Three-Dimensional Thermo-Fluid-Electrochemical Modeling of Planar SOFC Stacks Using the STAR-CD Commercial CFD Code

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Presented by: Kurt Recknagle

OUTLINE

- Background
- Methodology
- Geometry
- STAR-CD / Prostar
- User Subroutines
- Parallel Processing
- Post Processing
- Further Topics
  - Transition modeling
  - Multiple Cell Stacks

Background

▶ The Planar SOFC is a high temperature (600-1000 °C), fuel cell that is favorable for use in many applications due to it's compactness: active areas can be stacked in close proximity to yield high power density

▶ The primary mechanical design challenge related to high temperature operation: the design must minimize the non-uniform temperature distributions that contribute to stress in the planar components

▶ Fuel utilization, temperature distribution, and average cell temperature are controlled by the delivery rate and the temperatures of fuel and air to the cell
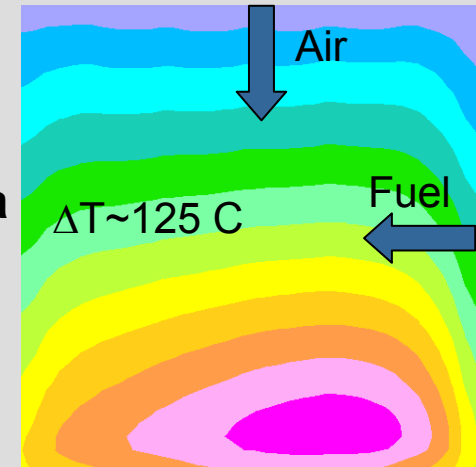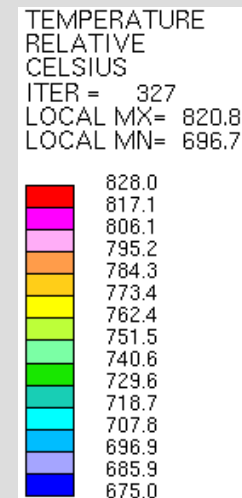
Background (continued)

▶ Increased fuel flow increases uniformity of the reaction rates on the active area but decreases fuel utilization.

▶ Decreased fuel flow increases fuel utilization, but can cause local fuel depletion and cold spots that exacerbate temperature non-uniformities.

▶ Management of the flow of air and fuel, and the distribution of each, is critical to stable operation of the cell.

▶ Reliable prediction of temperature distribution, using a Thermal-Fluid-Electrochemical (TFE) simulation tool, is key to successful analysis of potential designs
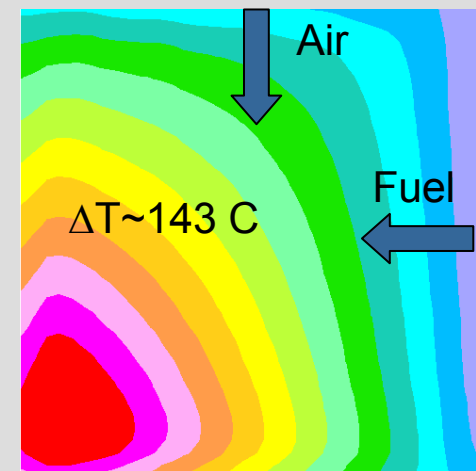
Background (continued)

▶ Example of difference in temperature distributions caused by difference in <u>fuel flow rate</u> only!

- Low fuel delivery
  - High fuel utilization
  - Decreased Power
  - Hot-spot near anode inflow
  - Smaller Delta-T
- High fuel delivery
  - Low fuel utilization
  - Increased Power
  - Hot-spot near anode outflow
  - Greater Delta-T

Active area of typical cross-flow cell

Air

Fuel

$\Delta T \sim 125$ C

Low fuel delivery rate

TEMPERATURE
RELATIVE
CELSIUS
ITER = 327
LOCAL MX= 820.8
LOCAL MN= 696.7

828.0
817.1
806.1
795.2
784.3
773.4
762.4
751.5
740.6
729.6
718.7
707.8
696.9
685.9
675.0

Air

Fuel

$\Delta T \sim 143$ C

High fuel delivery rate

Background (continued)

- Geometry is also key in establishing a well-operating cell. Distributions of Fuel & Temperature, and the fuel utilization are effected by:
  - Orientations of the fuel and airflows,
  - Mass and dimensions of the cell components,
  - Dimensions of flow channels and manifolds.
- In order to efficiently develop and optimize planar SOFC stacks, it is convenient to experiment numerically with the effects of geometric configurations on operation and performance.
- Will see examples of geometric effects later in this presentation.

Methodology: commercial code as platform

▶ Our methodology couples a validated electrochemistry calculation method (Chick et al, "Experimentally-Calibrated, Spreadsheet-Based SOFC Unit-Cell Performance Model") with the commercial computational fluid dynamics code STAR-CD (Computational Dynamics Ltd.).

▶ The resulting modeling tool is suitable for predicting the flow, distribution, composition, and utilization of anode and cathode gases, and the distributions of temperature and electric current in planar SOFC stacks with arbitrary three-dimensional geometries.

