Modeling & Simulation Tools for Solid Oxide Fuel Cells
SOFC-MP & Mentat-FC Training

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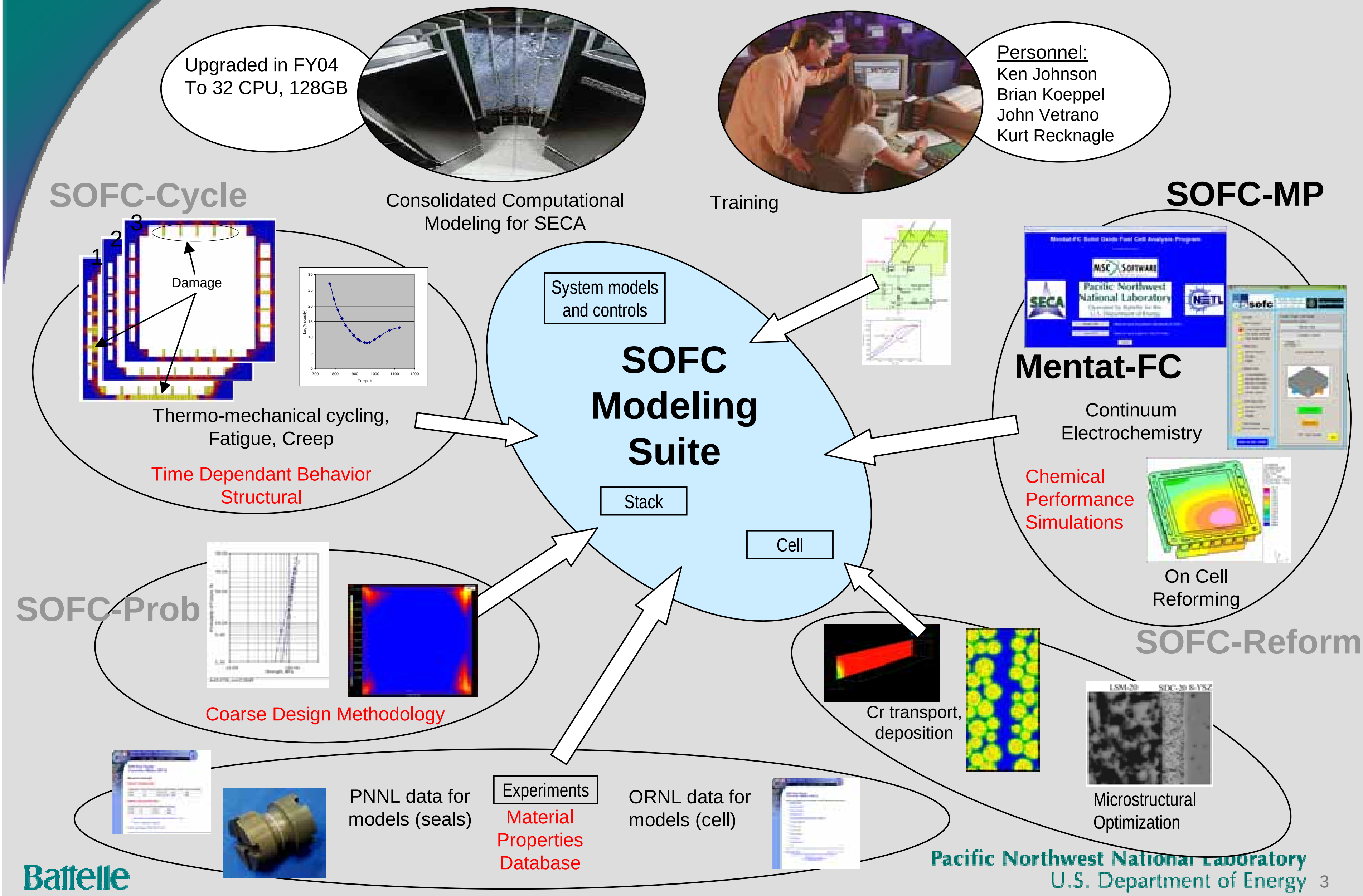
Seminar Outline

- PNNL Modeling Activities Overview (15-min)
  - Integrated Modeling Approach and the SOFC-Tools
  - Development Highlights - new capabilities
- Marc/Mentat Overview (15-min)
- Mentat-FC Training Presentation (~1hr)
  - Capabilities
  - Model Creation
  - Access to Tools
- Hands on Training & Live Demos (~1-1/2 hr)

