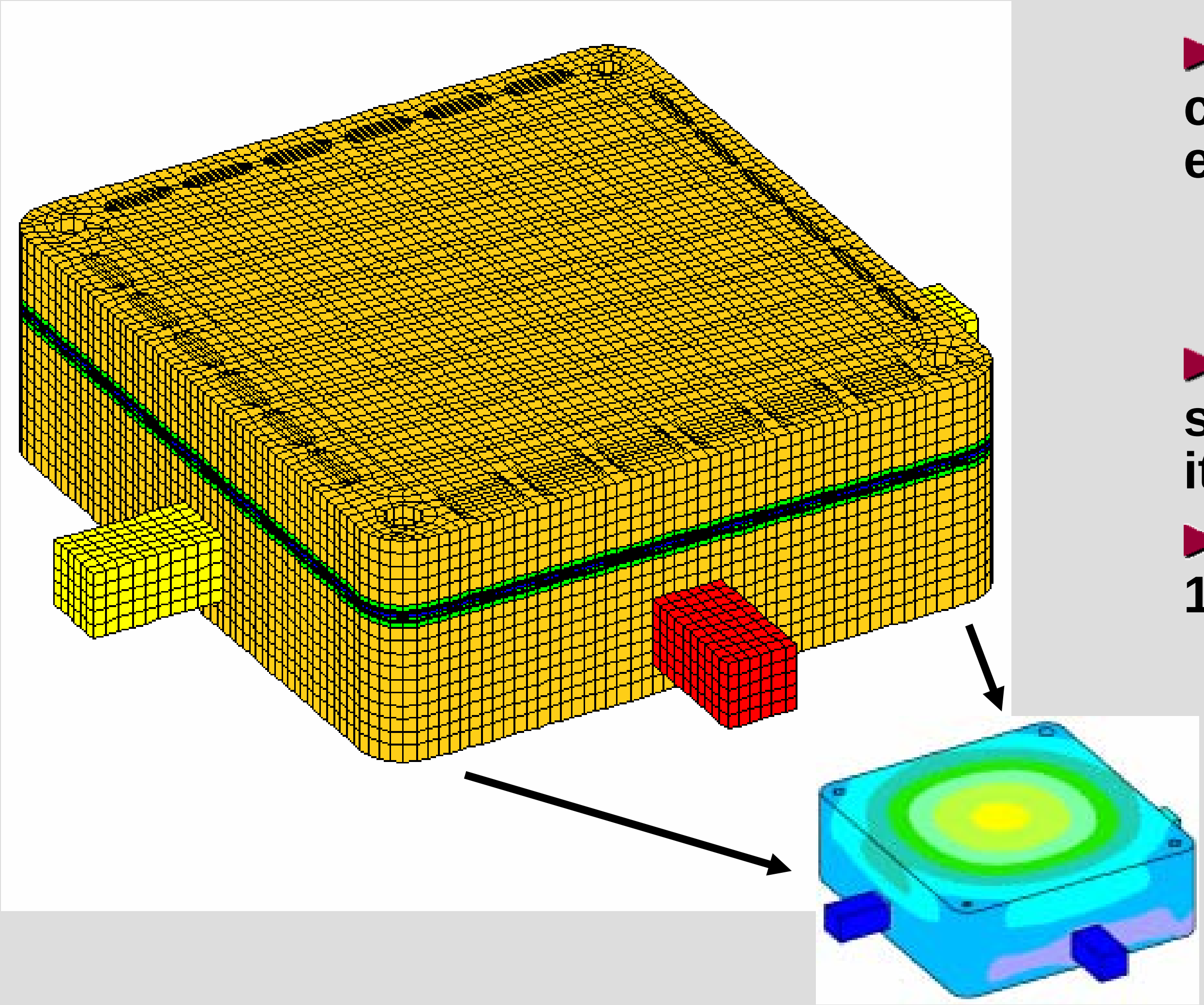
Cathode Air and PEN Elements



With Seals and Spacers



Full Model with Hearth and Top Plate



- **89000 computational elements**
  - 39000 fluid
  - 50000 solid
- **Converged solution in 140 iterations**
- **Compute time: 12-minutes**
  - Run on 8 HP/Linux “Itanium2” 1.5 GHz processors

Calculation Inputs & Conditions

Butler-Volmer Parameters:
alpha = 0.56
pre-exp = 1300
e-act = 133

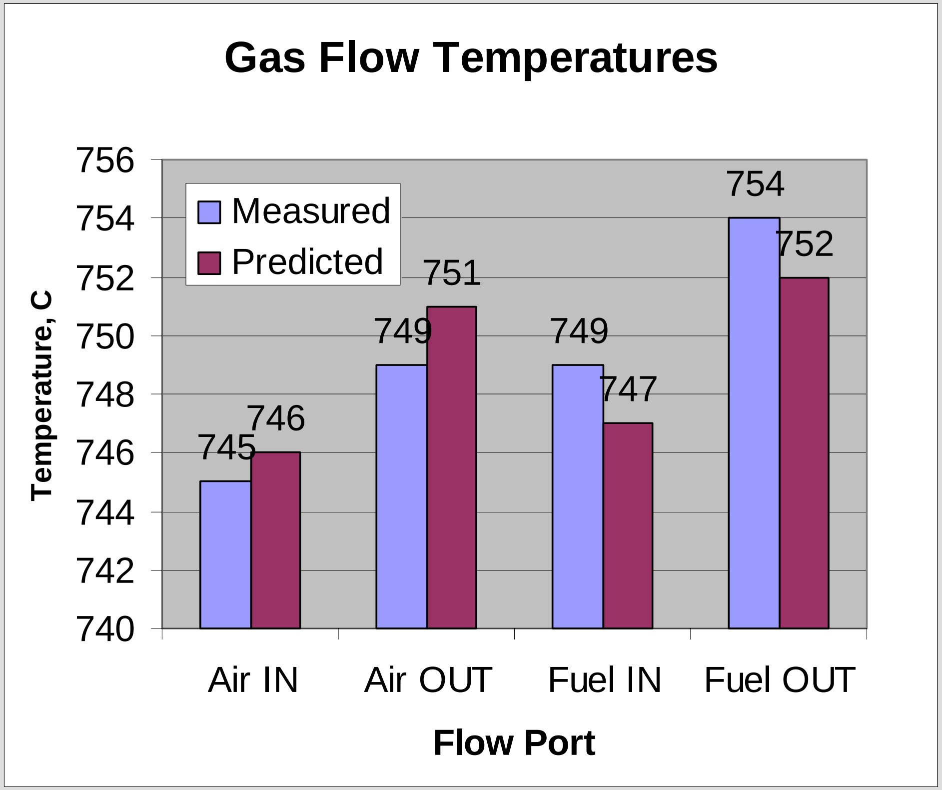
Inputs:

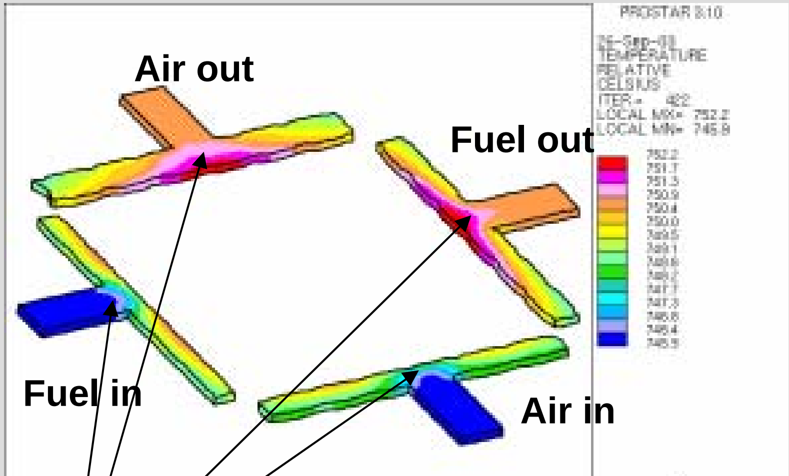
- Fuel: 2 slpm H_2 + 2 slpm N_2
- Air: 6 slpm Air
- Cell Voltage: 0.7
- Target operating temperature of 750 C yielded gas stream temperatures that were 5-8 degrees lower than those measured.
- Therefore: Target temperature set to ***760 C***
  - ***Resulted in slightly elevated power and fuel utilization*** & reasonable temperature match.

Outputs:

- Power & Fuel Utilization
  - Experimental: Power = 40 W (57 Amps @ 0.7 Volts), [20% fuel utilization]
  - ***Predicted: Power = 44 W (63 Amps @ 0.7 Volts), [22% fuel utilization]***
- ***Gas stream temperatures*** **(next slide)→**

Comparison of Measured and Predicted Gas Stream Temperatures





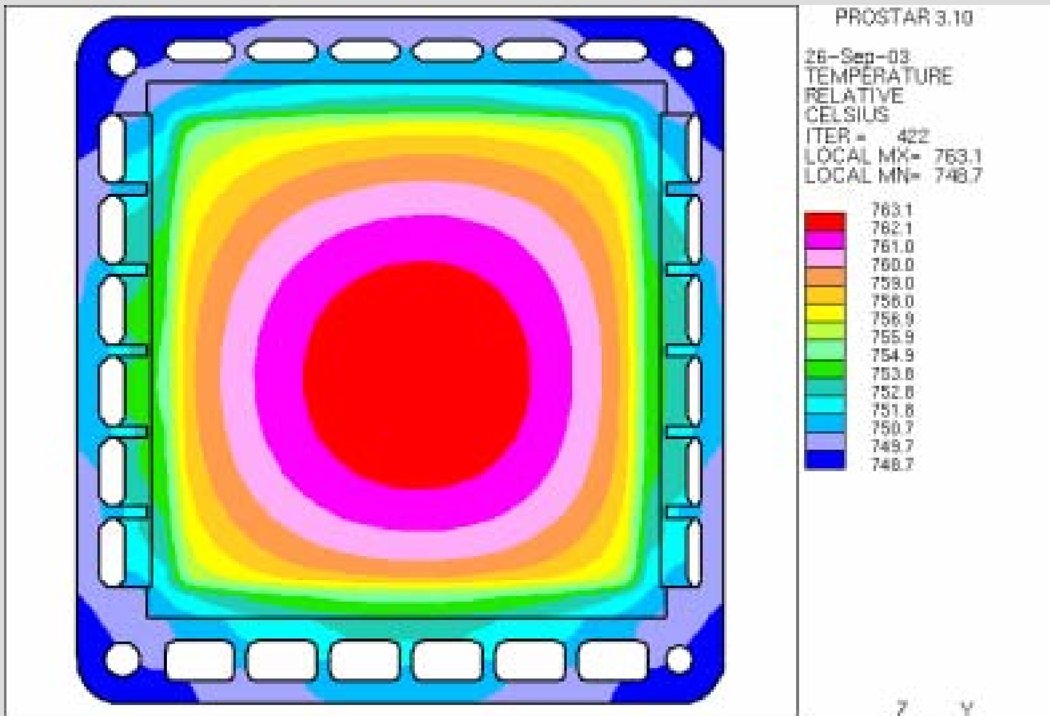
Temperature Plot: Subset of model containing air & fuel elements at level of ports

Gas temperatures taken mid-manifold, in line with ports – coinciding with Thermocouple locations.