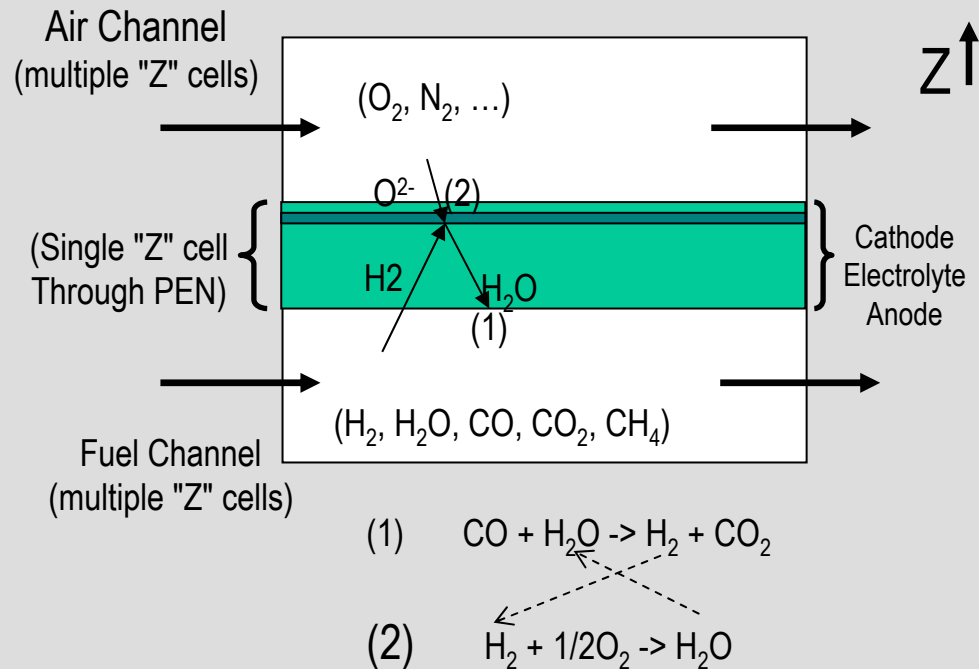▶ Presently, a FEA code is used to solve the stress distributions.

Methodology:
Why use commercial code as platform for TFE calculations?

▶ Built-in Capabilities to create complex cell geometries

- Ease in creating and comparing various flow configuration cases
- Enables parametric study of design features

▶ Built-in models to yield accurate prediction of scalar distributions including the temperature

- Transport equations for multi-component gaseous fluid streams
- Heat transfer models accommodate variable fluid stream properties (eg. 5:1 increase in fuel density from inflow to outflow boundary effects capacity to remove heat)

▶ Built-in models to calculate thermally induced stresses in solid parts

- Presently limited to finite element analysis codes

Methodology:
Hydrogen Combustion and Gas Water Shift Reaction

- Oxygen ions from the cathode side diffuse through electrolyte to the electrolyte-anode interface
- Hydrogen from the anode combusts with the oxygen and frees electrons which travel along the cell to an external circuit while water vapor generated by the combustion diffuses back to the anode side
- At the surface of the anode, the water vapor reacts with CO in the Gas-Water-Shift reaction generating more hydrogen and CO_2
- In the calculations, the shift reaction and combustion are assumed to be at equilibrium

Air Channel
(multiple "Z" cells)

$(O_2, N_2, ...)$

O^{2-} (2)

(Single "Z" cell Through PEN)

H2 H_2O

(1)

Cathode
Electrolyte
Anode

$(H_2, H_2O, CO, CO_2, CH_4)$

Fuel Channel
(multiple "Z" cells)

(1) $CO + H_2O \rightarrow H_2 + CO_2$

(2) $H_2 + 1/2 O_2 \rightarrow H_2O$

Methodology:
The Shift Reaction Procedure

▶ Assume that chemical equilibrium exists at every location

▶ Calculate the target (thermo-dynamic) equilibrium coefficient using

$$K_{eq} = \exp\left[-\frac{\Delta G(CO) + \Delta G(H_2O) - \Delta G(CO_2)}{RT}\right]$$

▶ Calculate the actual equilibrium coefficient using

$$K_{eq} = \frac{[CO][H_2O]}{[CO_2][H_2]}$$

▶ Adjust the shift reaction rate based on the difference between the two

▶ When steady, solution is converged
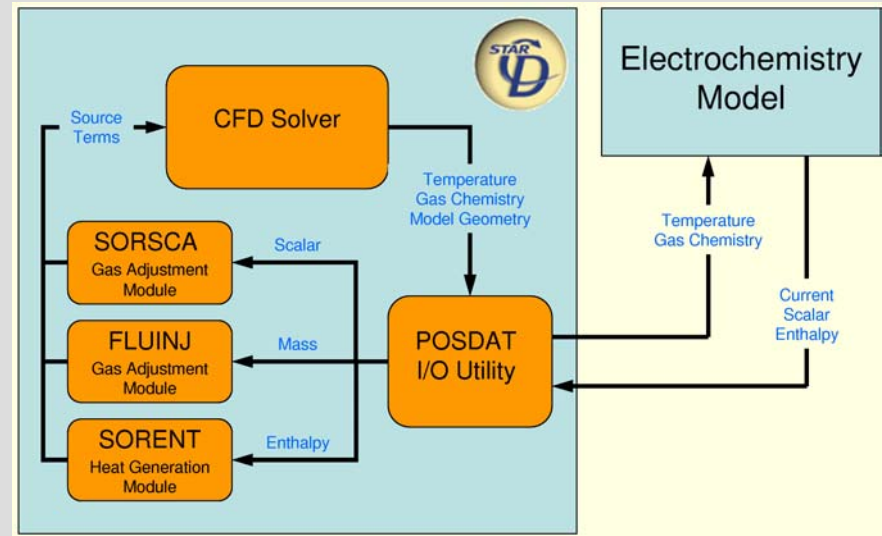
Methodology:
Electrochemistry - The I-V Relation

Term	**Description**
$V(i) = E_{nernst}$	Nernst potential
$- iR_i$	Ohmic resistances
$- b \sinh^{-1}(i/2i_0)$	Cathode Activation Polarization
$+ (RT/4F)\ln(1-i/i_{O2})$	Cathode Concentration Pol.
$+ (RT/2F)\ln(1-i/i_{H2})$	Anode Concentration Pol.
$- (RT/2F)\ln[1+p^0_{H2}i/(p^0_{H2O}i_{H2})]$	Anode Concentration Pol.

