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

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Pacific Northwest National Laboratory

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Battelle

Pacific Northwest National Laboratory
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Solution Flow

- *Mentat-FC*:

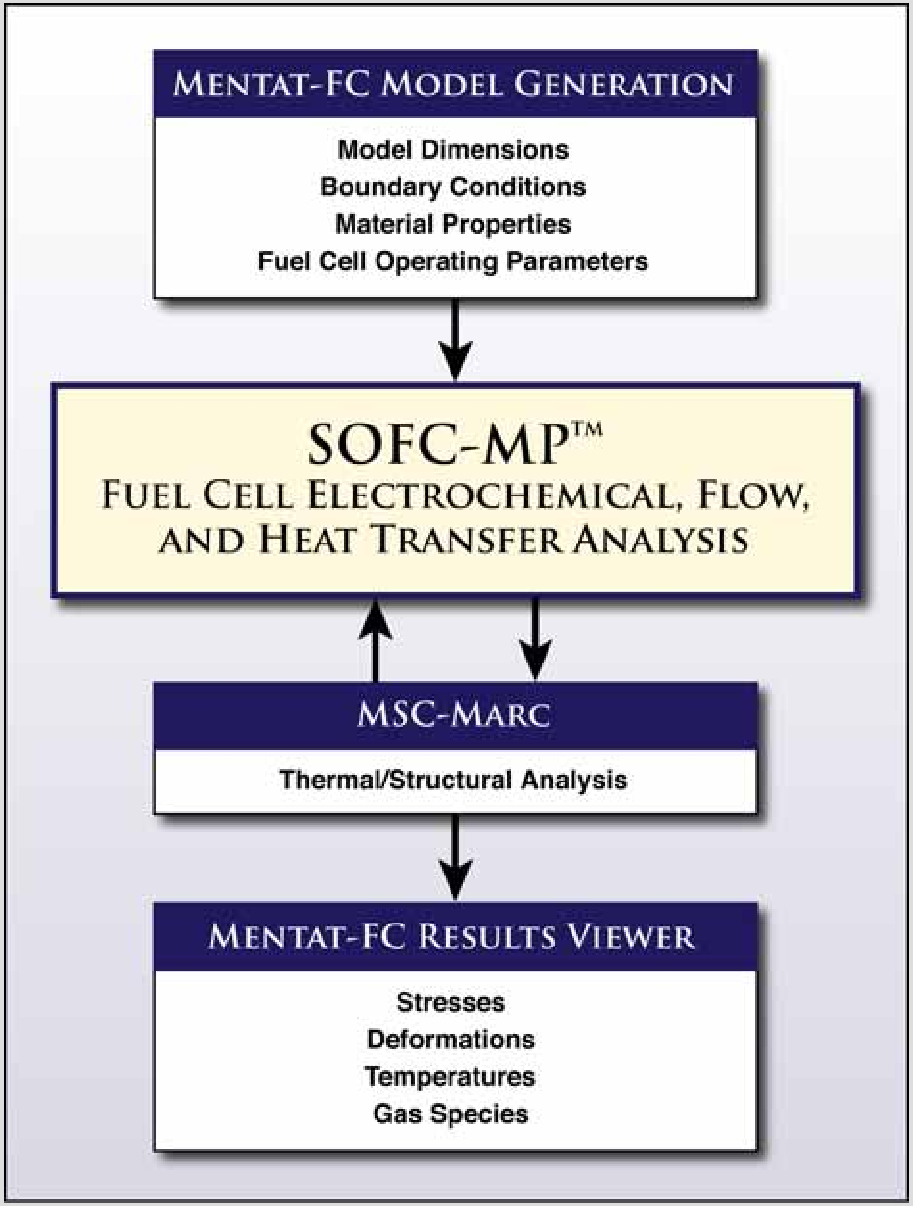
  Graphical User Interface for flexible finite element model generation.

- *SOFC-MP*:

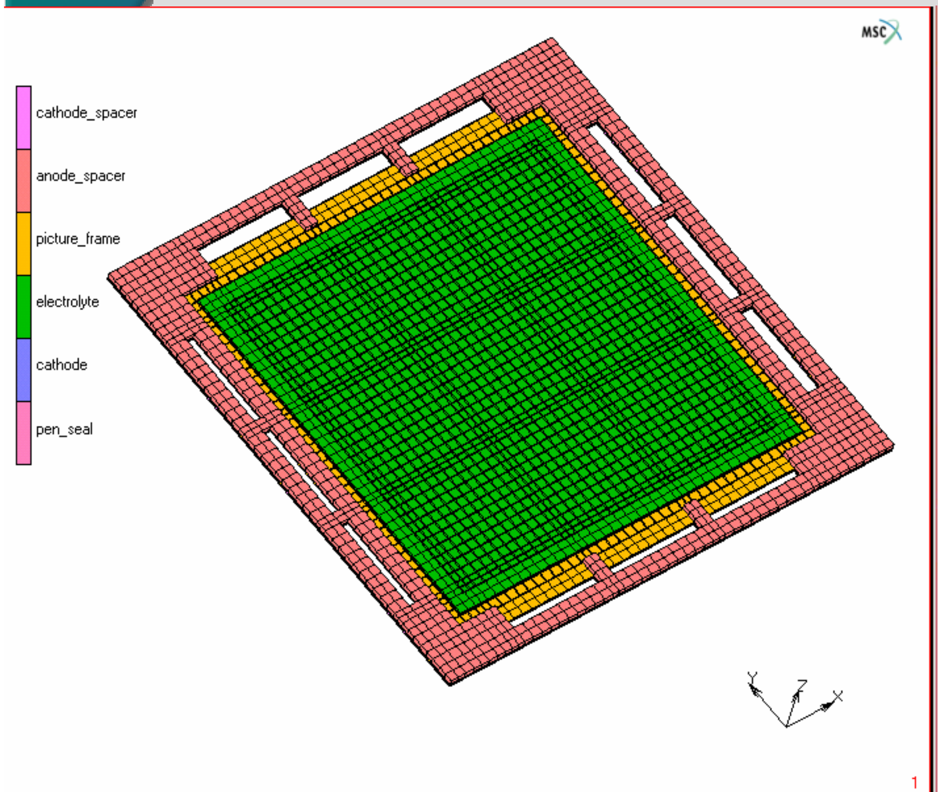
  Finite element based electrochemistry, flow and heat transfer solution.

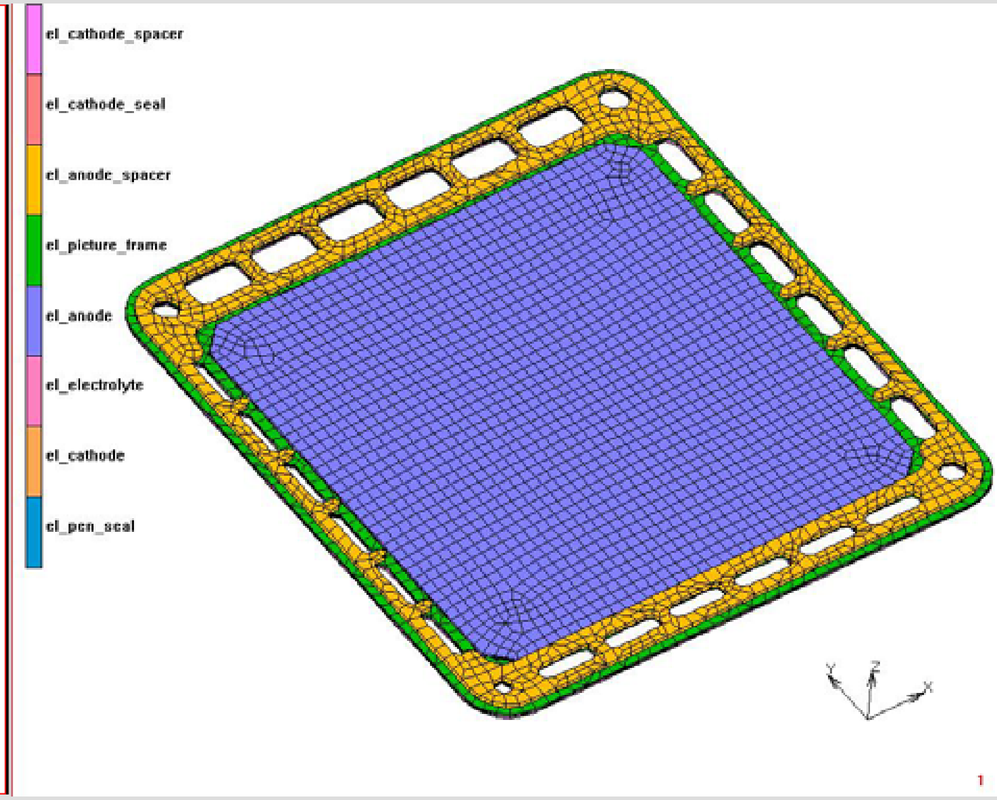
- *MSC.Marc:*

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



Mentat-FC:
Parametric and CAD based Models





Parametric

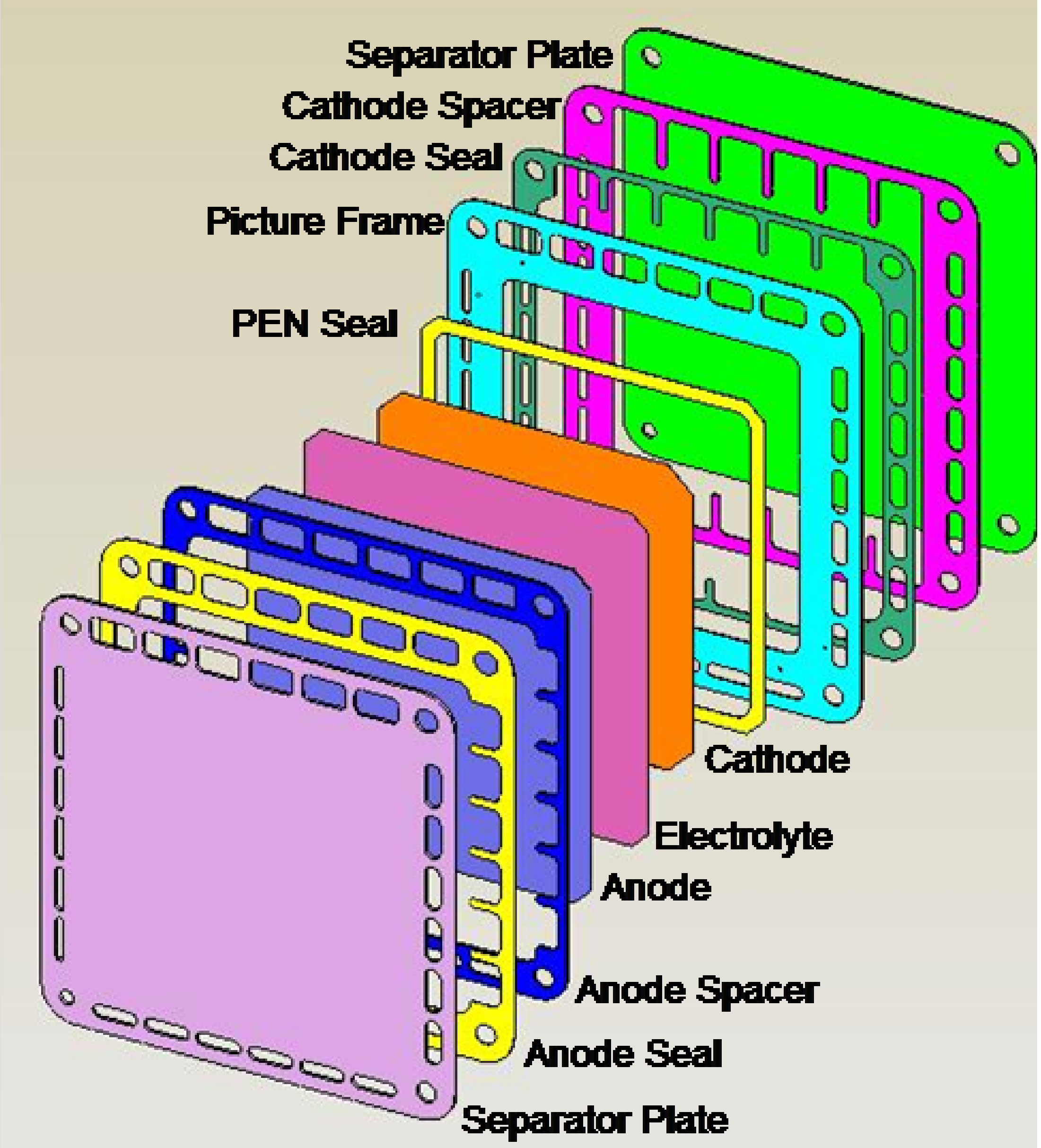
•Fixed SOFC designs
•Meshed from dimensional parameters
•Used for parametric design studies

CAD Based

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

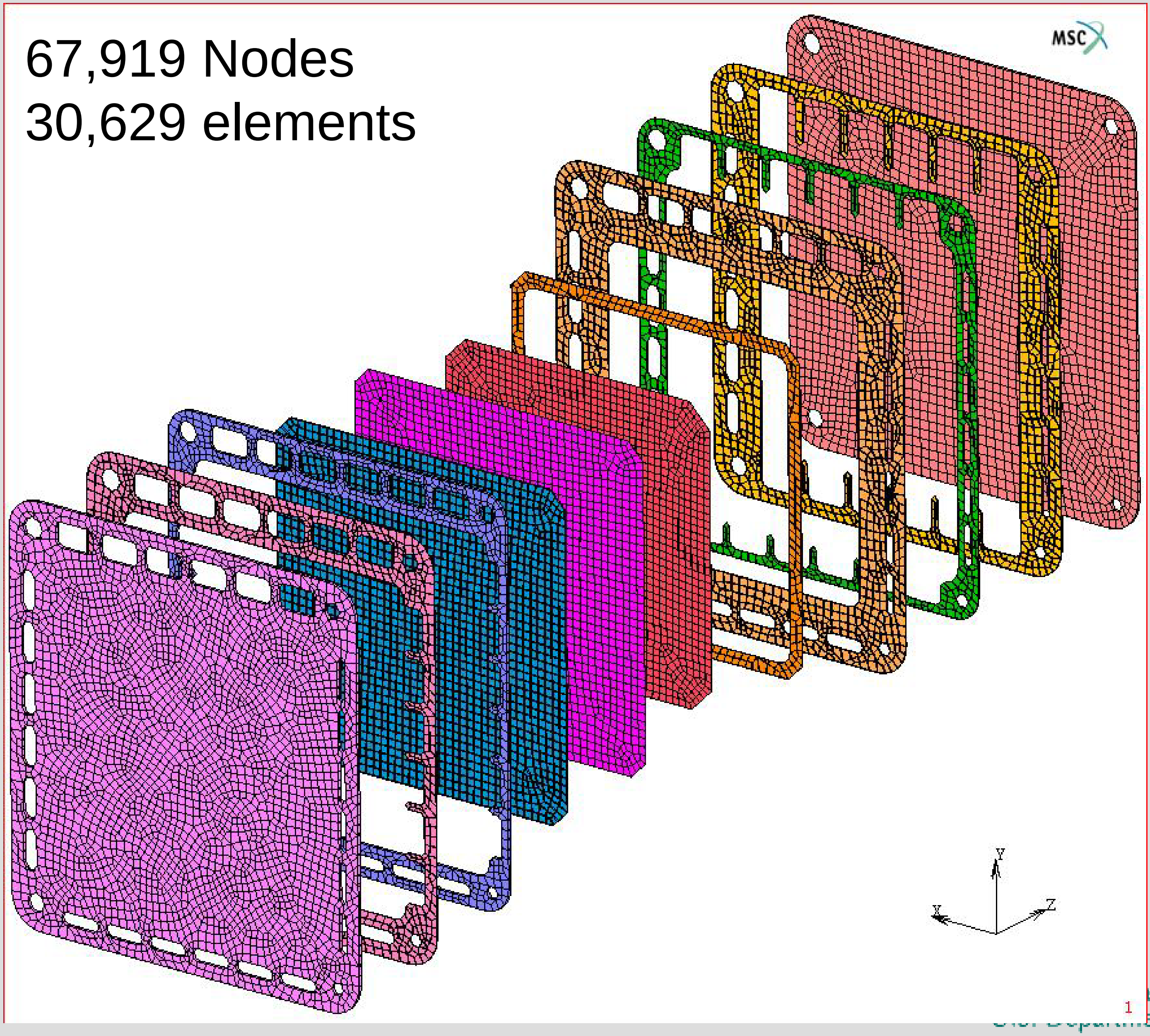
Mentat-FC: Model Generation from CAD Geometries

- 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.