Fuel Utilization:
- **Experiment: 20%** - **Model: 22%**
(current x 6.96 = cm3/min H2 burned)

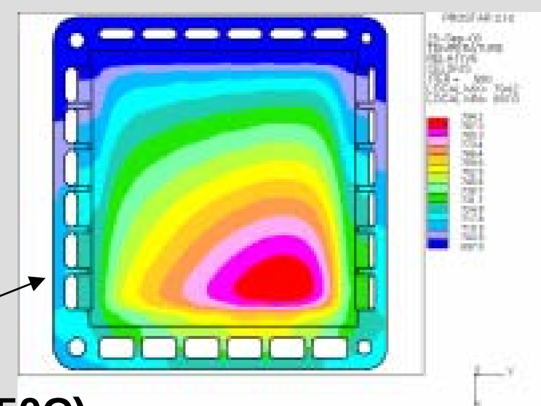
Predicted Temperature -
Inflow range: 744-749 C
Outflow range: 747-752 C

Cell/Stack Temperature Distribution



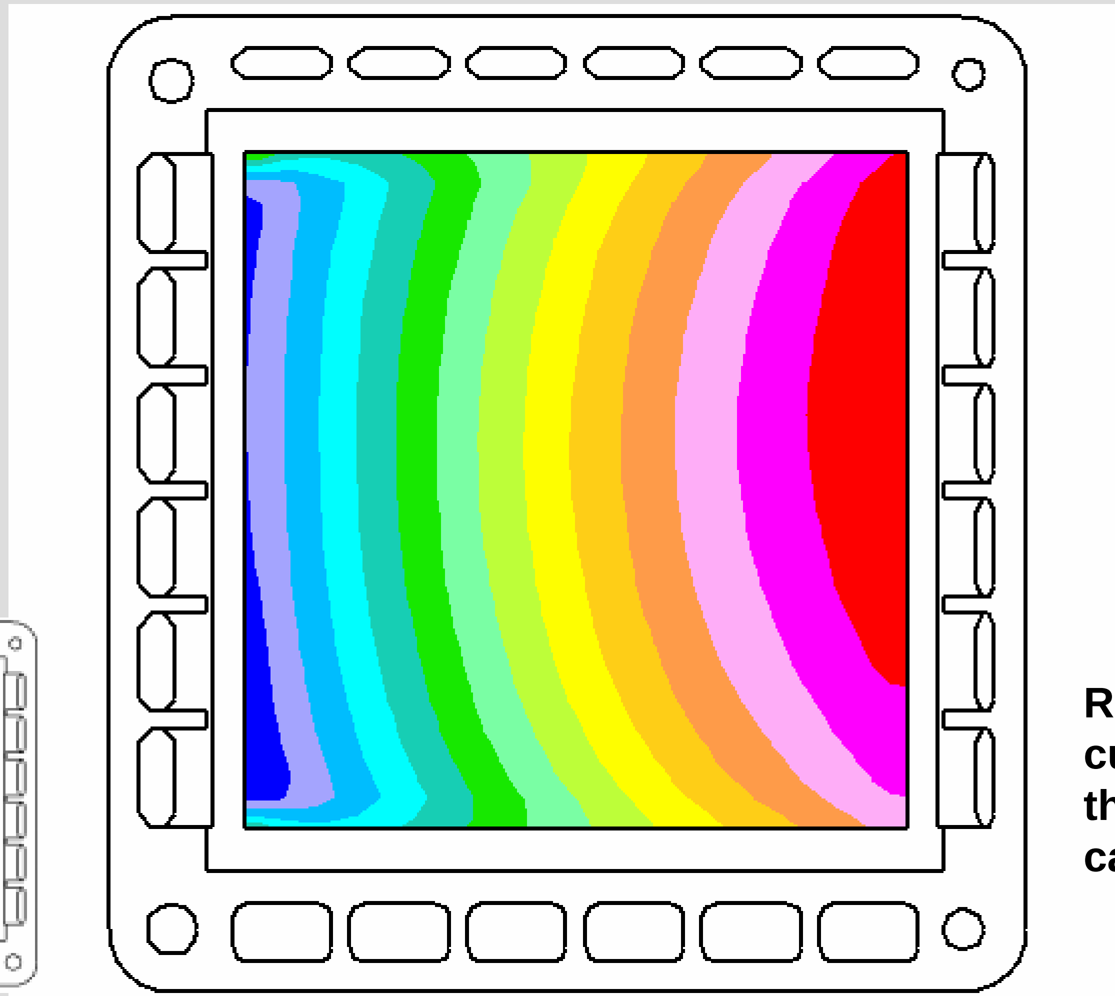
Stack in heated oven (present case)

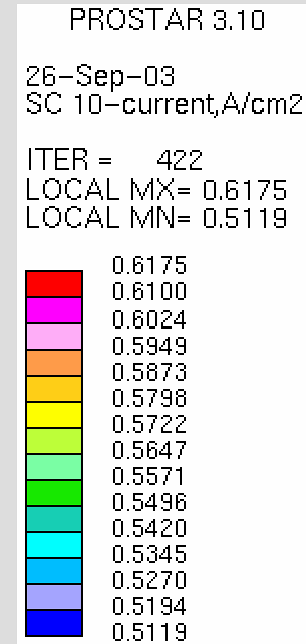
- Relatively isothermal compared to stack operating in insulated enclosure
  - ***15-degree C delta-T*** on present cell
  - ***94-degree C delta-T*** on insulated cell (fpc1c750.4gps.mdl)



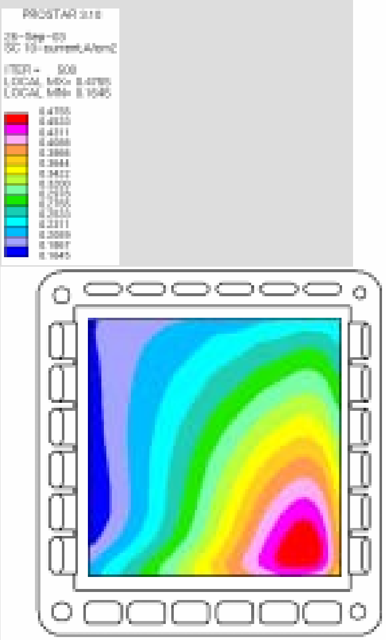
Stack in insulated enclosure with similar average temperature (750C) and 22 W (32 Amps @ 0.7 Volts)

Current Density



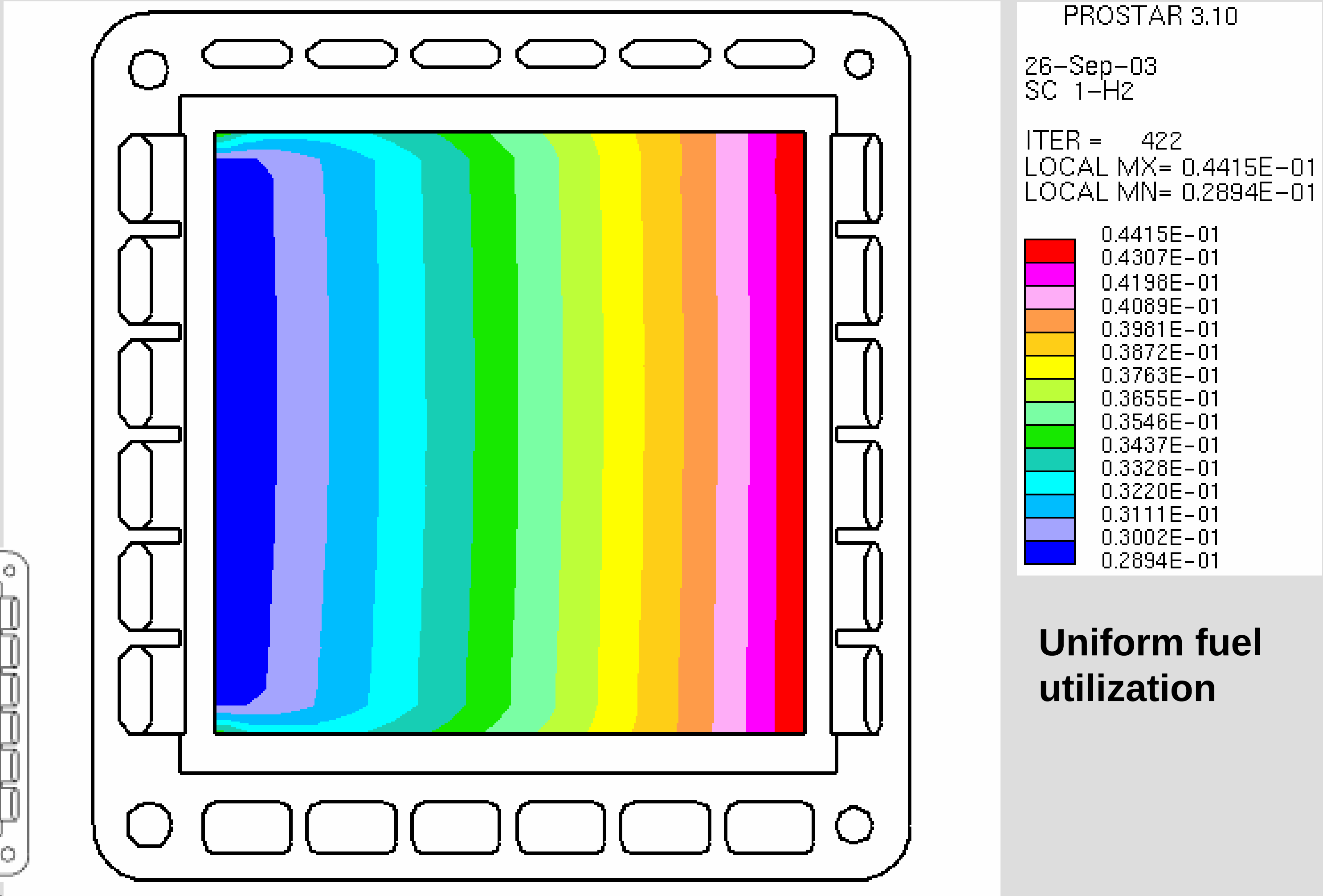


Relatively uniform current density in this "oven heated" case

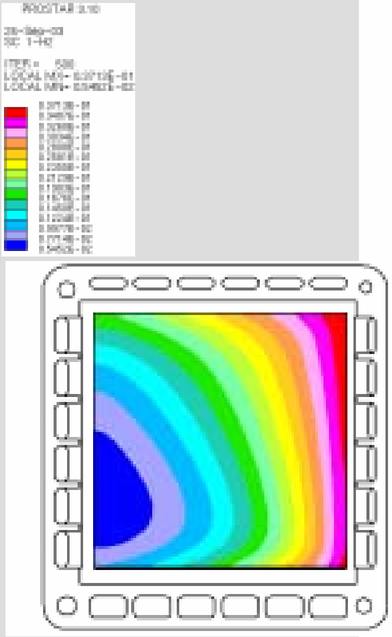


Insulated stack

Hydrogen Concentration



Uniform fuel utilization



Insulated stack

Conclusions

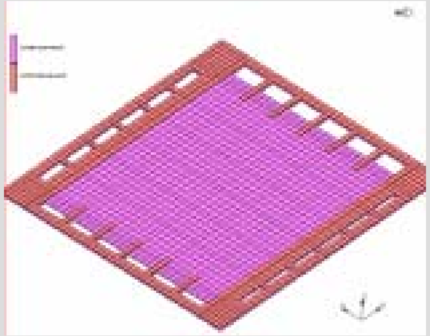
- Suitable gas stream temperature match achieved at elevated cell temperature – thus elevated power and fuel utilization
- Predictions matched inflow and outflow gas temperatures to within 2-degrees C
- Cell temperature of experimental “oven heated” stack relatively isothermal compared to “insulated” stack (15-degree ΔT, compared to 94-degree ΔT)
- Relatively uniform current density
- Uniform fuel utilization

Coupled Thermal, Electrochemistry and Flow Simulation for Full Geometry Planar SOFCs by Finite Element Analysis

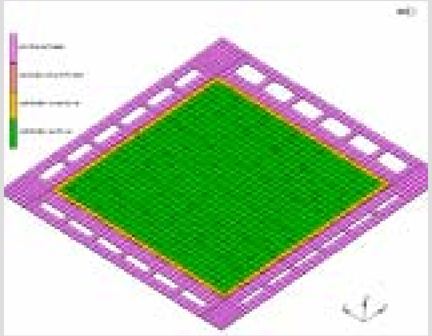
Purpose of Current Modeling Effort

- Develop multi-cell SOFC models in the *Marc* code.
- Extend previous electrochemistry-active-area-only SOFC models to include the intake and exhaust manifolds and the picture frames in the heat transfer and thermal stress solutions.
- Current models provide a platform for
  - linking PNNL’s electrochemistry module to a generic fuel cell model.
  - MSC development of a graphical user interface for industry partners to define their fuel cell models.
- Both heat transfer (with coupled EC) and thermal stress models have been developed.

