Progress of the NETL Solid Oxide Fuel Cell Research Portfolio

NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DOE Hydrogen and Fuel Cells Program 2020 Annual Merit Review and Peer Evaluation Meeting

Gregory A. Hackett, Ph.D. – Team Lead
NETL Research and Innovation Center

June 3, 2020

Harry Abernathy, Ph.D.
Shiwoo Lee, Ph.D.
Tom Kalapos, Ph.D.

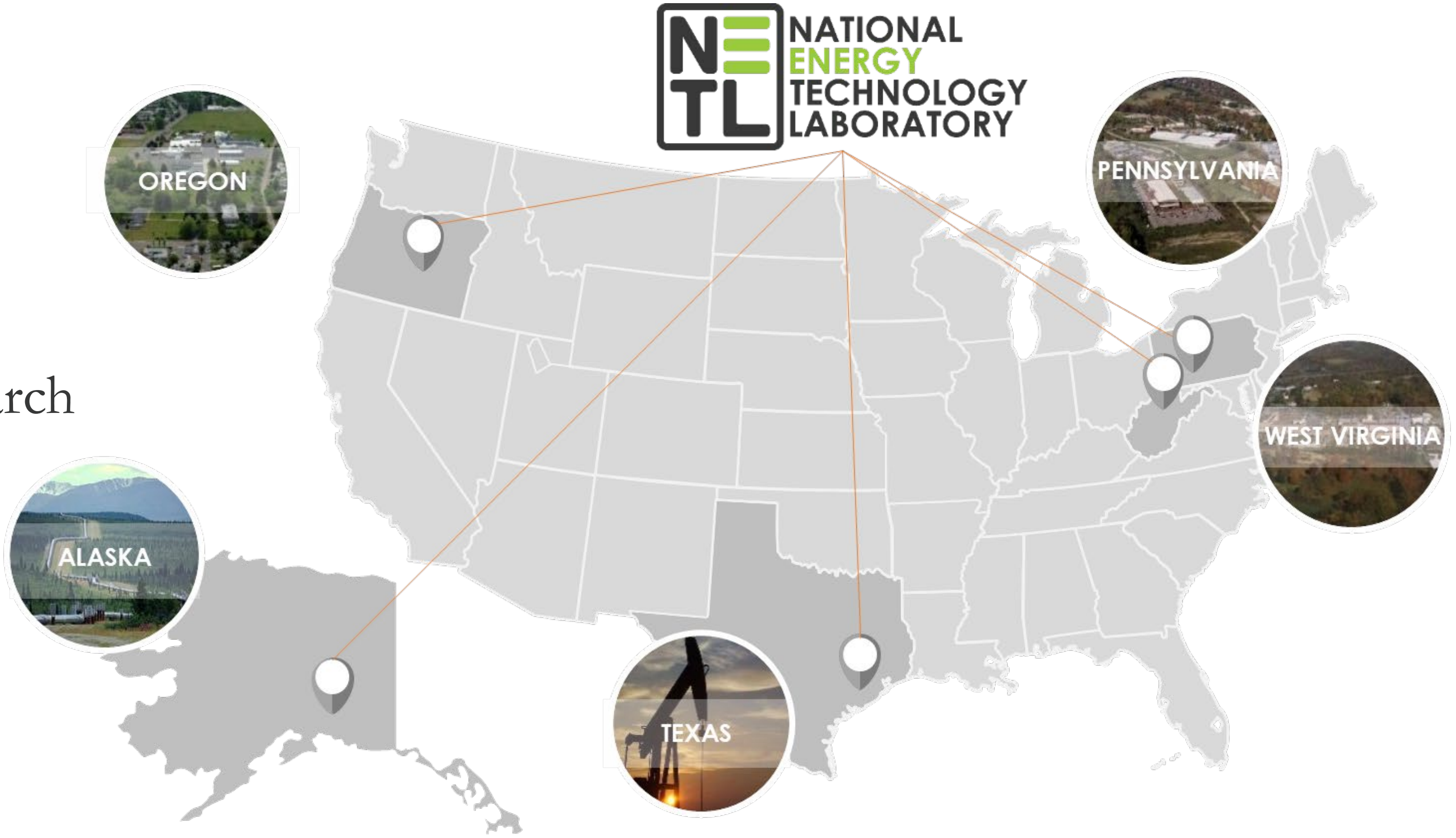
Solutions for Today | Options for Tomorrow

U.S. DEPARTMENT OF ENERGY

Outline

- **NETL SOFC Research Team (EY20)**

- **NETL SOFC Research Portfolio**
  - Electrode Engineering Research and Development Progress
  - Cell and Stack Degradation Evaluation and Modeling Progress
  - Systems Engineering and Analysis Progress



NETL SOFC Research Team

NATIONAL ENERGY TECHNOLOGY LABORATORY

NETL (Federal Staff)
- Gregory Hackett, Team Lead (NETL)
- Travis Shultz (NETL)
- Rich Pineault (NETL)
- Yves Mantz (NETL)
- Yuhua Duan (NETL)
- Slava Romanov (NETL)
- Youhai Wen (NETL)
- Dustin McIntyre (NETL)
- Jonathan Lekse (NETL)

West Virginia University
- Harry Finklea (Chemistry Emeritus)
- Ismail Celik (MAE Emeritus)
- David Mebane (MAE)
- Ed Sabolsky (MAE)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corporation)
- Bo Guan (WV Research Corporation)
- Jose Bohorquez (MAE, Student)

NETL (Site Support Team)
- Tom Kalapos (LRST)
- Harry Abernathy (LRST)
- Shiwoo Lee (LRST)
- Arun Iyengar (KeyLogic)
- Lynn Fan (LRST)
- Rick Addis (USSE2)
- Tianle Cheng (LRST)
- Youngseok Jee (LRST)
- Jian (Jay) Liu (LRST)
- Yueh-Lin Lee (LRST)
- Tao Yang (LRST)
- Yinkai Lei (LRST)
- Giuseppe Brunello (LRST)
- Billy Epting (LRST)
- Hunter Mason (LRST)
- Yoosuf Picard (LRST)

TARGETED FOCUS:
Collaboration
Technology Transfer
Open source tool development

Carnegie Mellon University
- Paul Salvador (MSE)
- Shawn Litster (MechE)
- Tony Rollett (MSE)
- Tim Hsu (MSE)
- Hokon Kim (MSE, Grad. Student)
- Randall Doane (MSE, Grad Student
- Elizabeth Holm (MSE)

Clemson University
- Kyle Brinkman (MSE - Chair)
- Jack Duffy (MSE)

Penn State University
- Long-Qing Chen (MSE)
- Yanzhou Ji (MSE, Student)

University of Wisconsin-Madison
- Dane Morgan (MSE)
- Ryan Jacobs (MSE)

Wake Forest University
- Michael Gross (Chemistry)
- Sixbert Muhoza (Post-Doc)

Western Carolina University
- Hayri Sezer (Engineering)

Currently 50+ SOFC Team Members

NETL SOFC Field Work Proposal Overview

Enabling SOFC Technology through Research and Development at NETL

Cell and Stack Degradation Modeling

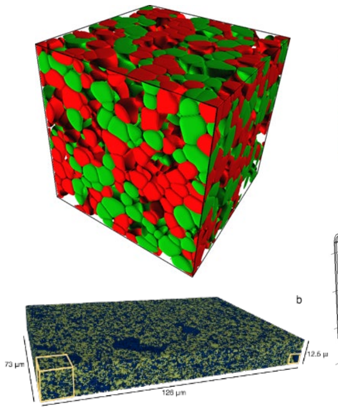
- Degradation Prediction Tools
- Atoms to system scale bridging
- Experimental Validation
- HT Fiber-Optic Sensors

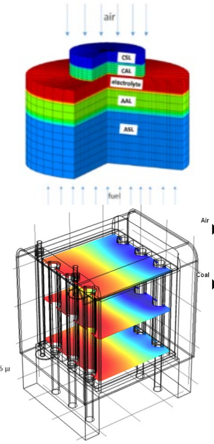
Electrode Engineering

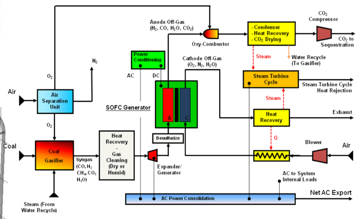
- Mitigation
- Microstructure Optimization
- Technology Transfer
- Reversible Operation

Systems Engineering and Analysis

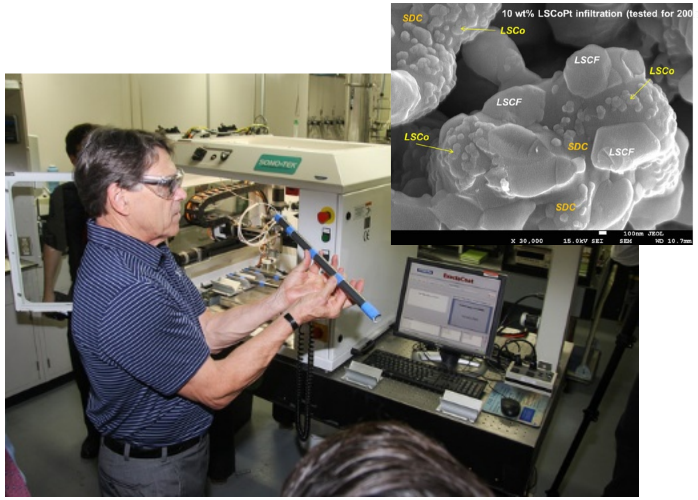
- Public Dissemination of Results
- Hybrid Configuration Assessment
- R&D Goals Evaluation

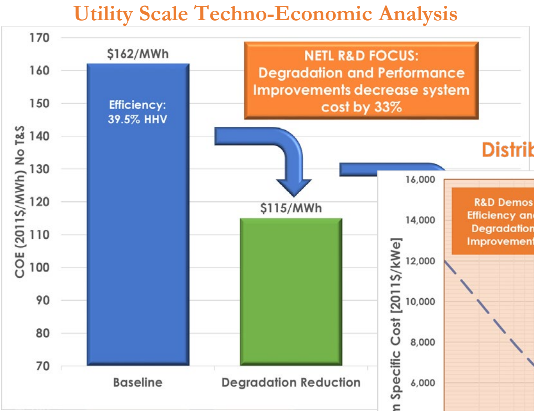


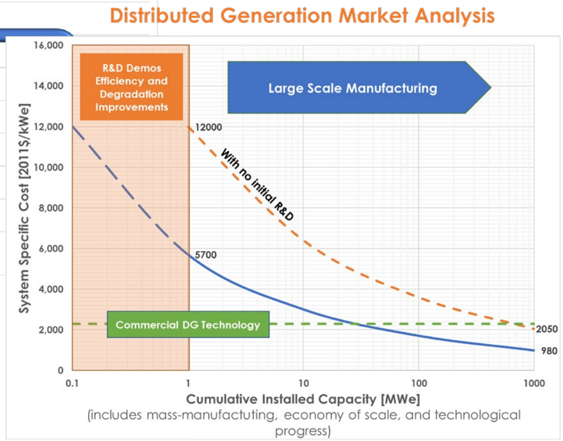




Increasing Scale







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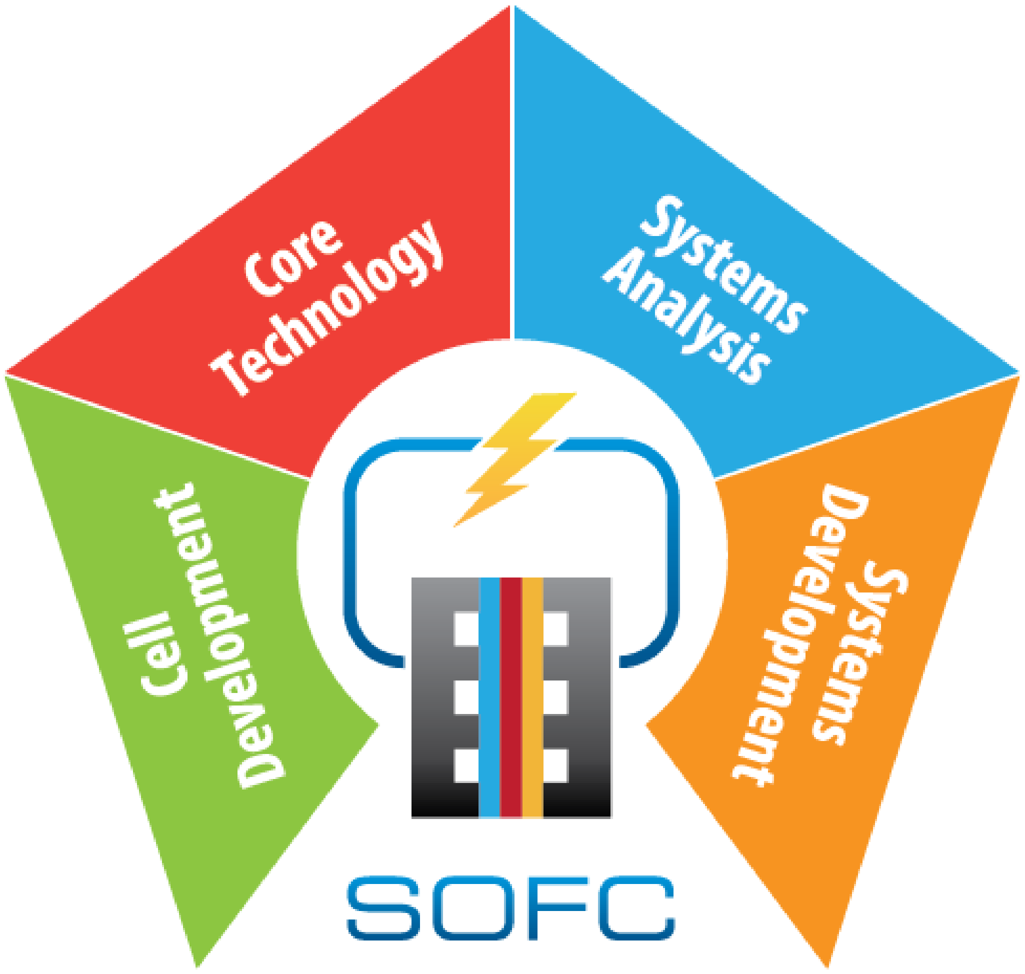
Performance Enhancement & Degradation Mitigation

