Progress of the NETL Solid Oxide Fuel Cell Research Portfolio

NATIONAL ENERGY TECHNOLOGY LABORATORY

U.S. DOE Hydrogen and Fuel Cells Program 2019 Annual Merit Review and Peer Evaluation Meeting

Gregory A. Hackett, Ph.D.

NETL Research and Innovation Center

April 30, 2019

Outline

- **NETL SOFC Research Team (EY19)**
- **NETL SOFC Research Portfolio Update**
  - Electrode Engineering Research and Development Progress
  - Cell and Stack Degradation Evaluation and Modeling Progress
  - Systems Engineering and Analysis Progress

A whirlwind of information coming your way!

NETL SOFC Research Team (EY19)

NETL (Federal Staff)

- Gregory Hackett, Team Lead (NETL)
- Travis Shultz (NETL)
- Rich Pineault (NETL)
- Yves Mantz (NETL)
- Paul Ohodnicki (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)
- Elizabeth Ridgeway (MAE, Undergraduate)
- Ed Sabolsky (MAE)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corporation)
- Ozcan Ozmen (MAE, Ph.D. Student)

NETL (Post-Doctoral Researchers)

- **Yueh-Lin Lee** (ORISE)
- Billy Epting (ORISE)
- Giuseppe Brunello (ORISE)
- Hunter Mason (ORISE)
- Tao Yang (ORISE)
- **Yinkai Lei** (ORISE)
- Beom Tak Na (ORISE-PM)
- TBD Experimentalist EY19

NETL (Site Support Contracts)

- 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)

Carnegie Mellon University

- **Paul Salvador** (MSE)
- Shawn Litster (MechE)
- Tony Rollett (MSE)
- Tim Hsu (MSE, grad. student)
- Rubayyat Mahbub (MSE, grad. Student)
- TBD EY19

Clemson University

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

Penn State University

- Long-Qing Chen (MSE)

University of Wisconsin-Madison

- Dane Morgan (MSE)
- Yipeng Cao (MSE)
- Ryan Jacobs (MSE)

Wake Forest University

- Michael Gross (Chemistry)
- Sixbert Muhoza (Chemistry, Ph.D Student)

POSTER

Currently 48 SOFC Team Members

Poster Session

Please stop by to see our posters!

Poster Session 6:30-8:00 PM

Location - Independence B

FE067 (Electrode Engineering Progress)

FE068 (Mesoscale Heterogeneity Impact)

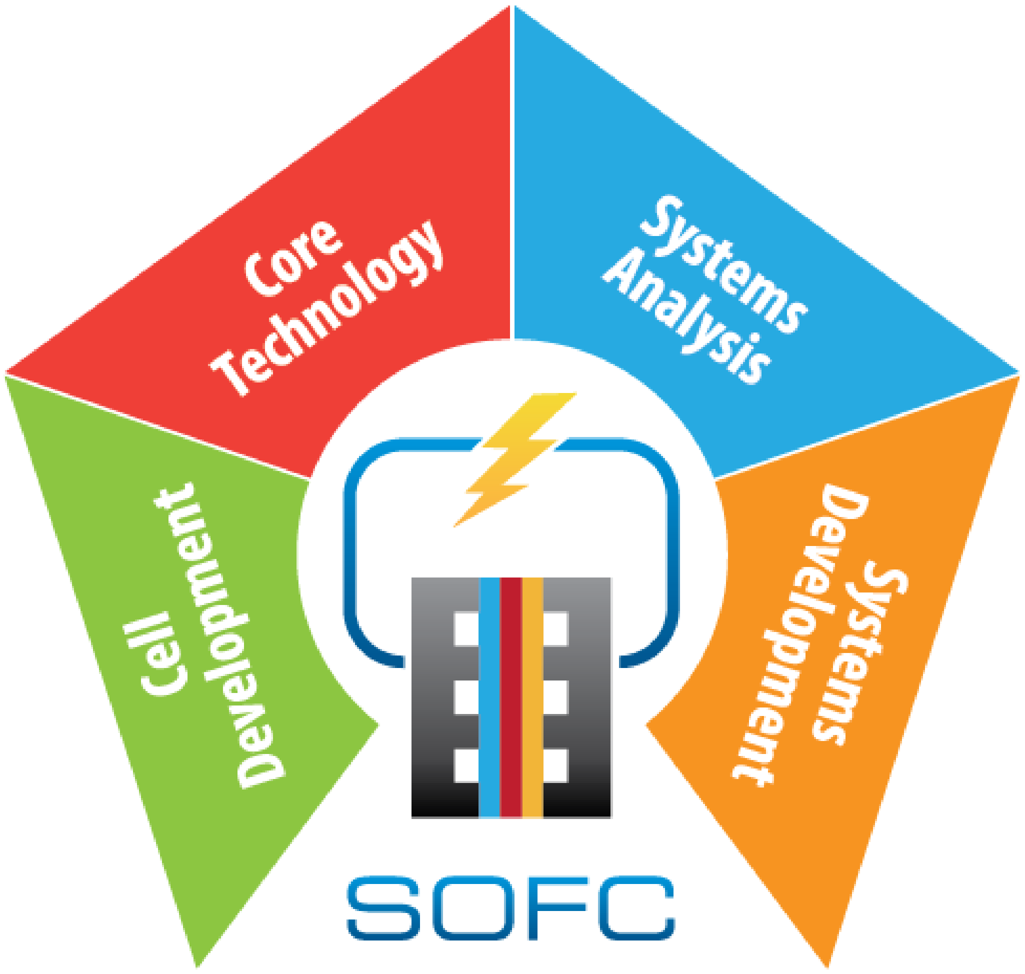
FE069 (Multiphysics Degradation Modeling)

FE070 (Effect of Hydrogen on Cation Diffusion)

FE071 (Microstructure Evolution Simulation)

Performance Enhancement & Degradation Mitigation

SOFC Electrode Engineering



SOFC Electrode Engineering Overview

Designing, Developing, and Deploying Advanced Electrode Engineering Techniques

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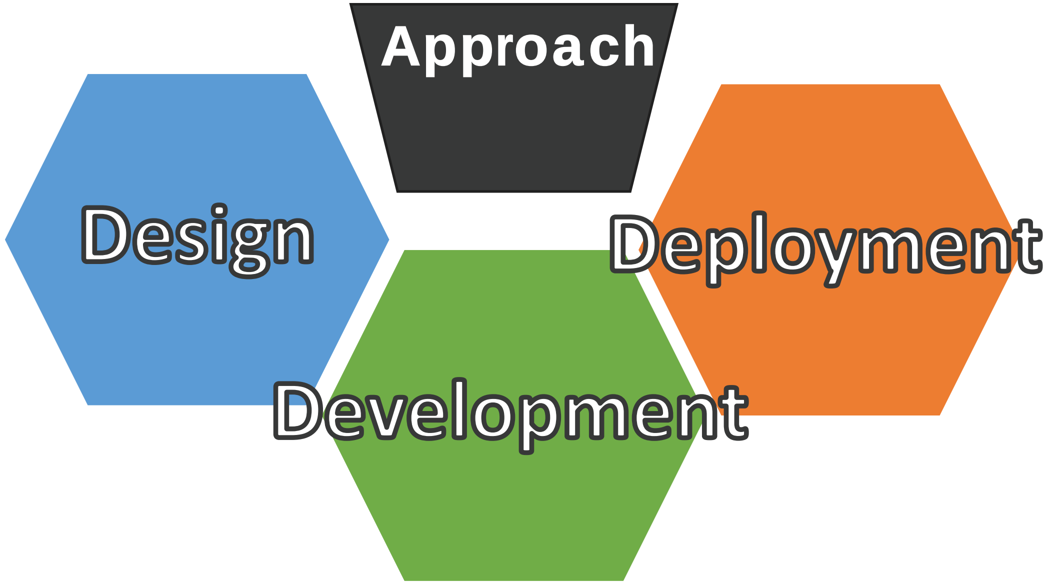
- **Objectives**
  - Enhancement of electrode performance and longevity
  - Materials engineering
  - Microstructure engineering
- **Benefits**
  - Stack cost reduction
  - Cell overpotential reduction
  - Thermo-chemical / thermo-mechanical stability increase

POSTER
FE-067

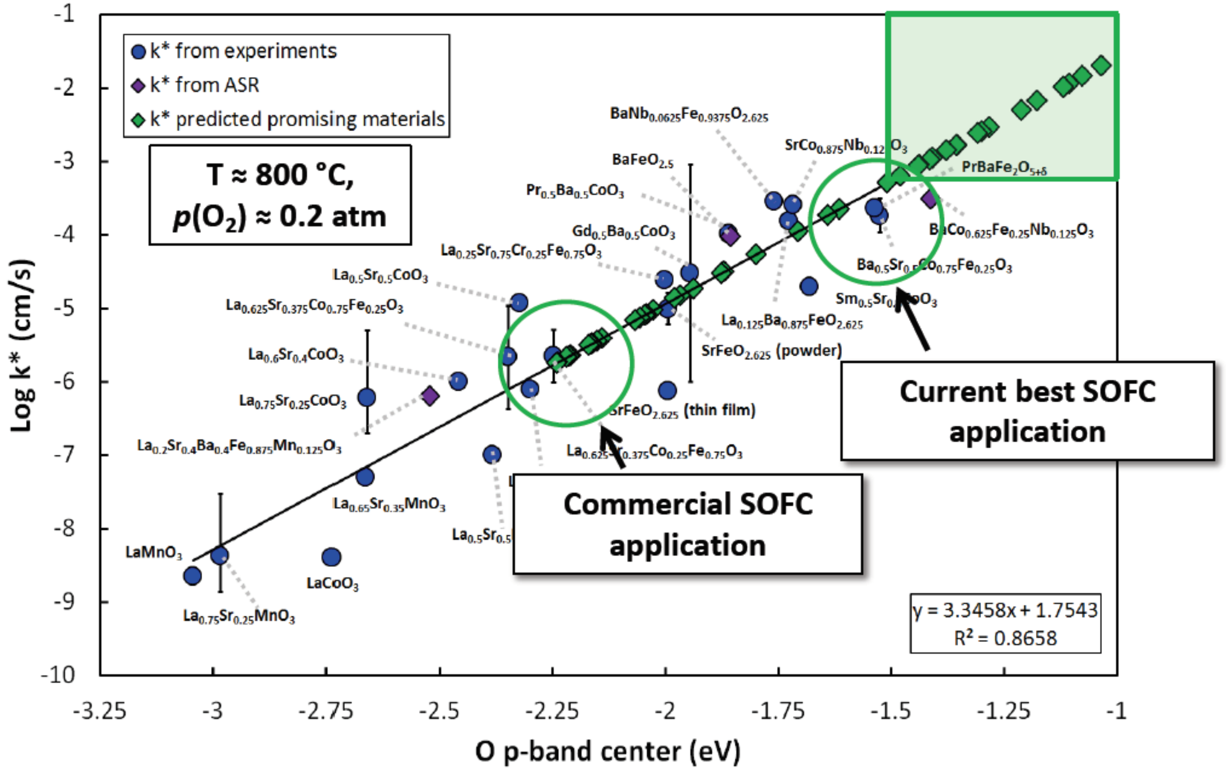


DESIGN of materials and nanostructures
DEVELOPMENT through tailored electrode construction
DEPLOYMENT in commercial SOFC systems