Integrated Modeling of Solid Oxide Fuel Cells



Development Highlights

- Material Properties Database Providing Foundation for Modeling
- Assisting Thermal Management of Stacks with On-Cell Fuel Reforming (SOFC-Reform)
- Preventing Seal Damage during Thermal Cycling (SOFC-Cycle)
- Designing Stack Components to a Common Survival Rate with a Probabilistic “Coarse Design Methodology” (SOFC-Prob)

Material Properties Database Providing Foundation for Modeling

- Present information is on fundamental SOFC material properties (such as strength, toughness and CTE)
  - Contributions by PNNL and ORNL
  - Available on NETL website
- These fundamental measurements support present structural model development
  - Thermal Cycling of Stacks
  - Coarse Design Methodology
  - Ongoing work in Mentat-FC
- Beginning to include time-dependent behavior and properties for life-prediction studies
  - Mechanical, electrical and physical degradation

Time-Dependent Material Behavior

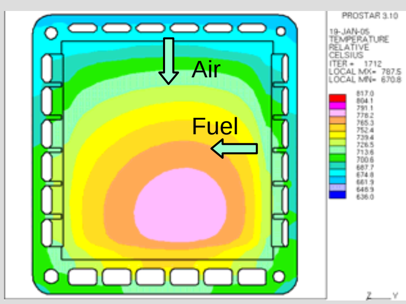
- Long times at high temperatures/stresses will affect the material
  - Strain, diffusion, oxidation, de-vitrification, fatigue
- Tests are underway at PNNL to examine time-dependent behavior of seal materials for input to models (creep, crack growth, fatigue)
- These data will allow better projections of behavior and help to prevent failure of SOFC stacks undergoing long operating times
  - Help SECA Industrial Team Members to meet long-term performance goals

Assisting Thermal Management of Stacks with On-Cell Reformation

- Validated Modeling Approach for Stack and Reformation Activity Design to:
  - Decrease Reformer Size Requirement
  - Decrease or maintain Air Blower Size Requirement
  - Assist in Stack Thermal Management
  - Minimize Thermal Stress within Cell components

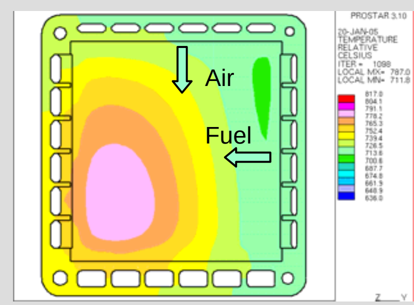
Ready for Mentat-FC now! Delivery Date Sept. 2005

Example: two stacks operating at the same electrical current, cell temperature, and gas flow rates. One with and one without CH_4



H_2 Fuel
Baseline case (Tin = 651C)
(../devNoDIRcase/fpcNoDIR.mdl)

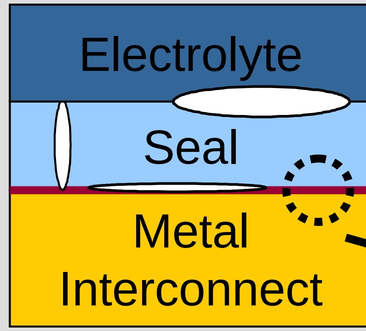
Case	Delta-T C	S1 max, Mpa Anode	S1 max, Mpa Seal	S1 max, Mpa Picture Frame
H2 Fuel	117	25	10.1	141.1
DIR	75	11.8	5.9	59.5

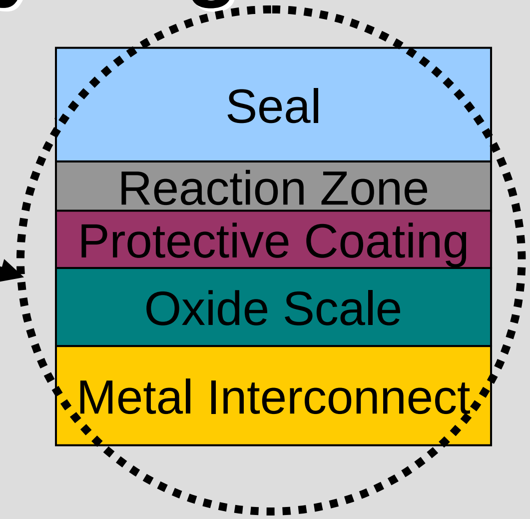


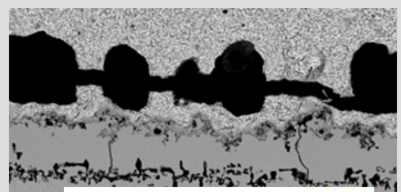
DIR (CH_4) S:C=3
decreased activity (Tin = 715C)
(../DIR-E114535-tconmod/fpcDIR2.mdl)

