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SOFC Development at PNNL: Overview

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Pacific Northwest National Laboratory, Richland, WA

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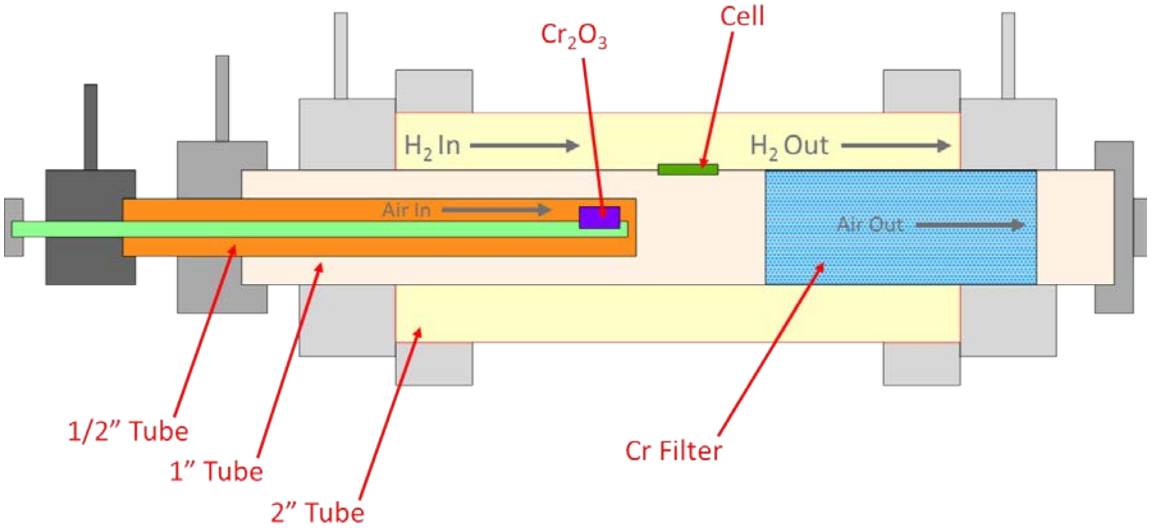
Scope of Work

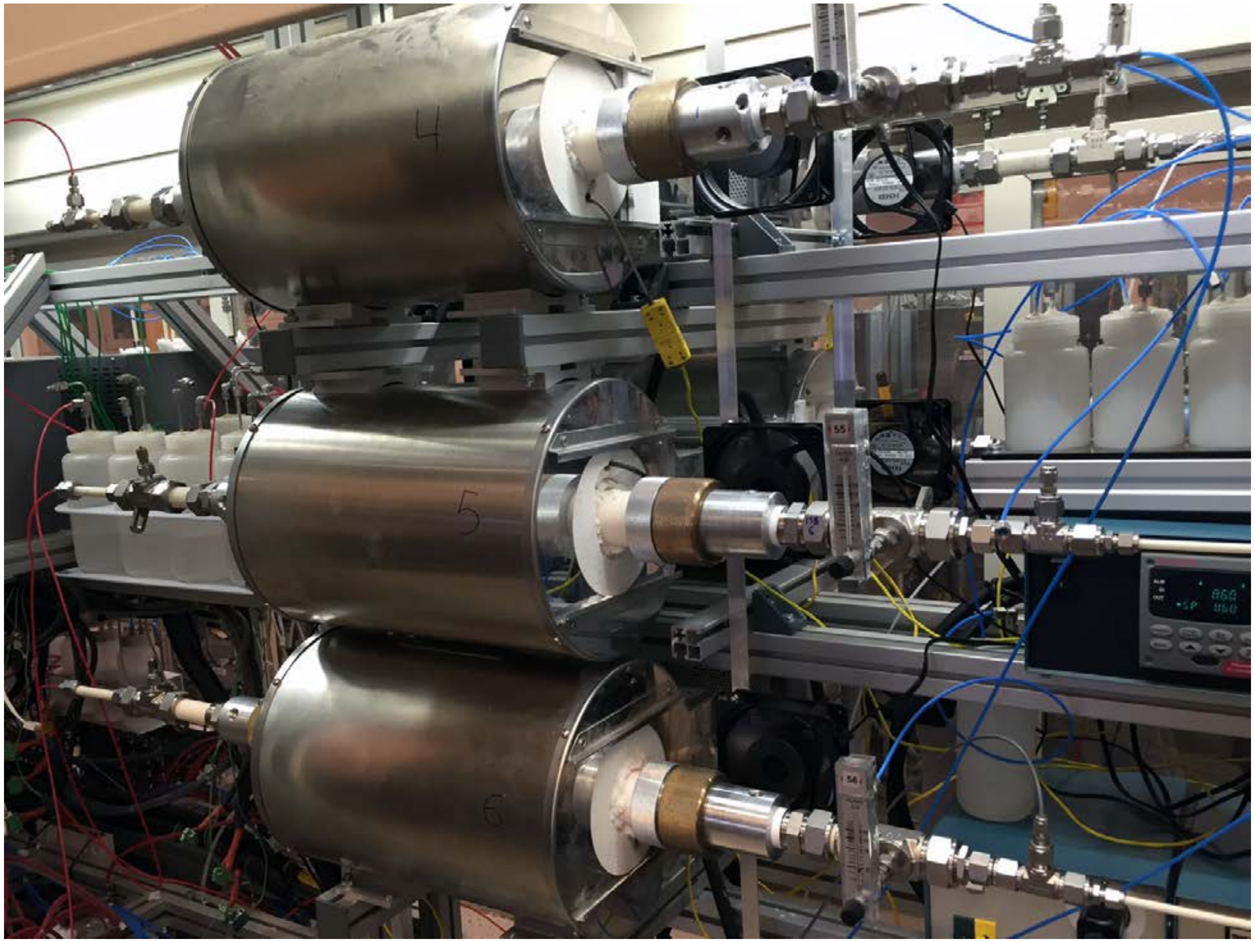
- Materials Development
  - Cathode materials and interactions
    - Effects of volatile Cr compounds on cathode performance
      - **Poster: Button Cell Tests with LSM/YSZ Cathodes in Air with Quantified Cr Concentrations (John Hardy)**
    - Improved density of ceria barrier layers
  - Mitigation of Cr poisoning
    - Evaluation of Cr capture materials
      - **Poster: Mitigation of Cr-Poisoning of Solid Oxide Fuel Cells (Matt Chou)**
  - Cathode contact materials
    - Enhancing reliability of cathode/contact materials interfaces
      - **Poster: Cathode Contact Development at Pacific Northwest National Laboratory (Matt Chou)**
  - Interconnects/BOP
    - Reactive air aluminization: Reduction of fabrication temperature
      - **Poster: The Effect of Kinetics and Element Additions on Lower Temperature RAA Process (Jung Choi)**
- Modeling/Simulation
  - SOFC Stack Modeling Tools
    - Reduced Order Models (ROM) for improved system modeling
      - **Poster: Improved Capability and Accuracy of a Reduced Order Model (ROM) for SOFC Stacks (Chao Wang)**
  - Modeling of Stack Degradation and Reliability
    - Reliability of cell and stack structures
    - Integration of lower-scale degradation data
      - **Poster: Electrode Coarsening and Temperature Distribution Effects on Long-Term Electrochemical Degradation of SOFC Stack (Brian Koeppel)**

Cathode Materials and Interactions: Effects of Volatile Cr Compounds

- Objective
  - Quantitatively assess effects of Cr on cell performance as function of cathode composition, Cr concentration, temperature, and time
- Approach
  - Anode-supported button cells with LSM/YSZ or LSCF cathodes
  - Correlate Cr dosing with cell performance (power density and stability) and cathode microstructure and chemistry.
  - Constant current testing with I-V and EIS sweeps
  - Post-test characterization: SEM/EDS/EBSD/XRD/TEM/APT

