

Systems Analysis of Fuel Cell Plant Configurations



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Systems Engineering and Analysis (SEA)

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18TH Annual SOFC Project Review Meeting

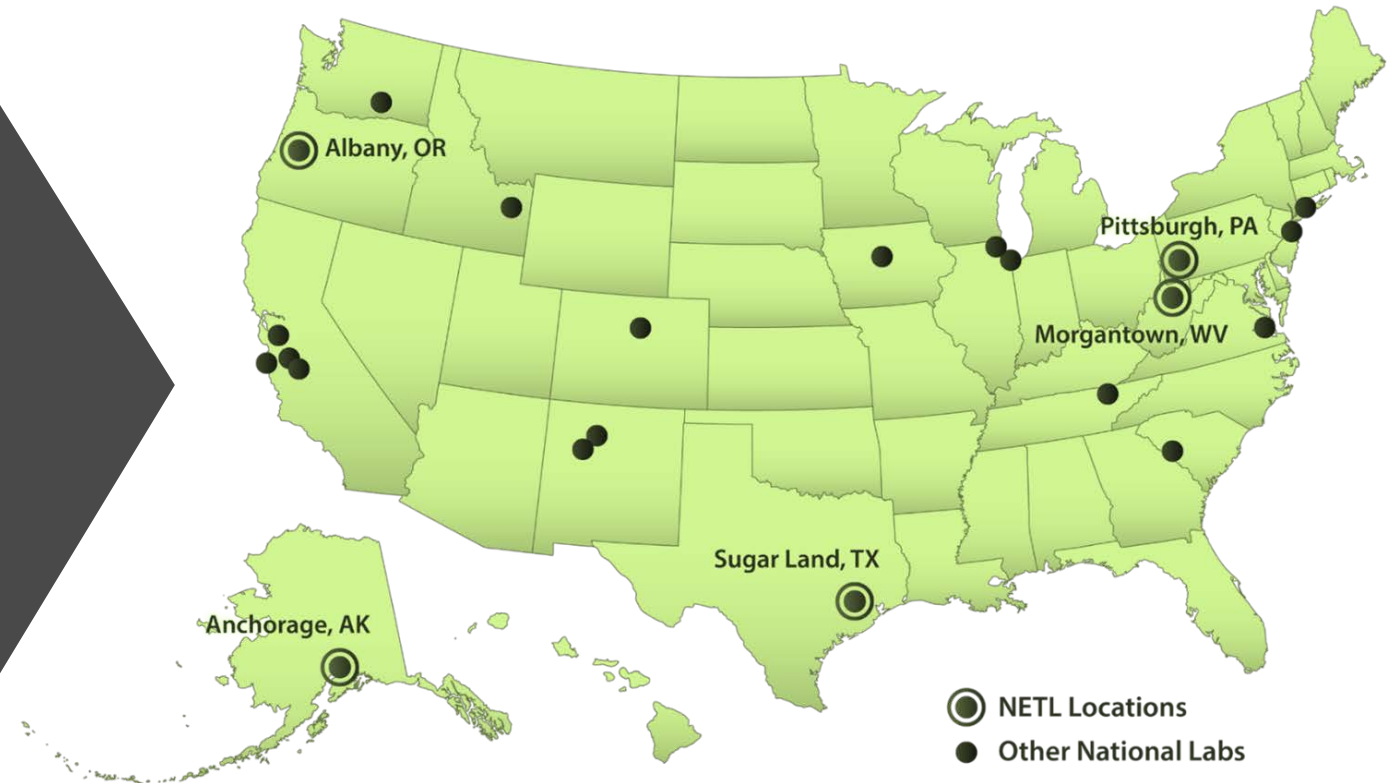


Solutions for Today | Options for Tomorrow



Outline

- SEA Primary Functions and Objectives
- SOFC Technology Development Plan
- Distributed Generation Market Analysis Update
- Pathway Studies
 - NETL Systems Model Enhancement



SEA Primary Functions and Objectives

- **Assess Technology Cost and Performance**

- Compare advanced technologies with current state-of-the-art (SOTA) and research and development (R&D) goals
 - Baseline studies* (current SOTA) – updated regularly
 - Screening studies for novel technologies
 - Technology pathway studies (e.g. IGFC, NGFC, IGCC, post-combustion CC)
- Identify integration, performance, and cost requirements as appropriate for advanced technology components
- Unbiased assessments of technology options

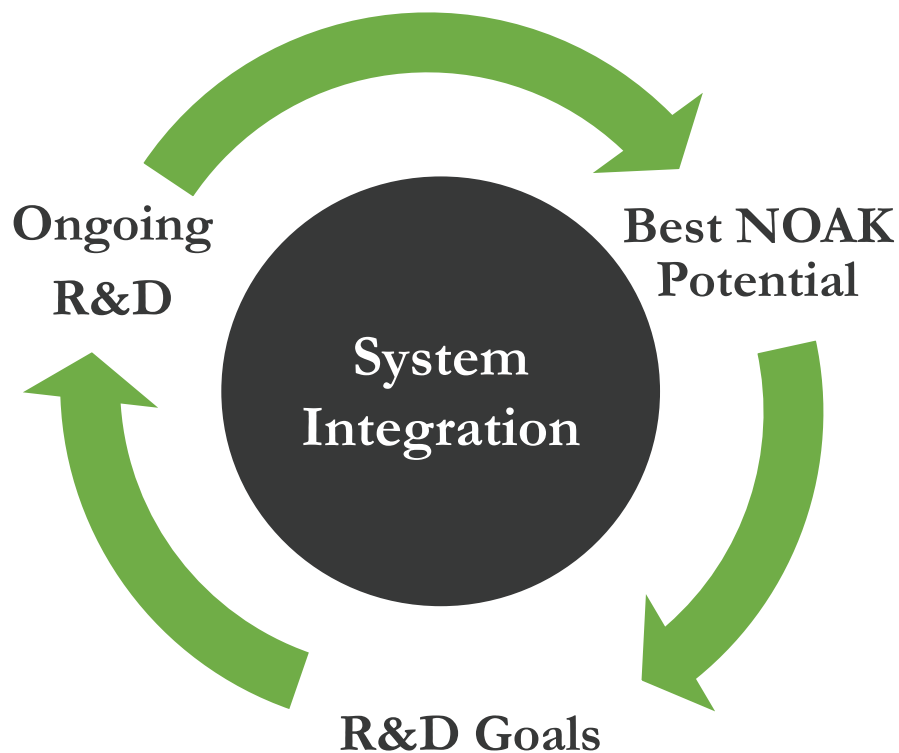
- **Assist NETL Science & Technology Strategic Plans & Programs**