Advanced Electrode Design

Collaboration: University of Wisconsin-Madison

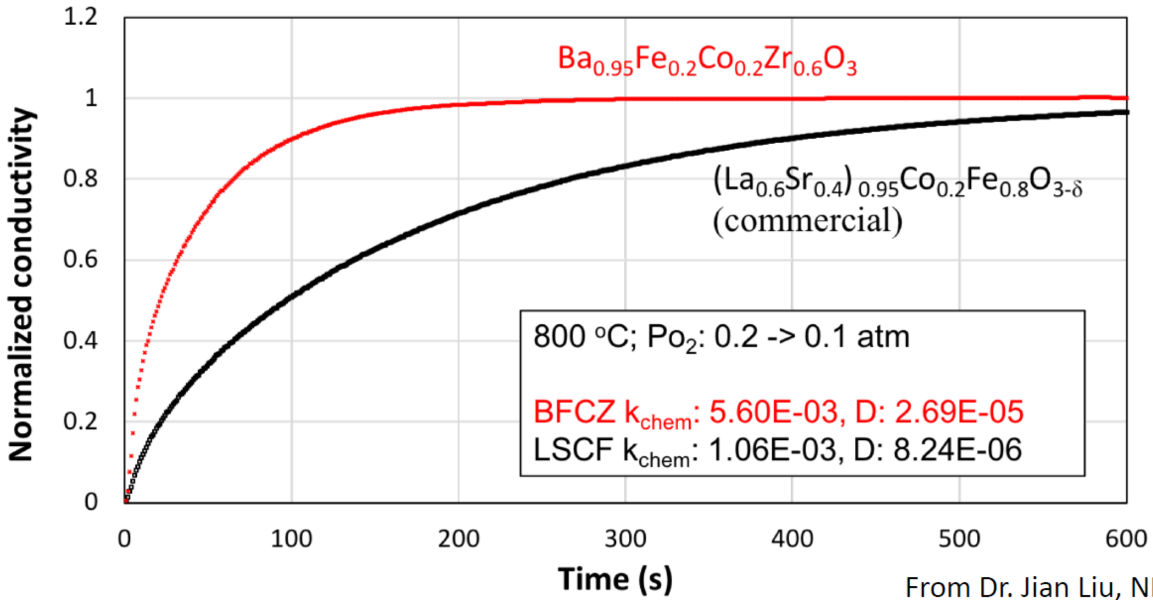
Bridging Theory and Reality



Surface exchange coefficient versus *O p*-band center

- R. Jacobs et al., *Adv. Energy Mater.* (2018)

- Electrical Conductivity Relaxation measurement of the calculated **$Ba(Fe_{0.2}Co_{0.2}Zr_{0.6})O_3$** resulted in 5× higher k_{chem} and 3× higher D_{chem} compared to LSCF



From Dr. Jian Liu, NETL

Advanced Electrode Design

Collaboration: Clemson University

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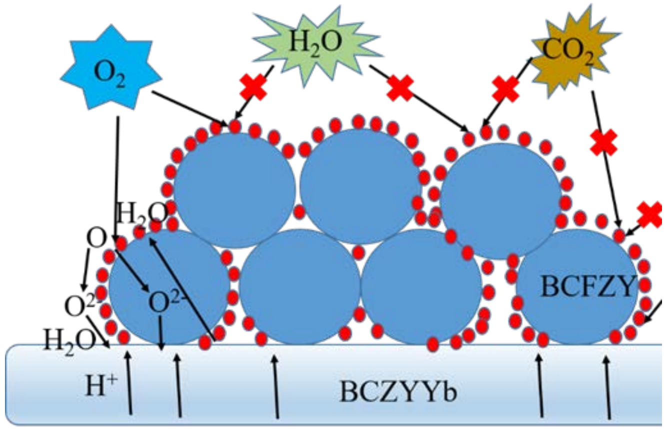
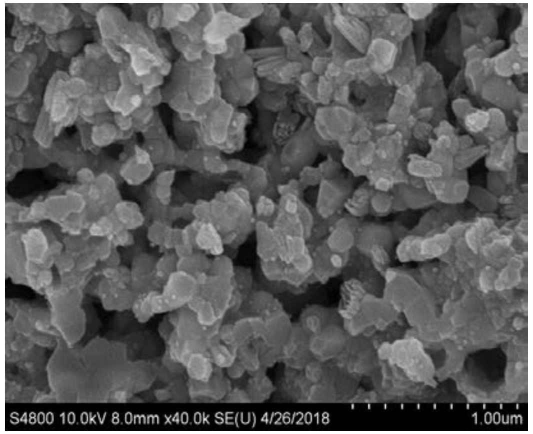
Proton Conducting SOFC Electrodes

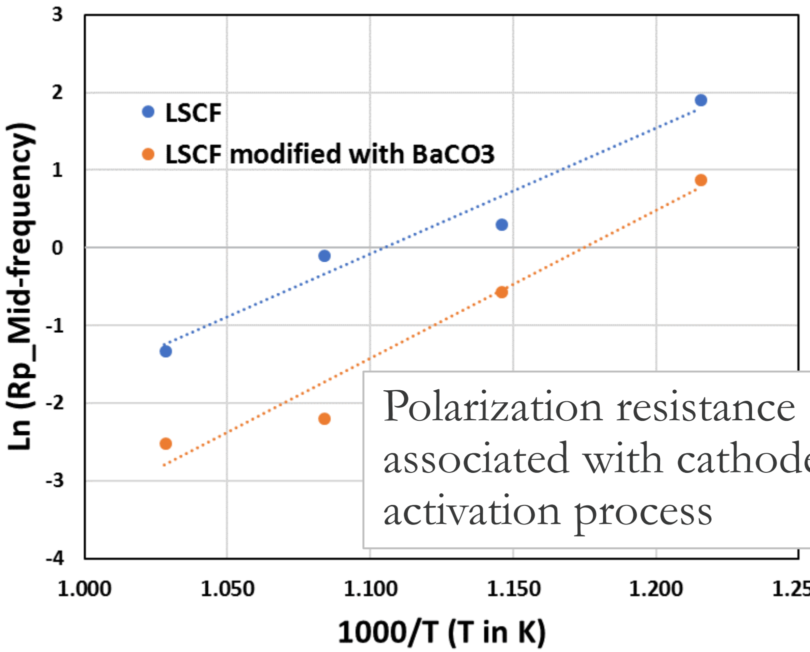
- Electrolyte: BCZYYb, Cathode: BCFZY or LSCF
- **Electrocatalyst: $BaCO_3$, nano-BCFZY, etc.**



Cathode infiltration in Proton SOFCs



LSCF electrode infiltrated with $BaCO_3$



Polarization resistance (R_P) associated with cathode activation process

- The ASR of the **$BaCO_3$-infiltrated LSCF cathode** (0.08 Ω•cm²) is significantly less than that of the pure LSCF cathode (0.27 Ω•cm²) at 700°C

Advanced Materials Property Characterization

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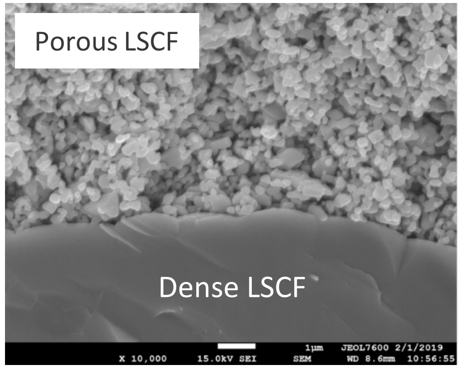
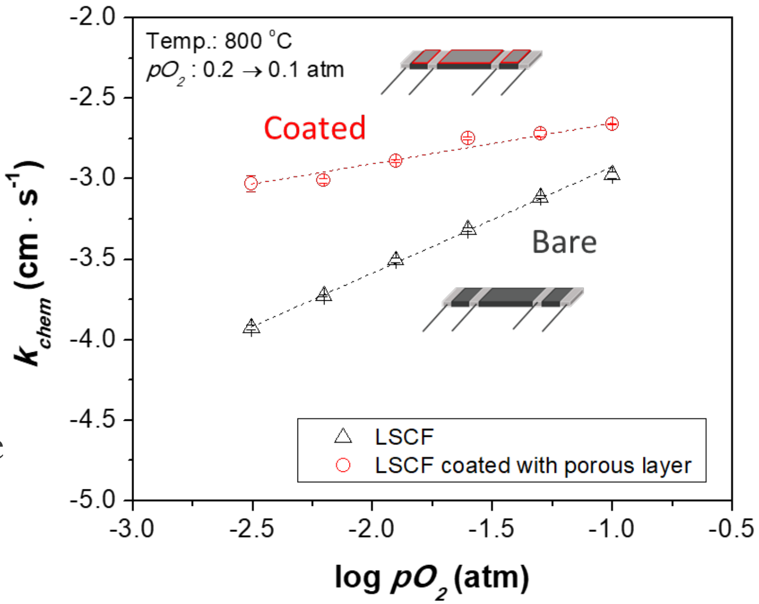
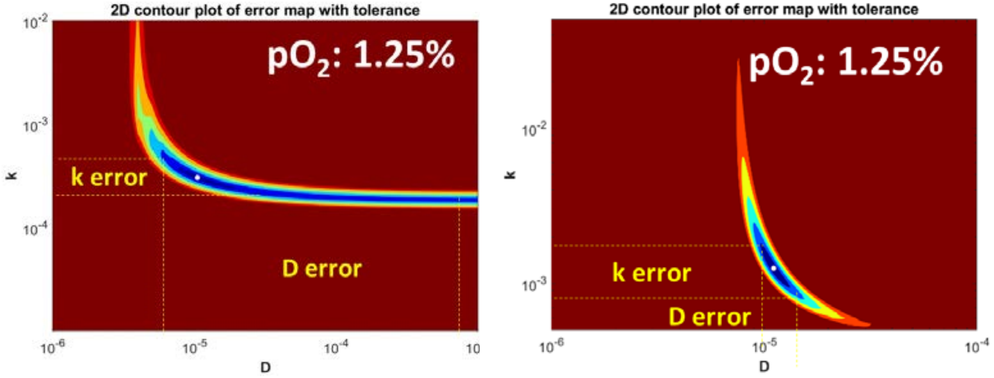
Modified ECR (Electrical Conductivity Relaxation)



