Reversible Solid Oxide Cell Degradation: Characterization, Simulation, and Mitigation

NETL FWP 1022411

Harry Abernathy, Ph.D.
Team Lead, NETL SOC R&D

23rd Annual Solid Oxide Fuel Cell Project Review Meeting

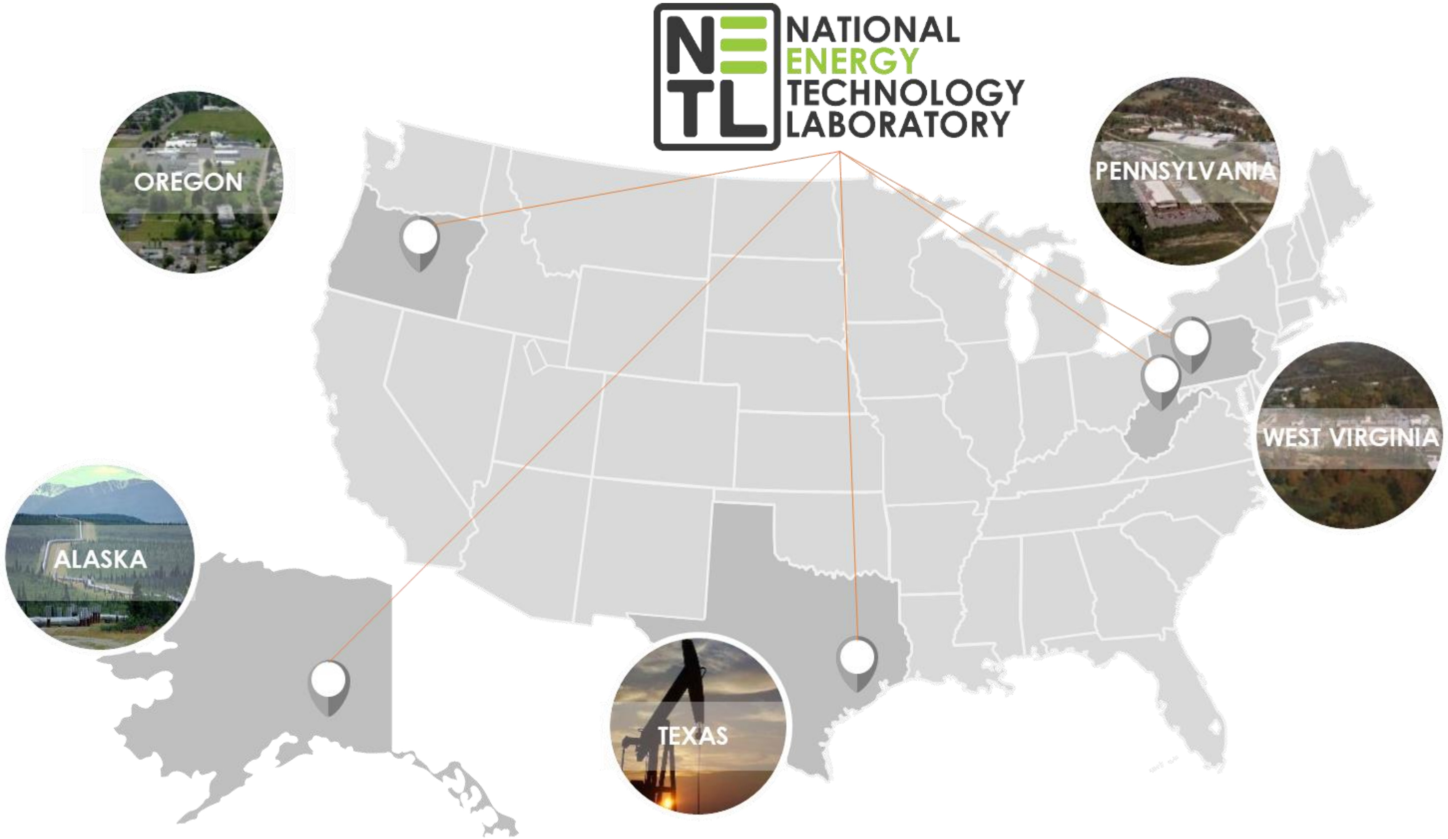
October 26, 2022

Outline

- **Introduction**

- **Recent Progress**
  - Cell and Stack Degradation Modeling and Simulation
  - Electrode Design and Engineering
  - Strategic Systems Analysis and Engineering

- **Wrap-Up**



SOFC FY22 FWP Personnel

NETL (Federal Staff)
- Anthony Burgard (PGH)
- Billy Epting (**Task 2 PI**, ALB)
- Gregory Hackett (**Task 4 PI**, MGN)
- Harry Abernathy (**TPL, Task 3 PI,** MGN)
- Jay Liu (MGN)
- Rich Pineault (MGN)
- Sam Bayham (**Task 5 PI**, MGN)
- Wissam Saidi (PGH)
- Youhai Wen (ALB)
- Yuhua Duan (PGH)
- Yves Mantz (MGN)

Carnegie Mellon University
- Paul Salvador (MSE)
- Liz Holm (MSE)
- Hokon Kim (PhD student)
- William Kent (PhD student)
- Rachel Kurchin (MSE)

Georgia Southern University
- Hayri Sezer (Eng&Tech)

NETL (Site Support Contracts)
- Alex Noring (KeyLogic/PGH)
- Arun Iyengar (KeyLogic/PGH)
- Biao Zhang (LRST/MGN)
- Bo Guan (LRST/MGN)
- Farida Harun (LRST/MGN)
- Fei Xue (LRST/ALB)
- Kyle Buchheit (KeyLogic/PGH)
- Lynn Fan (LRST/MGN)
- Rick Addis (SOS/MGN)
- Tao Yang (LRST/MGN)
- Tianle Cheng (LRST/ALB)
- Tom Kalapos (**PM**, LRST/PGH)
- Yinkai Lei (LRST/ALB)
- Yoosuf Picard (LRST/PGH)
- Youngseok Jee (LRST/PGH)
- Yueh-Lin Lee (LRST/PGH)

Clemson University
- Kyle Brinkman (MSE)
- Jack Duffy (MSE, PhD student)

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

University of Wisconsin-Madison
- Dane Morgan (MSE)
- Ryan Jacobs (MSE)
- Chiyoung Kim (MSE PhD student)

Wake Forest University
- Michael Gross (Chemistry)

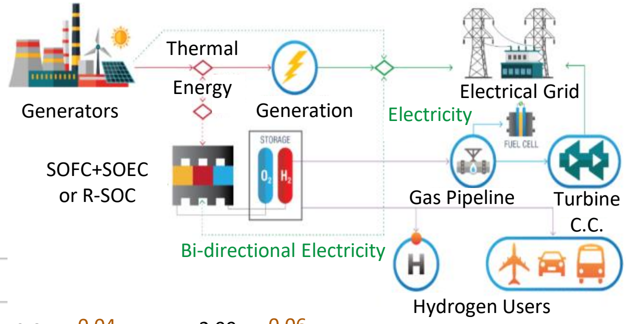
West Virginia University
- Harry Finklea (Chemistry)
- Ismail Celik (MAE)
- David Mebane (MAE)
- Ed Sabolsky (MAE)
- Joshua Tenney (PhD student)
- Xueyan Song (MAE)
- Xingbo Liu (MAE)
- Yun Chen (WV Research Corp.)

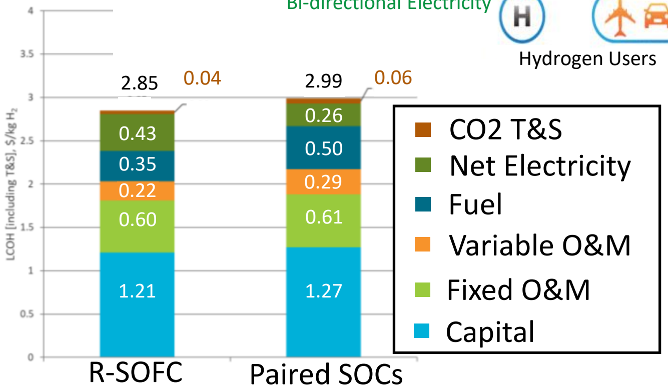
NETL SOC Capability Overview

CHALLENGE: SOC technology is cost prohibitive due to long-term performance degradation
APPROACH: Develop degradation modeling and mitigation tools to improve performance / longevity of SSEC

Systems Engineering and Analysis

- Techno-Economic Analysis
- Hybrid configuration assessment
- R&D Goals Evaluation

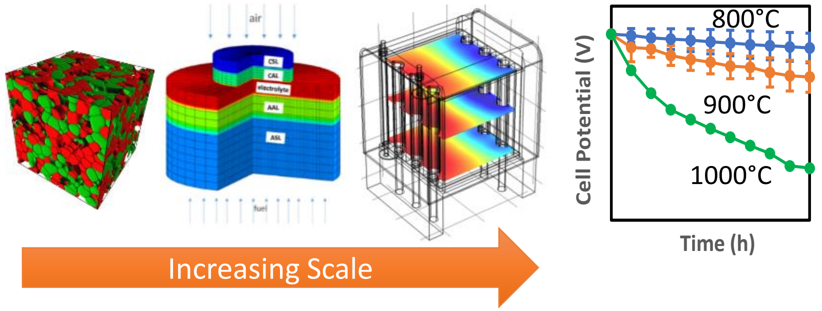




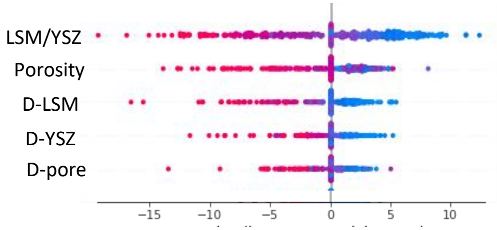
Levelized Cost of H_2 at $20/MWh Electricity

Performance Degradation Modeling

- Degradation prediction tools
- Atoms-to-System scale bridging
- Experimental validation
- Advanced Gas, Temperature Sensors



Machine learning-informed design tools

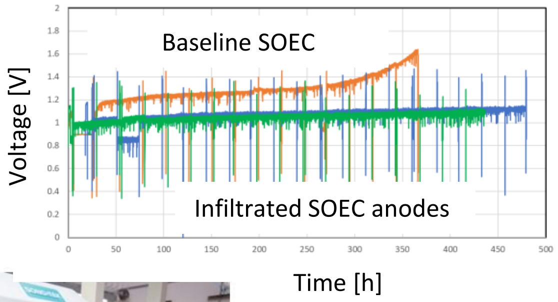


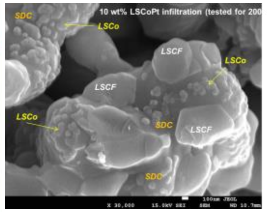
Impact of microstructural features on lifetime performance

Electrode Engineering

- Degradation mitigation
- Microstructure optimization
- Technology transfer to industry
- System demonstrations