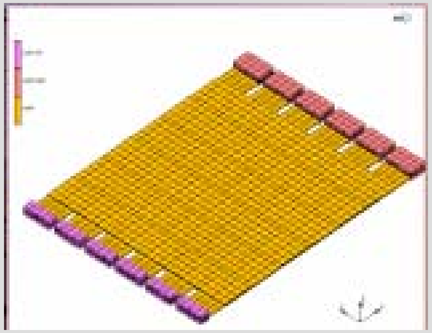
Layered Construction of Full-Feature Model



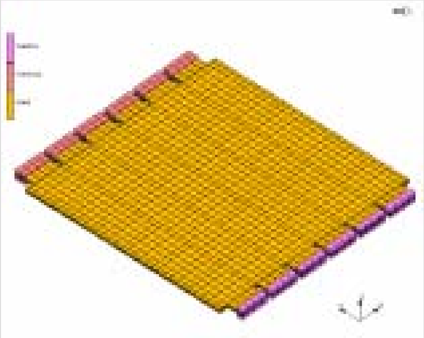
Interconnect and
Cathode Spacer



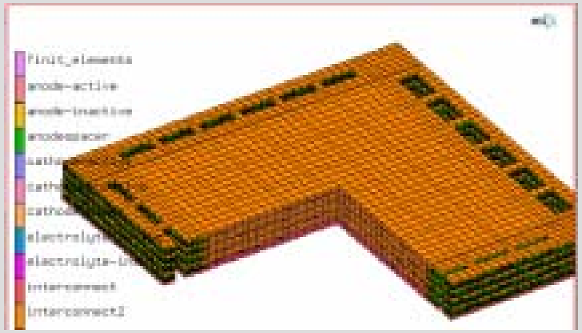
Pictureframe and PEN
layers



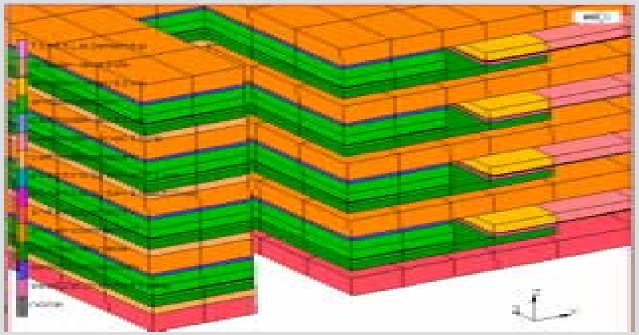
Air in Channel and
Manifolds



Fuel in Channel and
Manifolds



4-Cell Model Showing
Layered Construction



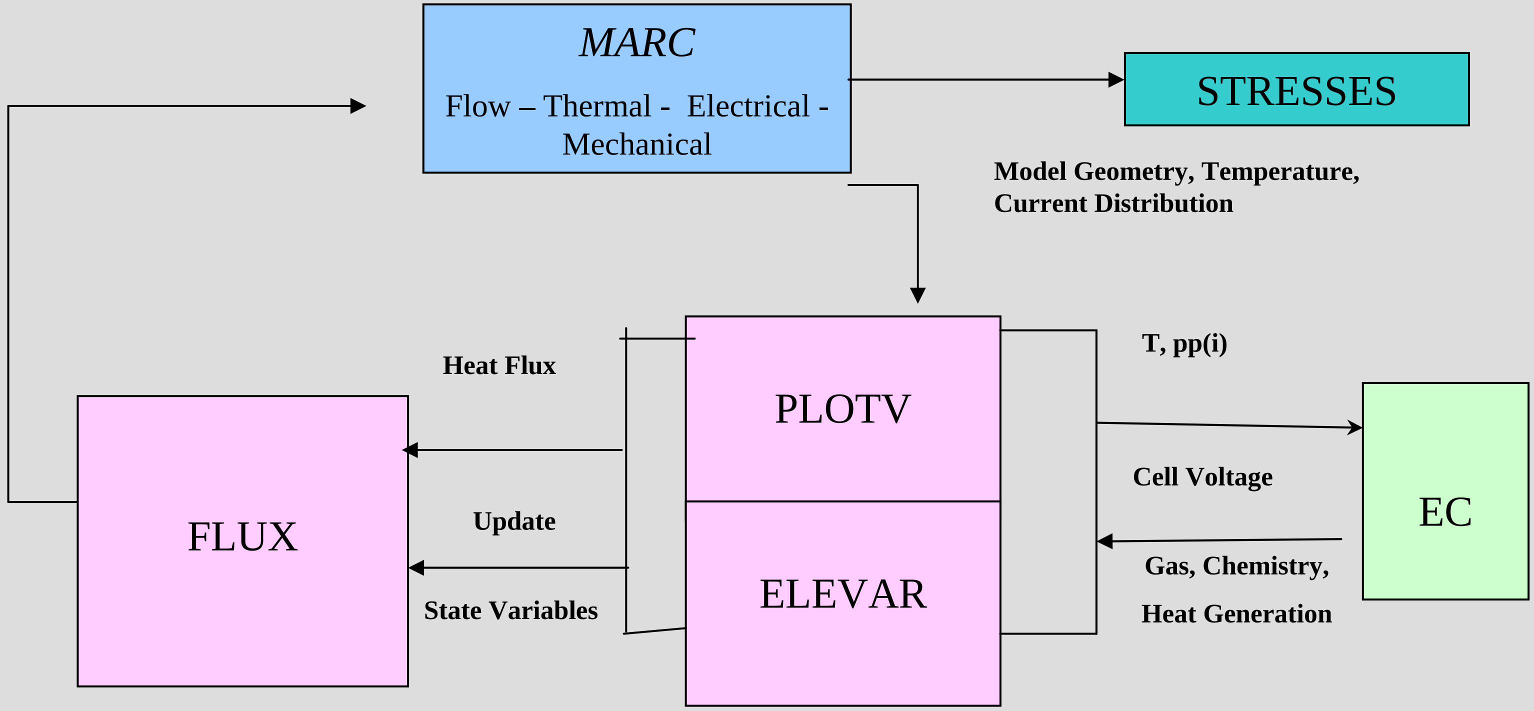
Closeup of Layers in Planar
Construction
of the 4-Cell Model

Linkage between EC module and *MARC*

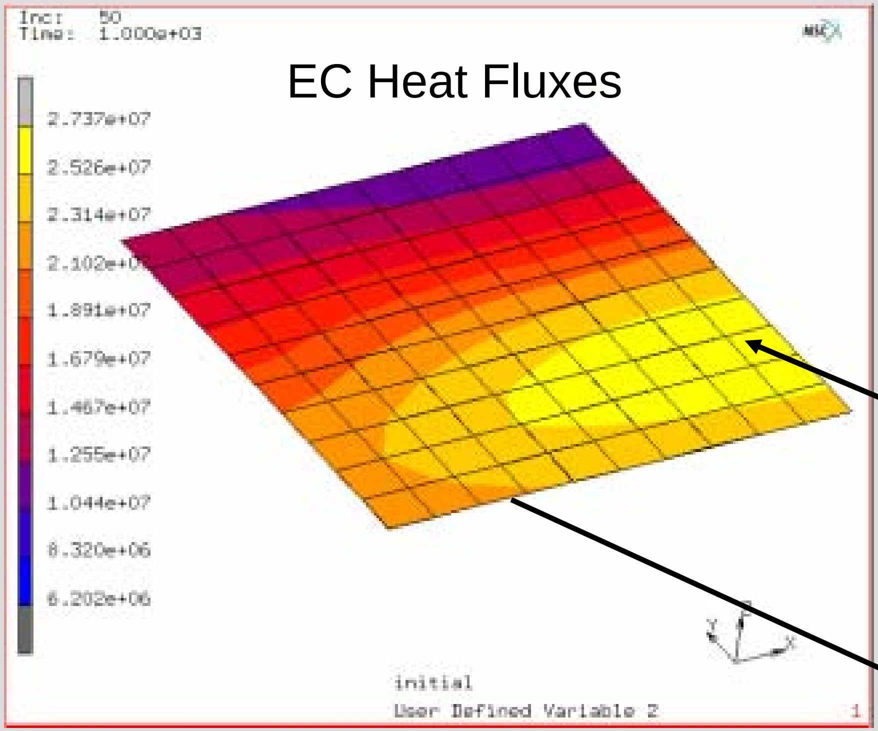
MARC source subroutine (flux(f,ts,n,time))

Input temperature profile and geometry info↓ ↑return heat flux and other state variables

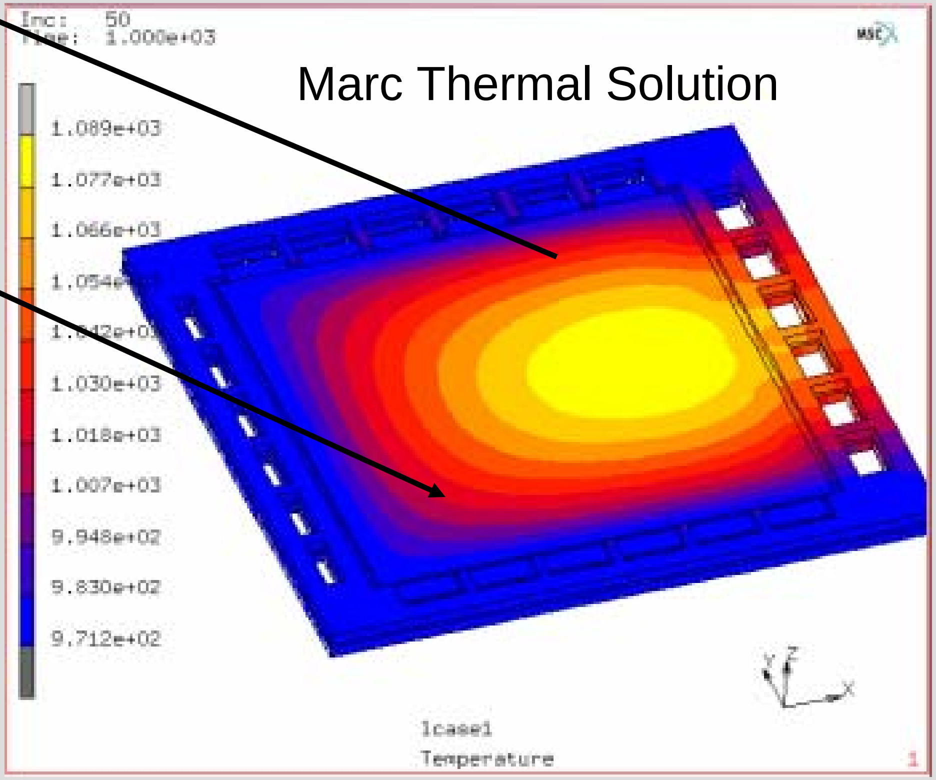
EC module interface subroutine



Coupling of EC to the Full-Feature *Marc* Model



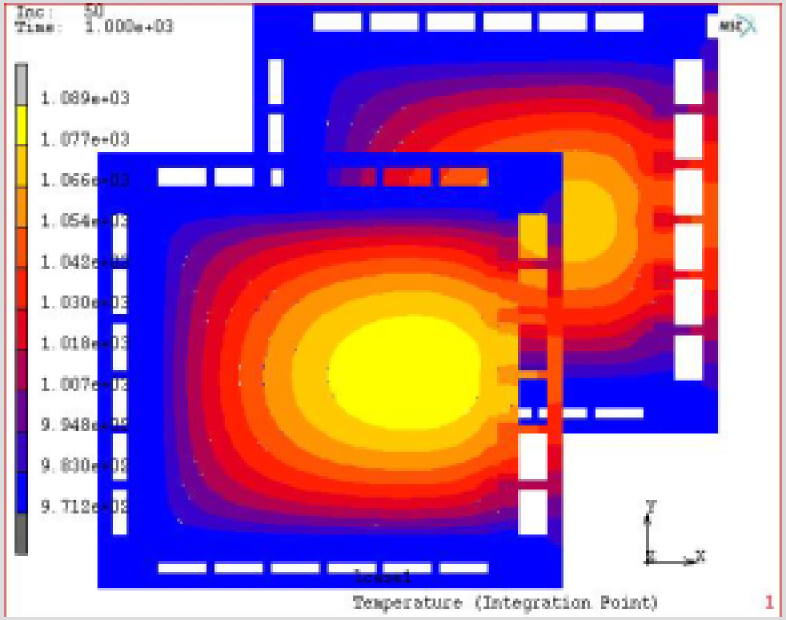
Marc calculates temperatures and stresses based on the EC heat fluxes and passes the temperatures back where they are mapped onto the EC internal mesh.