Porous LSCF layer on dense LSCF ECR sample



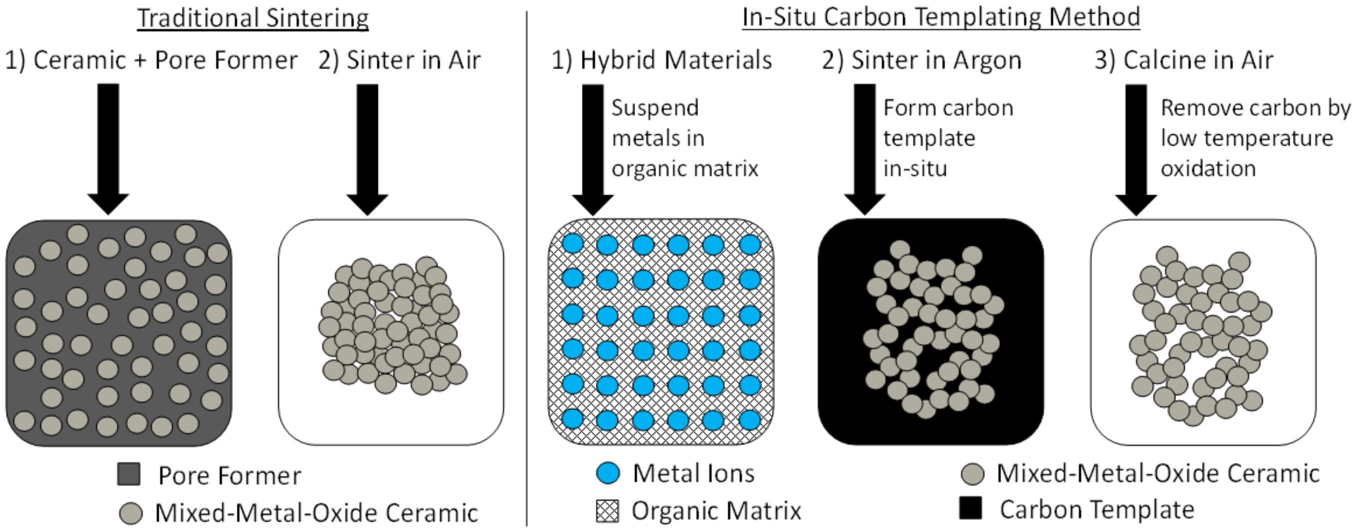


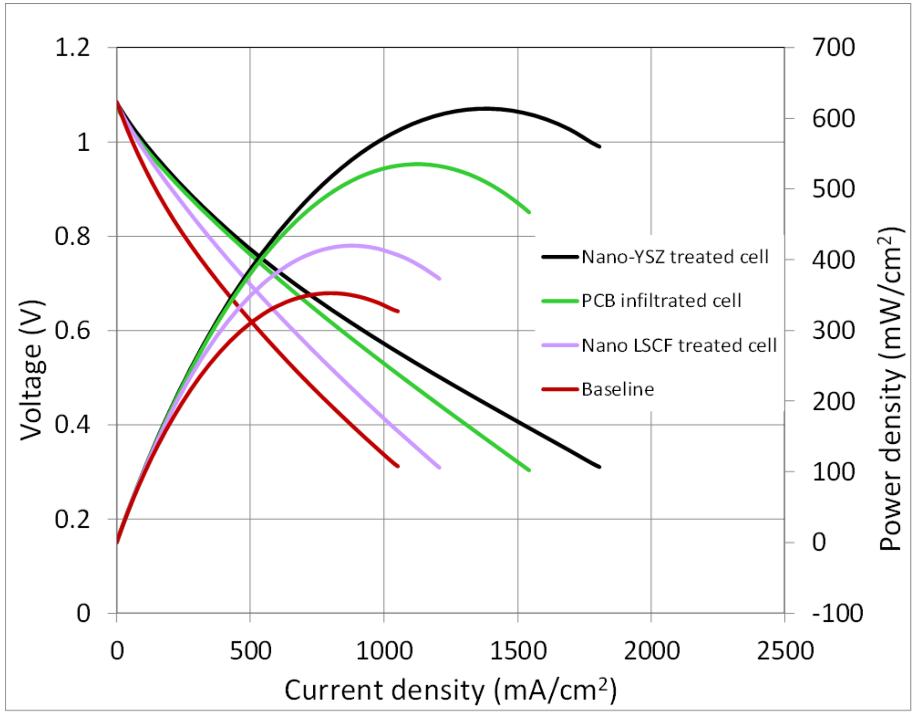
Error map for the calculated k_{chem} and D_{chem} at pO_2 = 1.25% (a) bare LSCF, (b) LSCF coated with porous layer.

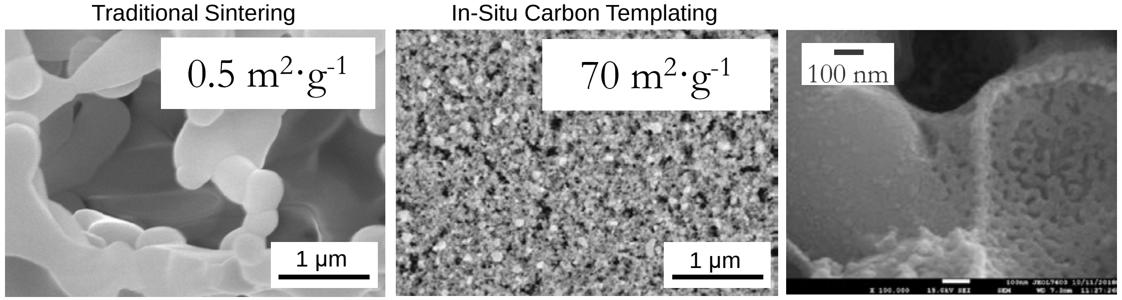
- A novel approach of determining bulk diffusion coefficient (D_{chem}) using the electrical conductivity relaxation (ECR) was developed.
- Coating the surfaces of bar samples with porous, in-kind particles (e.g. porous LSCF on dense LSCF bar sample) enabled reduction in the characteristic thickness (L_c) and determination of D_{chem} values with minimal error, which couldn't be achieved by conventional methods.

High Surface-Area Nanostructured Cathodes

via In-Situ Carbon Templating – Collaboration: Wake Forest University







Traditional sintering | In-situ carbon templating | Nano-YSZ infiltrated LSM-YSZ

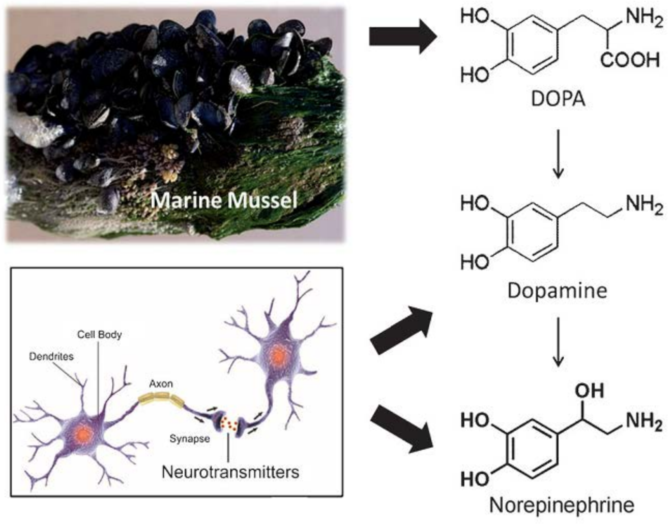
Nano-YSZ infiltrated LSM-YSZ cathode showed stable performance:

- **Nano-YSZ infiltrated: 0.67% over 200 h**
- **(PrBa)CoO_x infiltrated: 1.86% over 200 h**

Advanced Electrode Modification

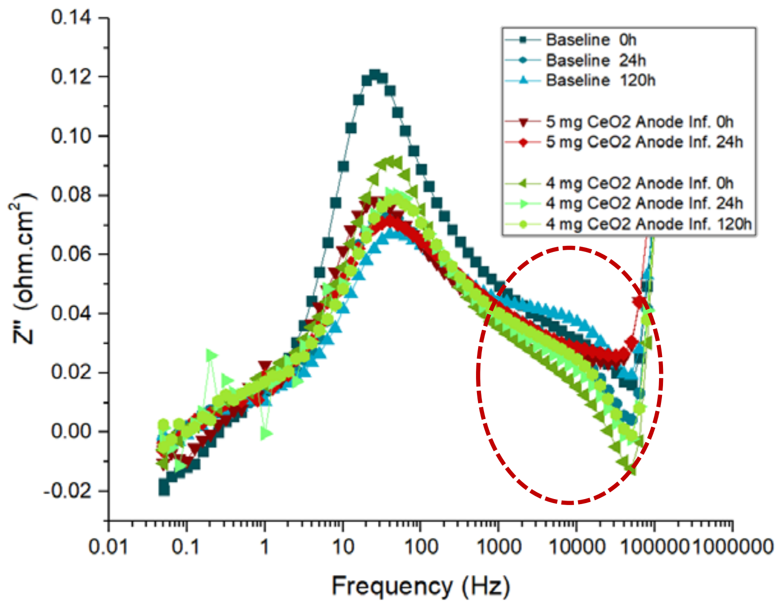
Collaboration: West Virginia University

Bio-Surfactant Assisted UN-REDUCED SOFC Anode Infiltration



- pNE offers smoother and more uniform coating

H. Lee, et al., *Angew. Chem. Int.*, (2013) 9187



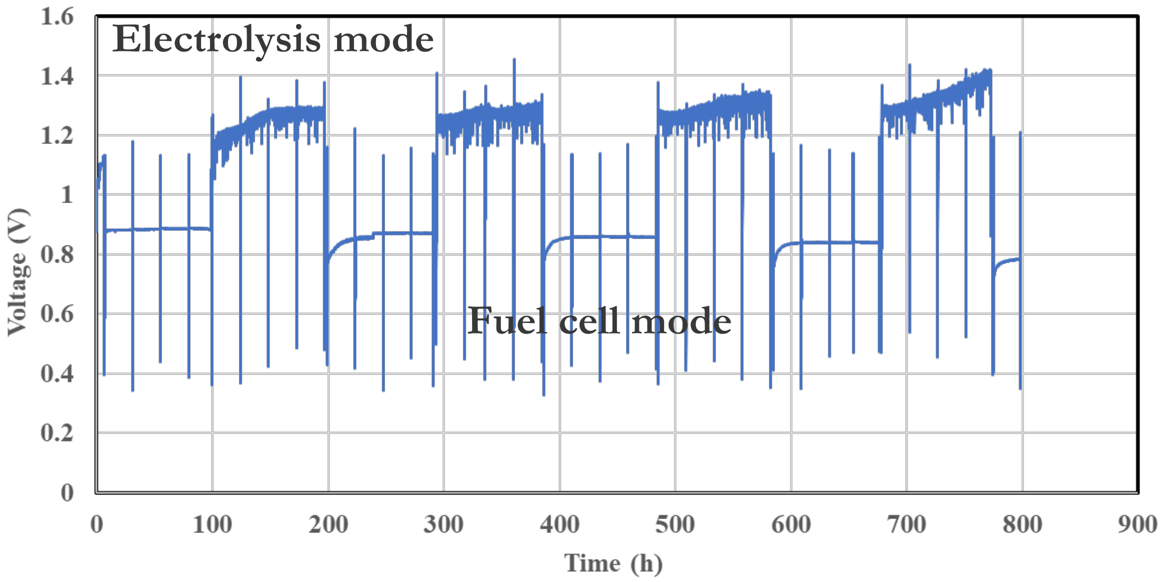
- Anode resistance of industry cells decreased by bio-surfactant assisted infiltration

