

# SOFC Development at PNNL

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Pacific Northwest National Laboratory

19<sup>th</sup> Annual Solid Oxide Fuel Cell Project Review Meeting

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## ▶ Core Technology Program: Materials Development

### ■ Cathode materials and interactions

#### ● Effects of volatile Cr compounds on cathode performance

- ◆ **Poster: LSM/YSZ Button Cell Tests in Cathode Air with Measured Cr Concentrations (John Hardy)**

#### ● Improved density of ceria barrier layers

### ■ Mitigation of Cr poisoning

#### ● Evaluation of Cr capture materials

- ◆ **Poster: Cr Mitigation by LSCF-based Materials for Solid Oxide Fuel Cells (Matt Chou)**

### ■ Cathode contact materials

#### ● Enhancing reliability of cathode/contact materials interfaces

- ◆ **Poster: Composite Approach to Tailoring Thermal Expansion of LSCo-based Ceramic Cathode Contact for Solid Oxide Fuel Cell Applications (Matt Chou)**

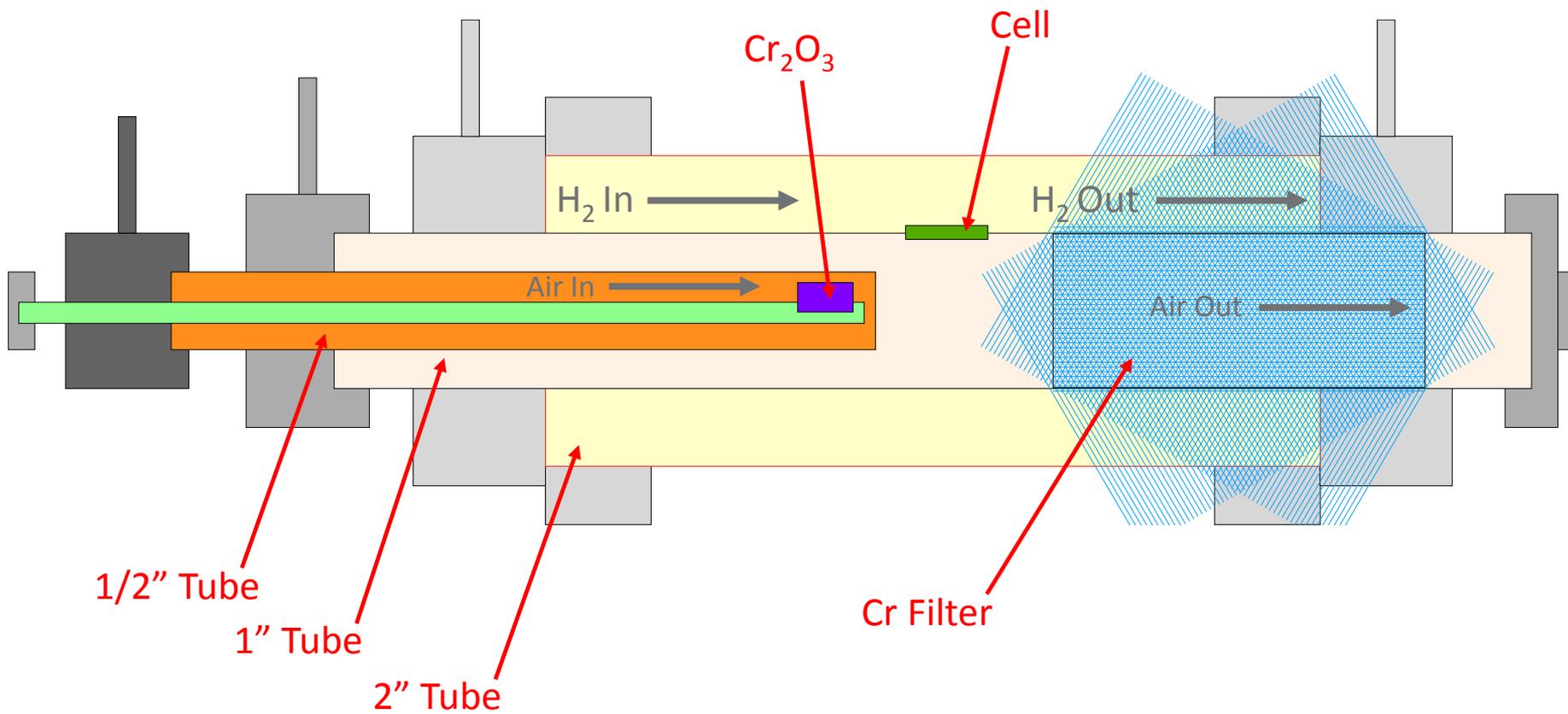
### ■ Interconnects/BOP

#### ● Reactive air aluminization

- ◆ **Poster: Long Term Stability Tests of Low Temperature and Standard Reactive Air Aluminization Process (Jung-Pyung Choi)**

- ▶ **Core Technology Program: Modeling/Simulation**
  - **SOFC Stack and System Modeling Tool Development**
    - **Poster: Advanced Reduced Order Model (ROM) Prediction and Error Quantification Framework for SOFC Stacks (Chao Wang)**
  - **Modeling of Stack Degradation and Reliability**
    - **Poster: Optimal Operating Conditions for Performance and Reliability of Solid Oxide Fuel Cells (Kurt Recknagle)**
  
- ▶ **Small-Scale SOFC Test Platform**
  - **Design and fabrication of SOFC power system for evaluation of performance and reliability of new stack technologies (1-10 kW)**
    - **Poster: Small-Scale Test Platform (SSTP) for SOFC Stacks (Brent Kirby)**
  
- ▶ **Industrial Collaborations**
  - **Cummins/Ceres**
    - **Effects of Fuel Contaminants on Anode Performance**
  - **TCF Project: Protective Spinel Coatings**
  - **TCF Project: Air Braze Optimization**
    - **Poster: Air Braze Optimization for Markets Targeted by Aegis Technology, Inc. (John Hardy)**

# Cr Poisoning: PNNL Test Fixture Design (Not to scale)



# Assembled Cr Test Fixtures

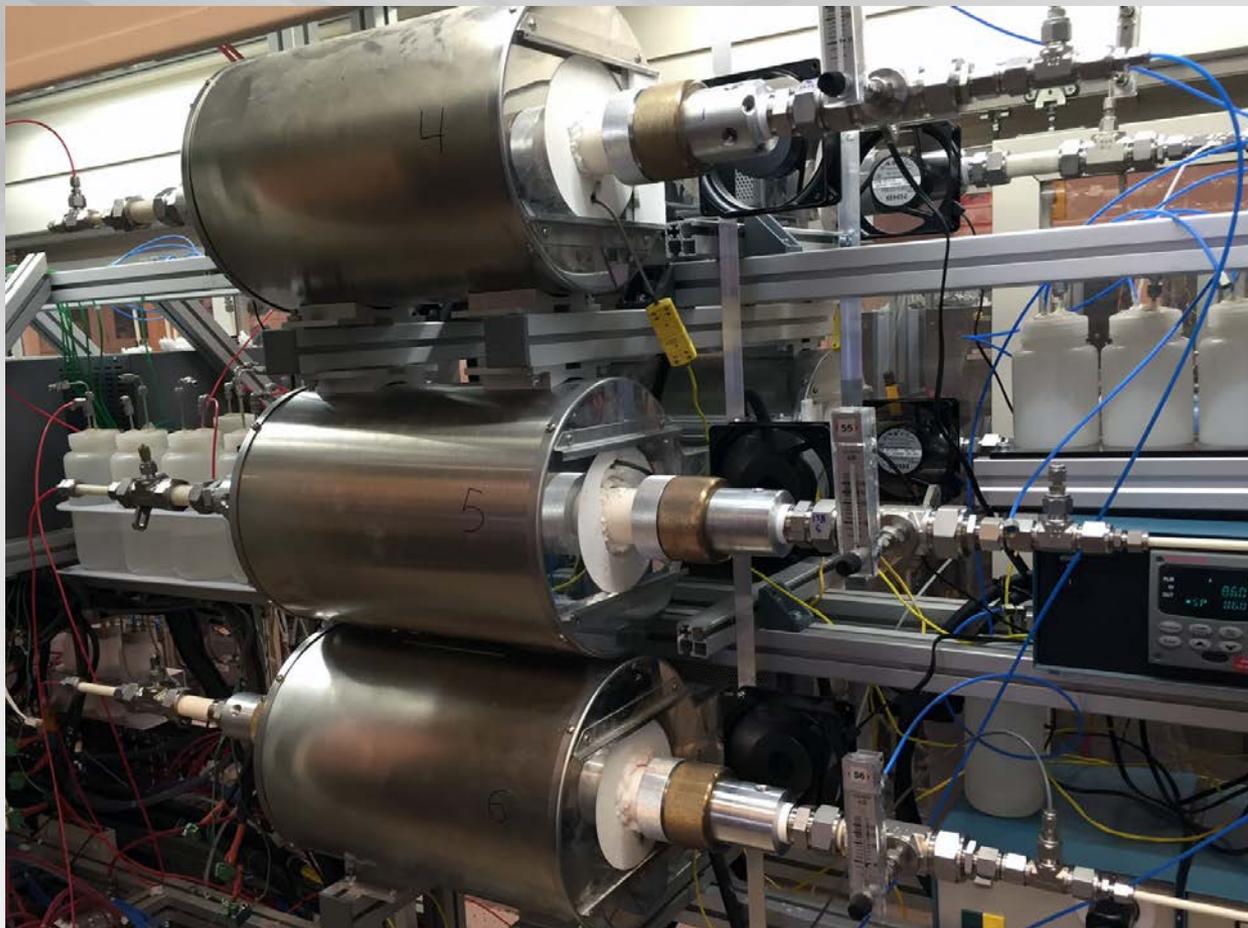


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Downstream filter



Chromia Pellet



Pacific Northwest  
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Proudly Operated by Battelle Since 1965

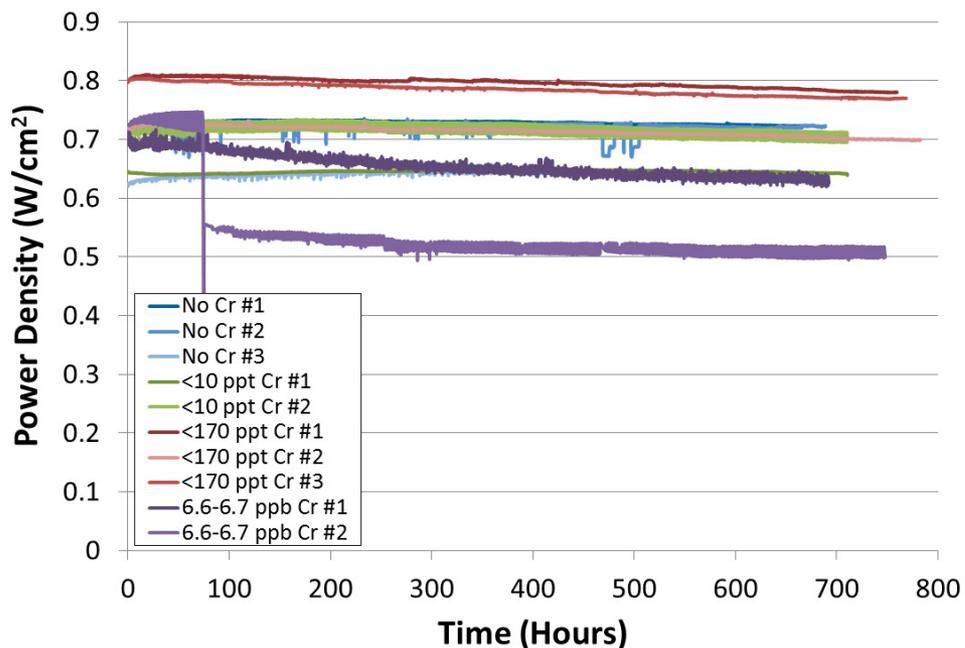
# Electrochemical Button Cell Tests

## ▶ LSM/YSZ Cathodes

■ LSM-20, A/B = 0.95

## ▶ Tested at 850°C

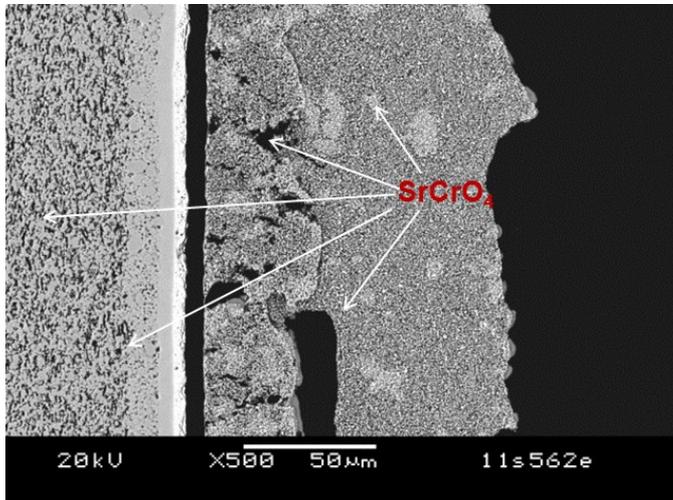
■ Cr concentration controlled by adjusting  $\text{Cr}_2\text{O}_3$  source temperature and moisture content of air



| Test Condition | # of cells | Ave. Degradation Rate (per kWh) |
|----------------|------------|---------------------------------|
| First Round    |            |                                 |
| No Cr          | 3          | -0.2%                           |
| ≤10 ppt Cr     | 2          | 2.2%                            |
| ≤170 ppt Cr    | 3          | 3.9%                            |
| 6.6-6.7 ppb Cr | 2          | 13.2%                           |
| Second Round   |            |                                 |
| ≤43 ppt Cr     | 3          | -0.8%                           |
| ≤164 ppt Cr    | 3          | 4.9%                            |
| ≤224 ppt Cr    | 2          | 3.9%                            |

# Mitigation of Cr Poisoning: LSCF as Cr-gettering Material

- ▶  $\text{SrCrO}_4$  observed throughout LSCF cathode layer.



