Finite Element SOFC Analysis with **SOFC-MP** and MSC.*Marc/Mentat-FC*

Ken Johnson, Speaker

Pacific Northwest National Laboratory

SECA 6th Annual Workshop, April 18-21, 2005

> Pacific Northwest National Laboratory Operated by Battelle for the U.S. Department of Energy



Solution Flow

Mentat-FC:

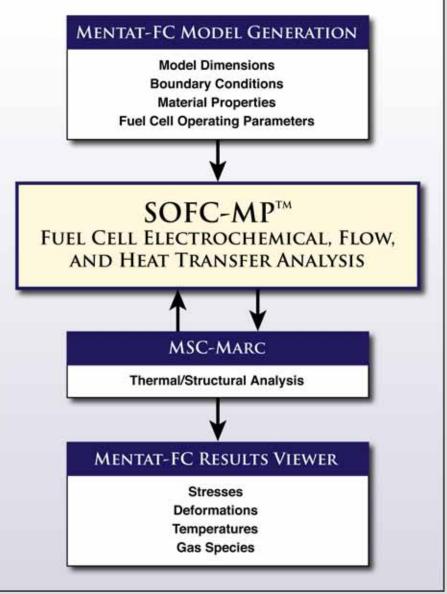
Graphical User Interface for flexible finite element model generation.

SOFC-MP:

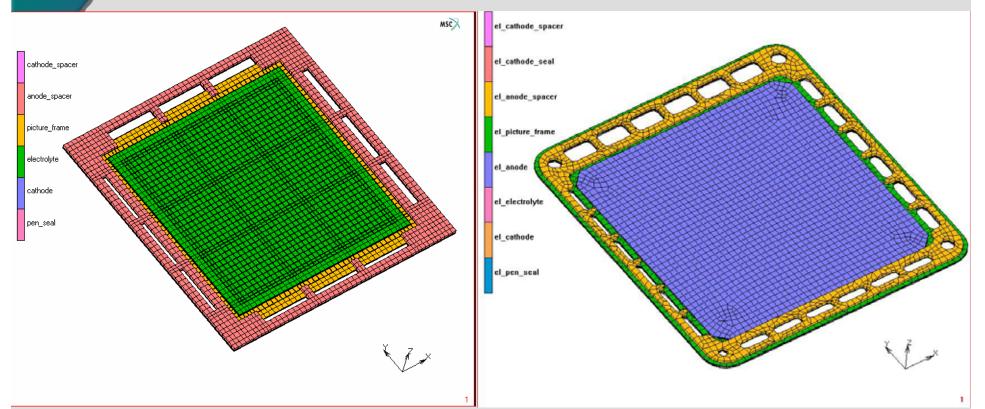
Finite element based electrochemistry, flow and heat transfer solution.

MSC.Marc:

Finite element stress analysis with temperatures from *SOFC-MP*.



Mentat-FC: Parametric and CAD based Models



Parametric

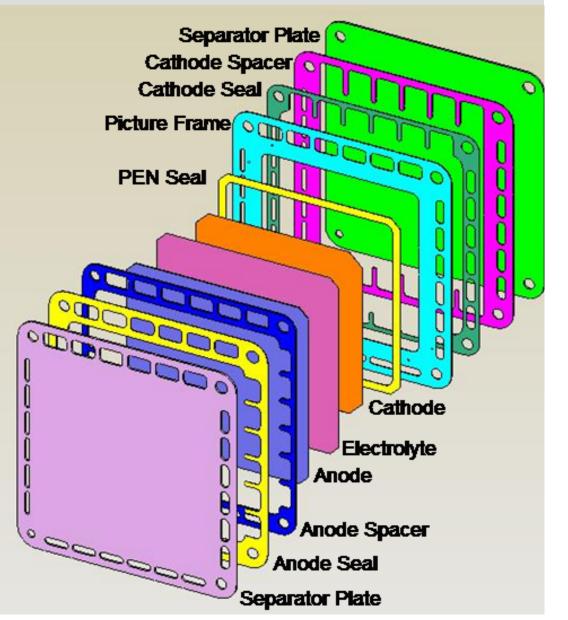
- •Fixed SOFC designs
- Meshed from dimensional parameters
- •Used for parametric design studies

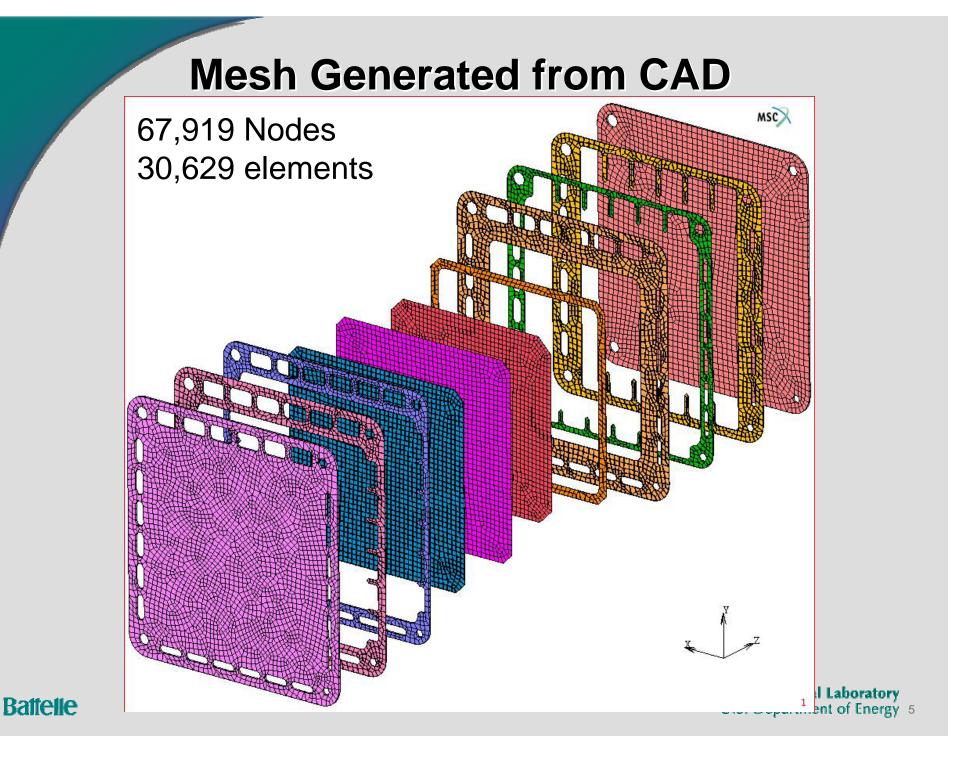
CAD Based

- •Meshed from user CAD files
- •Accepts existing FE meshes
- •Quick generation of very complex models

Mentat-FC: Model Generation from CAD Geometries

- Finite element grid meshed from CAD volumes.
- Generic ACIS file format used.
- Layers identified by name.
- Material properties assigned to components from the database.
- Contact and boundary conditions are defined.





Generic Model Regions are Defined for Meshing

Required Regions - define bounds of the electrochemical and flow calculations:

- PEN layers = Anode, Electrolyte, Cathode.
- Fuel = Inlet, Outlet, Anode flow channel.
- Air = Inlet, Outlet, Cathode flow channel.
- Separator plates.

Additional Regions – define the PEN Support Structure = components making up the manifolds, seals, and structure around the PEN.

- Anode and Cathode spacers.
- PEN support frame.
- Seals.