Model Parameters –Adjusted based on experimental cell data collected at PNNL

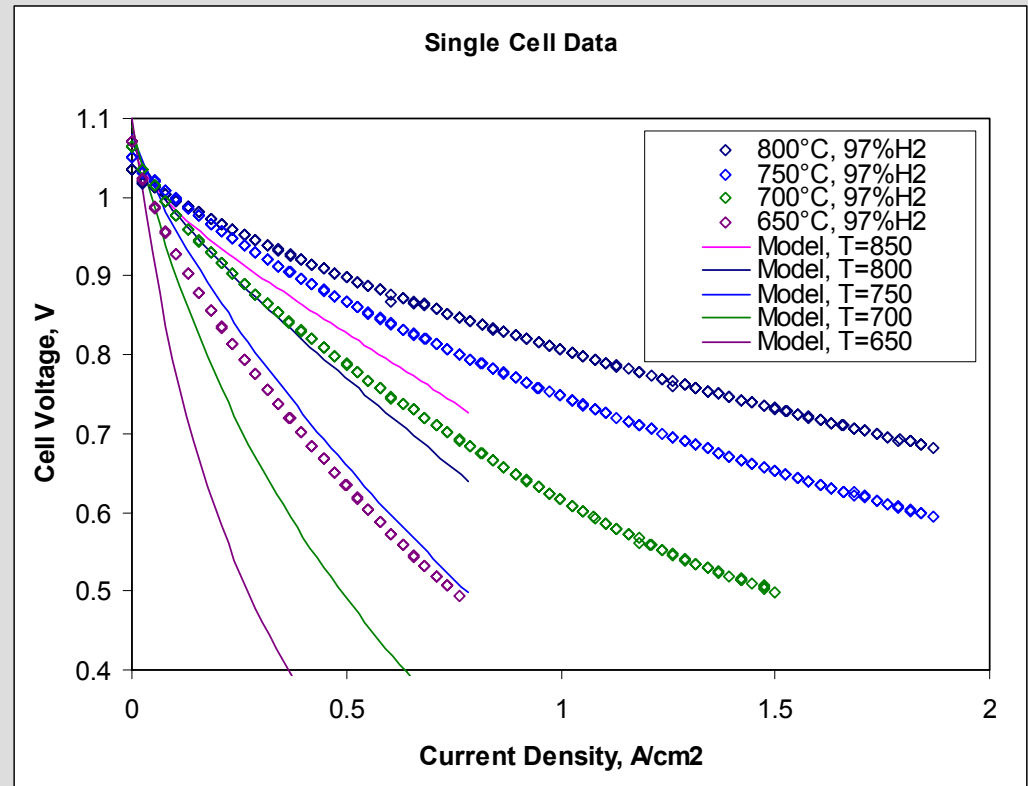|	
Nernst potential	$E_{nernst} = RT/4F \ln(Po2cath/Po2anode)$
Ohmic resistances	$R = R_p + R_e + R_n + R_{bipolar}$
Cathode Activation Pol.	b, i_O = Butler-Volmer parameters
Cathode Concentration Pol.	i_{O2} = cathode limiting current density
Anode Concentration Pol.	i_{H2} = anode limiting current density
Anode Concentration Pol.	p^0_{H2O} = partial pressure of water vapor

Methodology:
STAR-CD/EC Single-Cell Stack

- In the calculations, STAR-CD solves the Navier-Stokes and transport equations to obtain the flow, species concentrations and temperatures at each time step.

- The electrochemistry module calculates the local current distribution based on the applied voltage and local conditions. The current is used to calculate the local hydrogen combustion rates.

- The shift reaction rates are adjusted such that equilibrium conditions are satisfied at every location in the cell.

- Heat generation rates and species source rates are supplied to STAR-CD based on the local hydrogen combustion and shift reaction rates.

- Species concentration and temperature distributions are calculated for the next time step in STAR-CD.

Methodology:
The Spread Sheet, Chick, et al

- ▶ Spread sheet plots performance data from tests of a particular cell.

- ▶ Parameters of the I-V relation are adjusted to best fit the data.

- ▶ Thus a "cell specific" I-V relation is created.

- ▶ Electrochemistry routine in STAR-CD replicates the I-V relation determined by the spread sheet

Single Cell Data

Legend:
- ◇ 800°C, 97%H2
- ◇ 750°C, 97%H2
- ◇ 700°C, 97%H2
- ◇ 650°C, 97%H2
- — Model, T=850
- — Model, T=800
- — Model, T=750
- — Model, T=700
- — Model, T=650

Y-axis: Cell Voltage, V
X-axis: Current Density, A/cm2

Model Geometry – Cross-Flow Planar SOFC

- The repeating unit of a planar SOFC stack is constructed of a Positive electrode-Electrolyte-Negative electrode (PEN) and interconnect plates "stacked" together.

- Fig. 1 shows a schematic of an interconnect plate displayed as being transparent to show top and bottom features.

- The active cell area in Fig.1 is that formed by the intersection of air and fuel flows in the X-Y plane.

- A single-cell stack is formed when interconnects, similar to that in Fig.1, are placed above and below a PEN.

- Fig. 2 shows a partial schematic view of a vertical slice through a Y-Z plane of a multiple-cell, cross-flow stack. Air flows along the Y-direction. Fuel flow is along the X-direction (orthogonal to the page).

- The location of a cell unit along Z is shown at left in the figure.

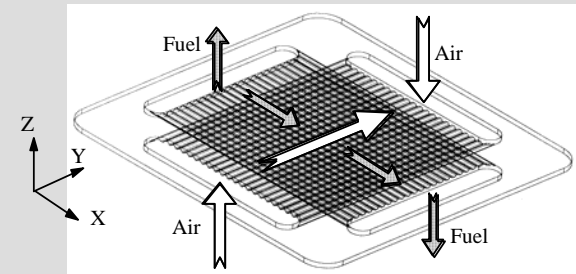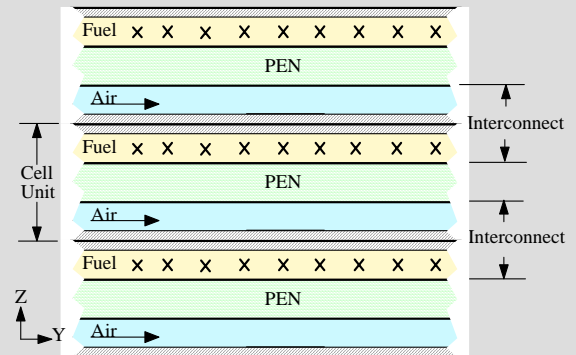Fig.1. Schematic view of a typical cross-flow planar interconnect plate.

Fig. 2. Schematic section view of a typical cross-flow stack. Xs in the fuel region represent fuel flow vectors perpendicular to the page.