## ▶ Potential Advantages

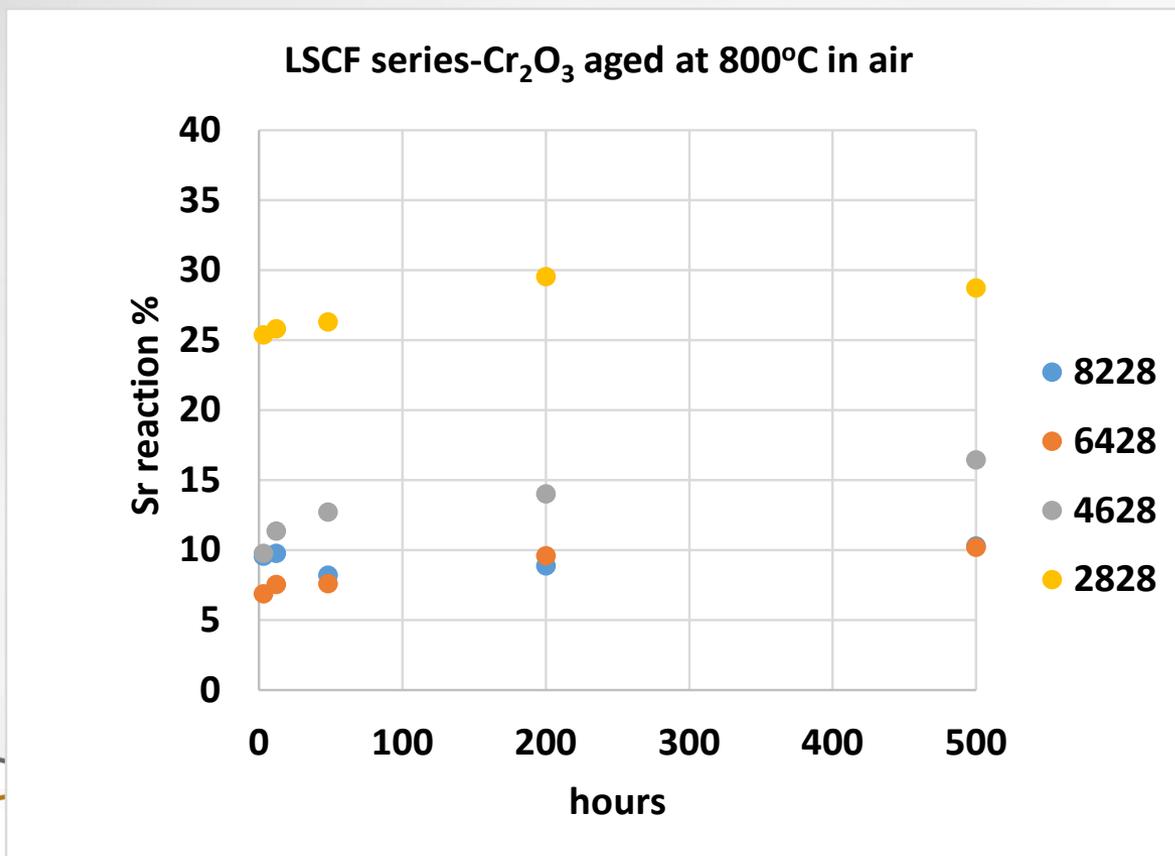
- Sr segregation from structure
- High electrical conductivity
- Chemical compatibility
- Thermal and phase stability
- Reasonable mechanical strength
- Tailorable La/Sr and Co/Fe ratios
  - Control Sr activity
- Commercially available

## ▶ 4 Compositions evaluated

- $\text{La}_{0.8}\text{Sr}_{0.2}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$
- $\text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$
- $\text{La}_{0.4}\text{Sr}_{0.6}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$
- $\text{La}_{0.2}\text{Sr}_{0.8}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_3$

# LSCF/Cr<sub>2</sub>O<sub>3</sub> Reaction at 800°C: Normalized Sr % Reacted

- ▶ SrCrO<sub>4</sub> wt% converted to Sr wt% then normalized with total Sr wt% in LSCF series as Sr % reacted.



# Cathode Contact Development

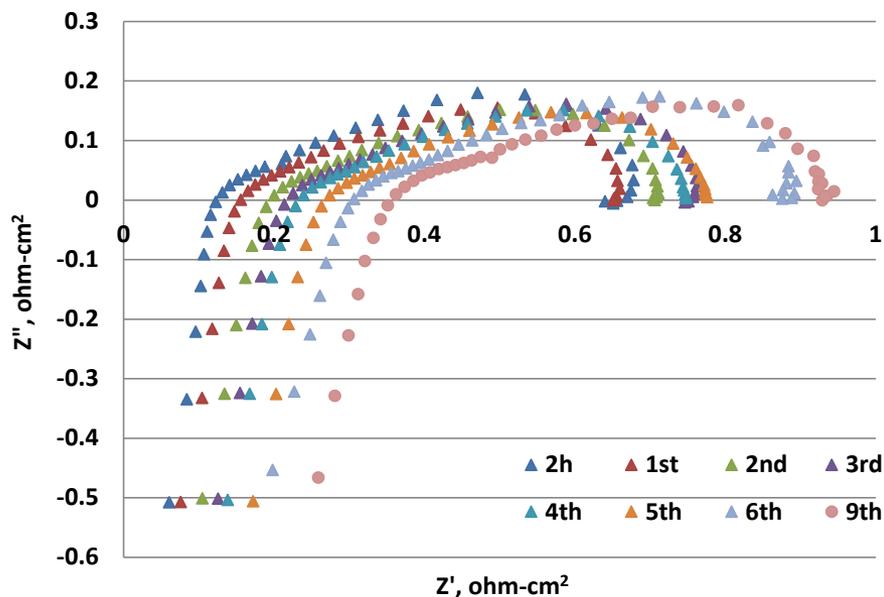
- ▶ Approach A: Impregnated Fibrous Substrates
- ▶ Approach B: Composite Mixtures to Tailor CTE

$$\sigma = E \Delta\alpha \Delta T$$

# Poor Thermal Cycle Stability of Ceramic Cathode Contact

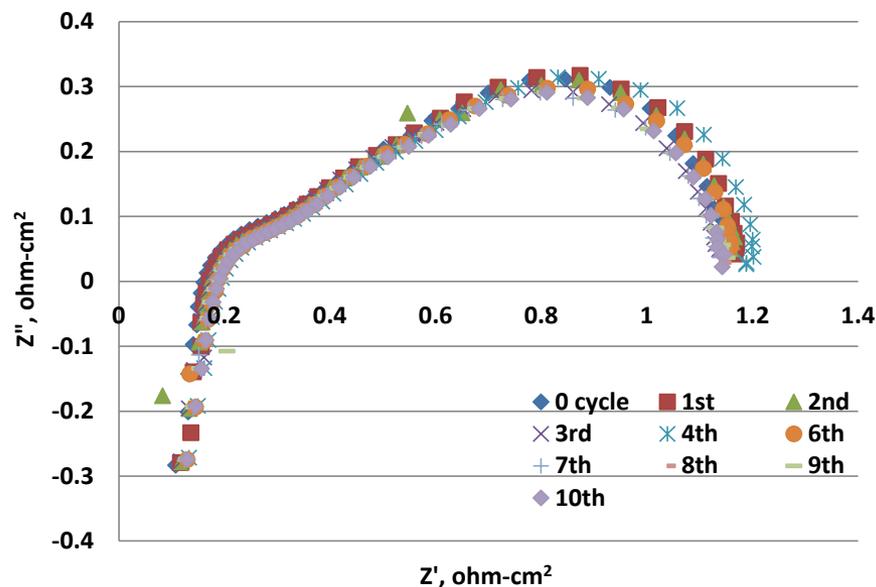
2"x2" LSM-based cell in stack test fixture during cycling between ~50°C and 800°C

cell #149, ASC3 plain LSM 800°C



Brittle cathode contact: LSM20

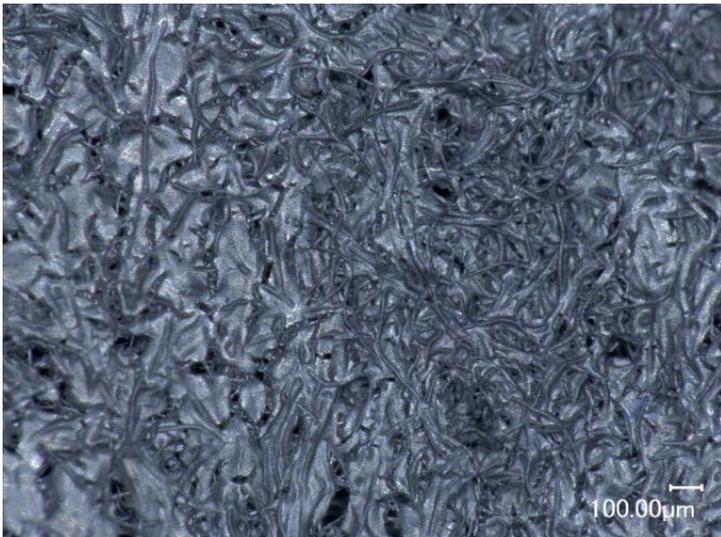
cell #153 ASC3 Ag paste, 800°C



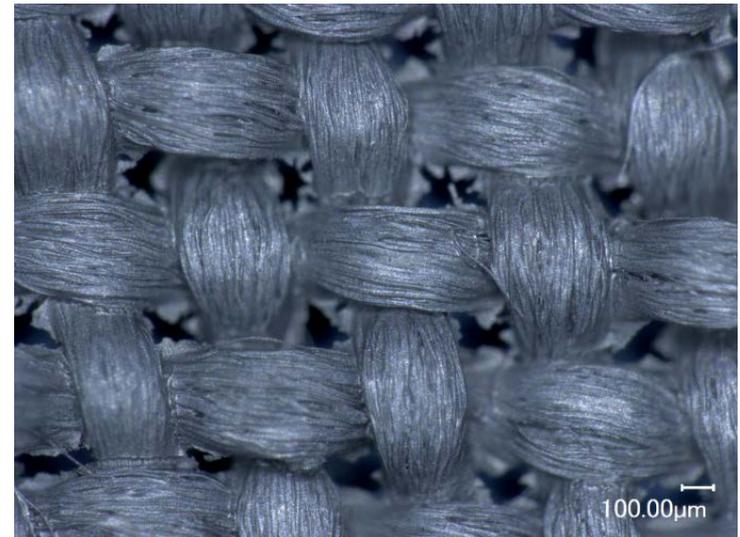
Ductile cathode contact: Ag

# Approach A: Impregnated Fibrous Materials

- ▶ Inert YSZ fibrous felt/woven cloth substrate
- ▶ Impregnate with conducting LSM20 or LSCo phase via dip-coating



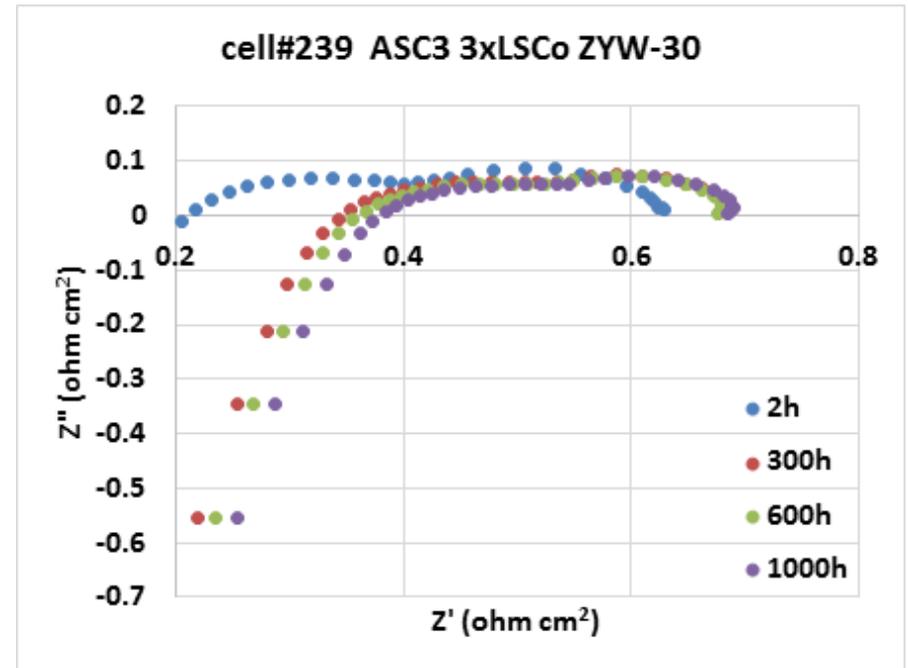
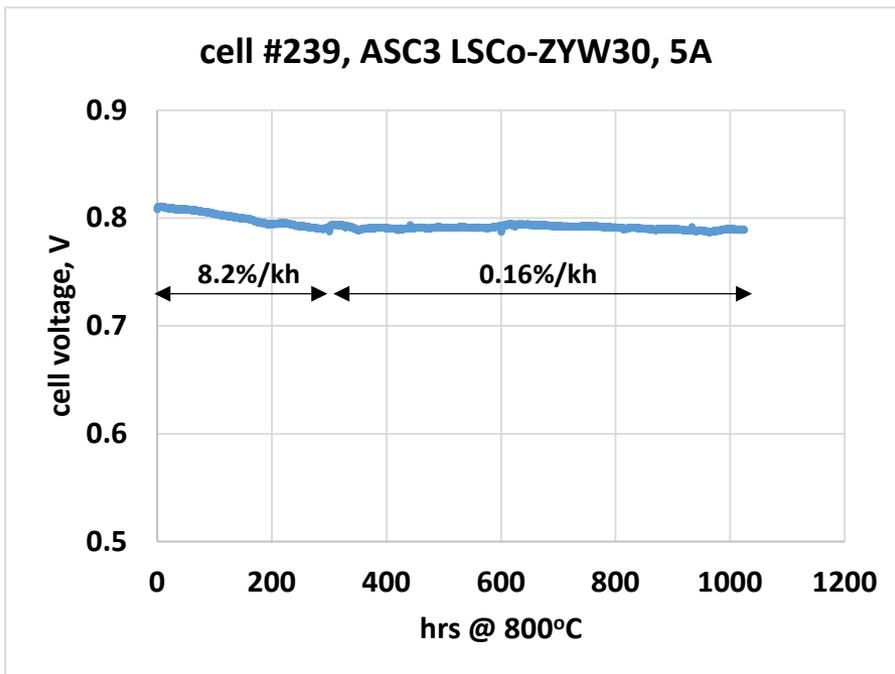
ZYF-50 ( $Y_2O_3$  10 wt% stabilized  $ZrO_2$ )  
(~0.05" thick, bulk porosity >96%)



ZYW-15 ( $Y_2O_3$  10 wt% stabilized  $ZrO_2$ )  
(~0.015" thick, square weave, bulk porosity >96%)