Material Data and Electrochemical Parameters

- Material data base for thermal, electrical, and structural properties is included for:
 - Metallic interlayers and support plates
 - Seals,
 - Anode, electrolyte, and cathode layers
- Electrochemistry parameters
 - I-V relationships
 - Fuel and Air composition and flow rates.
 - Startup conditions

Features of SOFC-MP

- Generic fuel and oxidants can be simulated. NASA's CEA code used for chemical equilibrium and species calculations.
- Finite element based flow, temperature and electrochemistry calculations. Thermal and structural solutions use the same mesh.
- Reduced dimensional analysis for fast flow solution.
- Contact algorithms treat incompatible meshes for contacting solids with different surface profiles.

Reduced Dimensional Approach for Fast Approximate Solutions

Reduced Analysis

Electrochemistry – 1D through thickness of the PEN

► Flow

- <u>Manifolds</u> Use an analytical pipe flow approximation
- <u>Channels across Cell</u> 2D with hydraulic approximation for varying channel height.
- Temperature 3D for solids, 2D in flow domains.

Full 3D Analysis

Stress and Distortion – 3D in solids.

Solution Performance

Algorithms are efficient for rapid analysis and extension to transient thermal-mechanical analysis.

Single cell examples on a single processor (Memory~1.5 Gb)

- Mentat-FC Mesh generation ~ 15 min.
- SOFC-MP solution ~20 min.
- MSC.Marc stress solution ~ 3 min.
- Coarse stack models with up to 3 cells have been run on the PC.
- Significant multi-cell analysis requires parallel processing for:
 - Increased memory
 - Reduced compute time.

Generating a Model from CAD files

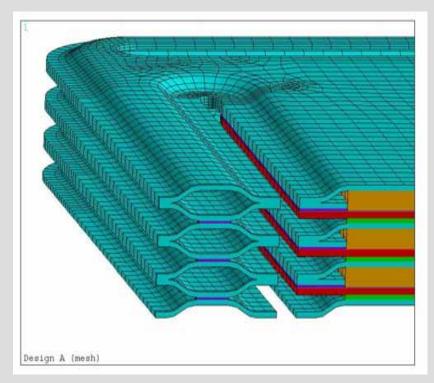
Required Components	Additional Components	Separator Plate
Separator Plate – Blank	Anode Seal	Cathode Spacer Cathode Seal Picture Frame
Fuel Flow	Anode Spacer	Picture Frame PEN Seal
Anode	Picture Frame	
Electrolyte	Pen Seal	
Cathode	Cathode Seal	
Air Flow	Cathode Spacer	
Separator Plate		Cathode
Fuel In		Electrolyte
Fuel Out		Anode Spacer
Air In		Anode Spacer Anode Seal Separator Plate
Air Out		Pacific Northwest National Laboratory

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Importing Existing FE Meshes

- User provides meshes identified for individual components.
- Can mix and match with CAD generated components.
- Fuel and Air cavities must also be meshed.
- Incompatible meshes are allowed through contact.
- Hex v.s. tetrahedral elements
 - Hex and wedge elements give smaller mesh and more accurate stresses in solid layers.
 - Tetrahedral mesh is sufficient for mapping temperatures in fuel and air.

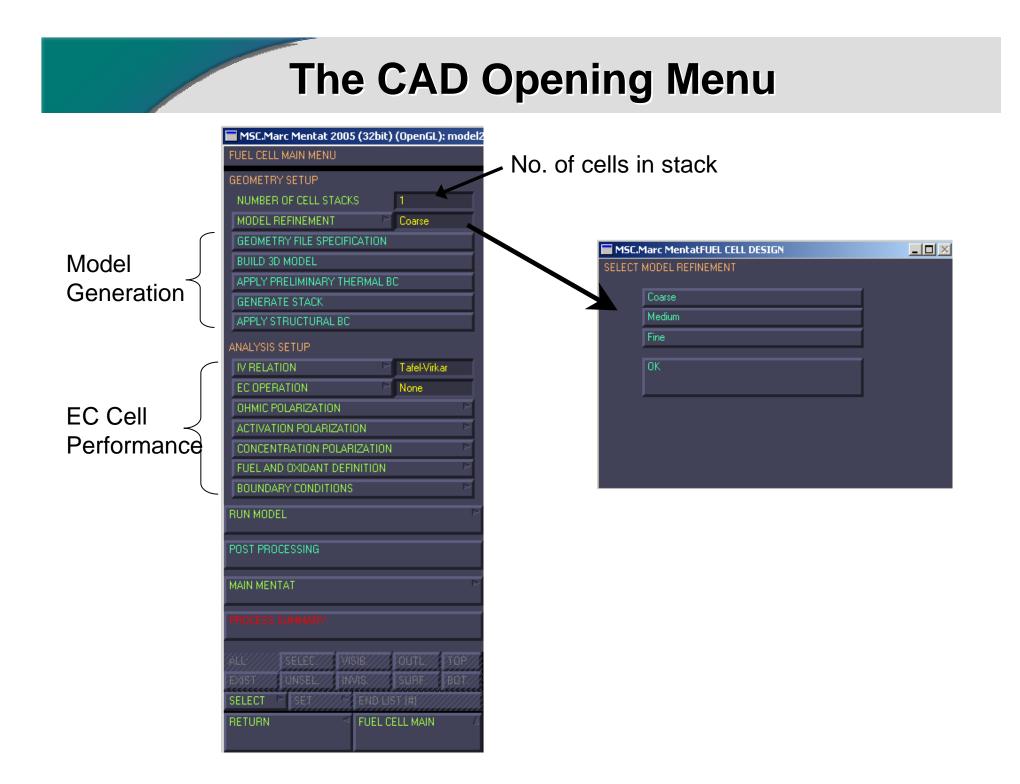


Example ANSYS mesh read into Marc

Starting Mentat-FC

Mentat-FC _ [] × Mentat-FC Solid Oxide Fuel Cell Analysis Program A cooperative effort between : MSC SOFTWARE SIMULATING REALITY **Pacific Northwest** National Laboratory Operated by Battelle for the U.S. Department of Energy Allows for input of parametric dimensions for SOFC Parametric SOFC Allows for input of generic CAD/FEA files CAD Input SOFC Cancel

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CAD file specification

		1 76 Major Componen	c Geometry Files Input
GEOMETRY SETUP NUMBER OF CELL STACKS	1	Component:	Require
MODEL REFINEMENT	Coarse	anode	D:/pnnl/phase2/phase
GEOMETRY FILE SPECIFICATION	Cualse	cathode	D:/pnnl/phase2/phase
		electrolyt	D:/pnnl/phase2/phase
BUILD 3D MODEL		separator	D:/pnnl/phase2/phase
APPLY PRELIMINARY THERMAL B	3C	separator_blank	D:/pnnl/phase2/phase
GENERATE STACK		fuel_in	D:/pnnl/phase2/phase
APPLY STRUCTURAL BC		fuel_out	D:/pnnl/phase2/phase
ANALYSIS SETUP		fuel_flow	D:/pnnl/phase2/phase
IV RELATION	Tafel-Virkar	air_in	D:/pnnl/phase2/phase
EC OPERATION	None	air_out	D:/pnnl/phase2/phase
OHMIC POLARIZATION	, richte	air_flow	D:/pnnl/phase2/phase
ACTIVATION POLARIZATION			
	1		
CONCENTRATION POLARIZATION			Specify so
FUEL AND OXIDANT DEFINITION			
BOUNDARY CONDITIONS			
RUN MODEL			
POST PROCESSING			
			nal Component Geometry
MAIN MENTAT			
		Component	Additic
PROCESS SUMMARY			Component 1 D:/pnnl/phas
			Component 2 D:/pnnl/phas
ALL VISIE	10477.//101	Additional 0	Component 3 D:/pnnl/phas
EXIST///UNSEL//UNVAS///	SUBE BO	111:	Component 4 D:/pnnl/phas
SELECT - SEX/// END/1	\$7/#}		Component 5 D:/pnni/phas
RETURN 4 FUEL C	ELL MAIN	Additional C	Component 6 D:/pnnl/phas