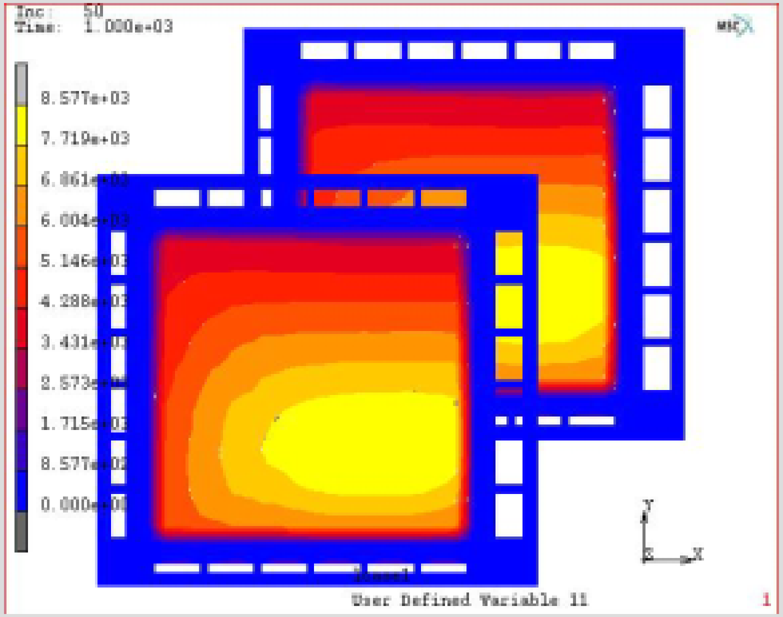
EC operates on an internal mesh and maps the heat fluxes in the PEN active area to the *Marc* mesh.

This is done for each cell.

Results for the 2-cell stack (Electrolyte and pictureframe)

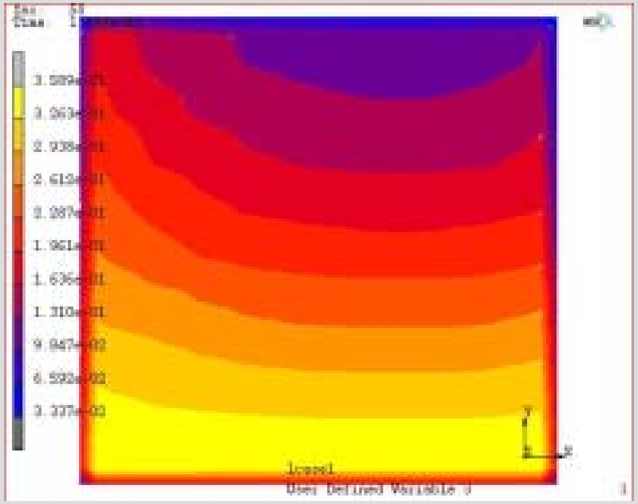


Temperature Profiles

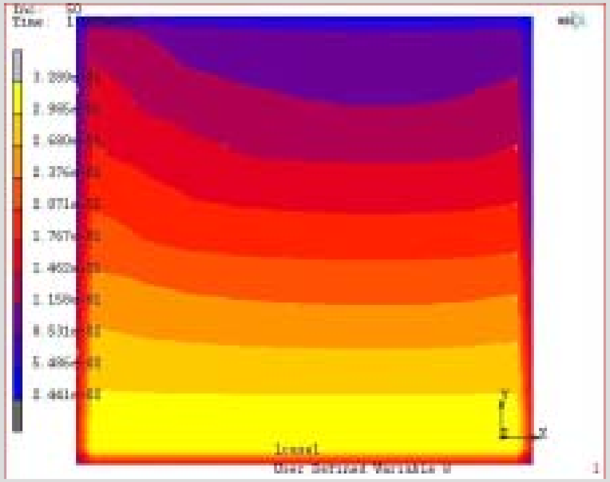


Current Density Profiles

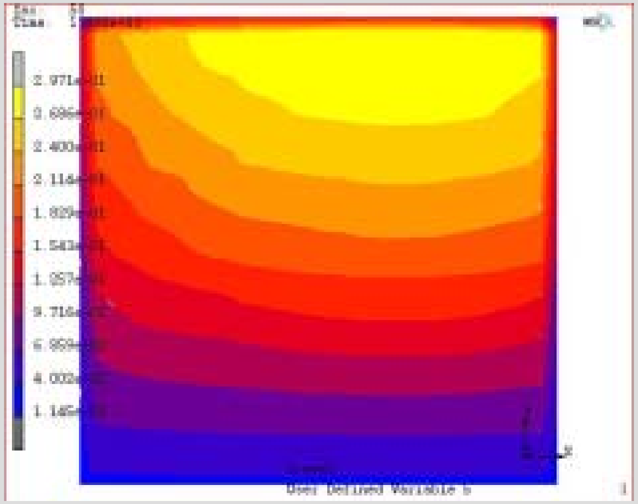
Species concentration calculated in active area



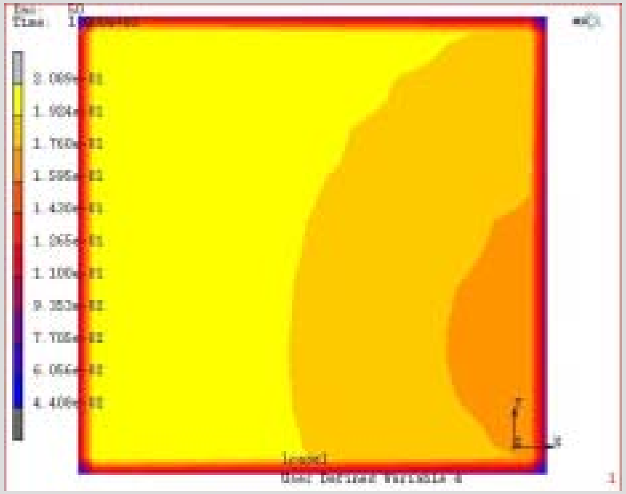
H2



CO



H2O

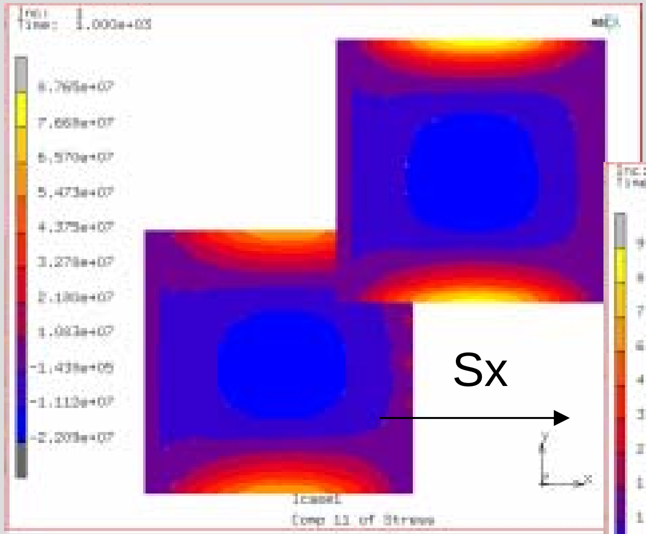


O2

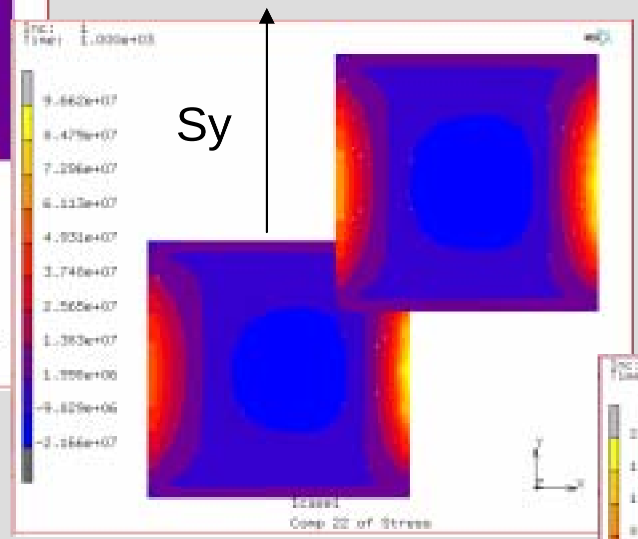
Thermal Stress Predictions from the *Marc*-EC model

- Temperature profiles from coupled *Marc*-EC model were applied to a structural model to predict thermal stresses.
- The model could also be run in a single coupled thermal-stress run.
- Air and Fuel elements are deactivated.
- Current model assumes all layers are connected.
- *Marc* contact capabilities can be used to analyse compression seal designs as well.
- Stresses in electrolyte shown, results in all other layers are available.

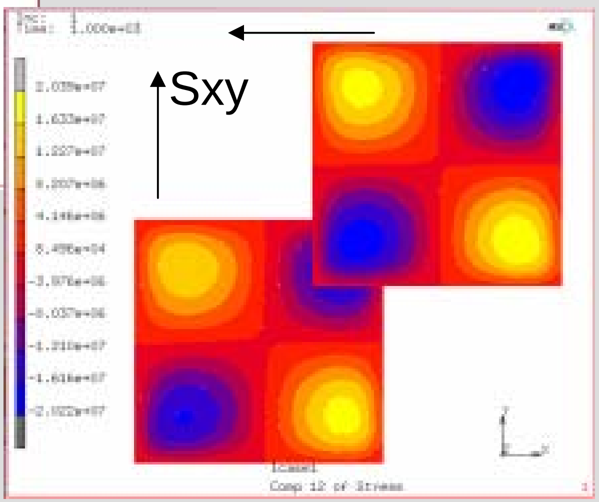
Stresses in electrolyte



X-direction stress



Y-direction stress



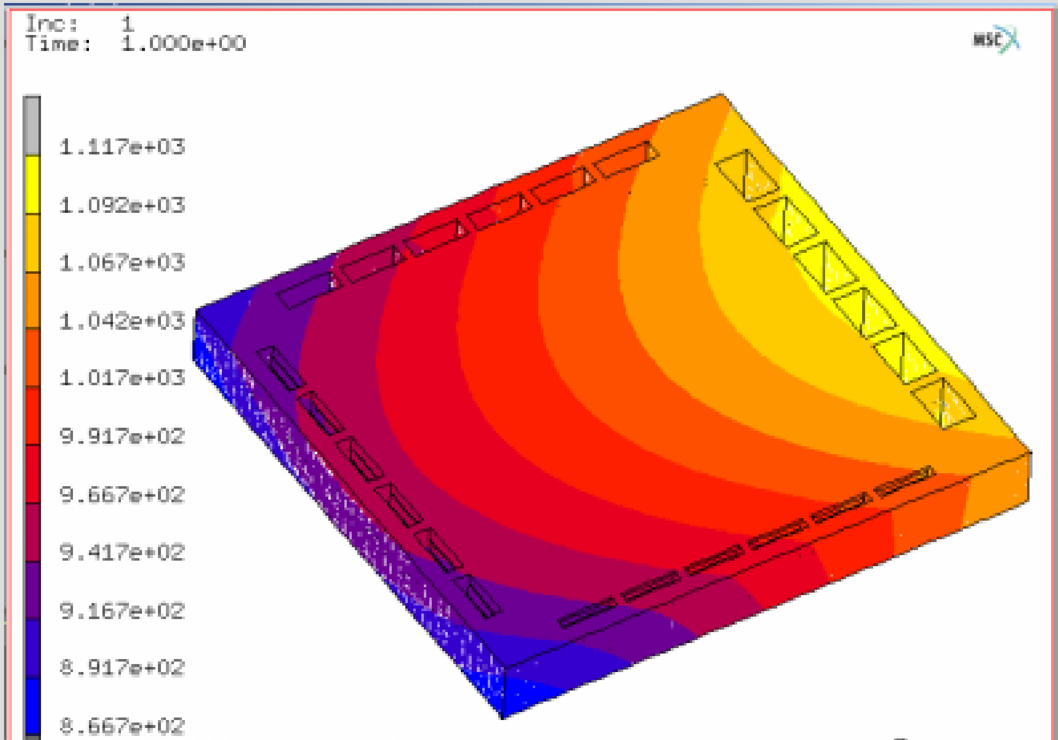
XY-direction stress

Thermal Stress Model of a 4-Cell Stack

The thermal stress model can be run with a specified temperature distribution.