Mesh Generated from CAD

67,919 Nodes
30,629 elements



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

Full 3D Analysis

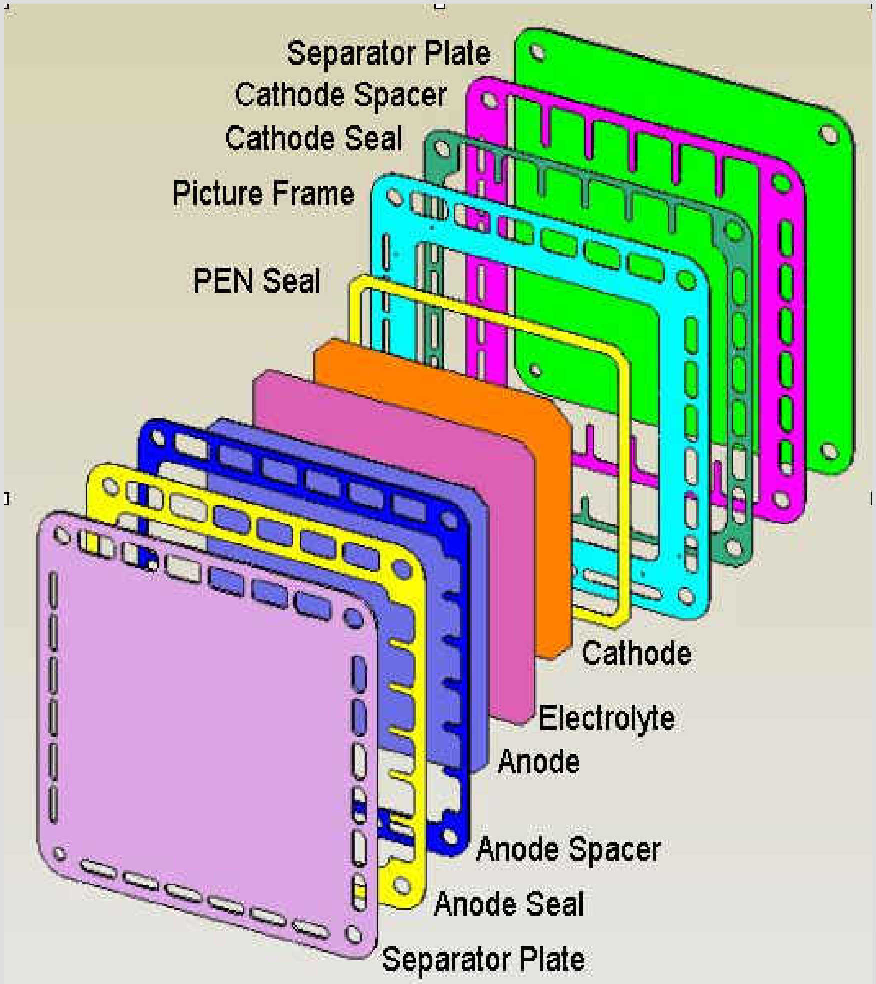
- Stress and Distortion – 3D in solids.

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.