Infiltrated Cells from **6** Partners





SOFC FWP Focus in FY22

- **Development and utilization of degradation modeling framework**
  - More degradation modes
  - Expansion to SOEC and r-SOC operation
  - New material sets
  - More big data analysis
  - Machine learning to develop more durable, higher performing electrodes
- **Proton-conducting SOC materials**
  - Computational chemistry studies
  - Experimental characterization
- **Reversible SOC studies**
  - Systems configurations
  - Experimental characterization

Output: 2022 Project Review Posters

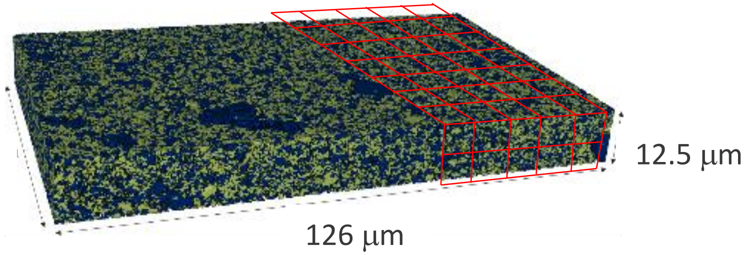
- H. Kim, et al., “Effect of Microstructural Variability and Operating Condition on Cr-poisoning in Solid Oxide Fuel Cell Cathode Using HPC Simulations”
- J. Liu, et al., “Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies”
- J. Tenney, et al., “Additive Manufacturing of Anode-Supported SOFCs through Aerosol Deposition”
- T. Yang, et al., “Numerical Study to Optimize the Microstructure of an LSM/YSZ Backbone for Nanoparticle Infiltration”
- W. Epting, et al., “Rapid Assessment of SOC Electrode Degradation Using Computer Vision and Machine Learning”
- Y. Chen, et al., “Sr Surface Segregation & Grain Boundary Degradation of LSCF/SDC Oxygen Electrode Operated in Both Fuel Cell and Electrolysis Mode”
- Y. Fan, et al., “Nanoparticles Infiltration in Air Electrode of LSM-YSZ/YSZ/Ni-YSZ Cells to Improve Performance and Mitigate Performance Degradation under Reversible SOFC/SOEC Operation”
- Y.L. Lee, et al., “Defect Thermodynamics and Transport Properties of Proton Conducting Oxide $BaZr_{1-x}Y_xO_{3-\delta}$ ($x \leq 0.1$) Evaluated Based on Density Functional Theory Modeling”
- Y. Lei, et al., “Modeling Ni Redistribution in the Fuel Electrode of Solid Oxide Cells”
- Y. Mantz, Y.L. Lee, “Surface Energies of $LaMnO_3$ High-Index Surfaces Obtained from Density-Functional Theory”

Cell and Stack Degradation Modeling

Simulation-driven design of advanced SOCs

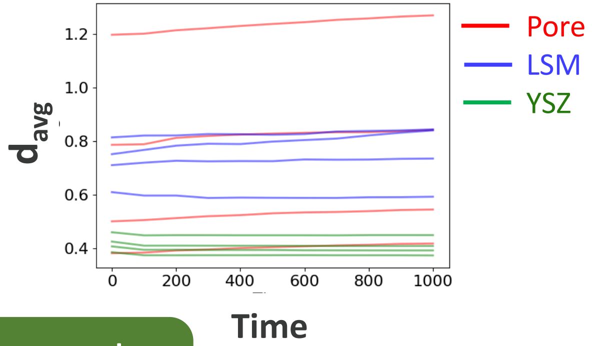
Integrated Cell Degradation Model

NATIONAL ENERGY TECHNOLOGY LABORATORY



3D Electrode Microstructures

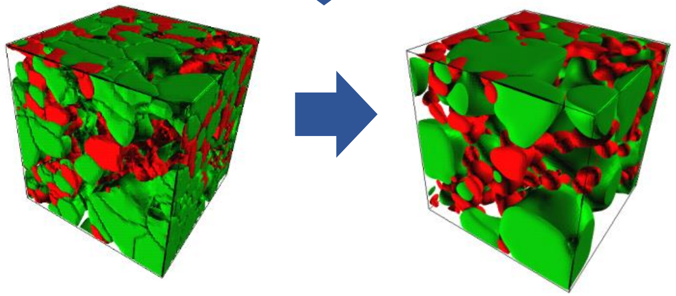
Microstructural Analysis



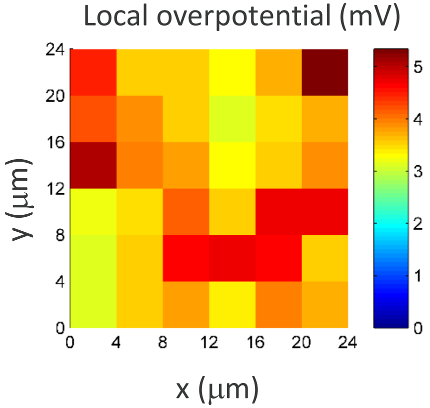
- Particle sizes
- Volume fraction
- Distributions
- Heterogeneity
- Tortuosity

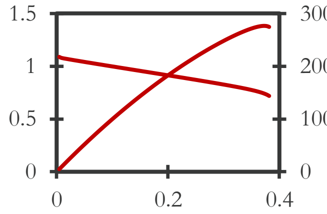
- Coarsening
- Secondary phases
- Poisoning
- Interdiffusion
- Cracking/delamination

Degradation models



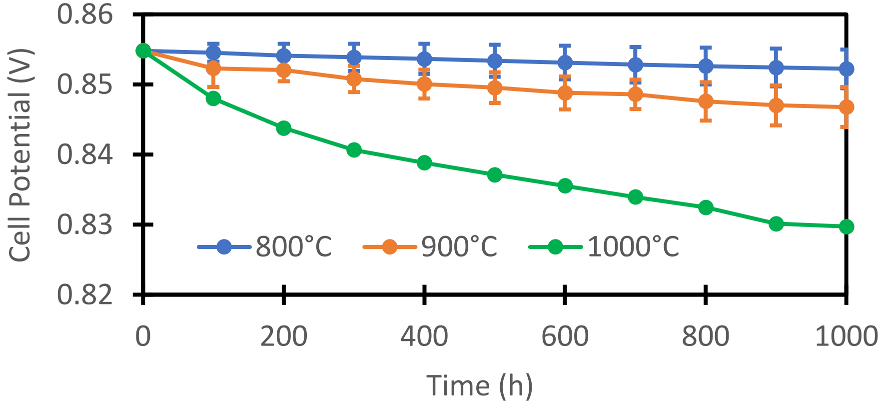
Multiphysics Performance Model





- Polarization curves
- Impedance spectra
- T, P Distributions
- Hotspots

Cell Lifetime Prediction



SOFC degradation from **coarsening** shown. Framework can be used in SOFC, SOEC, and r-SOC mode with multiple modes.

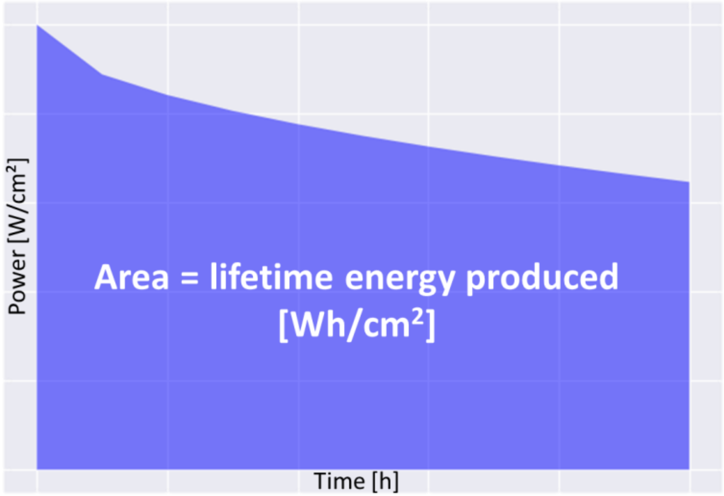
Analyzing performance degradation

- Simulations run on database of synthetic microstructure covering large matrix of microstructural parameter combinations
- How do you decide what's a good or bad electrode?

Need a single figure-of-merit that captures **both** **initial performance** and **stability**

Lifetime energy production chosen.

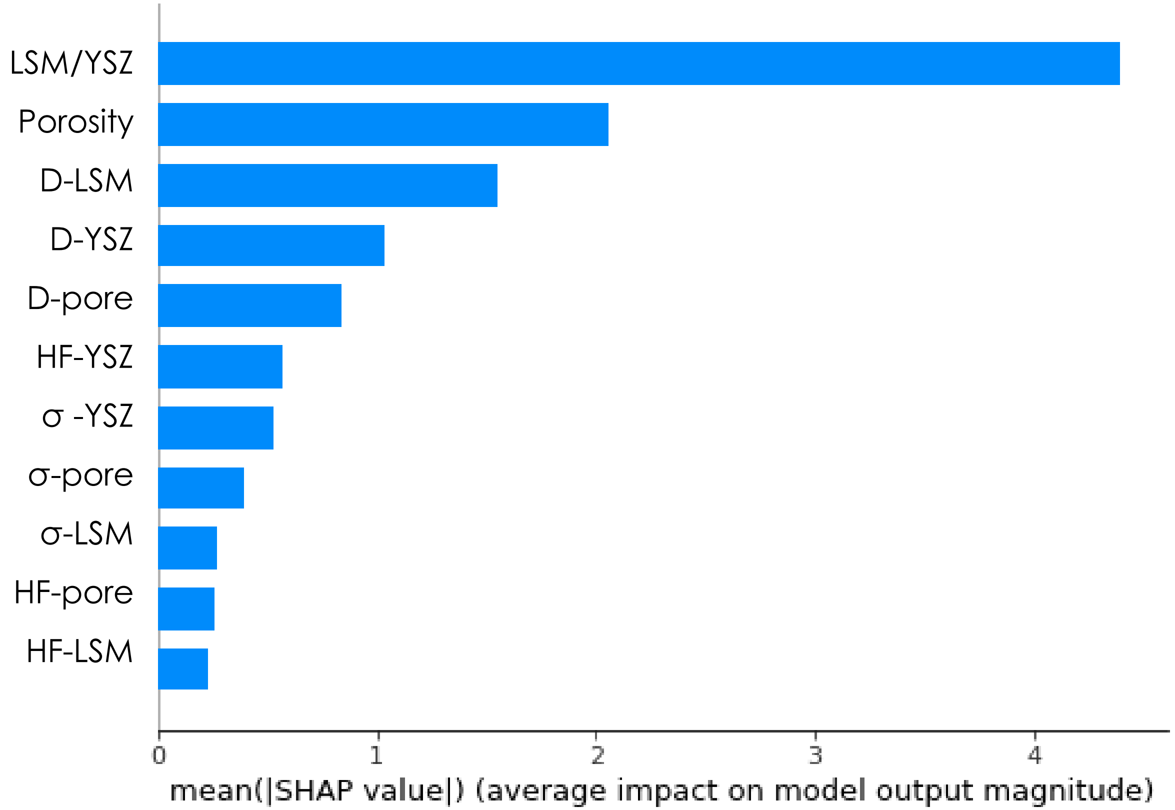
Presently: operation at a given current density, up to a given time



Cathode Feature Importance Ranking

NATIONAL ENERGY TECHNOLOGY LABORATORY

Each cathode feature's impact on lifetime energy produced at 400 mA/cm^2



Low LSM/YSZ ratio, low porosity, and small solid particles are beneficial

Machine Learning and Degradation

NATIONAL ENERGY TECHNOLOGY LABORATORY

- Use 11 initial microstructural values as “features” (inputs, known values for each sample)
- Lifetime energy produced at 400 mA/cm^2 as “target” (outcome, value to be predicted)

Training dataset

Features

	0	1	…	N
pf1	0.230081	0.23364		0.239156
pf23ratio	0.789111	0.824911		0.868857
davg1	0.363655	0.372662		0.37807
davg2	0.385066	0.40092		0.416845
davg3	0.413405	0.459561		0.525972
std1	0.138111	0.141968	…	0.139824
std2	0.140301	0.144869		0.14958
std3	0.148107	0.168732		0.204666
hf1	0.000676	0.000379		0.000674
hf2	0.000648	0.000861		0.000811
hf3	0.000678	0.000708		0.000945

Update model weights

ML model in training

Target

Lifetime Energy **Predicted**	Lifetime Energy **Actual**
344.20	332.3234
346.03	330.5791
…	…
320.77	327.9687

Repeat until satisfied

Aggregate error of 0.5%!