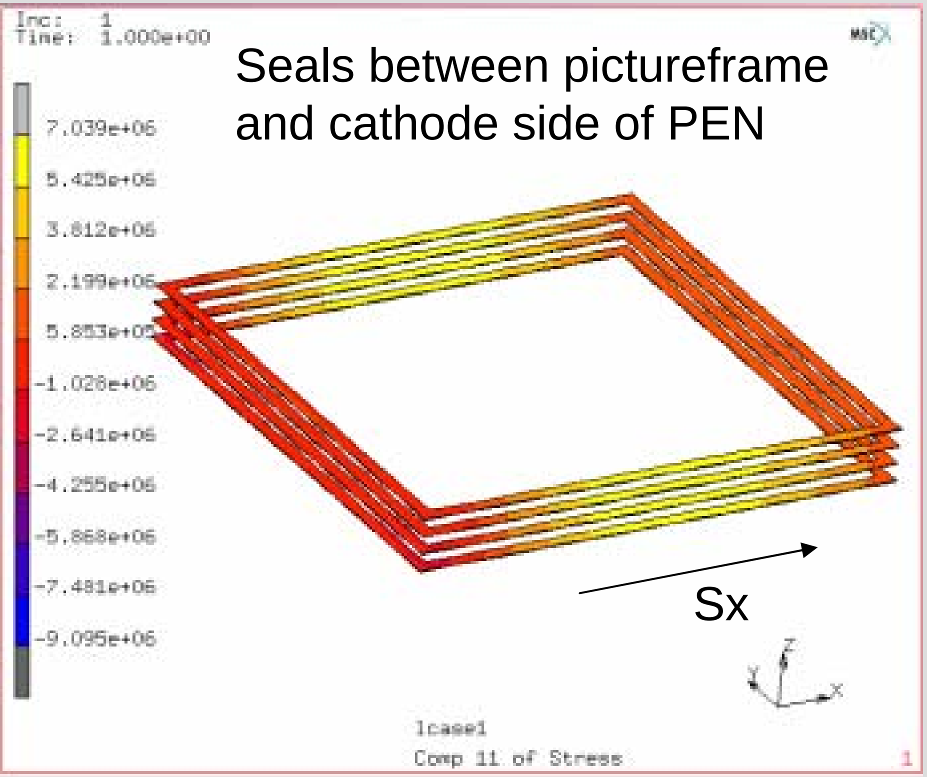
A 4-cell model was run to test memory size and solution times.

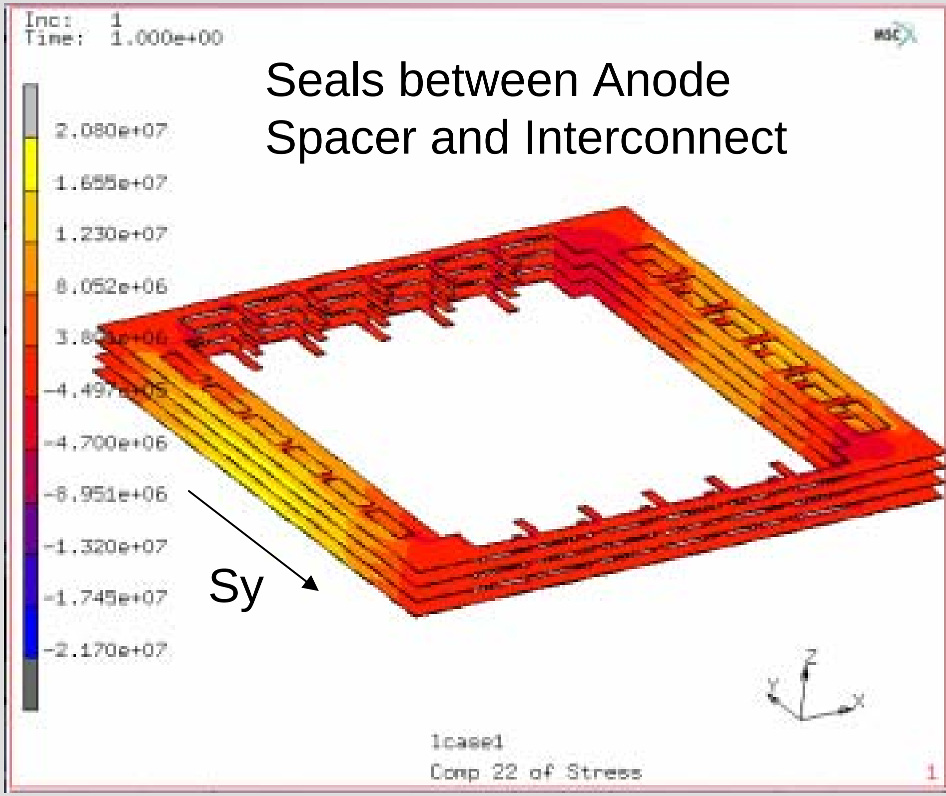
Seal stresses are presented on the next slide as example results.



Temperatures specified on the 4-cell stack model

Seal Stress


Inc: 1
Time: 1.000e+00
Seals between pictureframe and cathode side of PEN
7.039e+06
5.425e+06
3.812e+06
2.199e+06
5.853e+05
-1.028e+06
-2.641e+06
-4.255e+06
-5.868e+06
-7.481e+06
-9.095e+06
Sx
lcase1
Comp 11 of Stress


Inc: 1
Time: 1.000e+00
Seals between Anode Spacer and Interconnect
2.080e+07
1.655e+07
1.230e+07
8.052e+06
-4.700e+06
-8.951e+06
-1.320e+07
-1.745e+07
-2.170e+07
Sy
lcase1
Comp 22 of Stress

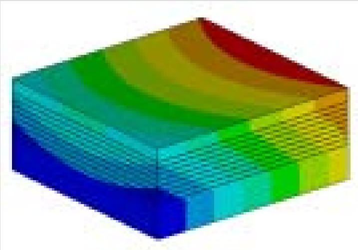
Thermal-Mechanical Stress Analysis of Compressive Seals in SOFC Stacks

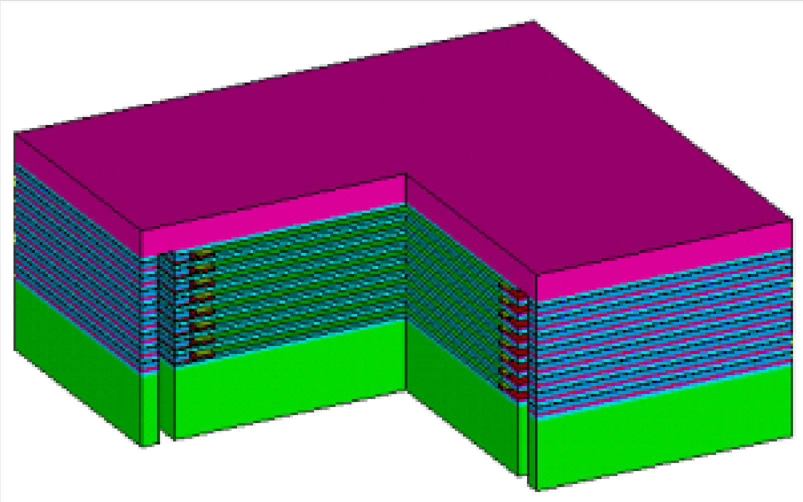
Compressive Seals: Objectives

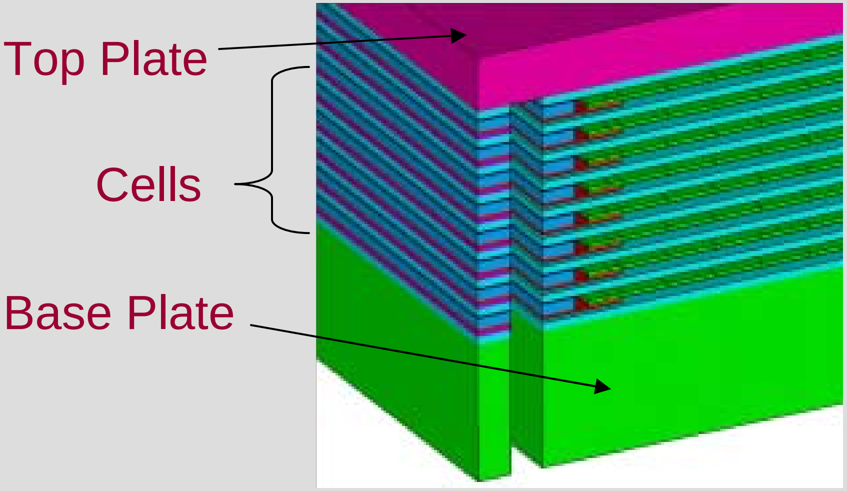
- Develop a method to analyze compressive seals
  - Permit components to slide relative to the seals
    - Numerical convergence more difficult
  - Include effects of compression set and thermal cycling
- Characterize compressive load distributions
- Characterize seal deformations and identify regions of potential seal damage
- Develop constitutive relations for identified degradation mechanisms of compressive seals
- Develop leak rate predictions based on leak path development and/or seal damage

Compressive Seals: Example Model

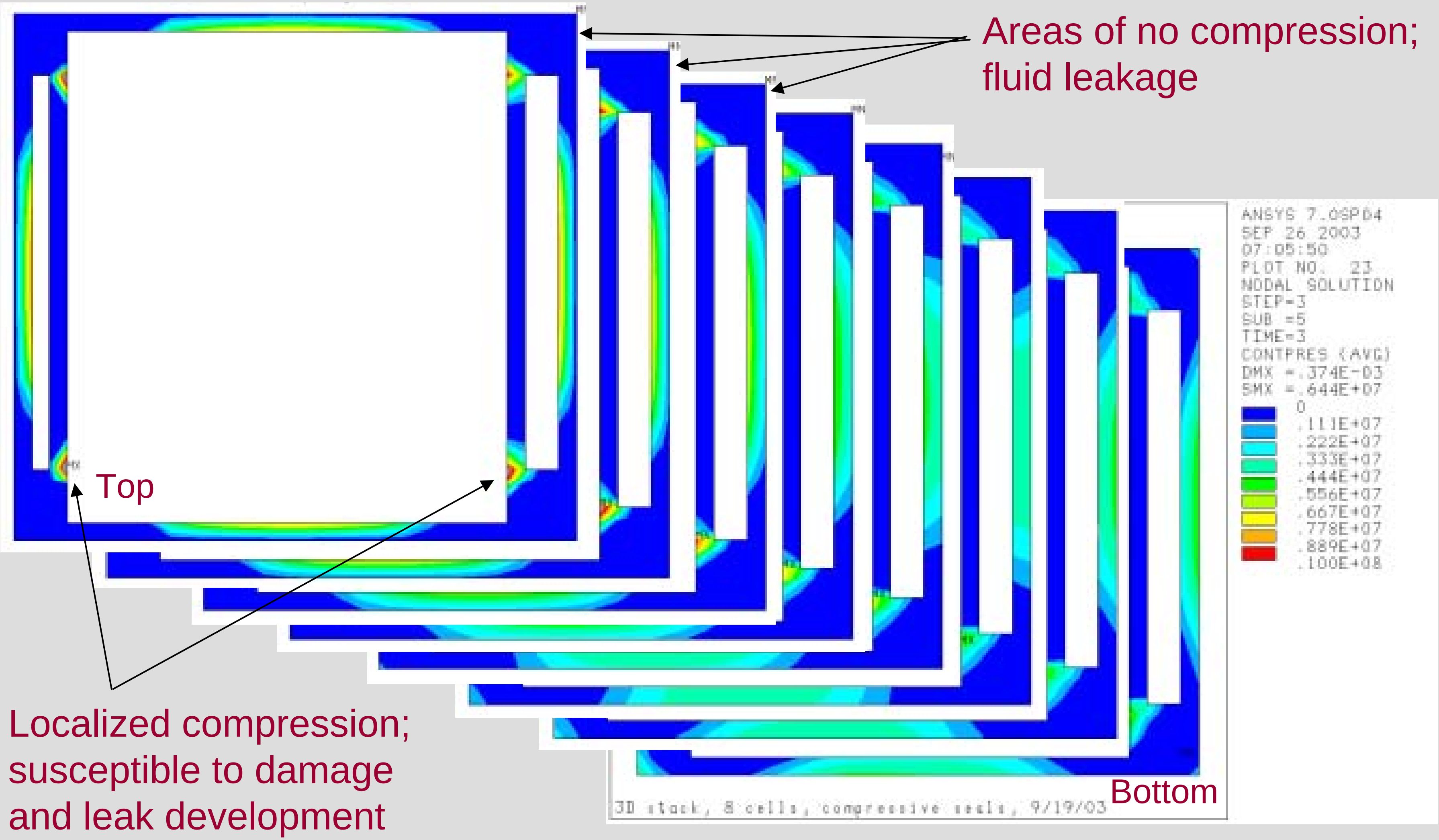
- 8-cell planar picture-frame design
  - 0.2 mm compressive mica seals at interconnect-anode spacer interface
  - Rigid seals at PEN-picture frame interface
- Frictional contact at compressive seal interfaces
- Load applied to top plate (nominal 200 psi compressive seal load)
- Simulated temperature profile