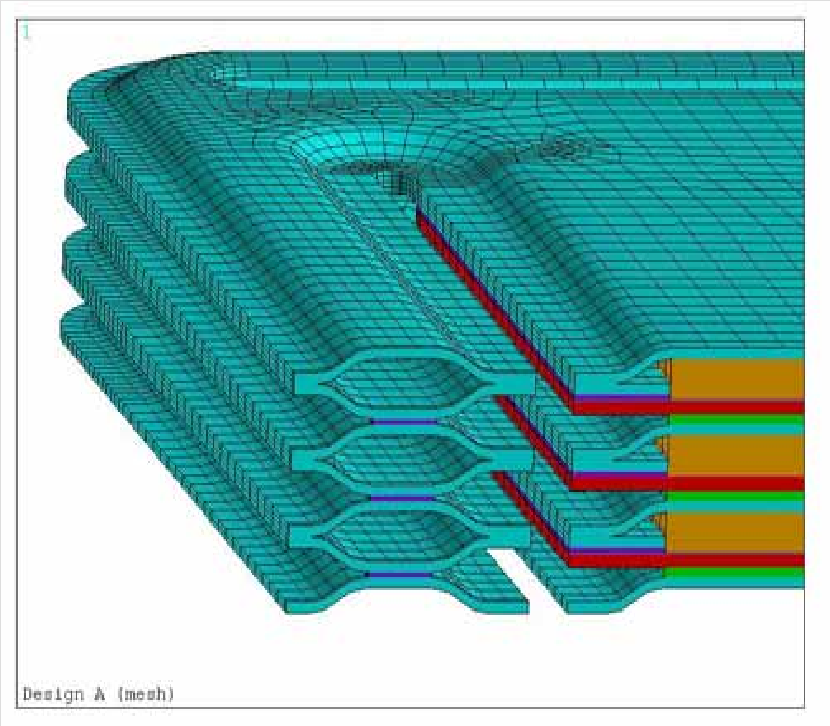
Generating a Model from CAD files

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



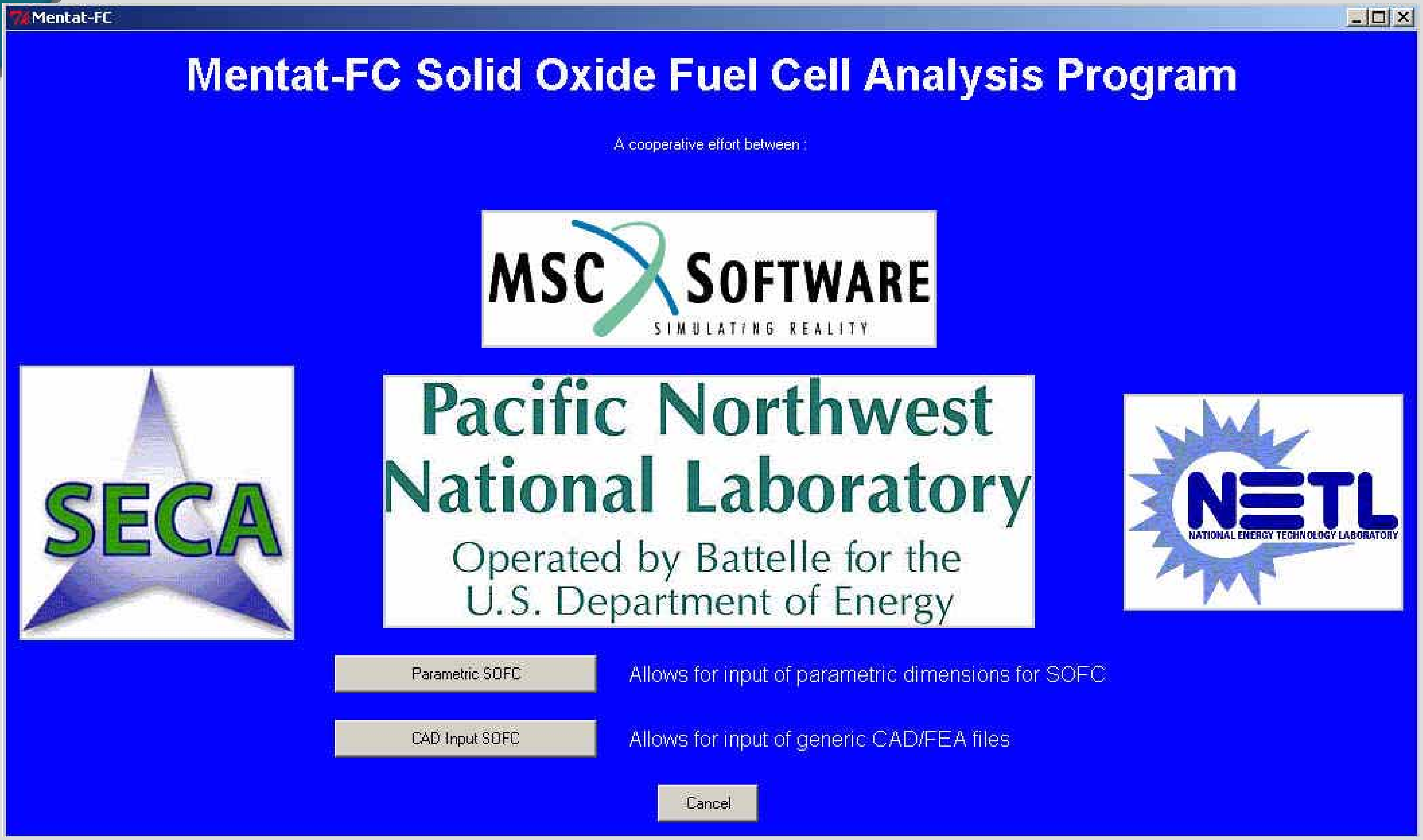
Importing Existing FE Meshes

- 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

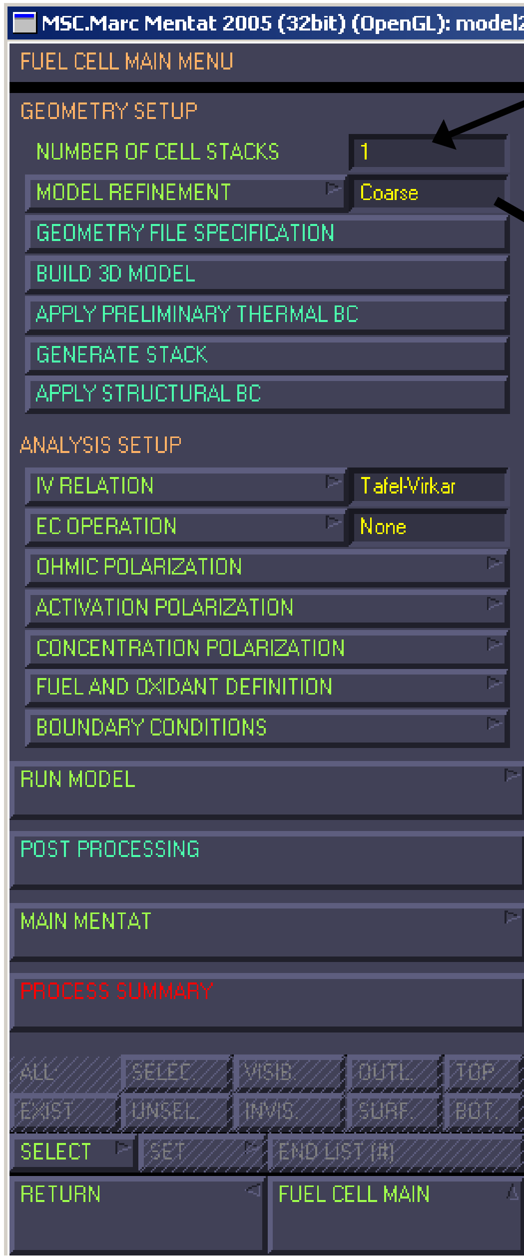
Starting Mentat-FC



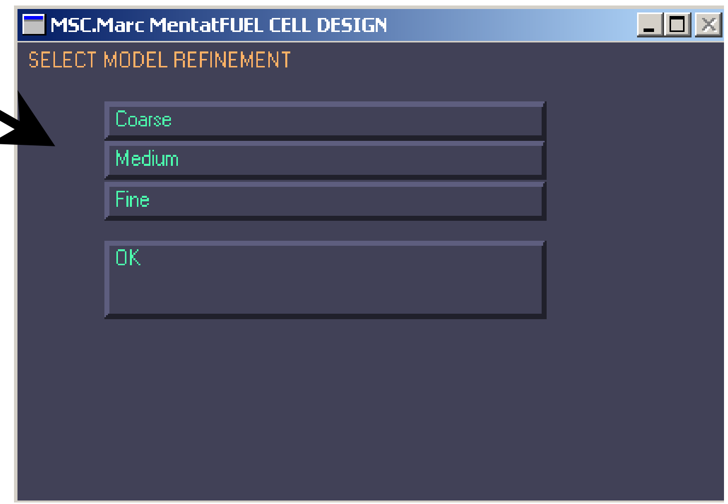
The CAD Opening Menu

Model Generation

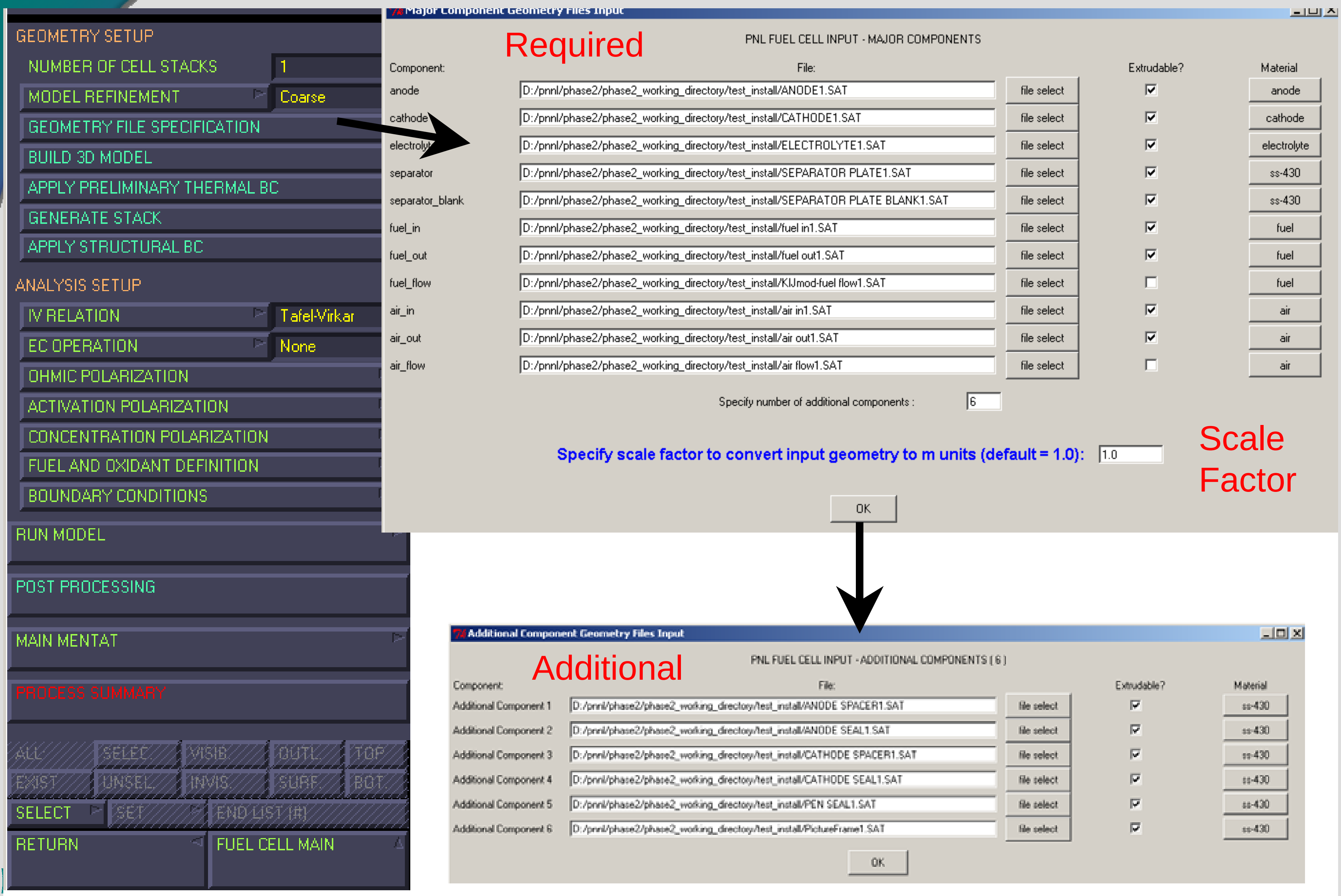
EC Cell Performance



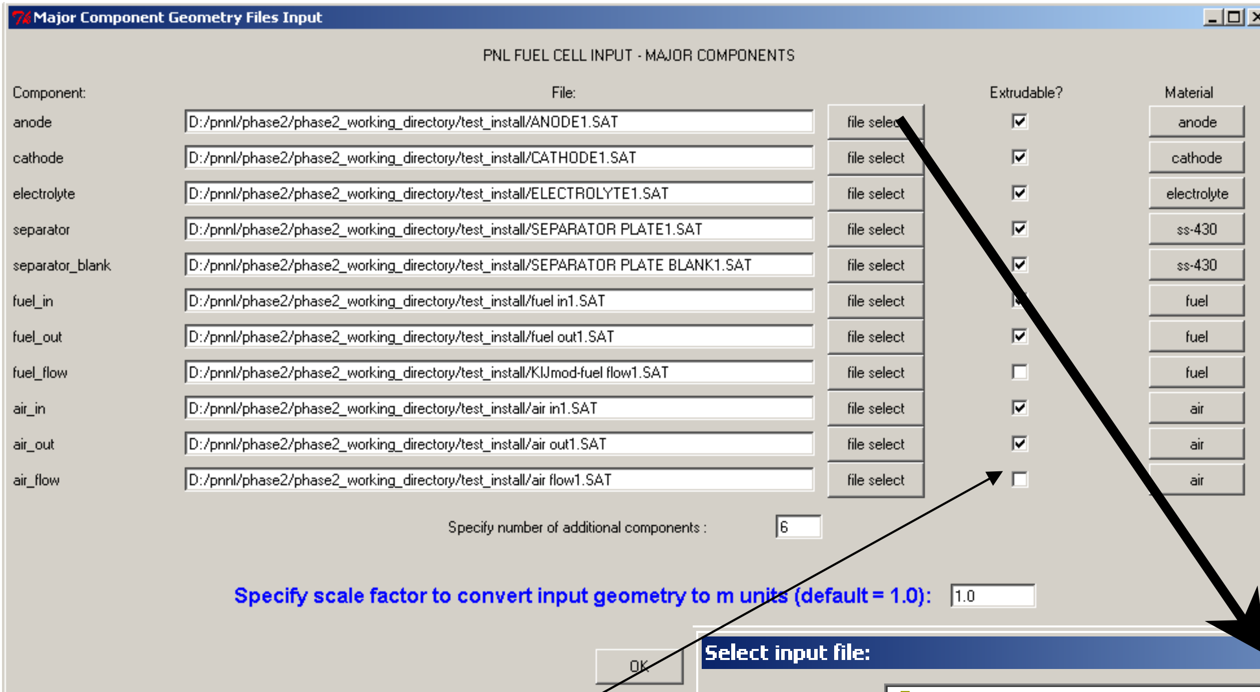
No. of cells in stack

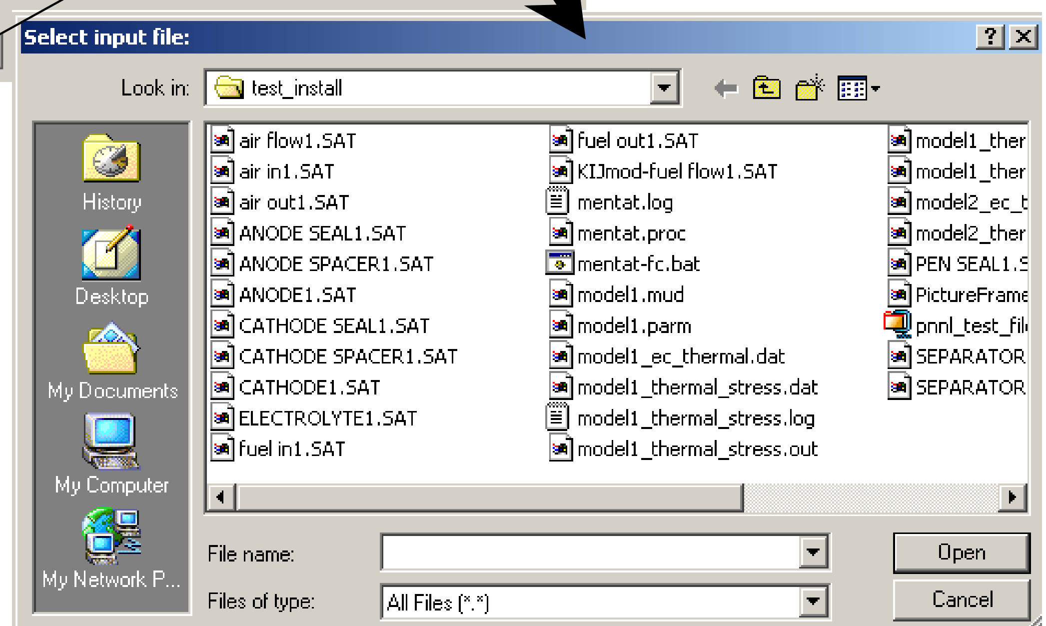


CAD file specification



CAD file specification (continued)

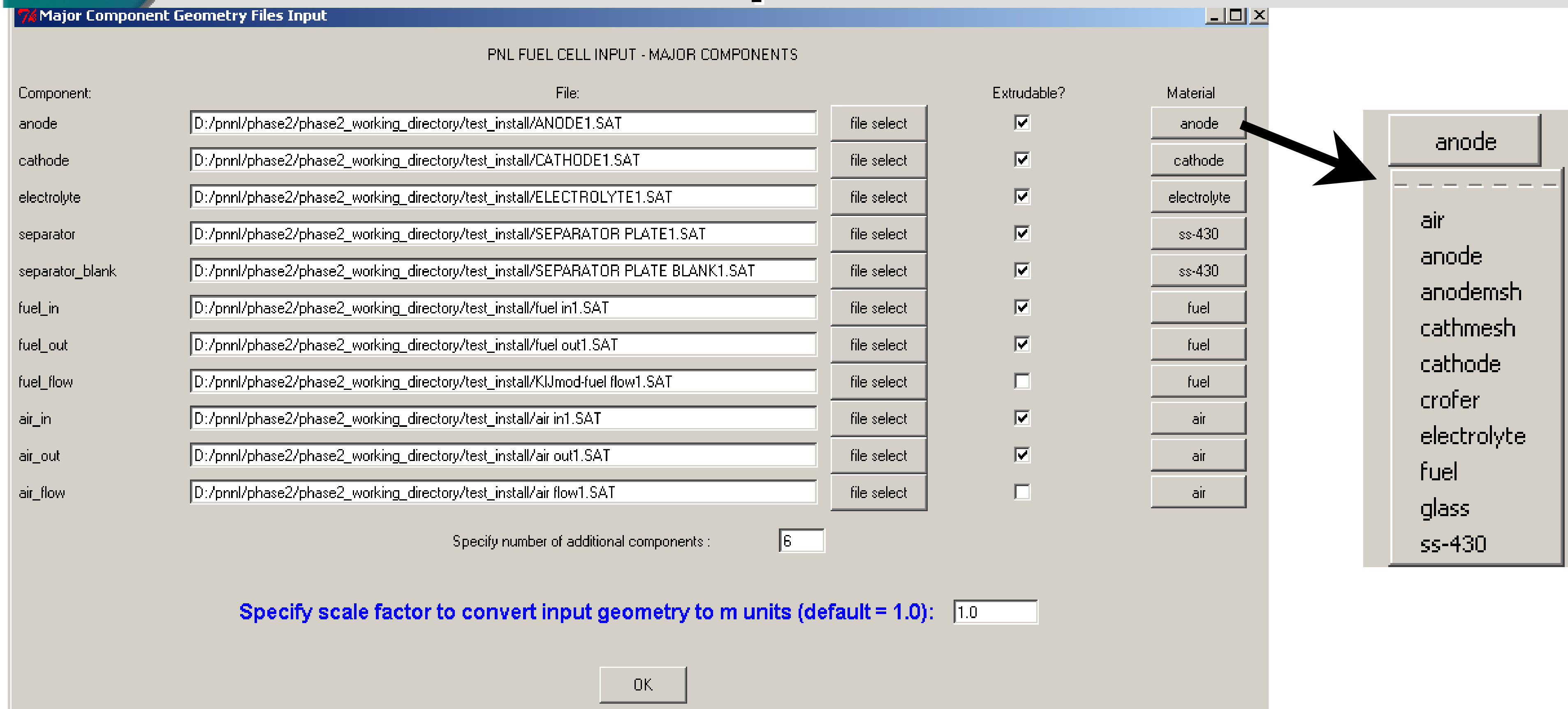




Extruded = surface mesh extruded through thickness

Non-extruded = Tetrahedral meshing of air and fuel solids

Material Specification

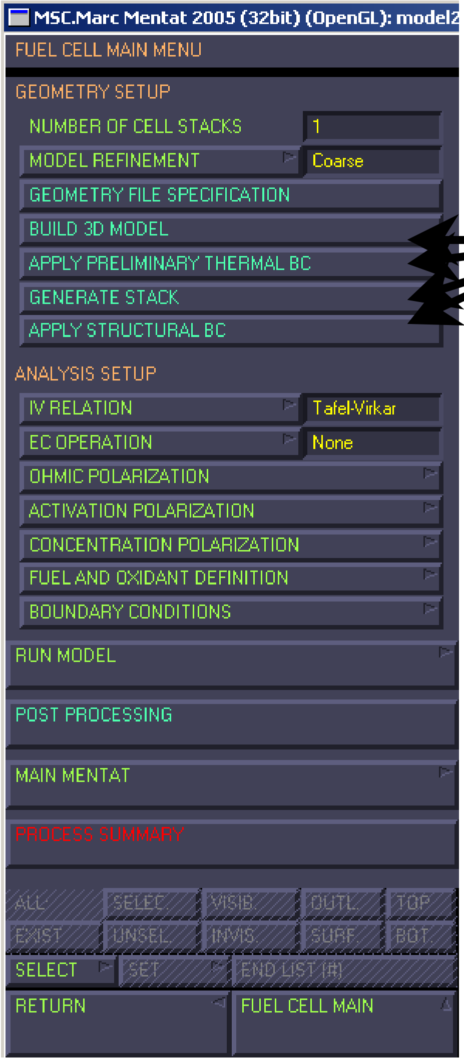


Material properties are from the SECA database:

•PNNL and ORNL data on cell materials.

•PNNL data on seal materials.