Electrocatalyst-infiltrated planar cells

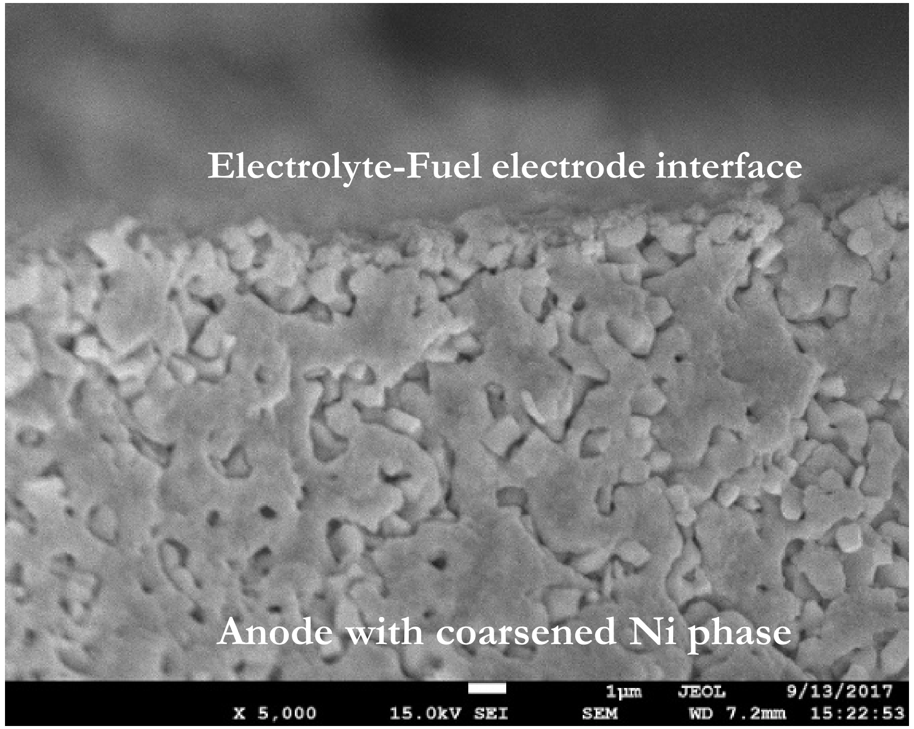
- The bio-surfactant assisted infiltration protocol was **verified on industrial planar fuel cells.**

Reversible Solid Oxide Cell Operation

- Cell: Commercial ASC w/ LSM-YSZ cathode
- Operation Temperature: 800°C
- Electrolysis (cathode): **H_2O – 60%, H_2 – 10%, N_2 – 30%**
- Fuel Cell (anode): **H_2 – 25%, N_2 – 75%**



Cell voltage variation under cyclic Fuel Cell/Electrolysis operation for 800 h

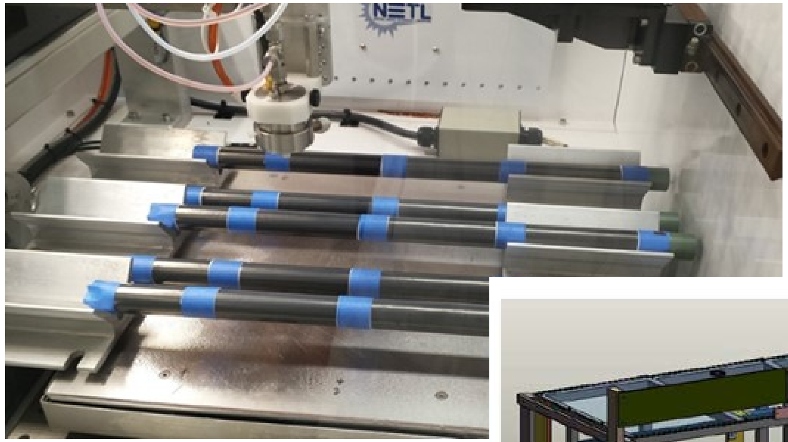


Delamination and Ni phase coarsening are evident from the fuel cell tested under electrolysis mode.

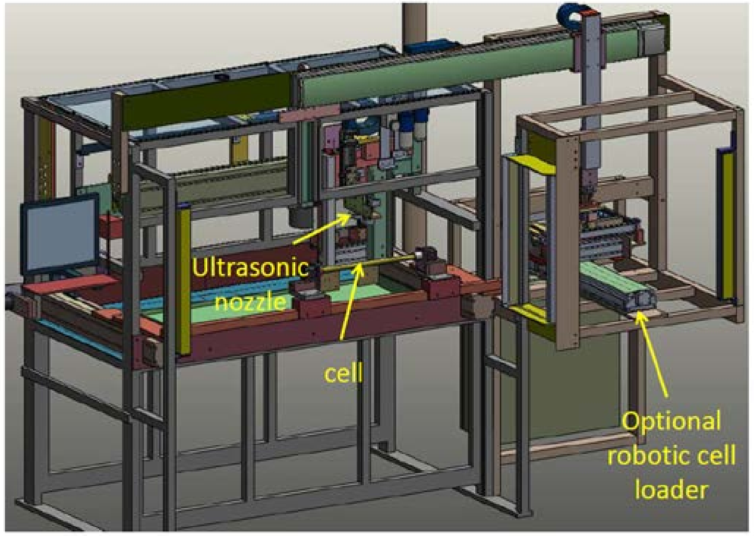
Advanced Electrode Infiltration Technique

NATIONAL ENERGY TECHNOLOGY LABORATORY

Technology Commercialization Fund Collaboration with Atrex Energy



Spray infiltration process at NETL

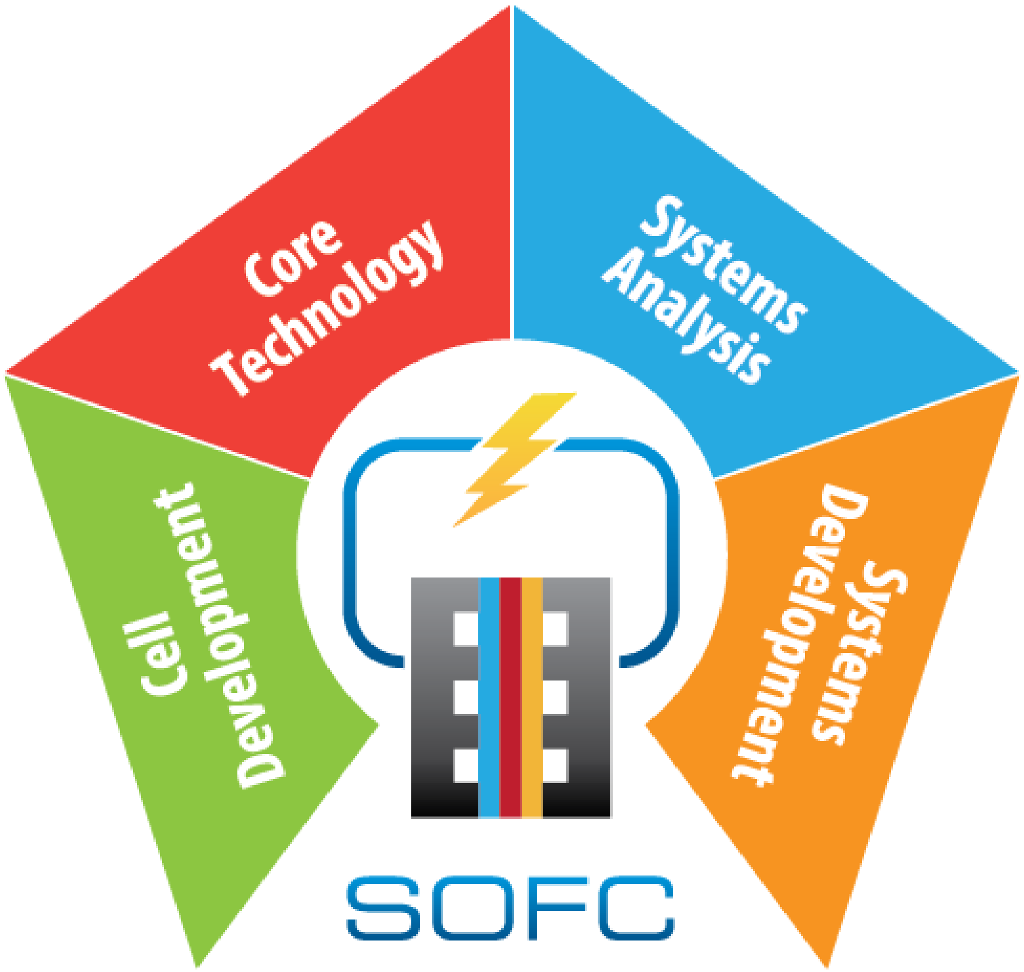


Factory-scale automatic spraying infiltration system installed at Atrex Energy

- Results showed the infiltration process applied to Atrex Energy tubular cells **reduced the processing time** required for cathode infiltration to one day.
- Atrex Energy has constructed a **factory-scale automatic spraying infiltration system** based on the NETL's technology.
- A **1.5 kW stack was tested** utilizing the infiltration process. The process improved the Atrex fuel cell stack performance **without noticeable degradation for 2,000 hours**.

Cell and Stack Degradation

Predictive Modeling Toolset Overview

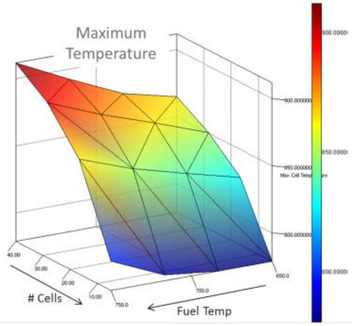


Background

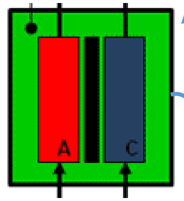
NETL/PNNL Collaboration to Complete Scaling Process

Need design and engineering at several scales to facilitate wide-scale SOFC commercialization

Link NETL and PNNL models at different scales to inform system level and life cycle analyses



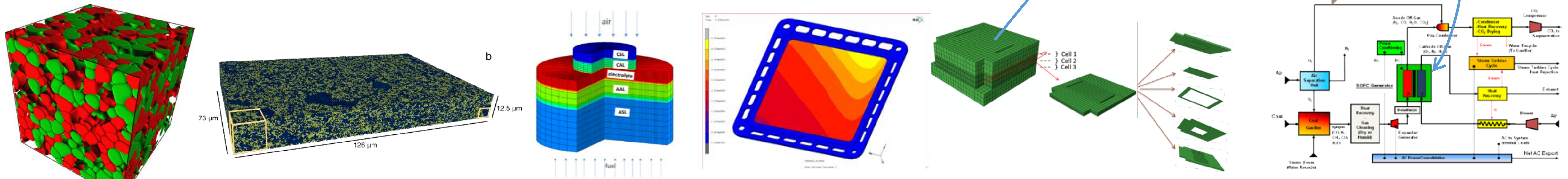
Response Surface Analysis



Reduced Order Model (ROM)