- Funding Opportunity Announcement preparation
- Proposal reviews
- Critiques of external system studies

SEA Primary Functions and Objectives

1
Assess technology
based on current data
from ongoing R&D

2
Based on initial
assessment, estimate best
possible NOAK
performance potential

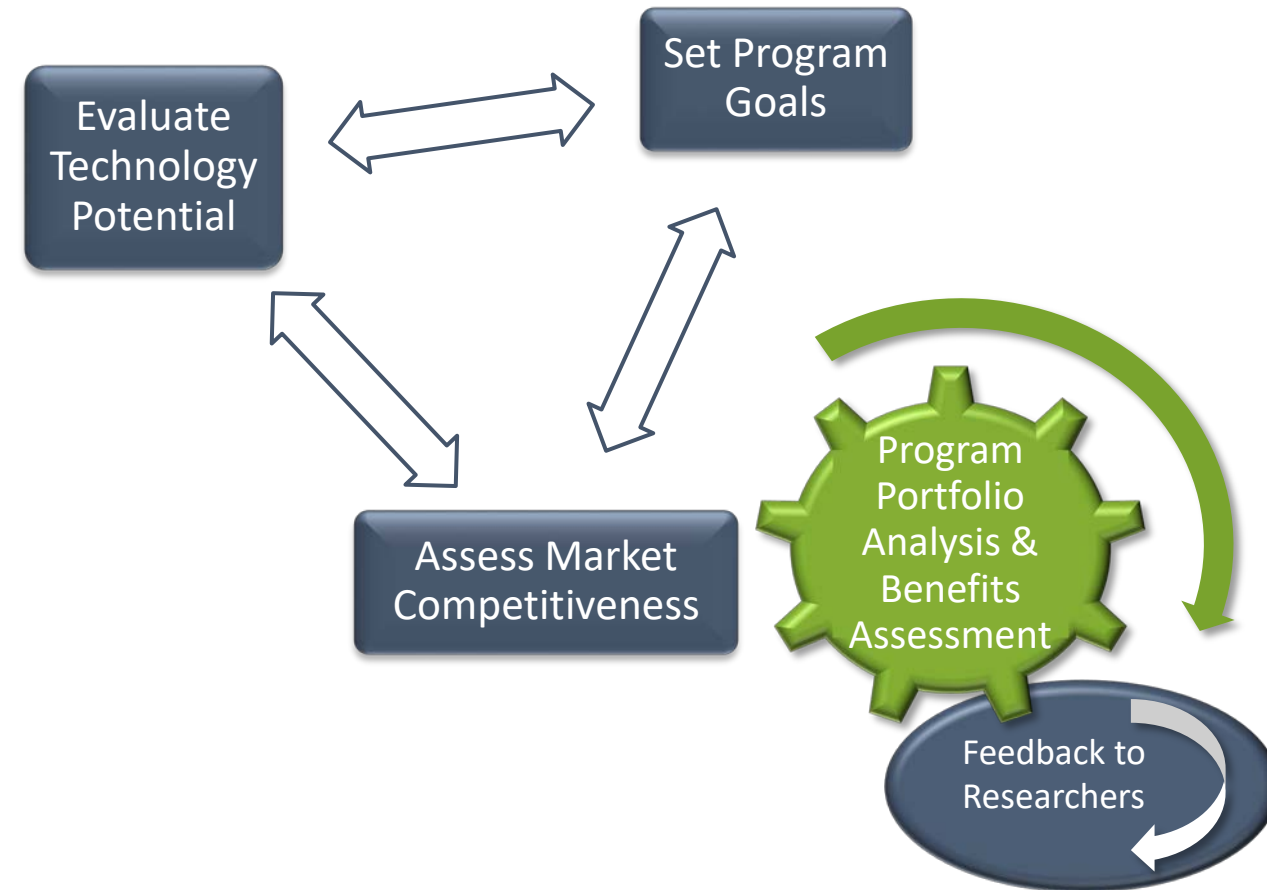


4
Provide feedback to
researchers

3
Compare best NOAK
performance to R&D goal;
determine if/how any
gaps can be closed

SEA and SOFC Program R&D at NETL

- How do SEA analyses directly impact SOFC research at NETL?
- **Systems Engineering and Analysis**
 - Informs Program of technology potential
 - Assists in establishing programmatic goals
 - Assess markets
- **Research and Development Efforts**
 - Directly addresses programmatic goals
 - Direct interaction with SOFC developers
 - Multi-disciplinary, collaborative effort



SOFC Technology Development Plan

CELL DEVELOPMENT (TRL 2-5)

R&D on individual cell components

Challenges

- Increase power density
- Lower degradation
- Reduce costs

Approach

- Innovative materials
- Increase cell area
- Automation

MODULE and BOP (TRL 2-5)

R&D on stack components, modules, and BOP

Challenges

- Thermal gradients
- Flow maldistribution
- Lower cost

Approach

- Modeling
- Robust/low cost materials
- In-stack fuel reformation

INNOVATIVE CONCEPTS (TRL 3-7)

R&D on second generation cell and stack technology

Challenges

- Reduce degradation
- Improve reliability
- Lower cost

Approach

- Modeling
- Compact design
- Advanced manufacturing

SYSTEMS INTEGRATION (TRL 6-8)