W. K. Epting et al., ECS Trans., 103, 909 (2021).
Z. Yan et al., Energy Convers. Manag. 198 (2019)

Machine Learning and Microstructure

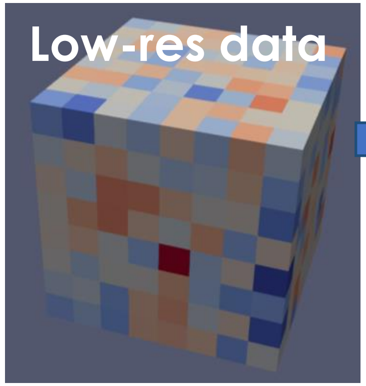
Getting hi-res properties from cheaper, more available low-res techniques

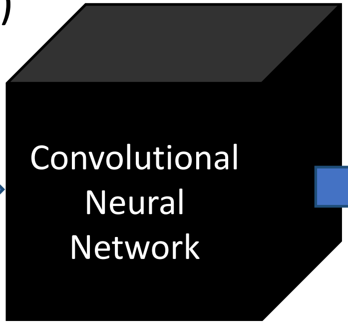
Super-resolution

3D analysis

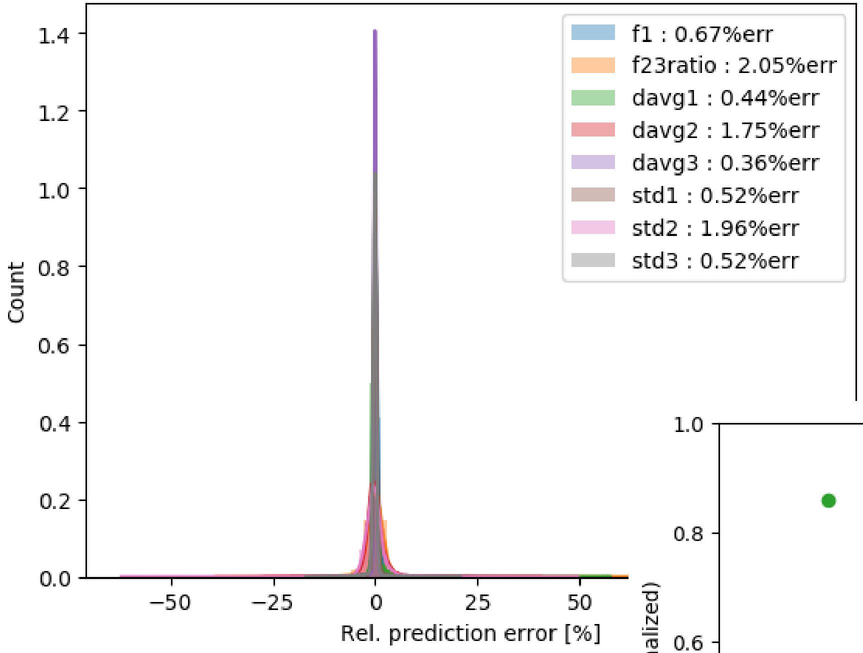
Properties	
Porosity	0.21
LSM/YSZ	0.8
Davg1	445
Davg2	610
Davg3	555
TPB	4.35
+ tortuosity, SA, etc	

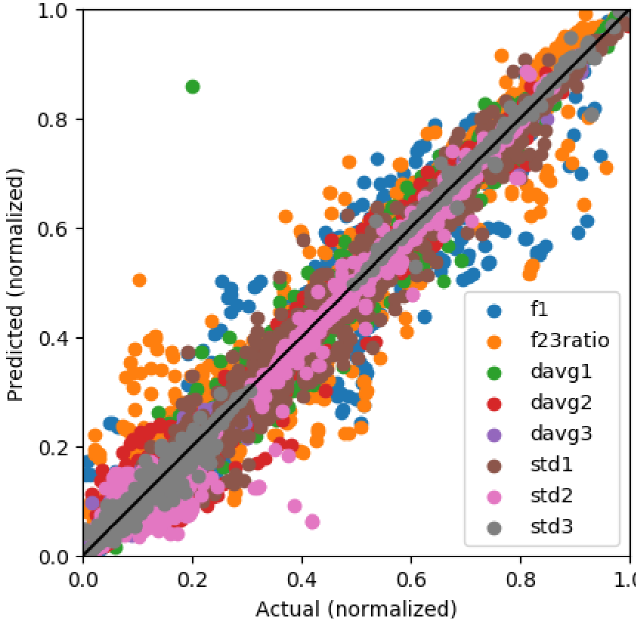
De-resolve x30
(1.5 μm voxels)





Properties	
Porosity	0.26
LSM/YSZ	0.86
Davg1	480
Davg2	660
Davg3	503
TPB	4.1
+ tortuosity, SA, etc	



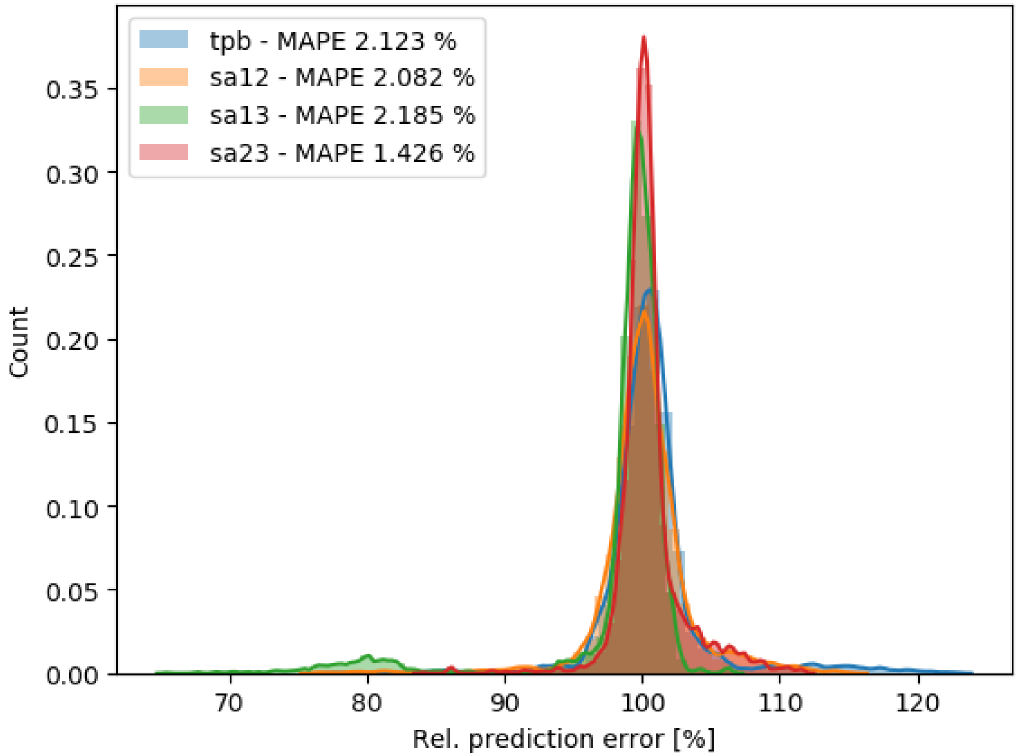


Machine learning vs. Percolation Theory

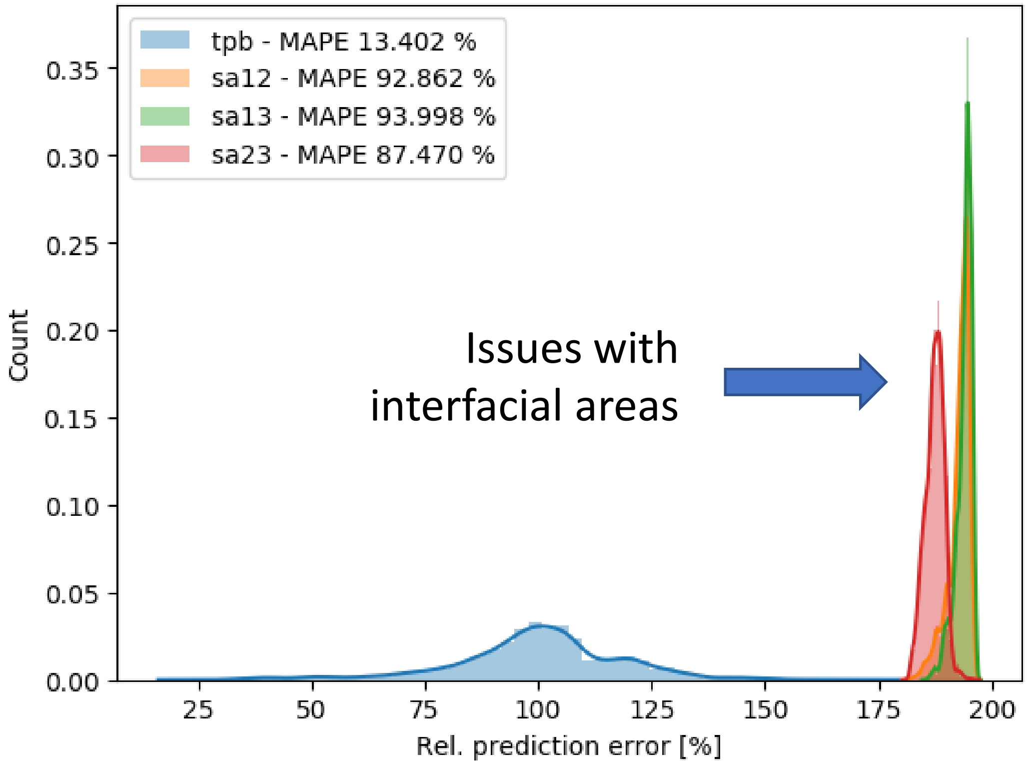
NATIONAL ENERGY TECHNOLOGY LABORATORY

Trained ML models can provide more reliable microstructural parameter input values for simulation studies