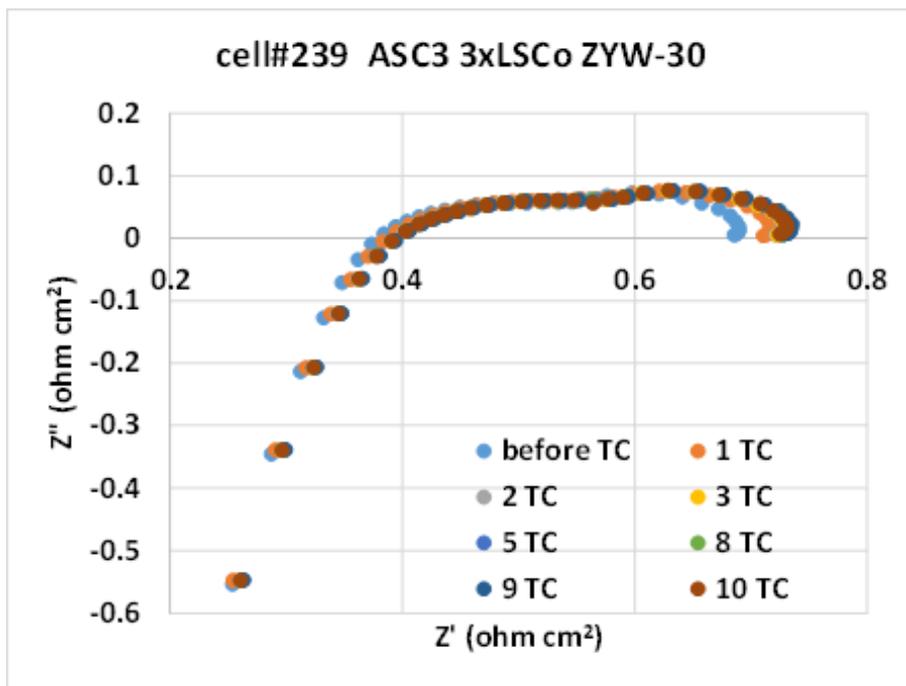
# Validation in a Generic Stack Fixture for Thermal Cycle Stability

- ▶ Standard LSM-based cell (2"x2") with 3x LSCo impregnated ZYW-30 woven cloth
- ▶ First tested at 800°C and constant current for 1000h then thermal cycled for ~10 times between ~50°C and 800°C

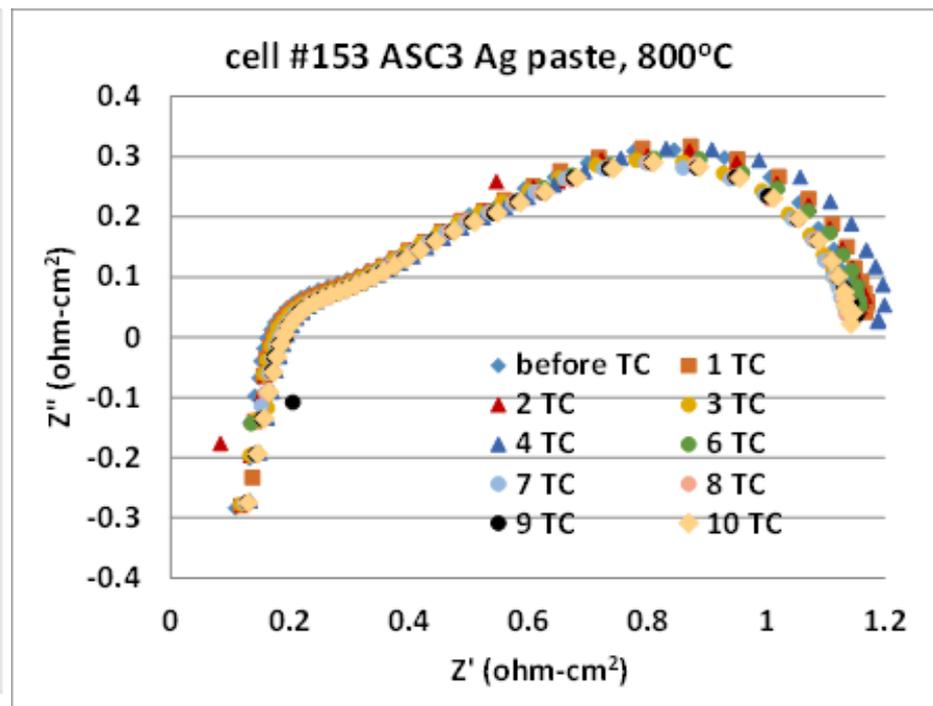


# Effect of Thermal Cycling

LSCo-impregnated YSZ cloth



Ag contact



# Approach B: Minimize Residual Stresses with Tailored CTE

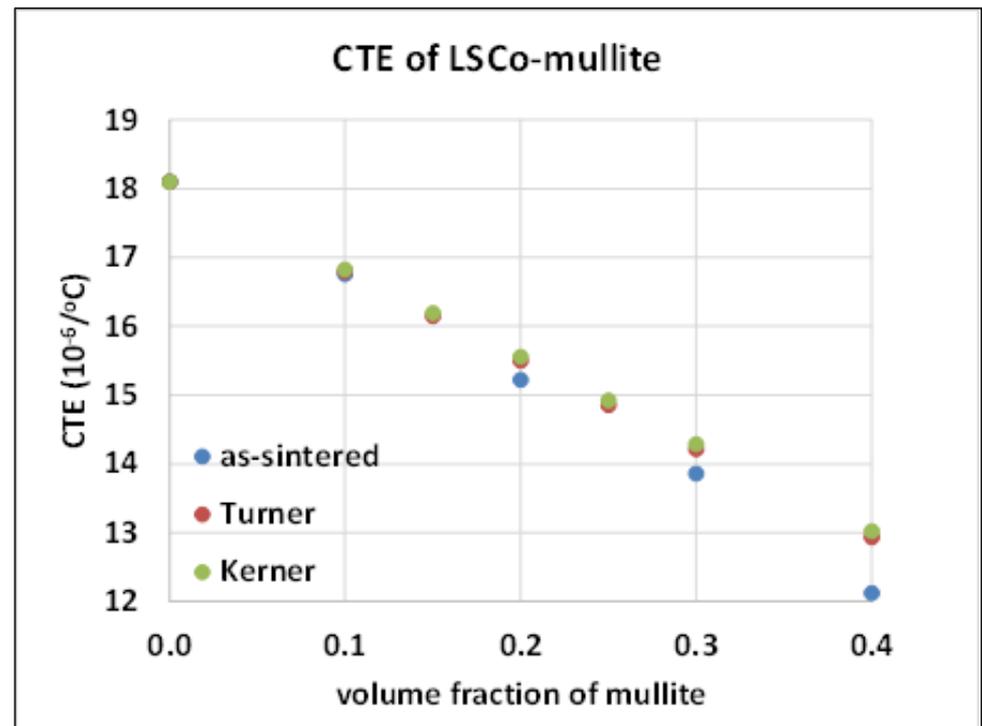
- ▶ LSCo20 perovskite offers high conductivity, but also very high CTE ( $\sim 18 \times 10^{-6}/^{\circ}\text{C}$ ), while CTE of typical cell and interconnect is  $12\text{-}13 \times 10^{-6}/^{\circ}\text{C}$ .
- ▶ Composite approach incorporating low CTE mullite ( $3\text{Al}_2\text{O}_3 \cdot 2\text{SiO}_2 - 2\text{Al}_2\text{O}_3 \text{SiO}_2$ ):  $\sim 5.5 \times 10^{-6}/^{\circ}\text{C}$ .

Turner's model (considers hydrostatic stress only)

Kerner's Model (hydrostatic + shear stress)

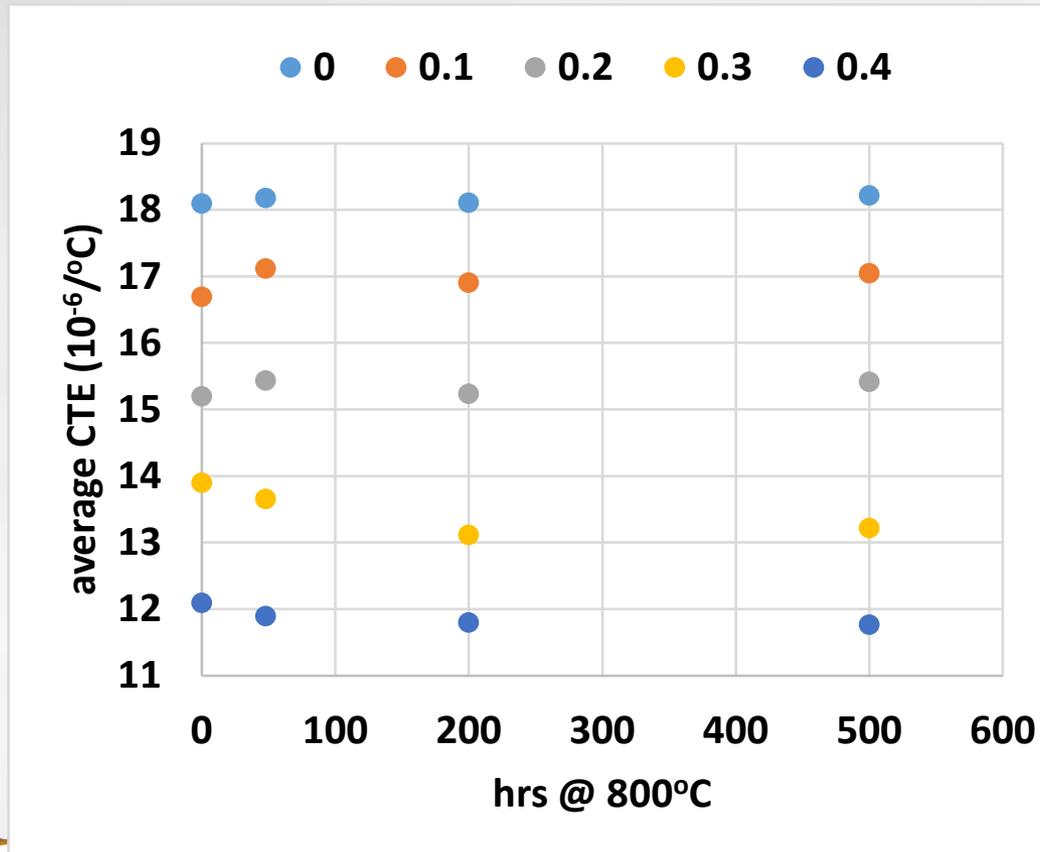
Measured values deviate from prediction at higher vol. fractions

Mullite received contains other phases (sillimanite and kyanite)



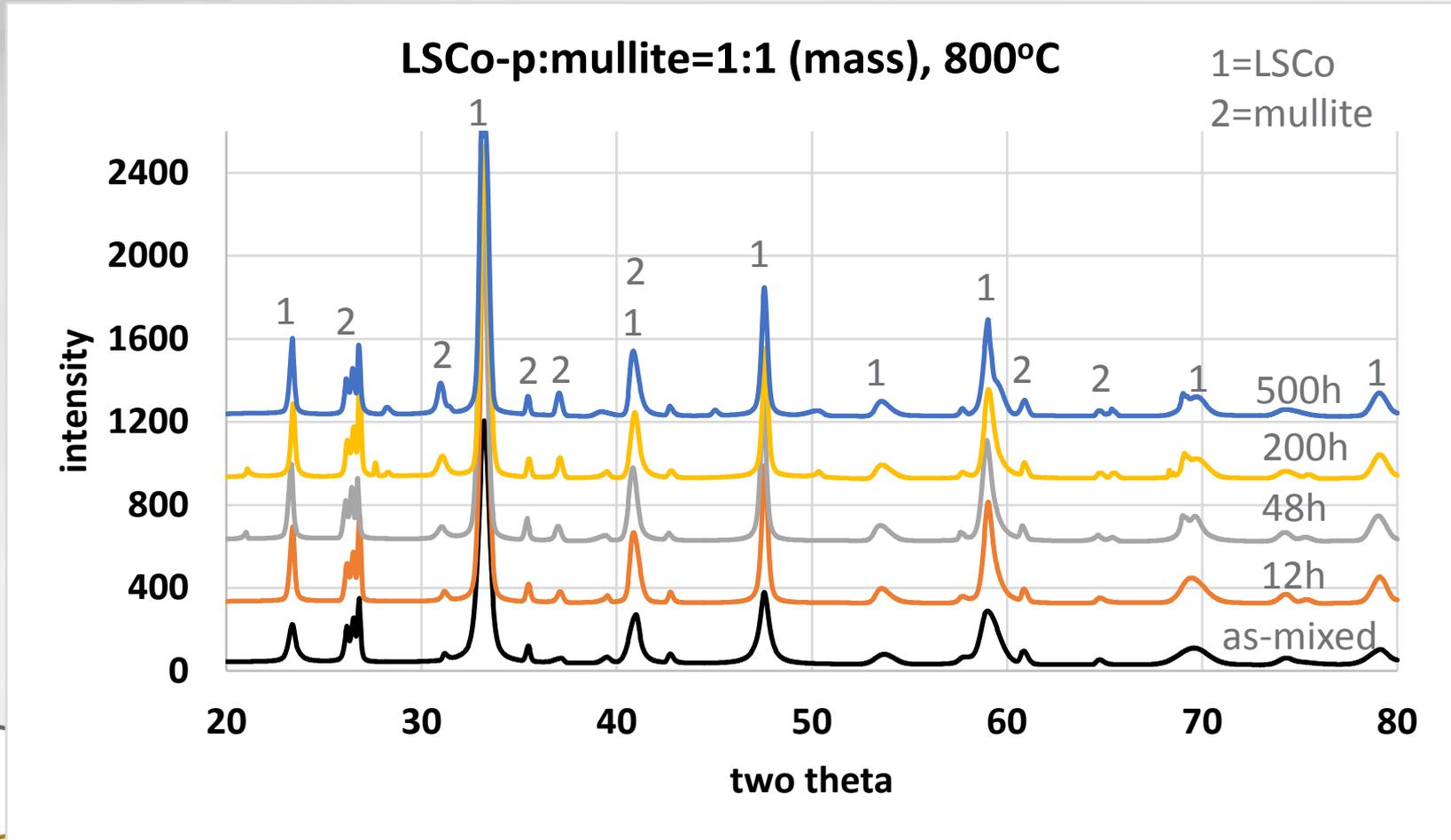
# Effect of Isothermal Ageing at 800°C

- ▶ Fairly stable with small changes over 500h ageing
- ▶ Indicating thermally stable and likely chemically compatible