Required PNL FUEL CELL INPUT - MAJOR COMPONENTS			
File:		Extrudable?	Material
D:/pnnl/phase2/phase2_working_directory/test_install/ANODE1.SAT	file select		anode
D:/pnnl/phase2/phase2_working_directory/test_install/CATHODE1.SAT	file select	V	cathode
D:/pnnl/phase2/phase2_working_directory/test_install/ELECTROLYTE1.SAT	file select		electrolyte
D:/pnnl/phase2/phase2_working_directory/test_install/SEPARATOR PLATE1.SAT	file select		ss-430
D:/pnnl/phase2/phase2_working_directory/test_install/SEPARATOR PLATE BLANK1.SAT	file select		ss-430
D:/pnnl/phase2/phase2_working_directory/test_install/fuel in1.SAT	file select		fuel
D:/pnnl/phase2/phase2_working_directory/test_install/fuel out1.SAT	file select		fuel
D:/pnnl/phase2/phase2_working_directory/test_install/KIJmod-fuel flow1.SAT	file select		fuel
D:/pnnl/phase2/phase2_working_directory/test_install/air in1.SAT	file select		air
D:/pnnl/phase2/phase2_working_directory/test_install/air out1.SAT	file select		air
D:/pnnl/phase2/phase2_working_directory/test_install/air flow1.SAT	file select		air

6

Specify number of additional components :

Specify scale factor to convert input geometry to m units (default = 1.0): 1.0

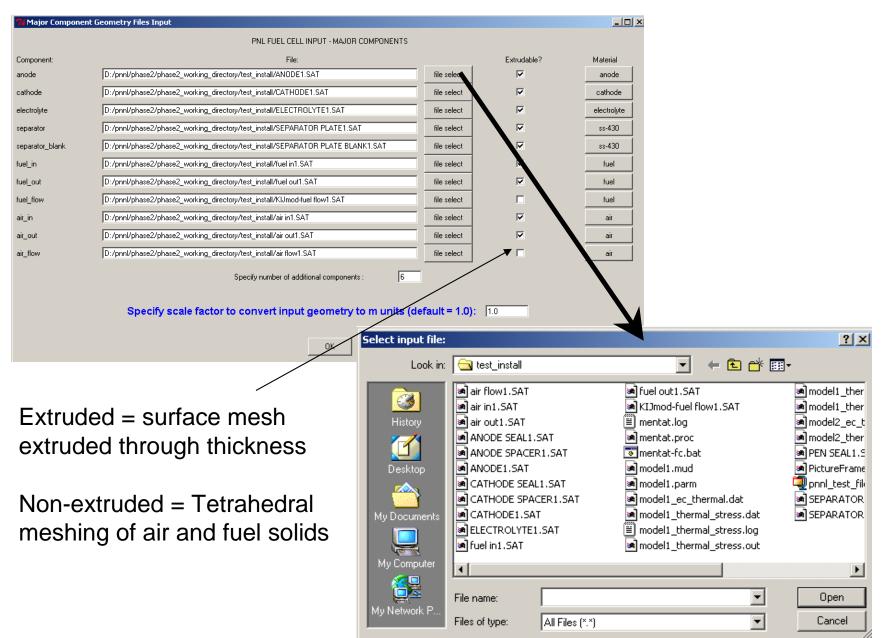
ΟK

Scale Factor

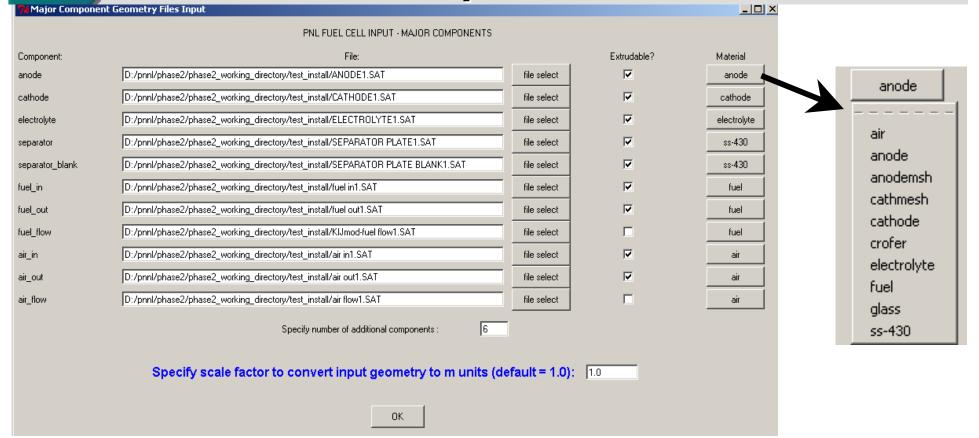
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7. Additional Compo	nent Geometry Files Input			_10
Component:	dditional PNL FUEL CELL INPUT - ADDITIONAL COMP	ONENTS (6)	Extrudable?	Material
Additional Component 1	D:/pnnl/phase2/phase2_working_directory/test_install/ANODE SPACER1.SAT	file select	1	ss-430
Additional Component 2	D:/pnnl/phase2/phase2_working_directory/test_install/ANODE SEAL1.SAT	file select	2	ss- 4 30
Additional Component 3	D:/pnnl/phase2/phase2_working_directory/test_install/CATHODE SPACER1.SAT	file select	2	ss-430
dditional Component 4	D:/pnnl/phase2/phase2_working_directory/test_install/CATHODE SEAL1.SAT	file select	2	\$\$-430
dditional Component 5	D:/pnnl/phase2/phase2_working_directory/test_install/PEN SEAL1.SAT	file select	9	ss-430
dditional Component 6	D:/pnnl/phase2/phase2_working_directory/test_install/PictureFrame1.SAT	file select	5	ss-430

CAD file specification (continued)



Material Specification



Material properties are from the SECA database:PNNL and ORNL data on cell materials.

•PNNL data on seal materials.