NN Regressor



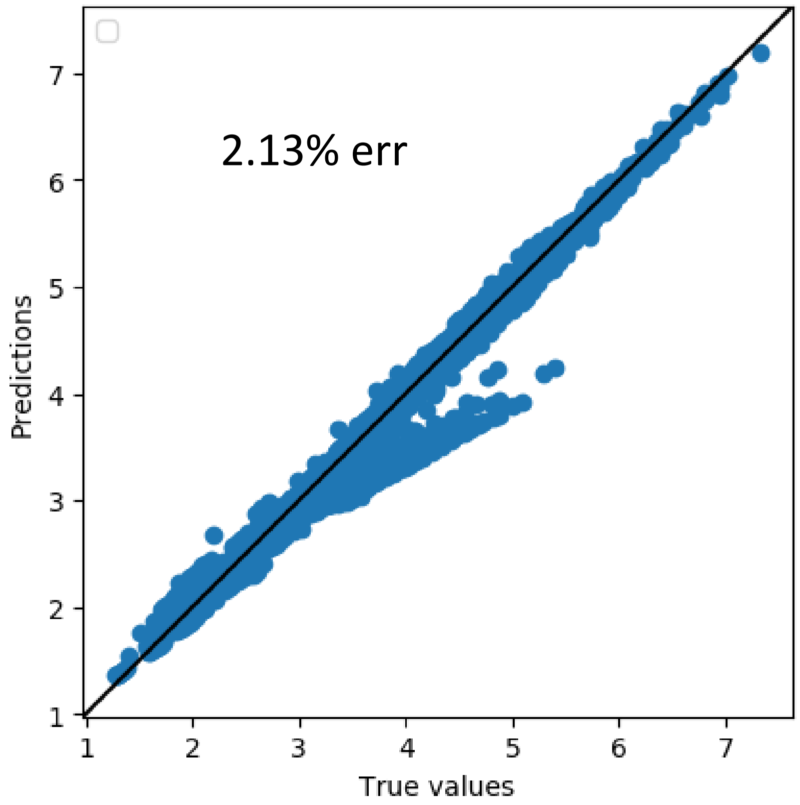
Percolation Theory



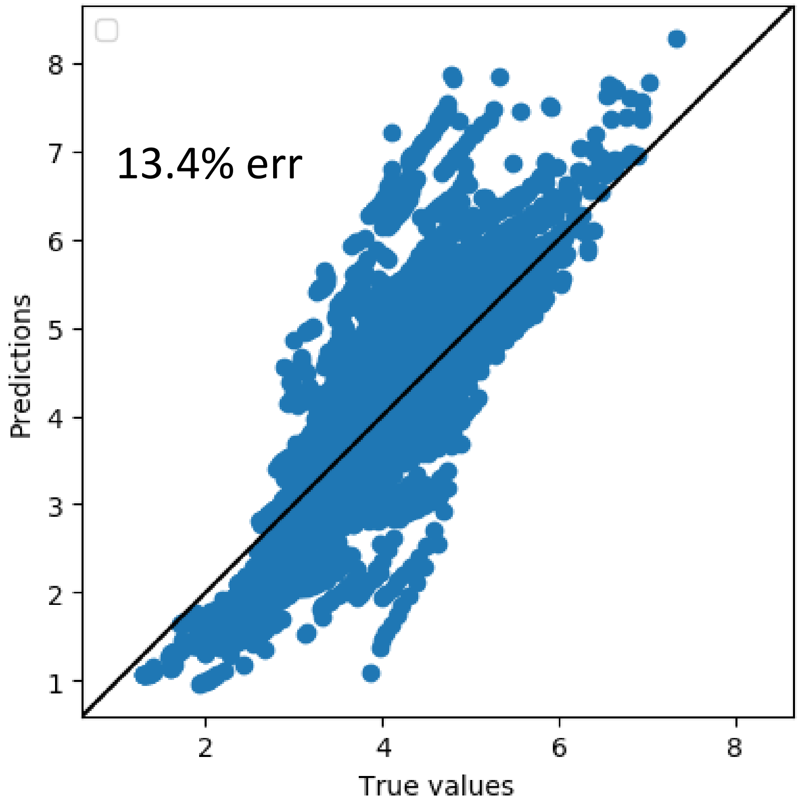
sa = Surface Area, tpb = Triple Phase Boundary Density

Comparison: TPB Density

NN Regressor

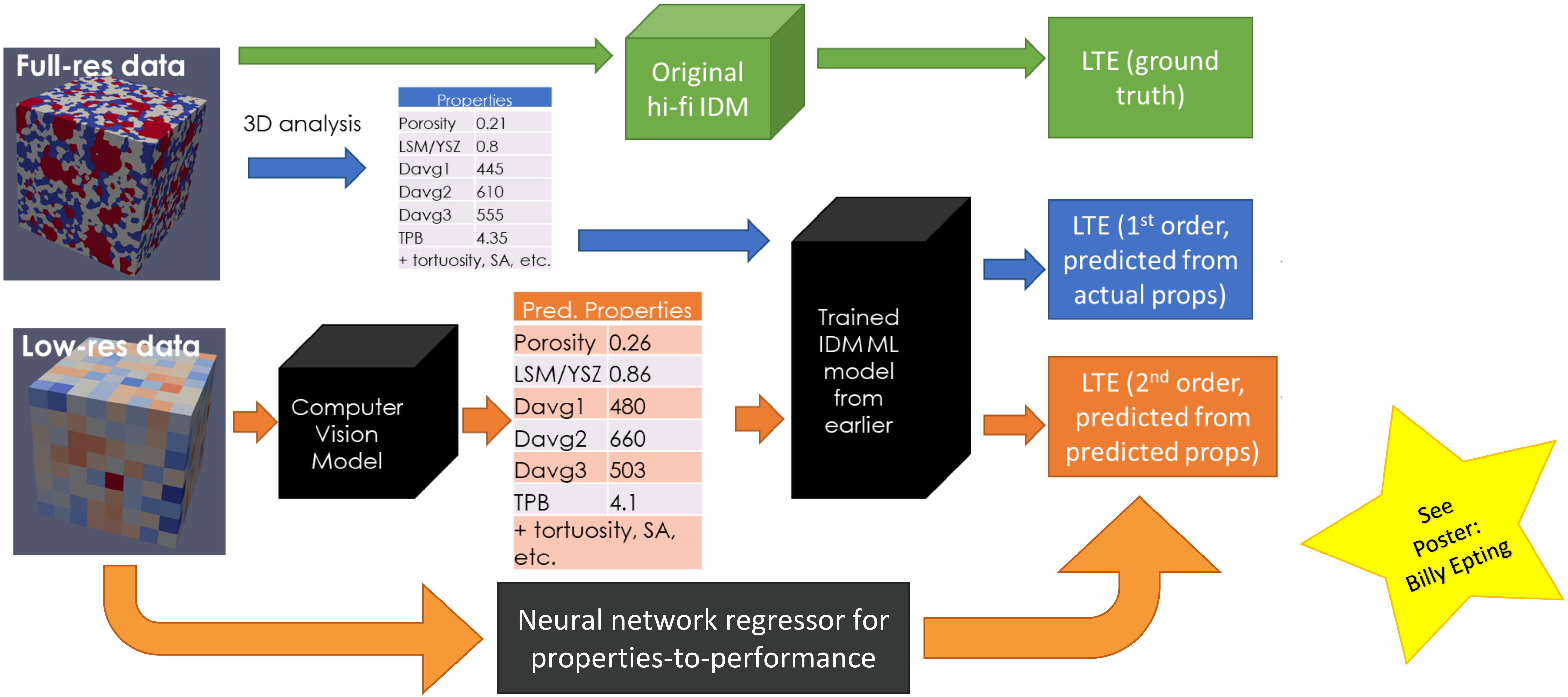


Percolation Theory



Predictions from Lower Quality 3D Data

Putting it all together

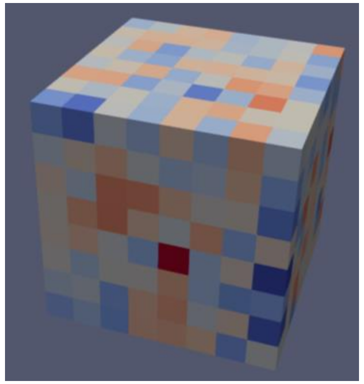


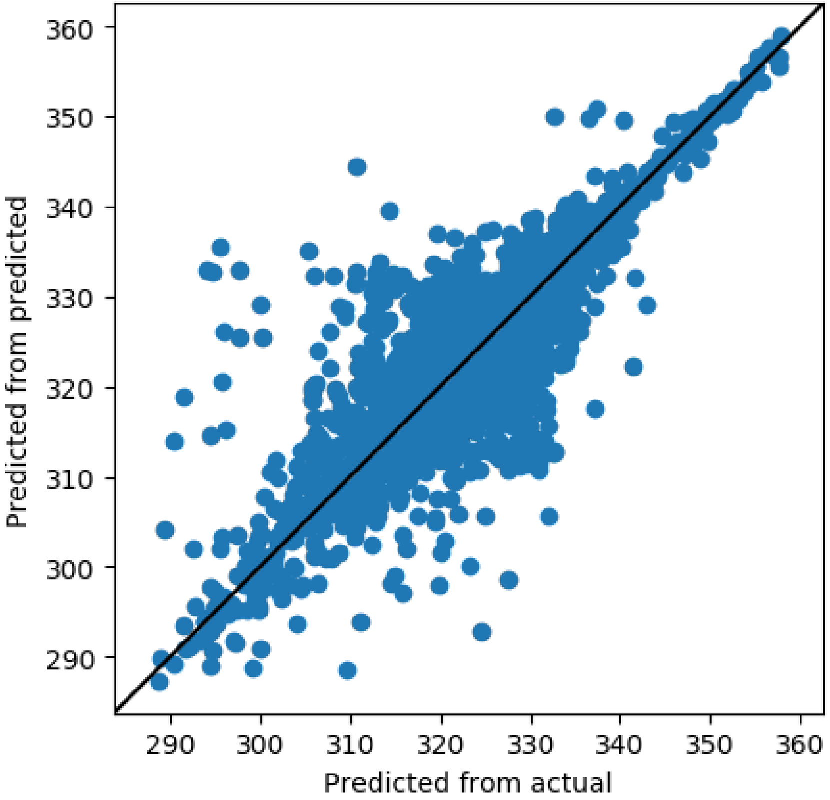
Properties	
Porosity	0.21
LSM/YSZ	0.8
Davg1	445
Davg2	610
Davg3	555
TPB	4.35
+ tortuosity, SA, etc.	