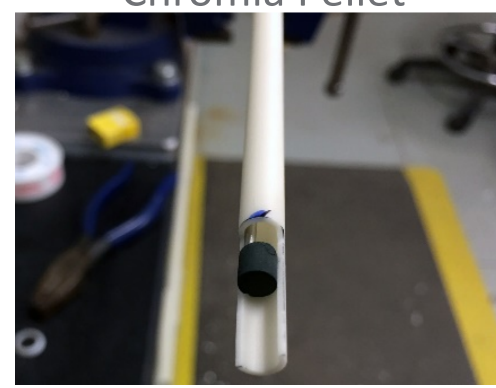


Assembled Cr Test Fixtures



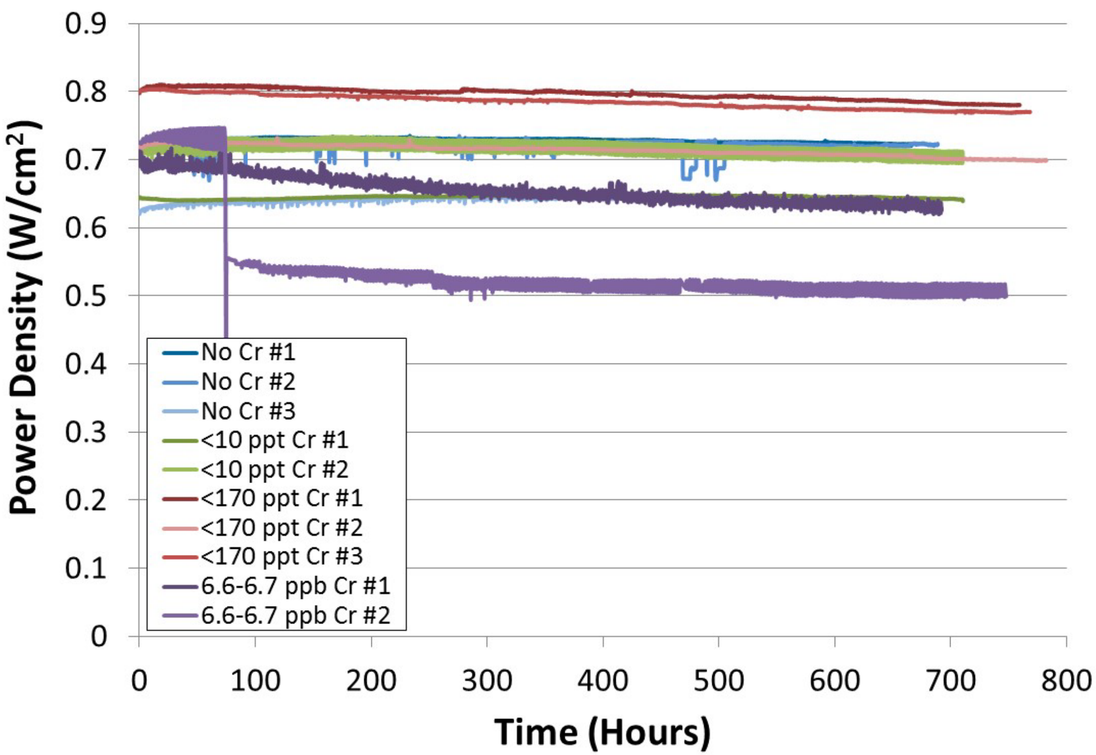
Downstream Filter

Chromia Pellet



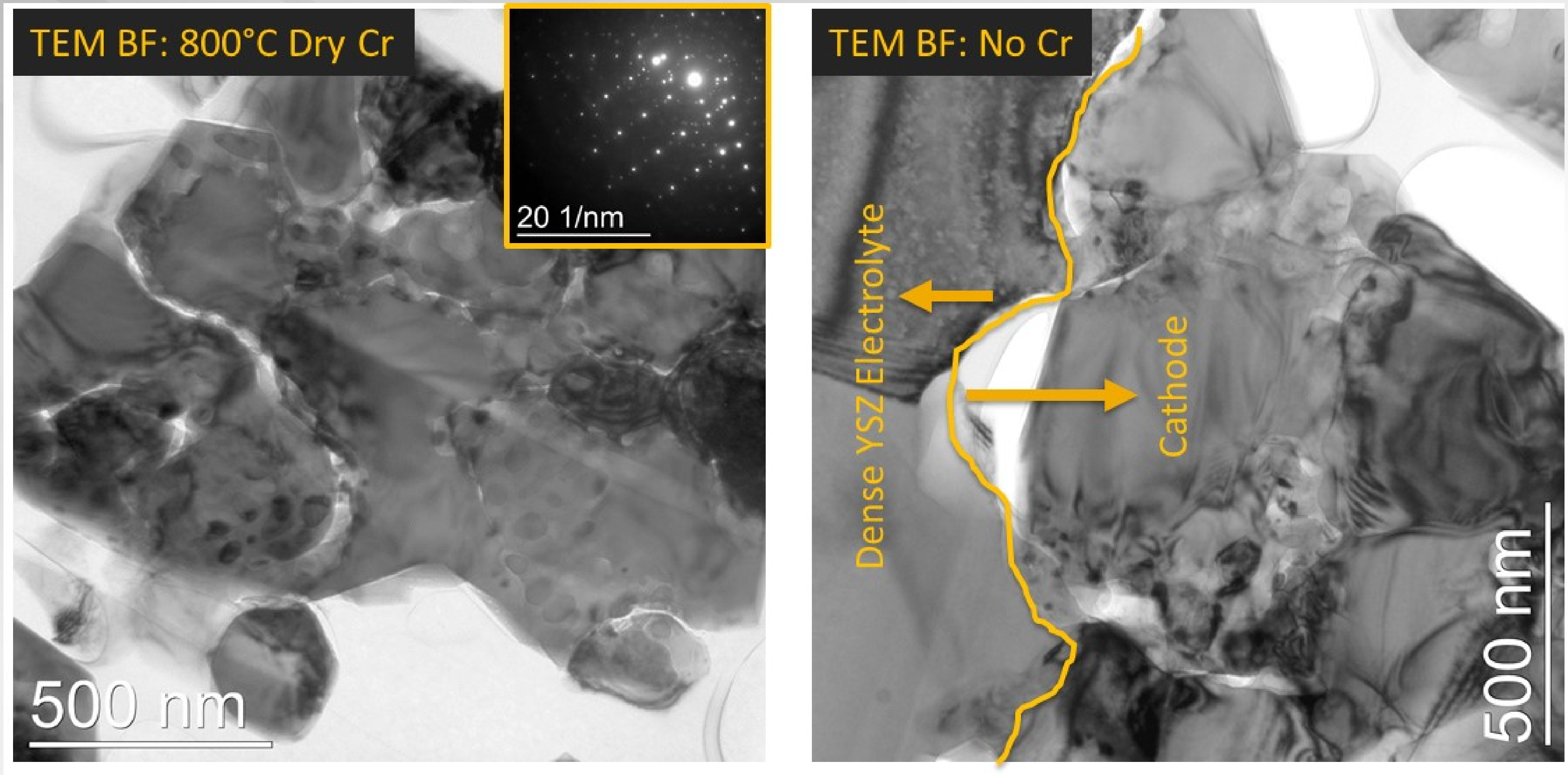
Electrochemical Button Cell Tests

- LSM/YSZ Cathodes
  - LSM-20, A/B = 0.95
- Tested at 850°C
  - Cr concentration controlled by adjusting Cr_2O_3 temperature and moisture content of air



Degradation Rates (per kh)			
Test Condition	0 h - 300 h	300 h - End	0 h - End
No Cr #1	-1.6%	3.0%	1.6%
No Cr #2	-1.5%	1.5%	0.2%
No Cr #3	-9.8%	3.3%	-2.4%
≤10 ppt Cr #1	-1.9%	2.9%	1.5%
≤10 ppt Cr #2	-1.5%	4.9%	3.0%
≤170 ppt Cr #1	0.8%	4.2%	3.2%
≤170 ppt Cr #2	0.8%	5.0%	3.7%
≤170 ppt Cr #3	6.0%	4.4%	4.8%
6.6-6.7 ppb Cr #1	20.7%	9.3%	12.3%
6.6-6.7 ppb Cr #2	29.1%	4.4%	14.0%

TEM Images: 800ºC Dry Cr vs No Cr



TEM suggests more attack at the interfaces between grains and potentially small precipitates have formed during Cr exposure. Precipitates may be thin platelets on the surface of the particles.

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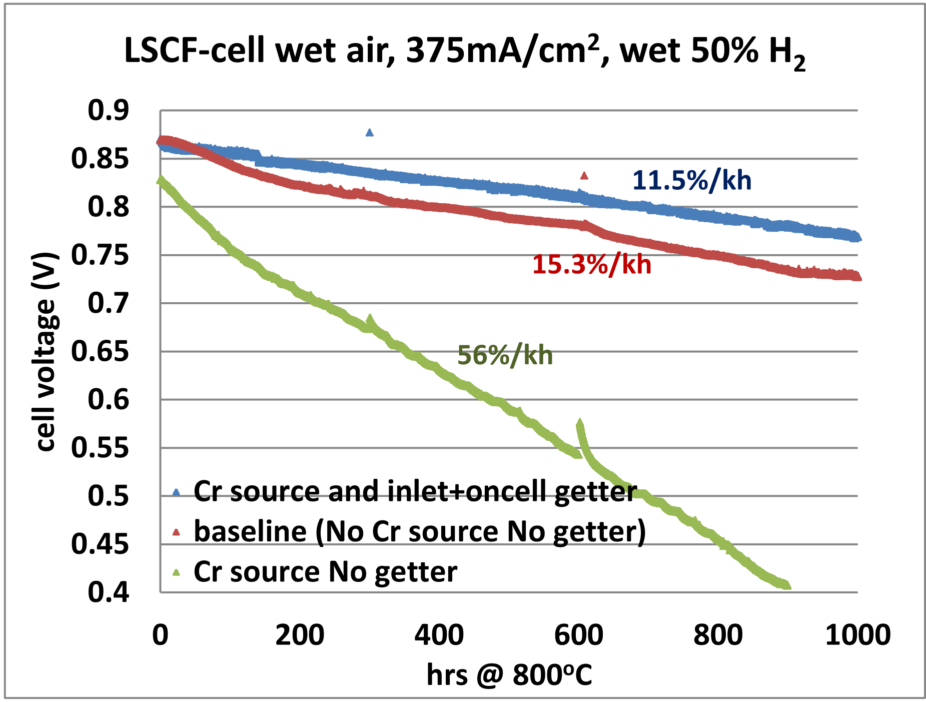
Mitigation of Cr Poisoning

- Objective
  - To validate/optimize a new Cr-capture material developed at U. Conn. by P. Singh's group
- Approach
  - Evaluate Cr-capture material under stack-like conditions in PNNL's stack test fixture
  - Optimize a solid state reaction process for preparation of the candidate Sr-Ni-oxide Cr-capture material
  - Evaluate Cr-getter structural options (e.g., porous monolithic structure, impregnated porous substrate)

Summary of validation tests with LSCF-based Cells

- The candidate Cr-capture material was validated with LSCF-based cells at 800°C for 1000h
  - Nominal composition: $Sr_9Ni_7O_{21}$
- With upstream Cr source and no Cr-capture material in cathode air stream, cell performance degraded drastically (~56%/kh) as compared to baseline cell (~15%/kh).
- The Cr-capturing behavior of Sr-Ni-oxide was verified in two cell tests
  - Cell degradation rates were similar to (actually slightly better -12.1%/kh and 11.5%/kh) than baseline (Cr-free) degradation (~15%/kh).
- EDS analysis detected no Cr within the cathode at the cathode/barrier layer interface.

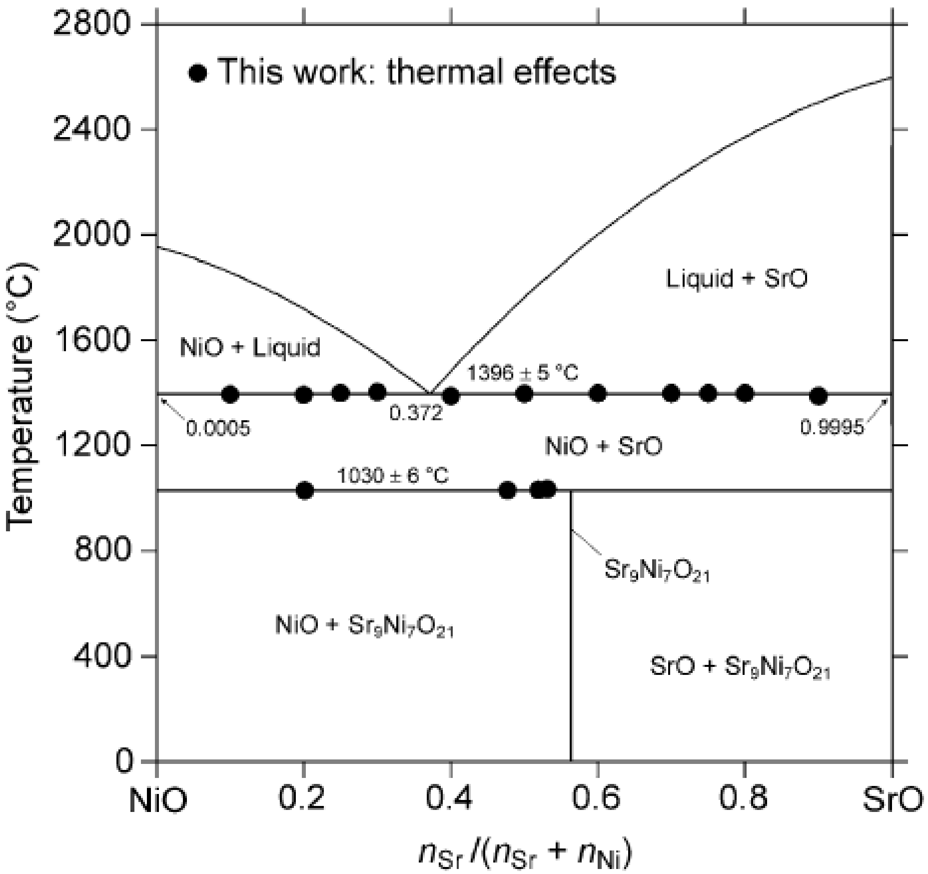


FY17 Activities

- Synthesis of Cr-gettering material via solid-state reaction
- Evaluation of alternative getter structures
- Validation of Cr-gettering materials in generic stack test fixture (LSM-based cells)
  - Electrochemical performance
  - Microstructure and chemical characterization of tested cells and Cr-gettering materials

Sr-Ni-O Phase Diagram

M. Zinkevich, J. Solid State Chemistry 178 (2005) 2818-2824



- Eutectic at ~1396 °C
- One ternary compound, $Sr_9Ni_7O_{21}$, below ~1030 °C
- $Sr_9Ni_7O_{21}$ decomposes to SrO and NiO above ~1030 °C