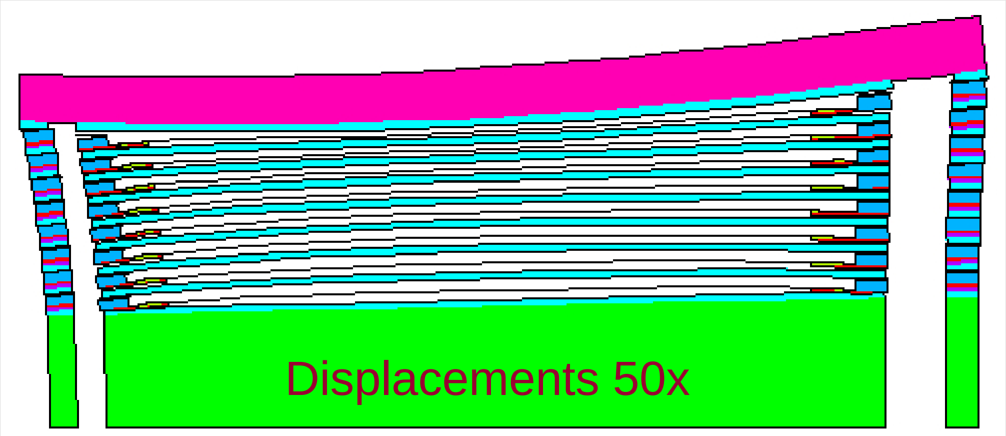


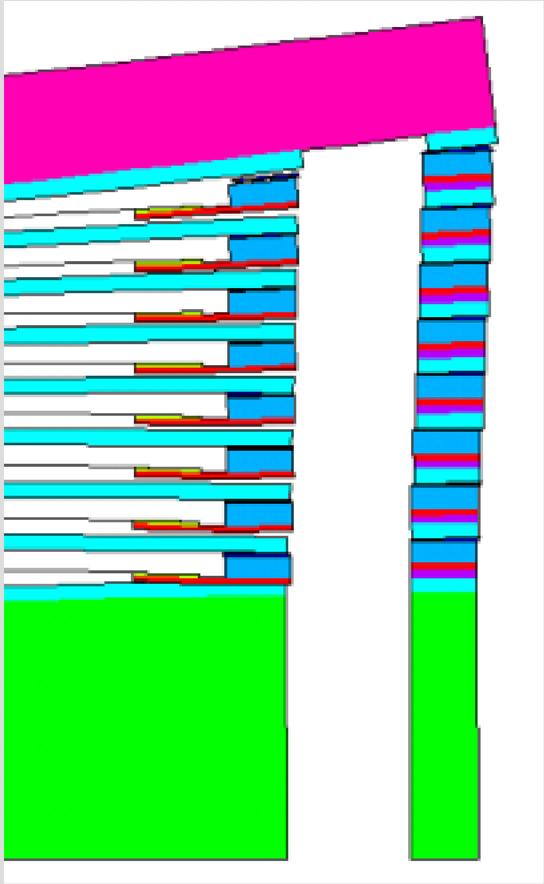


Compressive Seals: Results
Compressive Seal Pressure Distribution



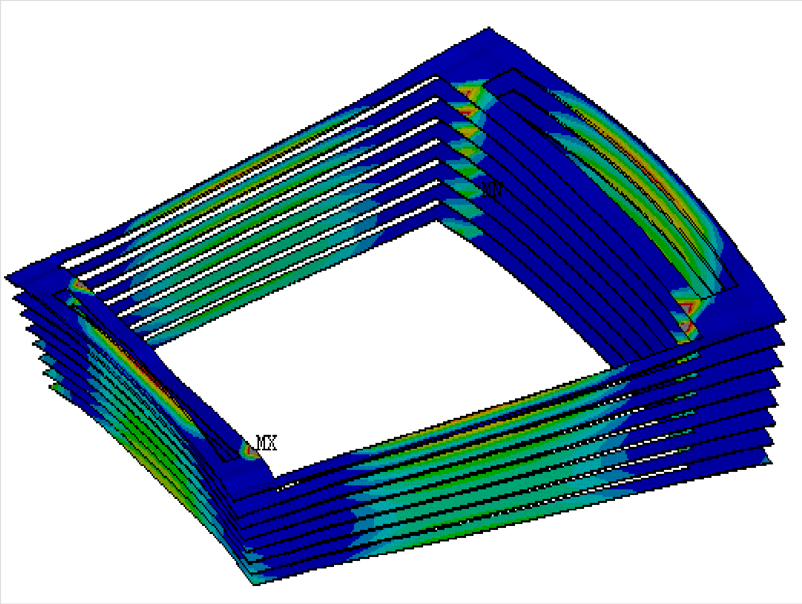
Compressive Seals: Results
Stack Deformation



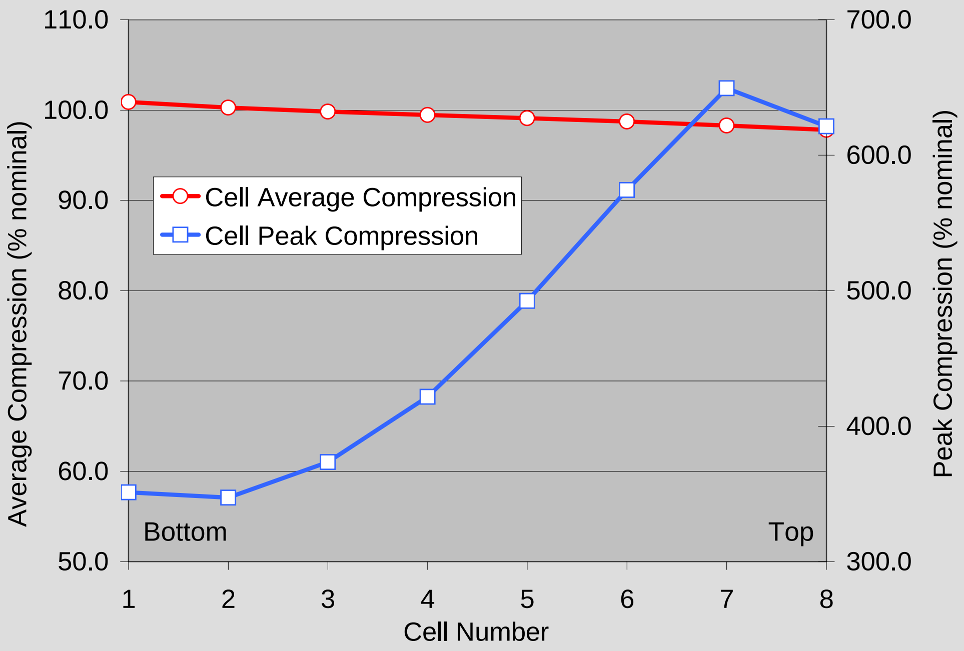


- Deflection in top plate influences stack deformations
  - Applied load was distributed uniformly
- Bending creates edge contact in the seals
  - Highly localized compression
  - Areas of no compression (separation)

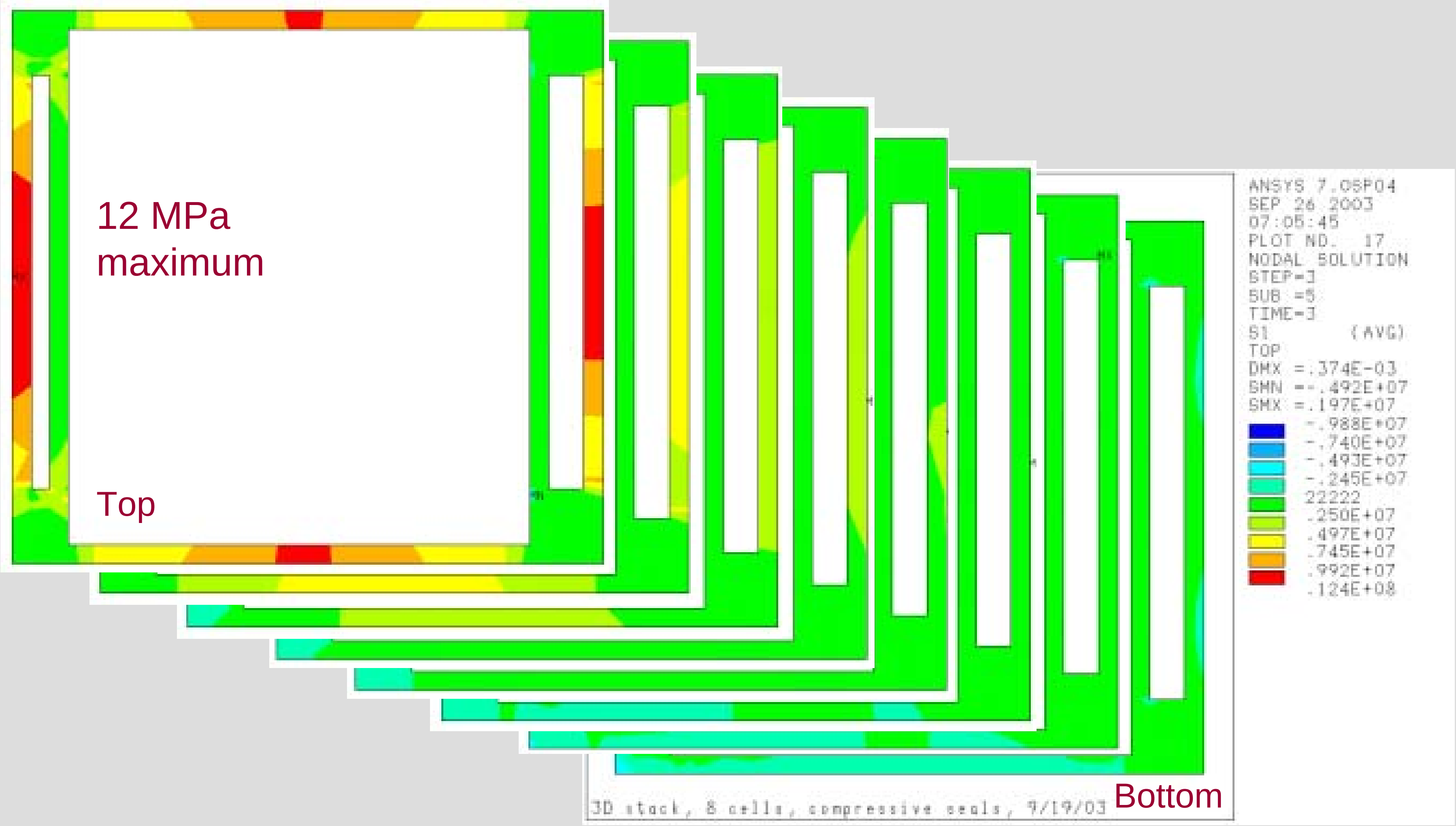
Compressive Seals: Results
Compressive Seal Pressure Variation