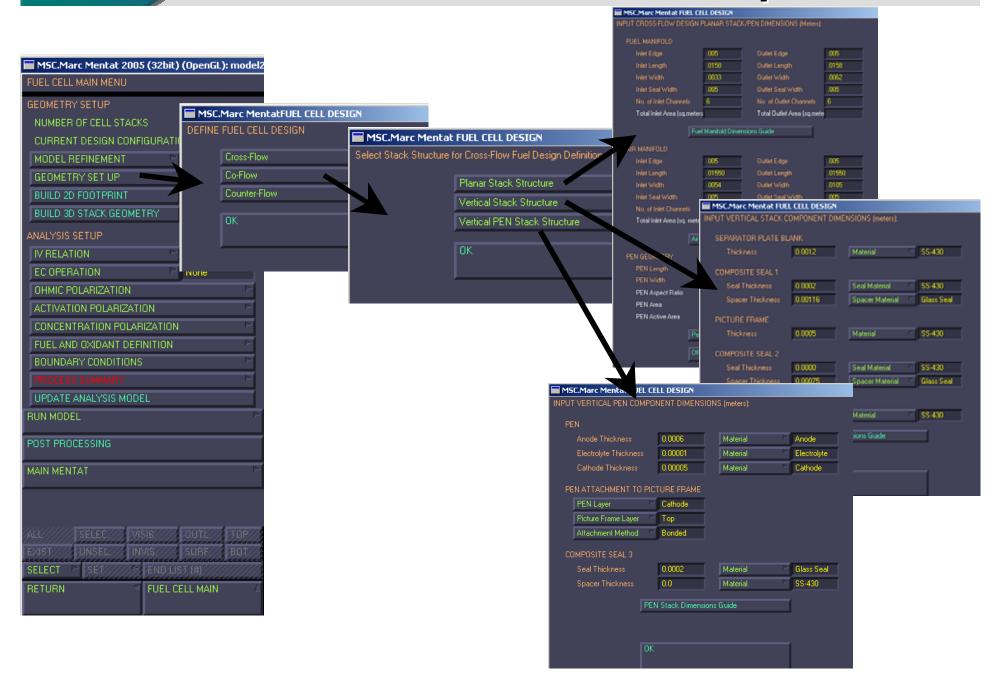
Finite Element Model Generation

EOMETRY SETUP NUMBER OF CELL STACKS MODEL REFINEMENT GEOMETRY FILE SPECIFICATION BUILD 3D MODEL APPLY PRELIMINARY THERMAL BC GENERATE STACK APPLY STRUCTURAL BC VALYSIS SETUP V RELATION Tatel-Virka EC OPERATION ACTIVATION POLARIZATION ACTIVATION POLARIZATION FUEL AND OXIDANT DEFINITION BOUNDARY CONDITIONS JN MODEL DST PROCESSING AIN MENTAT COLFESS SUMMARY C SELEC SET END UST (#MS SUBE	MSC.Marc Mentat		bit) (Up	enGL): I
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EC OPERATION None None OHMIC POLARIZATION ACTIVATION POLARIZATION ACTIVATION POLARIZATION FUEL AND OXIDANT DEFINITION BOUNDARY CONDITIONS UN MODEL OST PROCESSING AIN MENTAT SELECT VISIB OUTLAND SUBJECT OF SET OF	NALYSIS SETUP			
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BOUNDARY CONDITIONS JN MODEL DST PROCESSING AIN MENTAT TOCESS SUMMARY AUSSING SUBSECTION SUBSECTION SUBSECTION SUBSECTION	CONCENTRATION P	OLARIZAT	ION	
JN MODEL DST PROCESSING AIN MENTAT ROCESS SUMMARY AUSSIN UNSEL INVISIO (SUBE SUBE ELECT - SET	FUEL AND OXIDANT	DEFINITIO	DN .	
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	RETURN	<u> </u>	///////	7//////

• Four 'action' buttons to provide for complete fuel cell model generation

- 1. Mesh solids
- 2. Define exterior surfaces
- 3. for radiation and convection.
- 4. Duplicate cells for stack mesh
- 5. Apply structural boundary conditions

Parametric Based Model Input



Defini	ng Cell Perform	ance
ANALYSIS SETUP IV RELATION EC OPERATION OHMIC POLARIZATION ACTIVATION POLARIZATION	MSC.Marc MentatFUEL CELL DESIGN	MSC.Marc MentatFUEL CEL TOTAL VOLTAGE OPERATION Total Voltage = voltage * no. of cells in stack: Voltage (V): 0.7 No of Cells: 1 Total Voltage (V): 0.7 COMPUTE VOLTAGE OK
CONCENTRATION POLARIZATION FUEL AND OXIDANT DEFINITION BOUNDARY CONDITIONS UPDATE ANALYSIS MODEL	MSC.Marc MentatFr EL CEL	MSC.Marc MentatFUEL CEL TOTAL CURRENT OPERATION Total Current = current * acitve PEN area: Current (A/cm^2): 1.0 Active PEN area: Total Current (A): 0 COMPUTE CURRENT OK
Battelle		A MSC.Marc MentatFUEL CEL FUEL UTILIZATION OPERATION Fuel Utilization (%) 0.50 CK Ra

Ohmic Polarization

For TAFEL-VIRKAR Relation			
Electrolyte Conductivity (k=tT	[*prefactor*exp(eff act er		
Effective Activation Ener	rg 0.007355		
Prefactor	6.87e-7		
	Anode Parameters:	Cathode Parameters:	Interconnect Parameti
Temperature (K)	1273	1273	1273
Ohmic Resistance	3.33e-5	7.69e-5	4.0e-5
For BUTLER-VOLMER Relation			
Electrolyte Conductivity (k=A			
Electrolyte Conductivity (k=A			
Electrolyte Conductivity (k=A A			
Electrolyte Conductivity (k=A A B			
Electrolyte Conductivity (k=A A B C		Cathode Conductivity:	Interconnect Conduct
Electrolyte Conductivity (k=A A B C	.T^3+BT^2+CT+D):	Cathode Conductivity:	Interconnect Conduct
Electrolyte Conductivity (k=A A B C D	.T^3+BT^2+CT+D):	Cathode Conductivity:	Interconnect Conduct
Electrolyte Conductivity (k=A A B C D Activation Energy	.T^3+BT^2+CT+D):	Cathode Conductivity:	Interconnect Conduct

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Activation Polarization

MSC.Marc Mer	tatFUEL CELL [DESIGN			
ACTIVATION POLARIZATIO	N OPTIONS				
For TAFEL-VIRKAR Rela	tion				
Temperature (K):	Exchange Current (A/	Tafel Prefacto			
923	0.051e-4	0.031			
973	0.107e-4	0.028			
1023	0.113e-4	0.0248			
1073	0.132e-4	0.0247			
For BUTLER-VOLMER R	elation				
	vrefactor*exp(-act. energy/RT)	t:			
Activation Ene	ergy				
Prefactor					
Symmetry Fac	tor				
	OK		1		
L					
				orthwest Nationa	al Laboratory
				U.S. Departm	ent of Energy 22

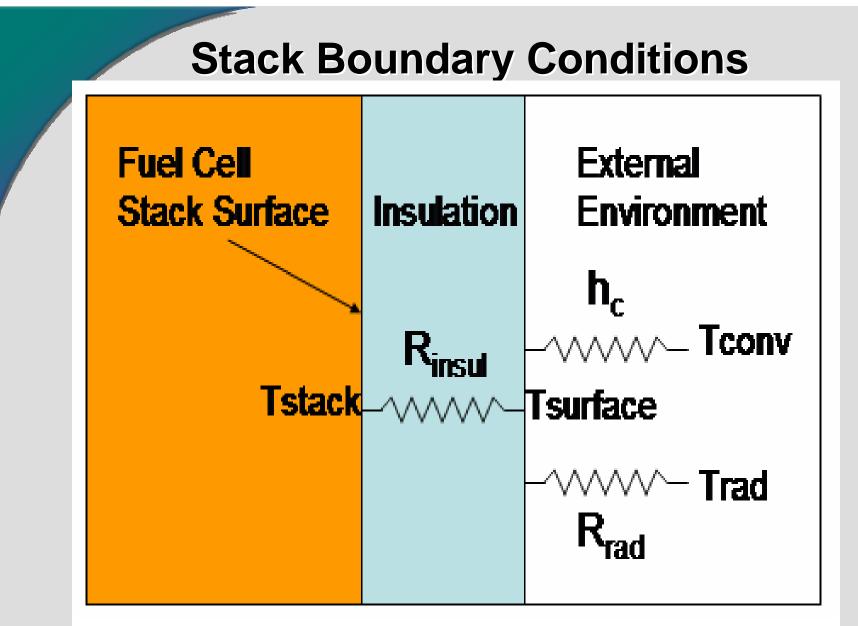
Concentration Polarization

NCENTRATION POLARI	NTATENT CELL DESIGN	
For TAFEL-VIRKAR Rela	stion	
Testing Fuel Pressure	e (atm):	
H2	0.96	
H20	0.04	
CO	0.0	
C02	0.0	
Temperature (K):	Anode Current Density (A/	
923	3.184e-4	
973	4.74e-4	
1023	4.953e-4	
1073	5.65e-4	
For BUTLER-VOLMER F		
Concentration r oranz	Anode Cathode:	
Porosity		
Tortuosity		
	ОК	