Cr-capture Material: Synthesis via Solid-State Reaction

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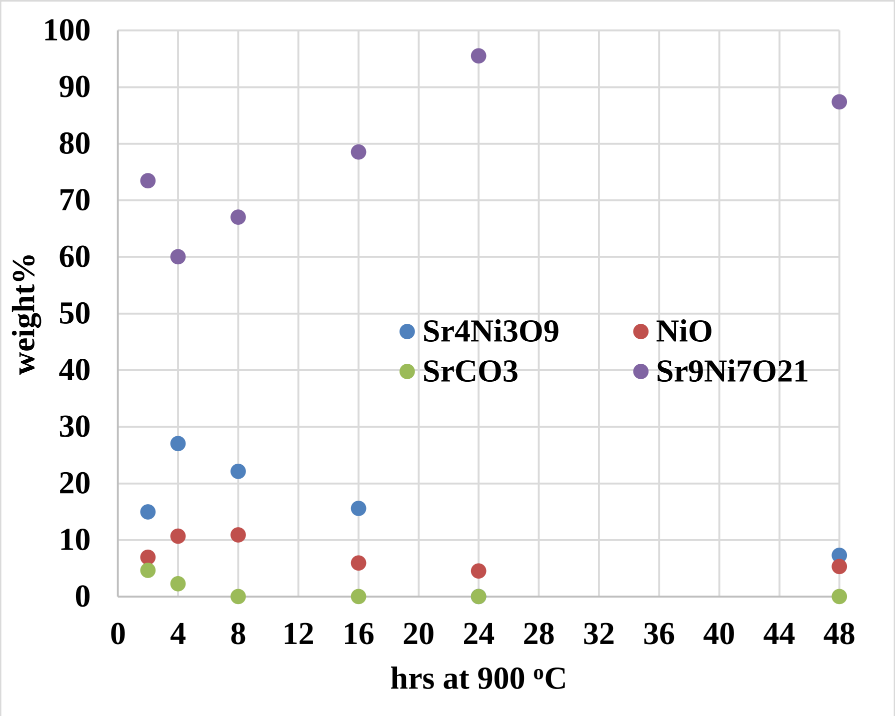
- Approach
  - Attrition milling 6 hrs of mixed oxides: SrO:NiO=9:7 (mole ratio)
  - Calcination at 600, 700, 800, 900, and 1000ºC for 2- 48 hrs
  - Grinding and sieving for XRD analysis with ZnO as internal standard for quantification
- Optimum condition to form $Sr_9Ni_7O_{21}$:
  - 900ºC for 24h: 95.5 wt% of desired phase (balance NiO)



Impregnation of Porous Substrate

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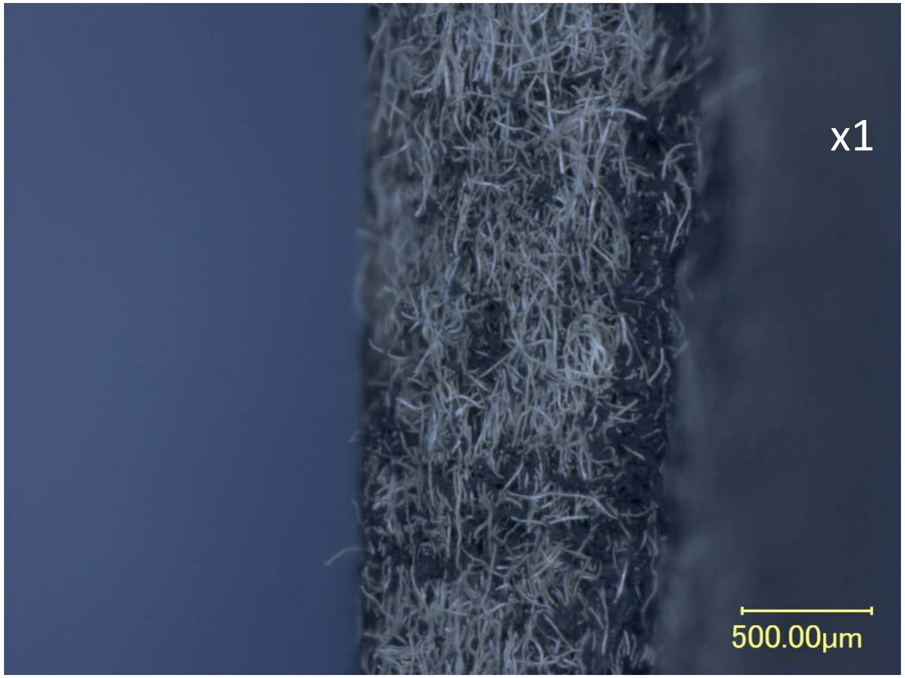
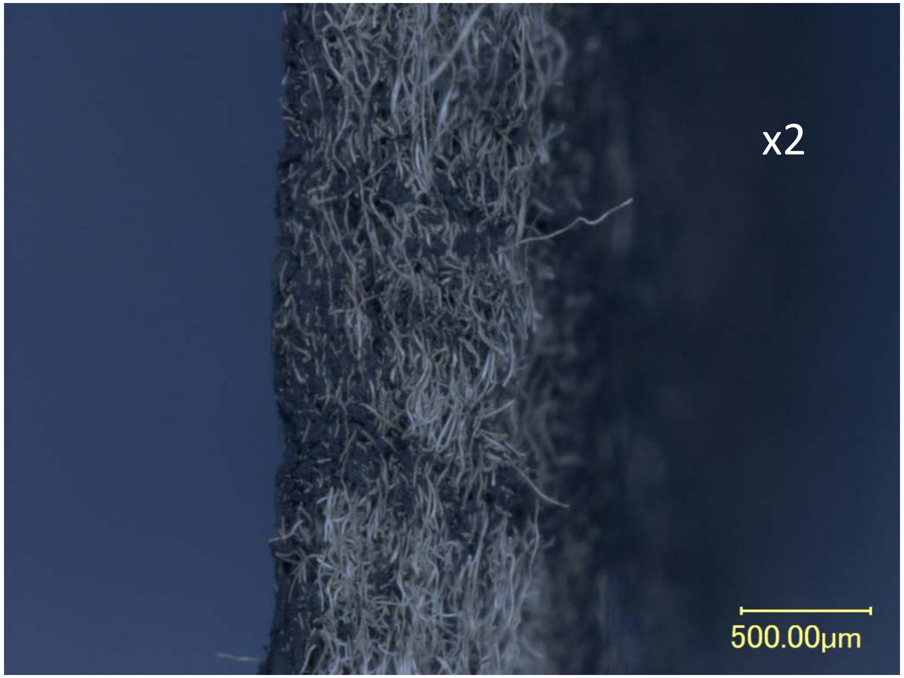
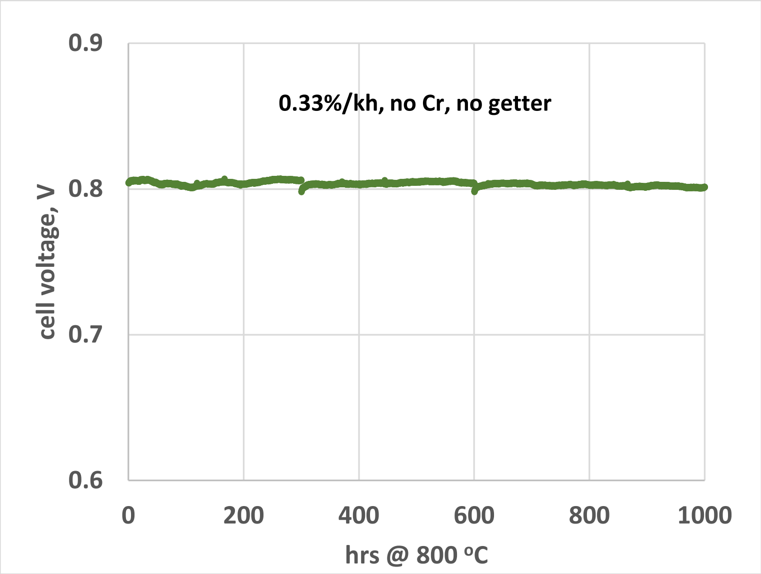
1. Impregnation via dip coating (1x or 2x); Attrition-milled Sr-Ni-O slurry
2. Sintered at 950 ºC 4h in air after drying
3. ZYF-50 zirconia felt (about 0.05” thick, bulk porosity 96%)

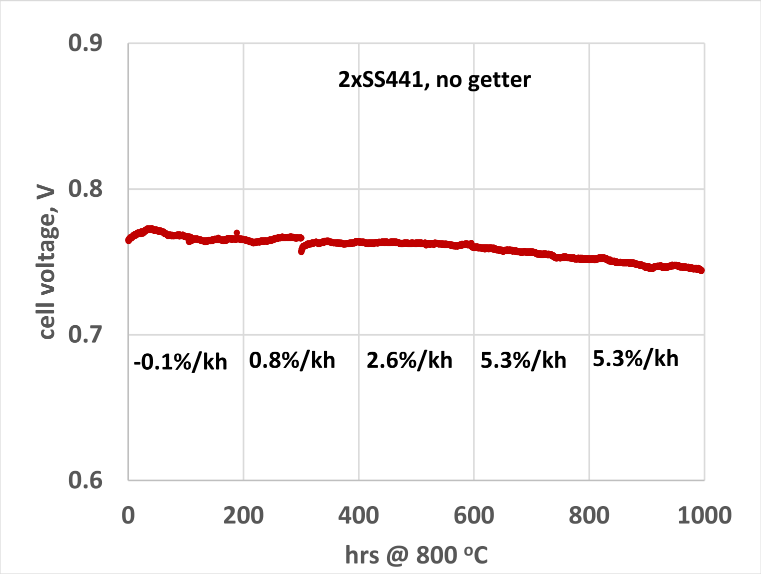




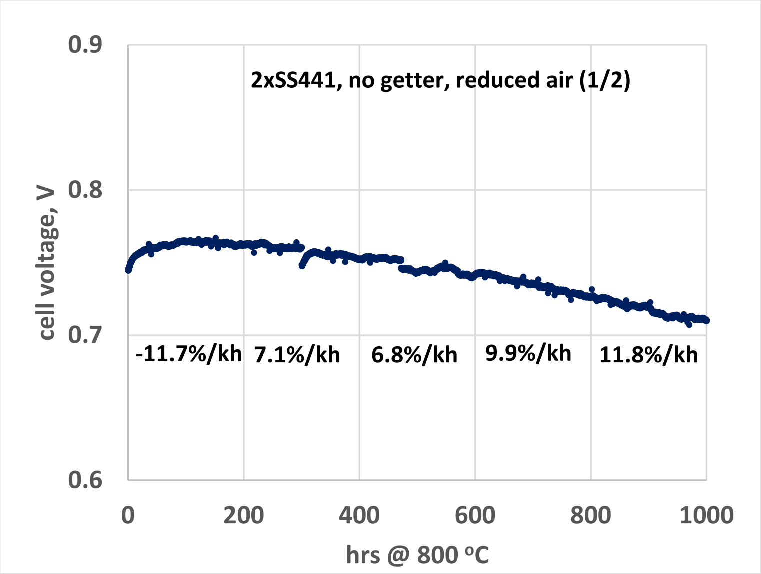
gm of Sr-Ni-oxide	dip coat x1	dip coat x2
per gm of coated ZYF-50	0.64	0.75
per cm^3 of coated ZYF-50	0.42	0.71

Evaluation of LSM-based Cells: Baseline with and without Cr source





1. **Cr-free baseline showed low degradation of 0.33%/kh.**
2. Presence of upstream Cr source (pre-oxidized SS441) resulted in higher degradation
3. Air flow rate affected degradation rate
4. Next step: Tests including Cr-capture material



Reactive Air Aluminization (RAA)

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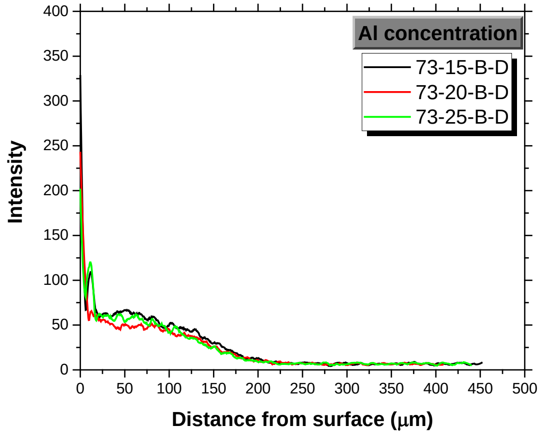
•Reaction between alkaline earths in glass seals and Cr in interconnect steel can form high CTE chromate phases (e.g., $SrCrO_4$), which degrade interfacial strength