RD&D leading to entry-into-service power systems

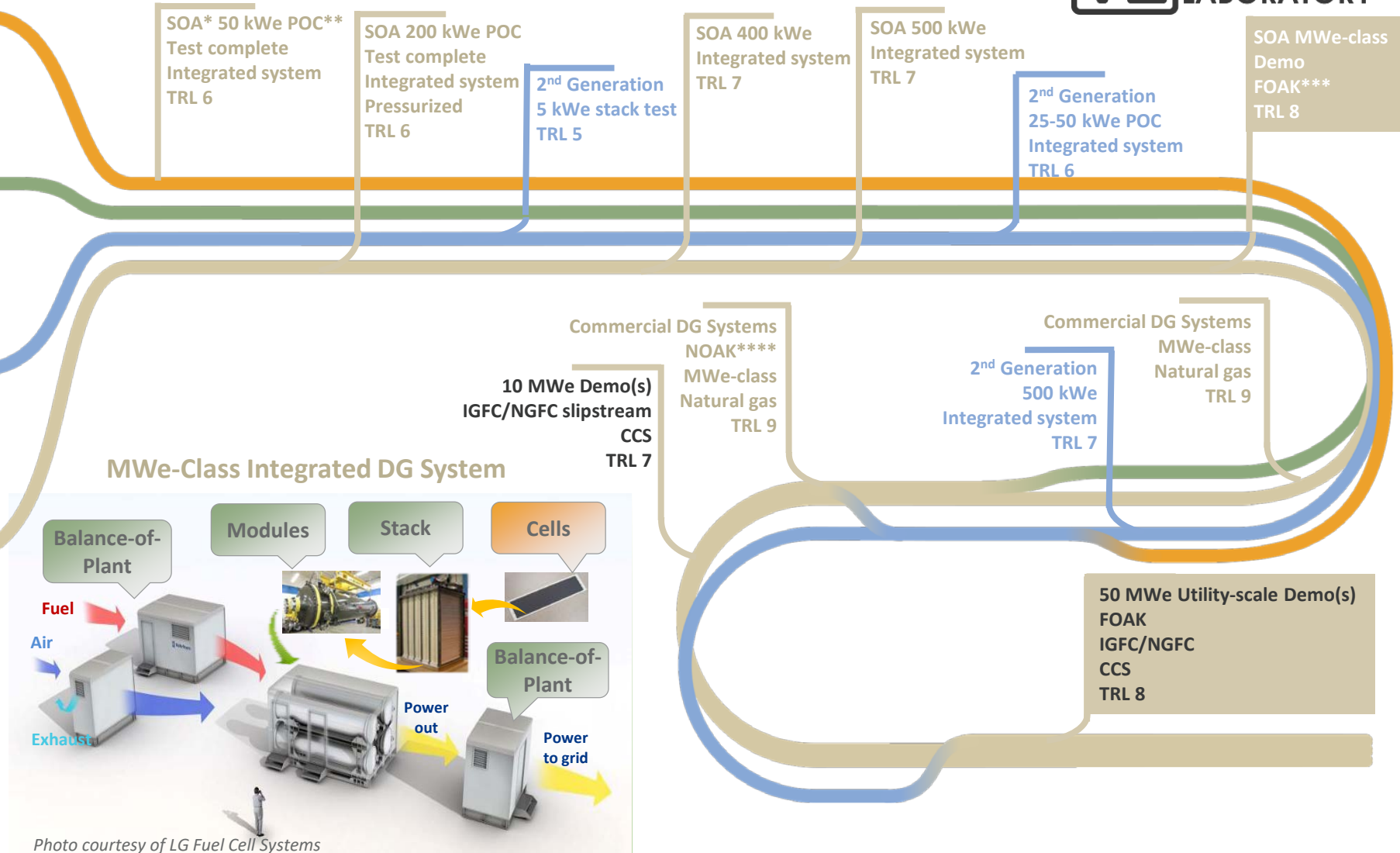
Challenges

- Integration of components
- Complexity
- Operating strategy

Approach

- Systems analysis
- Progressively larger system tests
- Multiple demonstrations

- * State-of-the-art
- ** Proof-of-concept
- *** First-of-a-kind
- **** Nth-of-a-kind



SOFC Major Development Targets

Distributed Generation (≈ 250 kW-1 MW) and Utility-Scale (550 MW)



- **Distributed Generation (DG)**

- Need to explore the DG market potential of SOFC
- An update to a previous market study is underway

- **Utility-Scale SOFC Plants (IGFC/NGFC)**

- Establish n^{TH} -of-a-kind performance and cost using experimental data from state-of-the-art SOFC and defining “advanced” SOFC performance for system models
- Sensitivity studies to determine and prioritize performance and cost parameters
- Pathway studies (previously released in 2014/15) will be updated

Distributed Generation Market Study Update

Distributed Generation Market Study



Background

- **The previous study* explored the DG market potential of SOFC**
 - DG market opportunity: electric power (250 kWe to MWe class units)
 - SOFC DG electric power application
 - Provides > 20-percentage-point gain in efficiency
 - Results in significant CO₂ emission reduction
 - Path charted to commercial, cost-competitive SOFC DG product
 - Consistent with technology development plan
 - ~ 25 MWe installed capacity to achieve competitive cost
 - Projected learning to achieve competitive cost is consistent with similar technology commercialization experience
 - Higher natural gas price: reduces time to commercialization
 - SOFC DG applications provide path to utility scale plants with >98% carbon capture with efficiencies > 60% HHV