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Fuel and Oxidant Definition

MSC.Marc Mentat		
IEL AND OXIDANT		
INLET FUEL		
Pressure (atm)	1.0	
Temperature (K)	967	
Flow Rate (gmol/sec)	4.236e-4	Stack Flow Rate
Composition (Molar Fraction %	9	
H2	0.95	
H20	0.05	
CO	0	\succ Fuel Composition
C02	0	
CH4	0	
INLET OXIDANT		
Pressure (atm)	1.0	
Temperature (K)	967	
Flow Rate (gmol/sec)	1.69e-2	Stack Flow Rate
Composition (Molar Fraction %	9	
02	0.21	Citical Composition
N2	0.79	
OK		
		Pacific Northwest National Laboratory U.S. Department of Energy 24



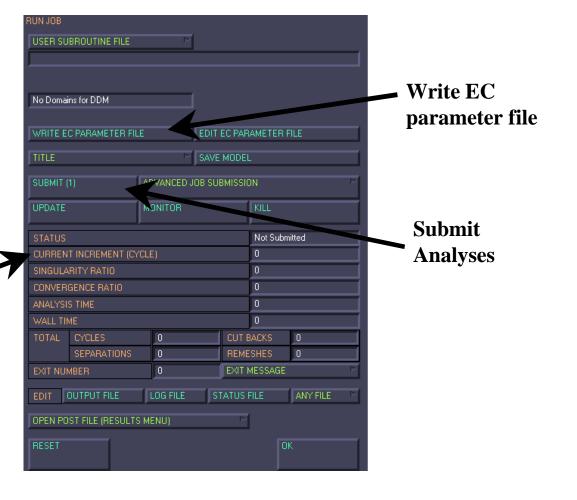
Boundary conditions defined on top, sides, and bottom of stack

Stack Boundary Conditions

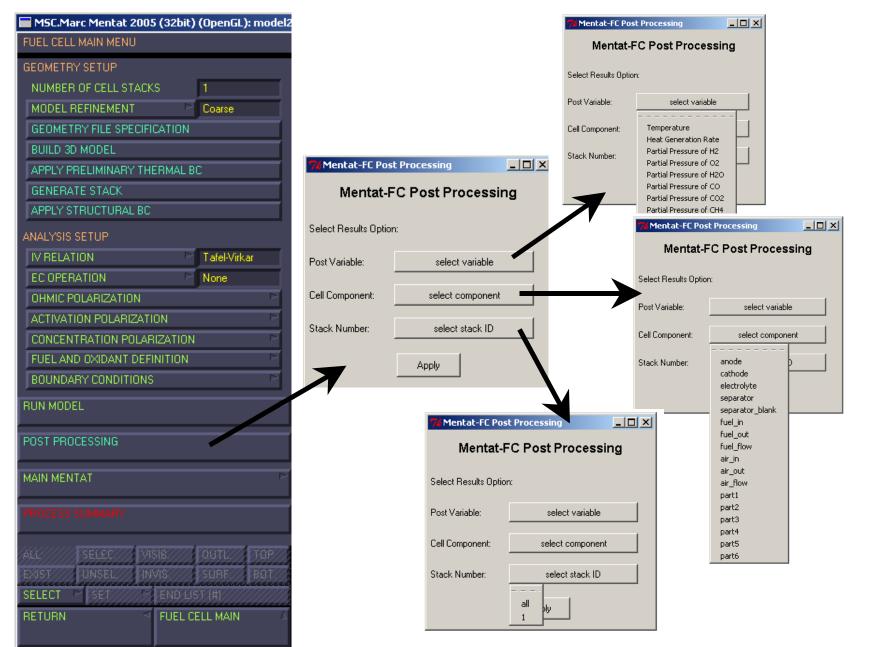
MSC.Ma	arc MentatFUEL CELI	DESIGN		
ERMAL BOUND	ARY CONDITIONS			
Initial Stacl	k Temperature (K)	950		
Surface He	eat Transfer:			
	SURFACE BEHAVIOR	Radiation/Convenction/Insulation	ı –	
1		,		
	STACK INSULATION			
		Тор	Bottom	Vertical Sides
	Thickness (m)	.01	.01	.01
	Conductivity (W/m-K)	.07	.07	.07
l				
	RADIATION			
		Тор	Bottom	Vertical Sides
	Emissivities (unitless)	.7	.7	.7
	Sink Temperature (K)	293	293	293
]	CONVECTION			
		Тор	Bottom	Vertical Sides
	Film Coef (W/m**2-K)	3.0	5.0	13.0
	Air Temperature (K)	293	293	293
CHANICAL BOU	JNDARY CONDITIONS			
Stress Free	e Stack Temperature (K)		950	
Include Cre	eep Effects - Event Duration (seconds)		0.0	
		ОК		

MSC.Marc Mentat 2005 (3 FUEL CELL MAIN MENU	zbit) (UpenGL): mode
GEOMETRY SETUP	
NUMBER OF CELL STACKS	1
MODEL REFINEMENT	Coarse
GEOMETRY FILE SPECIFICAT	ION
BUILD 3D MODEL	
APPLY PRELIMINARY THERM	IAL BC
GENERATE STACK	
APPLY STRUCTURAL BC	
ANALYSIS SETUP	
IV RELATION	P Tafel-Virkar
EC OPERATION	None
OHMIC POLARIZATION	
ACTIVATION POLARIZATION	⊳
CONCENTRATION POLARIZA	TION 🗠
FUEL AND OXIDANT DEFINIT	ion 🖻 🖻
BOUNDARY CONDITIONS	
RUN MODEL	
POST PROCESSING	
MAIN MENTAT	
ALL/////SELET///WISHE	//// OUTL/// TOP/
EXIST UNSEL INVIS	SÚRF. BOT.
SELECT P SET	ID LIST (#)
RETURN 4 FU	EL CELL MAIN

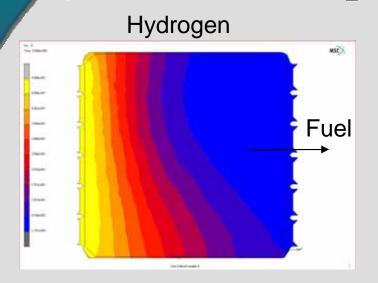
Model Solution



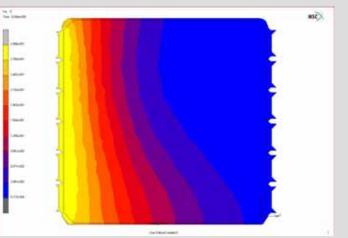
The Post Processing Menus

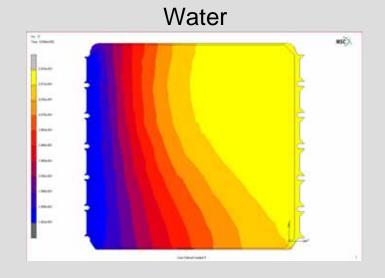


Fuel Species (Inlet Fuel: 0.6 H_2 , 0.1 H_2O , 0.3 CO, 0.1 CO₂)