SOFC Electrode Engineering



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SOFC Electrode Design and Engineering

Designing, Developing, and Deploying Advanced Electrode Engineering Techniques

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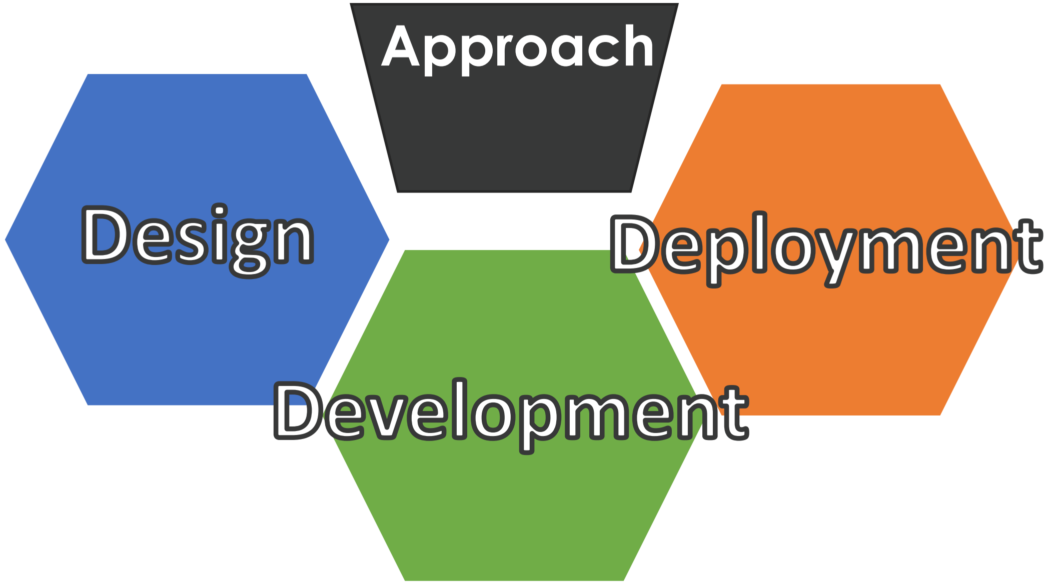
- **Objectives**
  - Enhancement of electrode performance and longevity
  - Materials engineering
  - Microstructure engineering
- **Benefits**
  - Stack cost reduction
  - Cell overpotential reduction
  - Thermo-chemical / thermo-mechanical stability increase



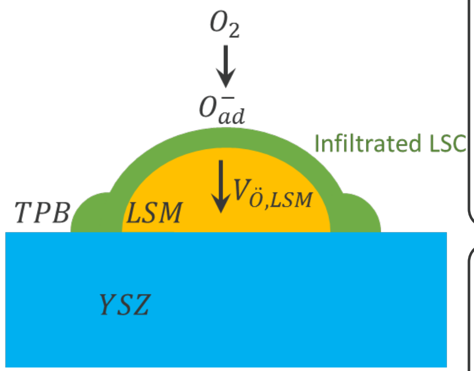
DESIGN of materials and nanostructures

DEVELOPMENT through tailored electrode construction

DEPLOYMENT in commercial SOFC systems

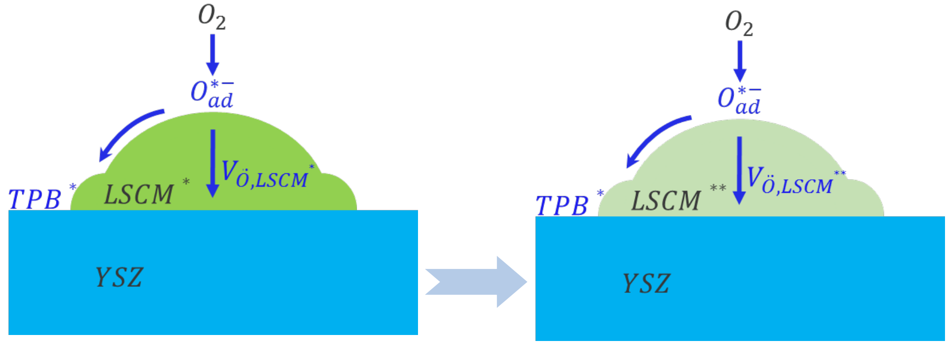
Modeling of Infiltrated Electrode

Performance of infiltrated LSM/YSZ composite cathodes is investigated via multi-physics simulations with a multistep charge transfer oxygen reduction reaction (ORR) mechanism.

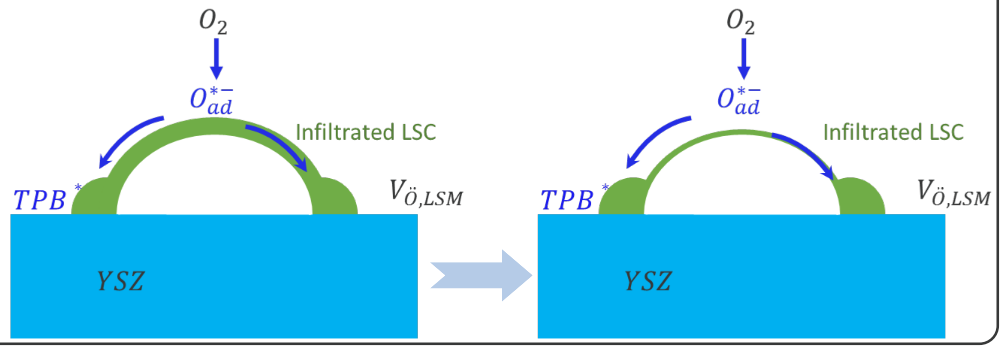


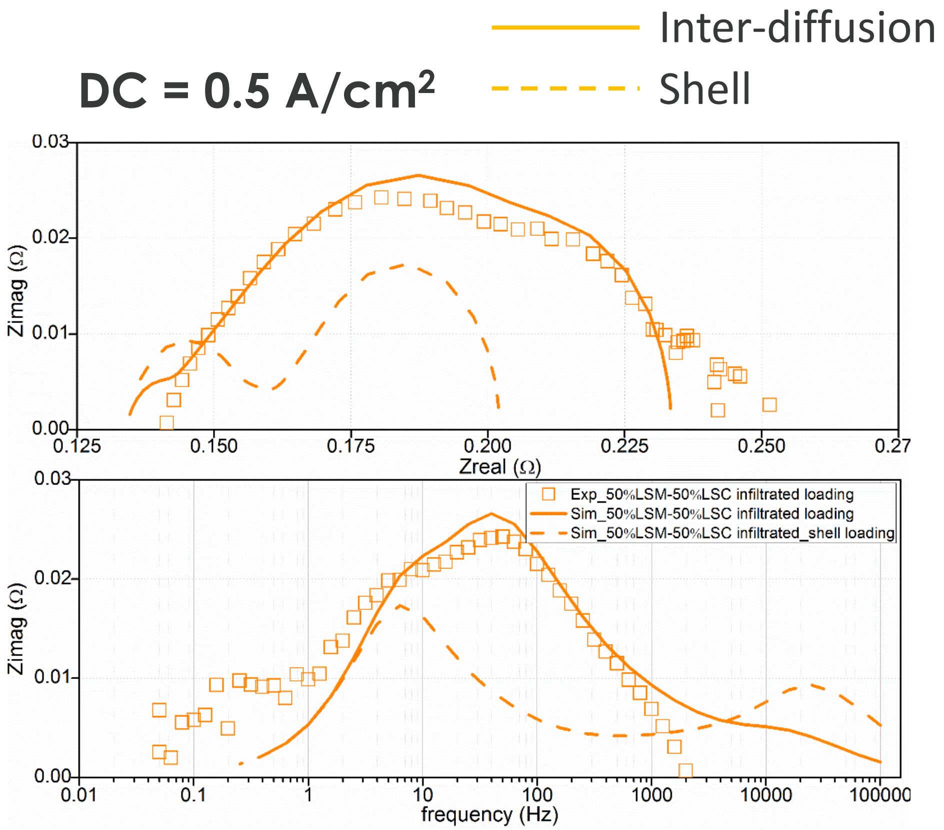
LSC infiltrated LSM/YSZ cathode: Inter-diffusion Model vs. Shell Model

Inter-diffusion model



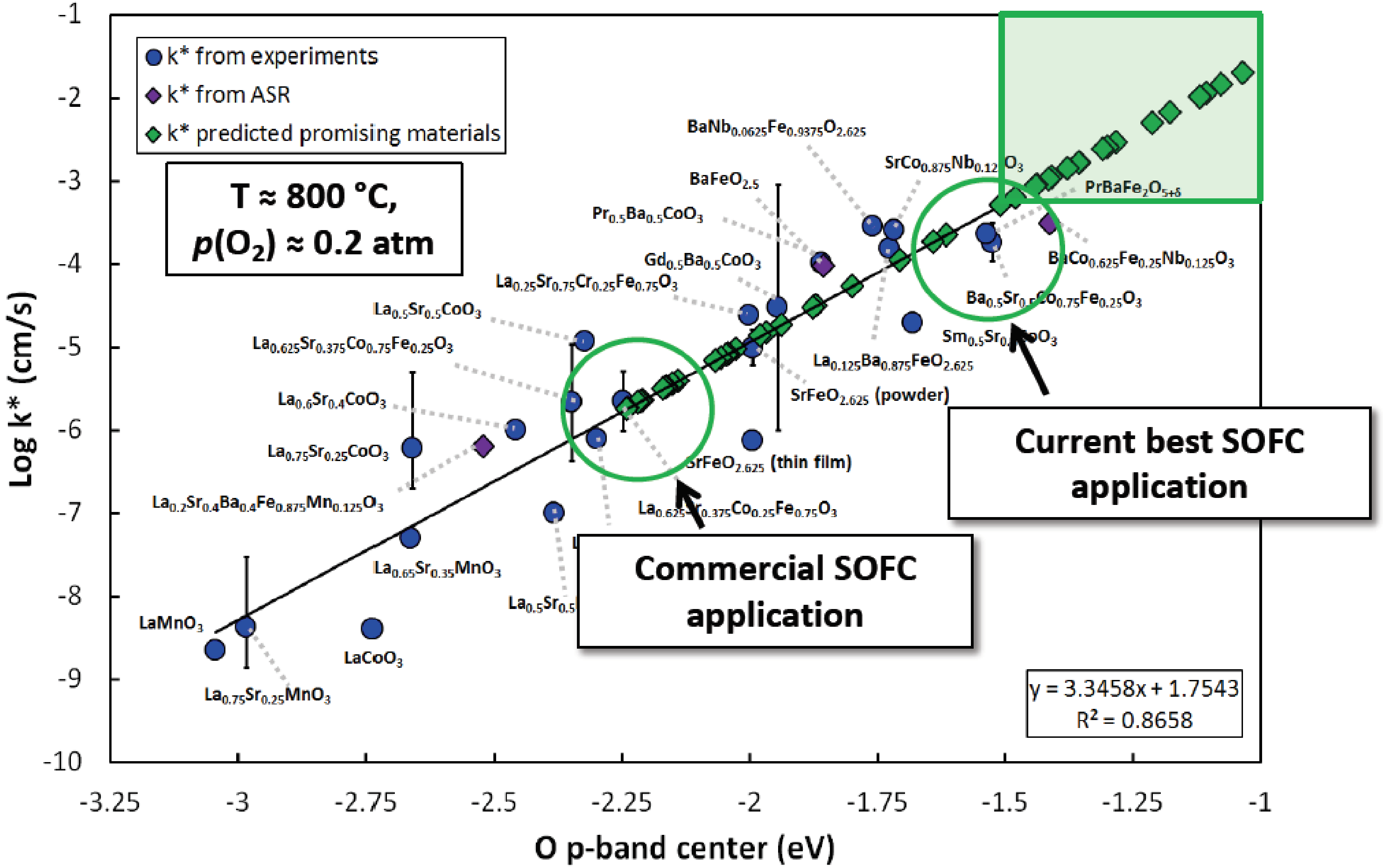
Shell model





Electrode Design and Engineering

Computational Design of Materials



- Utilizing computational chemistry techniques such as density functional theory, we can theorize a more active electrode material

- Theory shows that there are several materials with the potential to be exceptionally active compared to today's materials.