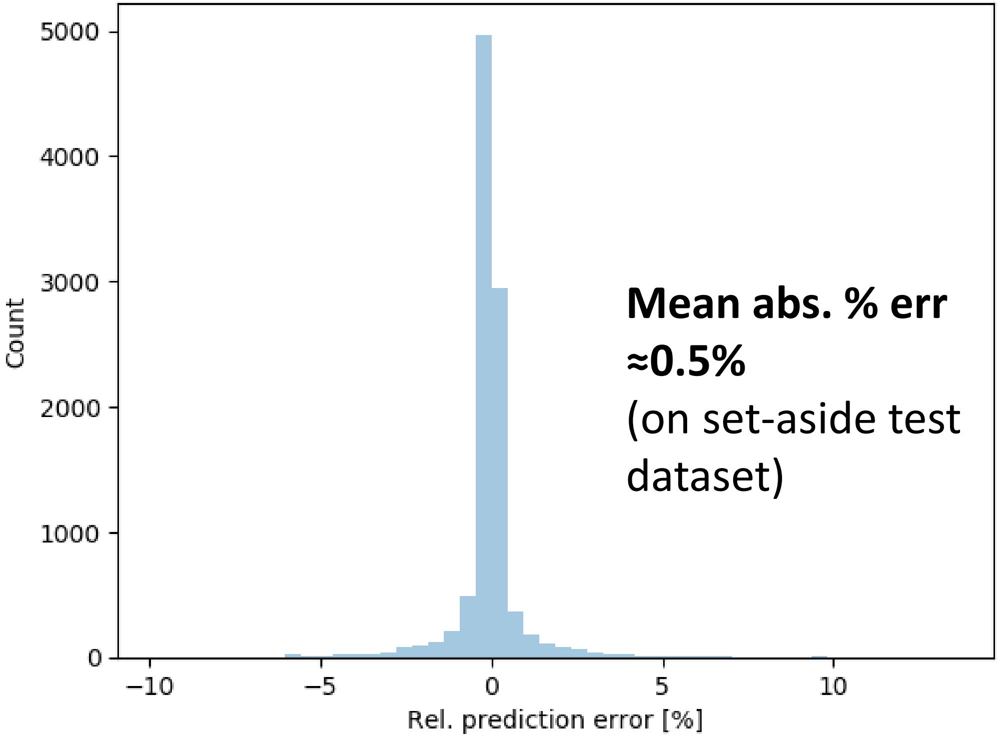
Pred. Properties	
Porosity	0.26
LSM/YSZ	0.86
Davg1	480
Davg2	660
Davg3	503
TPB	4.1
+ tortuosity, SA, etc.	

Predictions from Lower Quality 3D Data

Error analysis on 10,000 samples – Lifetime Energy Produced at 0.4 A/cm^2







Mean abs. % err ≈0.5%
(on set-aside test dataset)

Remains to be seen: How much the uncertainty increases over a wider operational space with more degradation modes

Additional Degradation Models

Simulation of Mechanical Degradation Considering Microstructures

- Last year: Phase field modeling of mechanical cracking from thermal and redox cycling
- This year: model expanded to include O_2 pressure buildup in air electrode during SOEC operation

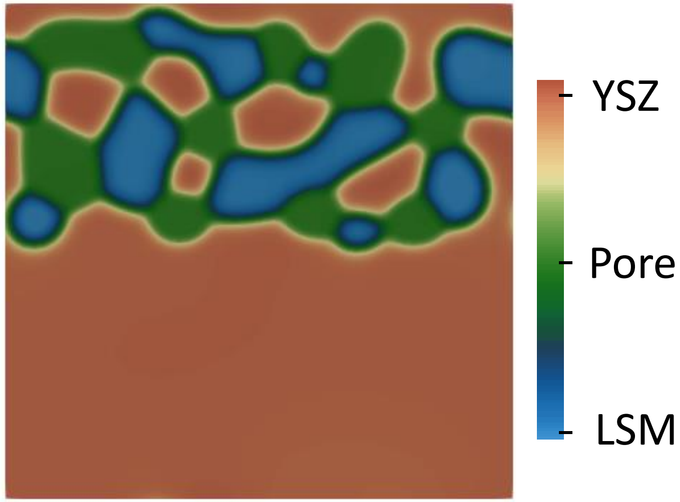
$$P_{O_2} = P_{O_2}^{Pore} \exp[\frac{4F}{RT}\eta_{anode}]$$

Modified Virkar model from **Int. J. Hydrog. Energy** 35(18) 9527, 2010.

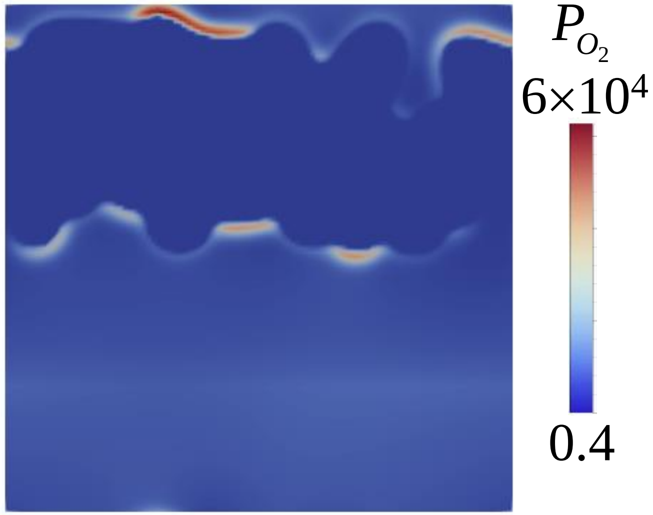
$$P_{O_2} = \sqrt{\frac{\pi \gamma E}{2(1-\upsilon^2)c}}$$

γ: Interfacial energy E: Young's modulus
ν: Poisson's ratio c: Initial crack size

Microstructure



Oxygen pressure (atm)



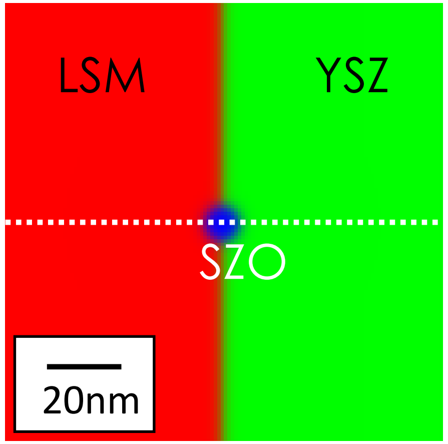
When c=0.5 μm and γ=1.75 Jm^{-2}, critical inner oxygen pressure P_{O2}=1.13*10^4 atm, and critical overpotential η_{anode}=237 mV

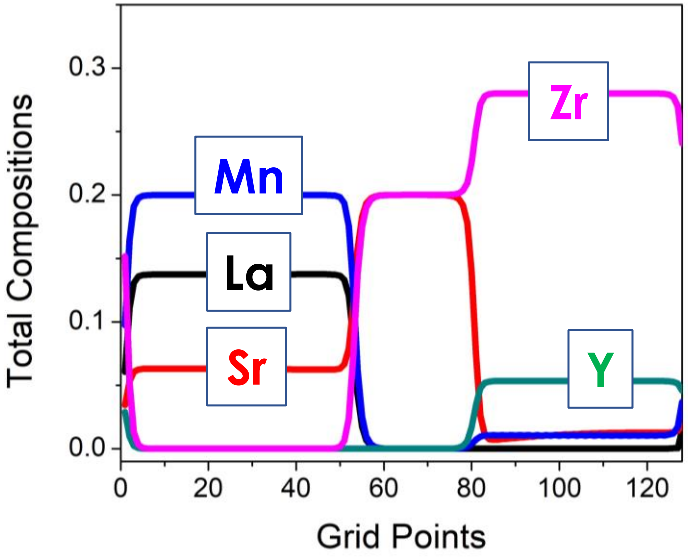
Additional Degradation Models

Simulation of secondary phase formation

- Developed a general thermodynamic model of non-stoichiometric phases, and applied it to SOFC systems, starting with LSM and LSCF.
  - Computer program developed to apply the thermodynamic model to given sublattice systems.
- Initially applied to simulate zirconate formation during sintering

Conditions (numbers)	Expressions
Site conservation (3)	$y^1_{La^{3+}} + y^1_{Sr^{2+}} + y^1_{Mn^{3+}} + y^1_{Va} = 1$ $y^2_{Mn^{2+}} + y^2_{Mn^{3+}} + y^2_{Mn^{4+}} + y^2_{Va} = 1$ $y^3_{O^{2-}} + y^3_{Va} = 1$
Charge neutrality (1)	$3(y^1_{La^{3+}} + y^1_{Mn^{3+}} + y^2_{Mn^{3+}}) + 2(y^1_{Sr^{2+}} + y^2_{Mn^{2+}}) + 4y^2_{Mn^{4+}} = 6y^3_{O^{2-}}$
Compositions (3)	$x_{La} = \frac{y^1_{La^{3+}}}{y^1_{La^{3+}} + y^1_{Mn^{3+}} + y^1_{Sr^{2+}} + y^2_{Mn^{2+}} + y^2_{Mn^{3+}} + y^2_{Mn^{4+}} + 3y^3_{O^{2-}}}$ $x_{Sr} = \frac{y^1_{Sr^{2+}}}{y^1_{La^{3+}} + y^1_{Mn^{3+}} + y^1_{Sr^{2+}} + y^2_{Mn^{2+}} + y^2_{Mn^{3+}} + y^2_{Mn^{4+}} + 3y^3_{O^{2-}}}$ $x_{Mn} = \frac{y^2_{Mn^{2+}} + y^2_{Mn^{3+}} + y^2_{Mn^{4+}} + y^1_{Mn^{3+}}}{y^1_{La^{3+}} + y^1_{Mn^{3+}} + y^1_{Sr^{2+}} + y^2_{Mn^{2+}} + y^2_{Mn^{3+}} + y^2_{Mn^{4+}} + 3y^3_{O^{2-}}}$