Seal Deformation



Compressive Seals: Results
Compressive Seal Principal Stresses



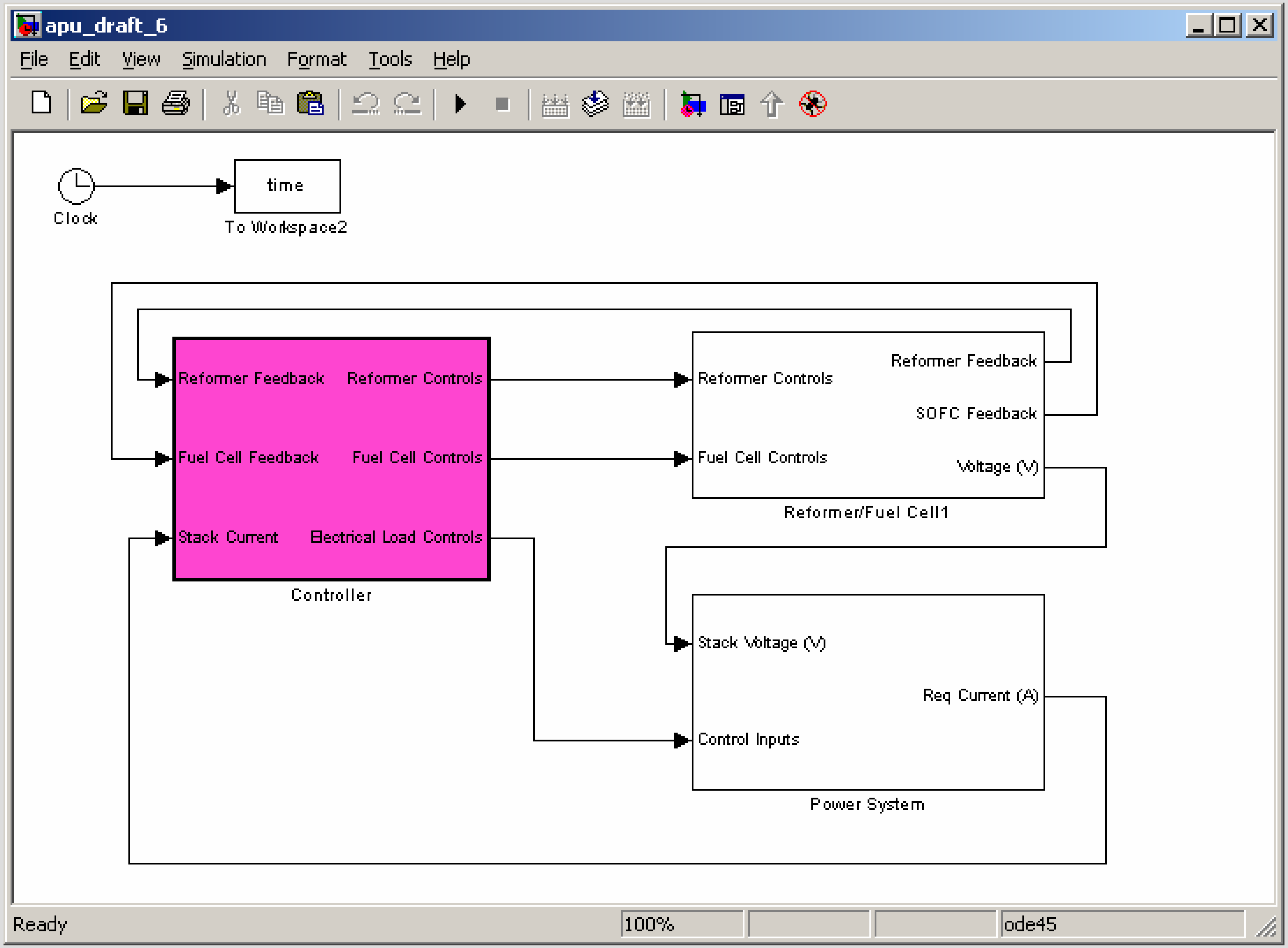
SOFC System Modeling and Controls

SOFC System Modeling and Controls

- **Purpose**: improve SOFC system efficiency and durability through better control techniques.

- **Goal**: develop system models and control techniques for a complete SOFC system.

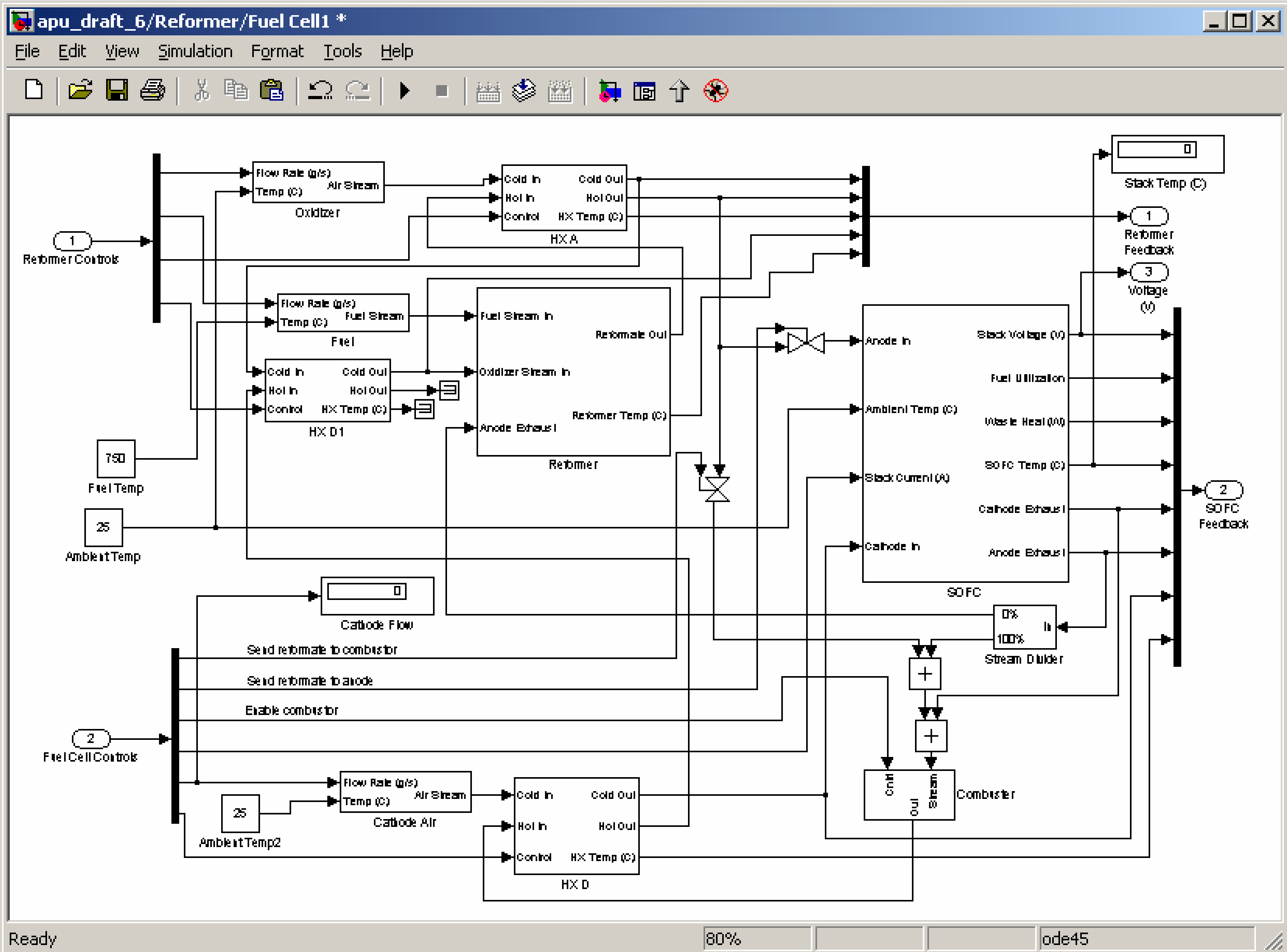
System Model



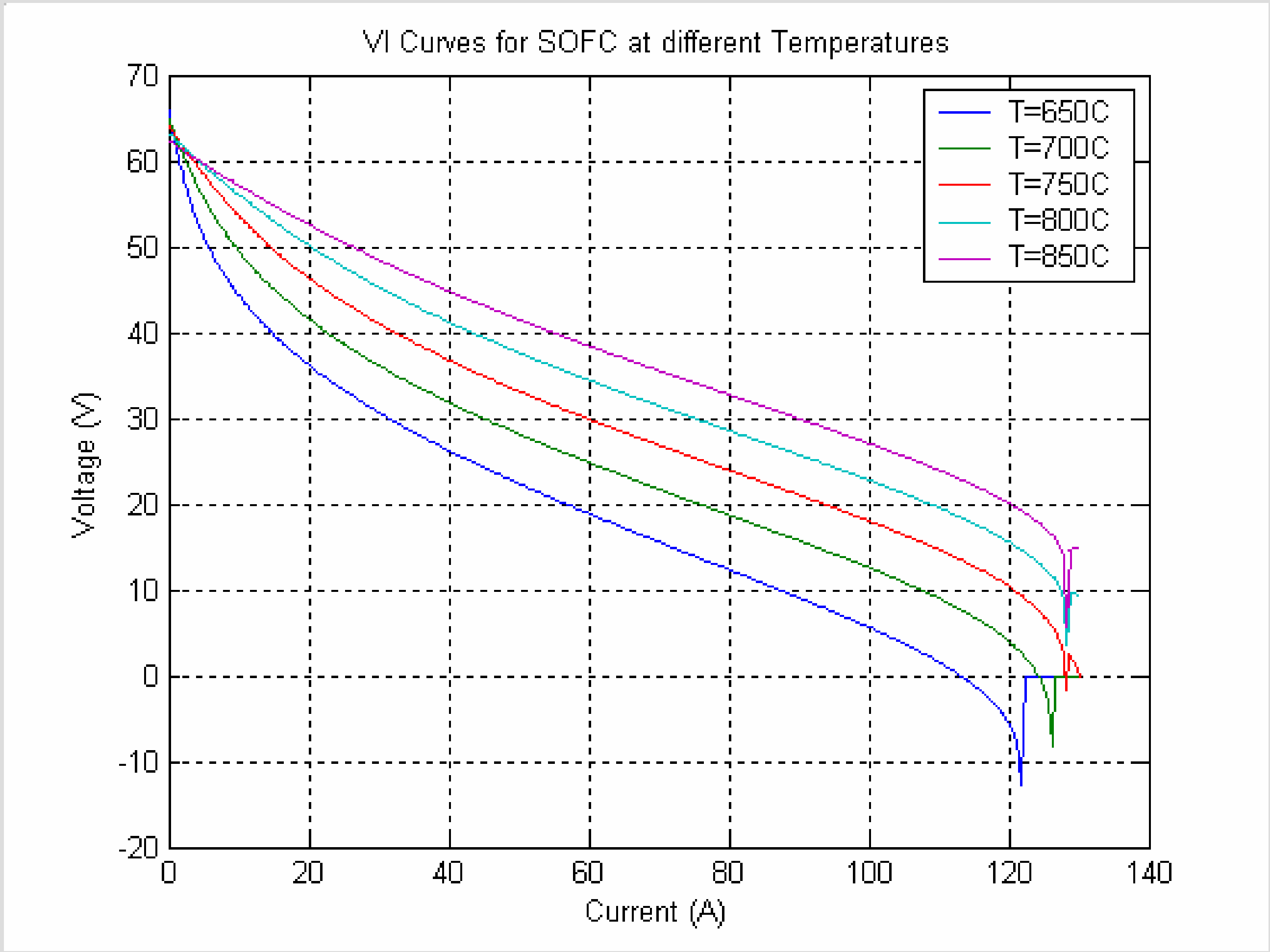
SOFC System Model

- Major system model components: controller, electrical system, reformer and SOFC stack.
- SOFC model is based on spreadsheet electro-chemical model. We extended the thermal aspects to deal with heat up phase and are adding dynamic components to the fuel utilization.
- Reformer model is a POx model and approximates diesel as $C_{12.95}H_{24.38}$ as fuel.
- Electrical system modeling models the power conversion electronics as well as the electrical loads such as air conditioning.