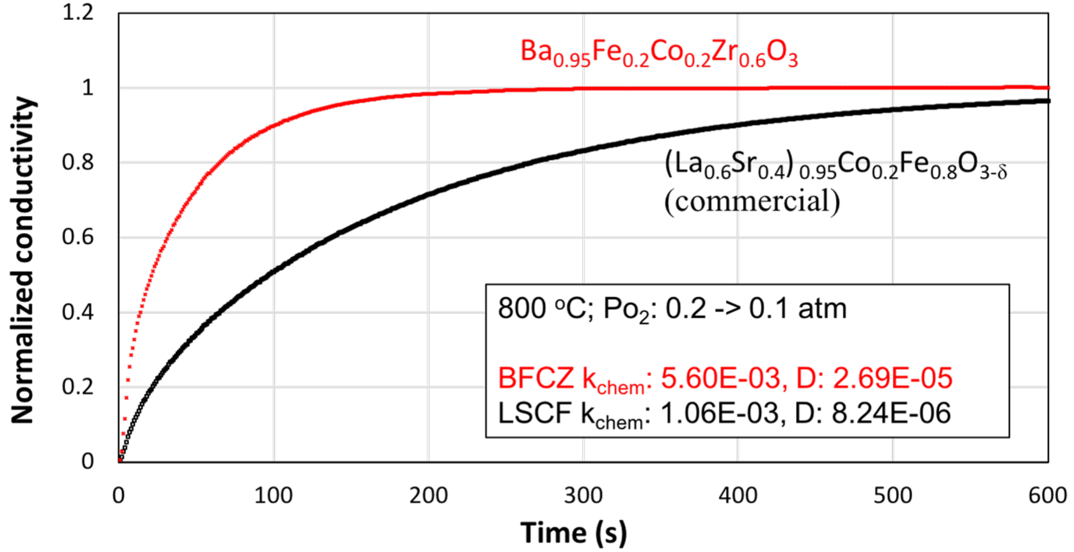
Linear correlation of k* and O *p*-band center [1]

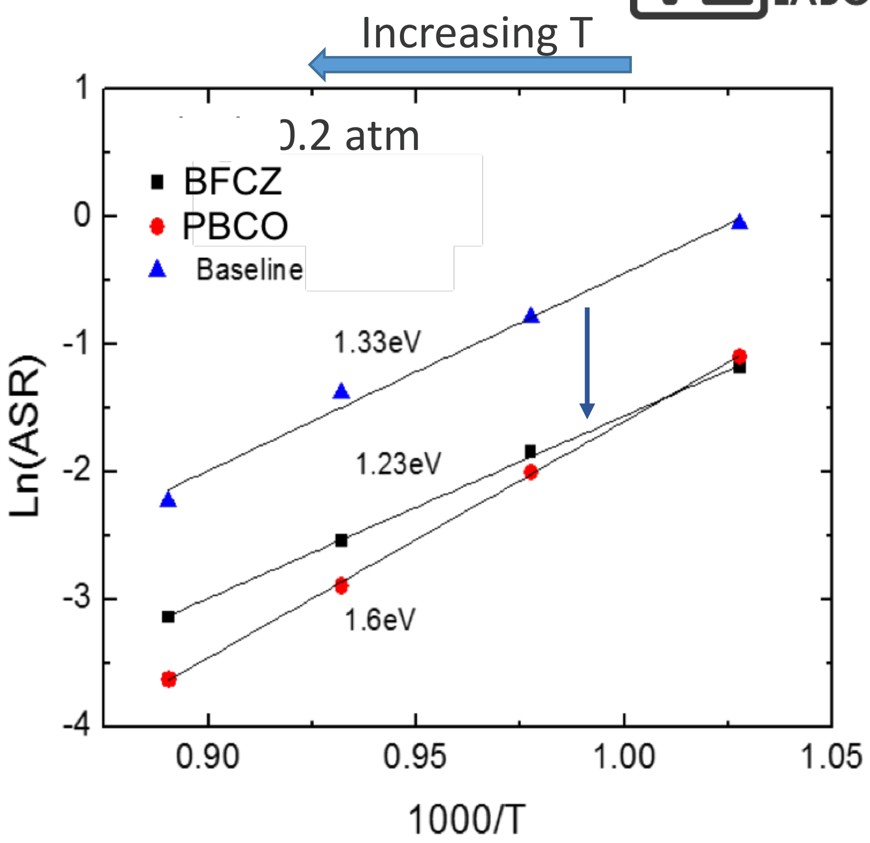
[1] R. Jacobs et al., *Adv. Energy Mater.* (2018)

Computational Design of Materials

Experimental Verification

ECR tests on $Ba_{0.95}Fe_{0.2}Co_{0.2}Zr_{0.6}O_3$ (BFCZ60)

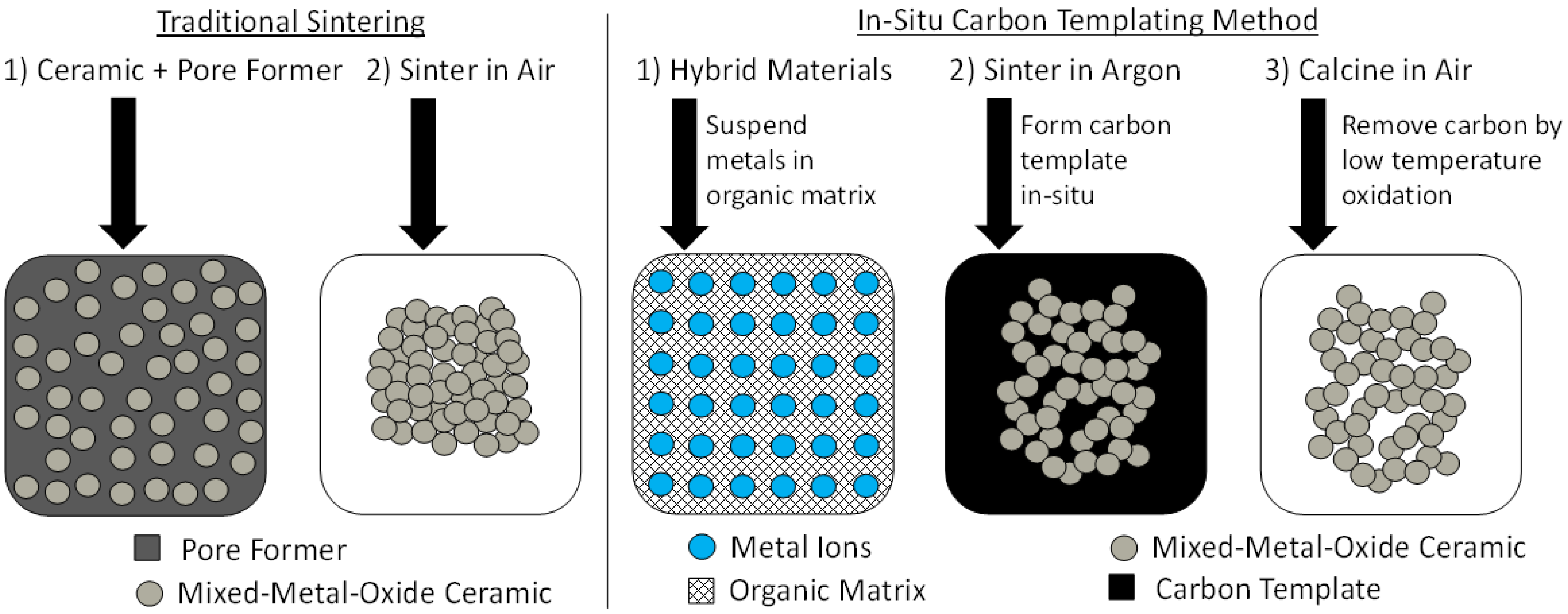


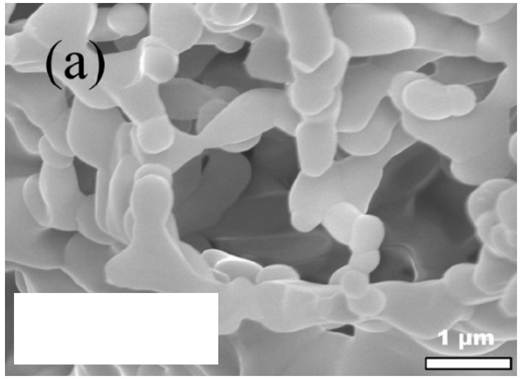


- ECR measurements on BFCZ containing 60% Zr resulted in 5× higher k_{chem} and 3× higher D_{chem} than LSCF
- Infiltration of LSM cathode with BFCZ containing 75% Zr resulted in reduced ASR by about 10×, and comparable performance to $(PrBa)_2Co_2O_{5+x}$