Stack Details

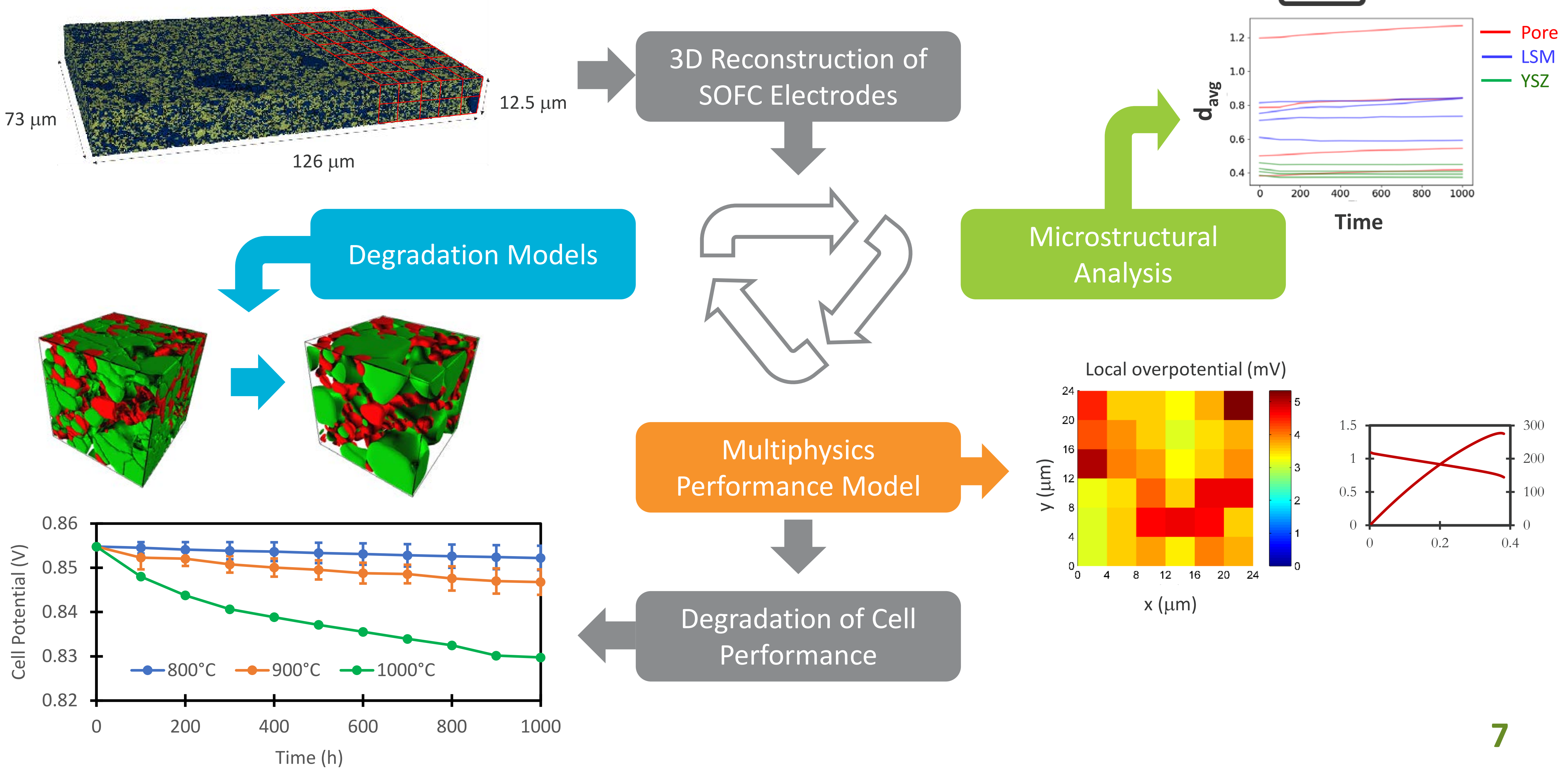
Increasing Scale



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

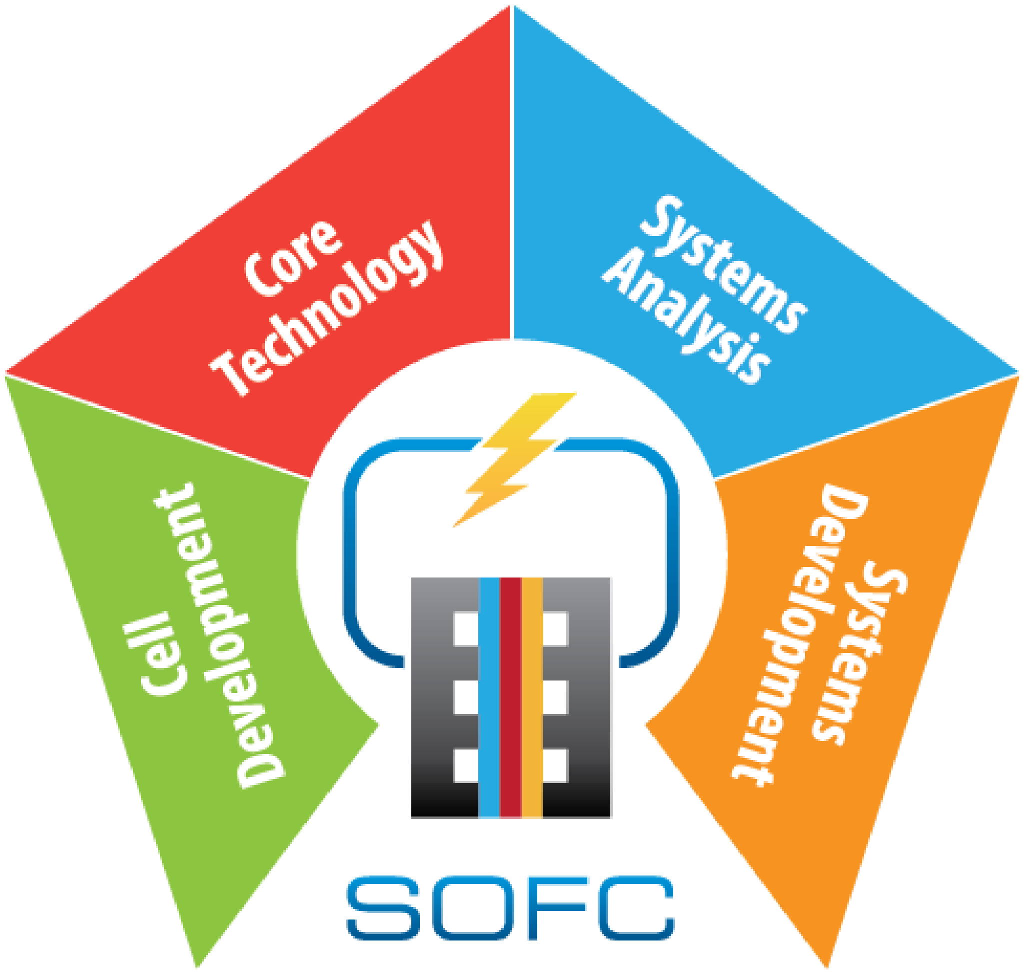
NETL | ***PNNL*** | ***NETL***

Integrated Cell Degradation Model



Cell and Stack Degradation

Technologies and Toolsets Under Development



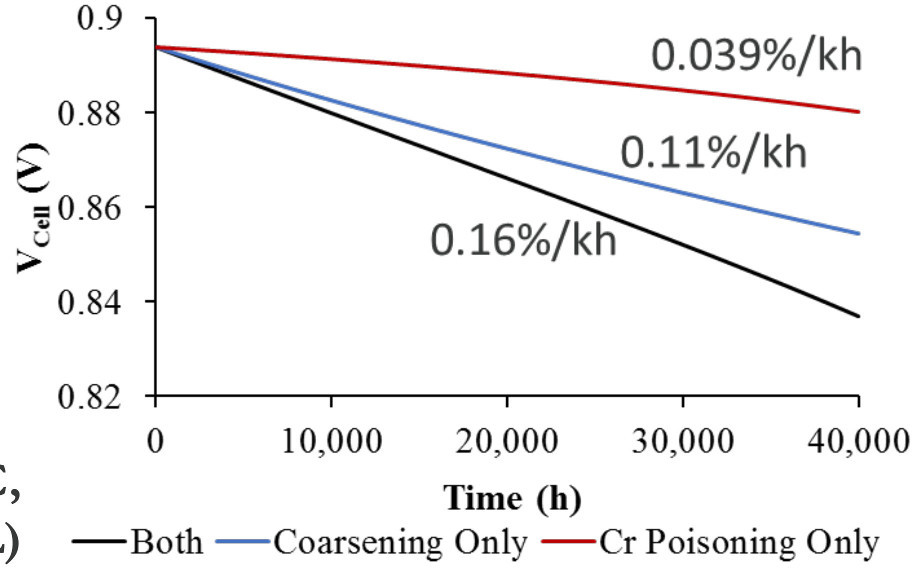
Degradation Modeling Overview

From Single to Multiple Degradation Modes

POSTER FE-069

POSTER FE-070

- **Last year:** Particle coarsening only (Temperature)
- **Current Efforts:**
  - Particle coarsening with gas phase transport of Ni (Temperature, Steam content)
  - Chromium poisoning of LSM (Temperature, Humidity, Potential)
  - Electrode delamination, cracking (No kinetic model yet)
- **Future Work:**
  - Initial toolset release
  - Interfacial phase formation
  - Reactions with fuel gas contaminants
  - Cation interdiffusion



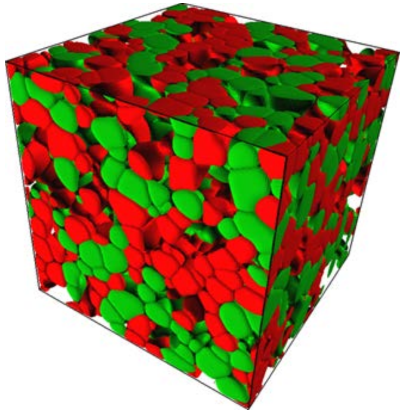
20×20 cm² cell, 0.5 A/cm² at 800°C, with 1% H_2O in air (Collaboration with PNNL)

See Poster "Performance degradation modeling of SOFCs using a multiphysics framework"
See Poster "Cation Diffusion in Bulk Tetragonal ZrO_2 for SOFCs"

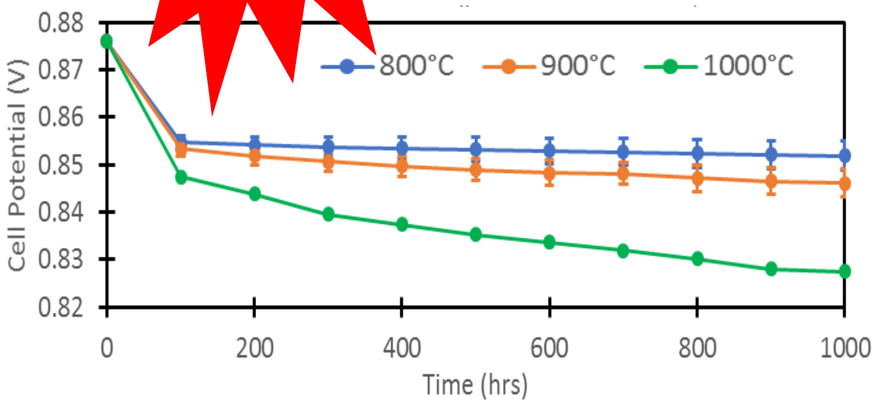
Performance Degradation Framework

Optimizing Electrodes for Performance and Lifetime

- **7,500 distinct electrode microstructures created with DREAM.3D**
  - Building blocks for 22,500 cathodes, 22,500 anodes with variety of phase fractions, phase fraction standard deviations (heterogeneity), particle sizes, particle size standard deviations
- **<u>Currently</u> running coarsening and performance simulations on 2,025 unique button cell microstructures**
  - Determine which factors play largest role in degradation
- **Future Work:**
  - Phase field coarsening replaced with calibrated ROM*
  - Inclusion of model parameters for LSCF
  - Publicly available tool for coarsening simulations
    - Workstation and supercomputer versions