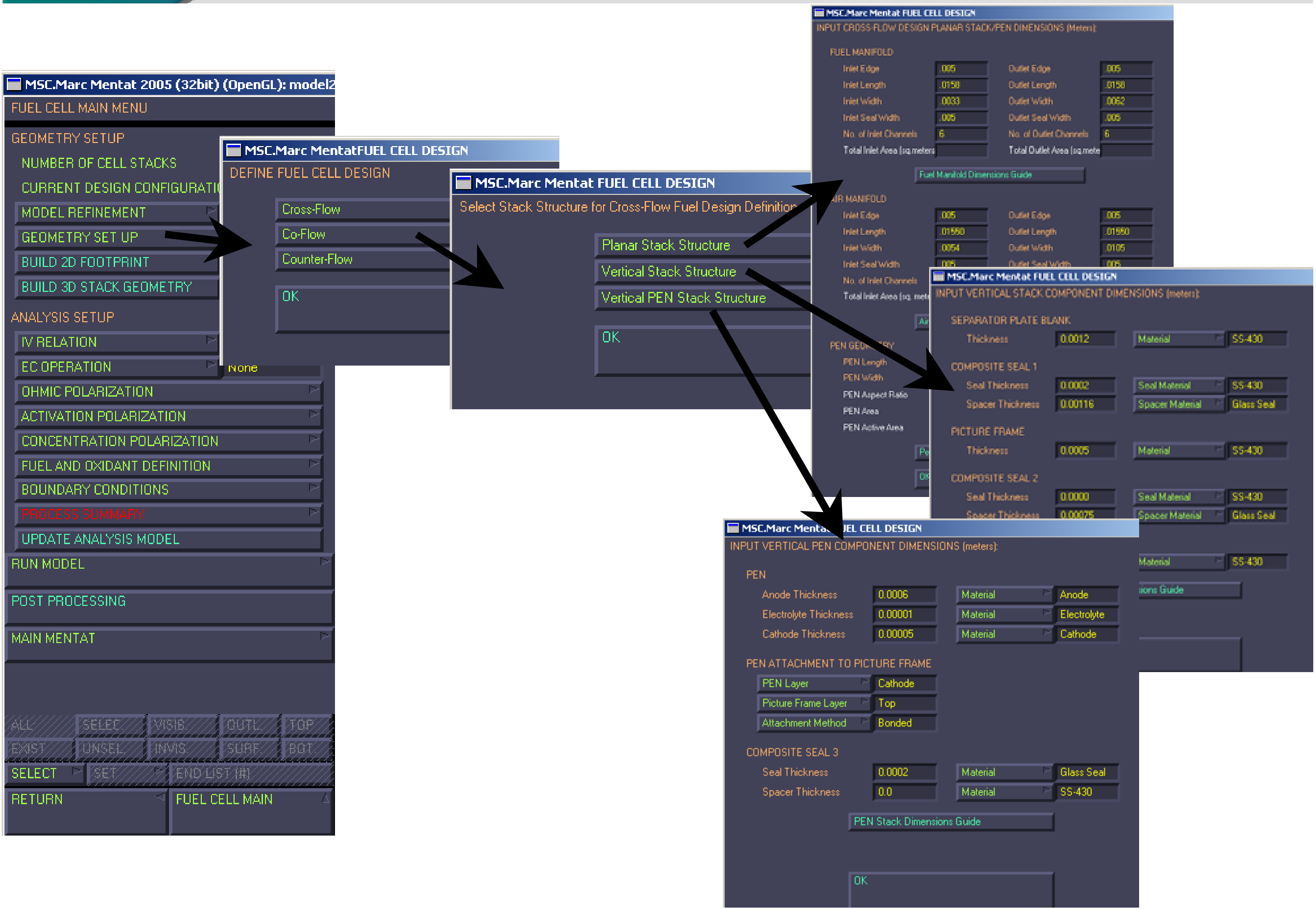
Finite Element Model Generation



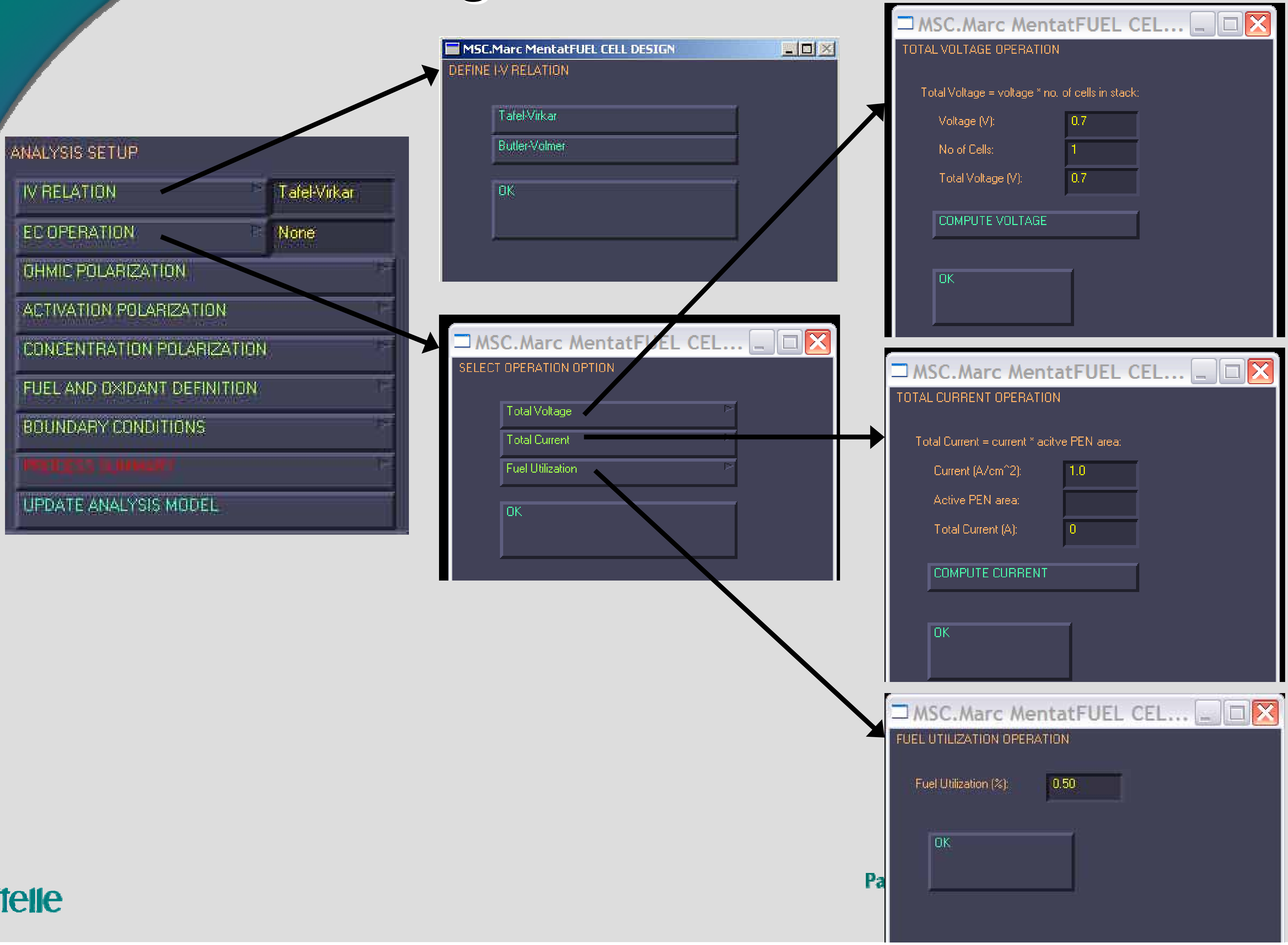
Four ‘action’ buttons to provide for complete fuel cell model generation