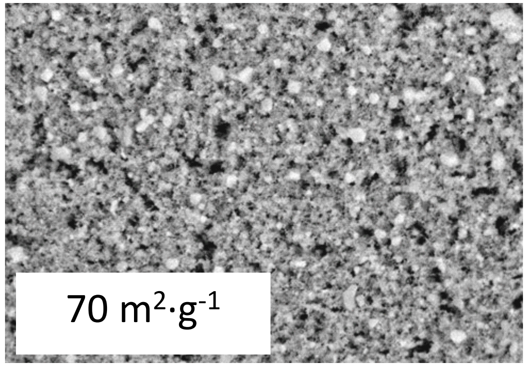
Electrode Design and Engineering

Hybrid Materials-Assisted Templating





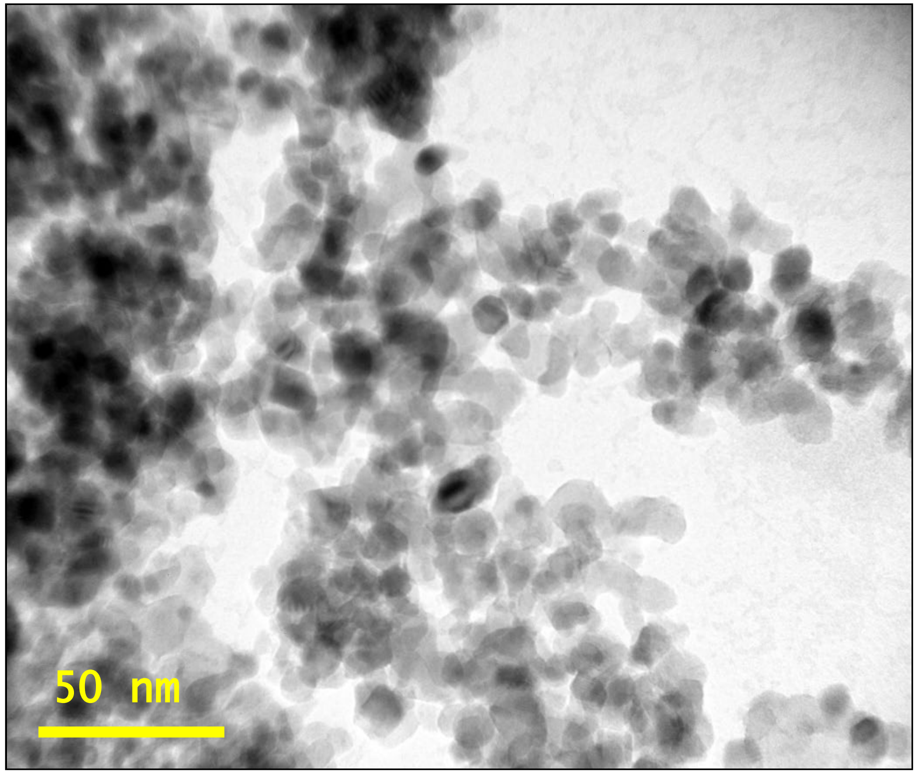
Traditional sintering



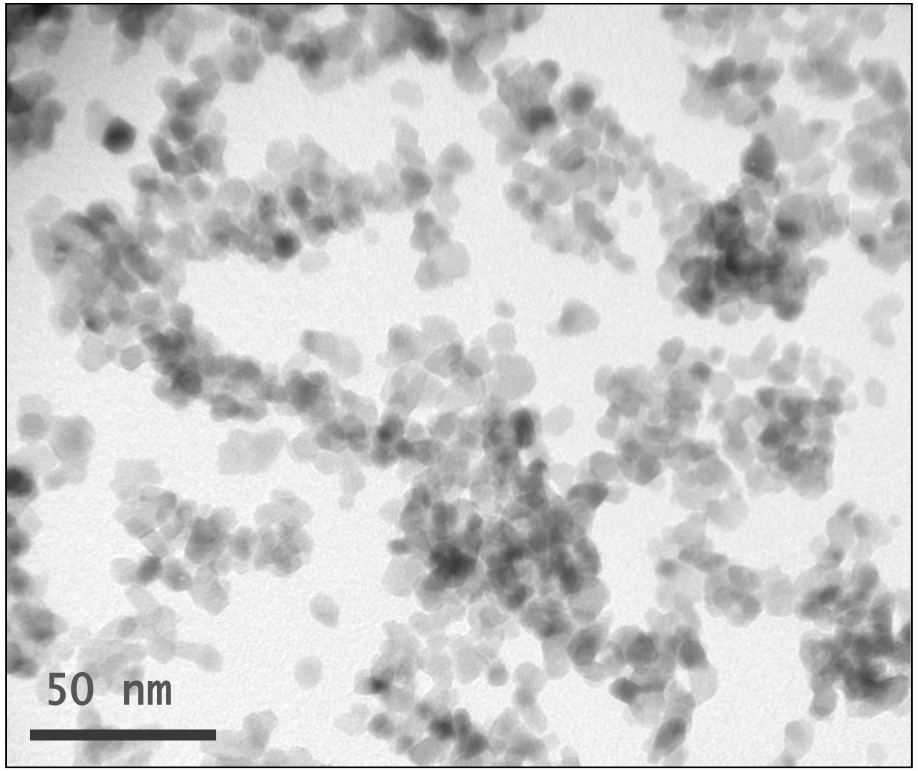
In-situ carbon templating

Hybrid Materials-Assisted Templating

YSZ - 850°C in N_2, 700° C in Air



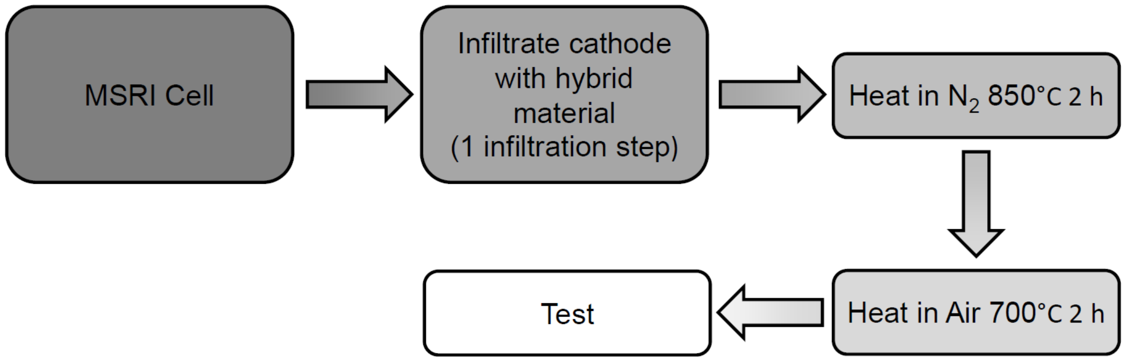
YSZ - 1250°C in N_2, 700° C in Air



The properties of the nanoparticles are controlled by varying the processing conditions

Hybrid Materials-Assisted Templating

<u>MSRI Cells Infiltrated with nanoLSCF or nanoYSZ</u>

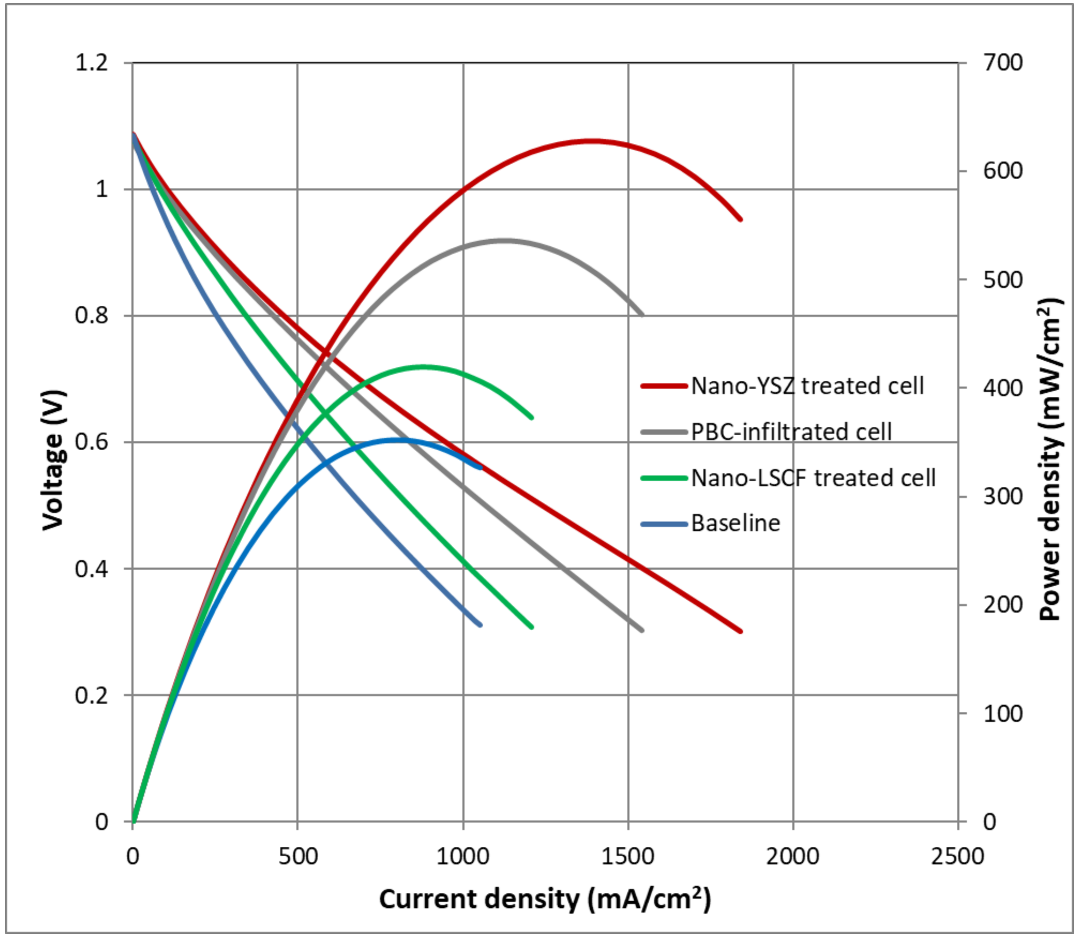


Degradation rate of cell voltage

PBC infiltrated cell: 3.1 % / 200 h

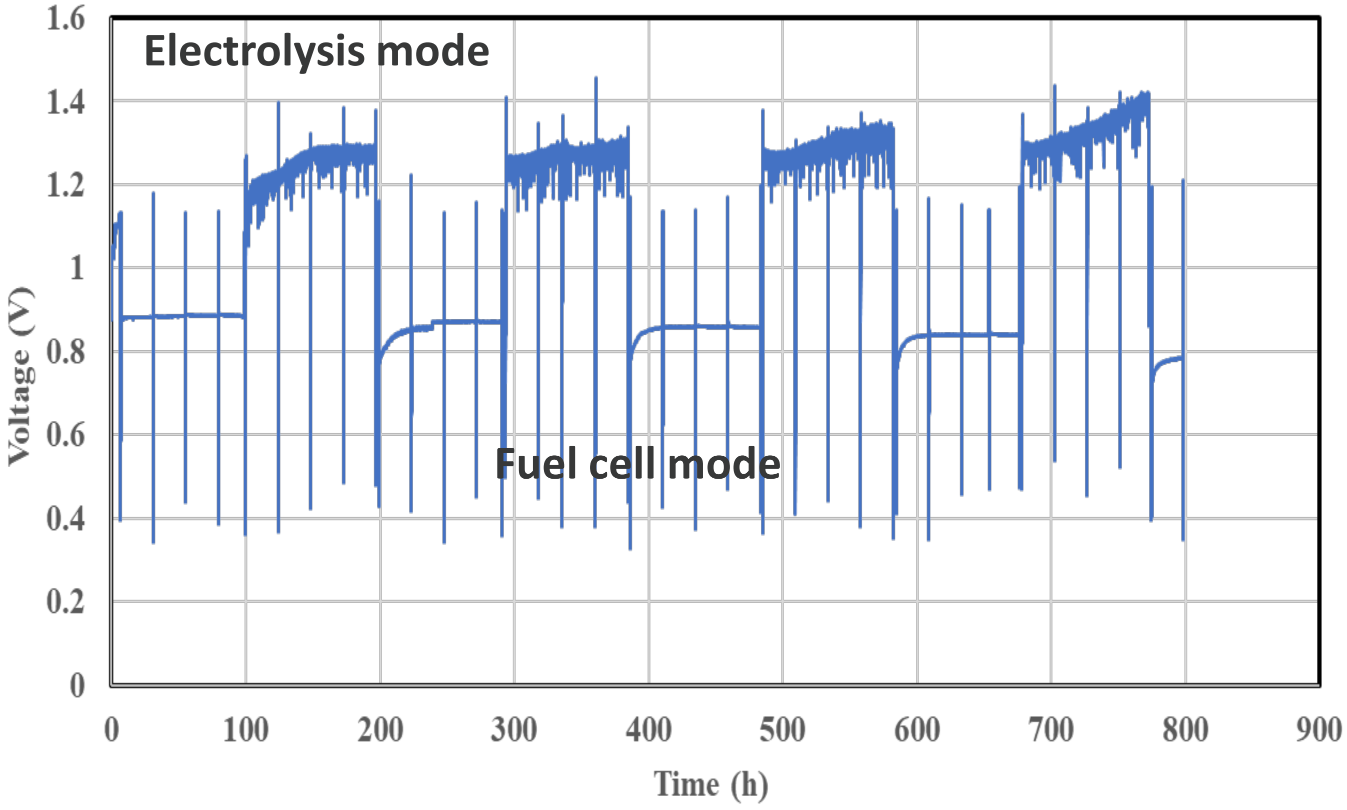
Nano-YSZ infiltrated cell: 0.7 % / 200 h

MSRI Cells Infiltrated with nanoLSCF or nanoYSZ

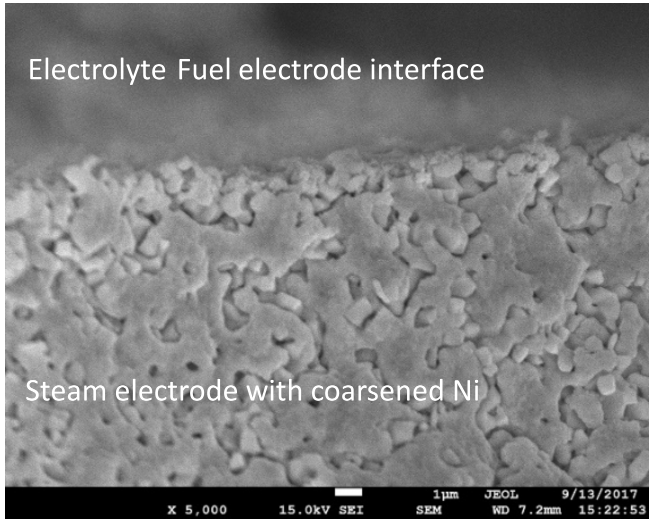


Reversible Mode Operation

New Effort – Reversible Mode Operation



- Anode-supported commercial cell (**LSM/YSZ cathode**)
- Temperature: **800°C**
- Electrolysis (cathode): **60% H_2O** – 10% H_2 - 30% N_2
- Fuel Cell (anode): **25% H_2 - 75% N_2**

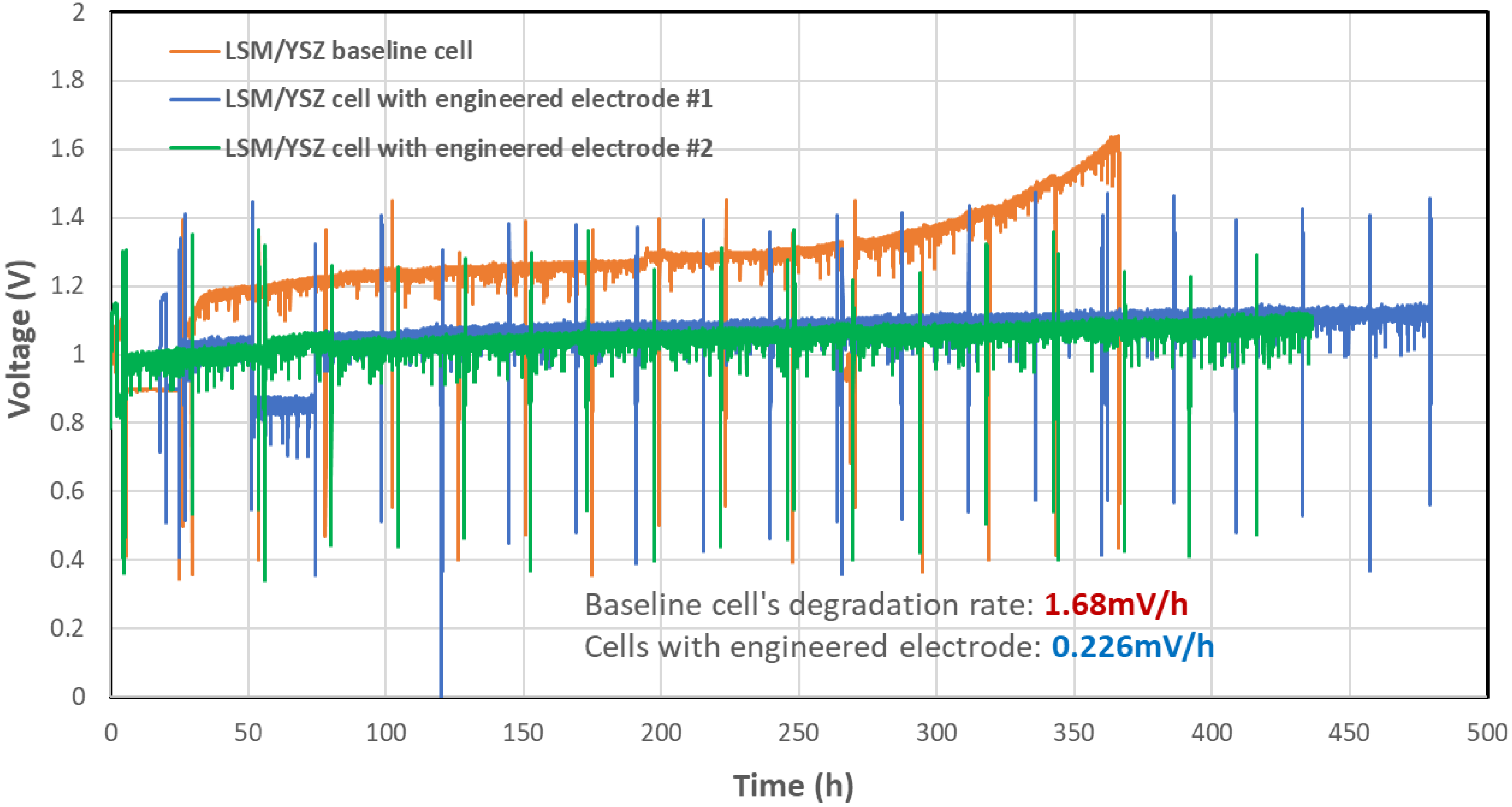


Delamination and Ni phase coarsening were evident from the cell tested under high steam conditions