Electrode Design and Engineering

Building better performing, longer lasting electrodes

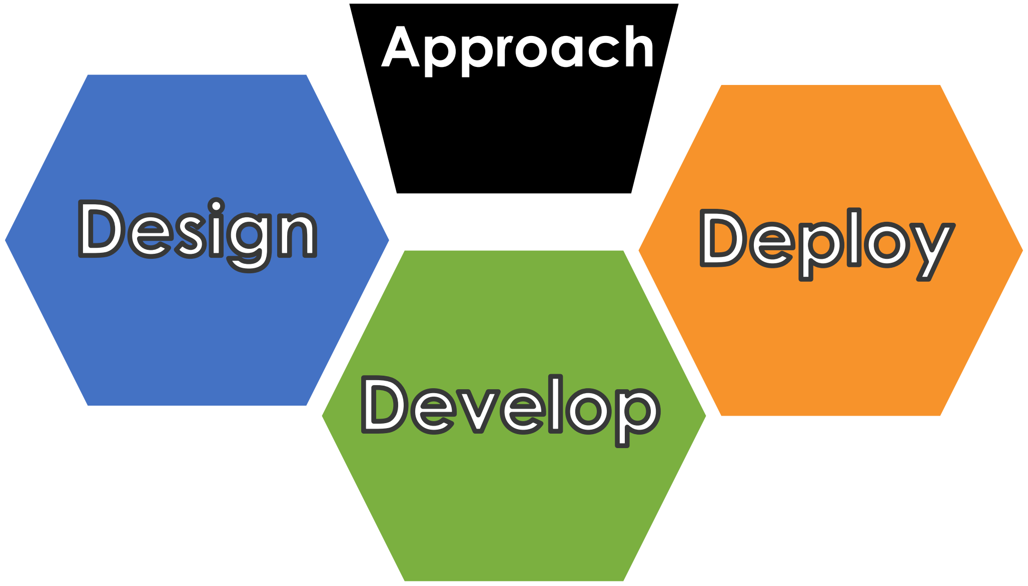
SOC Electrode Design and Engineering

Objectives

- Enhancement of performance and longevity
- Materials engineering
- Microstructure engineering

Benefits

- Cell/stack cost reduction
- Cell overpotential reduction
- Increased thermo-chemical/thermo-mechanical stability
- Reduced cost-of-electricity and/or cost of hydrogen



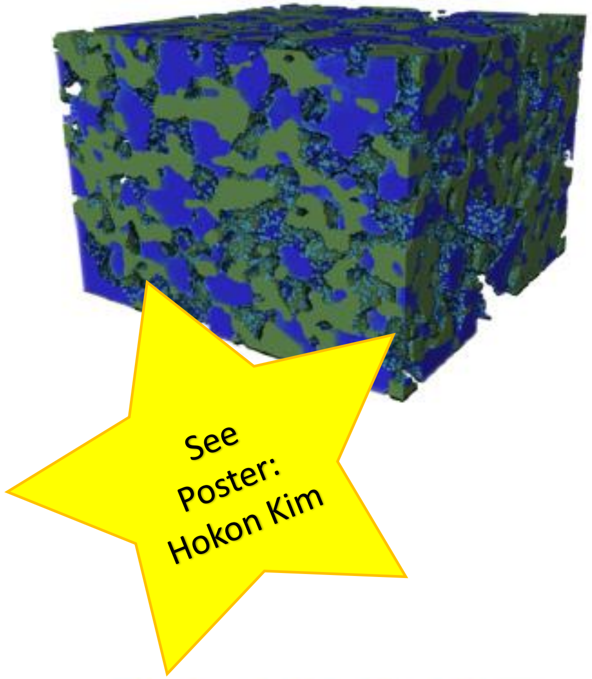
DESIGN new materials and structures

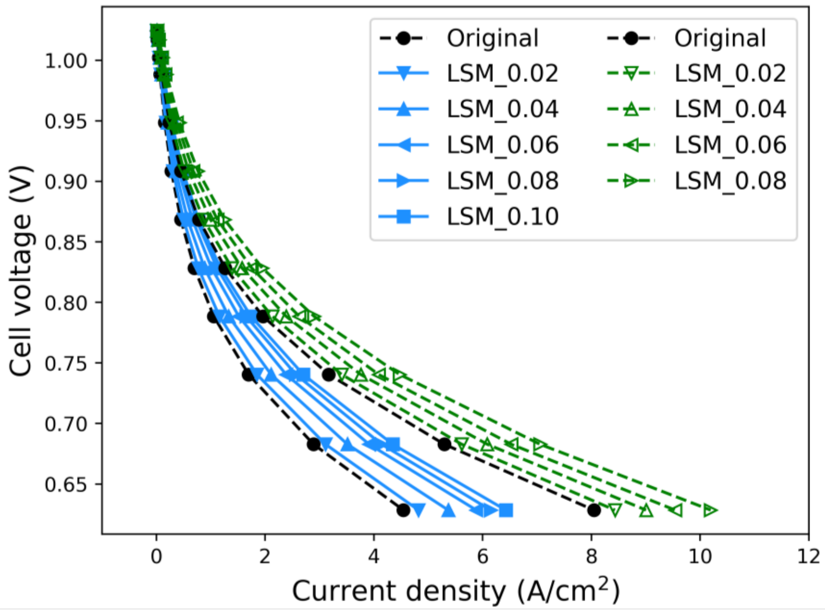
DEVELOP tailored electrode designs

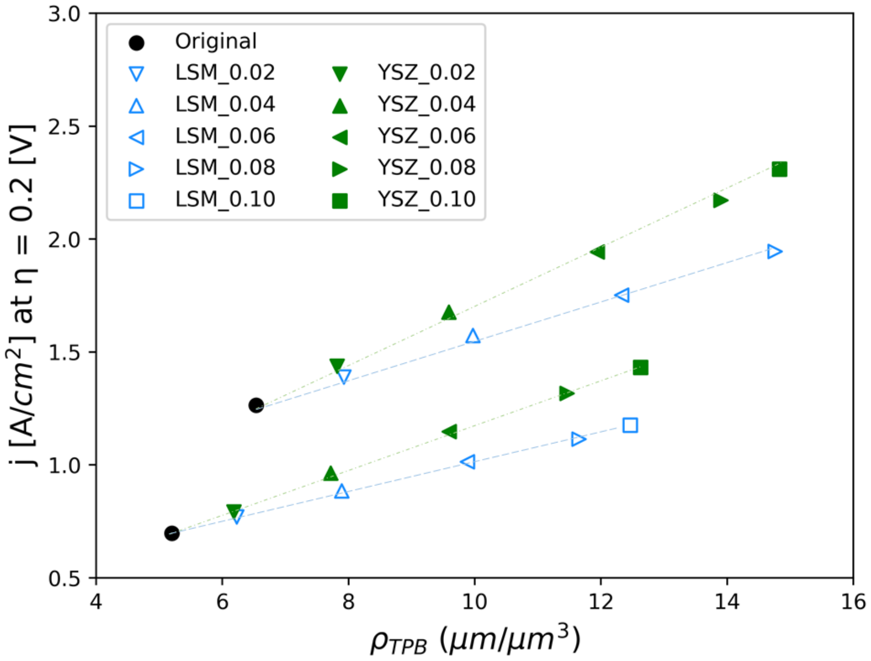
DEPLOY in commercial SOC systems

Simulating infiltrated electrodes: Sub-volumes

- Using ERMINE SOFC module in MOOSE platform for microstructurally resolved infiltration (individual nanoparticles) to how infiltrated particle parameters impact local electrochemical performance/degradation





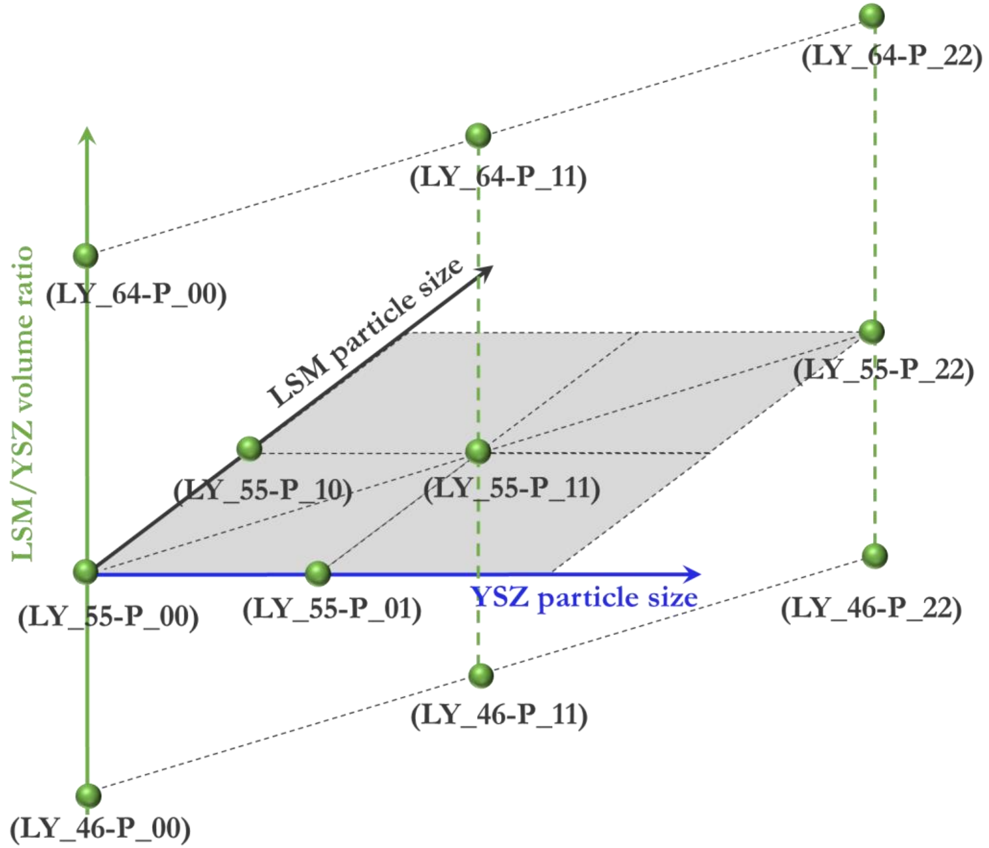


Comparing performance improvement on 2 selected LSM/YSZ subvolumes when infiltrating different loadings of LSM and YSZ nanoparticles

MOOSE *

Simulating infiltrated electrodes: Full cells

- Using in house DREAM SOFC code to optimize cathode performance by controlling infiltration and backbone structure
  - Optimal catalytic properties for a given backbone composition/structure
  - Optimal backbone composition/structure for given catalytic properties
  - Optimal lifetime performance based on backbone/infiltrated particle degradation