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

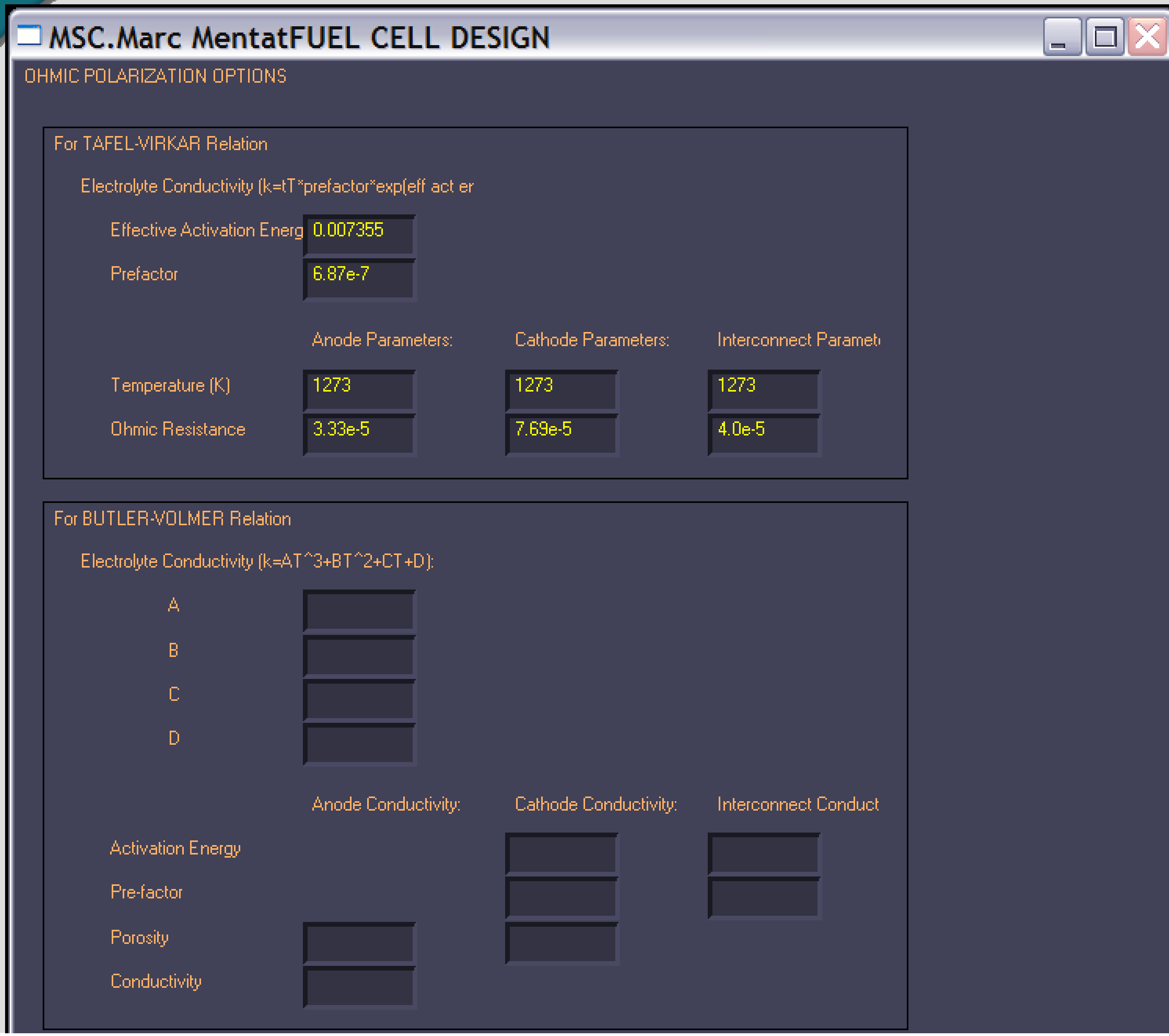
Parametric Based Model Input



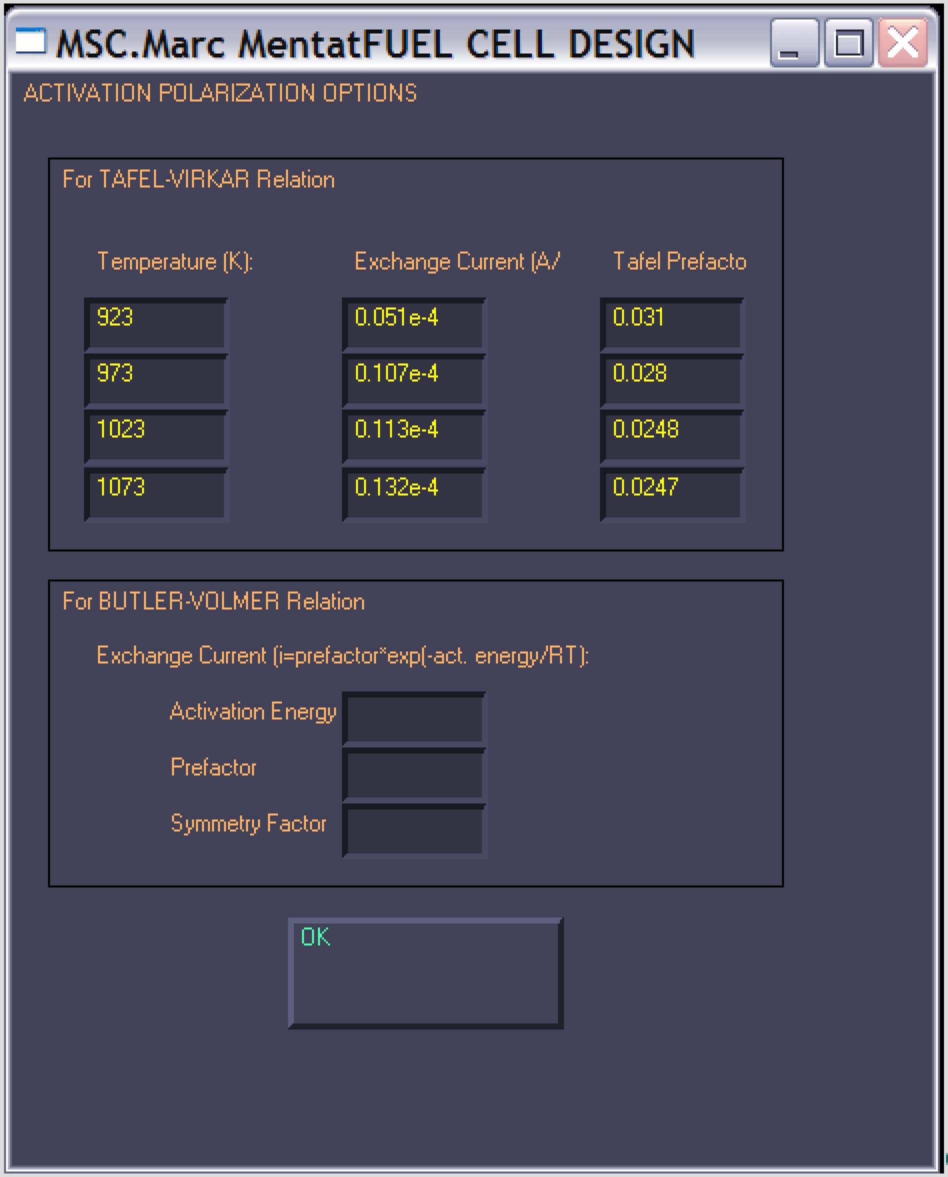
Defining Cell Performance



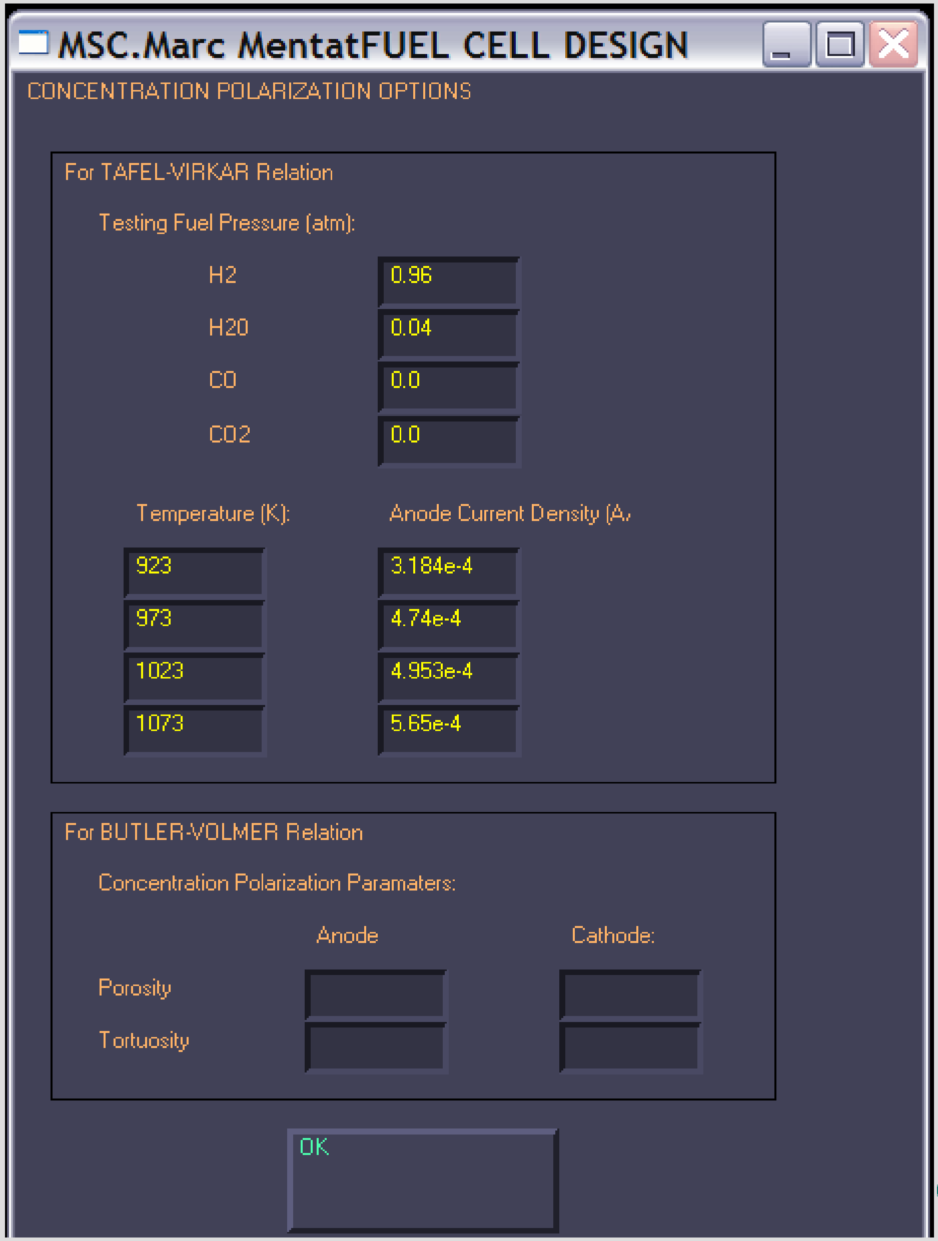
Ohmic Polarization



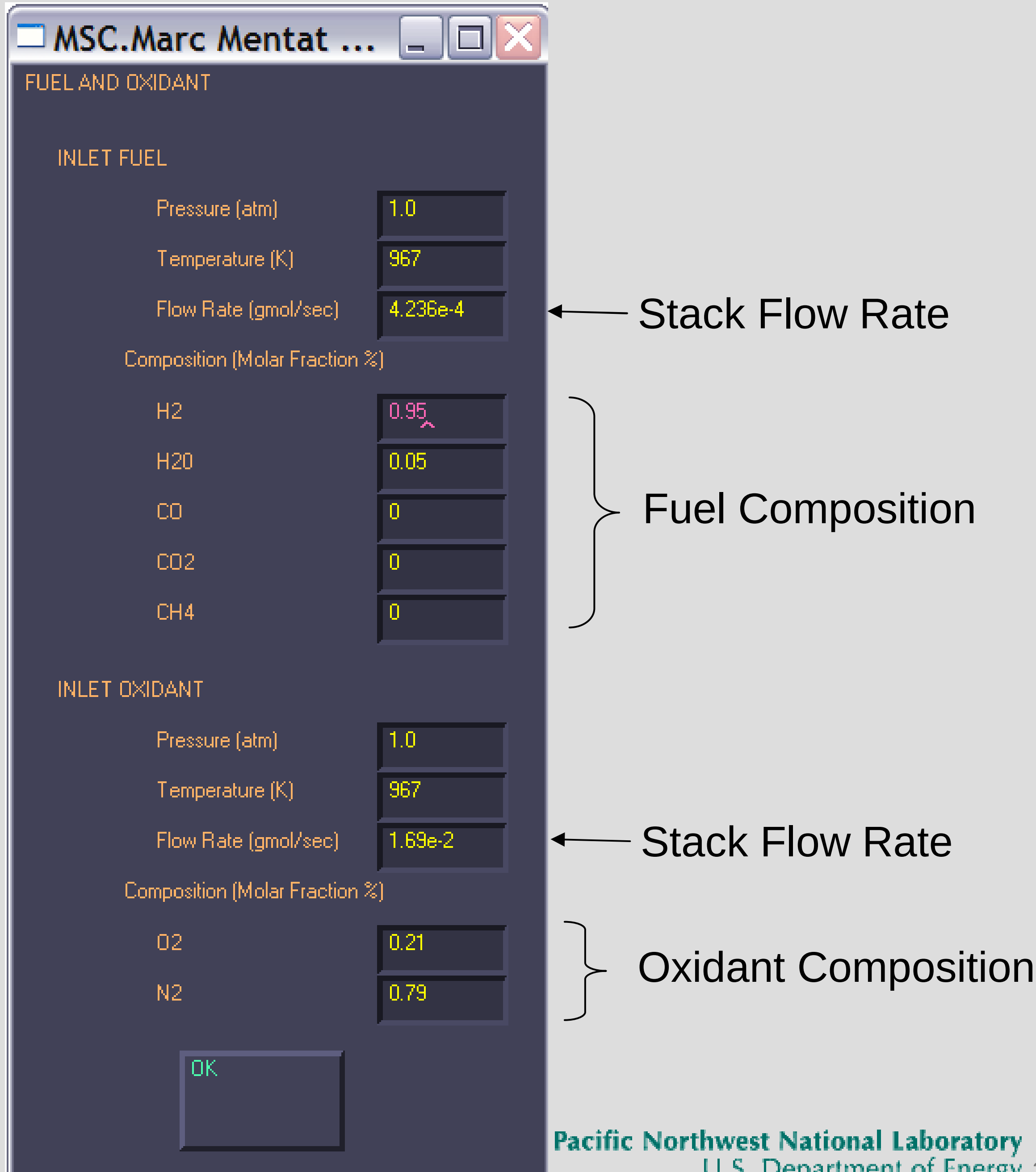
Activation Polarization



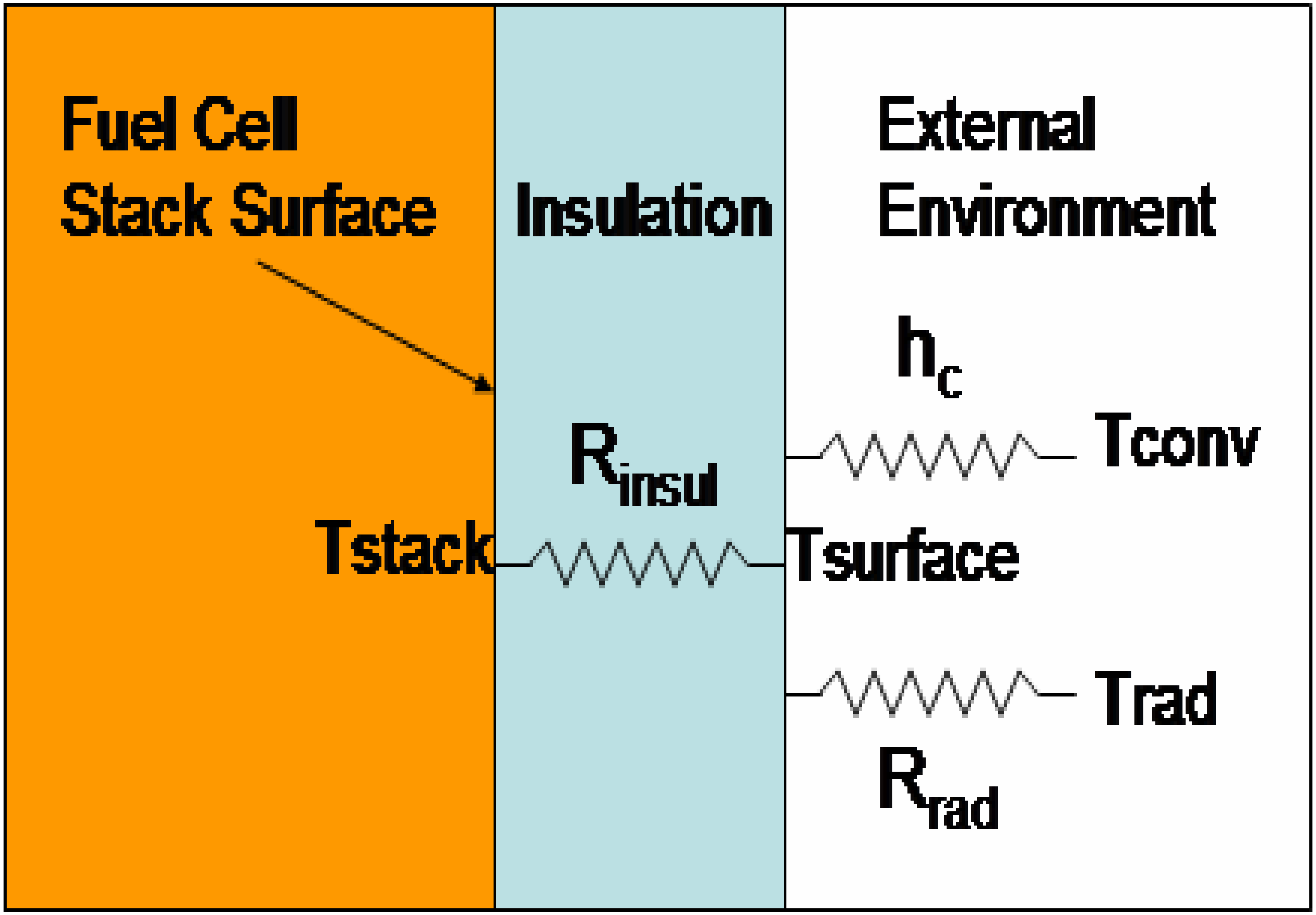
Concentration Polarization



Fuel and Oxidant Definition

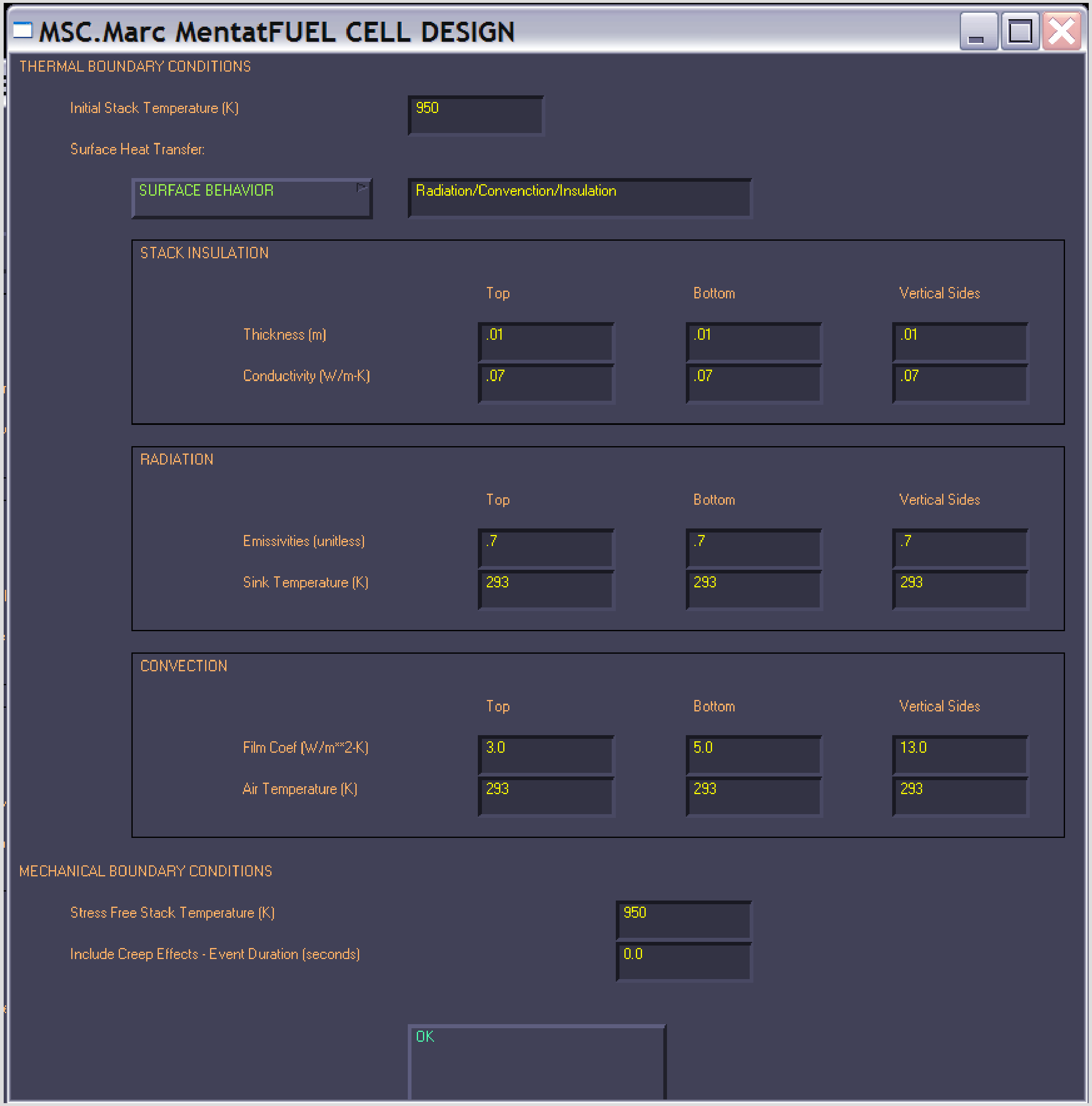