Electrode Design and Engineering

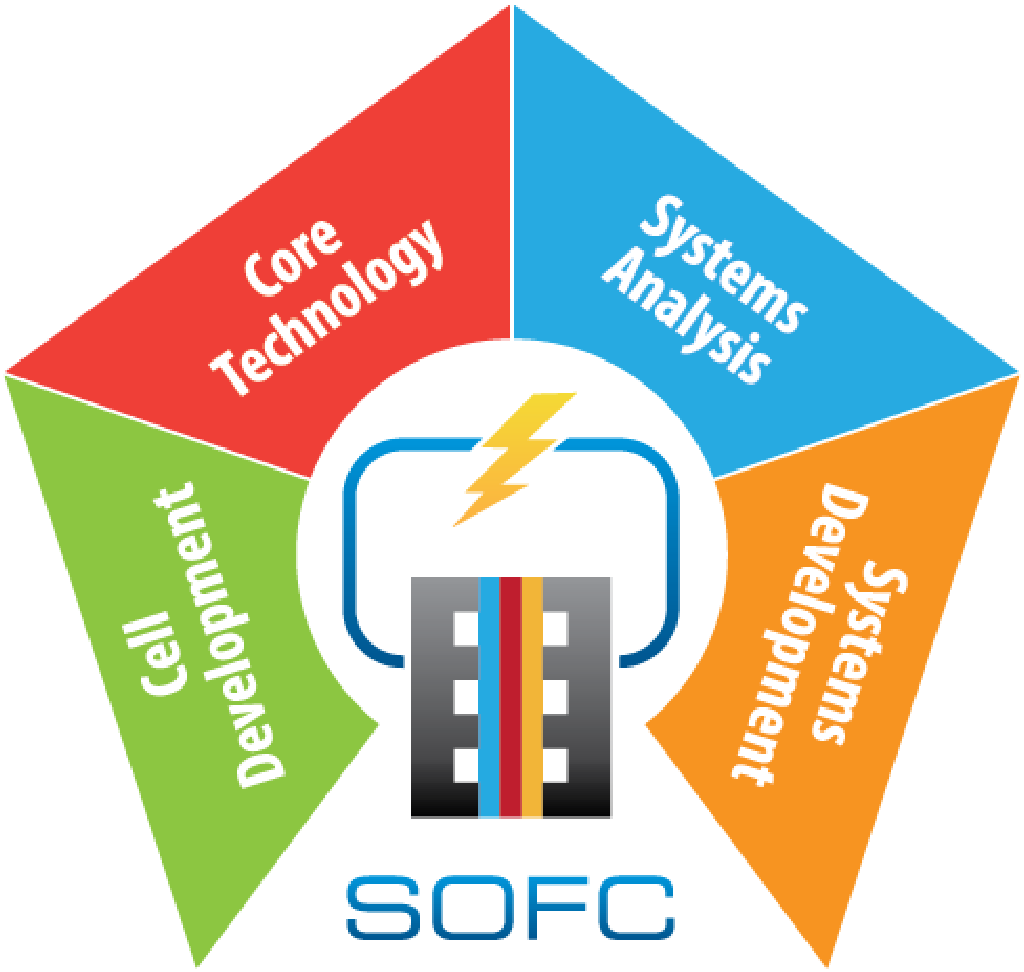
Solid Oxide Electrolysis Cell with Engineered Electrode

- An **LSM/YSZ** cell with engineered electrodes
- Temperature: **800°C**
- Electrolysis (cathode): **60% H_2O** – 10% H_2 - 30% N_2
- Fuel Cell (anode): **25% H_2 - 75% N_2**



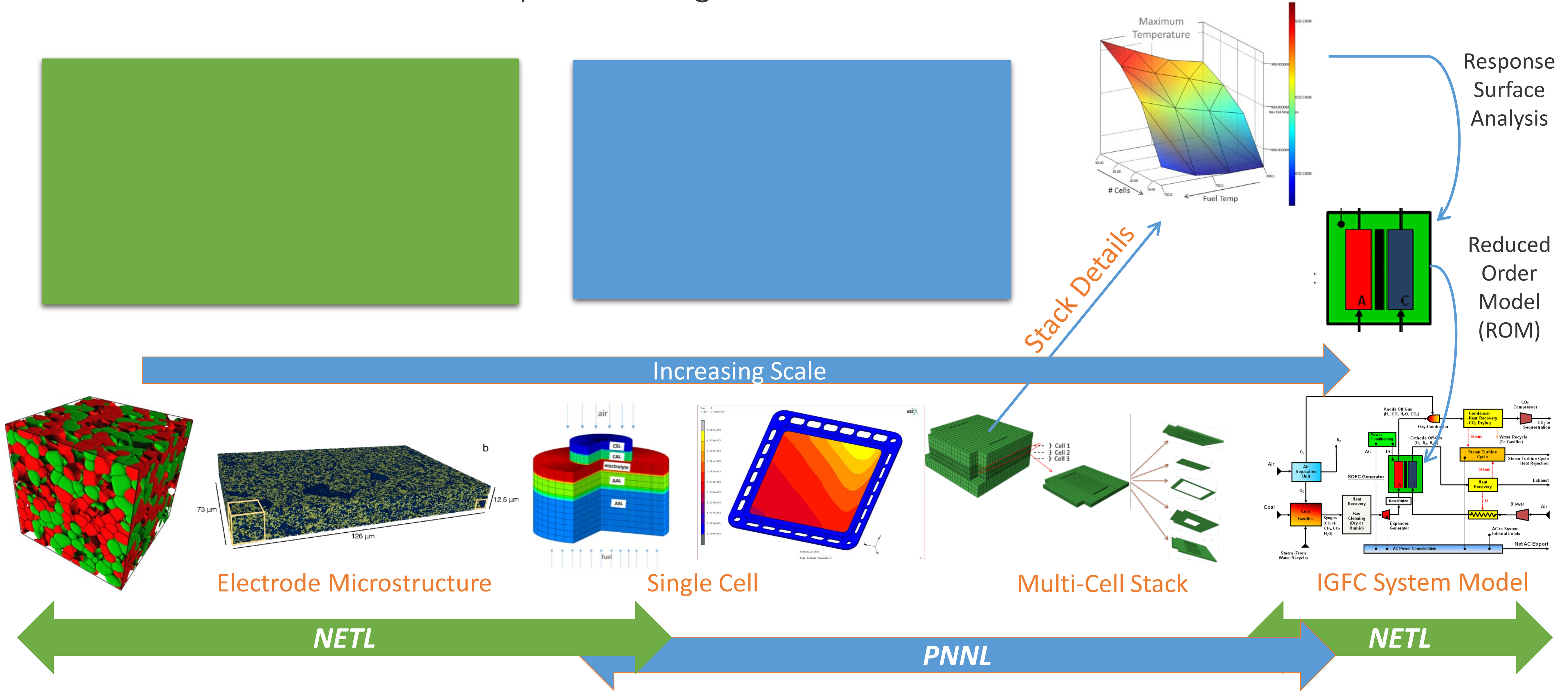
Cell and Stack Degradation

Technologies and Toolsets Under Development



Background

NETL/PNNL Collaboration to Complete Scaling Process



Enabling SOFC Technology through R&D at NETL

Predictive Modeling – Reduction of Cost for SOFC Systems

TOOL RELEASE
Release of SOFC Predictive Modeling Tool into public domain

DEMONSTRATION
Fully integrate all degradation models into SOFC operation model

MATURATION
Demonstration of degradation models integration into SOFC operation model

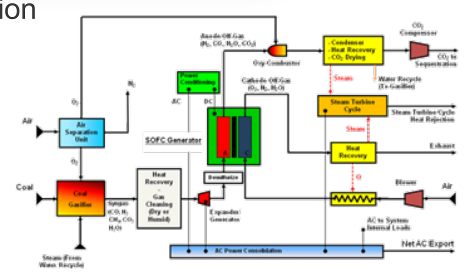
DEVELOPMENT
Critical SOFC degradation modes identified, expansion of SOFC operation model

DISCOVERY
Proof of Concept

Concept to Market Readiness

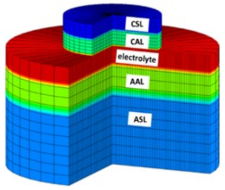
2020 — *Demonstrate how microstructure and operating conditions affect plant-level cost-of-electricity*

Integrated Gasification Fuel Cell System Model

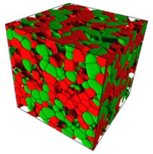


2018-19 — *Scale-bridge from microscale to cell to stack/system level (collaborate with PNNL)*

SOFC Operation "Multi-physics" Model



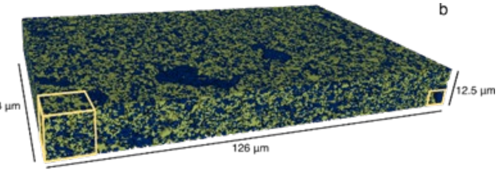
2015-18 — *Use of plasma-FIB to create world's largest reconstruction commercial developer cells*



Particle coarsening degradation model

2013-15 — *Use of focused-ion beam (FIB) to reconstruct electrodes, evaluate operationally-relevant properties*

Cathode microstructure reconstruction

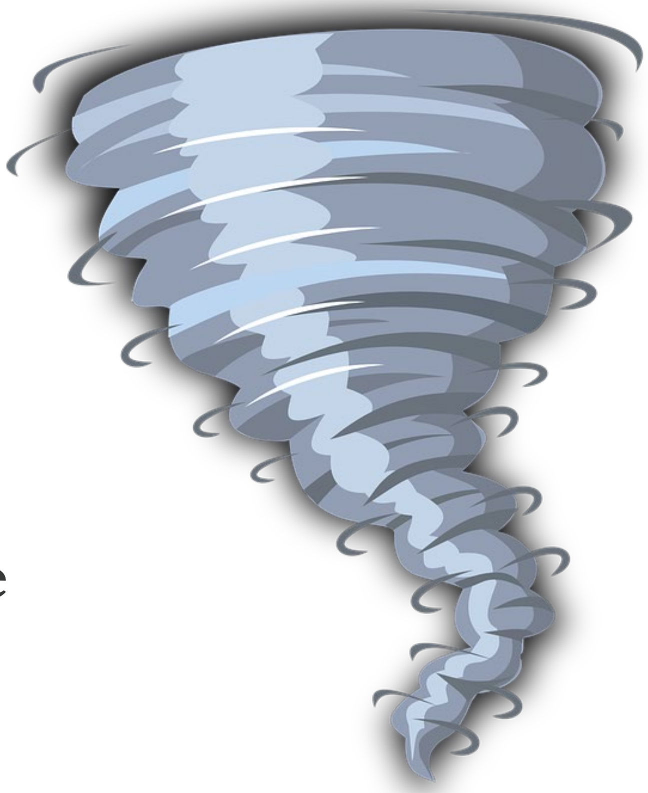


2012 — *Concept of Predictive "Hurricane" Model for SOFC*

Hurricane prediction concept

Recent Progress

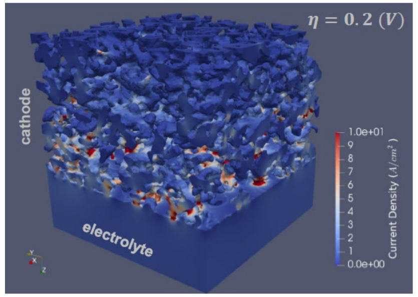
- **Converting modeling tools to open-source platform(s)**
- **Integrated multiple degradation modes into predictive framework**
  - Particle coarsening, secondary phase formation, contaminant interactions, etc.
  - Utilizing principle component analysis and machine learning to understand complex model parameter interactions
- **Working with SOFC commercial developer to demonstrate high-temperature fiber optic sensors via NDA**
  - Temperature and gas composition measurement
- **Predictive modeling tools scheduled for initial release by March 2021**