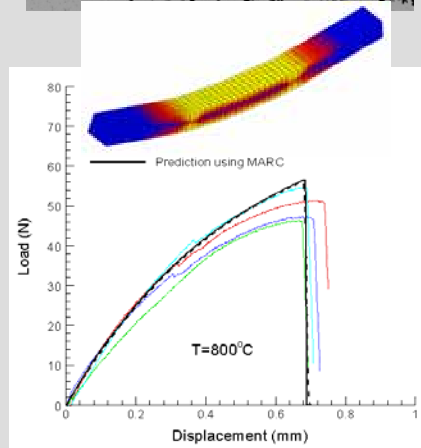
Preventing Seal Damage Caused by Thermo-Mechanical Cycling

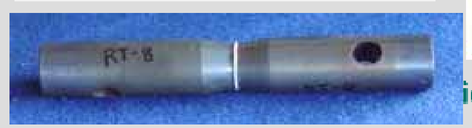
- Sealing remains critical Issue
  - Glass/Ceramic Seals are popular but prone to cracking
  - Model presently in Marc:
    - characterizes bulk G18 seal material damage (bend-bar)
    - Predicts critical areas in stack → seal failure
    - In Mentat-FC in June '05
  - Extending model with rate dependant behavior to characterize creep/relaxation
- Interconnect/Seal Interface
  - Data → Interface Strength < Bulk Strength
  - Interfaces weakened due to reactions, porosity, scale growth
  - Modeled in Marc
- Thermal Cycling
  - Example shows damage near rigid hearth, in narrow ligaments
  - Estimate leak rate → damage
  - Improve cell design for reliable sealing under multiple startup & shutdown cycles

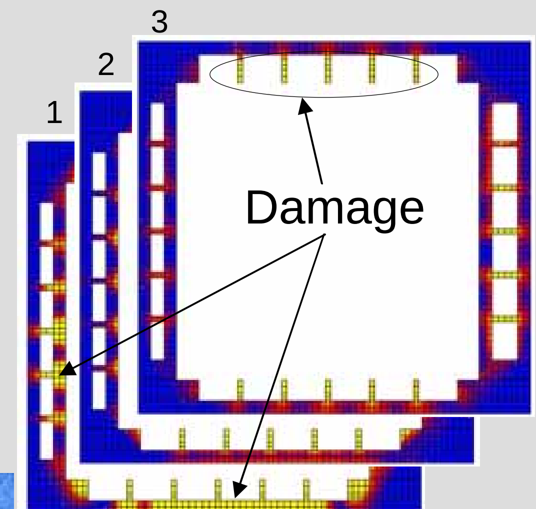










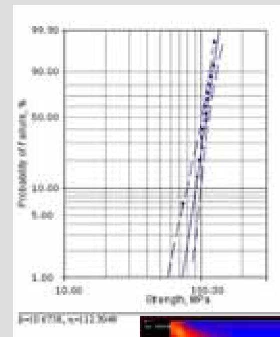


Designing Stack Components to a Common Survival Rate: a “Coarse Design Methodology”

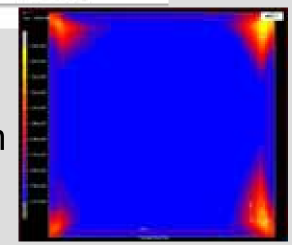
- Depending on the variability of a Load (S) – Stress, and Resistance (R) – Strength, There is an associated probability that a cell component will fail
- The Probability of failure for each individual component can vary widely
- The Designer must either decrease the load or increase the strength in order to achieve some desired probability of component survival
- PNNL is using an approach to “normalize” the expected survival of cell components

$$g(x) = r - s$$

$$P_f = \int_{g(x) \le 0} f_x(x)\, dx$$



Anode strength distribution



Anode maximum principal stress

Design: Anode Thickness (microns)	Load: Fuel flow (gmol/sec)	Component Failure Probability (Pf)		
		Anode	Electrolyte	Seal
600	0.00272	<1.0E-5	0.067	0.955
	0.000907	<1.0E-6	0.0003	0.684
720	0.00272	<1.0E-5	0.036	1.0
	0.000907	<1.0E-6	0.0003	0.53
	0.00068	<1.0E-6	<1.0E-5	0.633