POSTER
FE-071



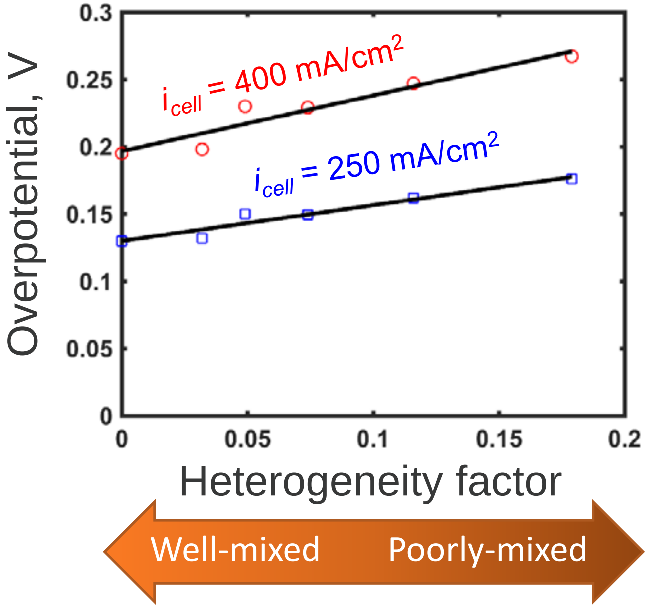
See Poster "ROM for microstructure evolution simulation in SOFC with dynamic discrepancy reduced modeling"

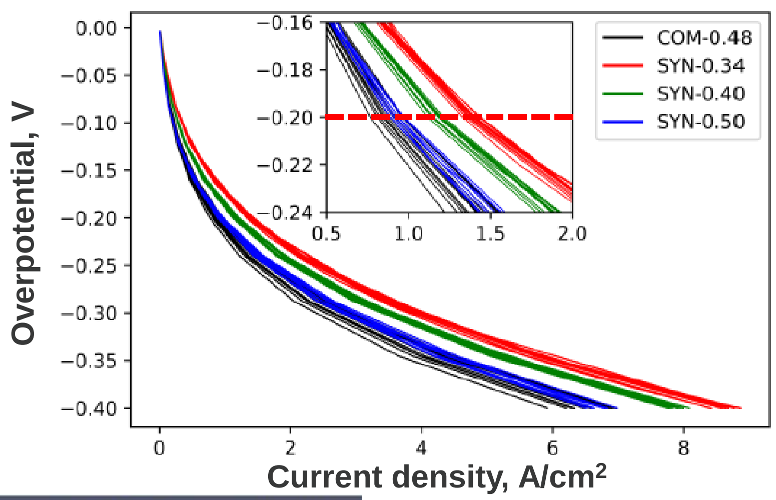
Heterogeneity and SOFC Performance

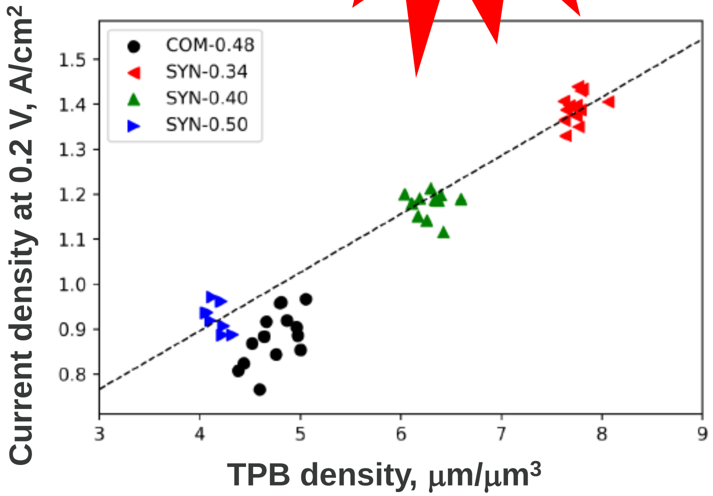
Collaboration: Carnegie Mellon University

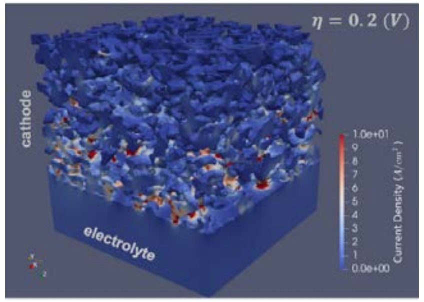
- Heterogeneity in composition impacts overpotential, degradation
- Tool: Developed ERMINE module for modeling SOFC subvolume performance within MOOSE framework

POSTER FE-068





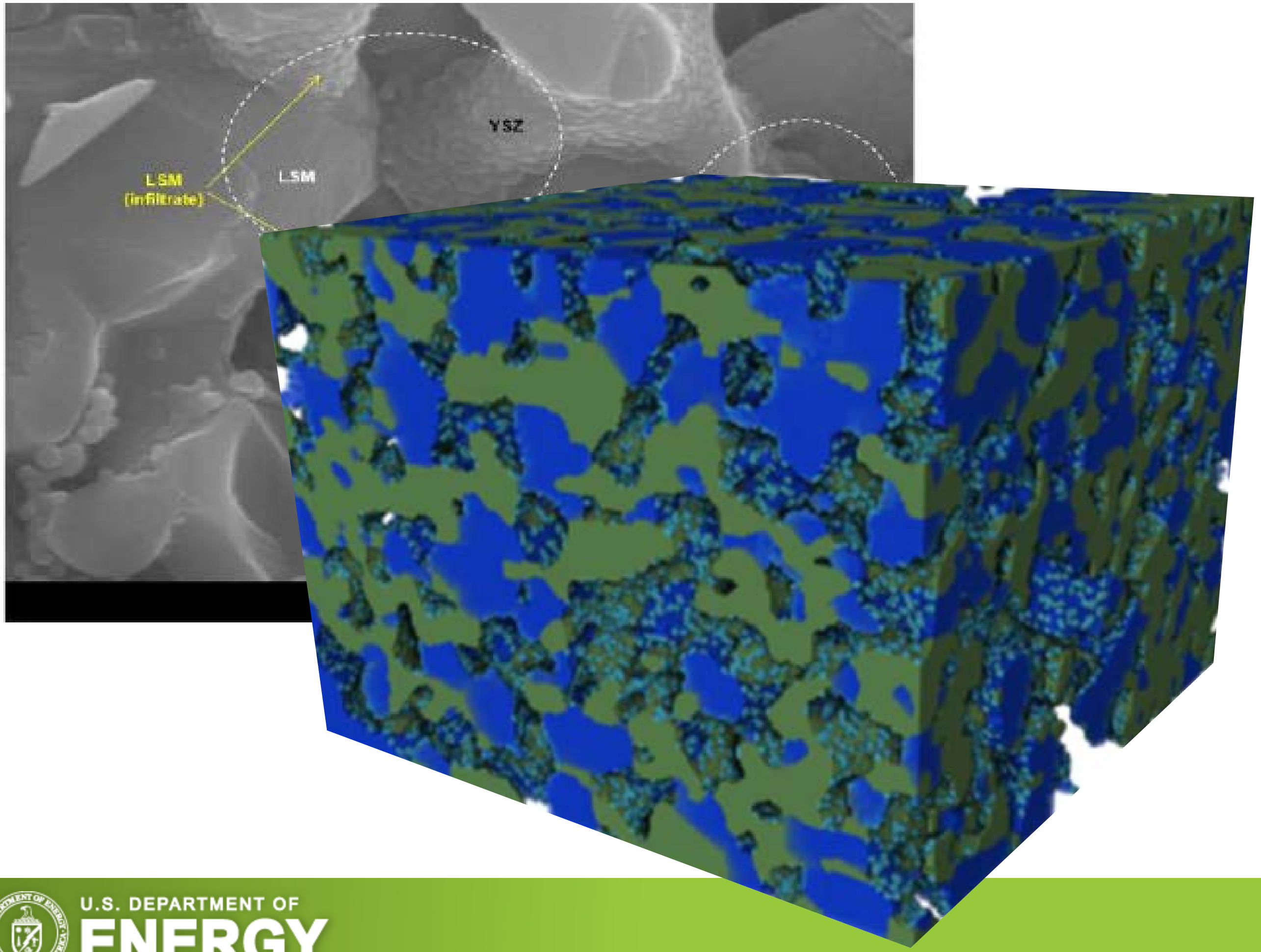


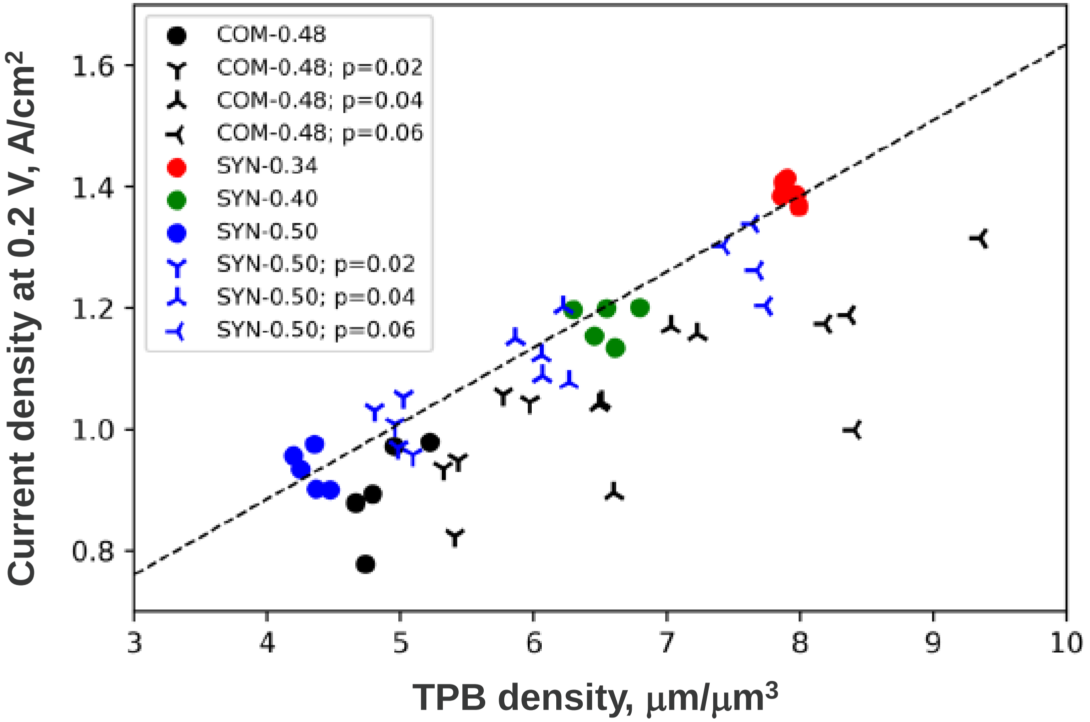


- Commercial cell subvolumes underperform synthetic cells of comparable micron-scale heterogeneity (other heterogeneity sources are present)

Electrode Infiltration Simulation

- Resolution of ERMINE subvolumes allows for infiltration of individual nanoparticles onto backbone