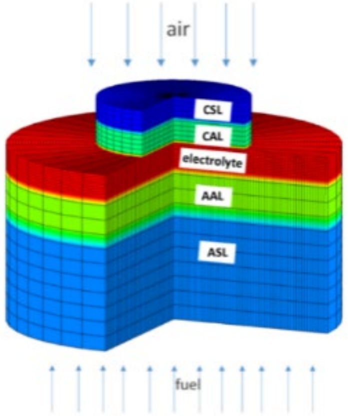


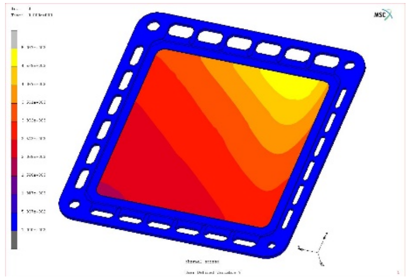
World Leading SOFC Research

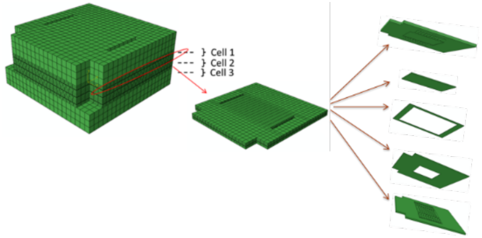
Modeling from Atoms to Cost-of-Electricity

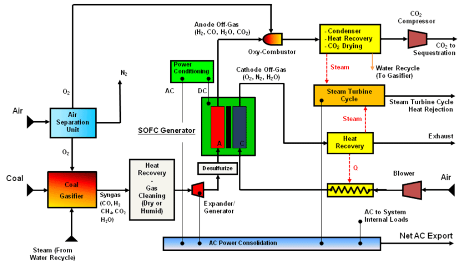
- **The SOFC group at NETL is the only solid oxide fuel cell research team capable of modeling from the atomistic scale to the system scale**
  - Atoms to cost-of-electricity











Electrode Sub-volumes

Single Cells

Multi-Cell Stack

IGFC System Model

NETL

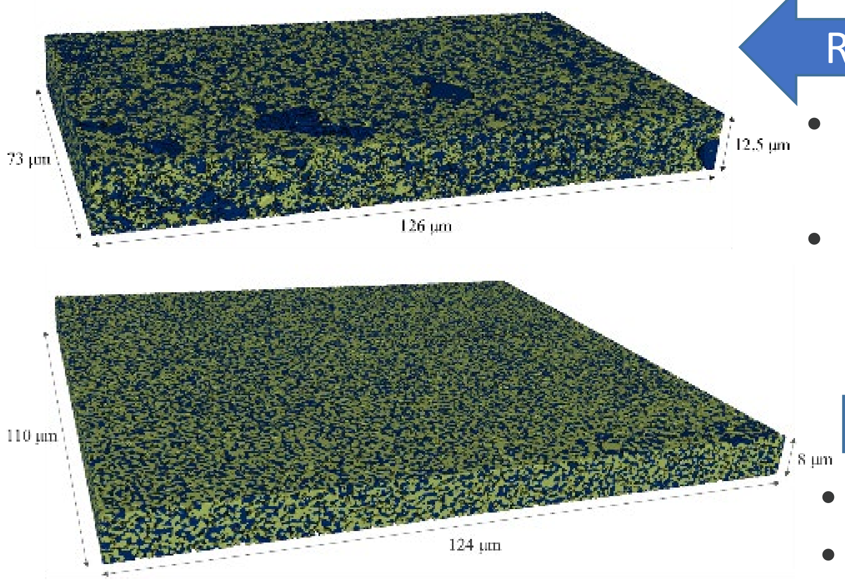
NETL

PNNL

World Leading SOFC Research

Production of High-resolution 3-D SOFC Microstructure Reconstructions

- **The SOFC group at NETL is the only solid oxide cell research team that has published high resolution electrode reconstruction datasets**
  - Crucial for accurate characterization of electrode heterogeneity

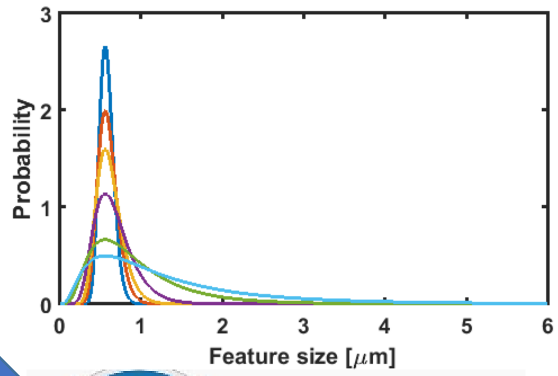


Real Microstructures

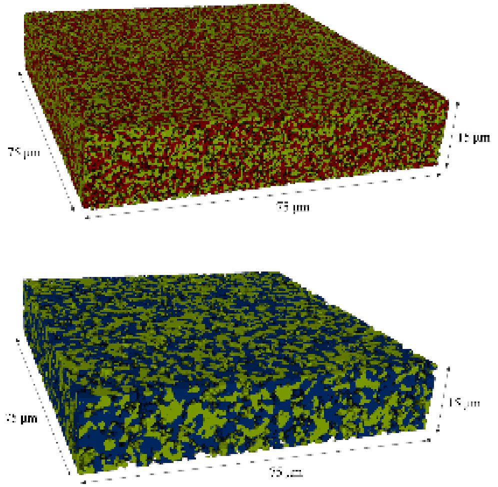
- Predict behavior of industrial cells
- Baseline for improving particular cell

Synthetic Microstructures

- Explore more features
- More efficient than creating/imaging 1000s of real cells



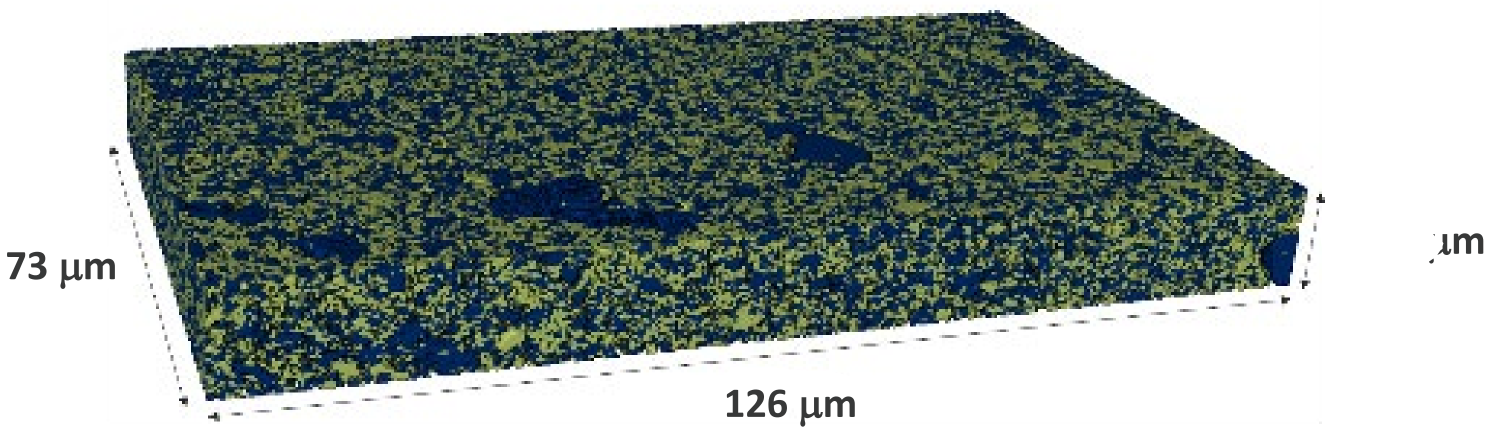
DREAM.3D BlueQuartz Software Edition

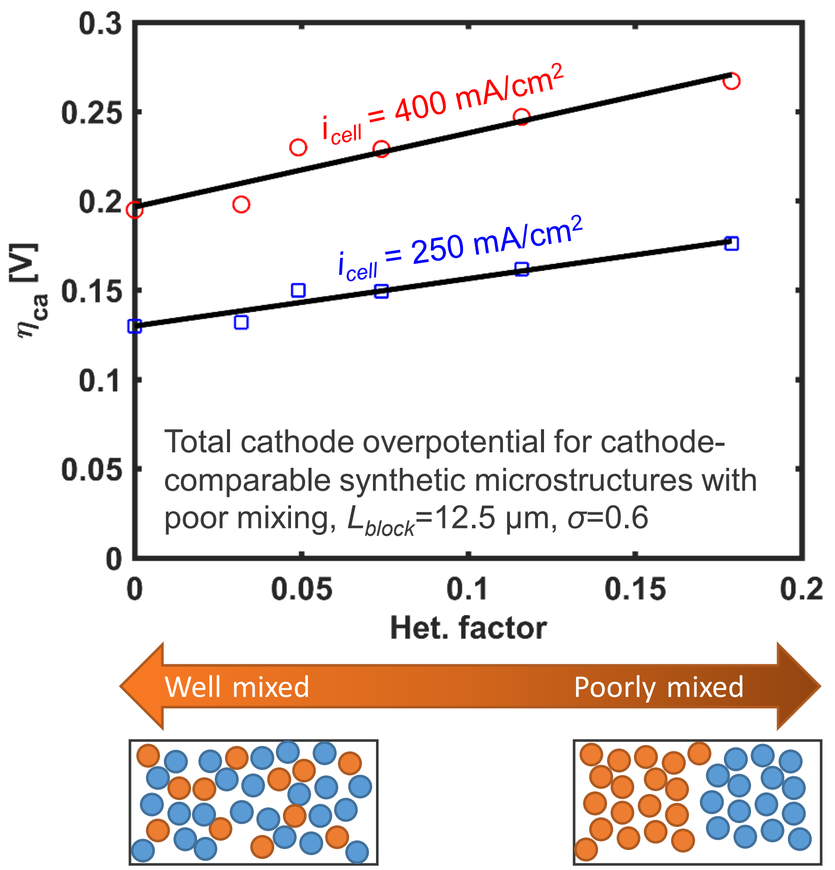


World Leading SOFC Research

Microstructural Heterogeneity Characterization and Simulation

- **The SOFC Group at NETL is the world leader in characterizing and simulating heterogeneity in porous electrodes**
  - First in using machine learning to create synthetic microstructures that more accurately capture heterogeneity in real electrodes