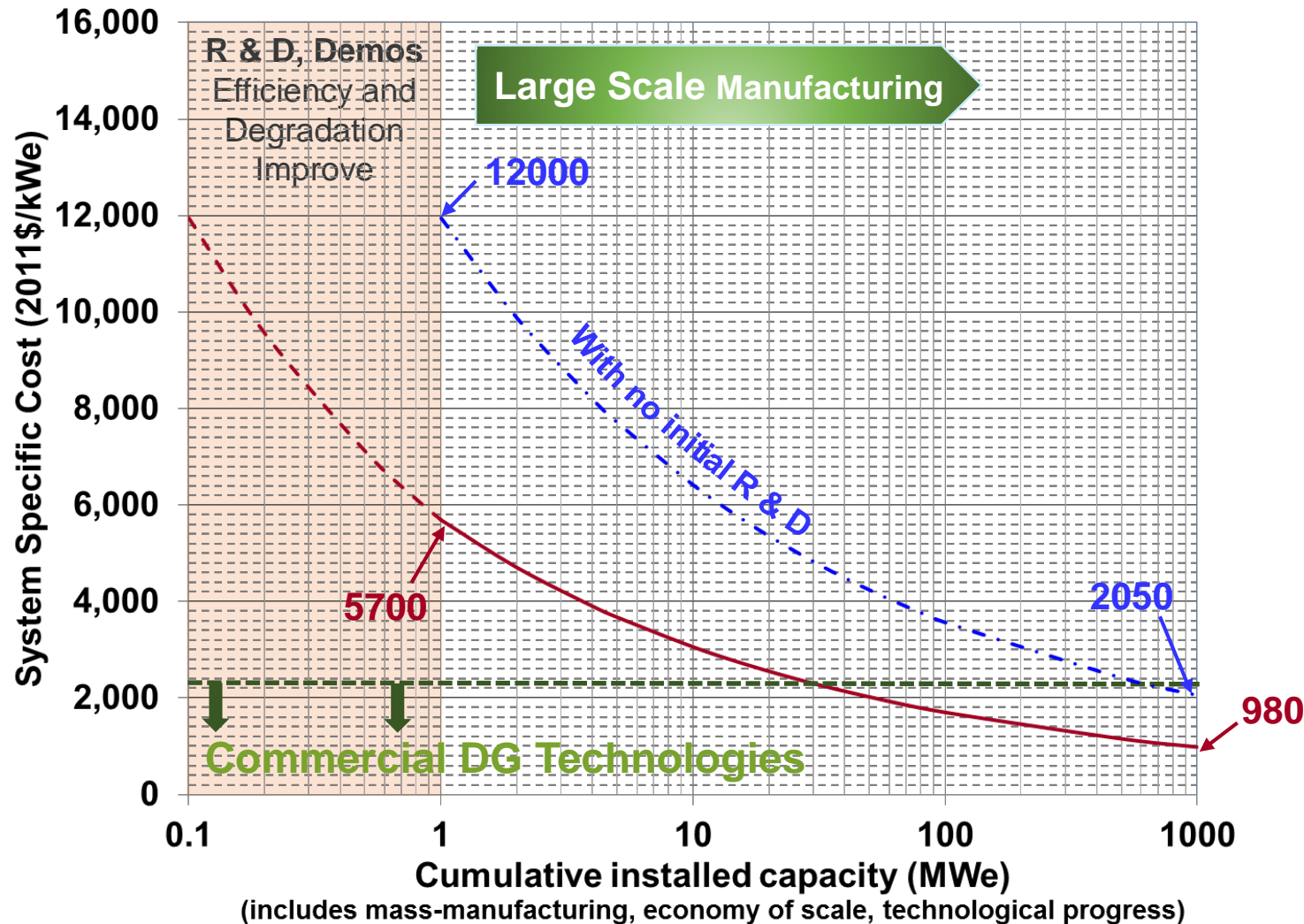
Distributed Generation Market Study

Objective

- **The objective of the present study is to update the previous analysis**
 - Update DG Market Projections
 - Identify appropriate market segment for SOFC
 - Integrate Department of Defense (DoD) opportunity analysis
 - Better represent competing technologies
 - Include renewable technologies – solar photovoltaics (PV), geothermal, wind, etc.
 - Update competing technologies costs data as available
 - Update subsidies/incentives
 - Update reference DG - SOFC system costs
 - Potentially include a reference pressurized system
 - Update learning curve analysis
 - Include learning curves for competing technologies
 - Installed capacity to achieve competitive cost
 - Update capacity/learning projected to achieve competitive cost