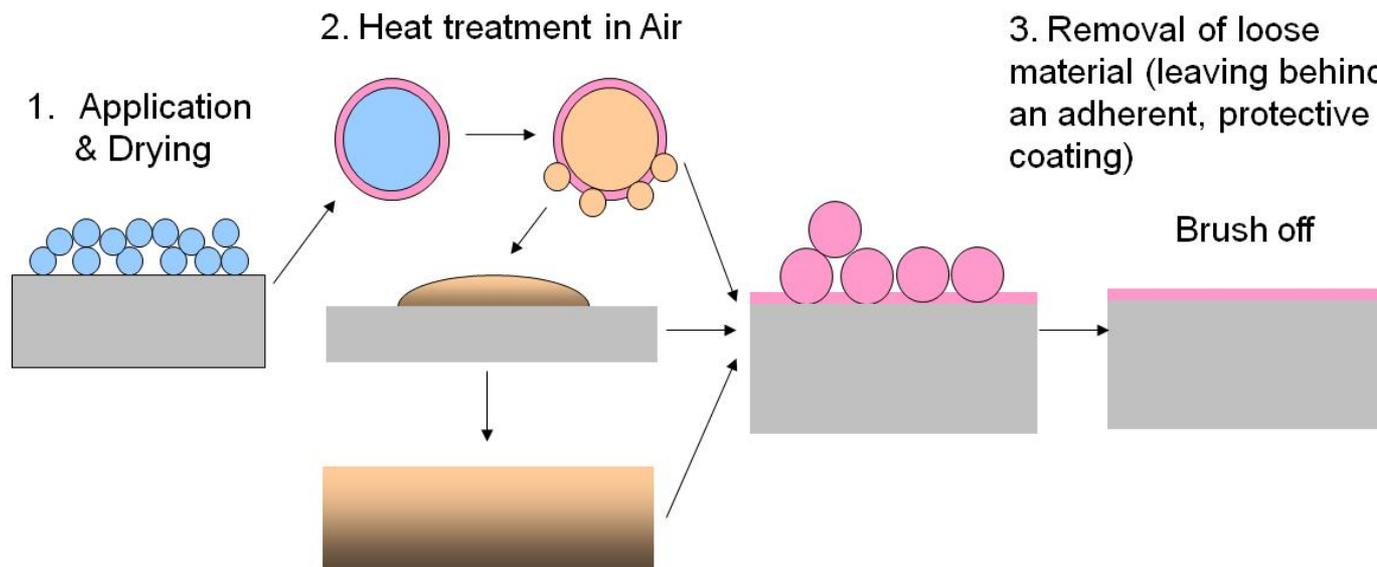
# Thermal Stability

- ▶ LSCo20:mullite at 1:1 ratio aged at 800°C for 12, 48, 200, and 500h in air



# Reactive Air Aluminization (RAA)

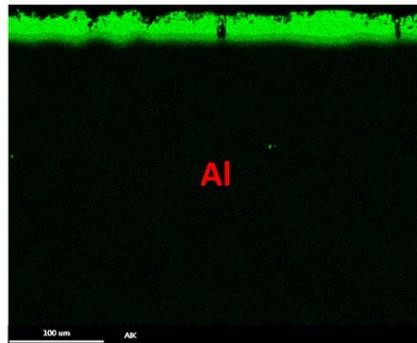
- Reaction between alkaline earths in glass seals and Cr in interconnect steel can form high CTE chromate phases (e.g.,  $\text{SrCrO}_4$ ), which degrade interfacial strength
- Cr volatility from alloys can poison cathodes
- Reactive Air Aluminization (RAA) offers a simple alternative to controlled atmosphere aluminization of interconnects (and BOP components)



# Low temperature RAA process

- Primary challenges to lowering process temperature using our standard slurry are incomplete/nonhomogenous alumina layer formation and excessive reaction/diffusion of Al into substrate
- Approach: Add additional elements to optimize oxidation kinetics and metal diffusion at lower temperatures (800-900°C) to form protective alpha alumina coating and “right-sized” Al reservoir in substrate to provide CTE gradient (to improve coating bond-strength) and self-healing capability.
- Results:
  - Seed elements (Mn, Ti, or Fe) enhance formation of cubic gamma phase at lower temperatures, which then accelerates formation of desired alpha phase.
  - Formation of thick gamma phase “egg shells” at temperatures below the melting point of the aluminum powder prevents excessive release and diffusion of the molten aluminum into the underlying substrate. During dwell time at temperature (e.g., 900°C), transition from gamma to alpha alumina is completed.

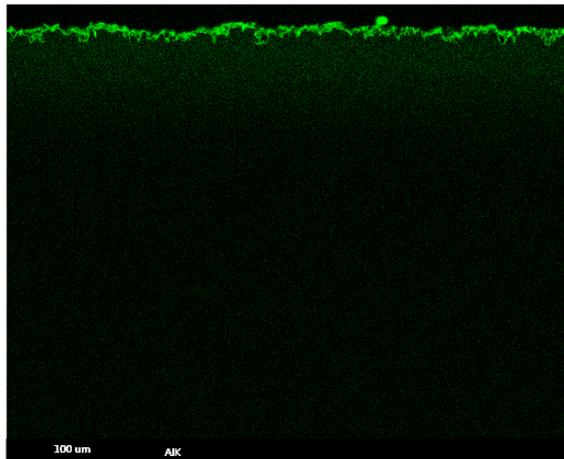
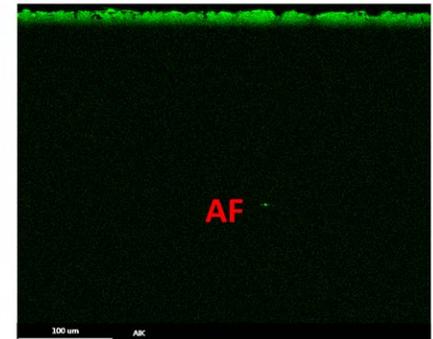
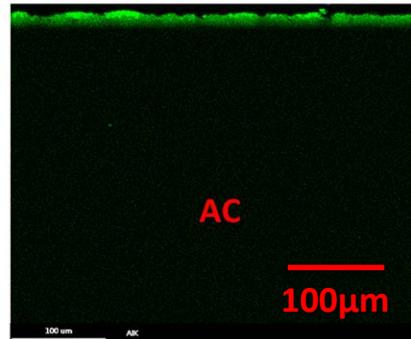
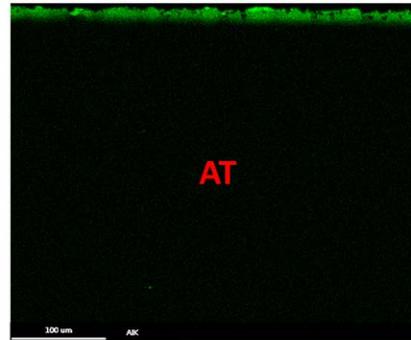
# Low temperature RAA process



800°C



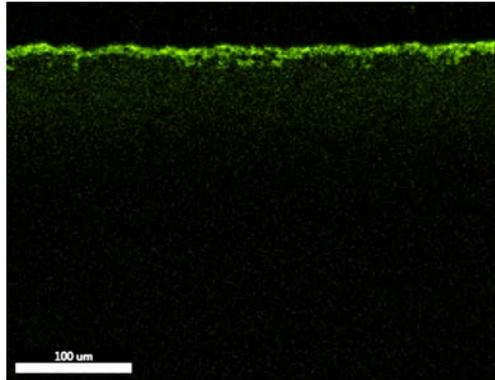
Same magnification



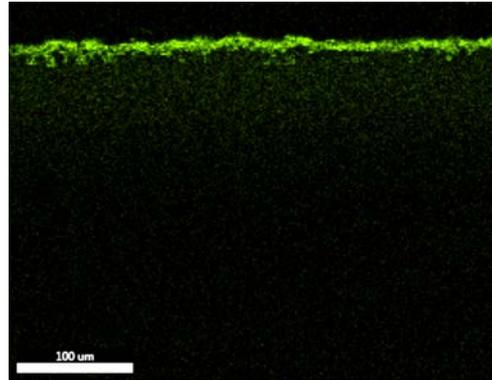
Standard RAA at 1000°C

# Long term stability test (Standard RAA)

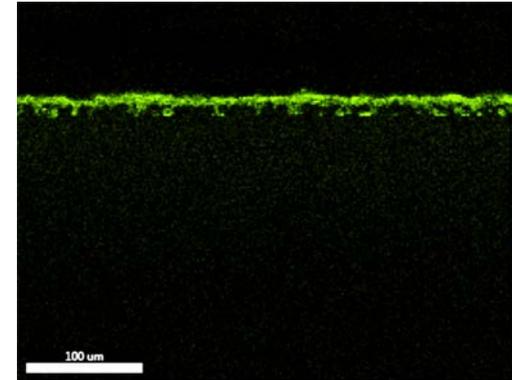
800°C



50 cycles

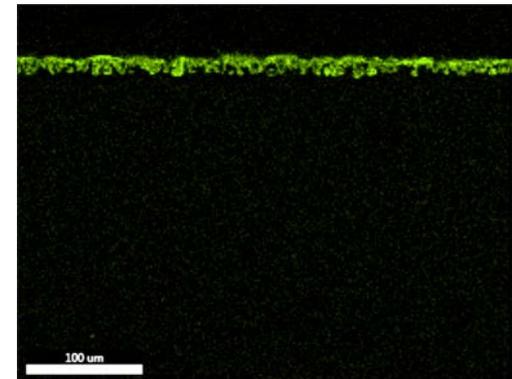
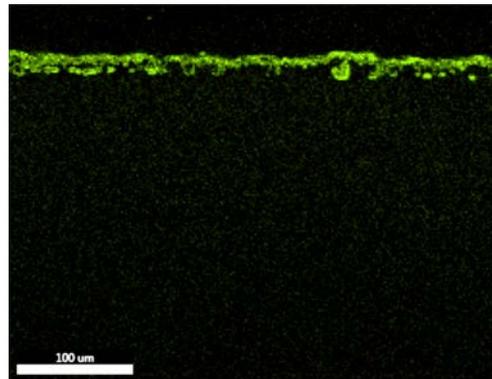
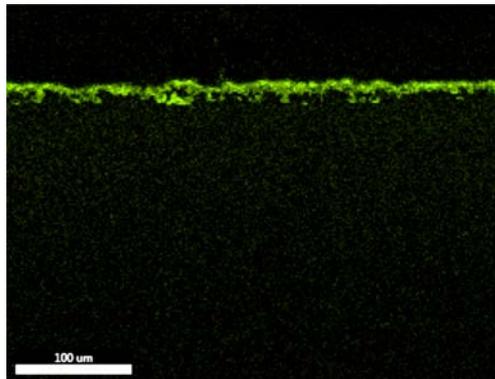


100 cycles



300 cycles

900°C



# Co-free Electrically Conductive Protective Coatings

- ▶ Objective: Develop Co-free, electrically conductive protective coatings for planar SOFC stack interconnects
- ▶ Based on previous studies,\* selected 3 ternary oxide systems for evaluation
  - Cu-Mn-O
  - Cu-Fe-O
  - Ni-Mn-O
- ▶ Approach:
  - Examine powder synthesis options
  - Develop/optimize a cost-effective manufacturing process (aerosol spray)
  - Evaluate long-term and thermal cyclic behavior (in terms of electrical conductivity and surface stability) of these candidate materials on inexpensive ferritic stainless steel substrates
- ▶ \*A. Petric and H. Ling, J. Am. Ceram. Soc., 90, 1515 (2007); S. Hosseini, F. Karimzadeh, M. Enayati, and N. Sammes, Solid State Ionics, 289, 95 (2016); N. Hosseini, F. Karimzadeh, M. Abbasi, and G. Choi, Ceramics International, 40, 12219 (2014); N. Hosseini, M. Abbasi, F. Karimzadeh, and G. Choi, J. Power Sources, 273, 1073 (2015); W. Huang, S. Gopalan, U. Pal, and S. Basu, J. Electrochem. Soc., 155, B1161 (2008); Z. Sun, S. Gopalan, U. Pal, and S. Basu, Surface & Coatings Tech., 323, 49 (2017); P. Wei, X. Deng, M. Bateni, and A. Petric, Corrosion, 63, 529 (2007); M. Bateni, P. Wei, X. Deng, and A. Petric, Surface & Coatings Tech., 201, 4677 (2007)

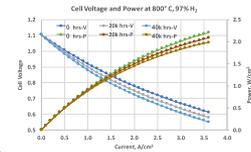
# FY18 Modeling Focus

- ▶ Recent modeling task activity continued to focus on **linking model results across length scales**
  - Utilize the **Reduced Order Model (ROM)** approach to improve the accuracy of power system models



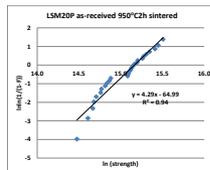
Micro/Meso-Scale Models

I-V Performance

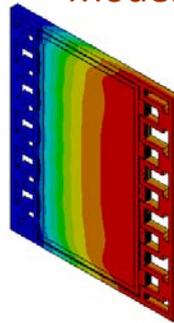


Cell Material Testing

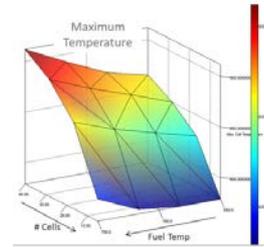
Property Data



Cell/Stack Models



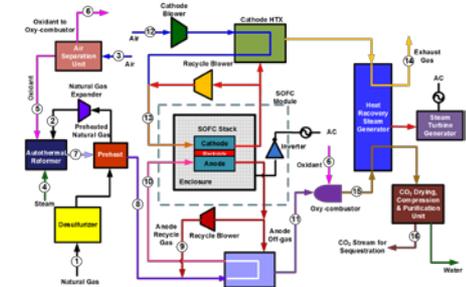
Response Surface Analysis



Performance:  
Electrical  
Thermal  
Mechanical



System Models



Reduced Order Model (ROM)