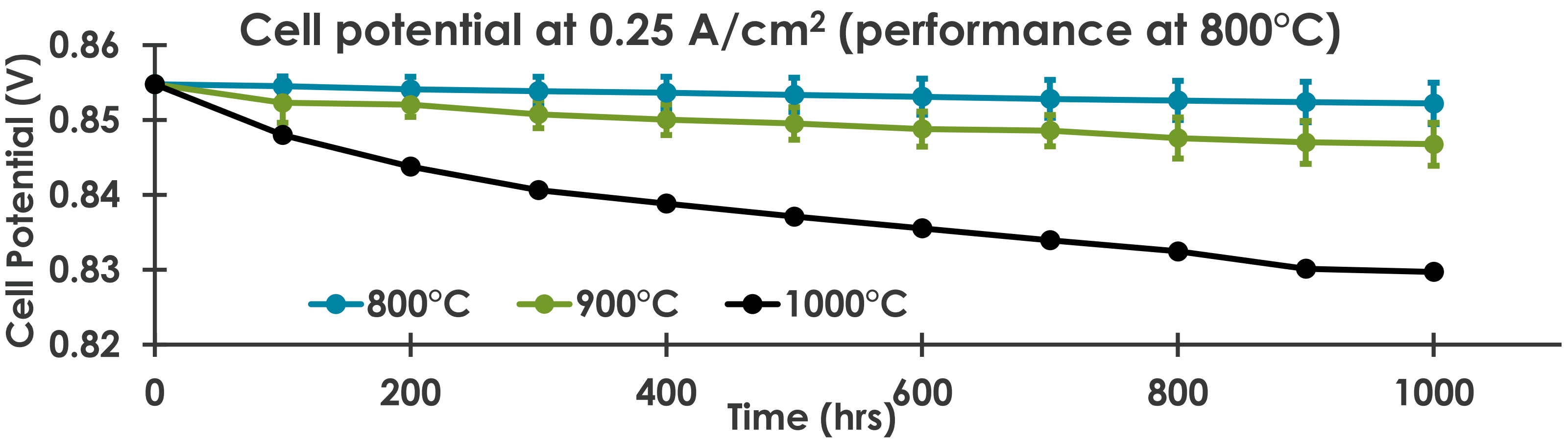


Multiphysics modelling by Dr. Hunter Mason

World Leading SOFC Research

Synthetic Microstructures Explored to Date

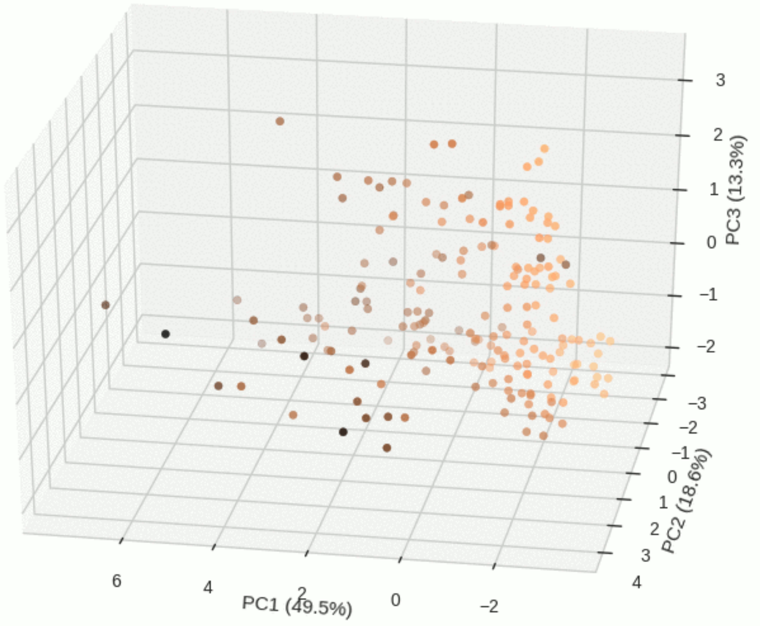
- **The largest and broadest bank of unique electrode microstructures (45,000) has been generated by NETL**
  - JOULE 2.0
  - Varied phase fractions, phase fraction distributions of three phases (COMPOSITION)
  - Varied particle sizes, particle size distributions (MICROSTRUCTURE)
- **Simulated particle coarsening of 500+ unique cathode microstructures**

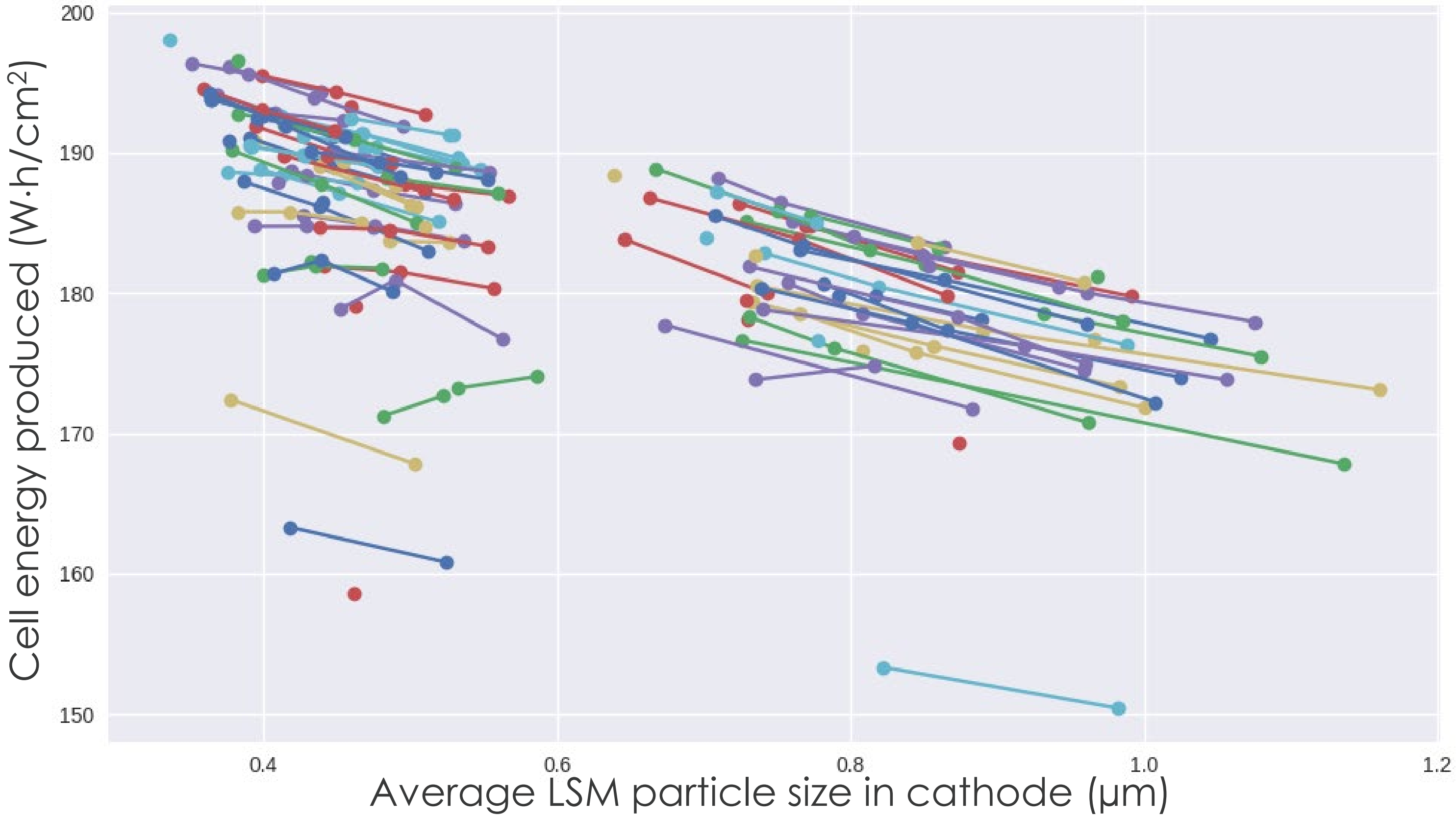


World Leading SOFC Research

Connecting Microstructure to Cost-of-Electricity

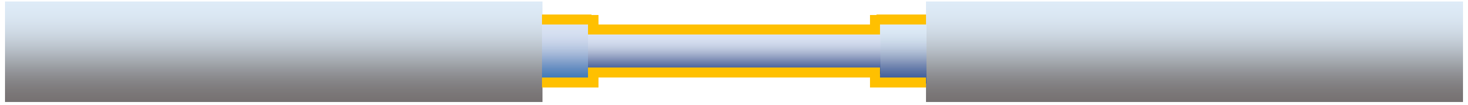
- **NETL has developed a sound methodology to connect microstructural changes to the cost-of-electricity**
  - Figure of Merit: W·h/cm²
  - Trends discovered via principal component analysis





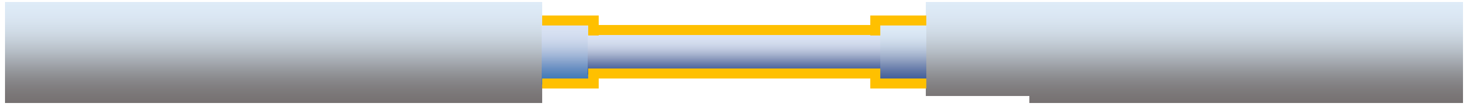
High Temperature Optical Fiber Sensor

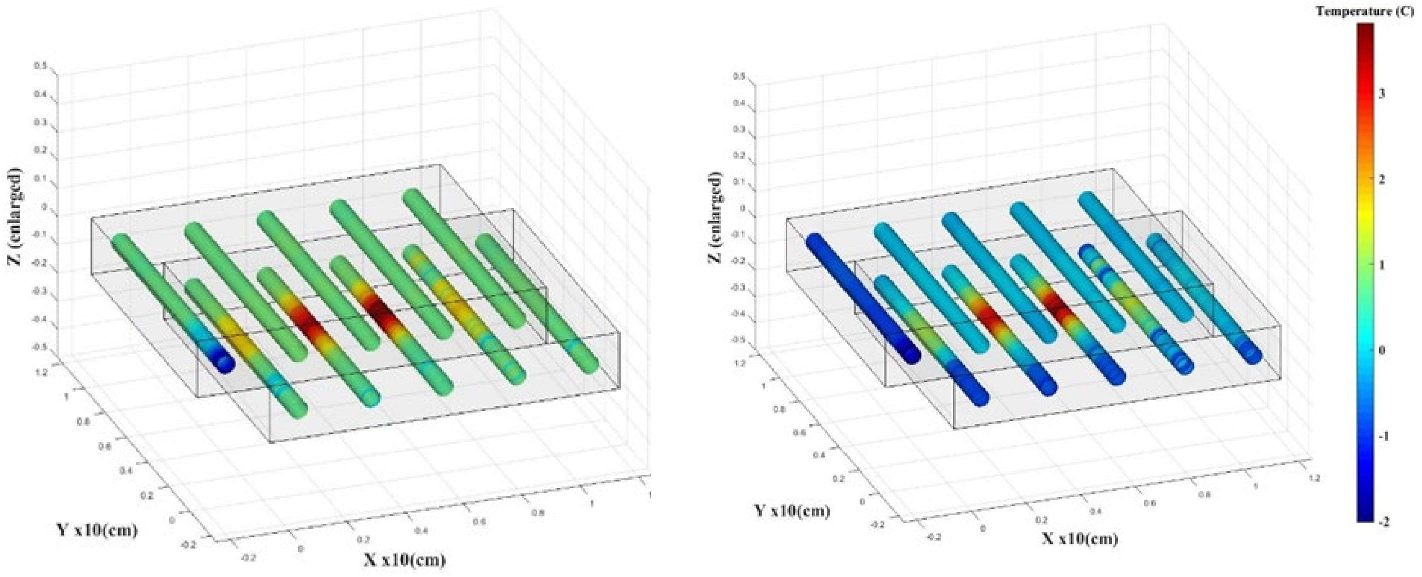
- **Multi-application technology under development for high temperature sensing**
  - Demonstrated in SOFC environment
- **In-situ sensing of**
  - Temperature distribution
  - Gas composition
    - CO, CH_4, H_2, CO_2
- **Novel coatings for optimal selectivity**
- **Of interest to several SOFC commercial developers**

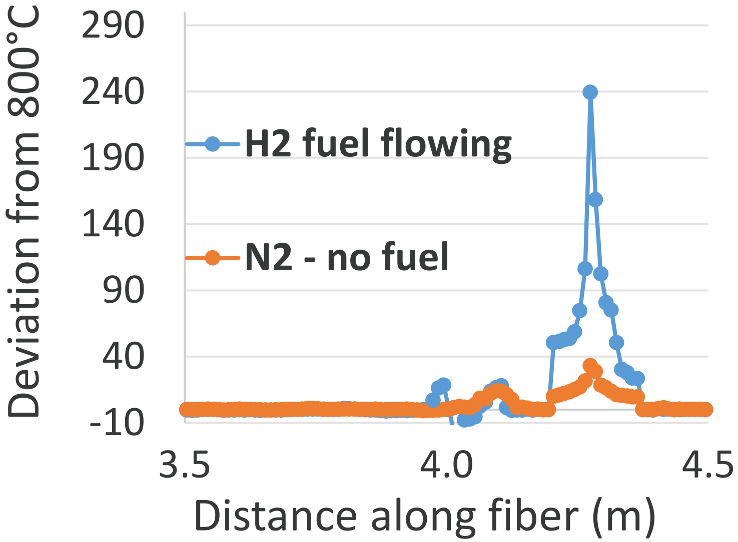


High Temperature Optical Fiber Sensor

Distributed In-situ Temperature and Gas Composition Sensing





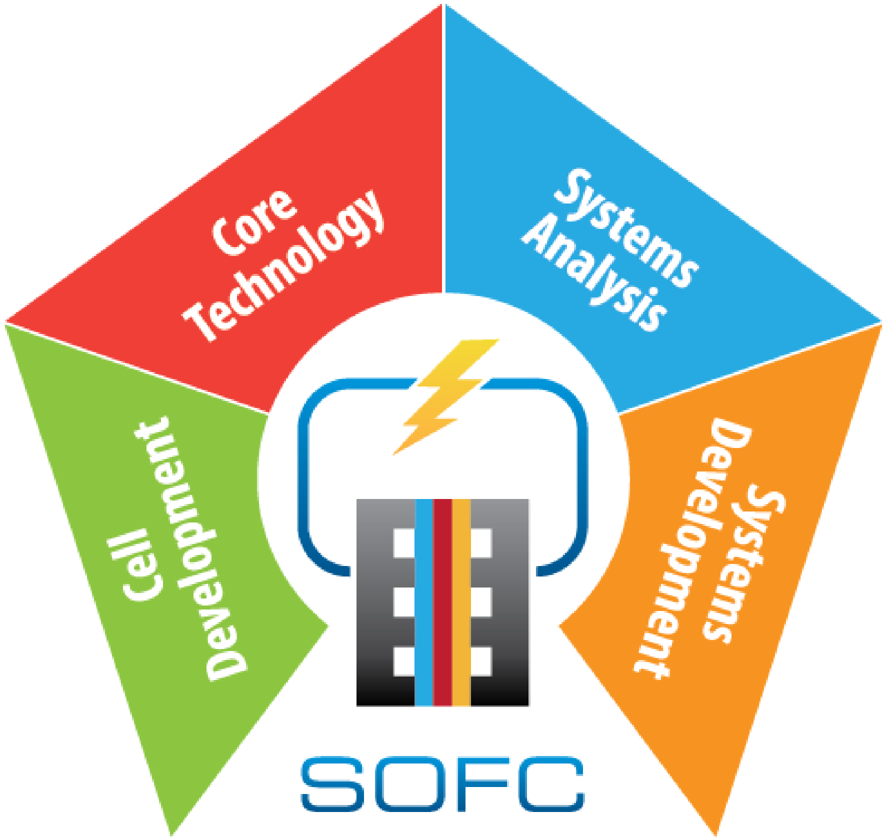


Thermal transients at 30 and 90 s from 5×5 cm^2 ASC at 750°C with H_2 fuel after 2A load