SOFC Learning Curve Analysis Update

Specific Cost versus Installed Capacity

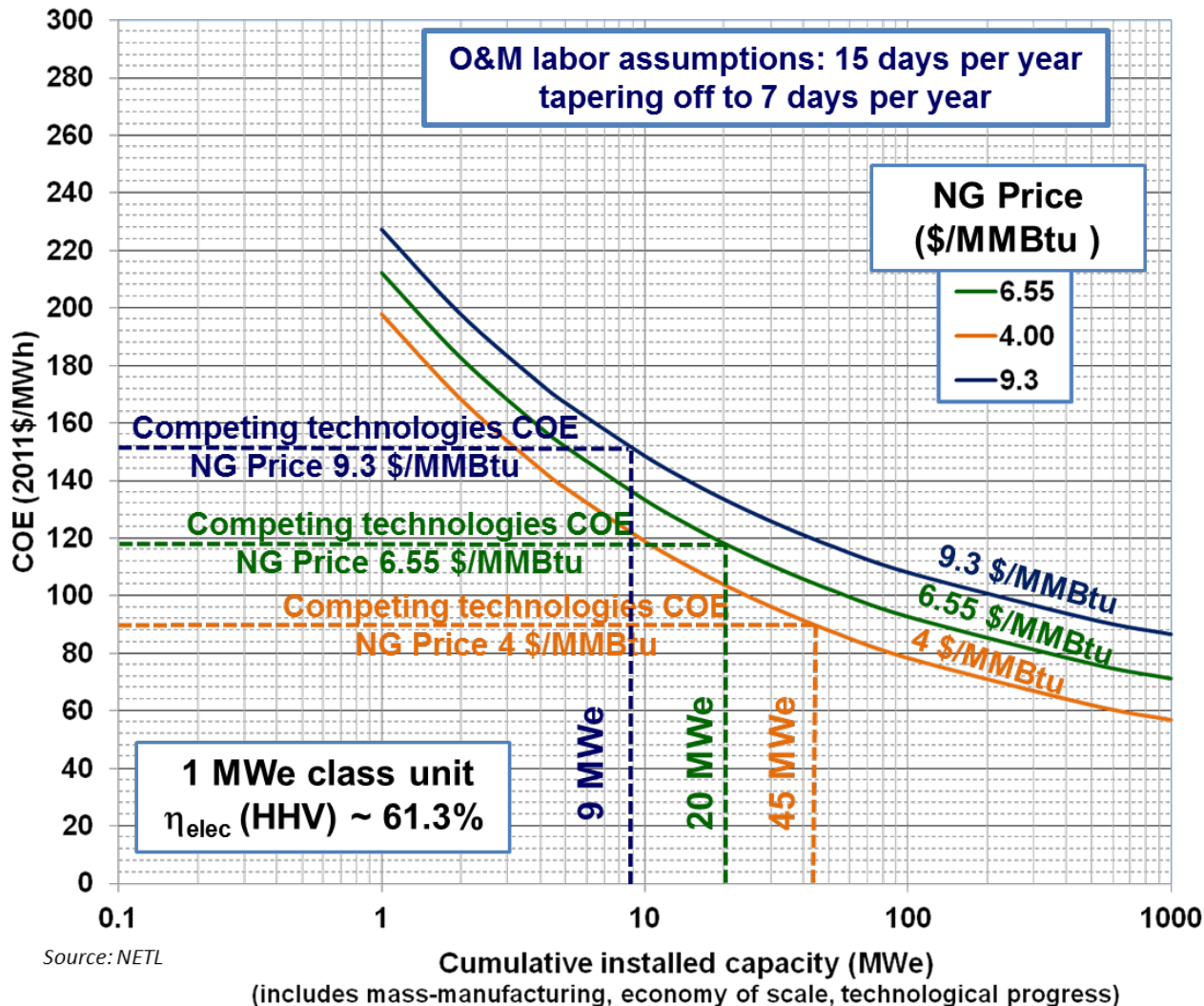


- Update learning curve to be consistent with the capital vs. installed capacity plot and the SOFC roadmap
- Include learning curve for competing commercial DG technologies

Source: NETL

SOFC Learning Curve Analysis Update

COE versus Installed Capacity



- Update the sensitivity of natural gas prices on cost-of-electricity (COE)
- As natural gas prices decrease, more installed DG SOFC capacity needed to be cost competitive

NETL SOFC System Model Enhancement

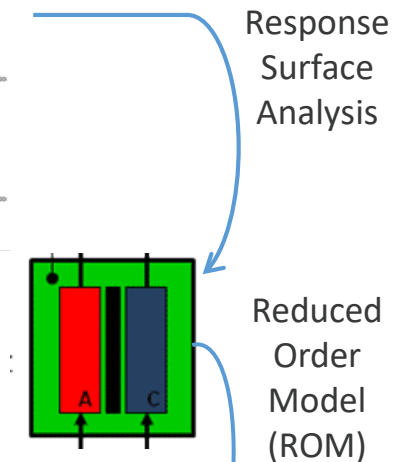
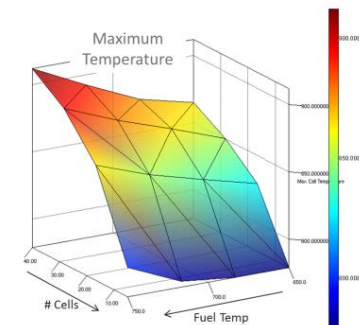
Incorporation of PNNL SOFC-MP Model

Background

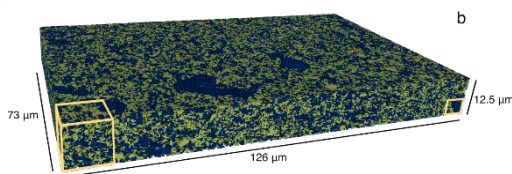
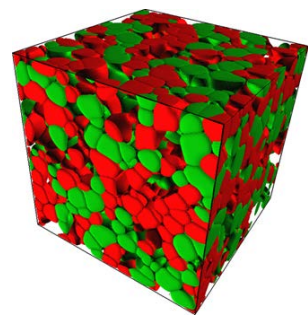
NETL/PNNL Collaboration to Complete Scaling Process

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

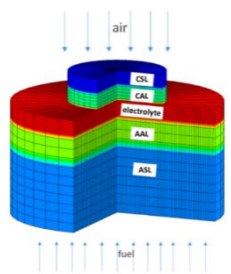
Link NETL and PNNL models at different scales to inform system level and life cycle analyses



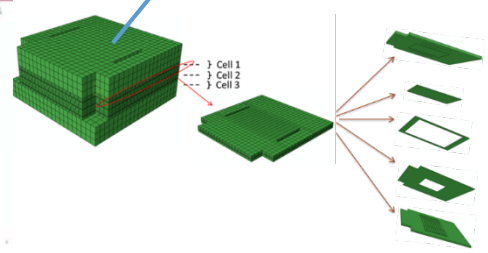
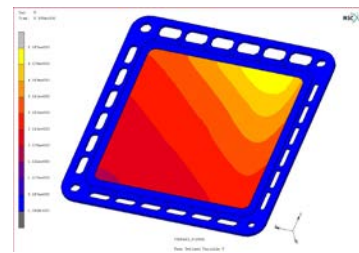
Increasing Scale



