Progress of the NETL Solid Oxide Fuel Cell Research Portfolio


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NETL Research and Innovation Center
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Solutions for Today | Options for Tomorrow
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)

Carnegie Mellon University
- Paul Salvador (MSE)
- Shawn Lister (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)

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)

Currently 48 SOFC Team Members
Posters 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

• Objectives
  • Enhancement of electrode performance and longevity
  • Materials engineering
  • Microstructure engineering

• Benefits
  • Stack cost reduction
  • Cell overpotential reduction
  • Thermo-chemical / thermo-mechanical stability increase

See Poster “Progress in Electrode Engineering of SOFC at NETL”
Advanced Electrode Design

Collaboration: University of Wisconsin-Madison

Bridging Theory and Reality

- Electrical Conductivity Relaxation measurement of the calculated \( \text{Ba(Fe}_{0.2}\text{Co}_{0.2}\text{Zr}_{0.6})\text{O}_3 \) resulted in \( 5 \times \) higher \( k_{\text{chem}} \) and \( 3 \times \) higher \( D_{\text{chem}} \) compared to LSCF

Surface exchange coefficient versus \( O \) \( p \)-band center

Advanced Electrode Design
Collaboration: Clemson University

Proton Conducting SOFC Electrodes

- Electrolyte: BCZYYb, Cathode: BCFZY or LSCF
- Electro catalyst: BaCO$_3$, nano-BCFZY, etc.

- The ASR of the BaCO$_3$-infiltrated LSCF cathode (0.08 $\Omega \cdot \text{cm}^2$) is significantly less than that of the pure LSCF cathode (0.27 $\Omega \cdot \text{cm}^2$) at 700°C
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.

Error map for the calculated $k_{chem}$ and $D_{chem}$ at $pO_2 = 1.25\%$ (a) bare LSCF, (b) LSCF coated with porous layer.
High Surface-Area Nanostructured Cathodes via In-Situ Carbon Templating – Collaboration: Wake Forest University

Traditional Sintering
1) Ceramic + Pore Former  2) Sinter in Air

In-Situ Carbon Templating Method
1) Hybrid Materials
   Suspend metals in organic matrix
2) Sinter in Argon
   Form carbon template in-situ
3) Calcine in Air
   Remove carbon by low temperature oxidation

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

- Nano-YSZ infiltrated: 0.67% over 200 h
- (PrBa)CoOₓ infiltrated: 1.86% over 200 h
**Bio-Surfactant Assisted UN-REDUCED SOFC Anode Infiltration**

- pNE offers smoother and more uniform coating
- Anode resistance of industry cells decreased by bio-surfactant assisted infiltration
- 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): $\text{H}_2\text{O} – 60\%, \text{H}_2 – 10\%, \text{N}_2 – 30\%$
- Fuel Cell (anode): $\text{H}_2 – 25\%, \text{N}_2 – 75\%$

Electrolysis mode

Fuel cell mode

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

Technology Commercialization Fund Collaboration with 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
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

NETL/PNNL Collaboration to Complete Scaling Process

Response Surface Analysis
Reduced Order Model (ROM)
Stack Details

Increasing Scale
Electrode Microstructure
Single Cell
Multi-Cell Stack
IGFC System Model

NETL
PNNL
NETL

PNNL Collaborators: Brian Koeppel and Kurt Recknagle
Integrated Cell Degradation Model

3D Reconstruction of SOFC Electrodes

Degradation Models

Microstructural Analysis

Multiphysics Performance Model

Degradation of Cell Performance
Cell and Stack Degradation
Technologies and Toolsets Under Development
Degradation Modeling Overview

From Single to Multiple Degradation Modes

• **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% H₂O in air (Collaboration with PNNL)

See Poster “Performance degradation modeling of SOFCs using a multiphysics framework”
See Poster “Cation Diffusion in Bulk Tetragonal ZrO₂ 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

• Currently 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

See Poster “ROM for microstructure evolution simulation in SOFC with dynamic discrepancy reduced modeling”
• Heterogeneity in composition impacts overpotential, degradation

• Tool: Developed ERMINE module for modeling SOFC subvolume performance within MOOSE framework

- 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 ($D_o$)
  • 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
• 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
$10,000/kW Stack cost, 80% UF, 0% IR

Reference (DG-0)

SOA Baseline (DG-1)

1st MWe Unit (DG-2)

Conventional Gasifier (IG-0)

IG-1

IG-2

IG-3

IG-4

IG-5

IG-6


VGR, 90% UF

BOP Enhancements

Enhanced Gasifier

Catalytic Gasifier

NOAK MW Unit (DG-4)

Carbon Capture

IGFC Reference without CCS

NGFC Reference without CCS

Commercial Unit (DG-3)

Reference (DG-4)

1st MWe Unit (DG-2)

Adv. cell, $6,000/kW, 0.2%/1000 h Degradation

60% IR, 1%/1000 h Degradation

0.5%/1000 h Degradation

100% IR, 85% UF, BOP enhancements, and $200/kW stack cost

$10,000/kW Stack cost, 80% UF, 0% IR

IR Fraction = Internal Reformation Fraction

UF = System Fuel Utilization

VGR = Vent Gas Recirculation


Source: NETL
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