•Cr volatility from alloys can poison cathodes

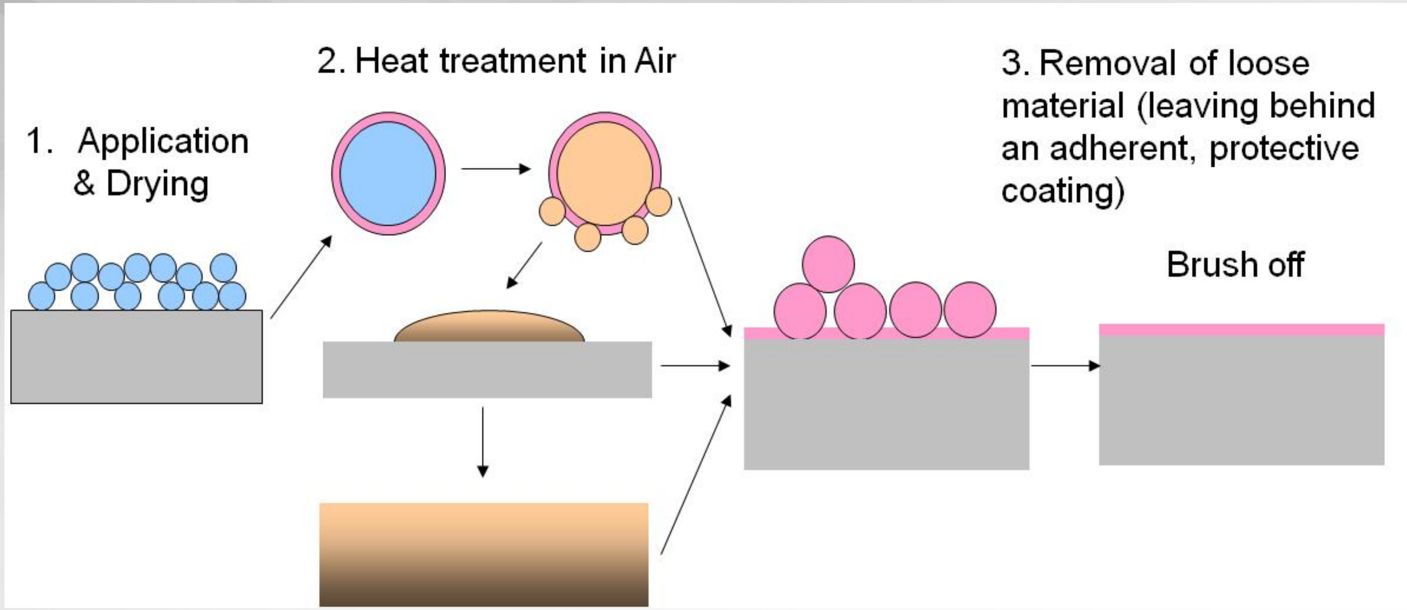
•Reactive Air Aluminization (RAA) offers a simple alternative to controlled atmosphere aluminization of interconnects (and BOP components)



- Simple process (aluminum powder slurry, single heat treatment in air)
- PNNL has developed screen-printing, aerosol spray, and dip-coating fabrication processes

- <u>Current emphasis:</u> Reduction of heat treatment temperature to <1000ºC

Reactive Air Aluminizing



- Aluminum powder slurry-based process
  - Spray, screen-print, dip-coat
- Heat treatment in air
  - 3ºC/min to 1000ºC
  - 1 hour dwell at 1000ºC
  - 3ºC/min cool-down

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Low temperature RAA process: Challenges

- Standard RAA process conditions (3°C/min to 1000°C, 1 hour dwell)
  - Average Al powder size: 3-4 μm
  - Very fine powders (0.1 μm): rapid oxidation and minimal Al diffusion into substrate leads to formation of weakly bonded alumina layer
  - Coarse powders (>10 μm): too much aluminum diffusion into substrate leads to cracking of alumina layer (CTE mismatch) and very irregular coating morphology (pros and cons)

- Primary challenges to lowering process temperature using our standard Al powder slurry are incomplete/nonhomogenous alumina layer formation and excessive reaction/diffusion of Al into substrate

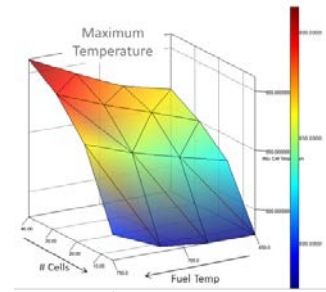
- Approach: Modify slurry to optimize oxidation kinetics and metal diffusion at lower temperatures to form protective alpha alumina coating and “right-sized” Al reservoir in substrate to provide appropriate CTE gradient (to improve coating bond-strength) and self-healing capability.

Future Work

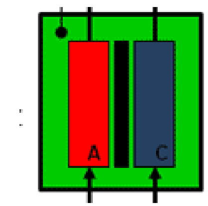
- Cr poisoning
  - Determine Cr concentration threshold below which cell performance and stability is not significantly affected for LSM/YSZ cathodes
  - Electrochemical tests at 800ºC on LSCF cathodes exposed to Cr
- Cr mitigation
  - Continued collaboration with Prof. Singh at U. Conn.
  - Development/evaluation of Cr-getter structural options
  - Complete stack fixture tests on LSM-based cells
- Reactive air aluminization
  - Durability testing of standard and reduced temperature RAA process

Modeling Background

- Need design/engineering at several scales to facilitate wide scale SOFC commercialization
- Program goal to *link models at different scales* to inform SOFC power generation system analyses
- Successfully used a *Reduced Order Model* (ROM) to increase the capability and accuracy of system models with an improved stack representation
  - Used SOFC-MP stack model results to simulate stack in an Aspen Plus model for NGFC system



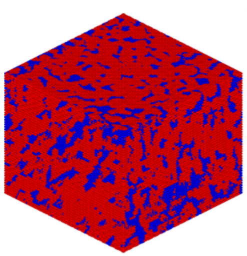
Response Surface Analysis

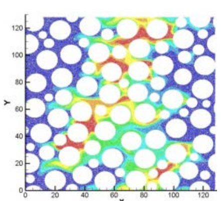


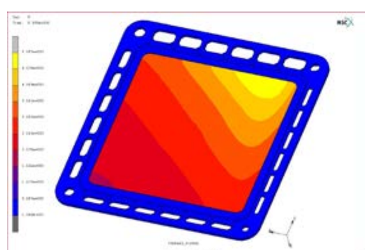
Reduced Order Model (ROM)

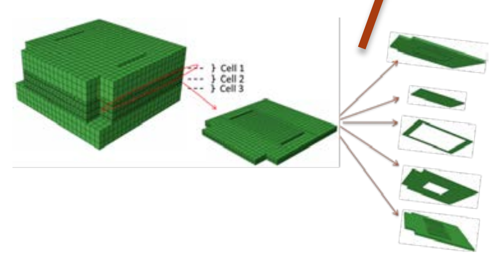
Stack Details

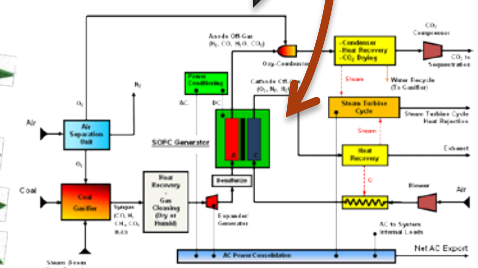
Increasing Scale











Electrode Microstructure | Single Cell | Multi-Cell Stack | IGFC Power System

NETL | *PNNL* | *NETL*

Overview: SOFC Stack ROM

- **Technical Challenge**: Use modeling results at different scales to inform design and cost studies performed with *system-scale models*

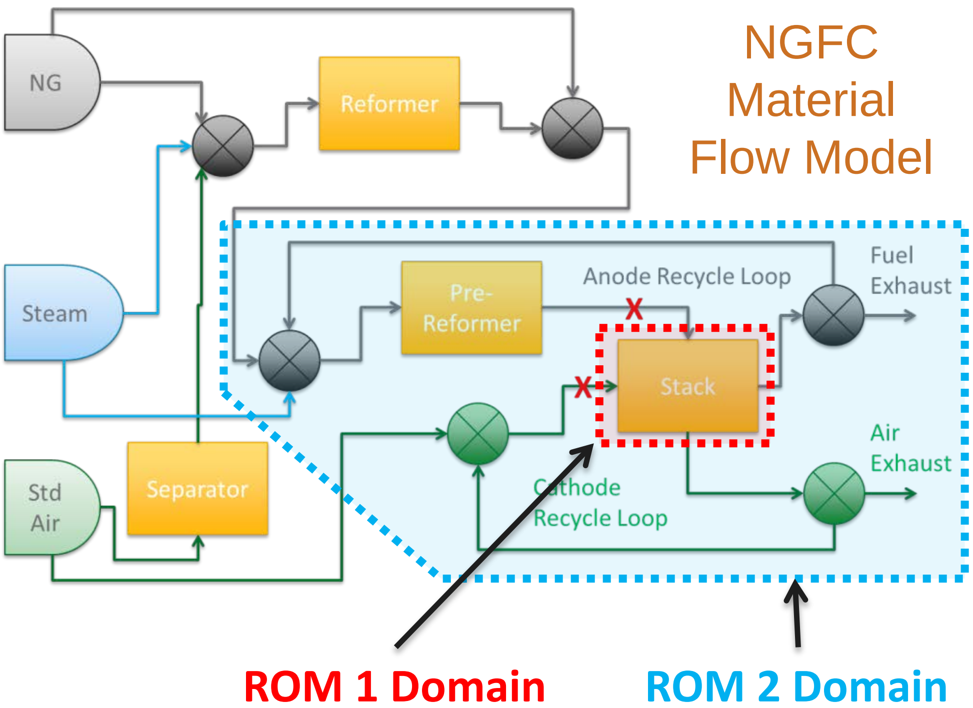
- **Objective**: To *improve the accuracy and capability* of NETL's Aspen Plus systems analyses using PNNL's stack model

- **Technical Approach**:
  1. Integrate detailed SOFC-MP stack model results into NETL's system models as an advanced *reduced-order model (ROM)*
     - Include recirculation and exhaust heat recovery directly in the ROM
     - Implement advanced ROM in the system model for NGFC (and IGFC)
     - Collaborate with NETL on design and performance studies
  2. Characterize the *accuracy* of the generated stack ROM and *reduce the error level* to acceptable ranges
     - Identify approach to best characterize and mitigate the approximation error
     - Develop procedure to identify and minimize regions with highest error
     - Evaluate Design of Experiment (DOE) methods to pre-identify sensitivity of the input parameters

Advanced ROM Features

- Collaborated with *NETL on advanced ROM includes the fuel and oxidant *recirculation loops*
- Implemented and tested the necessary SOFC-MP stack tool features identified in the initial ROM demonstration
  - Added fuel and oxidant recirculation loops to the stack model to account for *recycling* in the ROM directly
  - Added fuel and oxidant recuperators in the stack model to recover exhaust heat and determine the required *heat exchanger (HEX) effectiveness* values to achieve desired stack inlet temperatures
  - Included an in-loop pre-reformer to *eliminate the higher hydrocarbons* in the natural gas (NG) fuel source
  - Added capability for *pressurized* (non-atmospheric) stack I-V performance to support IGFC evaluations

NGFC Material Flow Model



- Updated the ROM software tool to accommodate the additional capabilities
- Generated an *advanced ROM* for a counter-flow stack in the atmospheric NGFC system