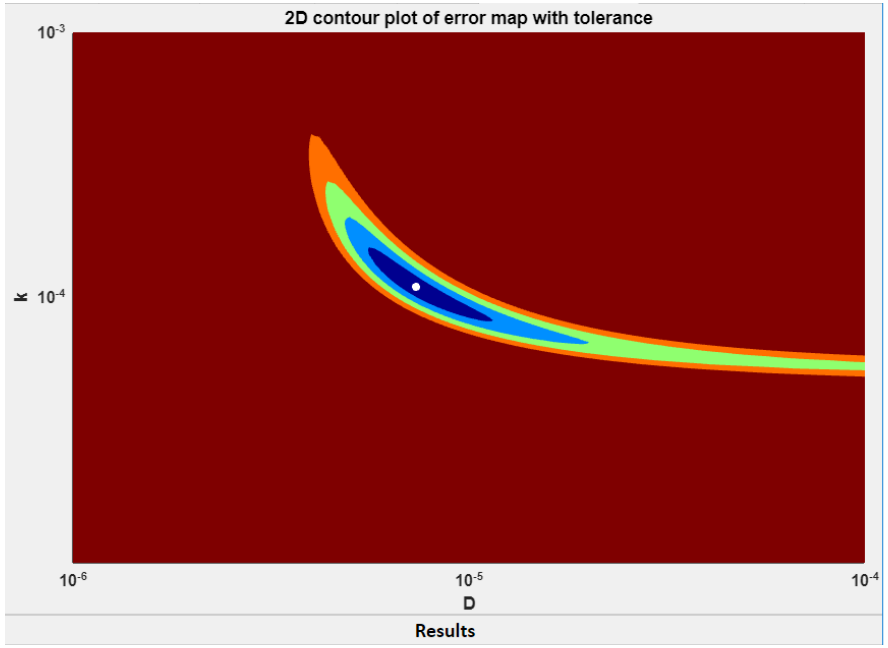


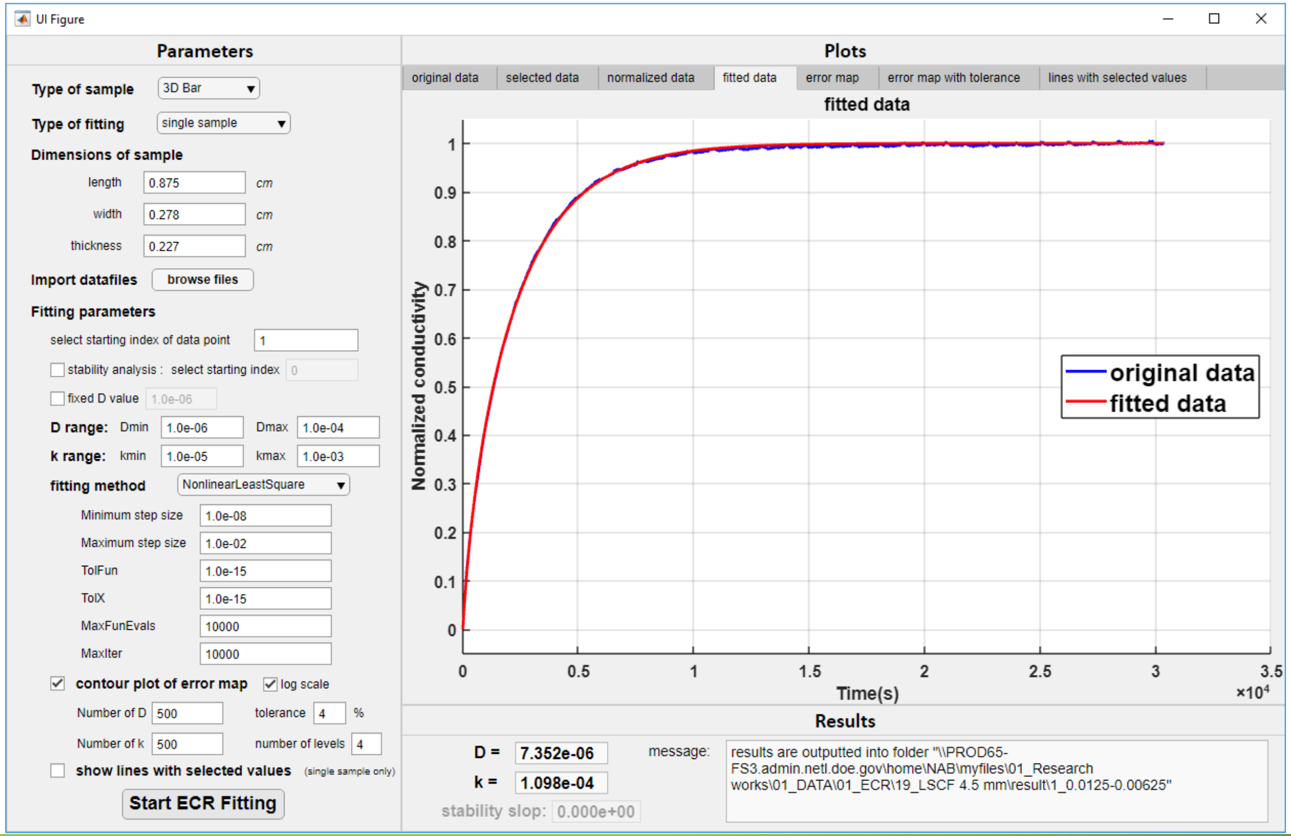


- Infiltration can achieve performance of more homogeneous microstructures

Data Analysis Tools

- **Developed tool for electrical conductivity relaxation (ECR) analysis**
  - Calculates surface exchange coefficient (*k*) and oxygen diffusion coefficient (D_0)
  - Calculates uncertainty map in *k*, *D* values
- **Next year: Release of impedance analysis tool for distribution of relaxation times (deconvolution)**

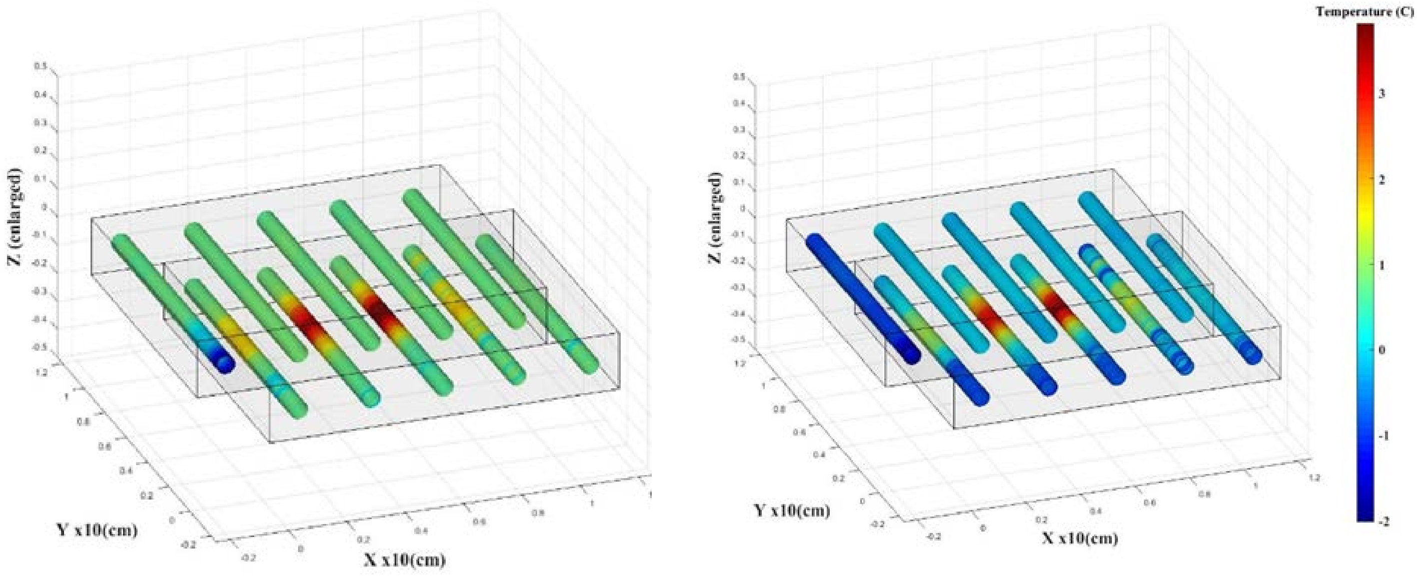




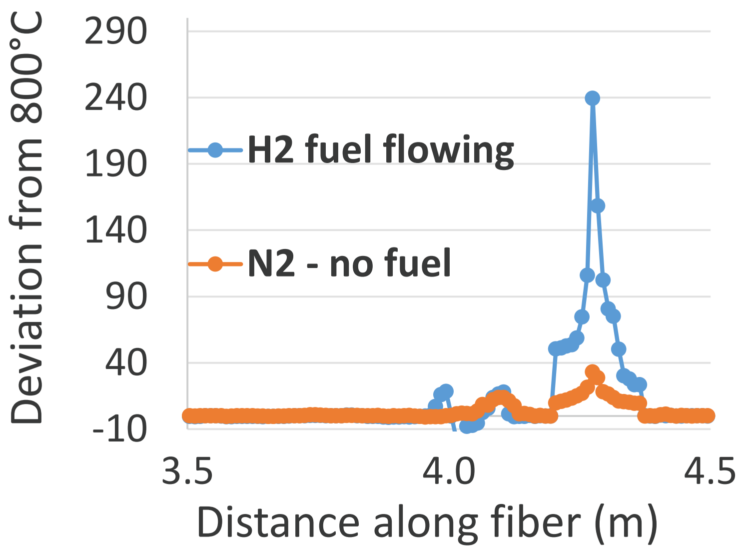
High Temperature Optical Fiber Sensor

Distributed In-situ Temperature and Gas Composition Sensing

- This year: Temperature, oxygen sensing tests on 25 cm^2 planar cells
- Next year: Temperature sensing in industrial planar and tubular cells



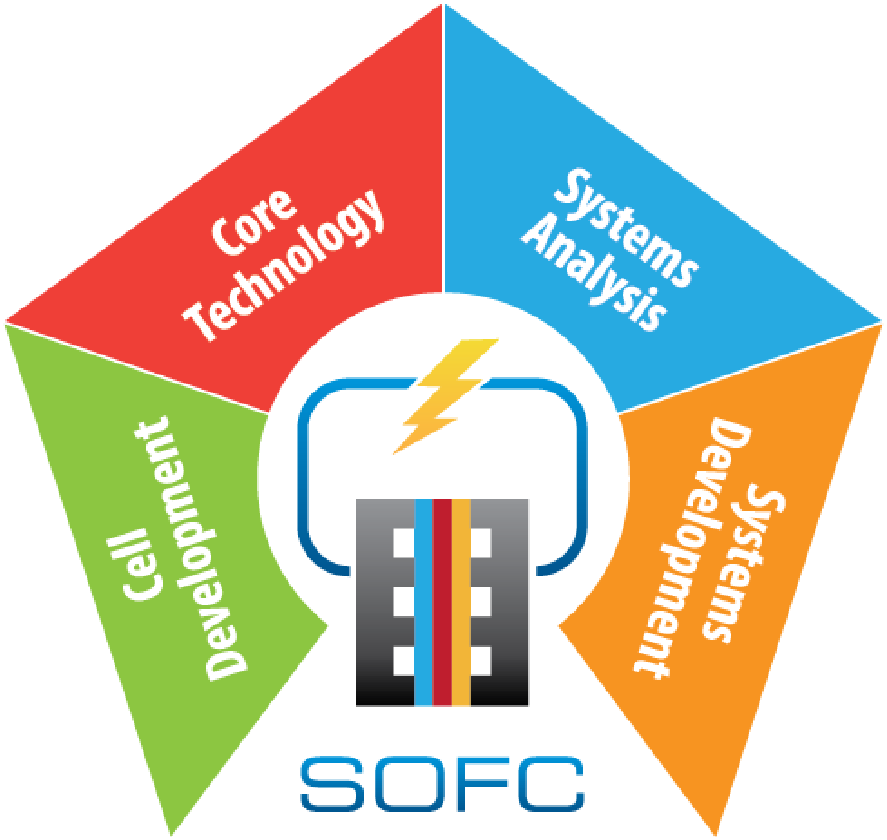
Thermal transients at 30 and 90 s from 5×5 cm^2 ASC at 750°C with H_2 fuel after 2A load