Failure detection: Temperature spike from cracked cell at 800°C

Systems Engineering & Analysis

Pulling It All Together



Systems Engineering and Analysis

Techno-Economic Analysis of Integrated Gasification Fuel Cell (IGFC) Systems

NATIONAL ENERGY TECHNOLOGY LABORATORY

Motivation: Techno-Economic Analyses (TEA) of SOFC systems are used to provide DOE-FE and the public with cost and performance information for SOFC technologies

Objective: This study updates performance, cost, and pathway information for IGFC systems to aid in the development of targeted R&D approaches for SOFC fueled by gasified coal

Study Details

Pathway cases are developed to demonstrate incremental progress from state-of-the-art to advanced SOFC performance

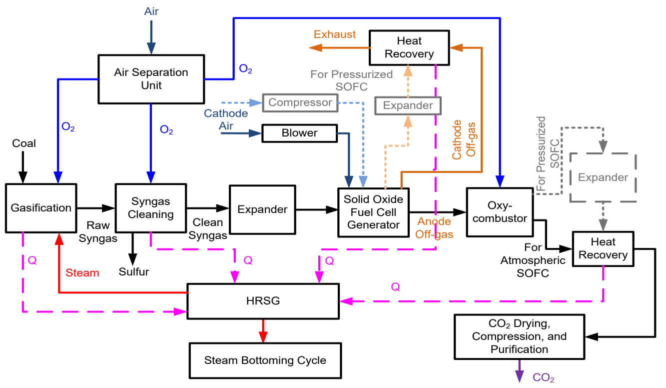
- Includes technology updates of other critical system components such as carbon capture, gasification units, etc.

Study updates a previously released report (2013). Updates include:

- Year dollar update to 2018$, performance data generated by PNNL stack model ROM, SOTA vs Advanced SOFC, vent gas recirculation concept, capture and non-capture cases, and updated gasification costs

Report to be Released June 2020

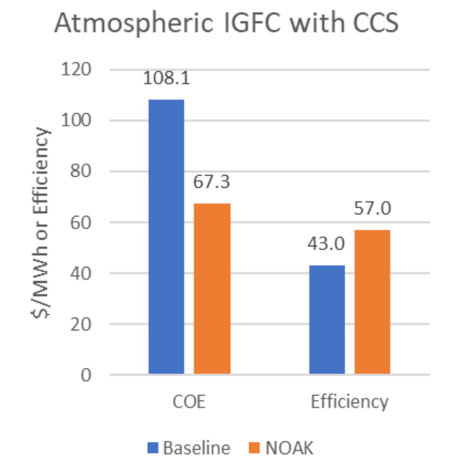
IGFC Configuration

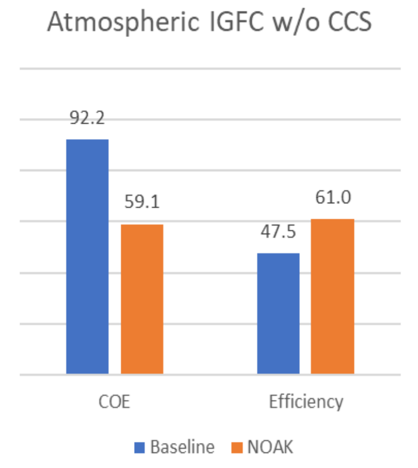


Principal Investigator

Gregory A. Hackett

Preliminary Results





Report includes detailed expansion of results for pressurized cases and more

Systems Engineering and Analysis

NATIONAL ENERGY TECHNOLOGY LABORATORY

Techno-Economic Analysis of Natural Gas Fuel Cell (NGFC) Systems

Motivation: Techno-Economic Analyses (TEA) of SOFC systems are used to provide DOE-FE and the public with cost and performance information for SOFC technologies

Objective: This study updates performance, cost, and pathway information for NGFC systems to aid in the development of targeted R&D approaches for SOFC fueled by natural gas

Study Details

Pathway cases are developed to demonstrate incremental progress from state-of-the-art to advanced SOFC performance

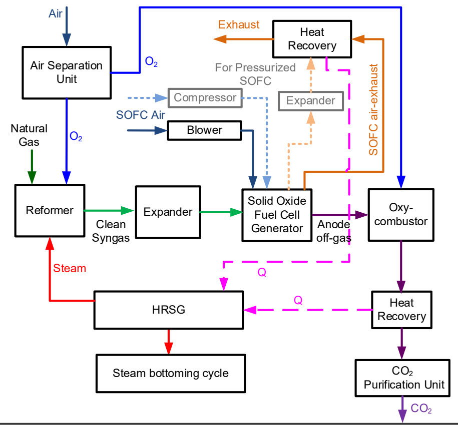
- Includes technology updates of other critical system components such as carbon capture, external reformers, etc.

Study updates a previously released report (2013). Updates include:

- Year dollar update to 2018$, performance data generated by PNNL stack model ROM, SOTA vs Advanced SOFC, vent gas recirculation concept, capture and non-capture cases, and on cell reforming percentage sensitivities

Report to be Released June 2020

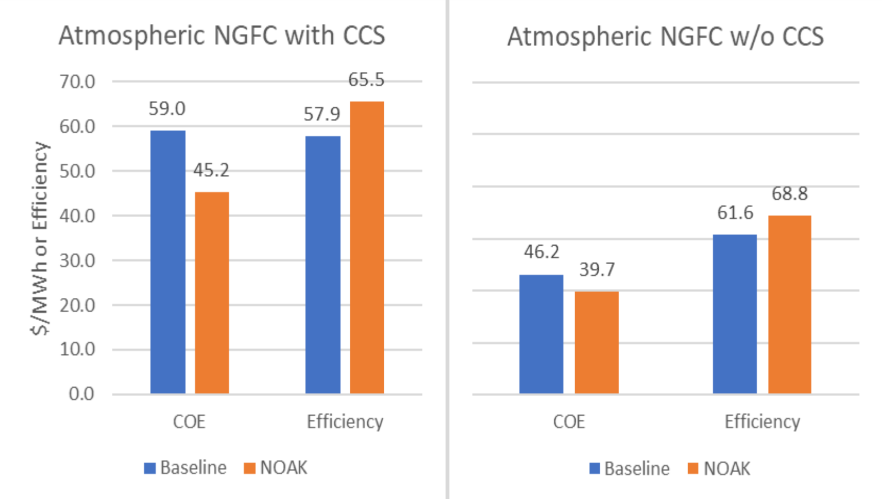
NGFC Configuration



Principal Investigator

Gregory A. Hackett

Preliminary Results



Report includes detailed expansion of results for pressurized cases and more

Systems Engineering and Analysis

NATIONAL ENERGY TECHNOLOGY LABORATORY

Distributed Generation (DG) as a Potential Market for SOFC

Motivation: DOE-FE's development plan for SOFC technology includes demonstration of commercial units at the DG scale (≈1 MW)

Objective: A market study is performed to describe how SOFC technology fits into a competitive DG market and projects cost reductions associated with demonstration of multiple units

Study Details

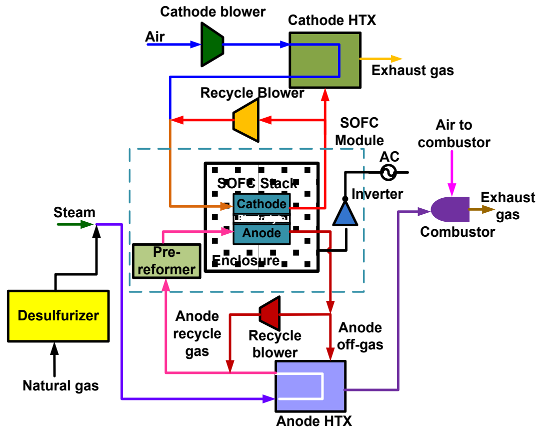
Document describes the current distributed generation market and the potential for SOFC technology within it

- Study analyzes several market studies, detailing the capacity potential for SOFC technology in the DG market
- Study projects how many DG demonstration units at 1-MWe are needed to reach the $900-$1000/kW cost target
- Sensitivities (such as natural gas price) applied for SOFC and other DG scale technologies for comparison

Incorporates anticipated penetration for other DG technologies including wind, solar, reciprocating engine, microturbines, etc.

Report Available Online (link below)

SOFC-DG Configuration



Principal Investigator

Gregory A. Hackett

Key Study Results

Parameter	Nth of a Kind SOFC DG Performance
Net AC Power [kWe]	1000
Operating Pressure [atm]	1.0
Operating Temp. [°C (°F)]	750 (1382)
Cell Voltage [V]	0.830
Current Density [mA/cm²]	400
Net AC Efficiency [HHV]	**61.3**
Module Cost [2011$/kWe]	452
BOP Cost [2011$/kWe]	531
Total System [$/kWe]	**983**

Study predicts 25-90 1-MWe units will be needed to reach this cost per kW

U.S. DEPARTMENT OF ENERGY

https://netl.doe.gov/energy-analysis/details?id=4375

Systems Engineering and Analysis

SOFC Cell and Stack Production Cost Study

NATIONAL ENERGY TECHNOLOGY LABORATORY

Motivation: DOE-FE's cost targets for SOFC require multiple (25+) demonstrations at the distributed generation scale (≈1 MW) for viability

Objective: Develop a comprehensive tool to assist SOFC commercial developers understand the costs associated with large scale production of solid oxide fuel cells and stacks

Tool Details

The SOFC cell and stack production cost tool is an Excel-based tool intended for public release

- Tool includes all of the necessary cost inputs including raw materials, equipment costs, labor costs, etc.
- Tool will allow for sensitivities to be conducted on parameters such as total production scale, materials costs, electricity costs, etc.
- Default values provided will serve as an example case study

Tool will be accompanied by a detailed user manual with instructions and a worked examples

- Can be easily modified to include the necessary materials for hydrogen producing SOEC

Tool scheduled for completion July/August 2020

Spreadsheet Tool Example

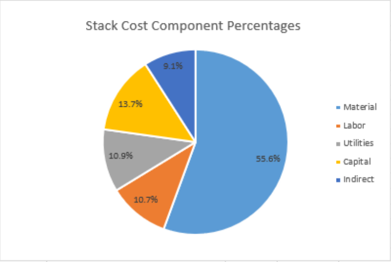
System Overview

Stacks per year	20000	
Capacity per year	107.95	MW/year
Power Density	0.34	W/cm2
Stack Power	5.40	kW

Cost Basis
2019

Cost Summary

Group	Description	Annual Cost ($)	Cost per stack ($/stack)	Cost per kW ($/kW)	Percentages of Total: Individual	Percentages of Total: Group
Material	Cell Costs	$ 4,636,220	$ 231.81	$ 42.95	17.6%	55.6%
	Interconnect Costs	$ 9,986,239	$ 499.31	$ 92.51	38.0%	
	Total	$ 14,622,459	$ 731	$ 135.45		
Labor	Direct Labor	$ 2,812,320	$ 140.62	$ 26.05	10.7%	10.7%
Utilities	Electricity	$ 2,879,014	$ 143.95	$ 26.67	10.9%	10.9%
Capital	Equipment	$ 2,000,060	$ 100.00	$ 18.53	7.6%	13.7%
	Building	$ 1,600,048	$ 80.00	$ 14.82	6.1%	
	Total	$ 3,600,108	$ 180	$ 33.35		
Indirect	Cell Fabrication Maintenance	$ 70,002	$ 3.50	$ 0.65	0.27%	9.1%
	Cell Fabrication Consumables	$ 14,000	$ 0.70	$ 0.13	0.05%	
	Cell Fabrication QA/QC	$ 2,800	$ 0.14	$ 0.03	0.01%	
	Stack Assembly Consumables	$ 14,000	$ 0.70	$ 0.13	0.05%	
	Indirect labor	$ 562,464	$ 28.12	$ 5.21	2.1%	
	Overhead	$ 1,729,393	$ 86.47	$ 16.02	6.6%	
	Total	$ 2,392,660	$ 120	$ 22.16		
Total Production Cost		$ 26,306,561	$ 1,315	$ 243.69		
		Annual Cost ($)	Cost per stack ($/stack)	Cost per kW ($/kW)		



Thank You!

VISIT US AT: **www.NETL.DOE.gov**

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