*Arun Iyengar

Advanced ROM Results

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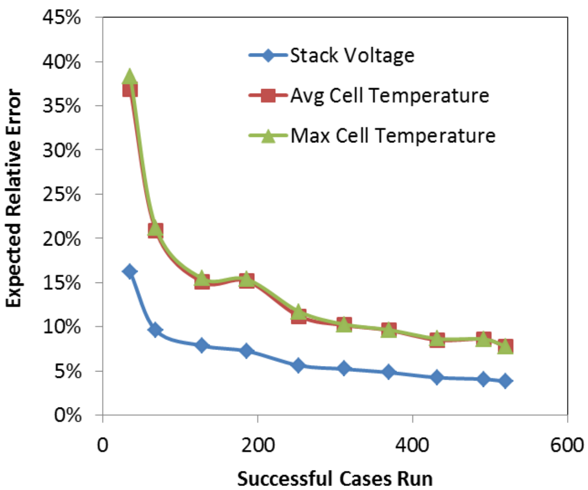
- Used wide range of potential operating conditions
- Obtained 520 successful cases
  - ~65% of random cases converged to viable solutions
- *Predicted Kriging mean error is moderate*
  - <4% for voltage, <8% for cell temperature over the entire design domain
- Actual error for test cases is very good
  - <1% for voltage and cell temperature
- Exported ROM provided to NETL for evaluation

Error Reduction with Number of Sampled Cases

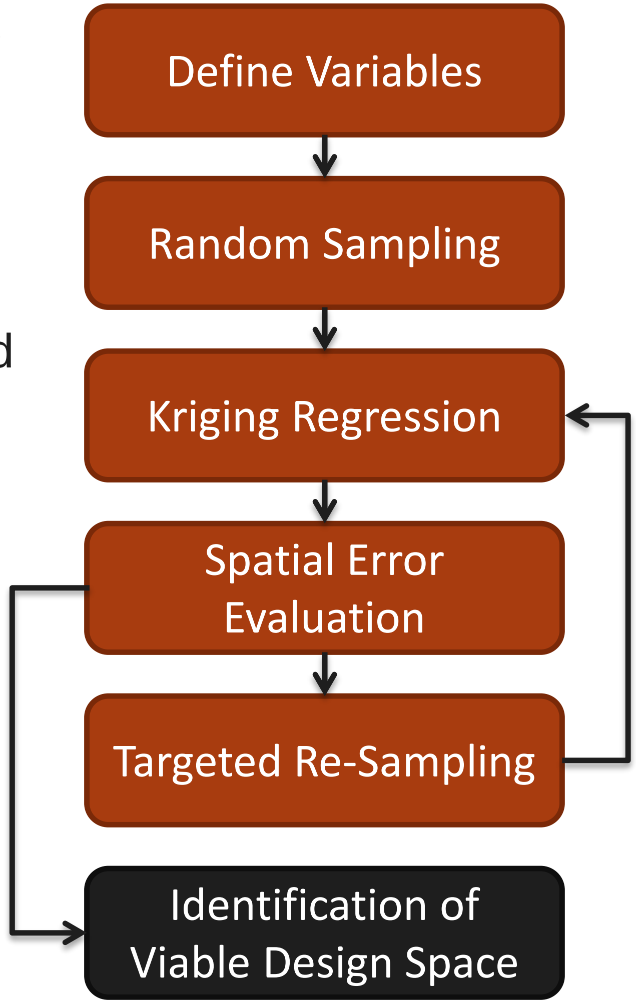


Input Ranges			Test Cases 1	Test Cases 2
Average Current Density	2000-6000	A/m^2	4000	4000
Internal Reforming	0-100%		90%	80%
Oxidant Recirculation	0-80%		27.7%	29.0%
Oxygen-to-Carbon Ratio Target @ Stack Inlet	1.5-3.0		2.6	2.1
Fuel Utilization (w/ recirculation loop)	40-95%		60%	60%
Oxidant Utilization (w/ recirculation loop)	12.5-83.3%		50%	50%
Oxidant Stack Inlet Temperature	550-800	°C	90	90
Fuel Loop Inlet Temperature	15-600	°C	709.4	718.7

Approximation Error	1	2
Current	0.1%	0.1%
Voltage	0.9%	0.7%
CD Max	-26.4%	-21.8%
Tcell Avg	-0.2%	0.5%
Tcell Min	-0.3%	0.4%
Tcell Max	-0.2%	0.1%
Tair Out	-0.2%	0.8%
Tfuel Out	-0.2%	0.2%

Framework to Minimize Regression Error

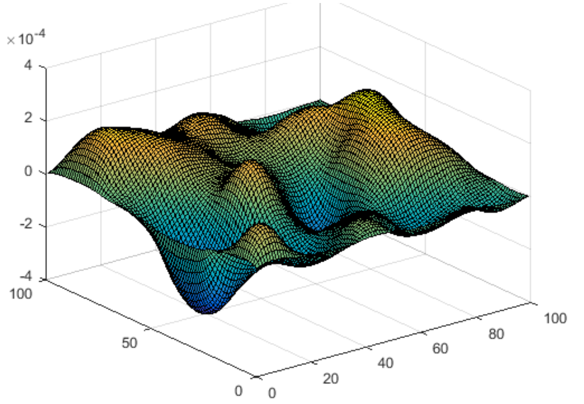
- Error for Kriging regression method is reduced currently through additional random sampling
  - *Clustered samples* not beneficial
  - Mean square error (MSE) of the prediction may even increase due to nonviable regions
  - Improved reduction of the MSE can be achieved through *targeted sampling*
    - Place additional samples in regions of high MSE predicted by Kriging
    - Identify the viable region in the design space and regions where no solution exists
- Implemented *improved sampling procedure*
  1. Initial random sampling
  2. Regression
  3. Error and domain evaluation
  4. Re-sampling



Error Quantification and Reduction

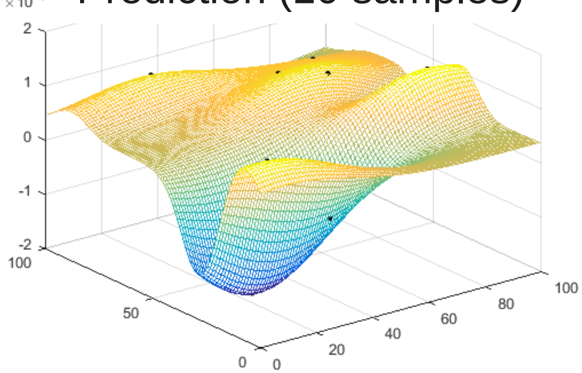
- Test function
  - Poisson equation: $\nabla^2 \varphi(x, y) = f(x, y)$
  - Two independent variables (x, y); one dependent variable (φ)
- Identified regions of highest estimated error and added targeted samples
  - Achieved lower overall MSE with less samples

True Solution of φ

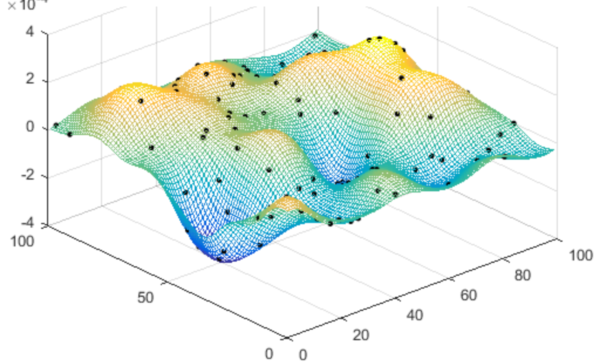


Add 76 targeted samples

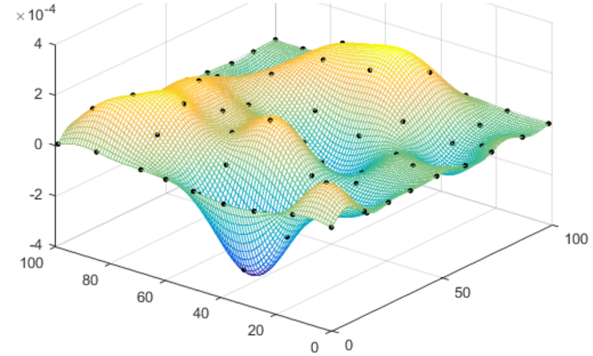
Prediction (10 samples)



Prediction (100 samples)



Prediction (86 samples)

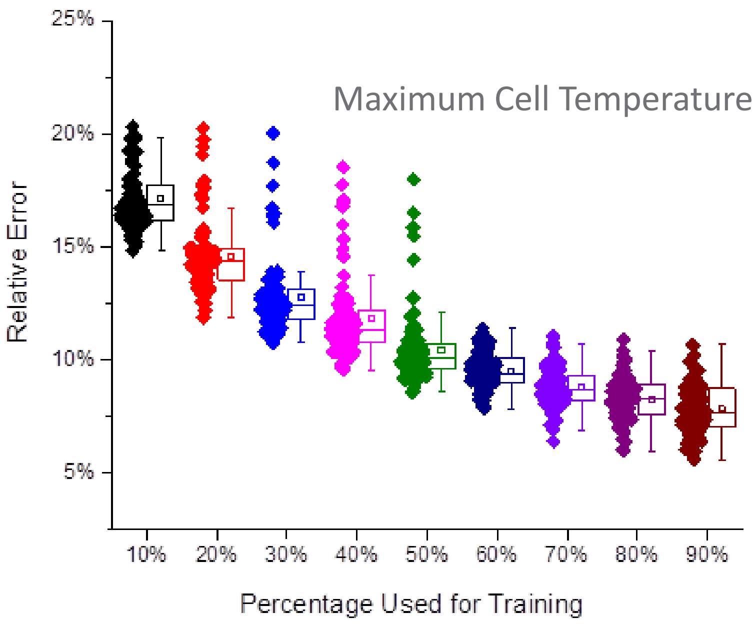


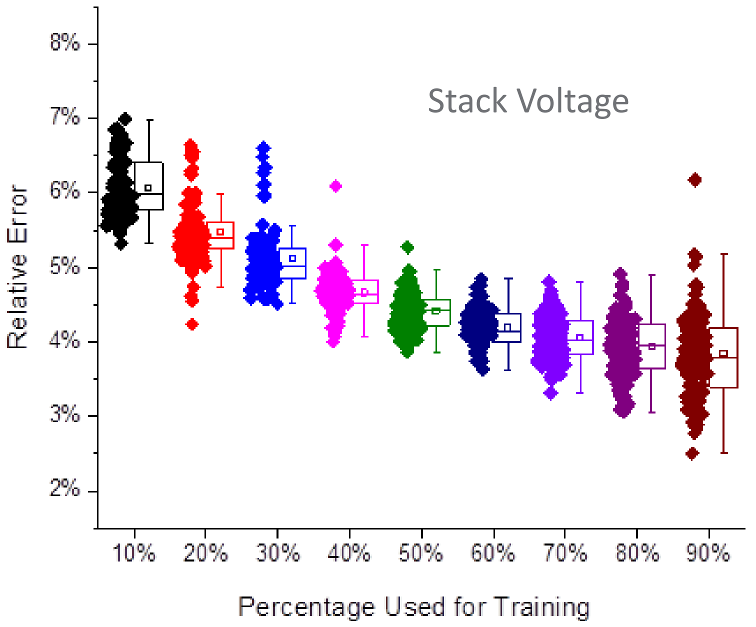
Add 90 random samples

ROM Error Distribution

- Previously, errors were minimized and refined using MSE
- Next, the difference between predicted and actual responses is computed
  - *Divide sampling pool with known actual responses into two partitions, i.e., training and validation set*
  - Training data set is used for Kriging regression to generate response surface
  - Relative error distribution is computed from the validation data set
    - Mean
    - Variance

$$relative\ error = \sqrt{\frac{\sum_1^N (True - predict)^2}{\sum_1^N (True)^2}}$$





Design of Experiments (DOE)