## ▶ SOFC *Modeling Tool Development*

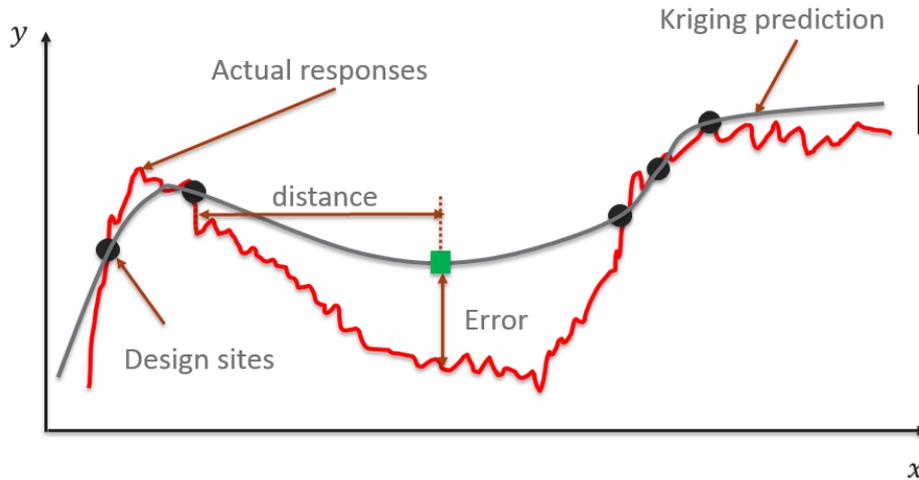
1. Response surface regression and error quantification
2. ROM tool for SOFC stacks
3. ROMs generated for NETL system analysis

## ▶ Modeling of *Stack Degradation and Reliability*

4. Short-term and long-term mechanical reliability
5. Optimal conditions for short-term reliability

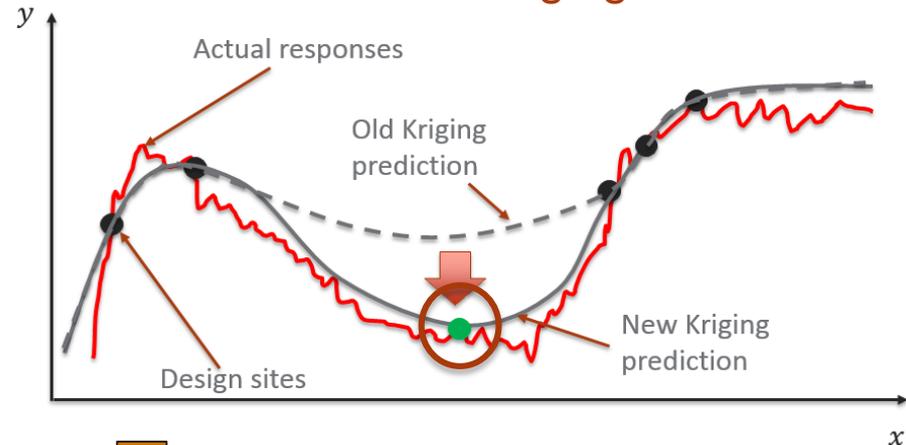
# Introduction of ROM Framework

## Initial Kriging regression

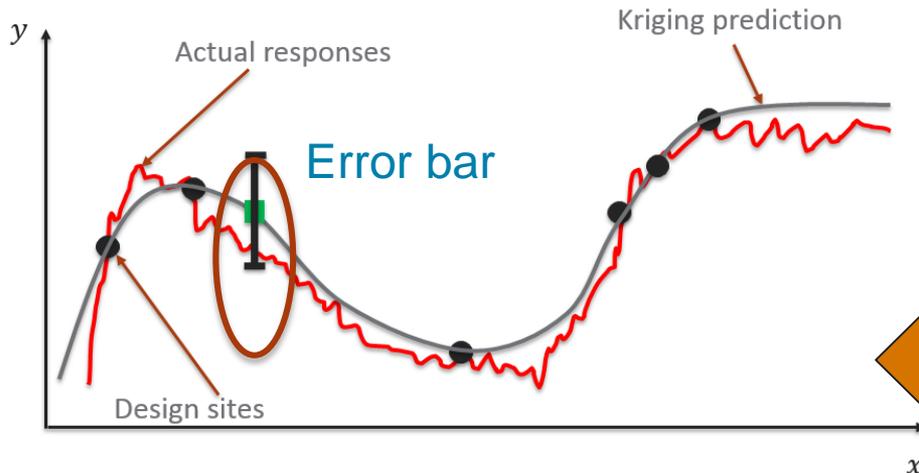


- *But how to select the best location to add additional design sites?*
  - *Need smart sampling*

Smartly add sampling points to reduce Kriging MSE



## Quantify the error of Kriging prediction

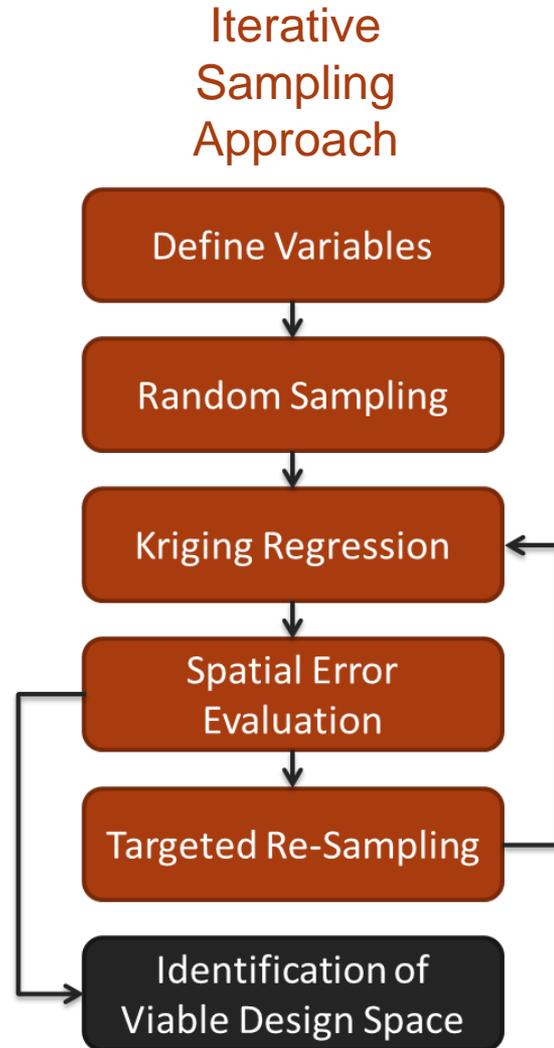


- *But how accurate is the prediction?*
  - *Need error bar*

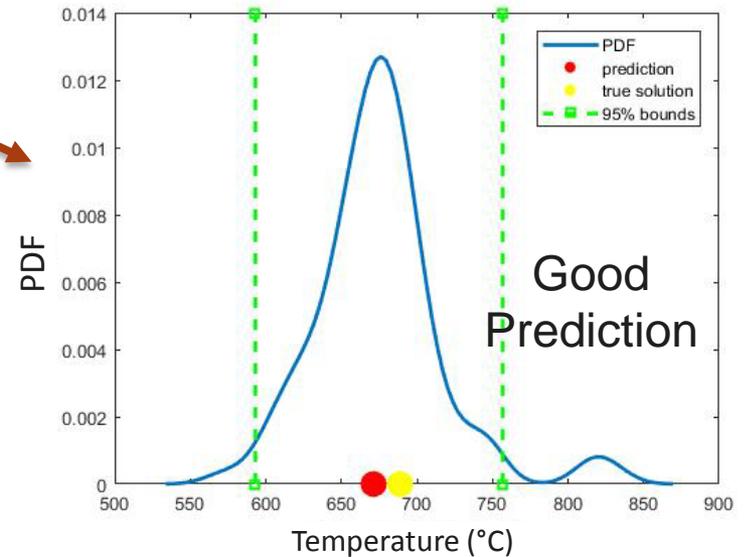
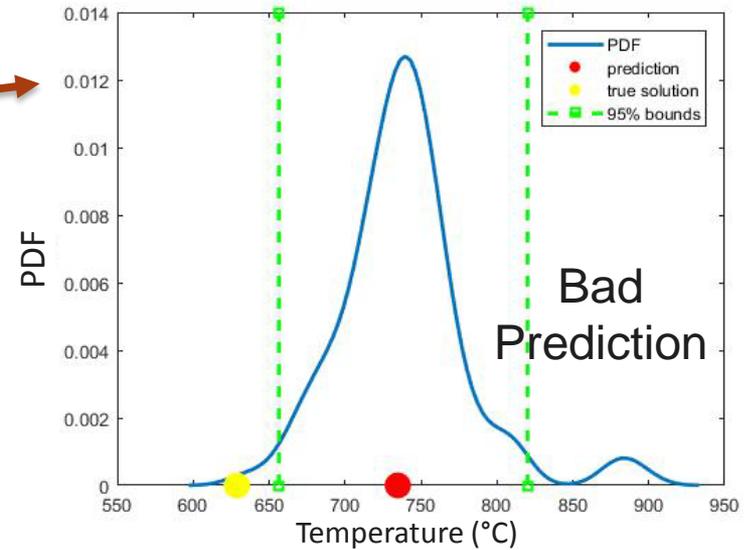
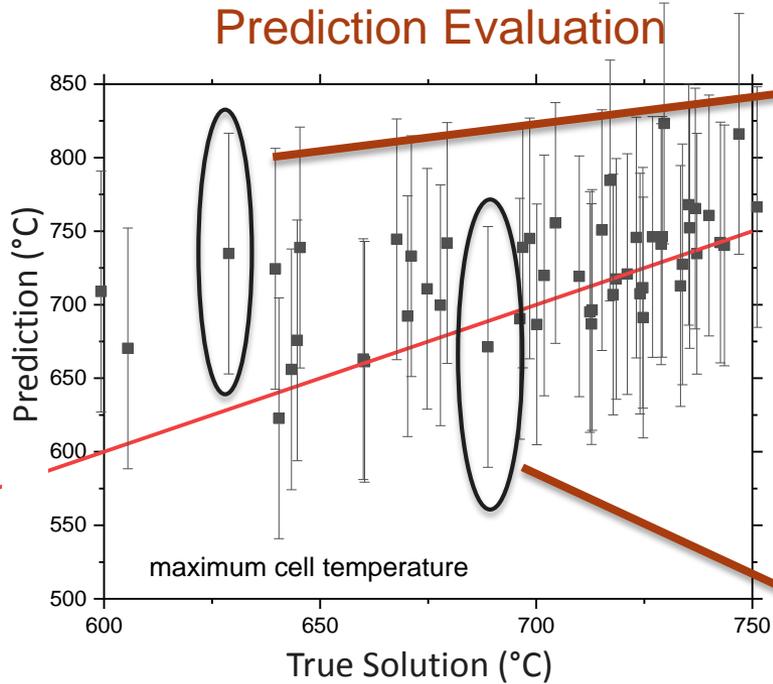
# Framework to Minimize Regression Error

- ▶ Demonstrate advantage of **adaptive smart sampling** versus traditional sampling using **NGFC stack model**
- ▶ Traditional sampling:
  - 11k random samples
  - Additional 1k samples for validation cases
  - Max voltage mean square error (MSE) of 3.0e-4
- ▶ Adaptive smart sampling:
  - 2k initial samples followed by MSE evaluation
  - Additional 2k targeted samples
  - Repeat iteration until desired MSE is reached
- ▶ **Same error** achieved with **~30% less samples** (<8k)

| Number of Samples | Maximum MSE   | MSE Ratio  |
|-------------------|---------------|------------|
| 2000              | 1.5e-3        | 487%       |
| 4000              | 4.2e-4        | 141%       |
| 6000              | 3.8e-4        | 126%       |
| <b>8000</b>       | <b>2.9e-4</b> | <b>96%</b> |



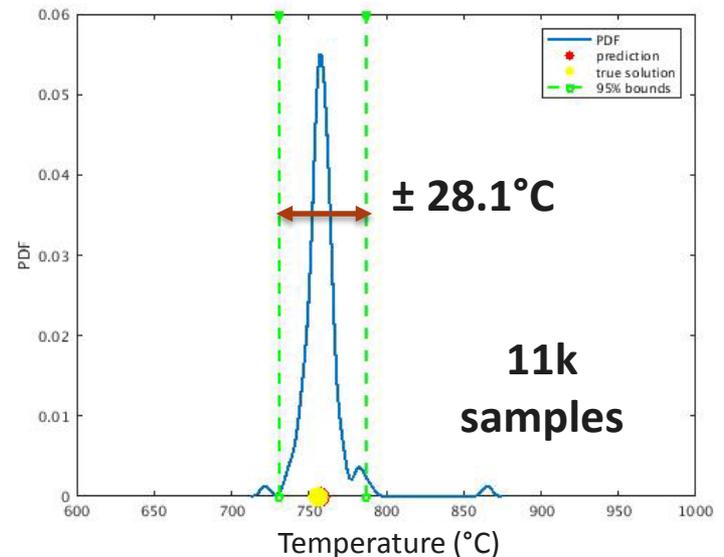
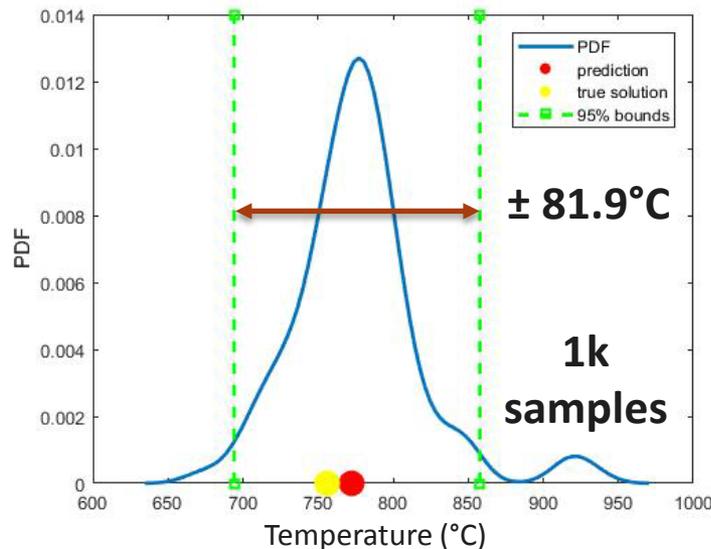
# ROM Error Quantification



- ▶ Prediction (black square) and 95% confidence interval (error bar) are shown
- ▶ Error bar crossing red line (100% match) indicates good prediction
- ▶ 48 out of total 50 predictions are good: 96% $\approx$ 95% **validates the quantified error**

# ROM Error Quantification (cont'd)

- ▶ Error quantification permits user to **obtain the required ROM accuracy**
- ▶ Evaluated the impact of sample size on **95% confidence interval (CI)**
  - Increase number of samples and perform cross-validation on maximum cell temperature
- ▶ Results:
  - Increased number of sample size by 11X, 95% CI range is reduced by 3X
  - Prediction is more accurate and closer to true solution
  - Allows user to choose desired range of 95% CI
- ▶ **Incorporating the error quantification framework in the ROM generation tool**



## ► **User interface** for stack simulations and ROM generation on **high performance computer (HPC)**

After creating all the simulations cases, use “Simulations on HPC” tab to run the simulations on Linux HPC clusters