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Specifying "Active" Elements for a STAR-CD Electrochemistry Calculation

- A partial schematic view of a typical STAR model of an SOFC is shown in the Figure.

- The green-shaded areas represent "cell" or PEN structure elements.

- Fluid elements comprising the cathode air and anode fuel streams are located adjacent to the PEN elements.

- Upon the first STAR time step, each element of the model is interrogated in search of PEN (Type 5) elements.

- When a PEN element is located, it's number and the numbers of it's nearest "fuel" (Type 11) and "air" (Type 10) neighbors are stored to an array as a group or "triple"

- At each time step (or iteration) the "triples" are invoked individually (for gas compositions of both the fuel and air elements, and PEN temperatures) for calculation of the local electrochemistry.

- When model geometry is decomposed for parallel processing, these "triples" must remain together in a "set" and available to the same processor.
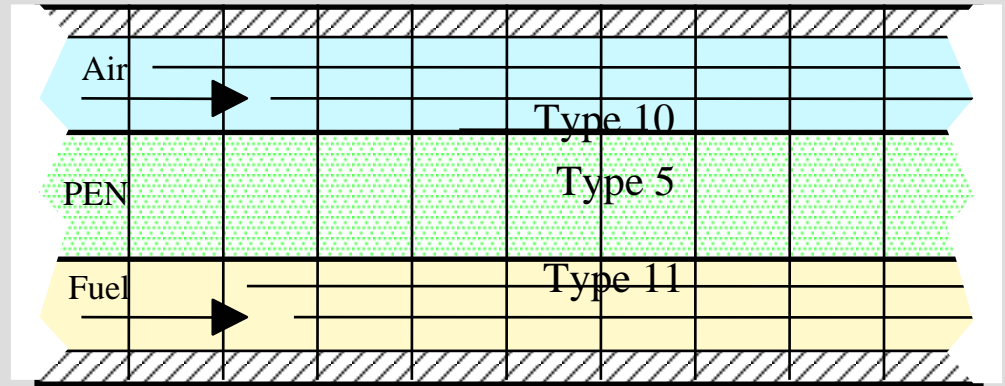
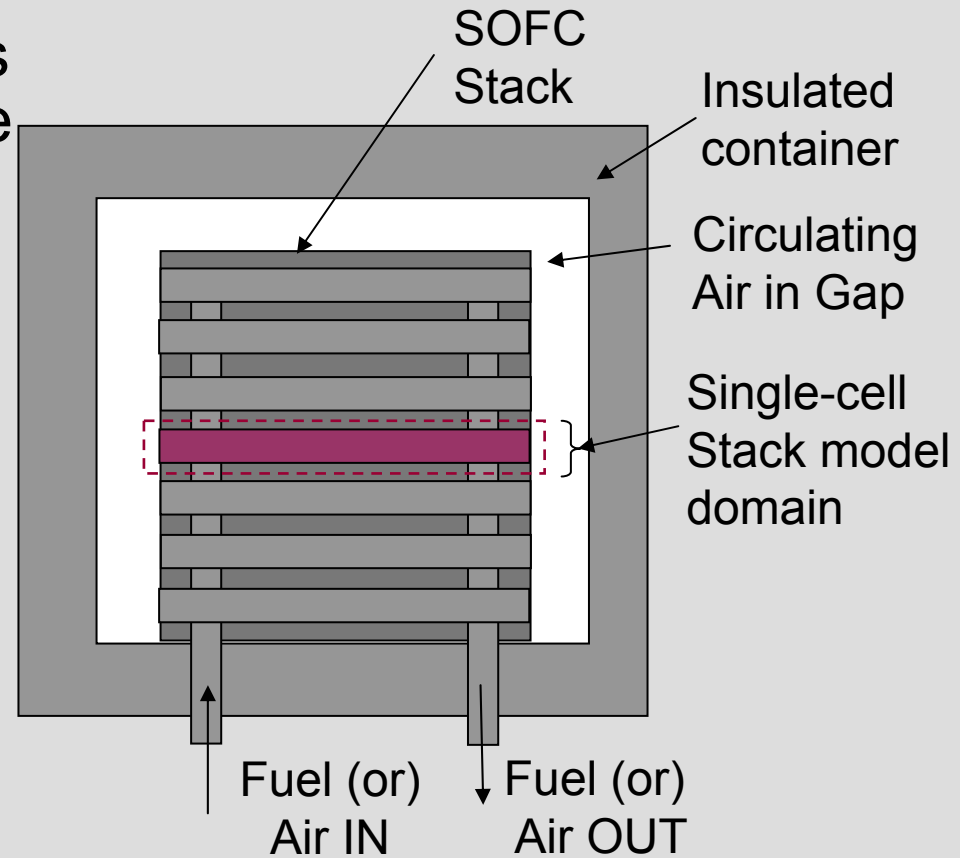# Typical Cross-Flow Cell Configuration & STAR-CD

► Start PROSTAR (pre- and post-processor for the STAR-CD code)
- prostar xm &

► Model geometry view
- cset all
- cplot

► Locate type 5, 10, and 11 cells discussed in previous slide.
- cset subset type 5 10 5
- cset add type 11
- cplot

► View the remaining cell types and materials in the model to understand how model geometry is assembled
- Use ctab button, and create new cell sets for viewing

Single-Cell Stack Model Boundary Conditions

▶ Cyclic Boundary conditions on top and bottom of single cell stack model (ie. cell resides within larger stack)

▶ Convection and Gap Radiation heat transfer to/from perimeter walls of model

▶ Constant Inflow boundary flow rates with variable temperature to control to desired operating temperature

SOFC Stack

Insulated container

Circulating Air in Gap

Single-cell Stack model domain

Fuel (or) Air IN

Fuel (or) Air OUT

Problem setup in Prostar

- ▶ "Select Analysis Features" – Steady State for this case, can be run in Transient mode
- ▶ "Create and Import Geometry" – Import Cad drawings, etc.
- ▶ "Create and Import Grids" –
  - Import meshes from ANSYS, Ideas, ICEM, Patran, Nastran, etc.
  - Create 2-D or 3-D meshes from scratch.
- ▶ "Check and Fix the grid" – warped faces, obtuse angles, zero or negative volumes, etc.
- ▶ "Locate Boundaries" – allows user to create boundaries on the model. Boundaries include inlet, outlet, pressure, symmetric, cyclic, wall, attach (for moving mesh), etc.