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- Evaluated traditional *Design of Experiment* (DOE) methods for the SOFC ROM procedure
  - Examines the impact (effects) of individual and interactions of independent variables (factors) on dependent variables (responses)
- Performed a full *factorial design* with data generated from SOFC-MP code
  - Three factors and two levels provide 8 cases (2^3)
  - Response is D- Maximum Cell Temperature
- Results of Yates analyses:
  - Main effect: Current Density (96% contribution)
  - Next effect: Oxidant Temperature (4% contribution)
  - Remaining factors and interactions are trivial
- Factorial design and Yates analyses can be implemented in the ROM generation procedure
  - Nonlinearity of response, high dimensionality for the SOFC ROM, and propensity for nonviable solutions makes it less useful than the random sampling approach overall
  - *Rank sensitivity* of input parameters
  - Can be used to *reduce dimensions* if necessary

Factors and Levels

Factor	Factor Levels	
	-1	+1
A- Average Current Density A/m²)	5000	4000
B- Fuel Inlet Temperature (°C)	700	600
C- Oxidant Inlet Temperature (°C)	700	600

Design Matrix

A	B	C	D
5000	700	700	871.5
4000	700	700	836.9
5000	600	700	869.7
4000	600	700	836.7
5000	700	600	876.0
4000	700	600	842.8
5000	600	600	878.8
4000	600	600	844.8

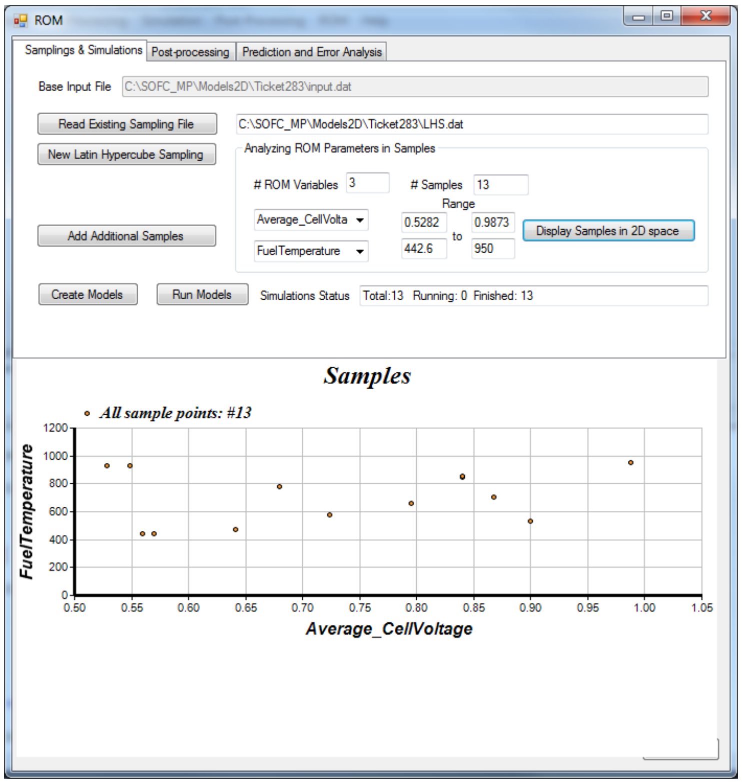
Table of Effects

Factors	Estimate of Effect	Sum of Squares	Percent Contribution
A	-33.73	2275.45	95.71
B	0.70	0.99	0.04
C	6.86	94.33	3.96
AB	0.21	0.09	0.00
AC	0.11	0.02	0.00
BC	1.68	5.66	0.23
ABC	-0.60	0.74	0.031

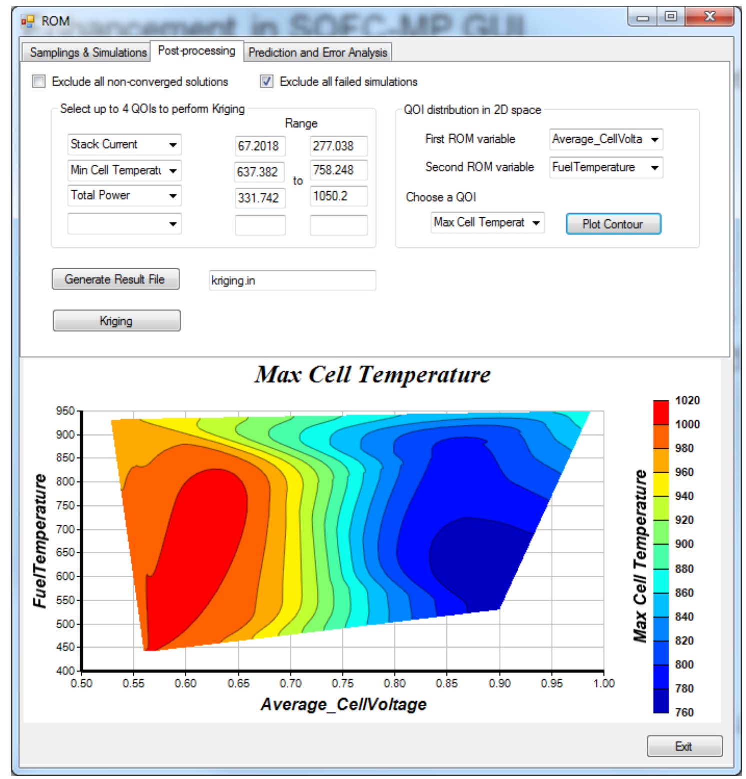
***See Poster**: Improved Capability and Accuracy of a Reduced Order Model (ROM) for SOFC Stacks*

Added ROM User Interface

- ROM being added to the existing SOFC-MP *graphical user interface* (GUI)
  - Latin Hypercube Sampling (LHS)
  - Kriging regression
  - Predictions using the response surface coefficients



- Features to add
  - Error distribution and confidence level
  - Display and analysis of predicted results
  - Augmentation of the sample set based on error analysis
  - ROM export for Aspen Plus



Summary & Next Steps: ROM

- **Summary**
  - Advanced ROM including recirculation loops was generated
  - ROM implementation in Aspen Plus for NGFC system is in progress
  - Method defined for quantifying actual error distribution of ROM using results partitioning
  - Framework defined for reducing Kriging MSE by targeted sampling
  - DOE approach useful for pre-identification of sensitive parameters and dimensionality needed in ROM generation
  - Use of the ROM approach still appears to be a beneficial solution for improving the accuracy of the system models

- **Next Steps**
  - Finalize the ROM framework with ***smart sample augmentation***
  - Develop ***user interface*** to perform ROM generation
  - Incorporate ***DOE approach*** in ROM analyses
  - Extend ROM analyses to ***pressurized system and IGFC*** configuration

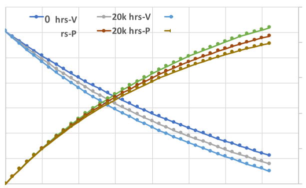
Modeling Background (cont'd)

Electrode Microstructural Changes

$$d_i^4 - d_{i,0}^4 = K_{D,i}\Delta t$$

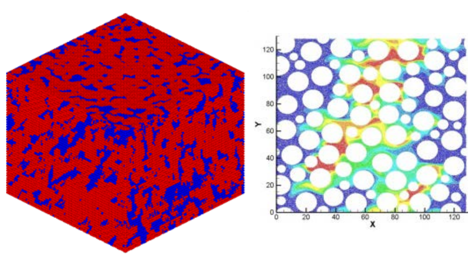
Model Details

Cell Performance

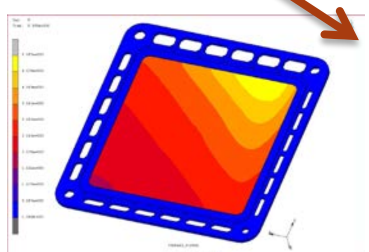


- Need design/engineering at several scales to facilitate wide scale SOFC commercialization
- Program goal to link models at different scales to inform SOFC power generation system analyses
- Implementing NETL electrode performance *degradation* models into PNNL stack models to simulate cell change over long time scales
  - End of Life (EOL) performance

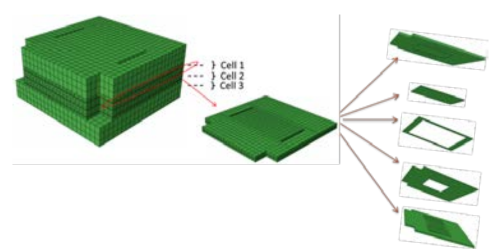
Increasing Scale



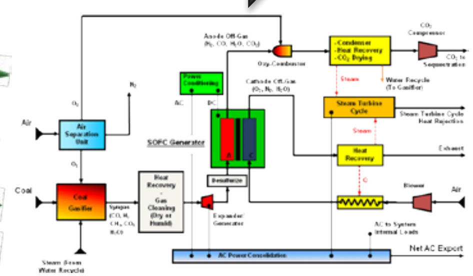
Electrode Microstructure



Single Cell



Multi-Cell Stack



IGFC Power System

NETL

NETL

PNNL

Overview: Degradation and Reliability

- **Technical Challenge**: Use modeling results at different scales to evaluate stack performance and reliability at *end-of-life* (EOL)
- **Objective**: Advance the stack modeling capability to enable identification of cell properties and operating conditions that will provide *optimal initial performance and minimal degradation*
- **Technical Approach**:
  1. Implement *lower-scale degradation models* into SOFC-MP stack model
     - Modify polarization dependencies in current-voltage (I-V) relationship for compatibility with NETL electrode coarsening models and incorporate
     - Implement evolution of multiple model parameters over time/temperature
     - Evaluate effects at the stack level
  2. Evaluate the *mechanical reliability* of stack structures
     - Determine probabilistic material strengths from testing and lower-scale models
     - Utilize 3D FEA stack models with CARES to evaluate mechanical reliability of contact interfaces, electrode structures, and seals at EOL degraded conditions
     - Evaluate effects of design, fabrication, and degradation on multi-cell stacks

Electrochemical Model for Degradation

- Collaborated with *NETL team to use their *electrode coarsening* model
  - *Solid particles* of both ion and electron conductors coarsen according to a power law with the mass transport coefficient based on an Arrhenius relation
  - *Triple phase boundary length decreases* as particles grow
  - *Pore size increases* with particle size
  - *Tortuosities increase* with particle size, and electrode *conductivity decreases* with increasing solid tortuosity

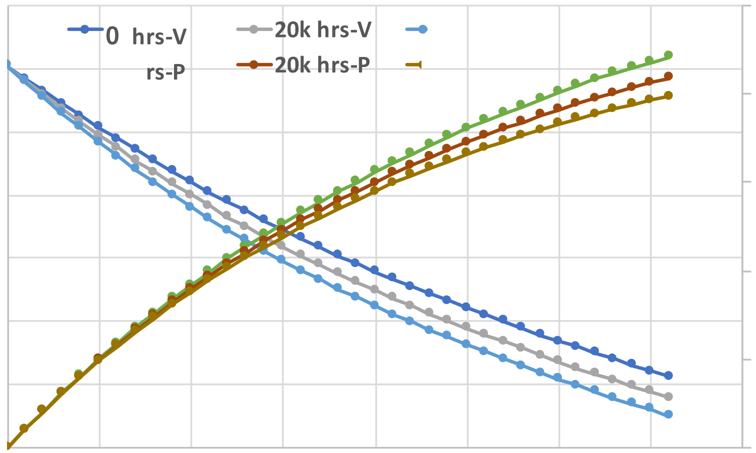
- Updated the *I-V relationship* in the SOFC-MP stack model
  - Concentration polarization: effective gas diffusivity is modified to include the effect of pore size per Knudsen diffusion
  - Activation polarization: triple phase boundary (L_{tpb}) is now used in calculating the limiting current
  - Ohmic loss: Conductivities now based on solid phase tortuosity and volume fraction in electrodes
  - Predicted performance now depends on microstructural parameters in addition to local temperature and species concentrations