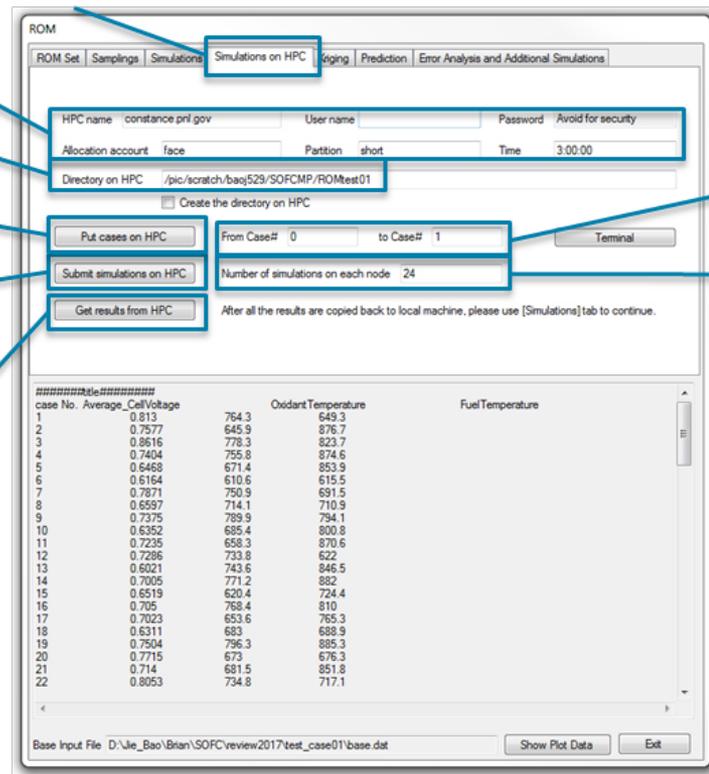
1. Account setup on HPC

2. Working direction on HPC

3. Copy data to HPC

4. Submit simulation jobs into queue on HPC. No need to keep connecting to HPC after submitting the jobs

5. Gather simulation results from HPC to local PC. List the cases without simulation results for tracking and/or rerun



ROM Set | Samplings | Simulations | **Simulations on HPC** | Logging | Prediction | Error Analysis and Additional Simulations

HPC name: constance.pnl.gov | User name: | Password: Avoid for security  
Allocation account: face | Partition: short | Time: 3.00.00  
Directory on HPC: /pic/scratch/bao529/SOFCMP/ROMtest01  
 Create the directory on HPC

Put cases on HPC | From Case# 0 | to Case# 1 | Terminal  
Submit simulations on HPC | Number of simulations on each node 24  
Get results from HPC | After all the results are copied back to local machine, please use [Simulations] tab to continue.

| case No. | Average_CellVoltage | Oxidant Temperature | Fuel Temperature |
|----------|---------------------|---------------------|------------------|
| 1        | 0.813               | 764.3               | 649.3            |
| 2        | 0.7577              | 645.9               | 876.7            |
| 3        | 0.8616              | 778.3               | 823.7            |
| 4        | 0.7404              | 755.8               | 874.6            |
| 5        | 0.6468              | 671.4               | 853.9            |
| 6        | 0.5164              | 610.6               | 615.5            |
| 7        | 0.7871              | 750.9               | 691.5            |
| 8        | 0.6597              | 714.1               | 710.9            |
| 9        | 0.7375              | 789.9               | 794.1            |
| 10       | 0.6352              | 685.4               | 800.8            |
| 11       | 0.7235              | 658.3               | 870.6            |
| 12       | 0.7286              | 733.8               | 622              |
| 13       | 0.6021              | 743.6               | 846.5            |
| 14       | 0.7005              | 771.2               | 882              |
| 15       | 0.6519              | 620.4               | 724.4            |
| 16       | 0.705               | 788.4               | 810              |
| 17       | 0.7023              | 653.6               | 765.3            |
| 18       | 0.6311              | 683                 | 688.9            |
| 19       | 0.7504              | 796.3               | 885.3            |
| 20       | 0.7715              | 673                 | 676.3            |
| 21       | 0.714               | 691.5               | 851.8            |
| 22       | 0.8053              | 734.8               | 717.1            |

Base Input File D:\ie\_Bao\Brian\SOFc\review2017\test\_case01\base.dat | Show Plot Data | Exit

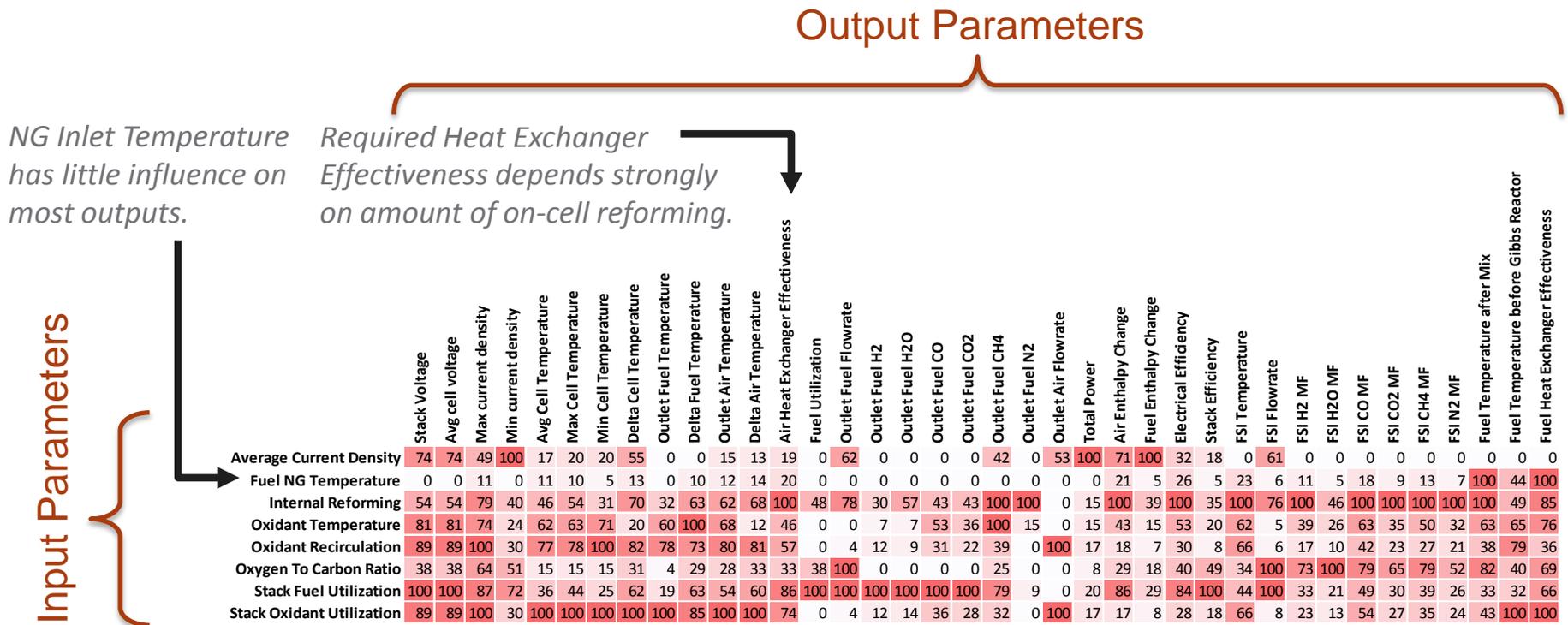
Specify the case/s run on HPC clusters for resume or rerun incomplete cases

SOFC-MP is a serial code. For fully use the capacity of compute node on HPC, specify the number of cases that can run simultaneously on each HPC node

# ROM Parameter Sensitivity Analysis

## ► Sensitivity scores

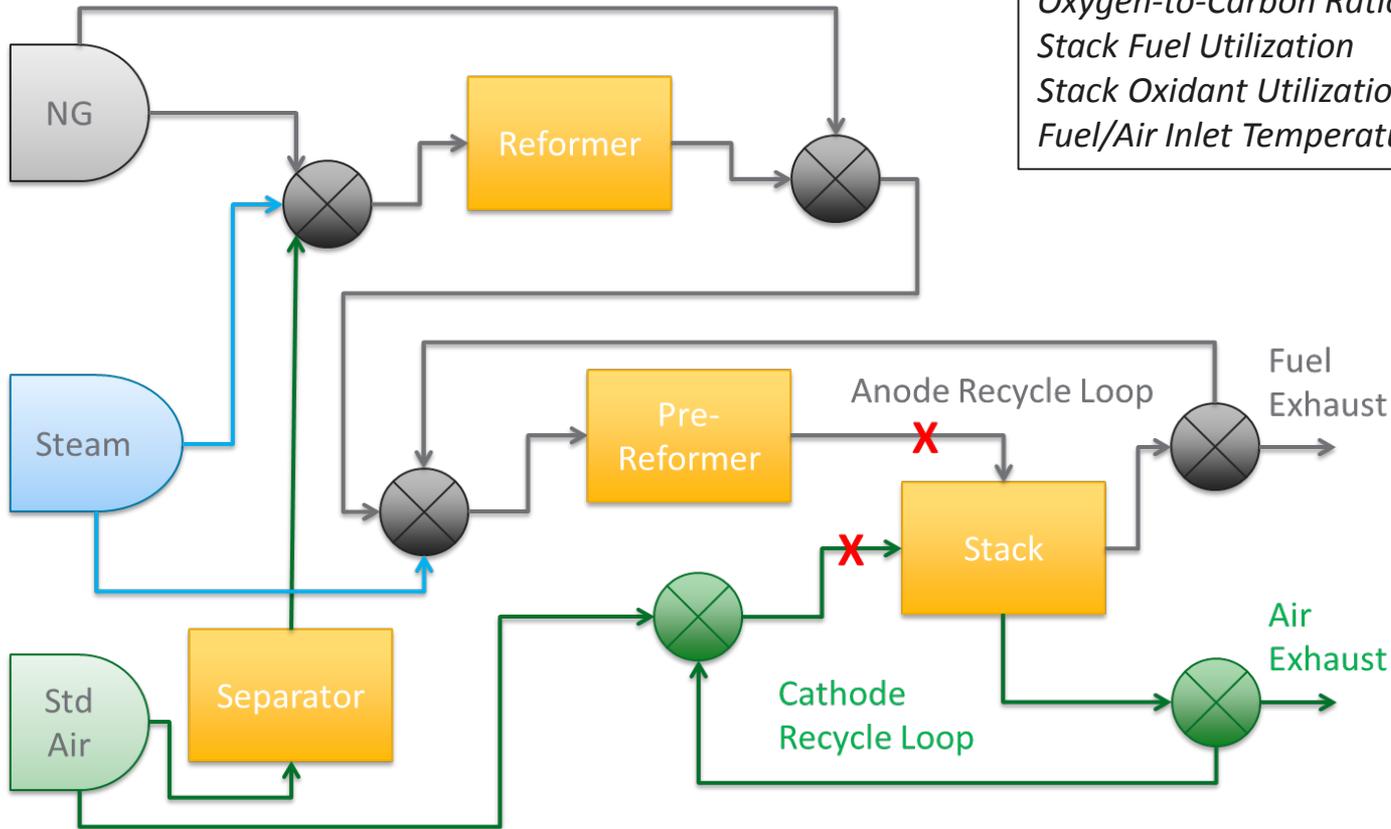
- Deviation between ROM predictions and SOFC-MP simulation results after removing each input parameter
- The parameter that induces the largest deviation after removing it from the ROM prediction has the highest sensitivity score (scaled to 100)



# ROMs for NETL System Analysis: NGFC Material Flowchart

► Baseline model is natural gas fuel cell (**NGFC**) system

■ 93% CH<sub>4</sub> requires external reformer



## ROM Input Parameters

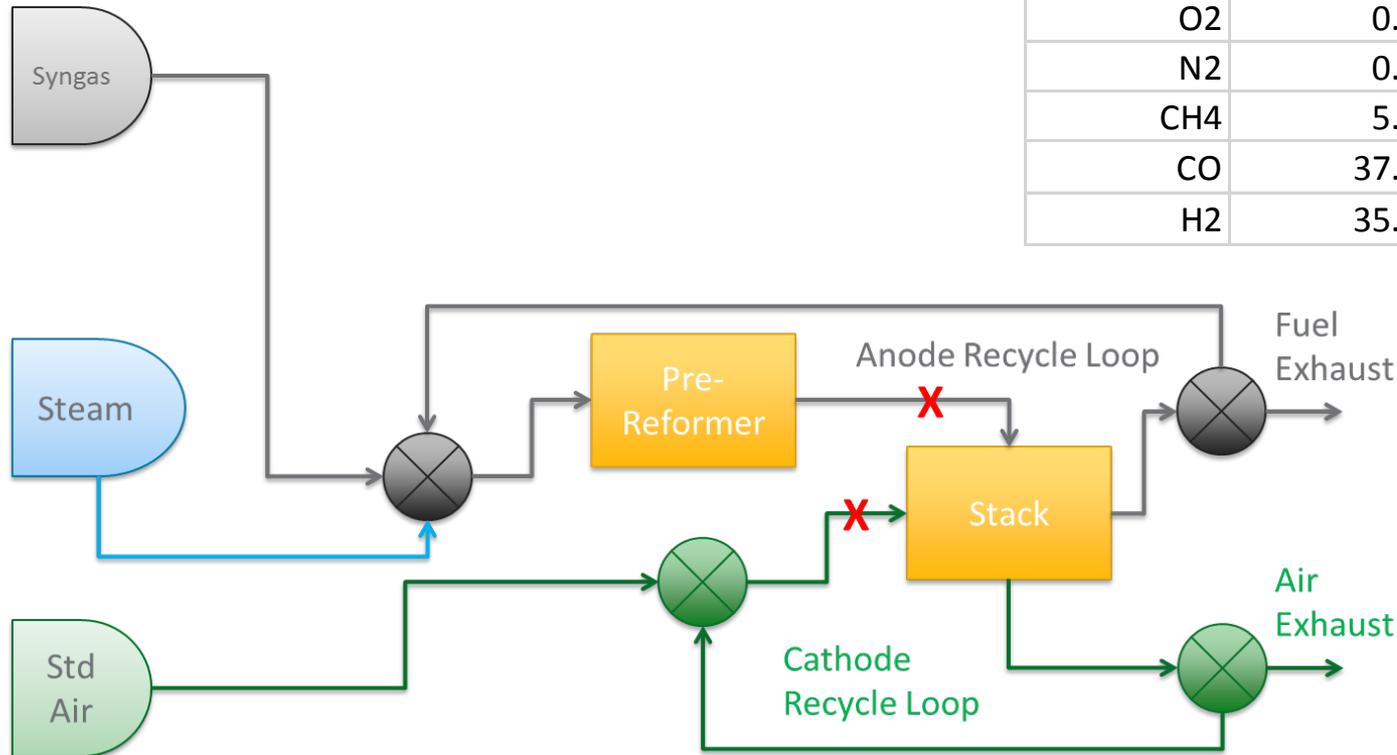
|                                   |                            |
|-----------------------------------|----------------------------|
| <i>Average Current Density</i>    | 2000-6000 A/m <sup>2</sup> |
| <i>Internal Reforming</i>         | 0-100%                     |
| <i>Oxidant Recirculation</i>      | 0-80%                      |
| <i>Oxygen-to-Carbon Ratio</i>     | 1.5-3.0                    |
| <i>Stack Fuel Utilization</i>     | 40-95%                     |
| <i>Stack Oxidant Utilization</i>  | 12.5-83.3%                 |
| <i>Fuel/Air Inlet Temperature</i> | 550-800°C                  |