- ▶ Discuss use of element "sets" for geometric domain decomposition and parallel processing (recall discussion of "triples" being intact within a "set")

Problem setup in Prostar (cont.)

- ▶ "Thermo physical Models and Properties" – define the physical characteristics of solids, fluids, species within the gas mixture, and porous media. Initial conditions, reference values, etc.
  - Thermal Options – conjugate heat transfer (solid conduction coupled to fluid convection) is on.
  - Liquids and Gases – molecular properties – Ideal gas density and multi-component specific heat.
  - Turbulence model – laminar in this example case
  - Thermal model – temperature calculation on
  - Additional scalars – active scalars used to setup the gaseous mixtures, and passive ones to store current density, and heat generation rate
    - Molecular Properties – molecular weight, density, specific heat, viscosity, conductivity, etc.
    - Binary Properties – Diffusivity, Schmidt Number (kinetic viscosity) / (molecular diffusivity)
    - Initialization – calculate the mass fraction of the gas species in the fuel (and air) mixture starting with mole fractions. One option is to use the utility spreadsheet "fuelconccalcGAScycl2.xls"
  - Solids – constant density, capable of user defined specific heat and conductivity

Problem setup in Prostar (cont.)

▶ "Define Boundary Conditions" – Set up inflow parameters, velocities, no slip, adiabatic, symmetric, cyclic, etc. Our problem uses:
- Inlet – user defined (posdat.f and bcdefi.f)
  - Use utility spreadsheet "fuel_mix_props.xls" to determine mixture density at temperature for calculating the inlet velocity from mdot=rho*U*A
- Outlet – flow split = 1
- Cyclic – top and bottom of cell modeled as if residing in middle of tall stack
- Wall (of stack) – user defined convection and gap radiation to 25 degree cooler insulated walls (for example problem) (posdat.f and bcdefw.f).

▶ Scalar Boundaries – set boundary concentration of scalars in inflowing anode and cathode gas streams.

▶ "Analysis Controls" – choose numerical solvers, relaxation factors, output options, turn on various user routines, etc.
- Solution controls – equation behavior – additional scalars – solve for scalar
- Output controls – analysis output – printed data – user subroutine (posdat.f)
- Other controls – Miscellaneous controls – source terms for scalars, mass and enthalpy (sorsca.f, fluinj.f, sorent.f)

Problem setup in Prostar (cont.)

- ▶ "Check Model Setup" –
- ▶ "Analysis Preparation and Running" – iteration count, convergence criteria, or time steps, new or restart, interactive or batch, etc.
- ▶ Save geometry file
- ▶ Save problem file
- ▶ Quit and Save

STAR-CD, Prostar File Structure

▶ Casename.mdl – the model definition file

▶ Casename.set – sets of elements which, when combined, make up the whole domain.

▶ Casename.geom – geometry definition file

▶ Casename.prob – simulation parameter problem file

▶ Param.prp – model parameter file (array sizes…)

▶ Ufile – directory containing all user routines

- posdat.f, sorent.f, sorsca.f, fluinj.f, bcdefi.f, bcdefw.f, electrochemistry.f, nom.inc

User Subroutines: POSDAT.F

► Search for "user" in the file to locate parameters which may need adjusting

- Number of fuel cells in stack – istack
- Initial and goal temperatures – told, tnew, tinflow, tgoal
- Nominal Cell Voltage –
  - vcell (istack) – multiple cell stack models
  - vgrid – single cell stack models
- Stack current – multiple cell stack models
- Cell layer thickness, Porosities, and Tortuousities – danode, dcathode, delec, poranode, porcath, torta, tortc
- Butler-Volmer Parameters – eactbv, pxbv, alphabv

User Subroutines: ELECTROCHEM.F

▶ Inputs: temperatures, partial pressures, voltage

▶ Outputs: current density, fuel/air specie source terms, enthalpy source term

▶ Within electrochem.f

- chemistry1 – pO2anode and other preliminary quantities
- diffus – specie diffusion in porous anode and cathode
- zbrent (solver) – calls to "comodel" to iterate on voltages in the Nernst equation to solve for local current density "igrid"
- chemistry2 – "igrid" determines moles of O2 consumed,
    - Shift in equilibrium with combustion of H2
    - => other species consumed/produced => fuel/air source terms
    - => net heat of reactions => enthalpy source term

User Subroutines: Others

► sorent.f – enthalpy source term to the PEN (type 5) elements for the energy equation

► sorsca.f – source terms for fuel/air stream components to the scalar transport equations

► fluinj.f – source terms for air/fuel streams (types 10, 11) for the "bulk fluid" and directed to the mass and momentum equations, equal in magnitude to the scalar source terms

► bcdefi.f – Inflow boundary condition settings – temperature adjusted to control stack (average PEN) temperature to desired value

► bcdefw.f – Wall boundary condition settings – temperature and resistance adjusted to reflect convection and radiation from stack walls to enclosure

Run PROHPC for Parallel Processing

▶ Start Prohpc - prohpc &

▶ Machine setup

▶ Problem setup

▶ Moving grid transients

▶ Run setup

▶ Post processing

▶ Utilities

STAR-CD Simulation

- Start STAR-CD simulation
- Monitor runtime parameters
  - tail –f "star-…log"
  - tail and pipe to grep for "ITV" in the 0001 directory .info
  - "Chem" in the 000x directory .info file
- Stop simulation prematurely and change run
  - prohpc ABORT
  - prohpc rmall ABORT
- Make simple change in Prostar – eg. post-processing dumps
  - prohpc putfile .prob
  - Restart simulation

Post Processing in Prostar

- Merge .pst file using prohpc
  - Prohpc merge .pst
- Start Prostar
  - Prostar xm &
- Post Processing module
  - Read .pst
  - Extract cell data
  - Make velocity vector plot
  - Make temperature contour plot
  - Make current density contour plot (others)

How to "Break" the code!