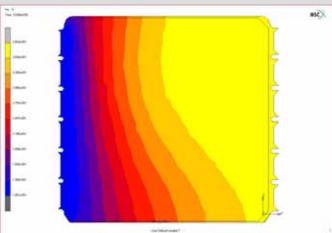




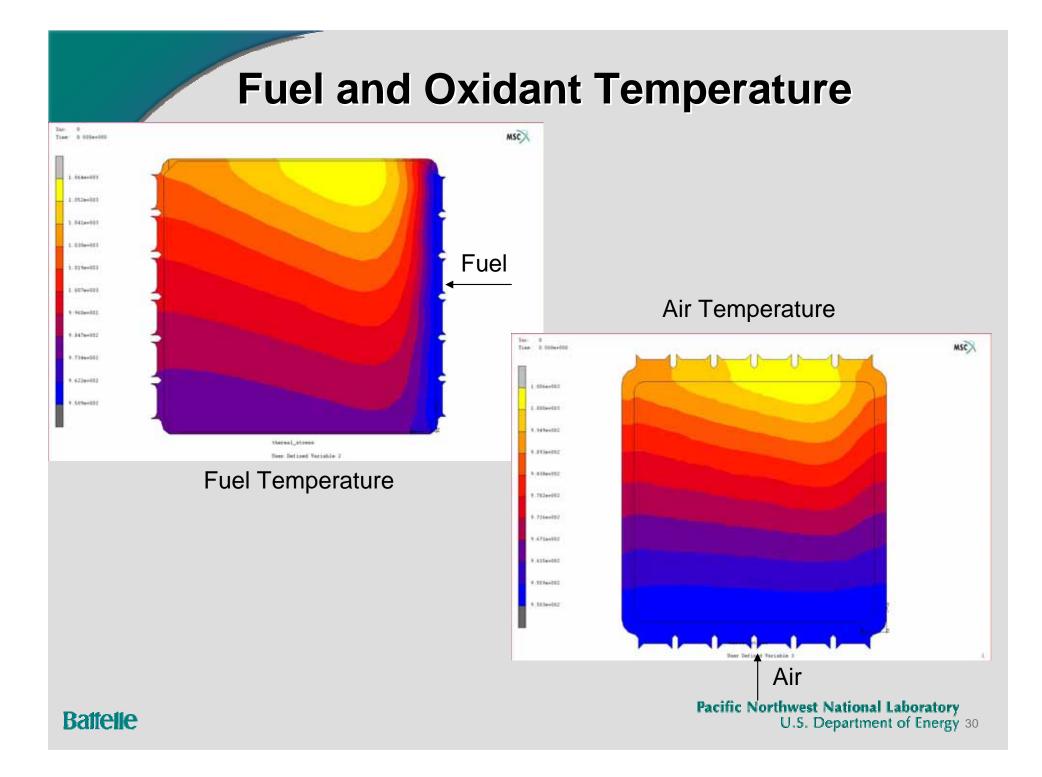


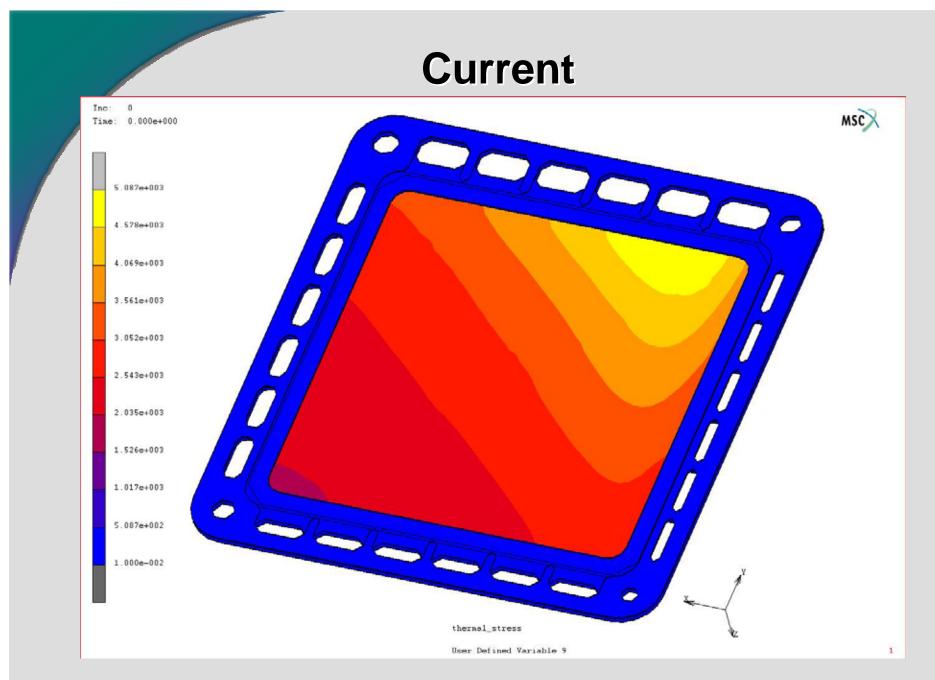






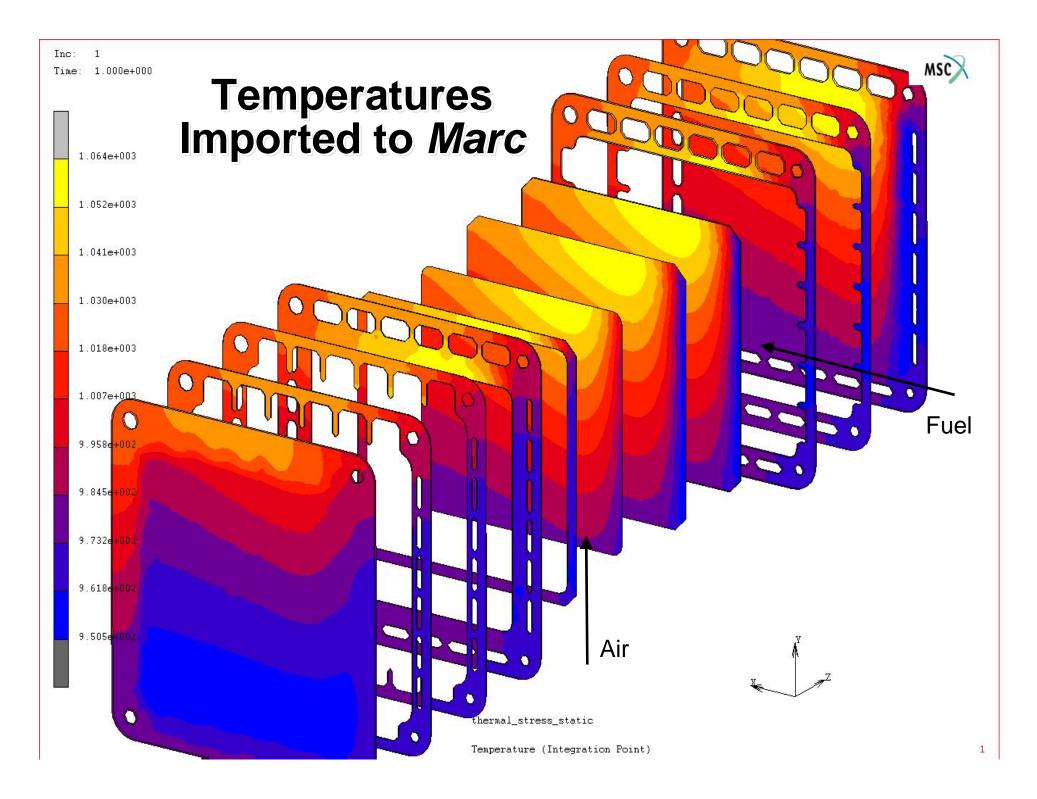
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