Designing Stack Components to a Common Survival Rate: a "Coarse Design Methodology"

$$Design\ goal:\quad stress < \alpha \times strength$$

Example design target: uniform component failure probability Pf=0.0014, safety index β=3.

$$\beta = \frac{\bar{R}_i - \bar{S}_i}{\sqrt{\sigma_{R_i}^2 + \sigma_{S_i}^2}}$$

- In this analysis, the probability of failure is chosen in advance
- Strength reduction factors for each component are calculated based on normal distributions of the associated variables
- The Designer uses the strength reduction factors directly in the "design goal" above to accommodate the stress

Design: Anode Thickness (microns)	Load: Fuel flow (mol/sec)	Component Strength Reduction Factor α		
		Anode	Electrolyte	Seal
600	0.00272	0.59	0.312	0.58
	0.000907	0.65	0.318	0.65
720	0.00272	0.58	0.31	0.62
	0.000907	0.60	0.32	0.65
	0.00068	0.65	0.3	0.65

Marc/Mentat Overview

Thank you

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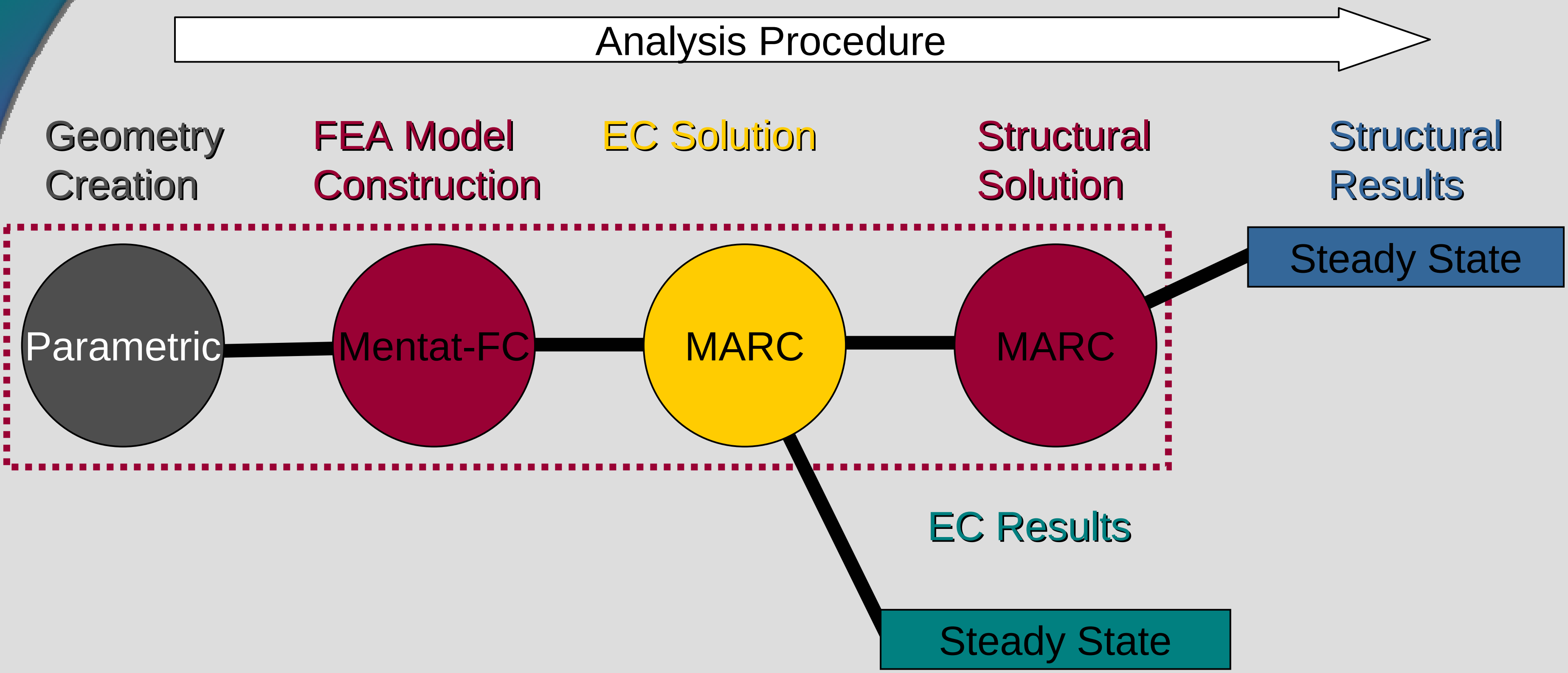
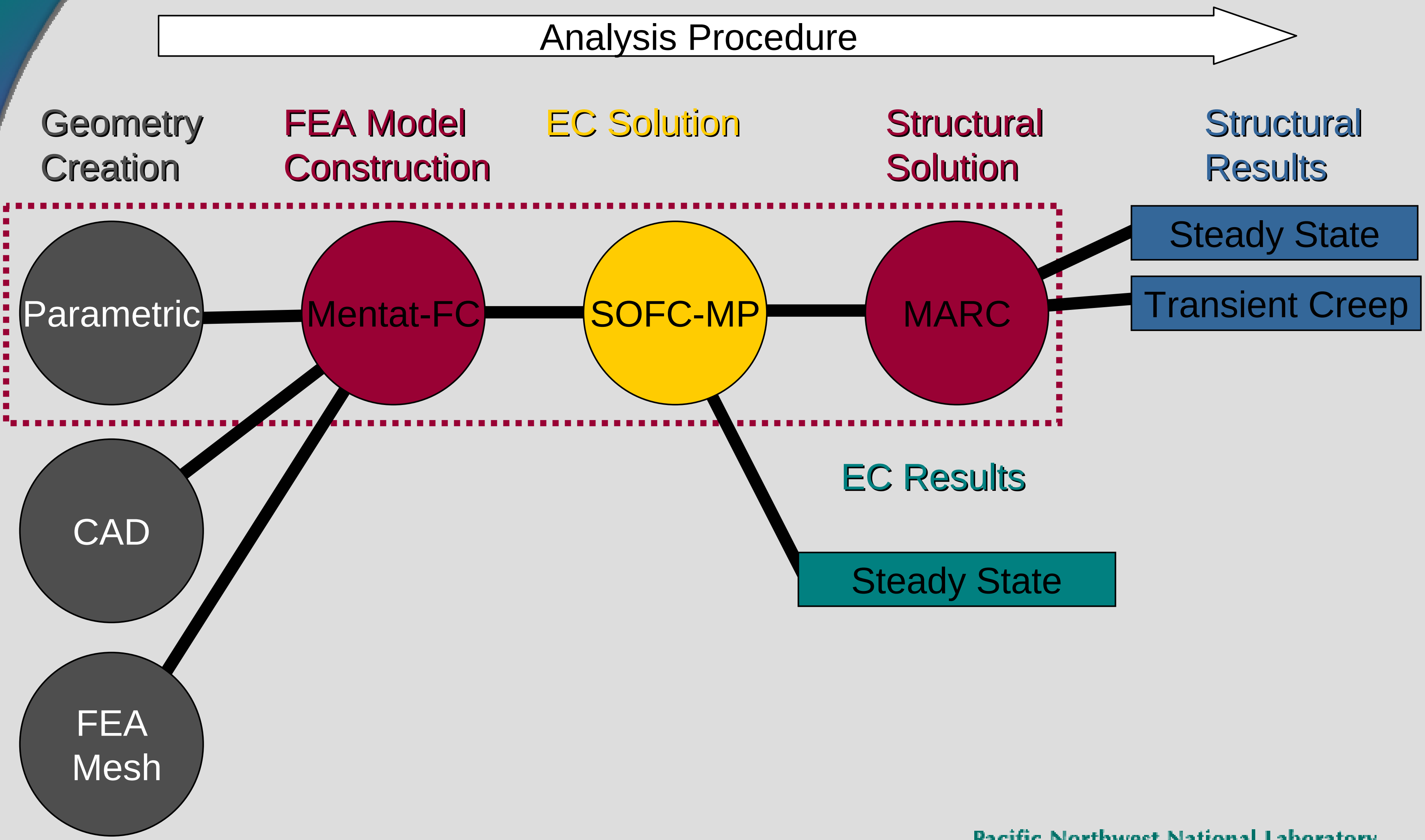
Status of the Mentat-FC Graphical User Interface