▶ Fuel Depletion
- In Prostar, make large decrease fuel inflow velocity

▶ High Temperature
- Modify "tgoal" in posdat.f to be 1123K (850C) or higher

▶ Too large a number for "sconst" in electrochem.f

Geometric Effect on Temperature Distribution – Single-cell stack

► 3 flow configuration cases

► Each case with similar average cell temperature and fuel utilization

► Results show very different temperature distributions

**Cross-Flow** **Counter-Flow** **Co-Flow**
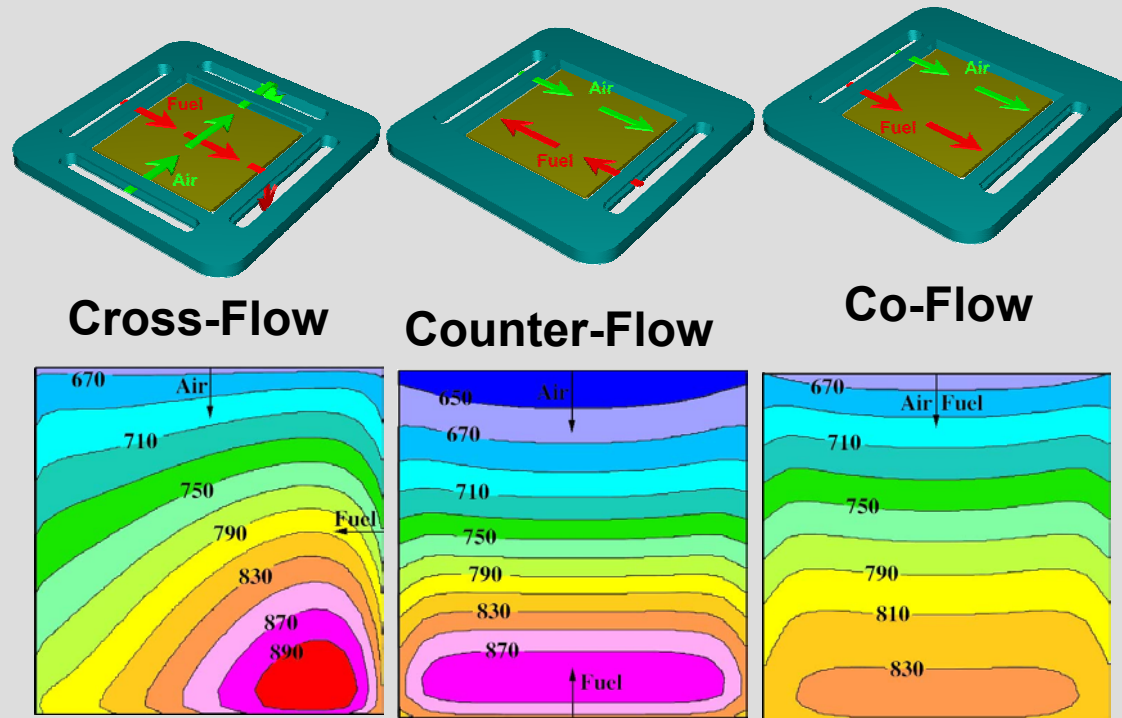
Transition from Startup to Steady

- In another modeling task we simulate stack startup

- Cathode air is used as heating source to heat the stack to the "startup" temperature

- The time to start is an important consideration in the design process for stacks used as auxiliary power sources

- To determine if we can abbreviate the startup time, and to ensure that the system will remain stable, we simulate the transition from startup to steady state

- For the transition, we use the startup temperature distribution as initial condition.
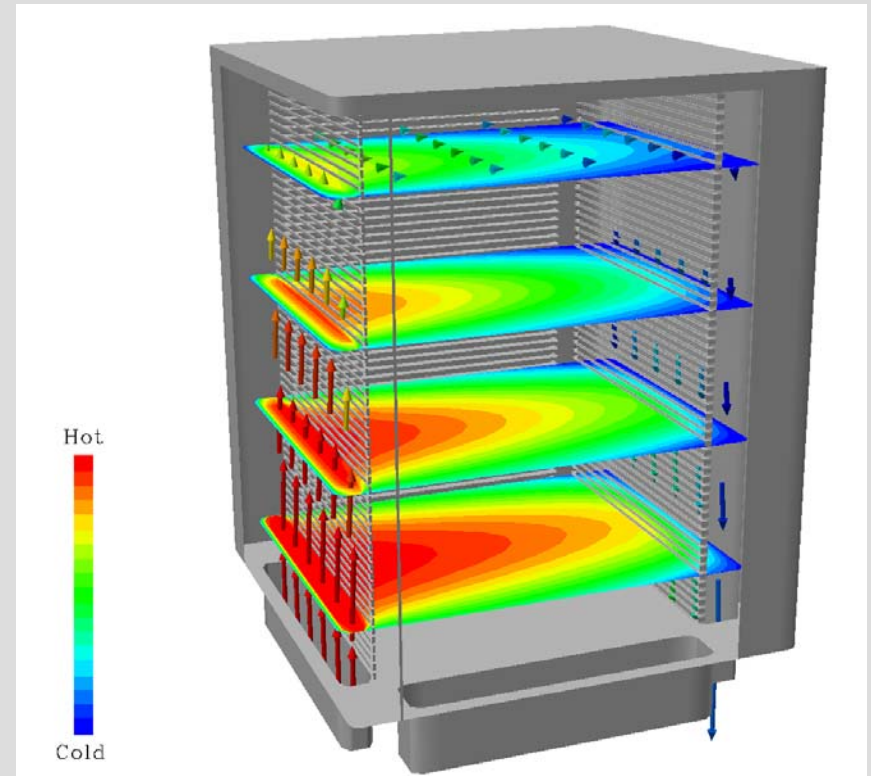
Example of an *early* startup model temperature result

Transition from Startup to Steady

- ▶ Run model fully transient from ambient – or – use initial temperature field from the end of a startup simulation

- ▶ If restarted using an initial temperature field from a separate model, restart using the SMAP option

- ▶ Run STAR-CD in transient mode

- ▶ Use artificially low specific heat – okay for preliminary test case to check problem stability, etc.