***J. Hunter Mason, Harry Abernathy**

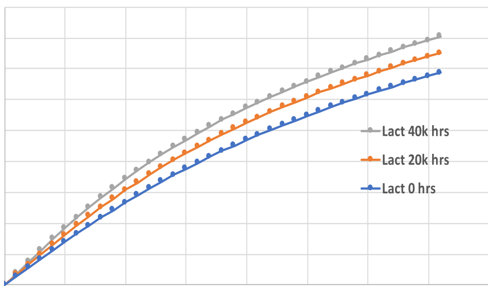
***See Poster**: Electrode Coarsening and Temperature Distribution Effects on Long-Term Electrochemical Degradation of SOFC Stacks*

Electrochemical Model for Degradation (cont'd)

- Voltage and power decrease over time (-11% @ 800°C)
- Majority of power degradation (94%), in this case, is due to *decreasing L_{tpb}* in anode and cathode combined, resulting in increased activation polarization
- Secondary effect is the anode concentration polarization accounting for 5.5%
- Cathode concentration polarization and ohmic losses combined represent 0.5% of the decrease

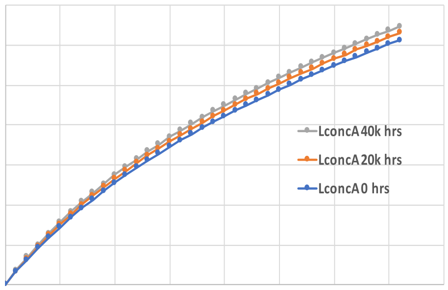


Activation Loss (V) at 800°C, 97%H_2



Current, A/cm^2

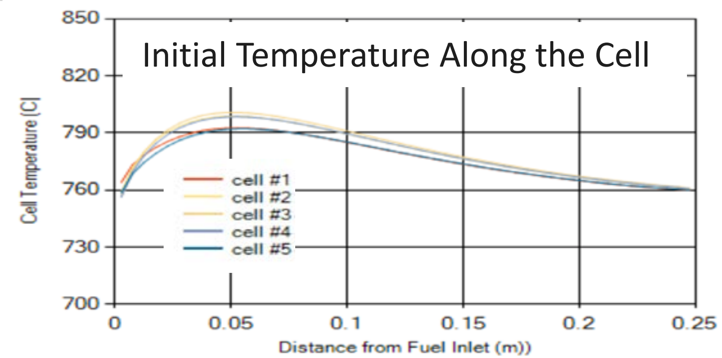
Concentration Loss (V) at 800°C, 97%H_2

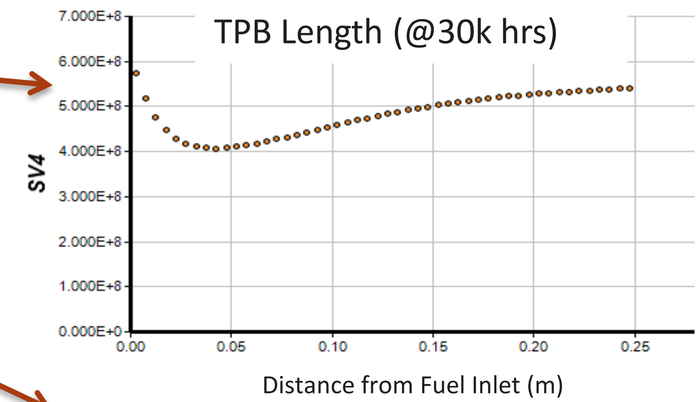


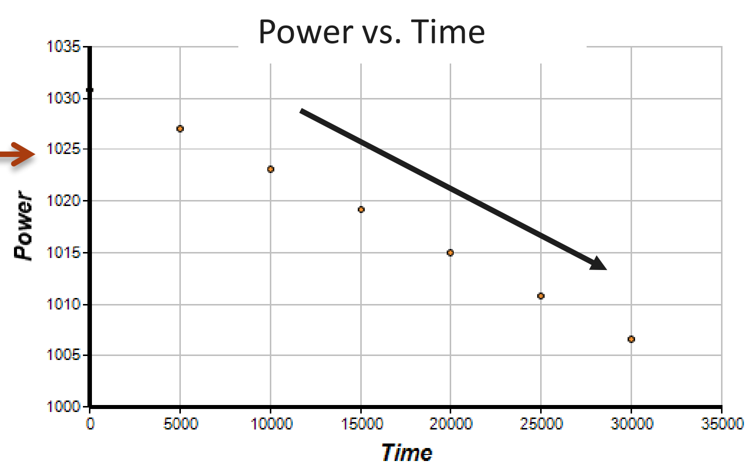
Current, A/cm^2

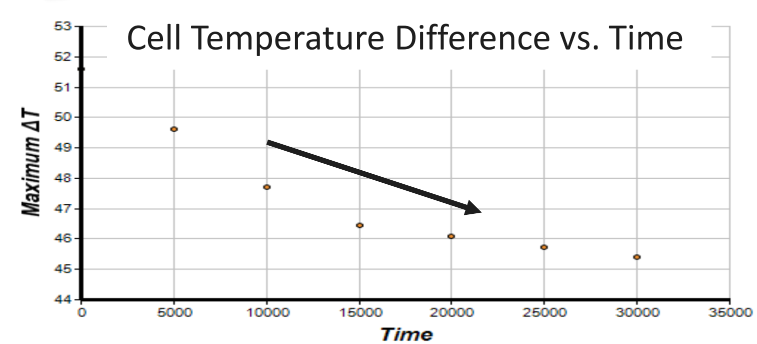
Demonstration of 2D SOFC-MP w/ NETL Degradation Model

- 5 cell counter-flow stack, 25x25 cm^2
  - 750°C enclosure, 700°C wet hydrogen and air
    - Uf = 93.8%, Ua = 43.4%
  - 0.81V cell voltage
  - 6 steps at 5000 hours/step
- Results
  - Total *power decreases* 2.4% over 30k hours
  - High local temperature *decreases L_{TPB}* and reactions resulting in decreased maximum temperature where it was initially highest
  - *Maximum cell temperature and cell temperature difference (ΔT) decrease* over time



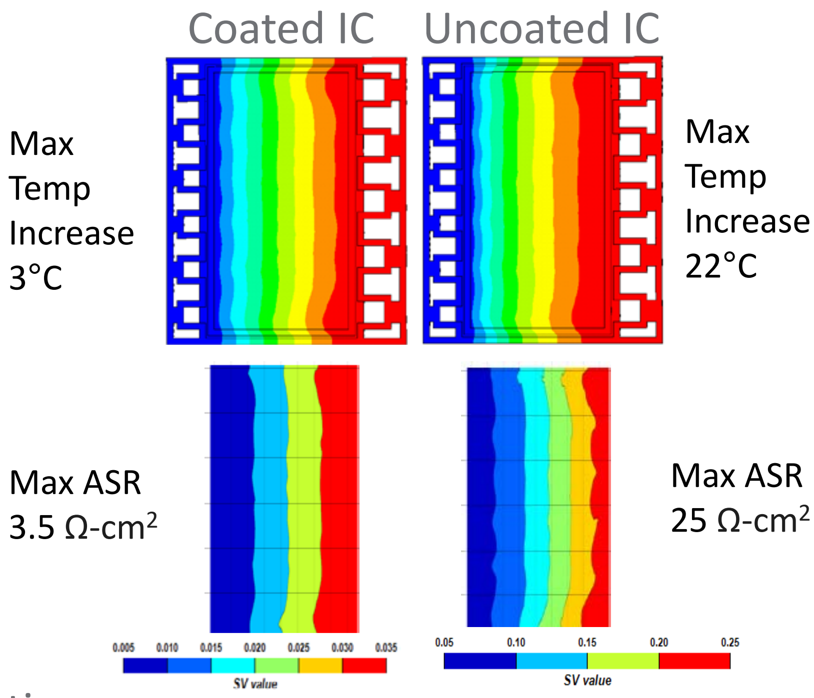




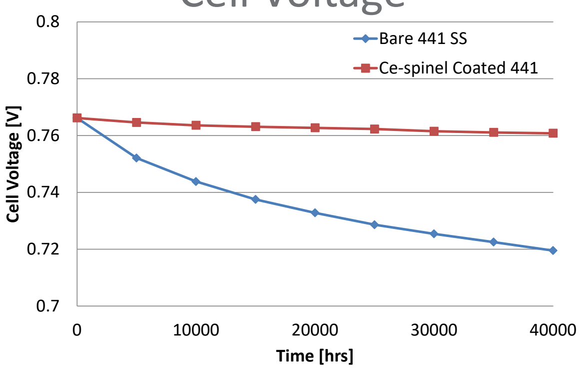


Stack Reliability with Degradation

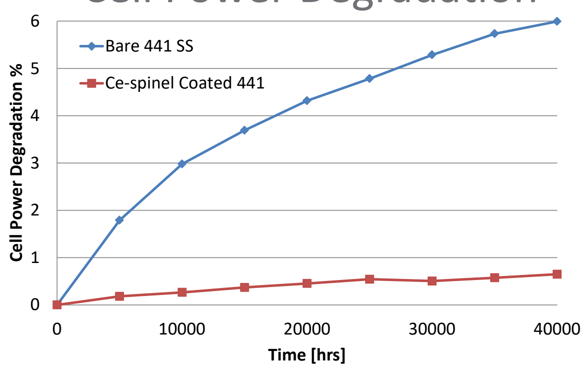
- Reliability was evaluated with *oxide scale growth* on cathode interconnect as an example of long term degradation
  - Scale thickness growth and ASR changes computed in SOFC-MP 3D
  - Bare IC degrades power 6% compared to less than 1% with coated IC for 40k hr
  - Minor changes to the thermal field caused no significant impact on structural reliability for both cases
- Coarsening model implemented and preliminary evaluations in progress



Cell Voltage



Cell Power Degradation



***See Poster**: Electrode Coarsening and Temperature Distribution Effects on Long-Term Electrochemical Degradation of SOFC Stacks*

Lower-Scale Interface Model & Reliability

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- Used the discrete element model (DEM) for rough interfaces to generate *stochastic strength estimates* for the rough LSM20 cathode contact material interface
  - Based on bulk and interfacial material test data
- Evaluated the interfacial stresses during stack operating conditions
- Evaluated the mechanical reliability of the contact material interface with the cathode
  - *Strength enhancement of roughness quantified*
  - Lower-scale modeling method is viable

Predicted Weibull Strengths

Contact Material & Cathode Interface	Weibull Modulus, α (unit less)	Scale Parameter, σ_0 (Pa. $(m^2)^{1/\alpha}$)	Characteristic Strength, β (Pa)
LSM20 (flat)	8.2237	204535	435471
LSM20 (rough)	8.4395	339443	708873

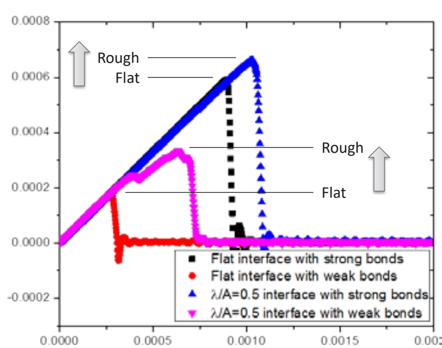
Predicted Cell Interface Reliability

Condition (surface)	Reliability (volume)	Reliability (interface)
Operating (flat)	99.4	70.6*
Operating (rough)	99.8	98.7*