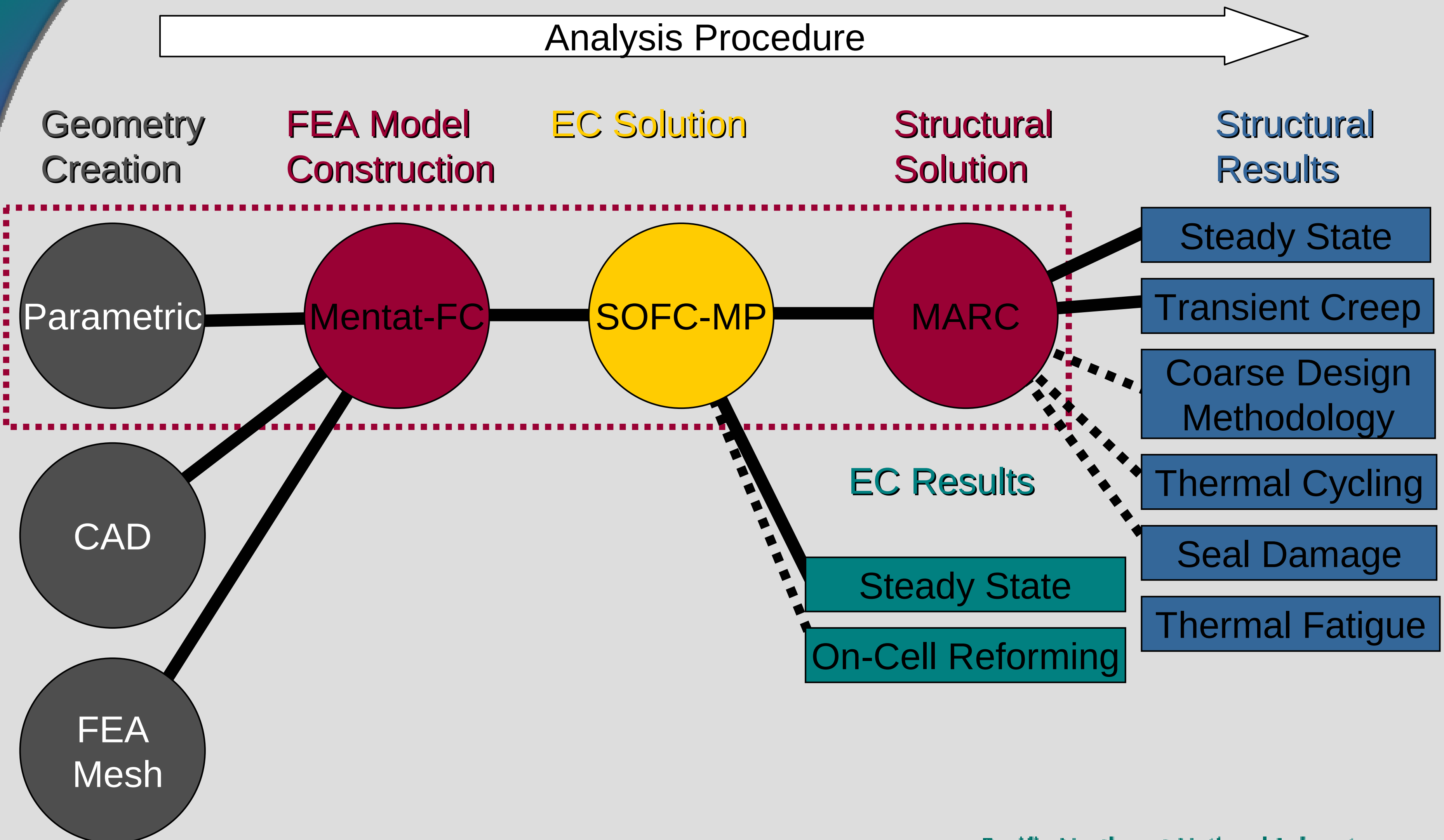
Mentat-FC: Original Parametric GUI



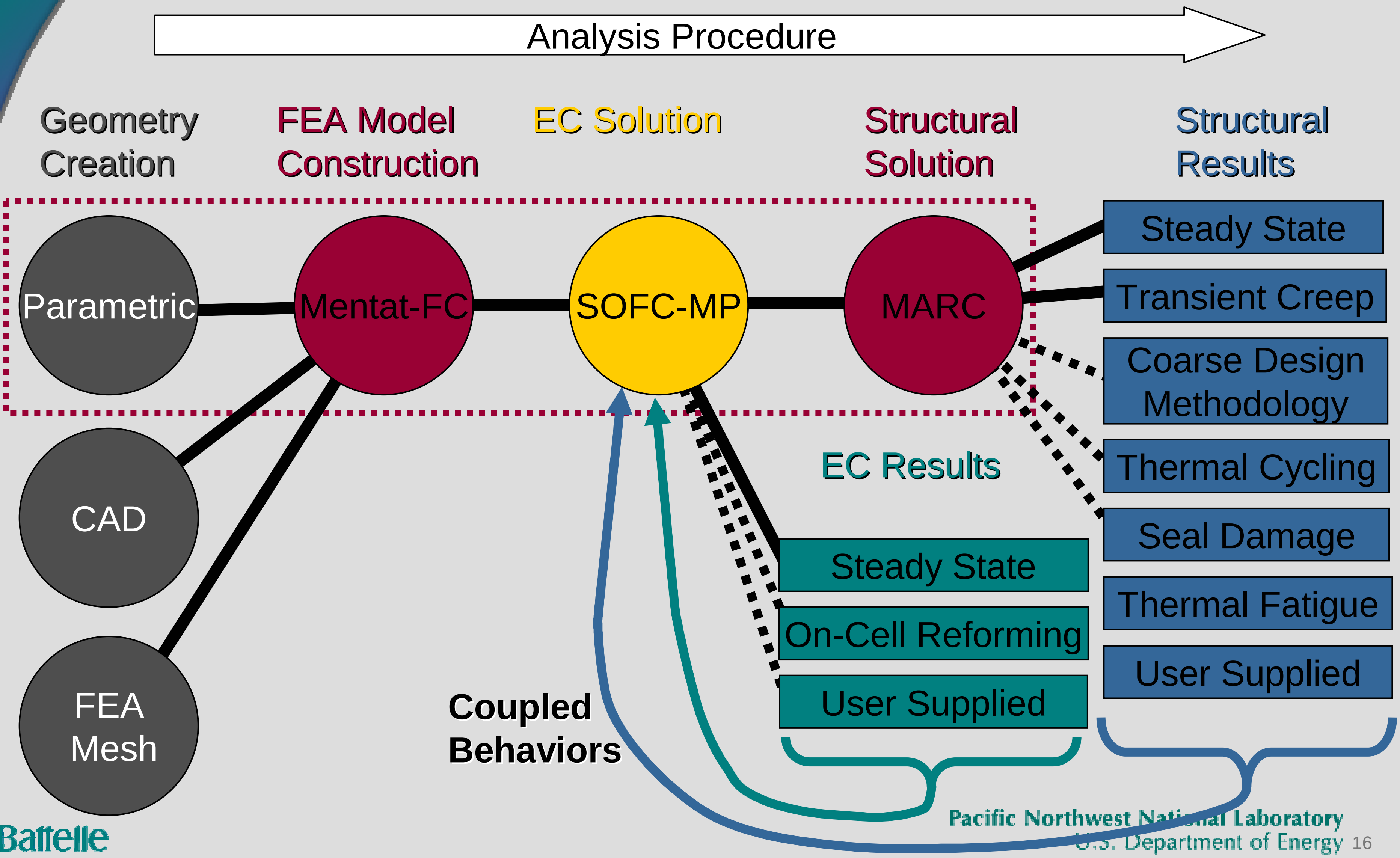
Mentat-FC: Present Modeling Tool



Mentat-FC: In-Progress Modeling Suite



Completed Modeling Suite



SOFC-MP/Mentat-FC Modeling Tools Overview

This section has the technical details of the tools. Based on Ken’s slides

Estimated Technical Targets

	Phase I	Phase II	Phase III
Efficiency	25% mobile 35% stationary	30% mobile 40% stationary	30% mobile 40% stationary
Steady State Test	<2% power degradation in 500 hr	<1% power degradation in 500 hr	<0.1% power degradation in 500 hr
Transient Test	<1% power degradation in 10 cycles	<0.5% power degradation in 50 cycles	<0.1% power degradation in 100 cycles
Design Lifetime	40,000 hr stationary 5,000 hr transportation	40,000 hr stationary 5,000 hr transportation	40,000 hr stationary 5,000 hr transportation

SOFC-MP

- Solid Oxide Fuel Cell Multi-Physics (SOFC-MP)
- A computationally efficient finite element solver for
  - Multi-species flow
  - Thermal
  - Electrochemical
    - Tafel-Virkar formulation
    - Butler-Volmer formulation
- Capabilities include
  - Multiple cell stacks
  - Contact algorithms for dissimilar meshes

Mentat-FC

- Mentat – Fuel Cells (Mentat-FC)
- An intuitive graphical user interface (GUI) to
  - Create SOFC geometry
    - Generic computer aided design (CAD) files
    - Existing finite element mesh files
    - Cross-, co-, or counter-flow planar parametric input
  - Create stack finite element model
    - Electrochemical behavior
    - Flow, thermal, and mechanical boundary conditions
    - Material properties database
  - Submit model to SOFC-MP solver
  - Post-process results
    - Species concentration, flow velocities, current density
    - Temperature
    - Stress, strain, & displacements