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

Systems Engineering & Analysis

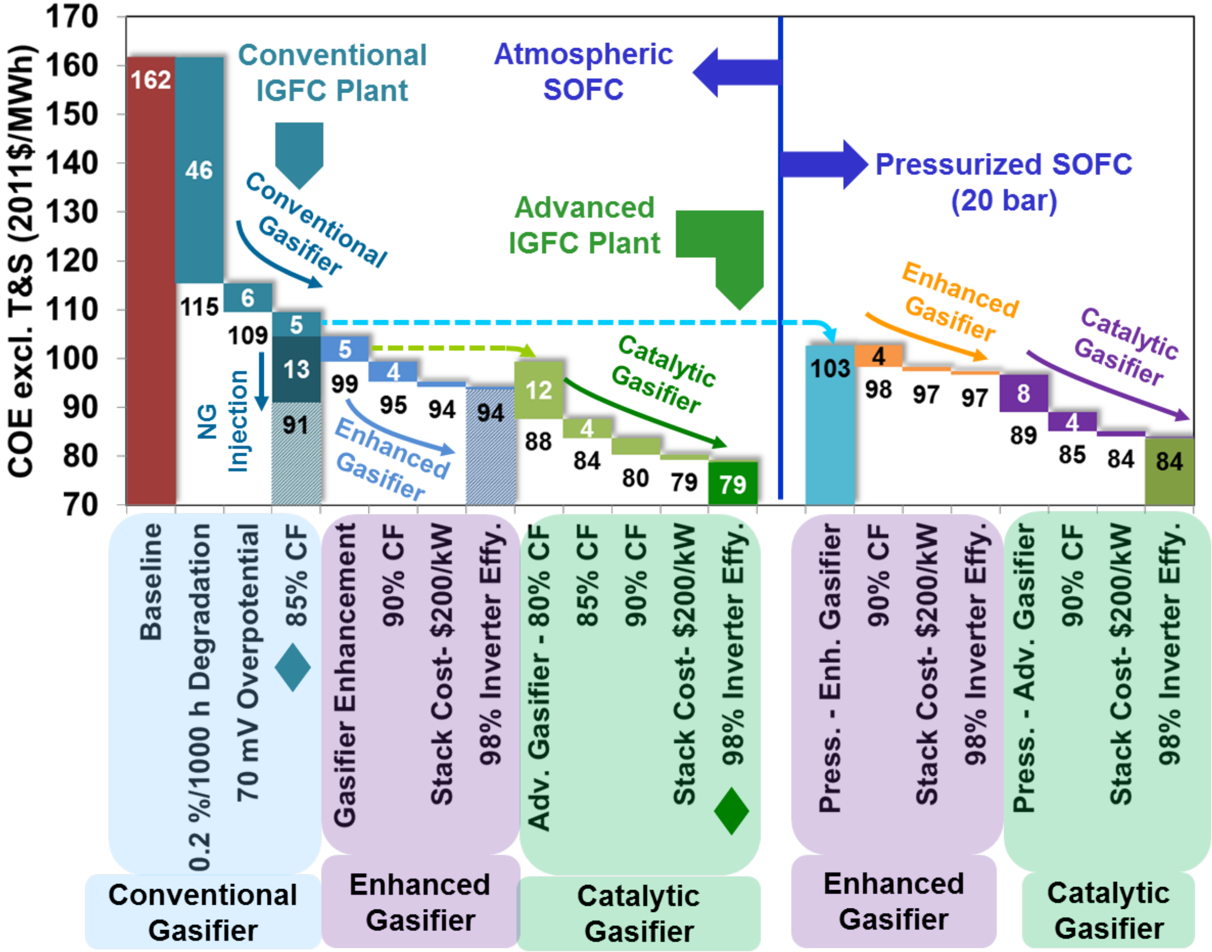
Pulling It All Together

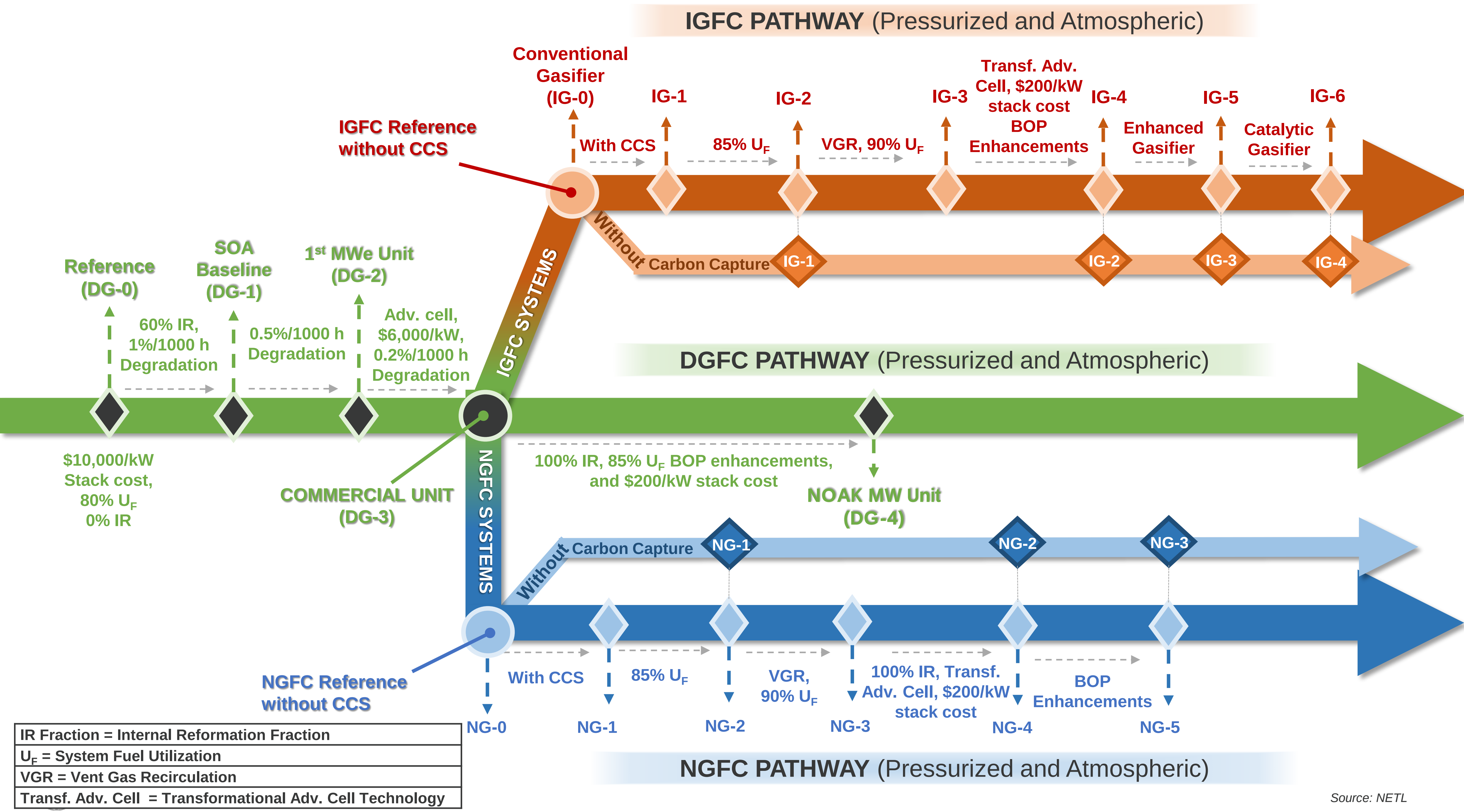


Systems Engineering & Analysis Efforts

Techno-Economic Assessment of SOFC Systems

- **Pathway Studies (Techno-Economic Assessment)**
  - Integrated Gasification Fuel Cell (IGFC) system
  - Natural Gas Fuel Cell (NGFC) system
  - Distributed Generation (DG) Fuel Cell system
- **Reports released to public by 10/31/2019**
- **Future Efforts (this coming year)**
  - Small Scale Fuel Cell systems
    - 5-, 10-, 50-kW





IGFC PATHWAY (Pressurized and Atmospheric)
Conventional Gasifier (IG-0)
IGFC Reference without CCS
With CCS
IG-1
85% U_F
IG-2
VGR, 90% U_F
IG-3
Transf. Adv. Cell, $200/kW stack cost BOP Enhancements
IG-4
Enhanced Gasifier
IG-5
Catalytic Gasifier
IG-6
Without Carbon Capture
IG-1
IG-2
IG-3
IG-4
IGFC SYSTEMS
Reference (DG-0)
60% IR, 1%/1000 h Degradation
SOA Baseline (DG-1)
0.5%/1000 h Degradation
1st MWe Unit (DG-2)
Adv. cell, $6,000/kW, 0.2%/1000 h Degradation
DGFC PATHWAY (Pressurized and Atmospheric)
$10,000/kW Stack cost, 80% U_F 0% IR
COMMERCIAL UNIT (DG-3)
100% IR, 85% U_F BOP enhancements, and $200/kW stack cost
NOAK MW Unit (DG-4)
NGFC SYSTEMS
Without Carbon Capture
NG-1
NG-2
NG-3
NGFC Reference without CCS
With CCS
85% U_F
VGR, 90% U_F
100% IR, Transf. Adv. Cell, $200/kW stack cost
BOP Enhancements
NG-0
NG-1
NG-2
NG-3
NG-4
NG-5
NGFC PATHWAY (Pressurized and Atmospheric)
IR Fraction = Internal Reformation Fraction
U_F = System Fuel Utilization
VGR = Vent Gas Recirculation
Transf. Adv. Cell = Transformational Adv. Cell Technology

Source: NETL

Contact Information

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Poster Session

Please stop by to see our posters!

NATIONAL ENERGY TECHNOLOGY LABORATORY

Poster Session 6:30-8:00 PM

Location - Independence B

FE067 (Electrode Engineering Progress)

FE068 (Mesoscale Heterogeneity Impact)

FE069 (Multiphysics Degradation Modeling)

FE070 (Effect of Hydrogen on Cation Diffusion)

FE071 (Microstructure Evolution Simulation)