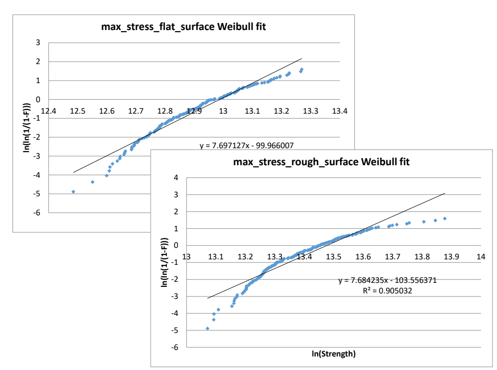
*localized high stresses observed

DEM Submodel Tension Test

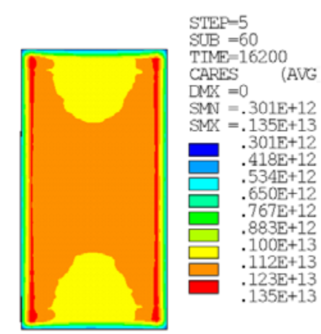
Interface Stress-Strain Response



Interface Weibull Parameters



FEA Stack Model and CARES Reliability



Multi-Cell Reliability with Sintered Contact

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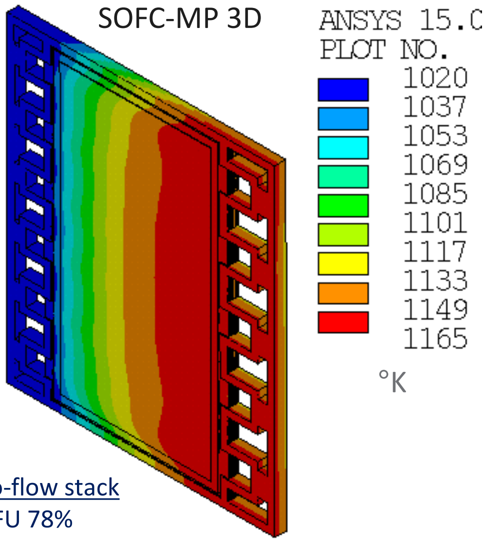
Temperatures from SOFC-MP 3D

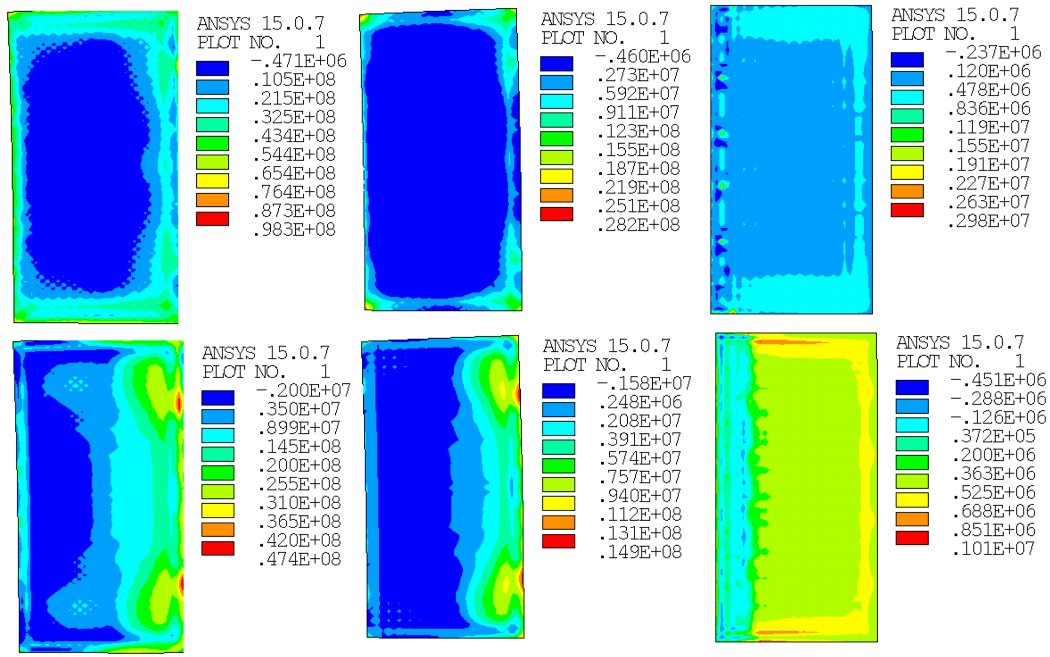


5 Cell Co-flow stack
- Avg FU 78%
- Avg AU 14%
- 4V (~0.8 per cell), 830 W
- Fuel: 42.1%H_2, 27.3%H_2O, 14.4%CO, 11.2%CO_2, 5%CH_4

Electrolyte — Cathode — Cathode Contact

S11 results from the Top cell (#5)

S11 results from the Bottom cell (#1)



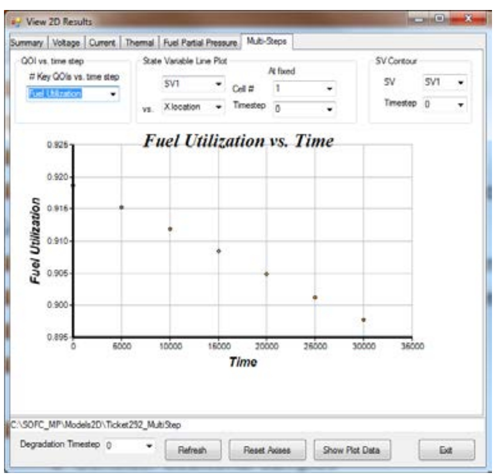
	Uniform Operating Temperature (750°C)		Realistic Operating Temperature (Avg. 820°C)	
Stack Component	Max. Stress (Pa)	Max. Cell P_f (%)	Max. Stress (Pa)	Max. Cell P_f (%)
Air Seal	4.22E+06	0	8.81E+06	0
Fuel Seal	4.65E+06	0	9.48E+06	0
PEN Seal	5.36E+06	0	5.09E+06	0
Electrolyte	4.67E+07	0.10	7.16E+07	3.3*
Anode	8.30E+06	0	7.29E+06	0
Cathode	8.15E+06	0	2.16E+07	18.8*
Cathode Contact	2.57E+06	1.99	4.07E+06	17.0*

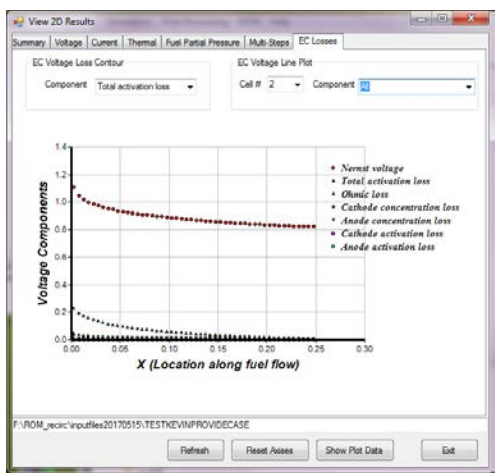
*High probabilities due to local high stresses in top cell components

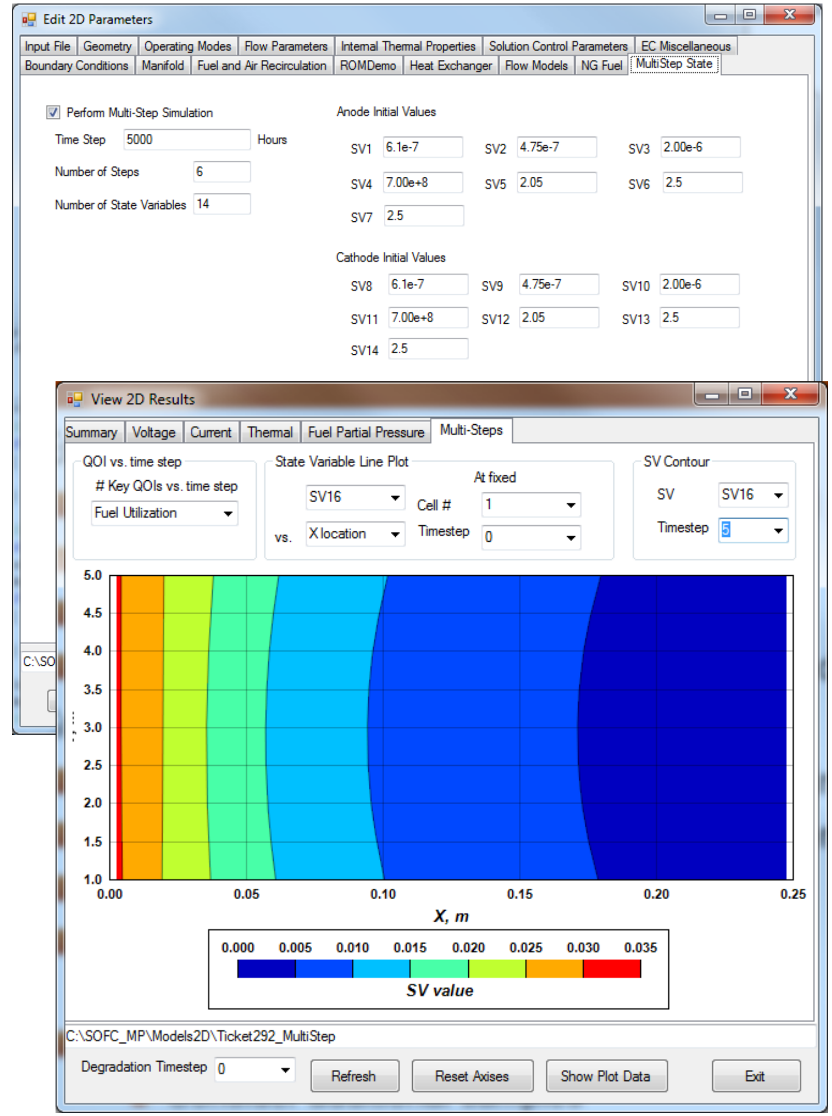
- Significant differences in the same component stresses noticed at different cell levels.
- *Stack end conditions affect the stresses* in the cells at various levels (loading affects contact sintering)
- High probability of failure could be due *to localized stresses* in one of the cell components
- Multi-cell stack reliability evaluations need design specific BCs and modeling (mid vs end cells)

Improved SOFC-MP User Interface

- Continue to improved user interface to support model enhancements
  - *Setup and pre-processing to of degradation models*
    - E.g. NETL coarsening model
  - Handling of degradation state variables and evolution equations
  - Display *time history* and distributions of simulation results and state variables
  - Display of *polarization losses* across the cell or stack for 2D and 3D modules







Summary & Next Steps: Degradation

Summary

- Adapted PNNL 2-D and 3-D stack models to incorporate the NETL time/temperature dependent electrode coarsening models
- Preliminary evaluations of degraded EOL stack conditions
- Defined procedure to utilize lower-scale degradation models in SOFC-MP 3D to study performance degradation and structural reliability of stacks.
  - The lower-scale interfacial strength DEM developed earlier was used to estimate strengths and evaluate reliability of the rough cathode contact interface
  - Degraded performance due to oxide scale growth was simulated

Next Steps

- Evaluate ***mechanical reliability of 3D stack model at EOL*** with electrode coarsening model
- Sensitivity studies with various parameters that influence electrochemical performance or stack reliability will be conducted stacks to ***identify favorable operating conditions for enhanced structural reliability***

Summary

- PNNL is using experimental and computational capabilities to accelerate the commercialization of SOFC power systems.

- Posters
  - Button Cell Tests with LSM/YSZ Cathodes in Air with Quantified Cr Concentrations (John Hardy)
  - Mitigation of Cr-Poisoning of Solid Oxide Fuel Cells (Matt Chou)
  - Cathode Contact Development at Pacific Northwest National Laboratory (Matt Chou)
  - The Effect of Kinetics and Element Additions on Lower Temperature RAA Process (Jung Choi)
  - Improved Capability and Accuracy of a Reduced Order Model (ROM) for SOFC Stacks (Chao Wang)
  - Electrode Coarsening and Temperature Distribution Effects on Long-Term Electrochemical Degradation of SOFC Stacks (Brian Koeppel)

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