Stack Boundary Conditions



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

Stack Boundary Conditions



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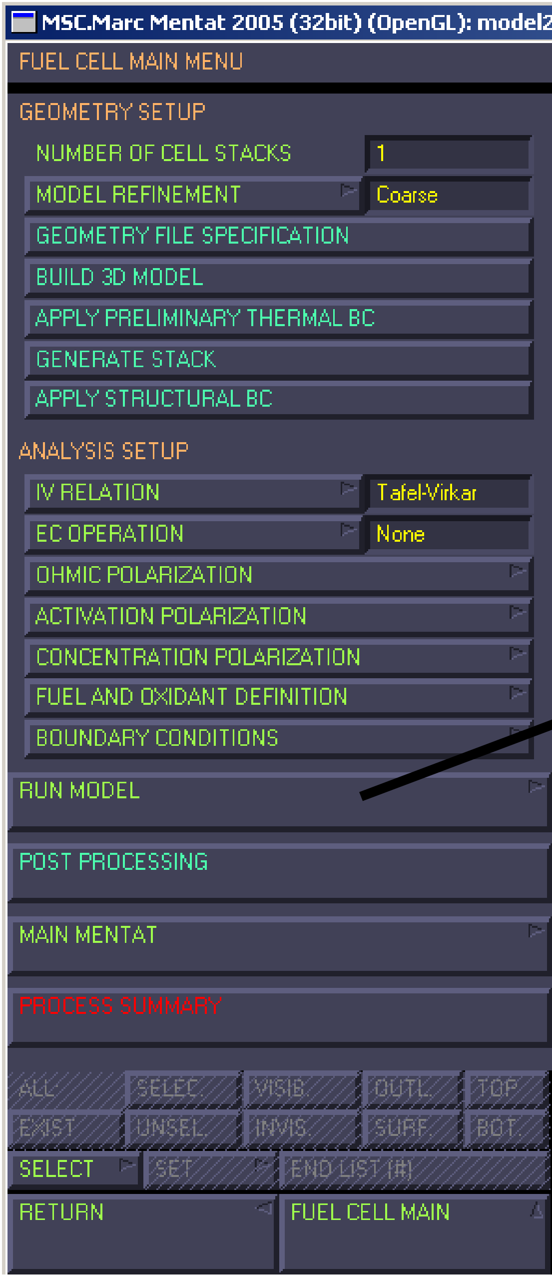
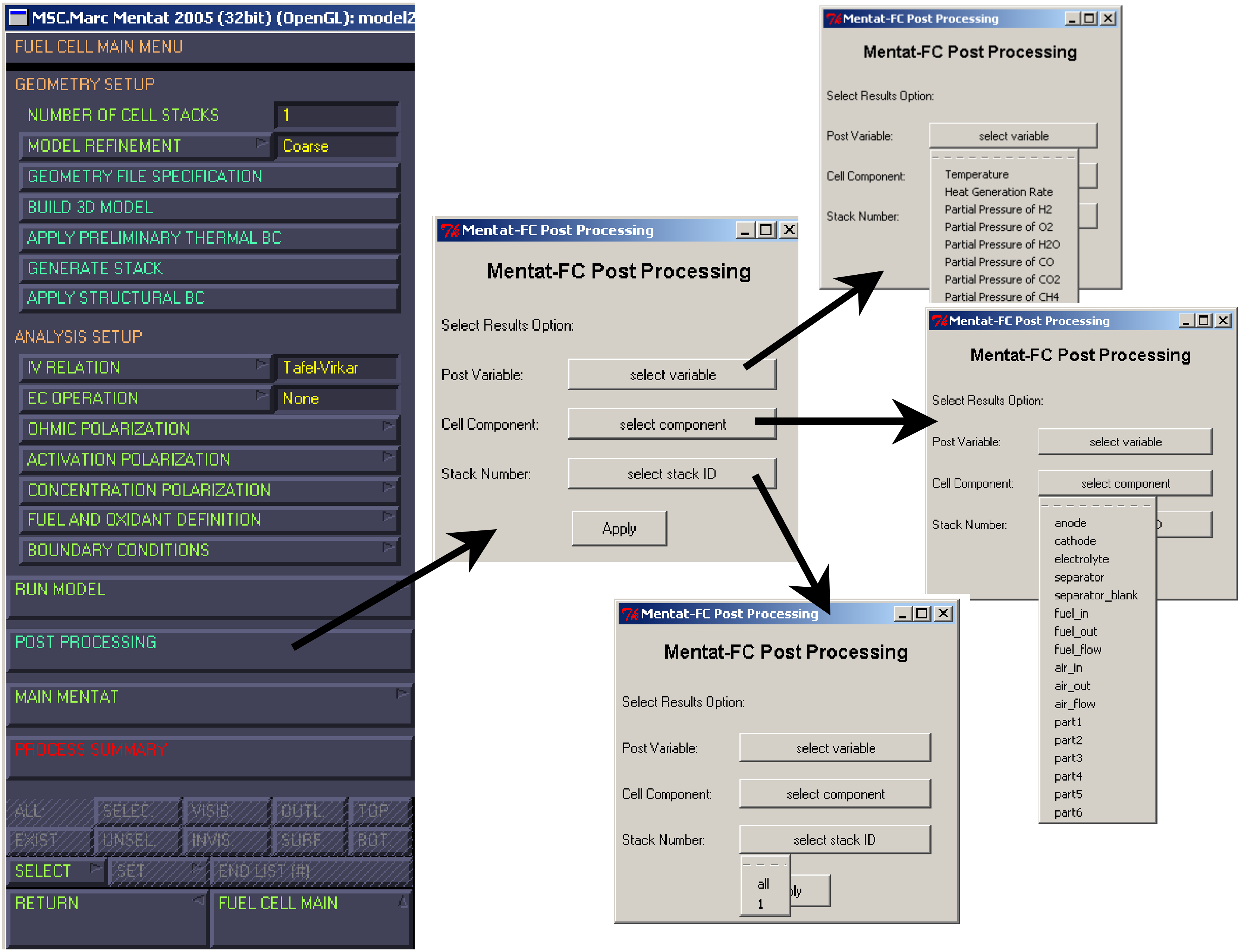
Model Solution



Write EC parameter file

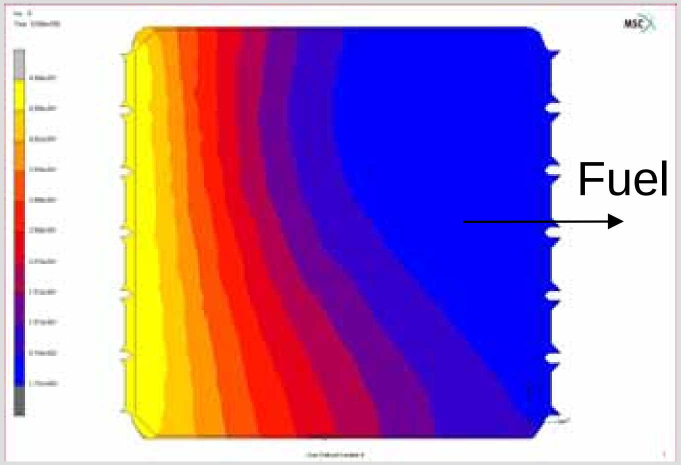
Submit Analyses

The Post Processing Menus

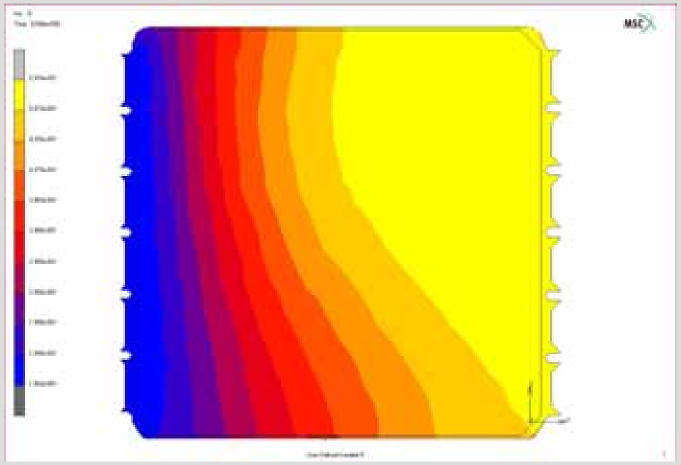


Fuel Species
(Inlet Fuel: 0.6 H_2, 0.1 H_2O, 0.3 CO, 0.1 CO_2)