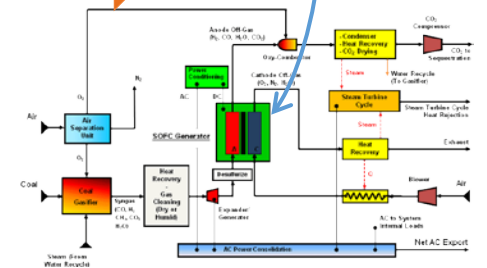
Electrode Microstructure



Single Cell



Multi-Cell Stack



IGFC System Model

NETL

PNNL

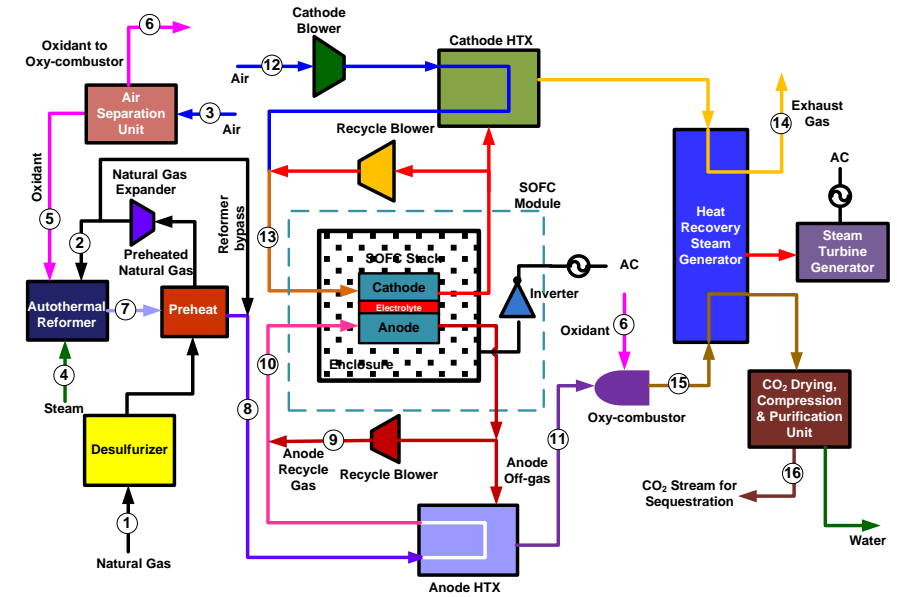
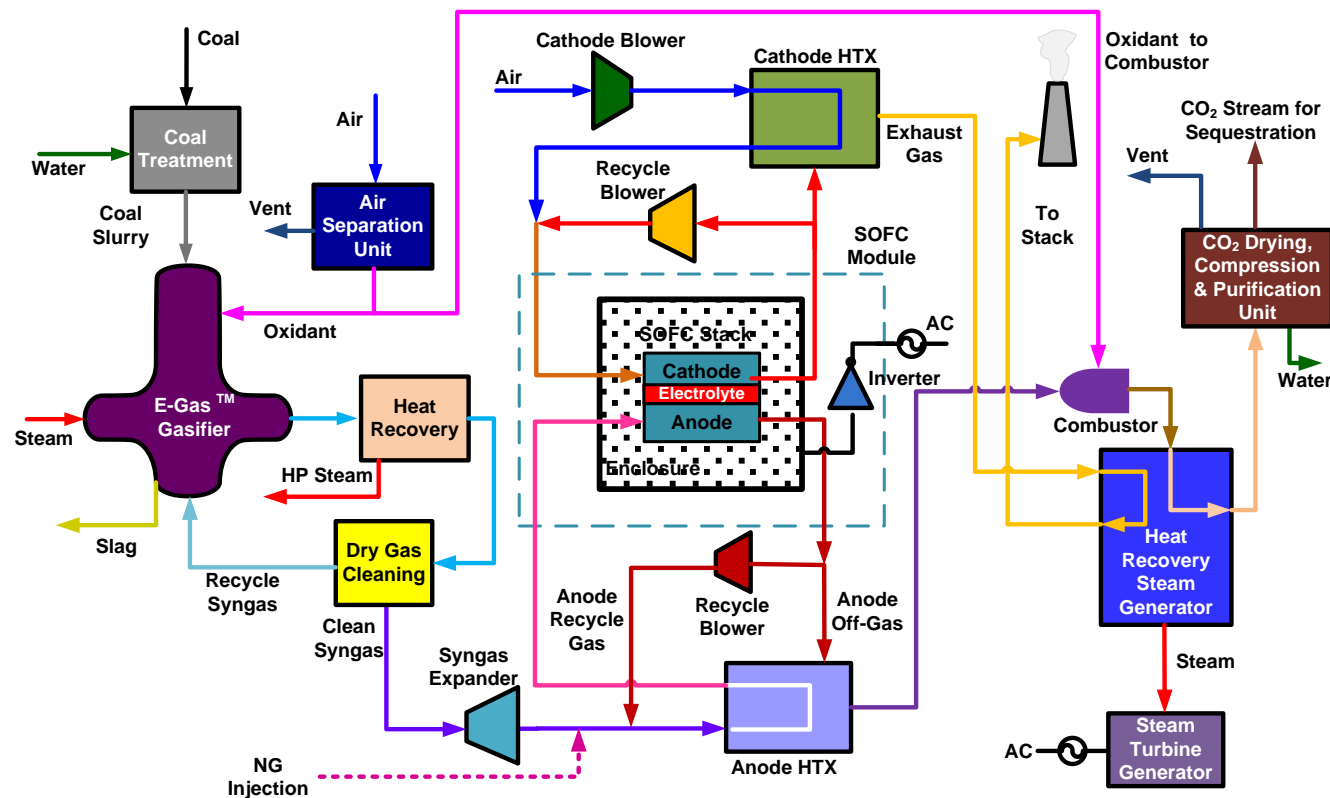
NETL

- **Pathway studies provide information on the significance that incremental improvements have toward reaching a technology's full performance/cost potential**
- **Cost and performance information at each step**
 - Evaluates several operating conditions/plant configurations and improvements to minimize COE/maximize efficiency
 - Ability to include performance degradation models developed at micro-scale
 - Includes program goals and targets
 - Provides apples-to-apples comparison to other technologies
 - Demonstrates the significance R&D has on technology commercialization