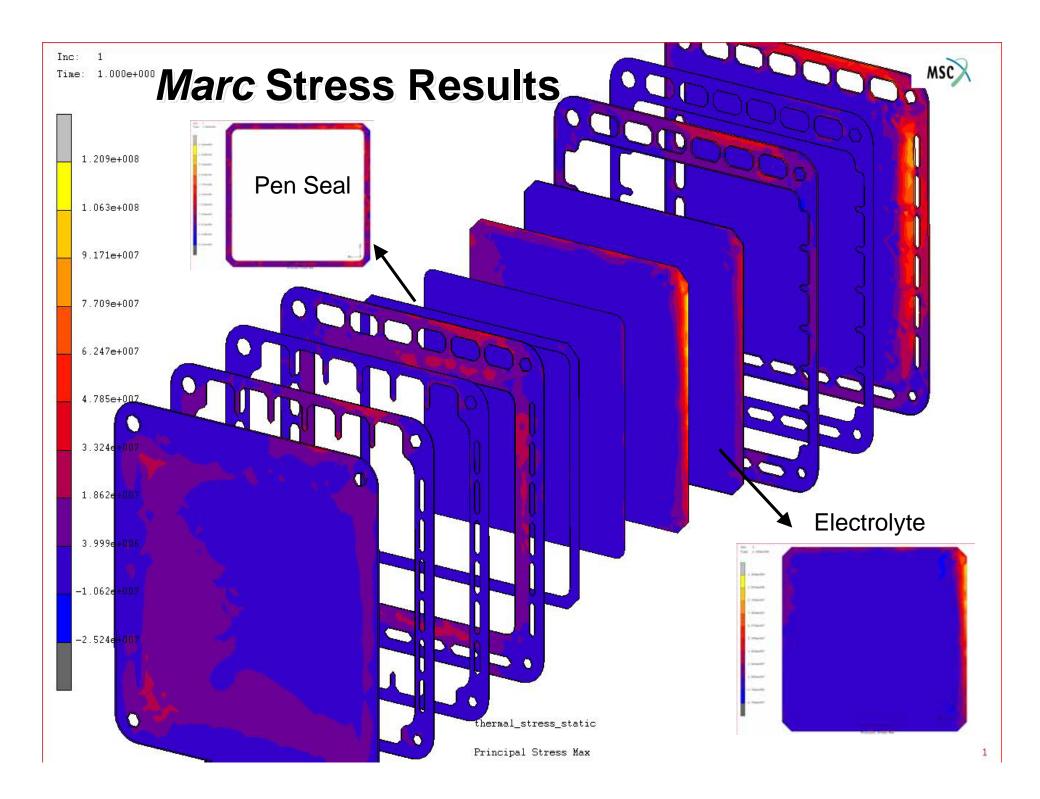




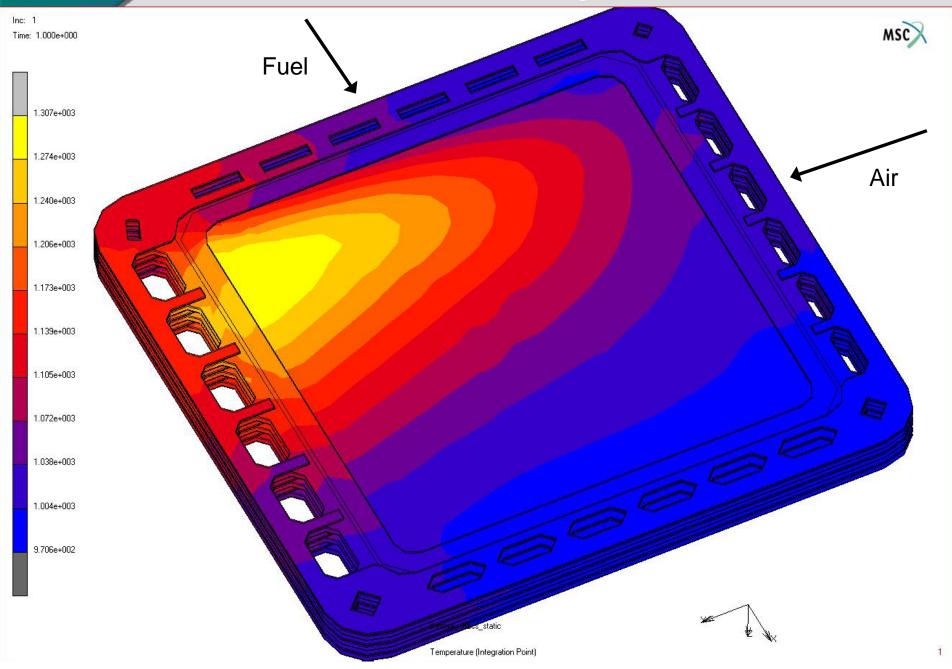
Battelle

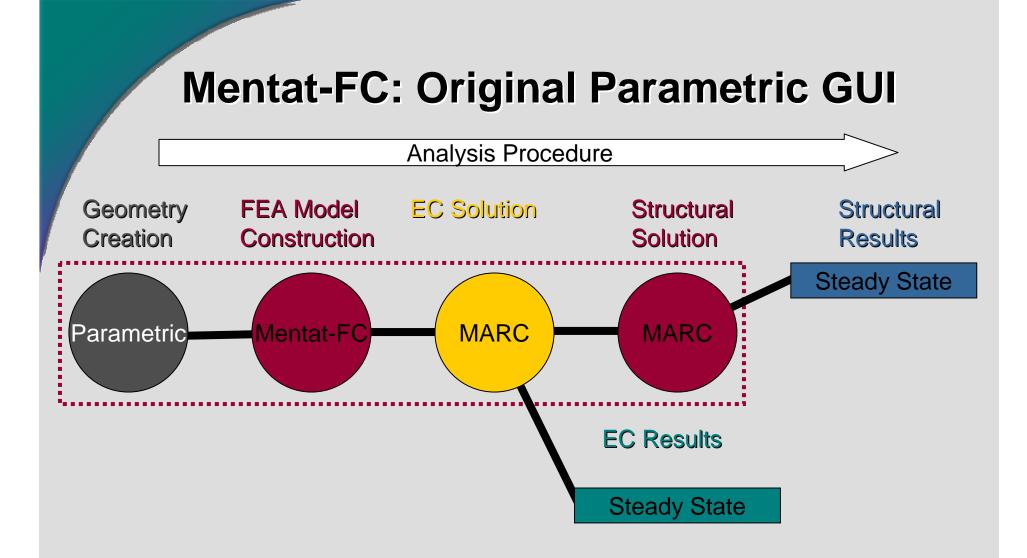
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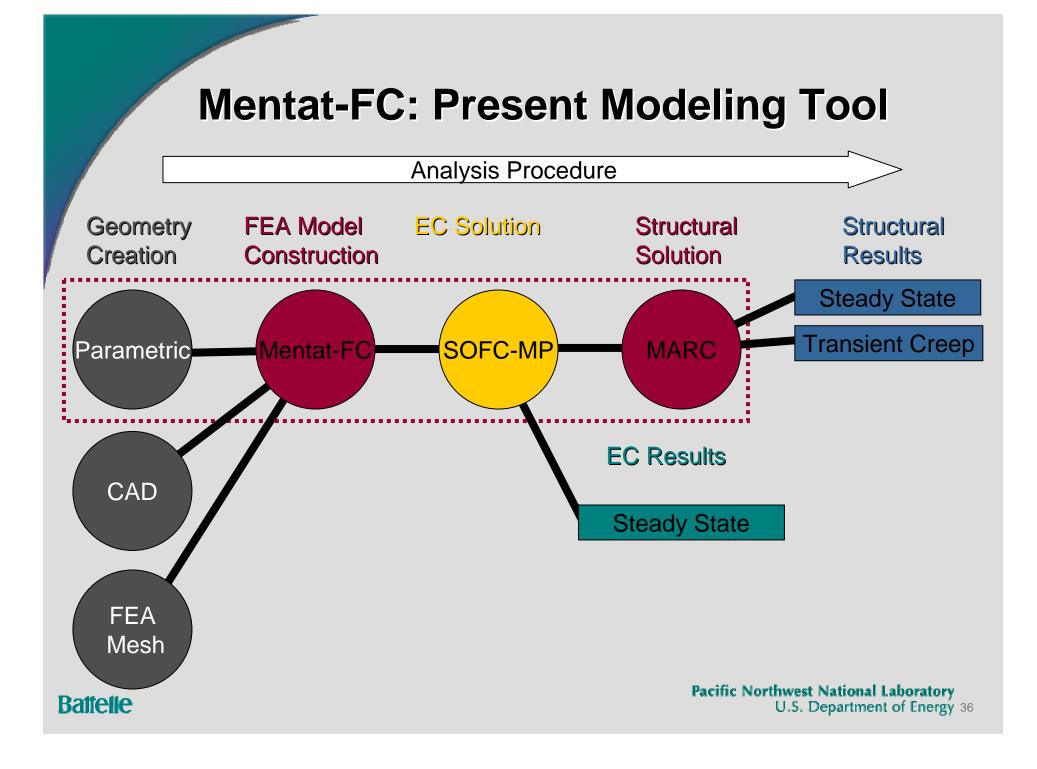