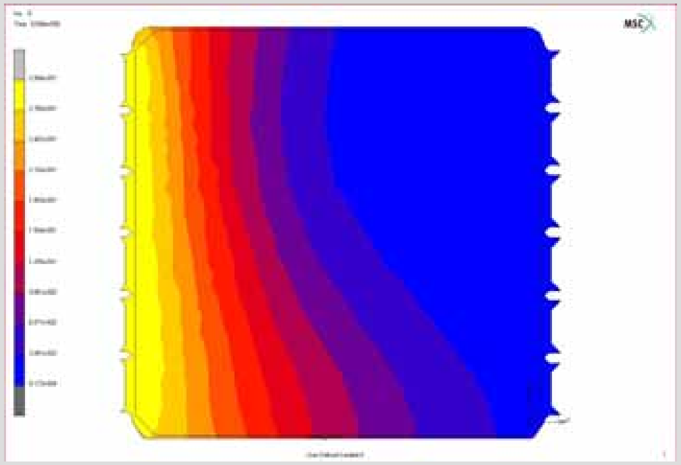
Hydrogen



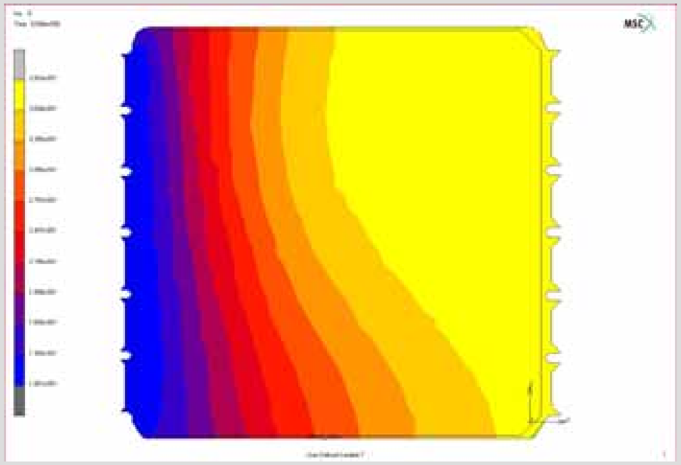
Water



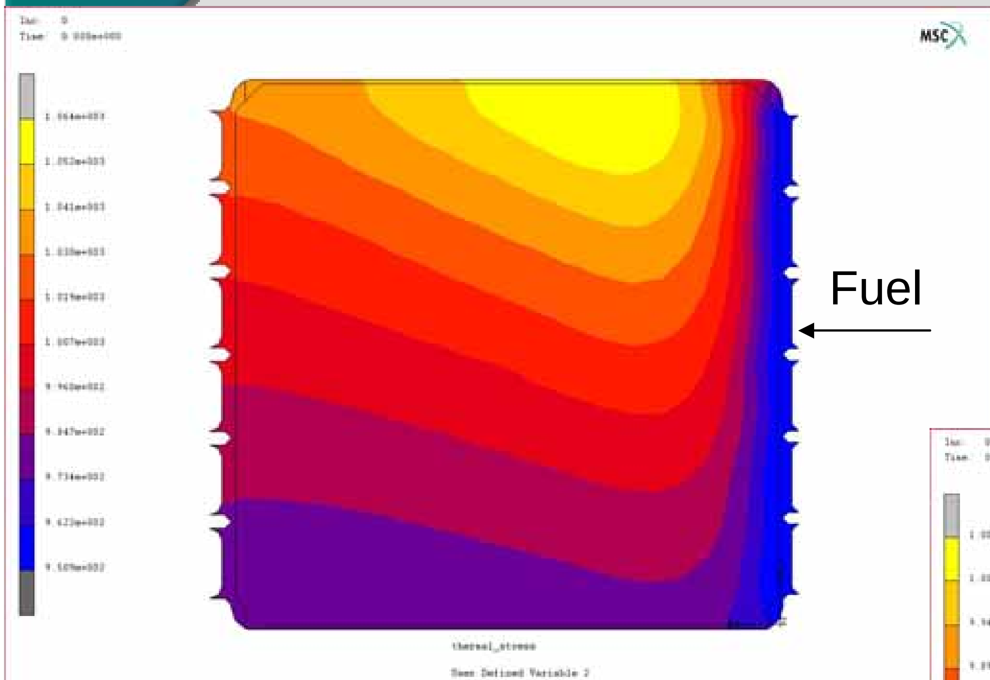
CO



CO_2

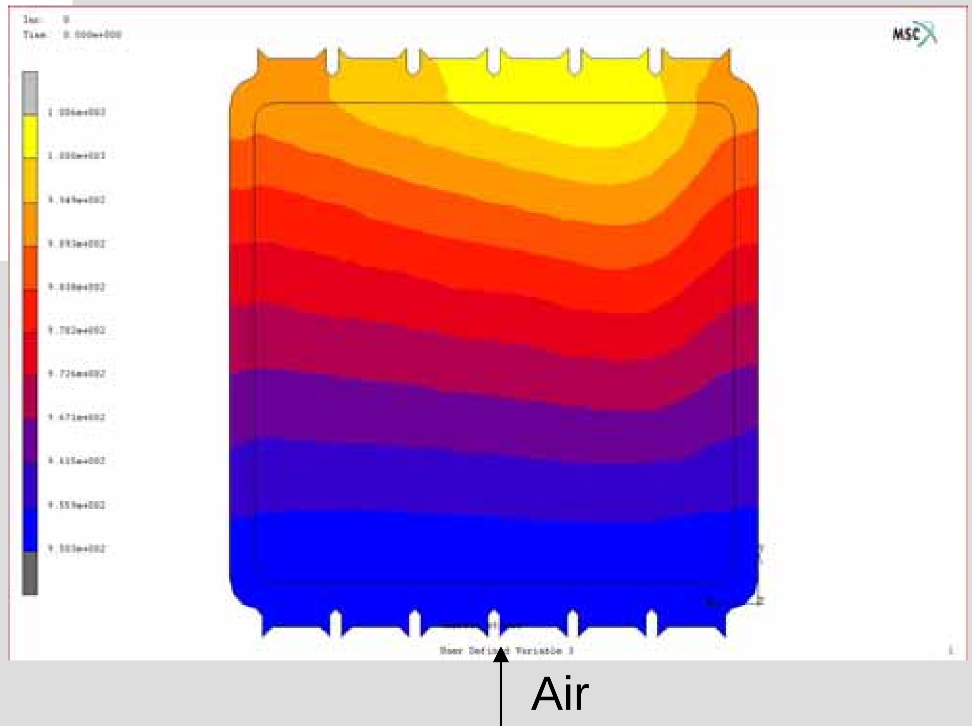


Fuel and Oxidant Temperature

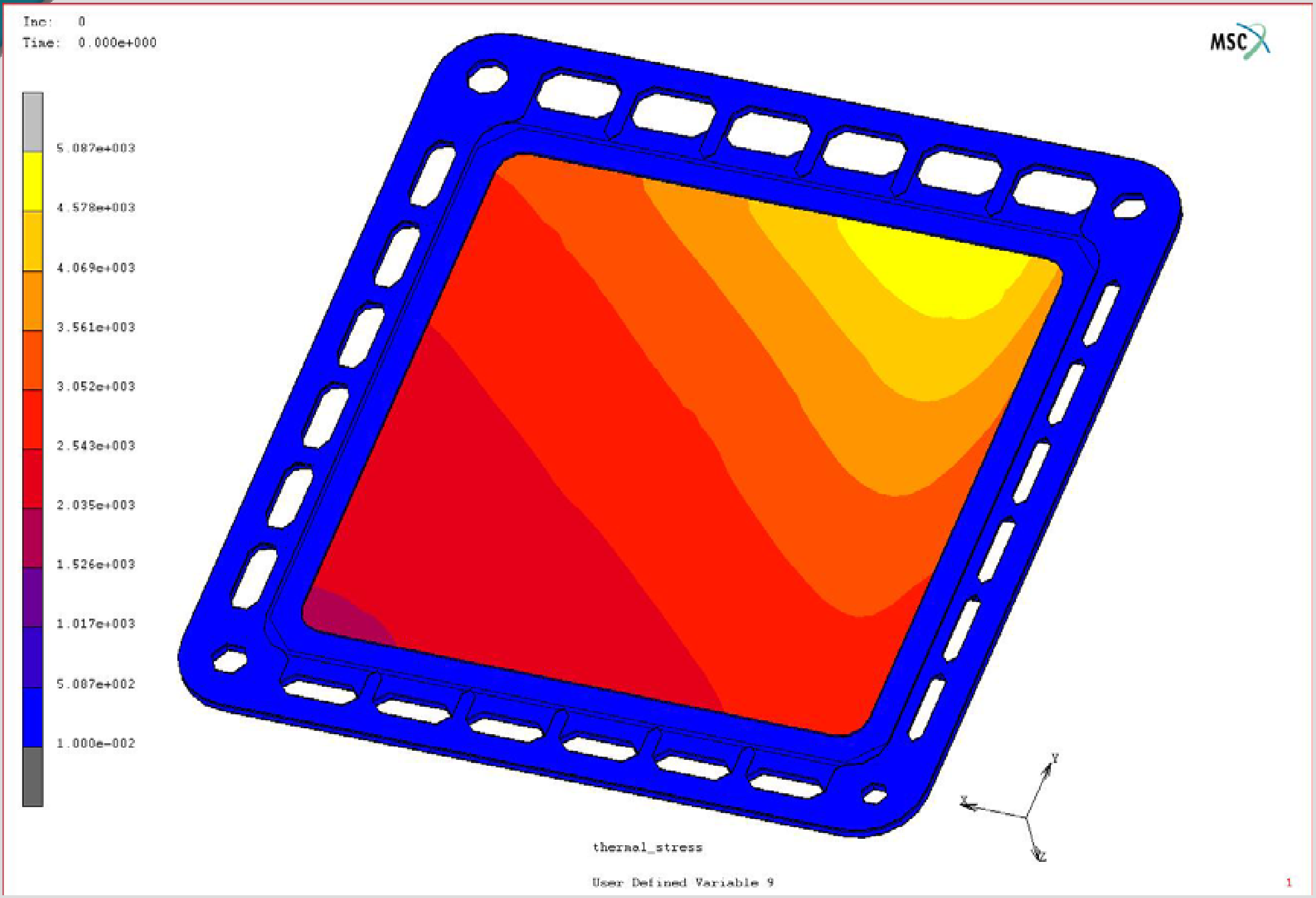


Fuel Temperature

Air Temperature

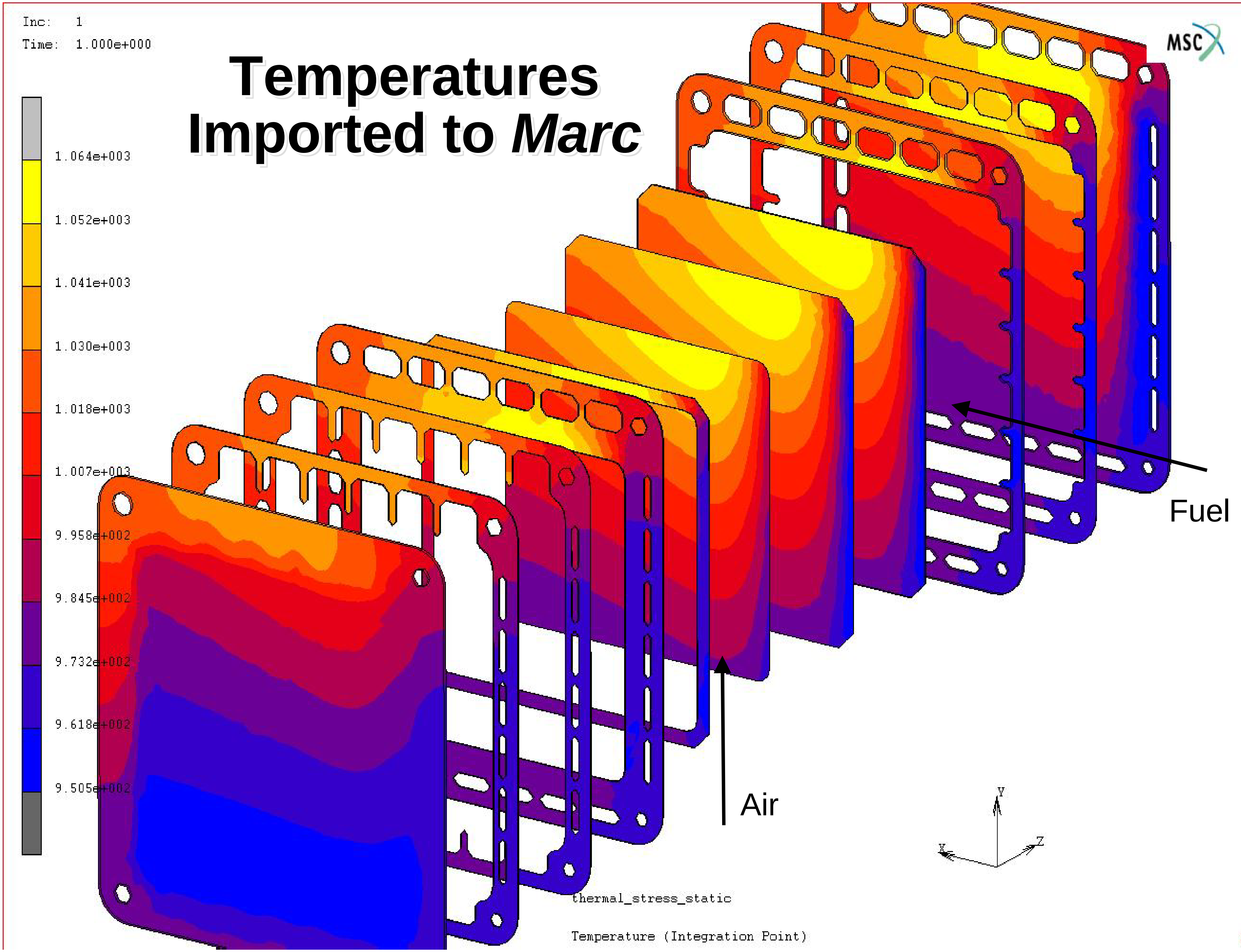


Current

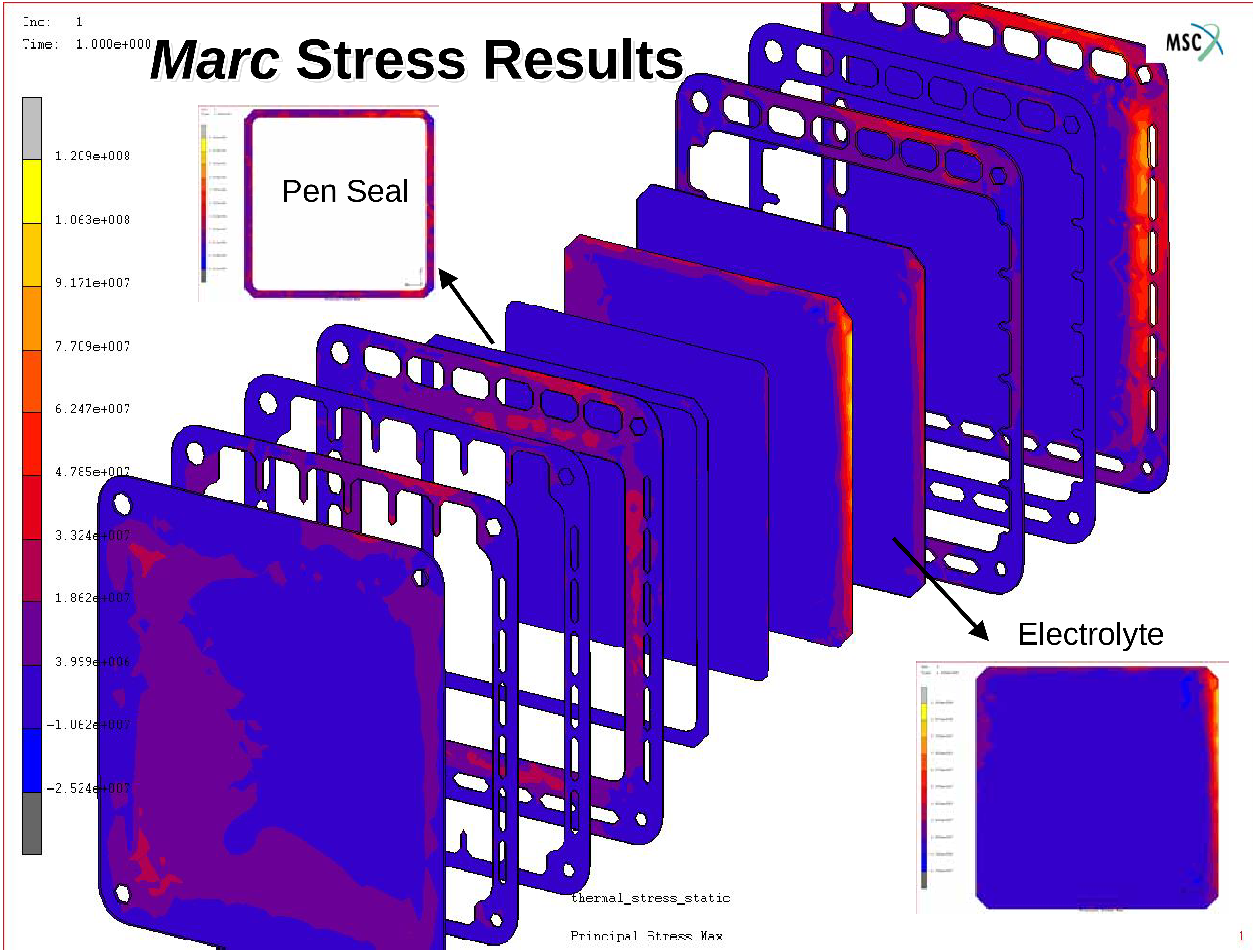


Inc: 0
Time: 0.000e+000
MSC
5.087e+003
4.578e+003
4.069e+003
3.561e+003
3.052e+003
2.543e+003
2.035e+003
1.526e+003
1.017e+003
5.087e+002
1.000e-002
thermal_stress
User Defined Variable 9
1