- ▶ Use correct properties for final, more accurate transient
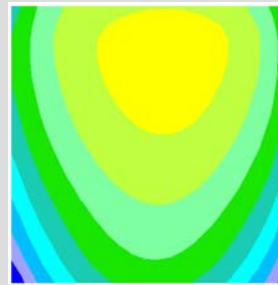
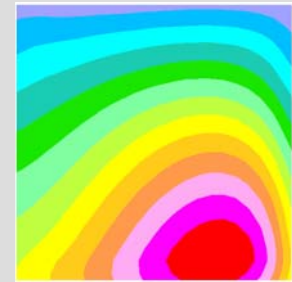**"Startup" Temperature Distribution (2% of transition time)**
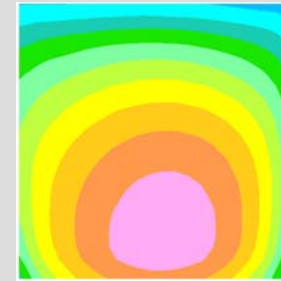
20%

40%

Run Model In Transient Mode

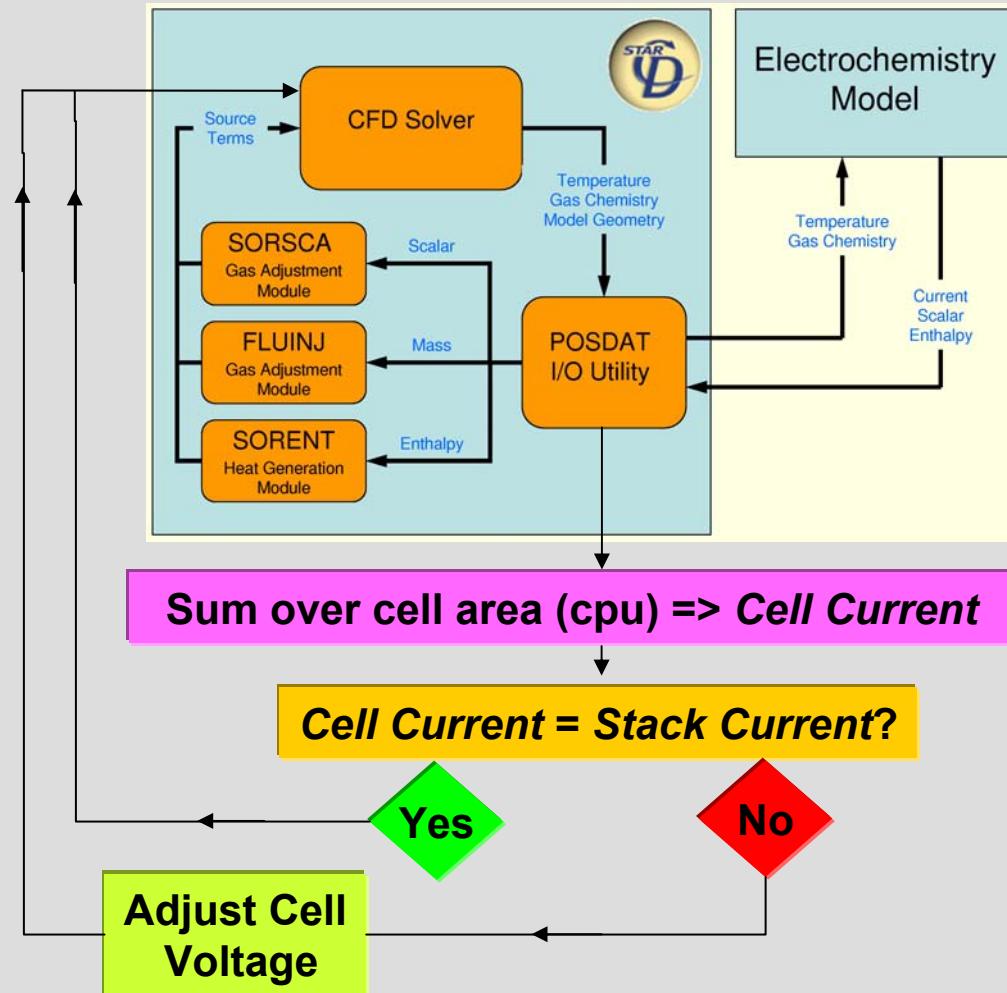**100% "Steady" Temperature Distribution**

Multiple-Cell Stack Model

▶ **Model domain is the full stack geometry**

▶ **Convection and Gap Radiation heat transfer to/from perimeter walls of stack/container included in the calculations**

▶ **Constant Inflow boundary flow rates with variable temperature to control to desired operating temperature**

▶ **Cell voltage adjusted such that stack current is satisfied –> stack voltage distribution resolved.**

SOFC Stack

Insulated container

Circulating Air in Gap

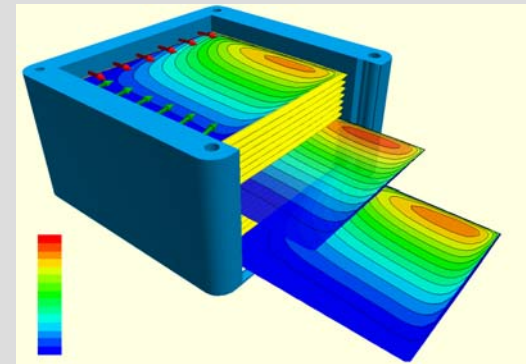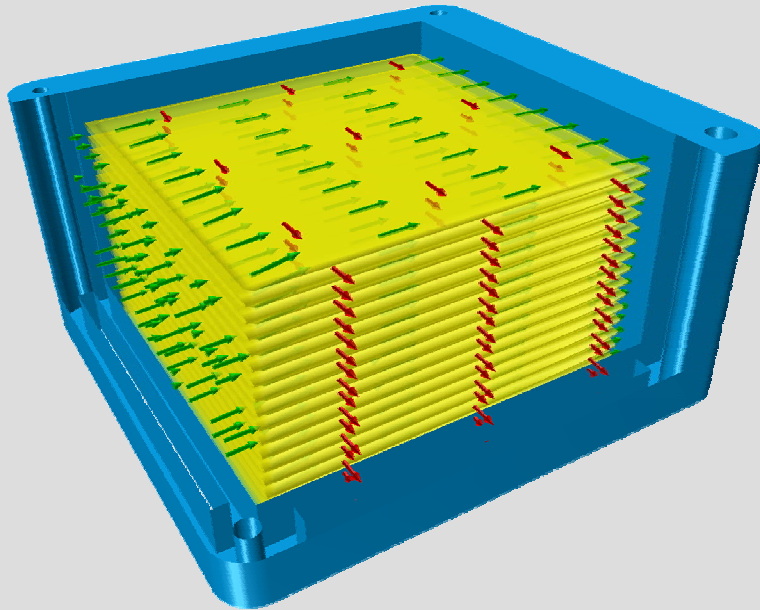**Multiple-cell Stack model domain**