Stack + Reformer Model



VI Curves


VI Curves for SOFC at different Temperatures
T=650C
T=700C
T=750C
T=800C
T=850C
Voltage (V)
Current (A)
70
60
50
40
30
20
10
0
-10
-20
0
20
40
60
80
100
120
140

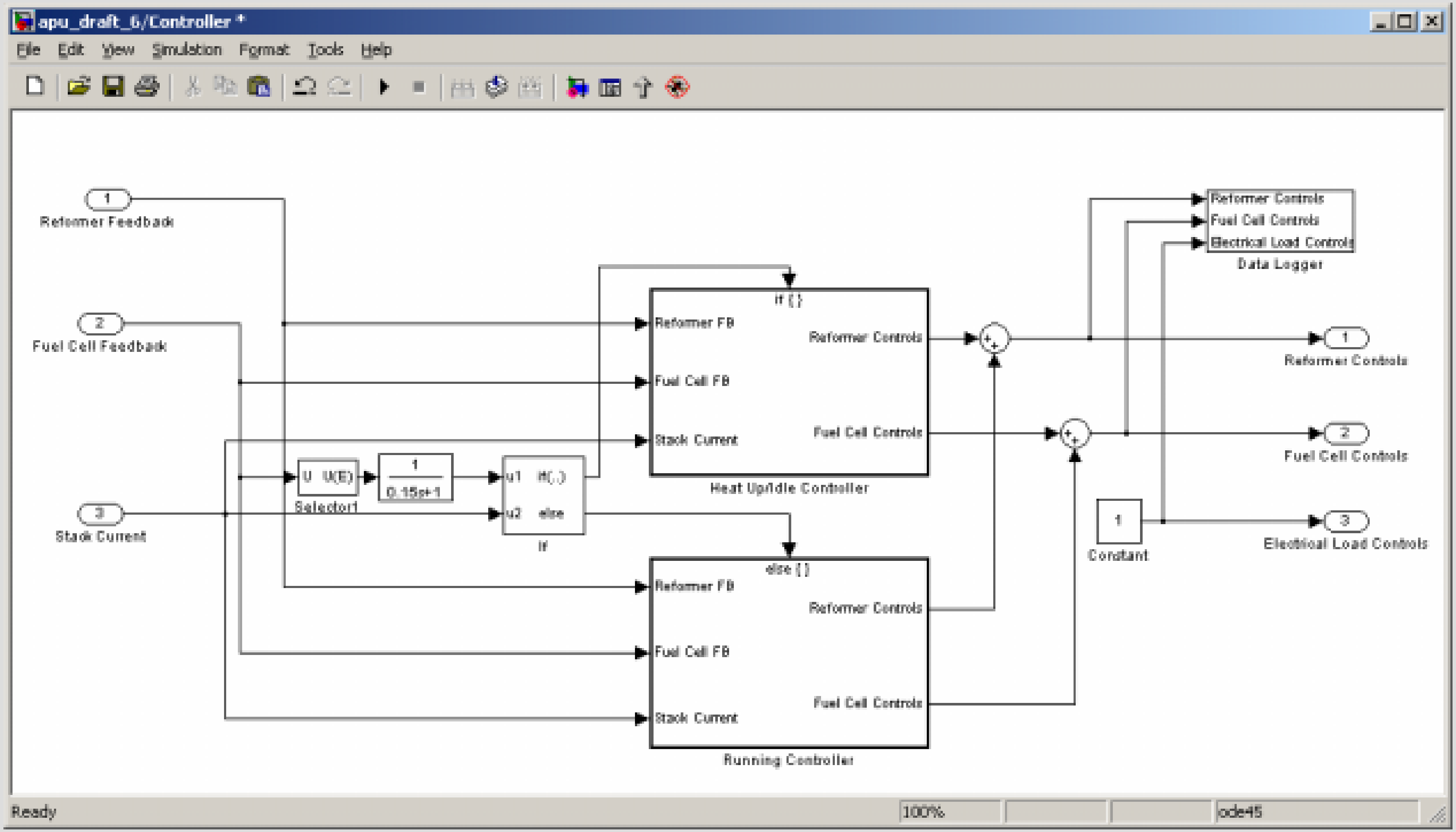
SOFC System Control

- The SOFC system is very complex and as electrical load demands change, the operating point of the reformer/fuel cell must be changed appropriately.
- A controller must control variables such as: fuel flow rate, reformate composition, cathode flow rate and temperatures throughout the system.
- Many of these variables are dependent on each other, and the controller must respond to potentially fast load changes.

Control Concept

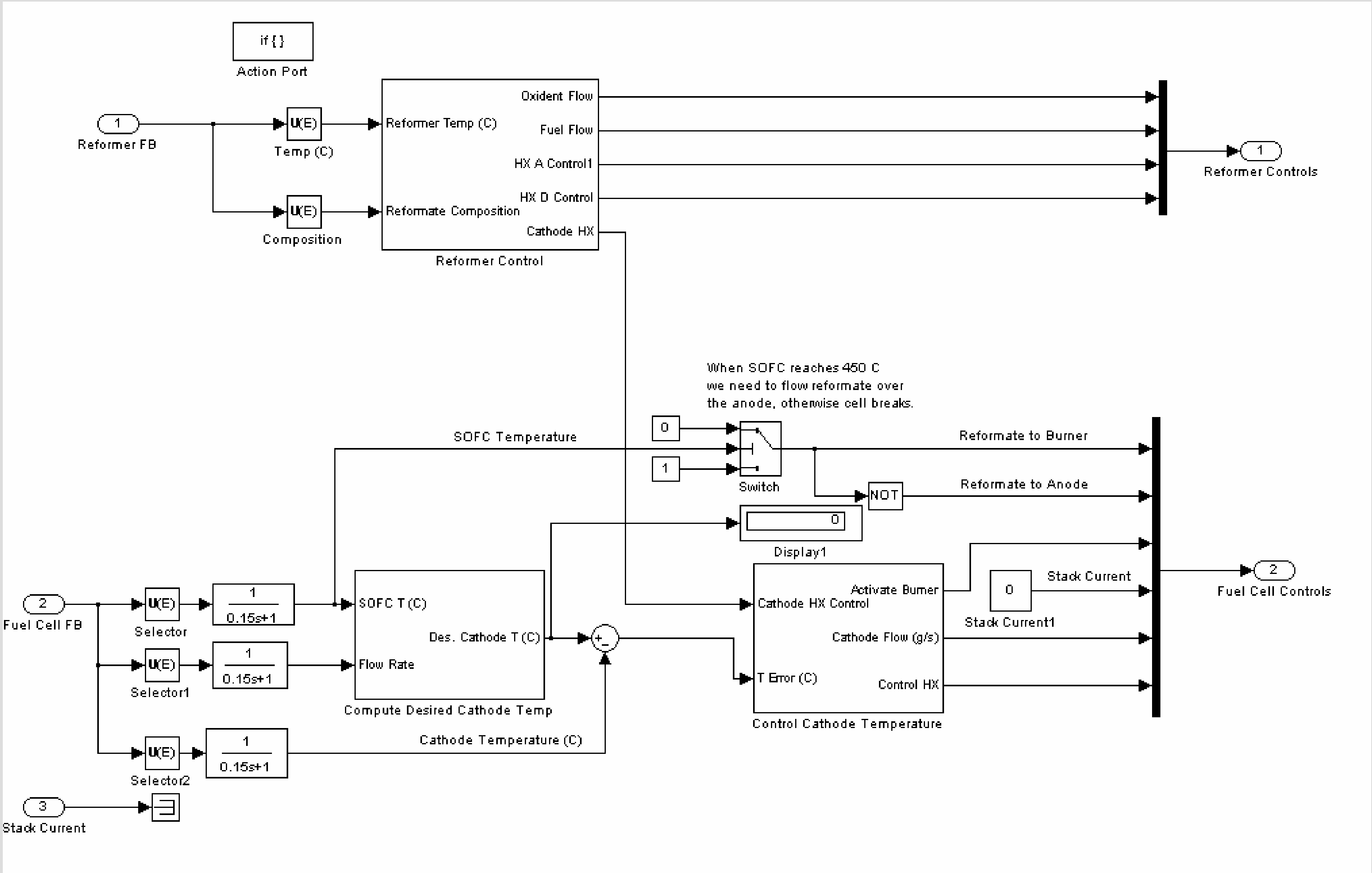
- Using a two phase controller – heat up/idle and operating.
- Heat up/idle controller
  - Uses a lookup table based on empirical data to specify desired cathode inlet temp based on stack temp and cathode flow rate.
  - Uses a PID controller to actuate HX bypass valve and control cathode temperature.
- Operating Controller
  - PID control of anode flow rate based on fuel utilization.

Controller

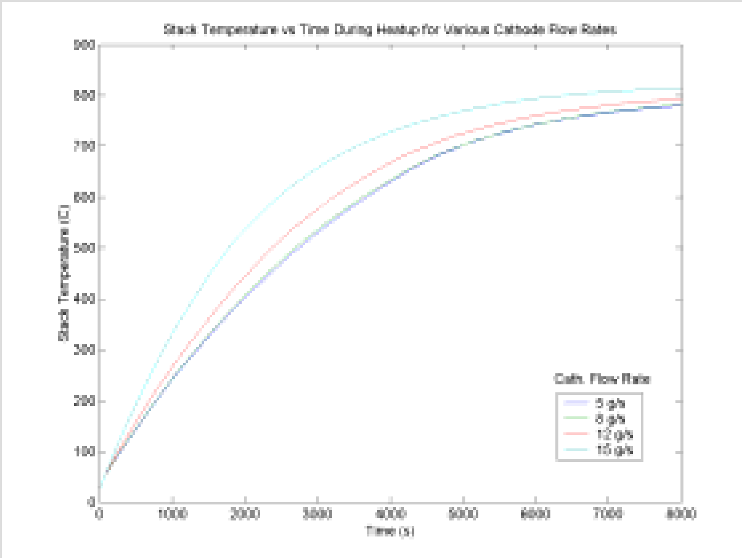


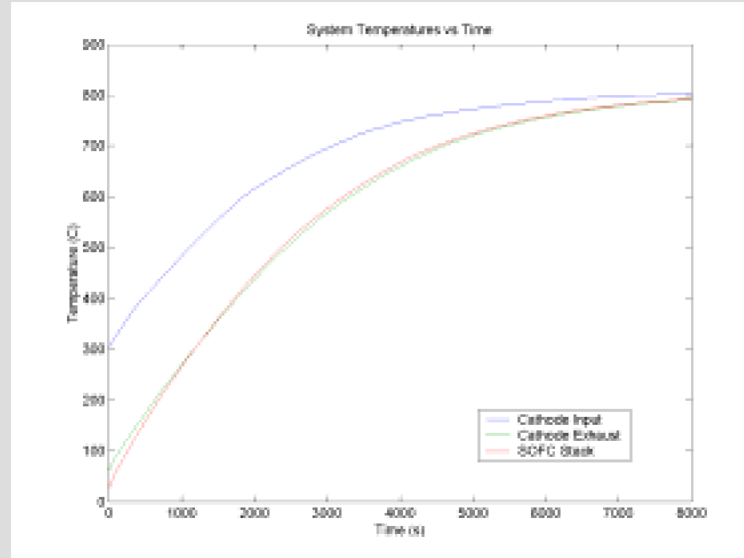
apu_draft_6/Controller *
File Edit View Simulation Format Tools Help
1
Reformer Feedback
2
Fuel Cell Feedback
3
Stack Current
U U(E)
Selector1
1
0.15s+1
u1 if(..)
u2 else
If
if { }
Reformer FB
Fuel Cell FB
Stack Current
Reformer Controls
Fuel Cell Controls
Heat Up/Idle Controller
else { }
Reformer FB
Fuel Cell FB
Stack Current
Reformer Controls
Fuel Cell Controls
Running Controller
Reformer Controls
Fuel Cell Controls
Electrical Load Controls
Data Logger
1
Reformer Controls
2
Fuel Cell Controls
1
Constant
3
Electrical Load Controls
Ready
100%
ode45

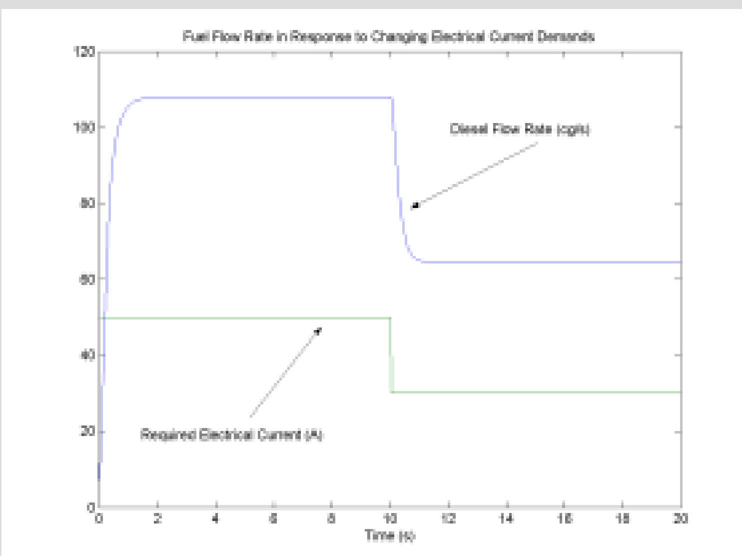
Heat Up/Idle Controller



Heat Up Controller Results







Fuel Utilization Controller Results

Future Steps - Compressive Seals

- Improve material model to include compressibility and recovery for compressible seal materials (e.g. mica gaskets)
- Improve material model to include creep effects
- Determine efficient contact element parameters
- Transfer model to MARC software environment
- Implement thermal cycling routines to account for degradation of seal compression
- Develop relations to predict leak rate for compressive seal designs

Future Steps – Next Quarter

- Work with the software vendor to complete the beta version of es-sofc and MARC-sofc software tools.
- Perform validation studies on 3 cell stacks.
- Develop constitutive relations and FEA models for rigid and compressive stacks.
- Create high level and optimal controllers for the SOFC system.
- Hold a workshop to establish technical activities regarding long-term degradations.
- Publish draft modeling and simulation roadmap (October 2003)