Data Collected on Bulk G18 Glass

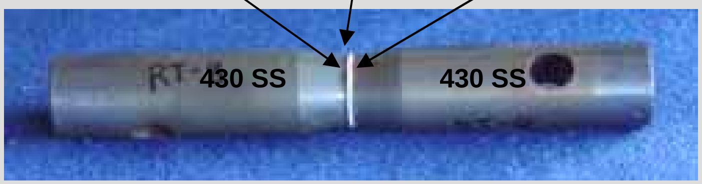
Test Temperature (C) (aging time)	Flexural Modulus (GPa)	Mean Strength (MPa)	Std Dev Strength (MPa)	Maximum Strain
25 (4 hr)	89	80	10	0.30-0.60%
600 (4 hr)	26	83	15	0.30-0.60%
700 (4 hr)	30	64	10	0.30-0.60%
800 (4 hr)	12	39	4	0.30-0.60%
				0.30-0.60%
25 (1000 hr)	64	43	3	0.30-0.60%
600 1000 hr)	56	42	6	0.30-0.60%
700 (1000 hr)	33	35	2	0.30-0.60%
800 (1000 hr)	20	31	2	0.30-0.60%

Test Temperature (C)	Condition (aging time @ 750 C)	Elastic Modulus (GPa)	Shear Modulus (GPa)	Flexural Modulus (GPa)	Poisson Ratio	Number of tests
25	4 hr.	80.5	31	89	0.3	4
25	1000 hr.	80.2	30.6	64	0.31	5
600	4 hr.			26		6
700	4 hr.			30		6
800	4 hr.			12		6
600	1000 hr.			56		6
700	1000 hr.			33		6
800	1000 hr.			20		6

Data From Seal Assembly Analogs

0.020” Crofer 22 washer (Ni brazed to 430) on both sides

Dispensed Glass



Tension

Torsion

Testing Method	Test Temperature (C)	Mean Failure Stress (MPa)	Number of Samples
Tension	25	22.8	2
	700	23.2	2
	750	16.5	6
	800	5.3	3
Torsion	25	46.7	6
	700	50.9	6
	750	22.8	6
	800	11	6

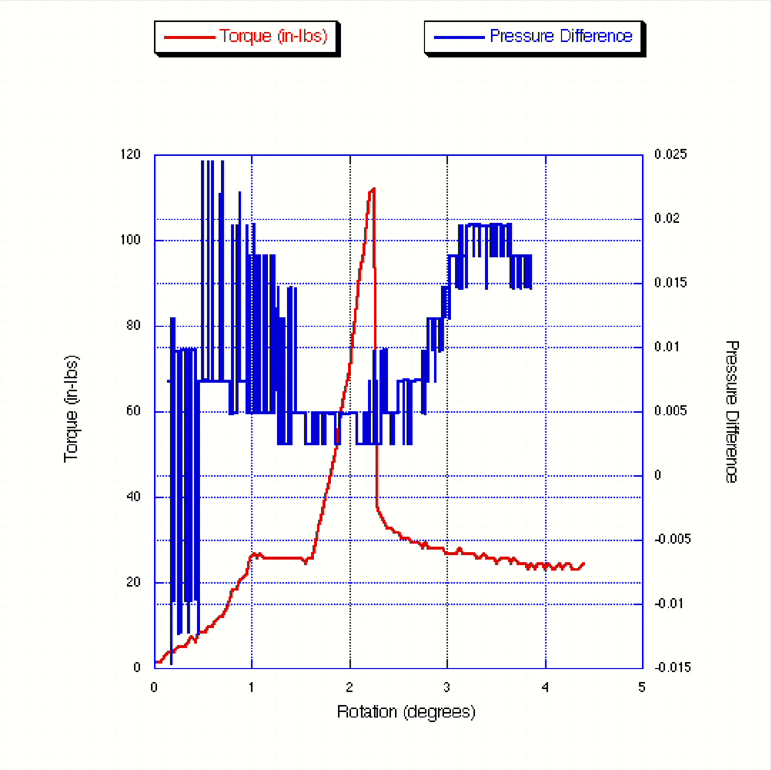
Thin-film analogs to test the entire seal assembly

Failure is generally interfacial rather than in the glass itself

Mica Seal Testing

8 mil thick phlogopite mica sheets with binder; cut to fit the torsion holders. 100 psi compressive force and 0.2 psig He pressure utilized during torsion testing

Initial Results on Mica Seals



Torsion-Leak test of Mica seals revealed that as the mica slides it may show slip-stick behavior and during the “stick” phase there might be some leakage. Preliminary tests show only small leaks.