Pathway Studies

Utility-Scale IGFC/NGFC Power Plants

- Pathway studies evaluate performance and cost of utility-scale (≈ 550 MWe) SOFC-based power plants



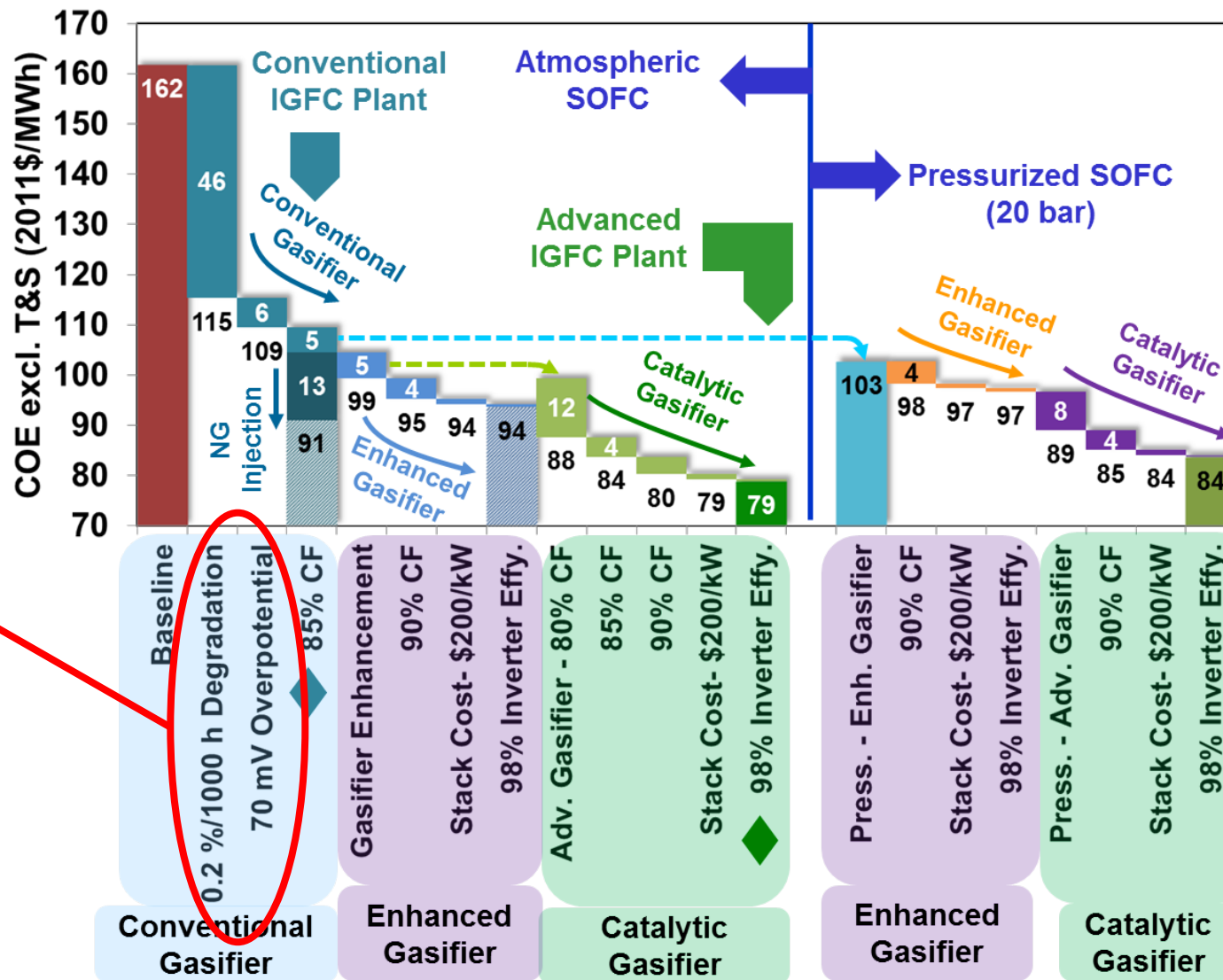
NETL, Techno-Economic Analysis of Integrated Gasification Fuel Cell Systems, November 2014, DOE/NETL-341/112613

NETL, Techno-Economic Analysis of Natural Gas Fuel Cell Plant Configurations, April 2015, DOE/NETL-2015/04082015

Pathway Studies

Cost of Electricity

REDUCE stack degradation
REDUCE cell overpotential



All cases include 90% CO₂ capture

Baseline	
Overpotential [mV]	140
Fuel Utilization [%]	90
Degrad. [%/1000 h]	1.5
Inverter Effy. [%]	97
Stack Cost [\$/kW]	225
CF [%]	80

0.2%/1000 h Degradation
70 mV Overpotential
85% CF

Gasifier Enhancement
90% CF
Stack Cost- \$200/kW
98% Inverter Effy.

Adv. Gasifier - 80% CF
85% CF
90% CF
Stack Cost- \$200/kW
98% Inverter Effy.

Press. - Enh. Gasifier
90% CF
Stack Cost- \$200/kW
98% Inverter Effy.

Press. - Adv. Gasifier
90% CF
Stack Cost- \$200/kW
98% Inverter Effy.