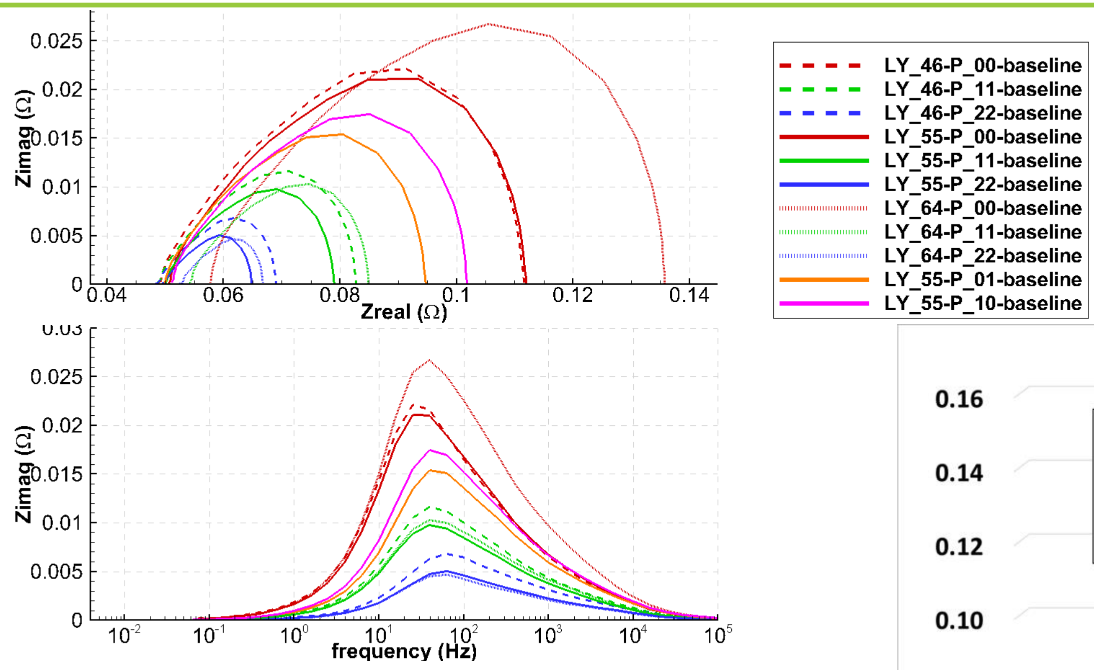


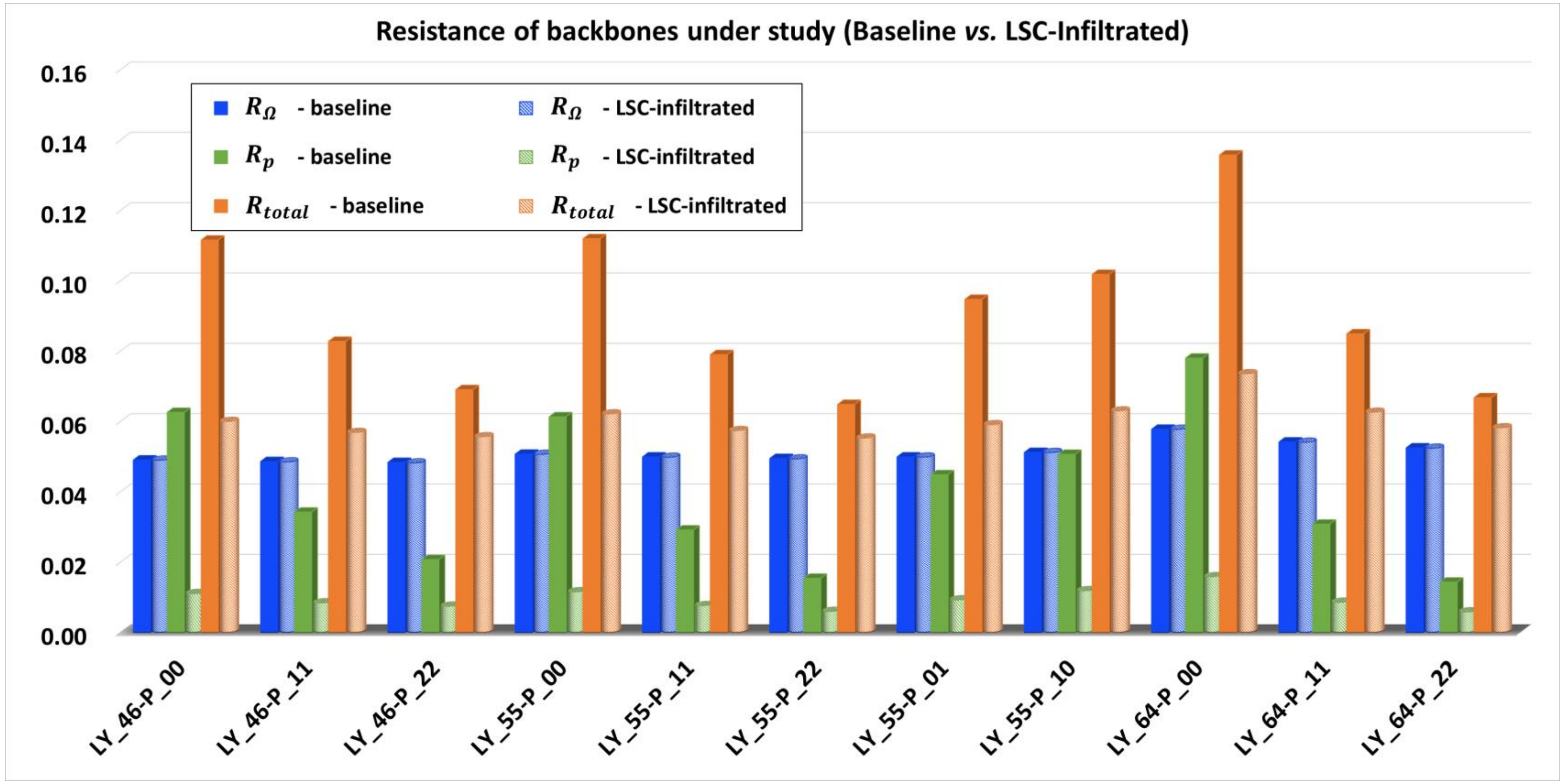
Volume fractions:	Particle size:
40:60	-1,0,1,2,3,4
50:50	0 = Baseline
60:40	-1 = Coarser
	1-4 = Finer

Notation: Backbone_LSM:YSZ-LSM/YSZ Particle size

Infiltrating LSC onto LSM/YSZ backbone

NATIONAL ENERGY TECHNOLOGY LABORATORY



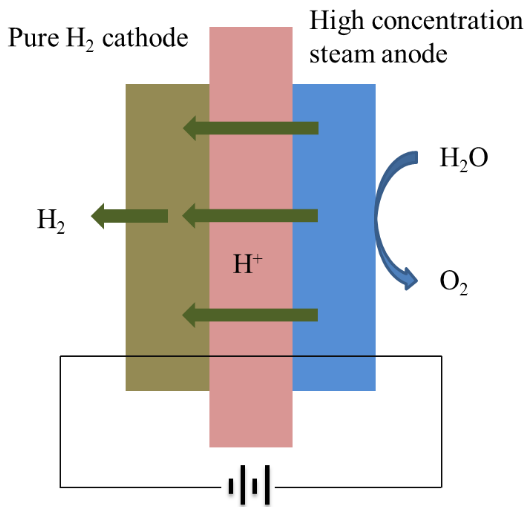


See Poster: Tao Yang

Proton-conducting SOCs

Expanding the degradation modeling framework's material sets

- **Proton-conducting SOCs can help lower operating temperatures, increase operational stability, and don't have a diluted H_2 stream**
- **Materials needs:**
  - More active electrodes
  - Electrolytes with higher σ, higher H^+ transference number
  - Less expensive thermal processing
- **SOEC, SOFC performance model code options created for proton-conducting systems**
  - *Model not fully calibrated due to lack of comprehensive calibration dataset*



Proton-conducting SOEC

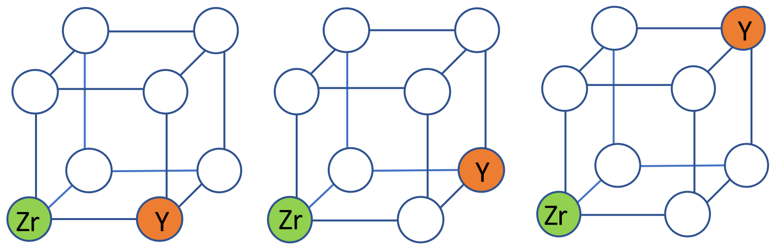
Proton-conducting materials studies

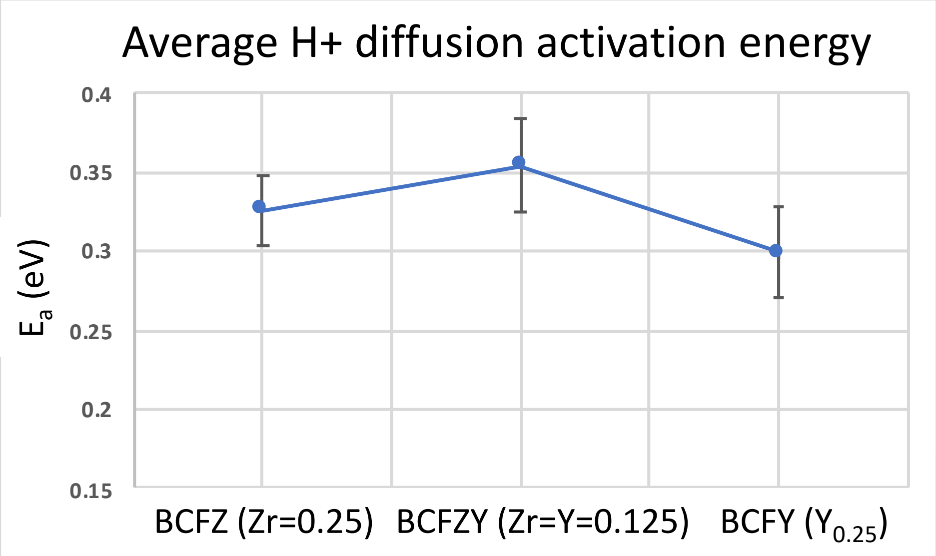
- **Electrolyte studies:**
  - Defect Thermodynamics and Transport Properties of Proton Conducting Oxide Electrolyte $BaZr_{1-x}Y_xO_{3-\delta}$ ($x \leq 0.1$)
  - Experimental measurement of conductivities and transference numbers of $BaZr_xCe_yY_zYb_{1-x-y-z}O_3$

See Poster: Yueh-Lin Lee

- **Triple-conducting oxide studies for electrodes:**
  - Computational study of H^+ transport in $Ba(Co, Fe, Zr, Y)O_{3-\delta}$ based on $[V_O^{\cdot\cdot}]$, cation arrangement, and amount of Y substitution
  - Experimental measurement of conductivities, H_2/O_2 permeation, and transference numbers of BCFZ/Y compositions