## NG Composition

|       |       |
|-------|-------|
| H2O   | 0.0%  |
| Ar    | 0.0%  |
| CO2   | 1.0%  |
| O2    | 0.0%  |
| N2    | 1.6%  |
| CH4   | 93.1% |
| CO    | 0.0%  |
| H2    | 0.0%  |
| C2H6  | 3.2%  |
| C3H8  | 0.7%  |
| C4H10 | 0.4%  |

# ROMs for NETL System Analysis: IGFC Material Flowchart

- ▶ Reduced CH<sub>4</sub> composition of integrated gasification fuel cell (**IGFC**) syngas (6-32%) does not require the external reformer



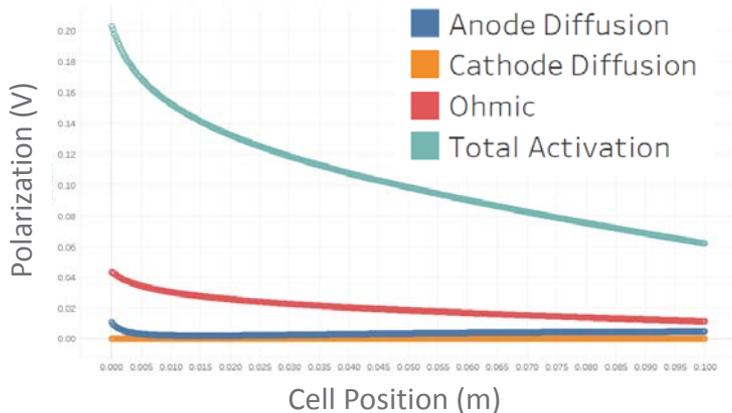
## Syngas Fuel Compositions

|                  | <u>Conventional</u> | <u>Enhanced</u> | <u>Catalytic</u> |
|------------------|---------------------|-----------------|------------------|
| H <sub>2</sub> O | 0.1%                | 0.1%            | 0.0%             |
| Ar               | 0.1%                | 0.1%            | 0.0%             |
| CO <sub>2</sub>  | 20.4%               | 24.2%           | 34.7%            |
| O <sub>2</sub>   | 0.0%                | 0.0%            | 0.0%             |
| N <sub>2</sub>   | 0.6%                | 0.6%            | 0.7%             |
| CH <sub>4</sub>  | 5.8%                | 10.2%           | 31.6%            |
| CO               | 37.7%               | 34.1%           | 9.1%             |
| H <sub>2</sub>   | 35.2%               | 30.6%           | 23.9%            |

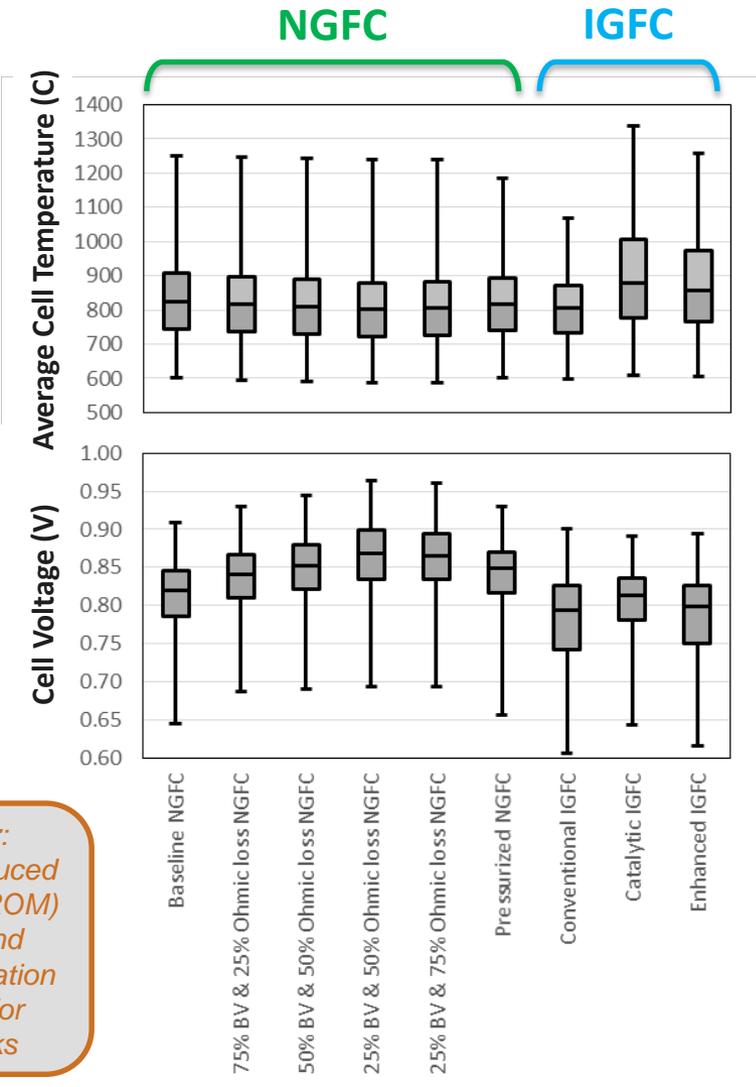
# ROM Usage for Power System Analysis

► **Collaborating with NETL** on ROMs for different stack operating performance levels and systems

- SOA atmospheric NGFC
- Future performance NGFC with reduced activation/ohmic losses
  - 25%-75% reduction combinations
- Pressurized NGFC
- IGFCs



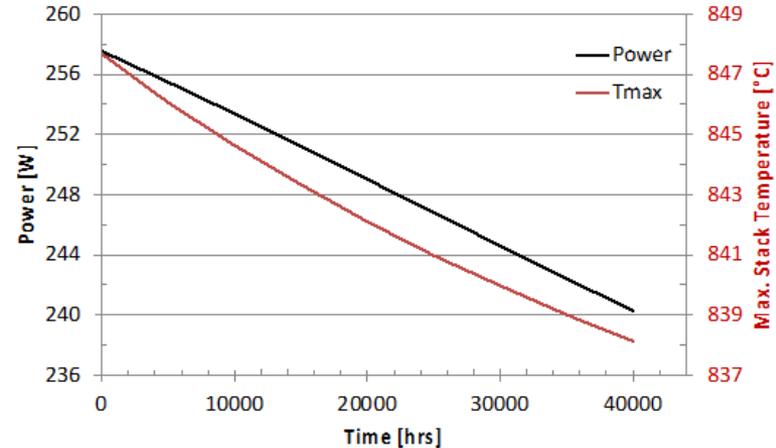
**See Poster:**  
*Advanced Reduced Order Model (ROM) Prediction and Error Quantification Framework for SOFC Stacks*



# Long-Term Stack Reliability: Degradation by Grain Coarsening

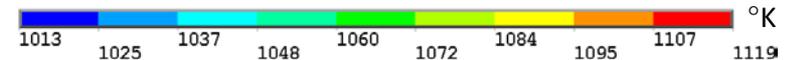
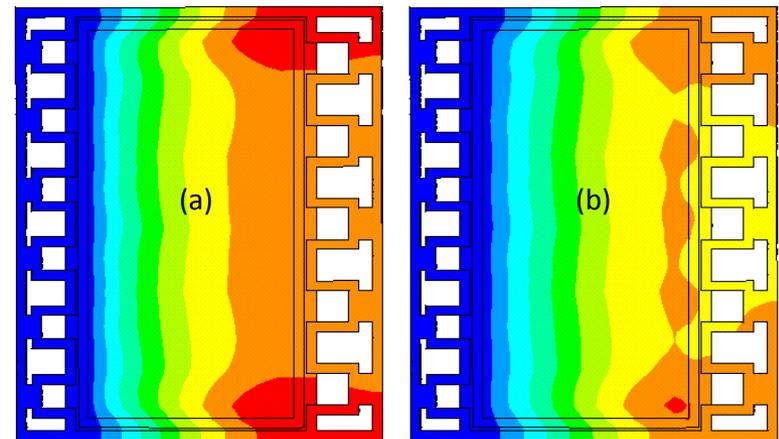
- ▶ Baseline 3D model for **single-cell, co-flow** cell operating at 750°C average temperature.
- ▶ Reliability evaluated at the beginning and end of operating life w/ **grain coarsening**.
- ▶ **Structural reliability increase** is predicted after long-term degradation due to **reduction in the stack peak temperatures and thermal gradients** at end-of-life conditions.

Power Degradation with Electrode Grain Coarsening



At t = 0 hours

At t = 40,000 hours



Initial and Degraded stack component reliability

| Stack Component              | Initial (t = 0 hrs) |                                      | Degraded (t = 40,000 hrs) |                                      |
|------------------------------|---------------------|--------------------------------------|---------------------------|--------------------------------------|
|                              | Max. Stress [Pa]    | Prob. Of Failure, P <sub>f</sub> (%) | Max. Stress [Pa]          | Prob. Of Failure, P <sub>f</sub> (%) |
| Air Seal                     | 4.70E+06            | 0                                    | 4.82E+06                  | 0                                    |
| Fuel Seal                    | 6.00E+06            | 0                                    | 6.05E+06                  | 0                                    |
| PEN Seal                     | 3.92E+06            | 0                                    | 3.90E+06                  | 0                                    |
| Electrolyte                  | 7.20E+07            | 3*                                   | 7.14E+07                  | 2*                                   |
| Anode                        | 8.10E+06            | 0                                    | 8.10E+06                  | 0                                    |
| Cathode                      | 9.71E+06            | 0                                    | 7.67E+06                  | 0                                    |
| Cathode Contact              | 1.95E+06            | 10                                   | 1.09E+06                  | 2                                    |
| Stack Overall P <sub>f</sub> | 12%                 |                                      | 4%                        |                                      |

NOTES: \*Localized risk of rupture at corners observed

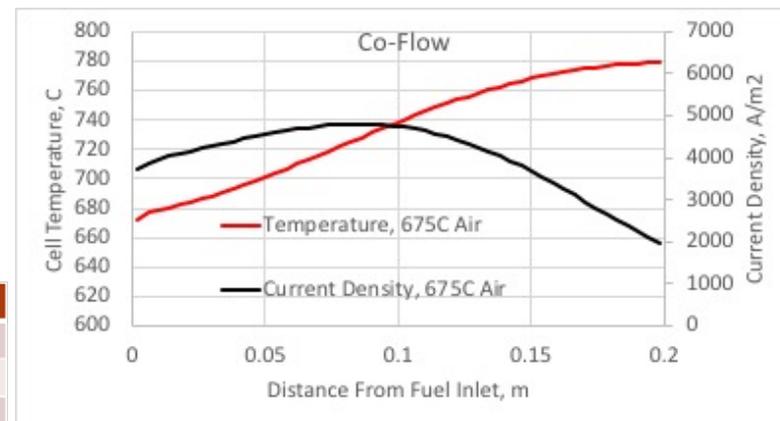
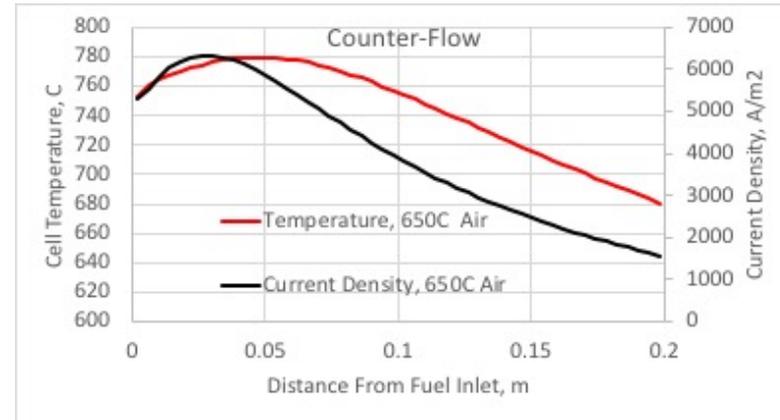
# Short-Term Reliability Study: Scoping Simulations w/ 2D Model

- ▶ Parameter ranges selected to focus structural simulation cases near **likely operating points** from the NGFC pathway evaluations
  - **Targeted 750°C average and 800°C maximum temperatures** at 400 mA/cm<sup>2</sup>
  - SOA and future NGFC operations (100% IR)
- ▶ Outputs of 2-D simulation sets show cathode inlet air temperature ranges can be focused down to a 50°C range
  - Use full range of fuel and air utilizations
  - Use three NG fuel compositions

## Input Parameters for 3D Model Cases

|                       | Counter-flow |         | Co-flow |         |
|-----------------------|--------------|---------|---------|---------|
|                       | Minimum      | Maximum | Minimum | Maximum |
| T <sub>air</sub> , °C | 650          | 700     | 675     | 725     |
| UA(stack), %          | 13.0         | 16.1    | 13.0    | 16.1    |
| UF(stack), %          | 68.8         | 84.4    | 68.8    | 84.4    |
| Fuel Composition      | All          | All     | All     | All     |

## Set #1 Case Results



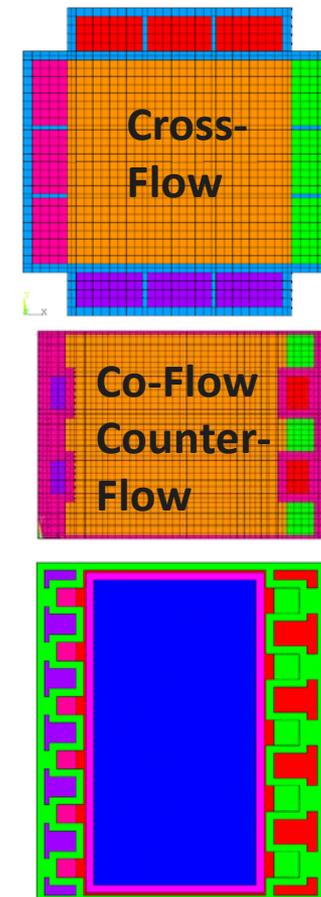
**See Poster: Optimal Operating Conditions for Performance and Reliability of Solid Oxide Fuel Cells**