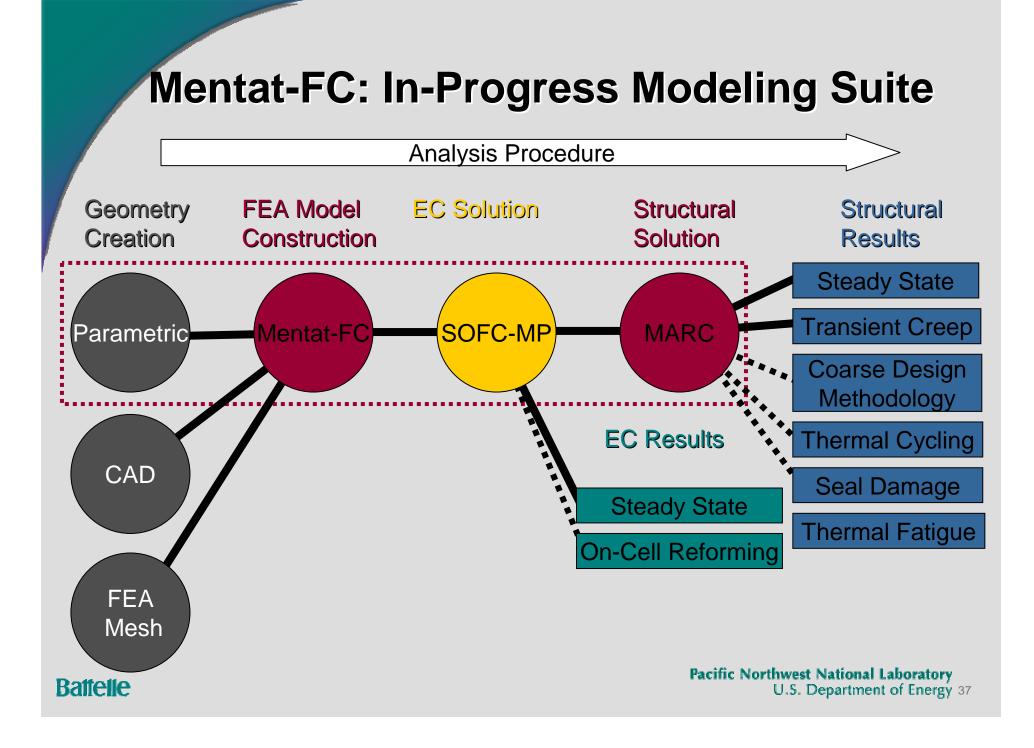


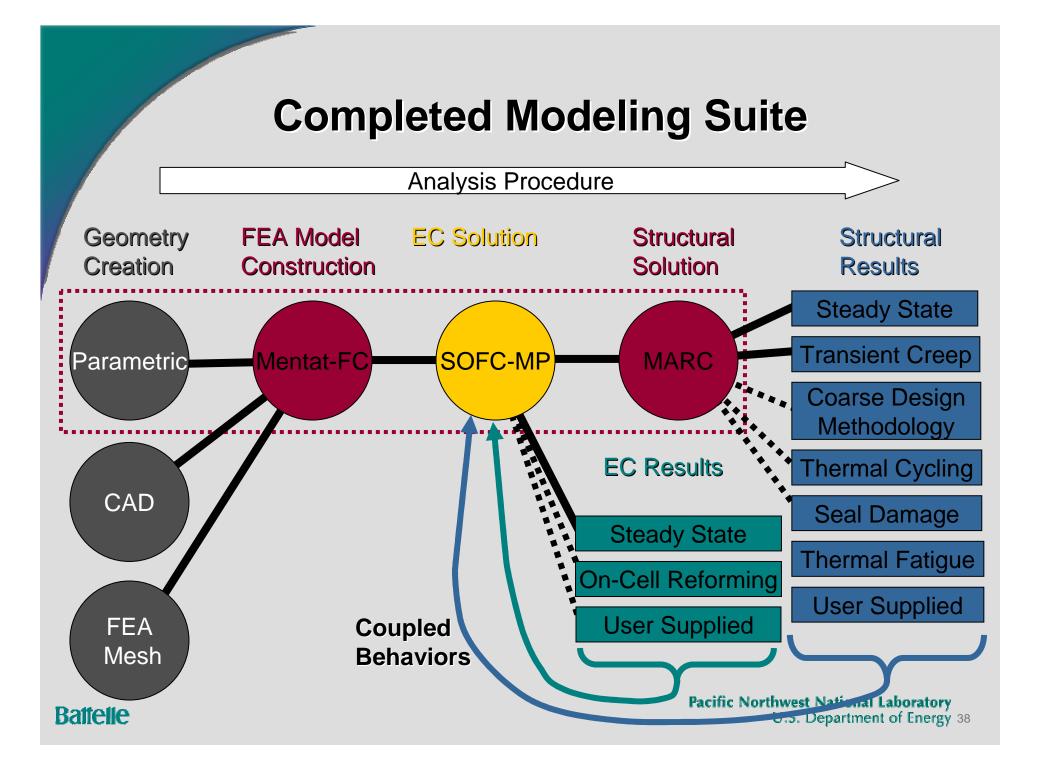
3-Cell Model directly from CAD











How to get this software and more training

MSC Evaluation Licenses

PNNL Summer Workshop



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Questions?

5-minute break before starting

the live demo of

SOFC-MP and MSC.Marc/Mentat-FC

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Test Problems

- 1-Cell course model from CAD
- ► 3-Cell model from existing ANSYS mesh files.
- 1-Cell cross-flow parametric model
- 1-Cell co-flow parametric model
- 1-Cell counter-flow parametric model