Fuel/Air IN

Fuel/Air OUT
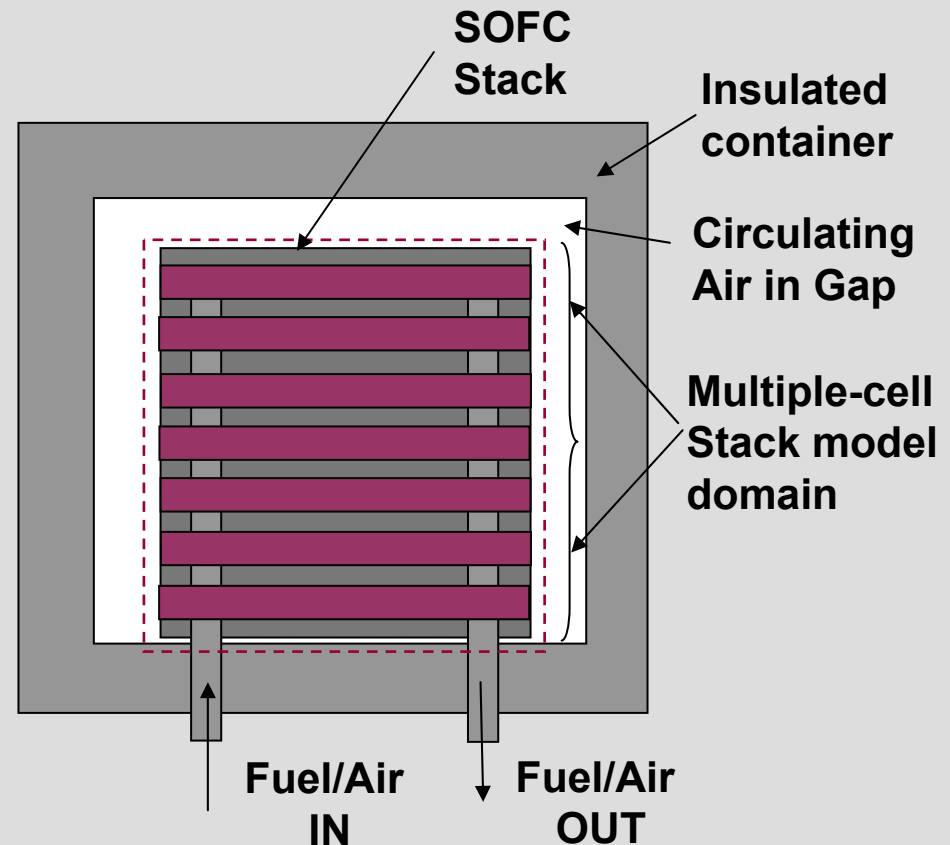
Methodology: Multiple-Cell Stack

- Multiple-Cell stack model is an extension of the single-cell stack calculation
- Additional loop adjusts cell voltages such that stack current is satisfied
- In present implementation, the domain is decomposed to one cell per processor (using "sets")
  - Simplifies "bookkeeping" and summation of scalars over each cell
- Convergence criteria remains the equilibrium of the combustion and shift reactions

Electrochemistry Model

CFD Solver

Source Terms

Temperature Gas Chemistry Model Geometry

Temperature Gas Chemistry

SORSCA Gas Adjustment Module — Scalar

FLUINJ Gas Adjustment Module — Mass

SORENT Heat Generation Module — Enthalpy

POSDAT I/O Utility

Current Scalar Enthalpy

Sum over cell area (cpu) => *Cell Current*

***Cell Current = Stack Current*?**

Yes **No**

Adjust Cell Voltage

Multiple-Cell Stack Model & Results

Temperature (C)

▶ Average cell temperatures increase with height in stack (away from inflowing gas source).

▶ Cell temperature difference is maximum low in stack near cooler source gases
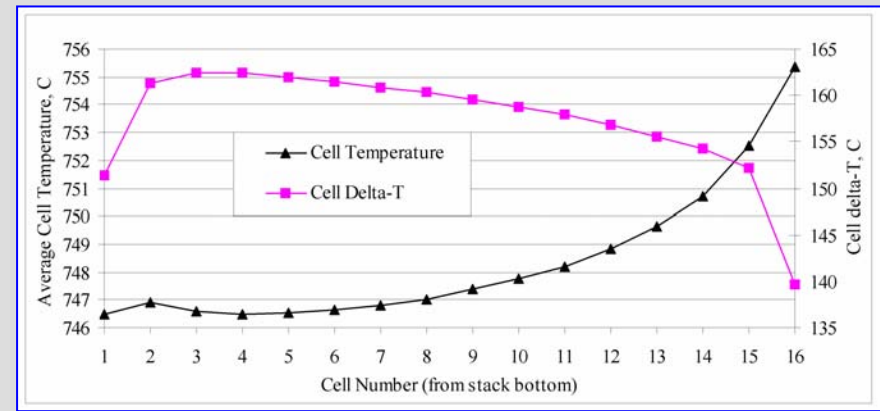
Multiple Cell Stack Models

► The Multiple-Cell model is an extension of the single-cell stack to a "full stack" model

► Wall boundary conditions at stack ends remove cyclic assumption

► Calculates voltage distribution and temperature distribution including stack end effects

► Domain is decomposed one cell per processor (bring up model to demonstrate sets)

► Adjustments to posdat routine (istack, stacki)