Source: NETL

NETL SOFC System Model Enhancement



Objective

- **Improvement of the accuracy and capability of NETL's ASPEN-based SOFC system analysis**
 - To produce a variety of optimization and what-if studies to guide the SOFC R&D Program
- **NETL analysis of SOFC systems is limited to what can be described as a “black box” SOFC module with the current ASPEN system model**
 - Two reactors (cathode/anode) with heat and oxygen transfer
 - Specified overpotential estimates
 - Limited potential to optimize on system level

NETL SOFC System Model Enhancement



Objective

- **Solution – Integrate the PNNL SOFC-MP model into NETL’s system model as a reduced-order model (ROM)**
 - Increase the accuracy of SOTA SOFC analysis
 - Reduce computational time and complexity versus full model
 - Allow for additional optimization studies (COE, etc.)
 - Allow for the ease of incorporation of other models
 - Such as degradation models, etc.
 - Facilitate development of a high fidelity SOFC tool for system analysis
 - An NETL/DOE/PNNL vision
 - SOFC industry team use

NETL SOFC System Model Enhancement

Description

• Stack Model

- Planar, adiabatic stack is used for input into ROM process
- Stack is modeled using PNNL's SOFC-MP software
 - Solves for gas species, temperature, and current density
- 550 cm² active area anode-supported cell with metal interconnects
- Counter-flow configuration
- Assumes water-gas shift reaction is in equilibrium
- Uses a first-order kinetic expression for the slower on-cell steam reforming of methane with a Ni-YSZ anode

NETL SOFC System Model Enhancement

Description

- **Electrochemical Model**

- Current-voltage relationship for the cell is defined by a user-defined function that returns a voltage based on the local temperature, species concentrations, and current density at each location of the cell's active area
- The coefficients used in the polarization equations provide an I-V response representative of high performing SOTA planar cells
- Provides 0.8 V at 400 mA/cm² for a wet H₂ fuel, with 75% U_F, and 12.5% U_A

NETL SOFC System Model Enhancement

ROM Parameters



Variable	Range	Description
Average Current Density	2000-6000 A/m ²	Cell operating current
Internal Reforming	0-100%	The degree of external reforming
Oxidant Recirculation Fraction	0-80%	Fraction of cathode exhaust recirculated
Oxygen-to-Carbon Ratio	1.5-3.0	Defines the fuel exhaust recirculation needed to achieve the desired O/C ratio at stack inlet
System Fuel Utilization	40-95%	Overall fuel utilization
System Oxidant Utilization	12.5-83.3%	Overall oxidant utilization
Fuel Inlet Temperature	550-800°C	Fuel temperature at stack inlet
Air Inlet Temperature	550-800°C	Oxidant temperature at stack inlet

NETL SOFC System Model Enhancement



Test Case Results

	Input/Output	Test Case 1	Test Case 2
Average Current Density	Input	4000 A/m ²	4000 A/m ²
Internal Reforming	Input	60%	60%
Cathode Exhaust Recirculation Fraction	Input	50%	50%
Oxygen-to-Carbon Ratio	Input	2.6	2.1
System Fuel Utilization	Input	90%	80%
Cell Maximum Temperature	Input Constraint	750°C	750°C
Cell ΔT	Input Constraint	100°C	100°C
Fuel Recirculation	Output	56.0%	44.9%
Stack Oxidant Utilization	Output	27.73%	23.04%
Fuel Inlet Temperature	Output	550°C	550°C
Air Inlet Temperature	Output	627°C	688.5°C
Cell Voltage	Output	0.958 V	0.966 V
NGFC System Efficiency (HHV)	Output	56.5%	53.9%

NETL SOFC System Model Enhancement



Next Steps

- **NETL was recently supplied with an improved ROM to incorporate into the system model**
 - Includes more unit ops within the ROM envelope
 - Extension to different fuel compositions (i.e. coal syngas)
- **NETL is working to identify an advanced SOFC performance electrochemical model to generate a ROM**
- **Begin generating data to update IGFC/NGFC Pathway studies (FY18)**
 - Include results from recent studies
 - Vent-gas recirculation configuration
 - Operating pressure sensitivity
 - Other incremental improvements

Acknowledgments



NETL

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Arun Iyengar

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NETL SOFC Group Posters

- Multi-physics Modeling of Solid Oxide Fuel Cells with Parallel Oxygen Reduction Reaction Pathways, **Tao Yang**
- Density-Functional Study of the $\text{La}_2\text{Zr}_2\text{O}_7$ Low-Index Faces, **Yves Mantz**
- Nanostructure Degradation of LSM/YSZ Interface from the Active Layer of the SOFC Cathode Operated with Elevated Steam Content, **Xueyan Song**
- Noninvasive Optical Sensor Development for Real-Time Solid Oxide Fuel Cell Monitoring Applications, **Youngseok Jee**
- High Performance Computation of Local Electrochemistry via TPB and MIEC Pathways in SOFCs based on Morphology-Preserving Microstructural Meshes, **Yu-Ting (Tim) Hsu**
- Quantitative Mesoscale Analysis of SOFC Electrodes Based on 3D Reconstructions Using Xe-Plasma Focused Ion Beam (pFIB) Coupled with SEM, **Rubayat Mahbub**
- Capacitance and Electrochemical Impedance Spectroscopy of a Solid Oxide Fuel Cell Interface using Phase Field Theory, **Yinkai Lei**
- Nano-Catalyst Infiltration by Bio-Surfactant Modification of Anode Supported SOFC Electrodes, **Özcan Özmen**
- Bayesian Calibration of Models of SOFC Electrode Materials, **Giuseppe Brunello**
- Phase Field Modeling on Initial Microstructure Effect on Grain Coarsening and Concomitant Property Degradations in SOFC Electrodes, **Yinkai Lei**
- Classifying Heterogeneity in SOFC Electrodes, **William K. Epting**
- Atomistic Modeling of Cation Diffusion in Transition Metal Perovskite $\text{La}_{1-x}\text{Sr}_x\text{MnO}_{3\pm\delta}$ for Solid Oxide Fuel Cell Cathode Applications, **Yueh-Lin Lee**
- Cation Segregation Analysis in SOFC – a Transmission Electron Microscope Based Study, **Yang Yu**
- Prediction of Performance Degradation Due to Grain Coarsening Effects in Solid Oxide Fuel Cells, **Jerry Hunter Mason**
- Improved Performance Stability of Solid Oxide Fuel Cells Achieved through Sr-Fe-O Infiltration of LSM/YSZ Cathode, **Yueying Fan**
- The Electrochemical Performance of LSM with A-site Non-Stoichiometry Under Cathodic Polarization, **Jian Liu**