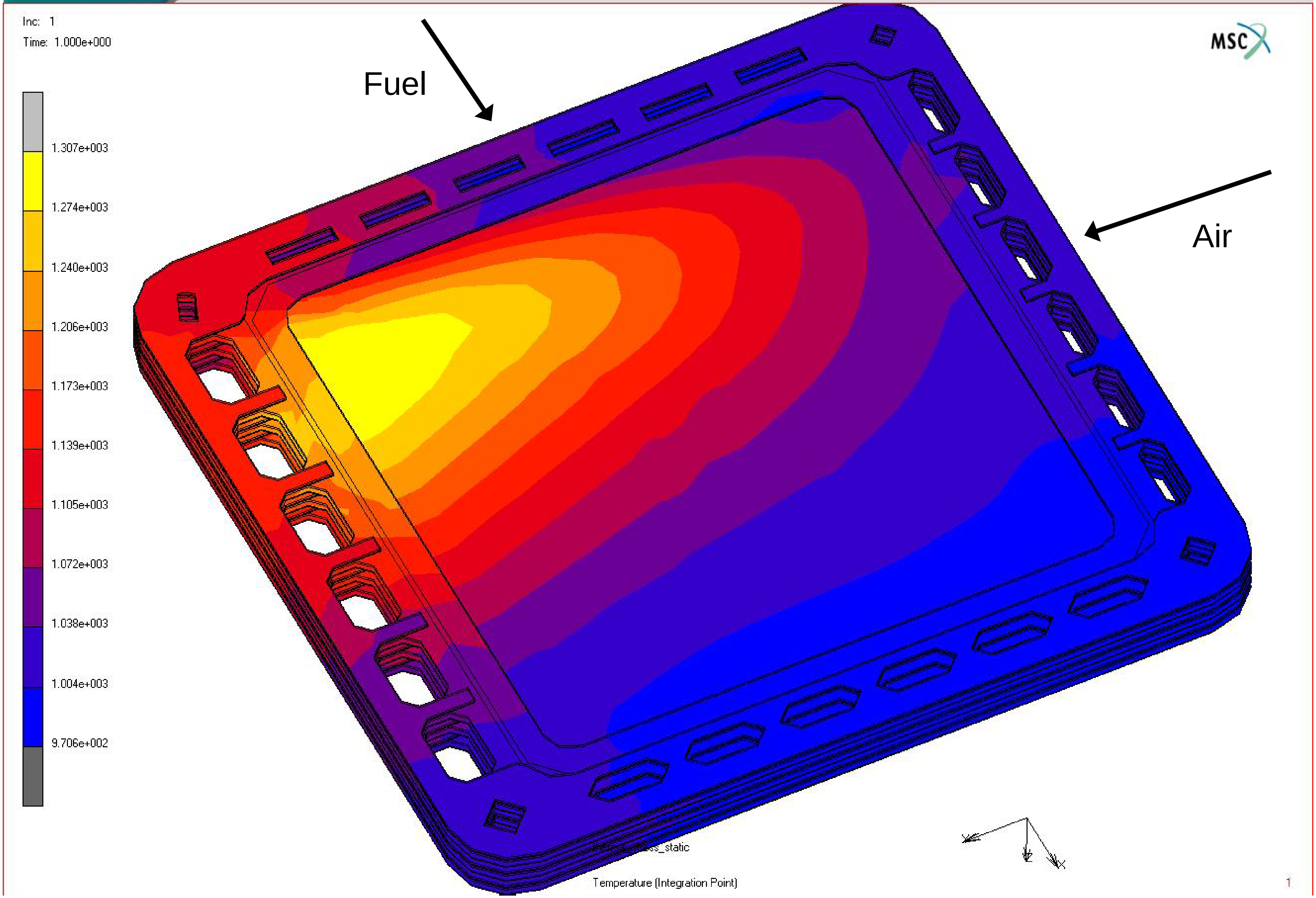
Temperatures Imported to *Marc*



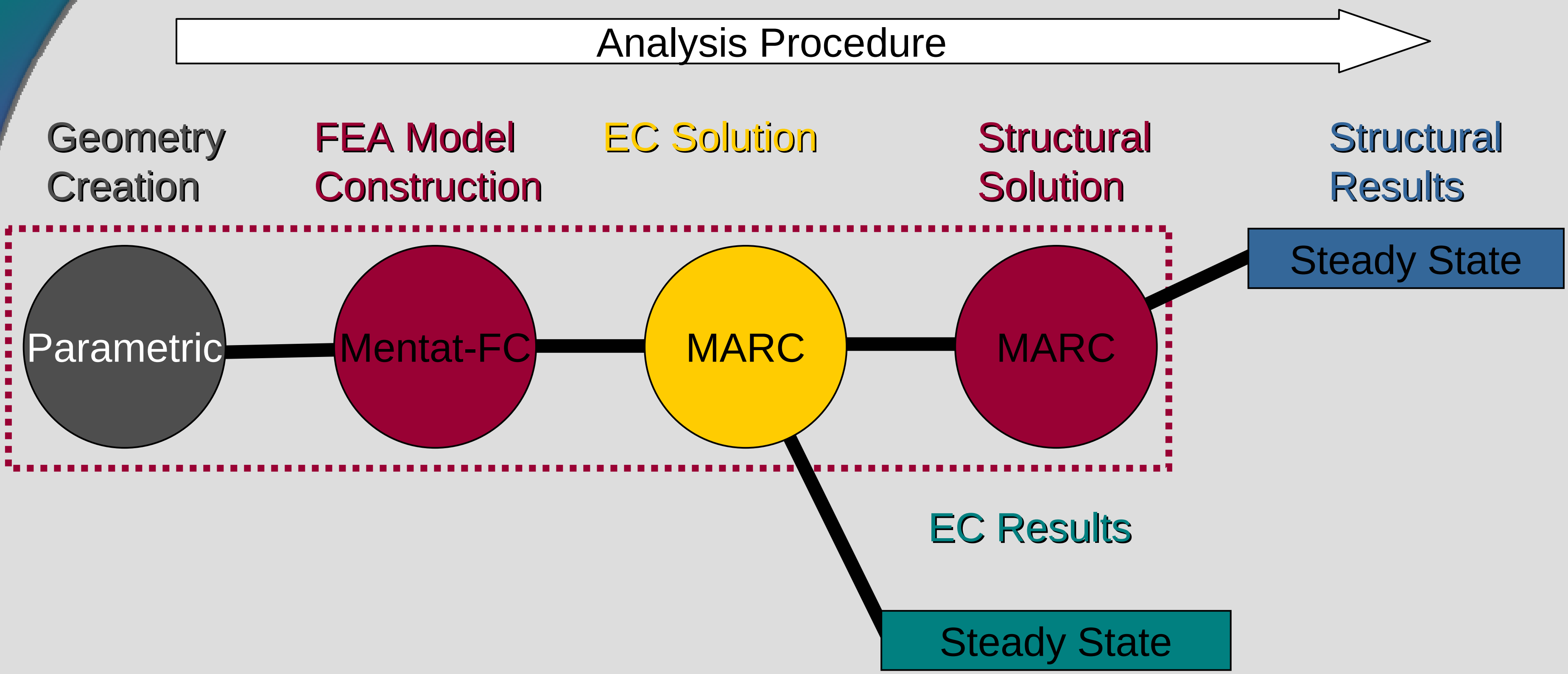
Marc Stress Results



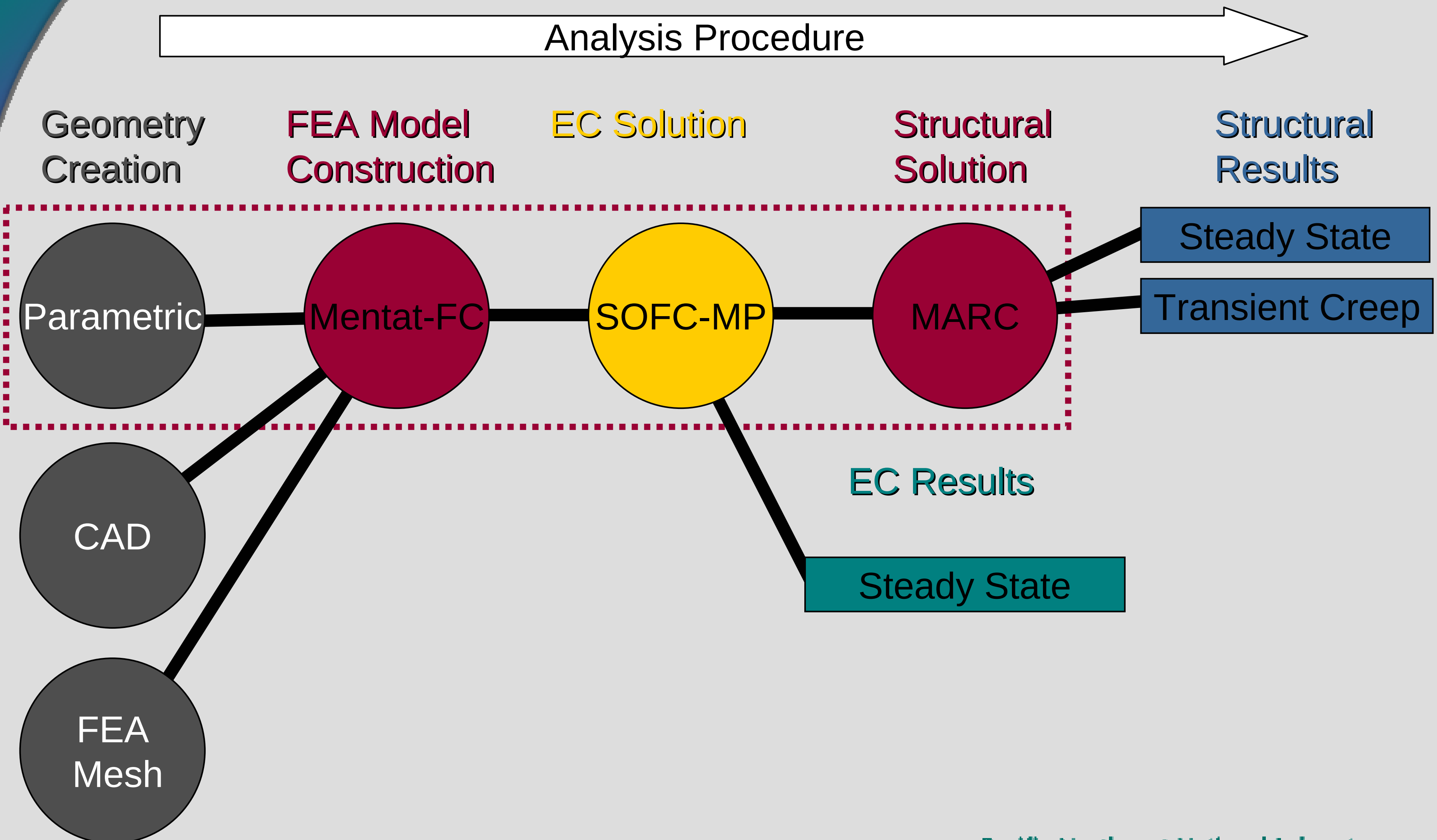
3-Cell Model directly from CAD



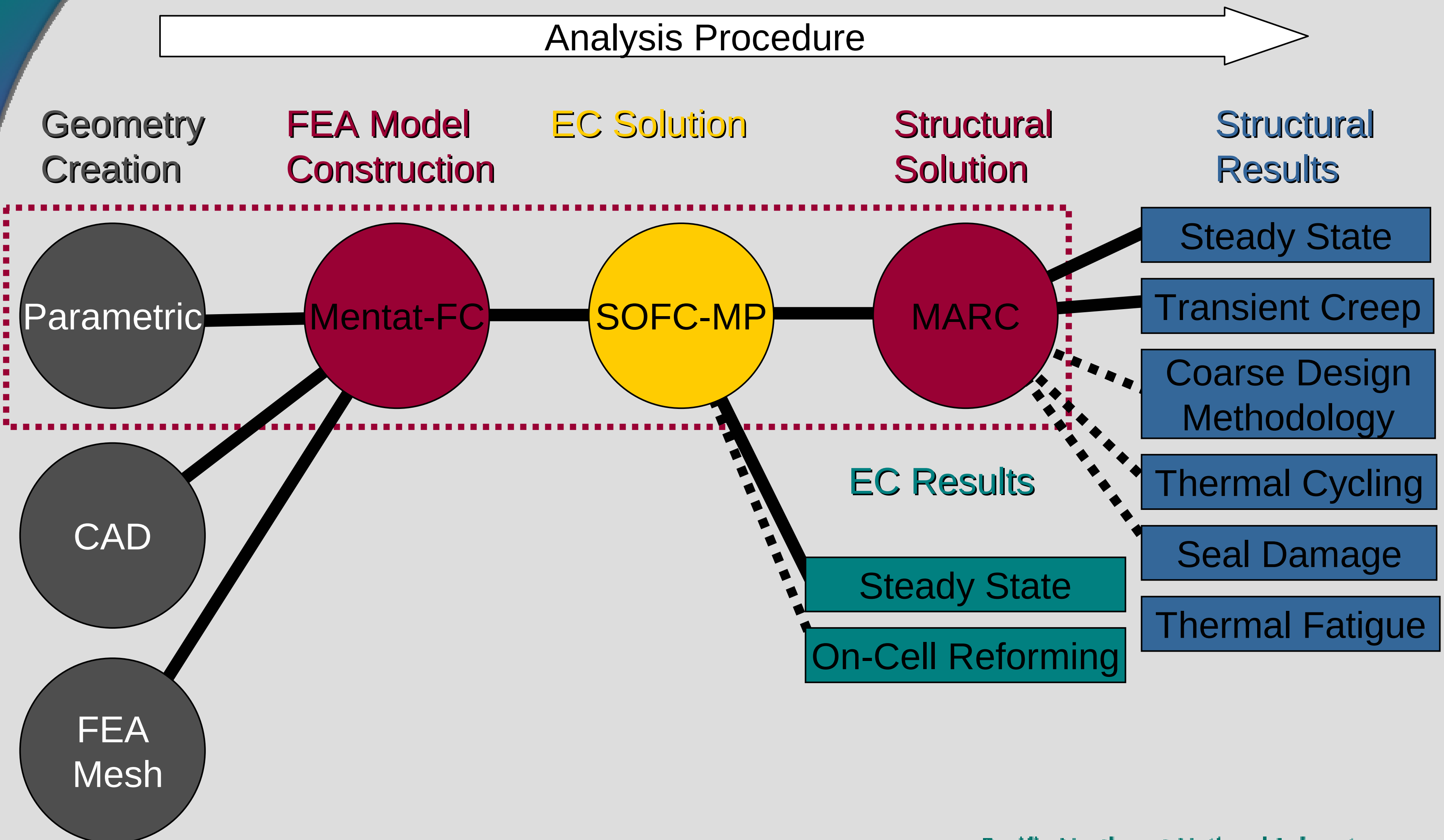
Mentat-FC: Original Parametric GUI



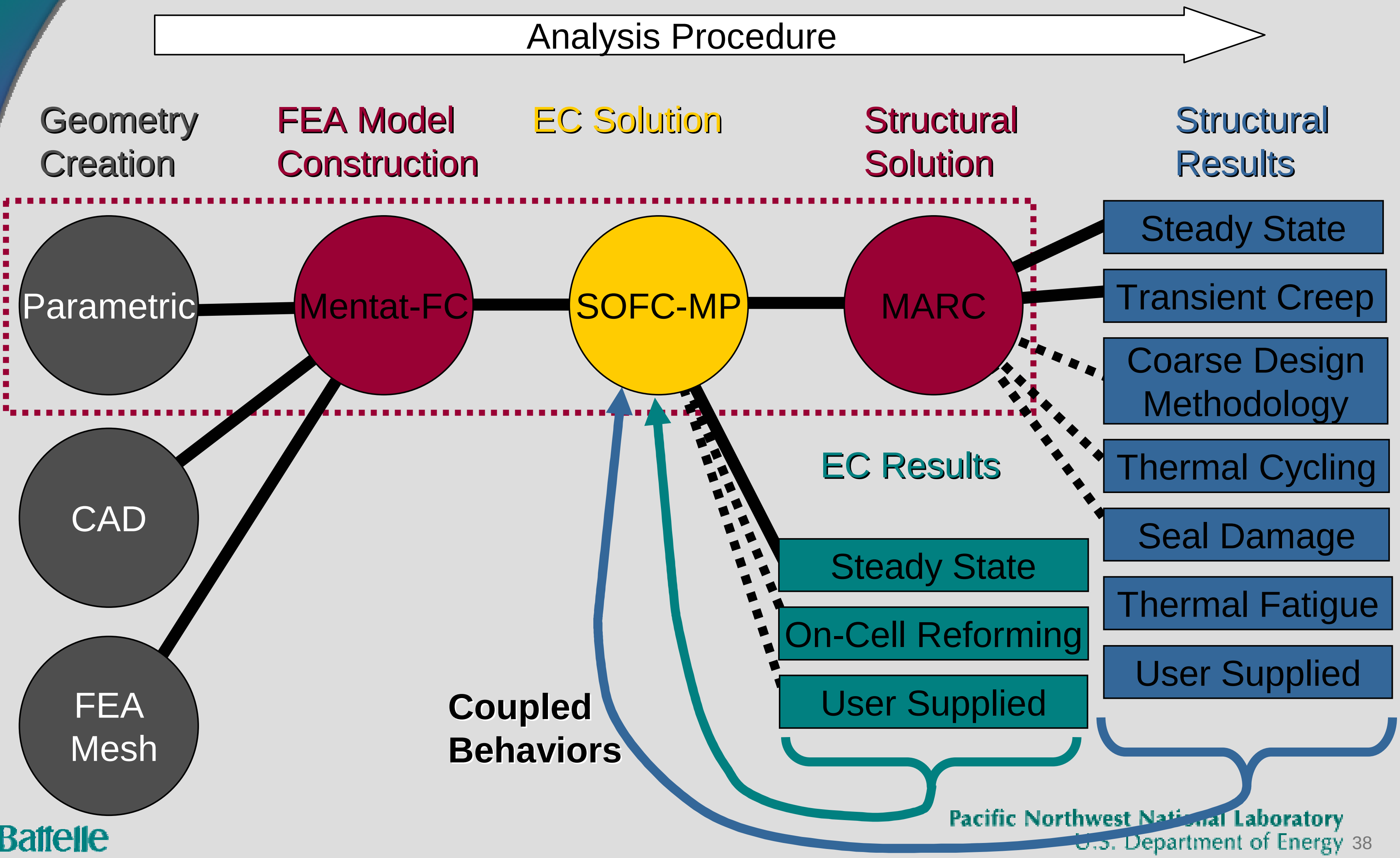
Mentat-FC: Present Modeling Tool



Mentat-FC: In-Progress Modeling Suite



Completed Modeling Suite



How to get this software and more training

- MSC Evaluation Licenses
- PNNL Summer Workshop

Questions?

5-minute break before starting

the live demo of

SOFC-MP and MSC.Marc/Mentat-FC

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

Fuel Species