# Design of Experiments (DOE) Approach: Effect of Fuel Compositions & Geometry

## Fuel Compositions and Flow Rates (20% Pre-Reformed with Anode Recycle)

| Species %                                               | Fuel species entering the stack (high UF) |                                   |                                    |
|---------------------------------------------------------|-------------------------------------------|-----------------------------------|------------------------------------|
|                                                         | Composition #1<br>60% IR, 2.1 OCR         | Composition #2<br>60% IR, 2.6 OCR | Composition #3<br>100% IR, 2.1 OCR |
| H <sub>2</sub> O                                        | 32.65                                     | 41.44                             | 36.25                              |
| Ar                                                      | 0.02557                                   | 0.0243                            | 0                                  |
| CO <sub>2</sub>                                         | 15.65                                     | 19.22                             | 22.79                              |
| O <sub>2</sub>                                          | 0                                         | 0                                 | 0                                  |
| N <sub>2</sub>                                          | 0.5620                                    | 0.5356                            | 0.6514                             |
| CH <sub>4</sub>                                         | 9.165                                     | 6.393                             | 12.37                              |
| CO                                                      | 10.77                                     | 8.304                             | 7.259                              |
| H <sub>2</sub>                                          | 31.18                                     | 24.09                             | 20.67                              |
| C <sub>2</sub> H <sub>6</sub>                           | 0                                         | 0                                 | 0                                  |
| C <sub>3</sub> H <sub>8</sub>                           | 0                                         | 0                                 | 0                                  |
| C <sub>4</sub> H <sub>10</sub>                          | 0                                         | 0                                 | 0                                  |
| Fuel flow rate, mol/s-cell (20x20 cm <sup>2</sup> cell) |                                           |                                   |                                    |
| High UF                                                 | 1.250E-03                                 | 1.792E-03                         | 1.362E-03                          |
| Low UF                                                  | 1.557E-03                                 | 2.447E-03                         | 1.956E-03                          |

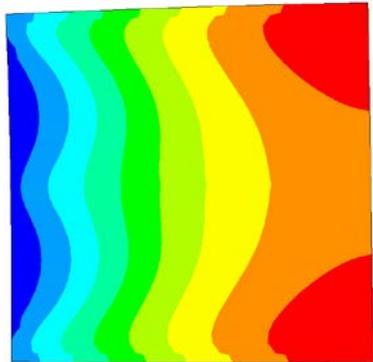
## Cell Geometry



# Effect of Composition on Reliability

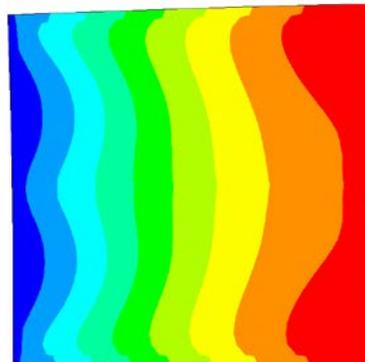
- ▶ **Significant variation in cell reliability** for **similar power output** under varying combination of air temperature and fuel/air flow rates
- ▶ Higher OCR fuel (with higher flow rates) increased reliability
- ▶ Fuel with 100% internal reforming significantly increased reliability

Comp1: 60%IR, 2.1 OCR



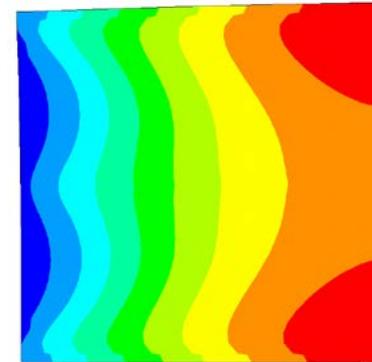
$T_{avg} = 789^{\circ}\text{C}$

Comp2: 60%IR, 2.6 OCR

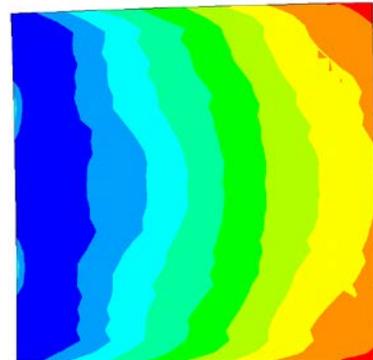


$T_{avg} = 782^{\circ}\text{C}$

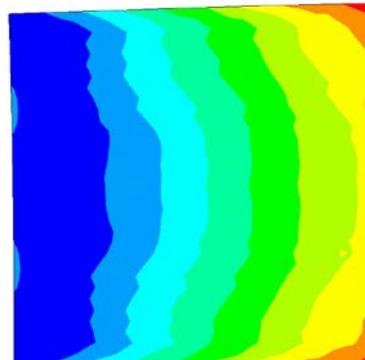
Comp3: 100%IR, 2.1 OCR



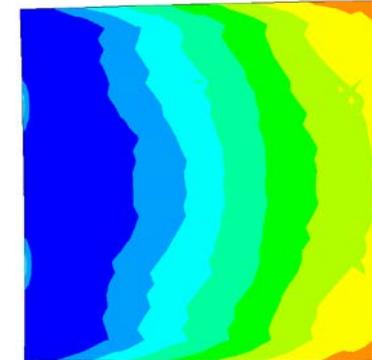
$T_{avg} = 763^{\circ}\text{C}$



$P_f = 11.5\%$   
54 MPa



$P_f = 5\%$   
51.2 MPa



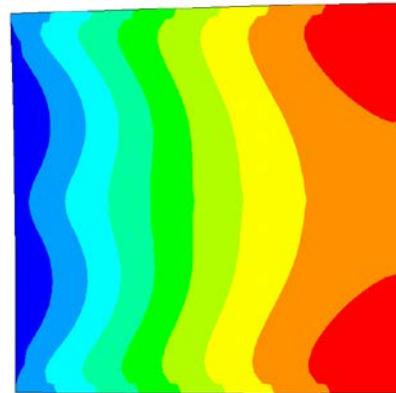
$P_f = 0.1\%$   
34 MPa

# Effect of Flow Configuration on Reliability

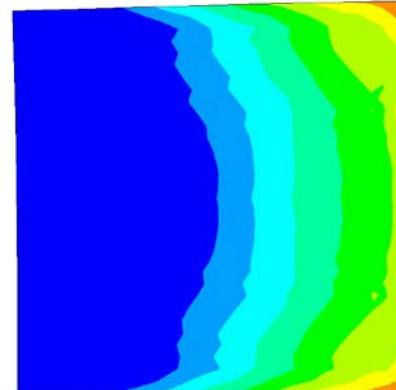
- ▶ Evaluated Composition 1 (60% IR, 2.1 OCR) for co- and counter-flow geometry
- ▶ **Similar power output could be produced in counter flow configuration with lower air temperatures**
- ▶ When same conditions of air temperature, air and fuel flow rates are maintained, the counter flow configuration produced **lower  $T_{avg}$  but higher  $P_f$  because of increased temperature gradient** across the cell.

## Co-flow

$$P = 132W$$
$$T_{avg} = 737^{\circ}C$$
$$\Delta T = 112^{\circ}C$$

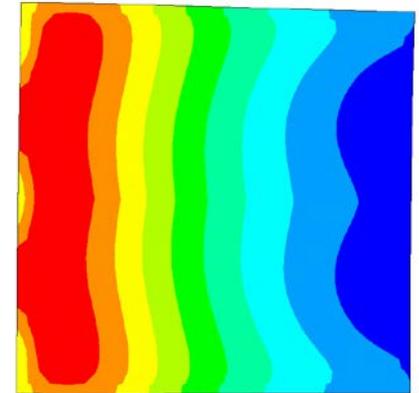


44 MPa max,  $P_f = 0.2\%$

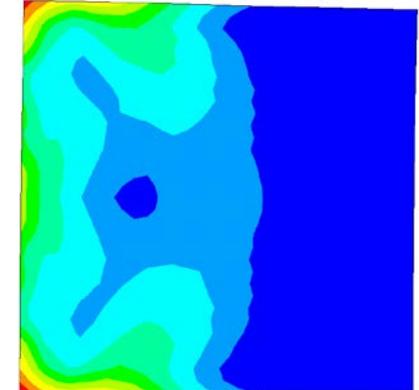


## Counter-flow

$$P = 133W$$
$$T_{avg} = 732^{\circ}C$$
$$\Delta T = 123^{\circ}C$$



59 MPa max,  $P_f = 1.1\%$



# Domain for Co-flow Design (Composition 1)

► **Desirability function approach** to find optimal solution

► Optimization Constraints:

- Power > 130 W
- $P_f < 5\%$
- $T_{avg} < 750^\circ\text{C}$
- $\Delta T$  not constrained

► **Optimal solution** of  $D=0.87$

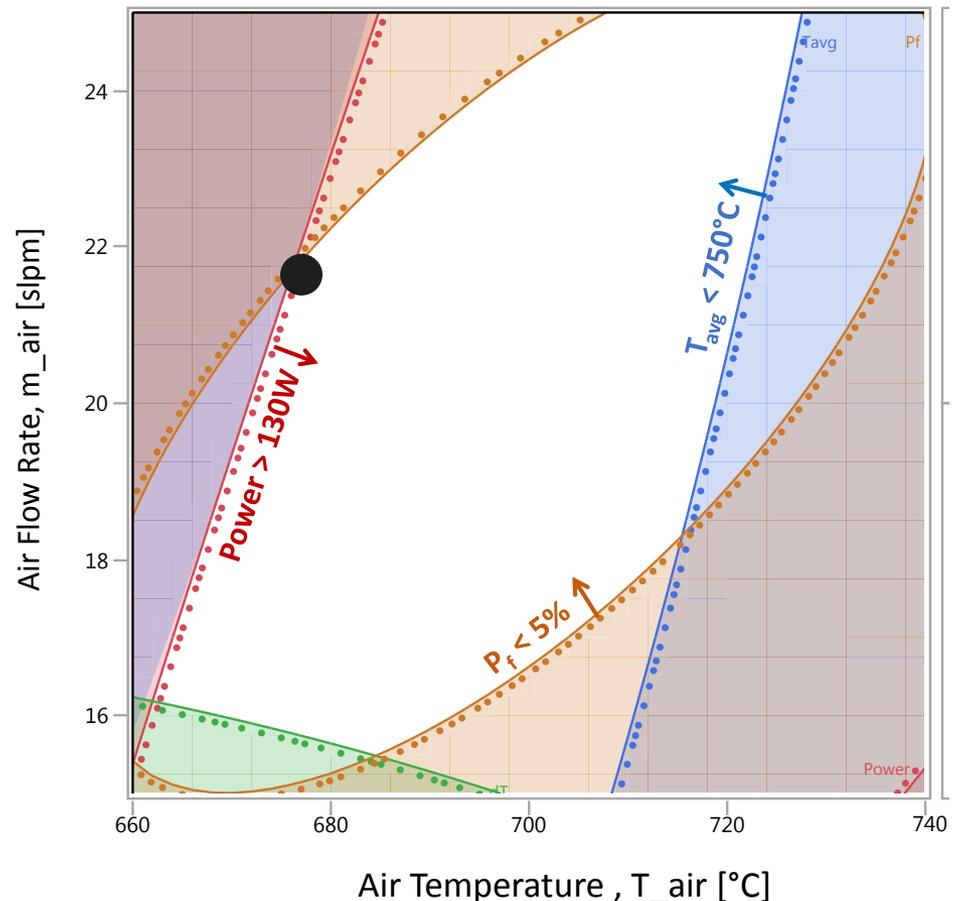
► Required Input:

- $T_{air} = 675^\circ\text{C}$
- $m_{air} = 21.26$  slpm (AU $\approx$ 15%)
- $m_{fuel} = 2.8$  slpm (FU $\approx$ 77%)

► Optimal Output:

- $P = 133.5\text{W}$
- $P_f = 4\%$
- $T_{avg} = 729^\circ\text{C}$

| Response | Contour | Current Y | Lo Limit | Hi Limit |
|----------|---------|-----------|----------|----------|
| Power    | 133.35  | 130.26248 | 133.35   | 140      |
| dT       | 125     | 86.593723 | 75       | 125      |
| Tavg     | 775     | 702.19036 | 728.7    | 775      |
| Pf       | 0.05    | 0.5046274 | -1       | 0.05     |



# FY18 Modeling Summary: Accomplishments and Next Steps

## ▶ Accomplishments

- Developed ***adaptive sampling*** approach to improve response surfaces
- Used cross-validation technique to quantify the ***error distribution*** and generate ***point and interval estimates***
- ***Developed tools and user interface*** for ***high performance computing*** for stack simulations and ROM generation
- ***Provided ROMs to NETL*** for system design and COE analyses
  - SOA and future performance for different system configurations
- Evaluated ***effects of operating conditions and flow geometry*** on electrical and structural performance
  - Identified ***local optimal condition*** for the cell based on ***mechanical reliability***

## ▶ Next Steps

- Continue to ***work with NETL*** staff to use the modeling tools to help ***identify target performance goals*** for SOFC power systems.
- ***Complete ROM tool GUI*** with error quantification this year
- Incorporate ***structural reliability performance*** in the ROM tool

- ▶ PNNL is using experimental and computational capabilities to accelerate the commercialization of SOFC power systems.
  
- ▶ Posters
  - LSM/YSZ Button Cell Tests in Cathode Air with Measured Cr Concentrations (John Hardy)
  - Cr Mitigation by LSCF-based Materials for Solid Oxide Fuel Cells (Matt Chou)
  - Composite Approach to Tailoring Thermal Expansion of LSCF-based Ceramic Cathode Contact for Solid Oxide Fuel Cell Applications (Matt Chou)
  - Long Term Stability Tests of Low Temperature and Standard Reactive Air Aluminization (Jung-Pyung Choi)
  - Advanced Reduced Order Model (ROM) Prediction and Error Quantification Framework for SOFC Stacks (Chao Wang)
  - Optimal Operating Conditions for Performance and Reliability of Solid Oxide Fuel Cells (Kurt Recknagle)
  - Small-Scale Test Platform (SSTP) for SOFC Stacks (Brent Kirby)
  - Air Braze Optimization for Markets Targeted by Aegis Technology, Inc. (John Hardy)

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