Yttrium in $H_{0.125}BaCo_{0.375}Fe_{0.375}(Y/Zr)_{0.25}O_{2.5}$



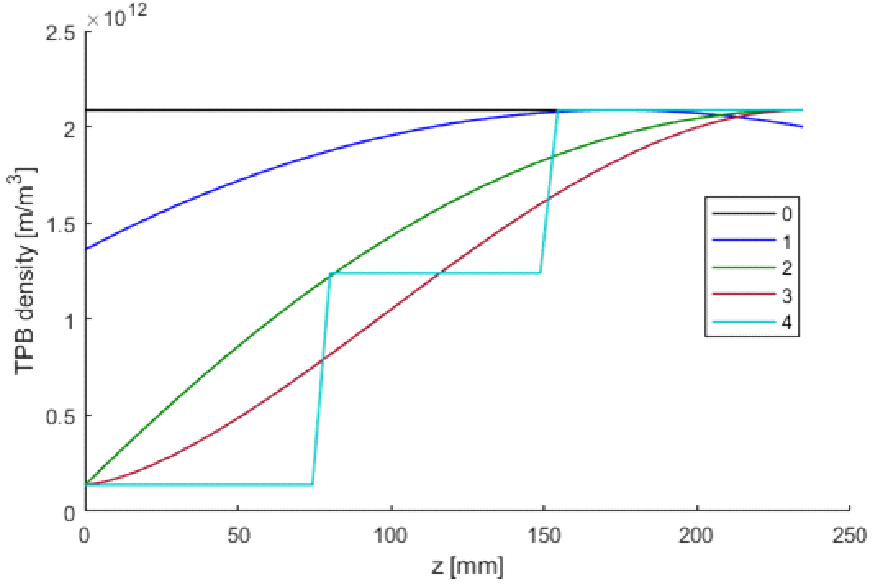


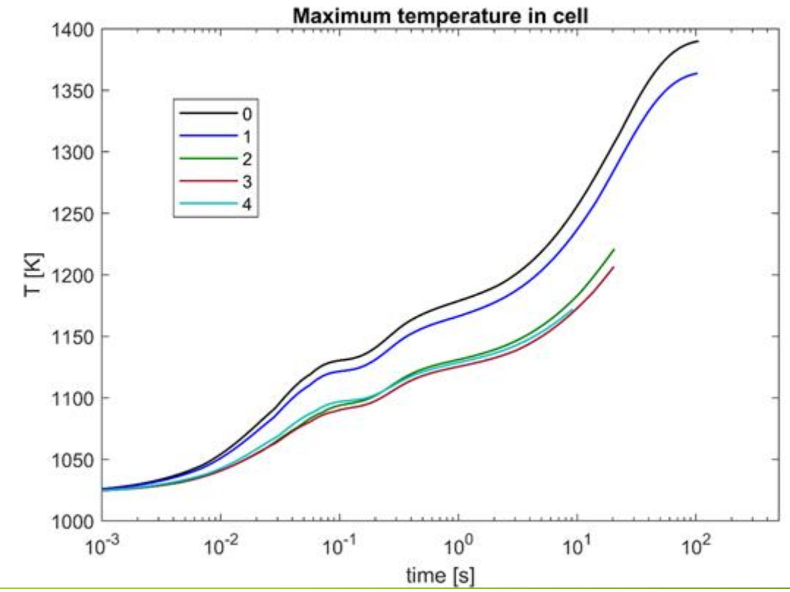
Motivation: Reducing gradients in planar cells

Mitigating long-term degradation through advanced electrode design

#	Description	Porosity (ε_p)	Ni/YSZ Ratio
0	Baseline	0.25	0.5
1	Porosity 0.1-0.3	$\varepsilon_p = 0.2\left(\frac{z}{L}\right) + 0.1$	0.5
2	Ni/YSZ 0.27-0.5	0.25	$R_{Ni} = 0.23\left(\frac{z}{L}\right) + 0.27$
3	Ni/YSZ 0.27-0.5 ^ 1.5	0.25	$R_{Ni} = 0.23\left(\frac{z}{L}\right)^{1.5} + 0.27$
4	Ni 0.25 0.37 0.50	0.25	$R_{Ni} = \begin{cases} 0.27 & 0 \le z < L/3 \\ 0.35 & L/3 \le z < 2L/3 \\ 0.5 & 2L/3 \le z \le L \end{cases}$

Temperature gradient can be reduced by varying Ni:YSZ ratio from inlet to outlet



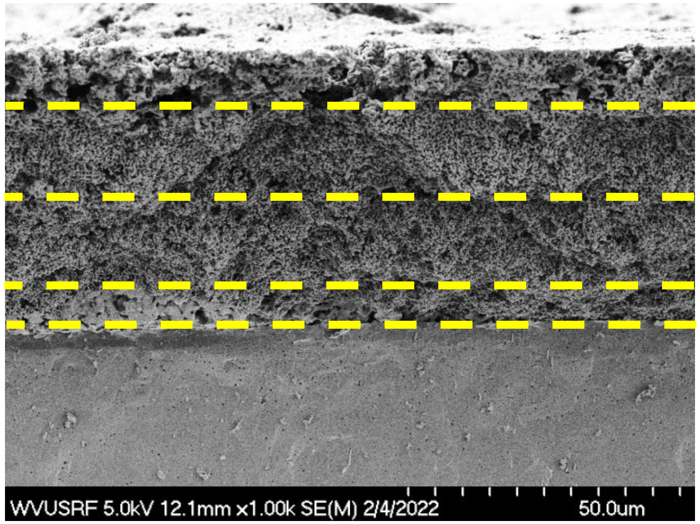


Additive manufacturing of SOC electrodes

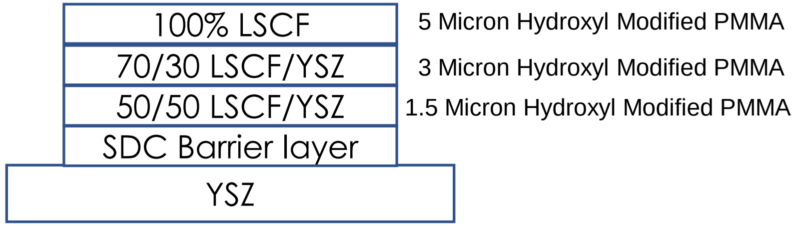
Creating 3D gradients in composition, microstructure

- Automated aerosol spray deposition system built at WVU to fabricate SOC electrodes and electrolytes
  - Feedstocks provide precursors with varying compositions, particle sizes
  - Started with 4 feedstocks that could be pumped through spray nozzle
  - Upgraded to in situ mixing system for wider range of compositions
- Ongoing studies to deposit both electrodes, electrolyte, and barrier layers to support layer
- System coupled with simulations to optimize long-term performance in planar cells

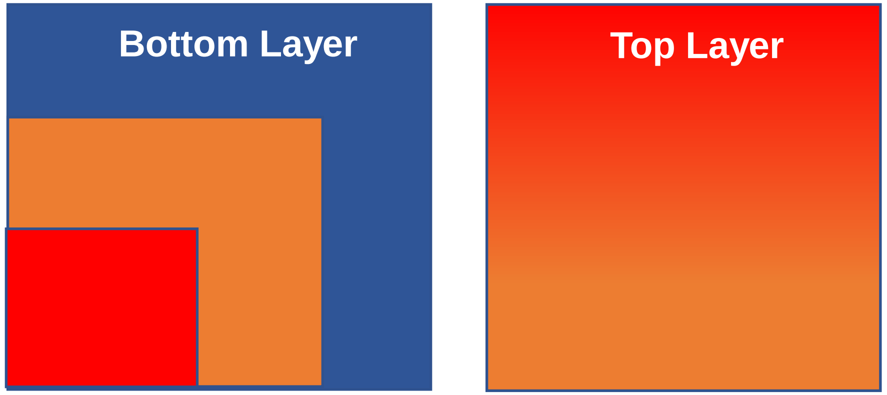
See Poster: Josh Tenney



Note: YSZ used in demonstration for cost considerations



Spray deposited electrode layers with varied electrode composition and pore size on top of electrolyte substrate



Example layout of 5x5 cm^2 electrode with 3D gradients in composition and microstructure

Strategic Systems Analysis and Engineering

Defining SOEC, SOFC, and R-SOC operation in the modern grid

SOC Cell and Stack Cost Production Tool

- Previous SOFC cell and stack production cost tool was expanded to include SOEC production and additional cell geometries
- Spreadsheet tool includes all necessary cost inputs
  - Raw materials, equipment, energy, etc.
- Sensitivity studies can be conducted on SOFCs and SOECs
  - Total production, materials costs, etc.
- Detailed guidance document/instructions available

OSTI Identifier: 1842511
Report Number: DOE/NETL-2022/3230

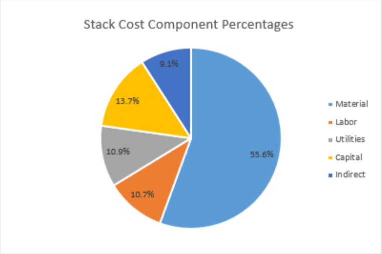
System Overview

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)		



Cell Characteristics

Cell Voltage	0.85	V
Cell Current Density	0.4	A/cm²
Power Density	0.34	W/cm²
Cell Side Length	15	cm
Total Cell Area	225	cm²
Active Area Percentage	90%	
Active Area	202.5	cm²
Power per Cell	68.85	W

Stack Characteristics

Cells per Stack	80	
Cell to Cell Resistance	1.00E-04	Ohm-cm²
Stack Voltage Loss	3.16	mV
Ratio of average cell voltage to nomical cell	98.00%	
Stack Power	5.40	kW

Stack Production

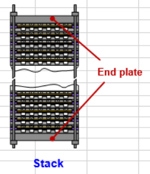
Stacks per year	20,000	
Capacity per year	107.95	MW/year

Yields

Tape Punching Yield	90%
Completed Cell Yield	97.7%

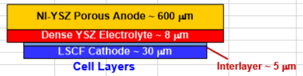
Total Stack Material Cost

$ 731.12



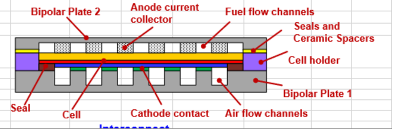
Cell Layers

Layer	Material	Thickness (u	Porosity	Density (g/cm3)	Weight per Cell (g	Weight w/ Losse	Cost per Cell	Cost per Stack
Cathode contact layer	LSCF	10	0%	6.30	1.28	1.31	$ 0.12	$ 9.50
Cathode current collector	LSCF	30	20%	6.30	3.06	3.13	$ 0.29	$ 22.81
Cathode active layer	LSM-YSZ	20	10%	6.50	2.37	2.43	$ 0.16	$ 12.98
Cathode interlayer	Gd/Sm	5	5%	7.90	0.76	0.78	$ 0.05	$ 4.00
Electrolyte	8YSZ	8	0%	6.10	0.99	1.01	$ 0.04	$ 3.46
Anode active layer	Ni-YSZ	25	10%	5.56	2.53	2.59	$ 0.10	$ 7.99
Anode support	Ni-YSZ	600	35%	5.56	48.79	55.49	$ 2.14	$ 171.06
								$ 231.81



Interconnect

Part	Material	Percent of Cell Area	Part Area + Scrap Area (cm2)	Thickness (mm)	Density (g/cm3)	Weight Required per Unit (kg)	Cost per Unit	Units per Stack	Cost per Stack
Frame	SS-441 Sheet	120%	270.00	1	6.81	0.18	$ 0.49	80	$ 39.36
Separater Plate	SS-441 Sheet	120%	270.00	1	6.81	0.18	$ 0.49	80	$ 39.36
Anode Flowfield	SS-411 Mesh	100%	225.00	0.5	1.70	0.02	$ 1.83	80	$ 146.36
Cathode Flowfield	SS-411 Mesh	100%	225.00	0.75	1.70	0.03	$ 2.74	80	$ 219.53
Spacers	Borosilicate glass	20%	45.00	1	2.23	0.01	$ 0.02	160	$ 3.44
End Plates	SS-441 Sheet	125%	281.25	50	6.81	9.58	$ 25.63	2	$ 51.26



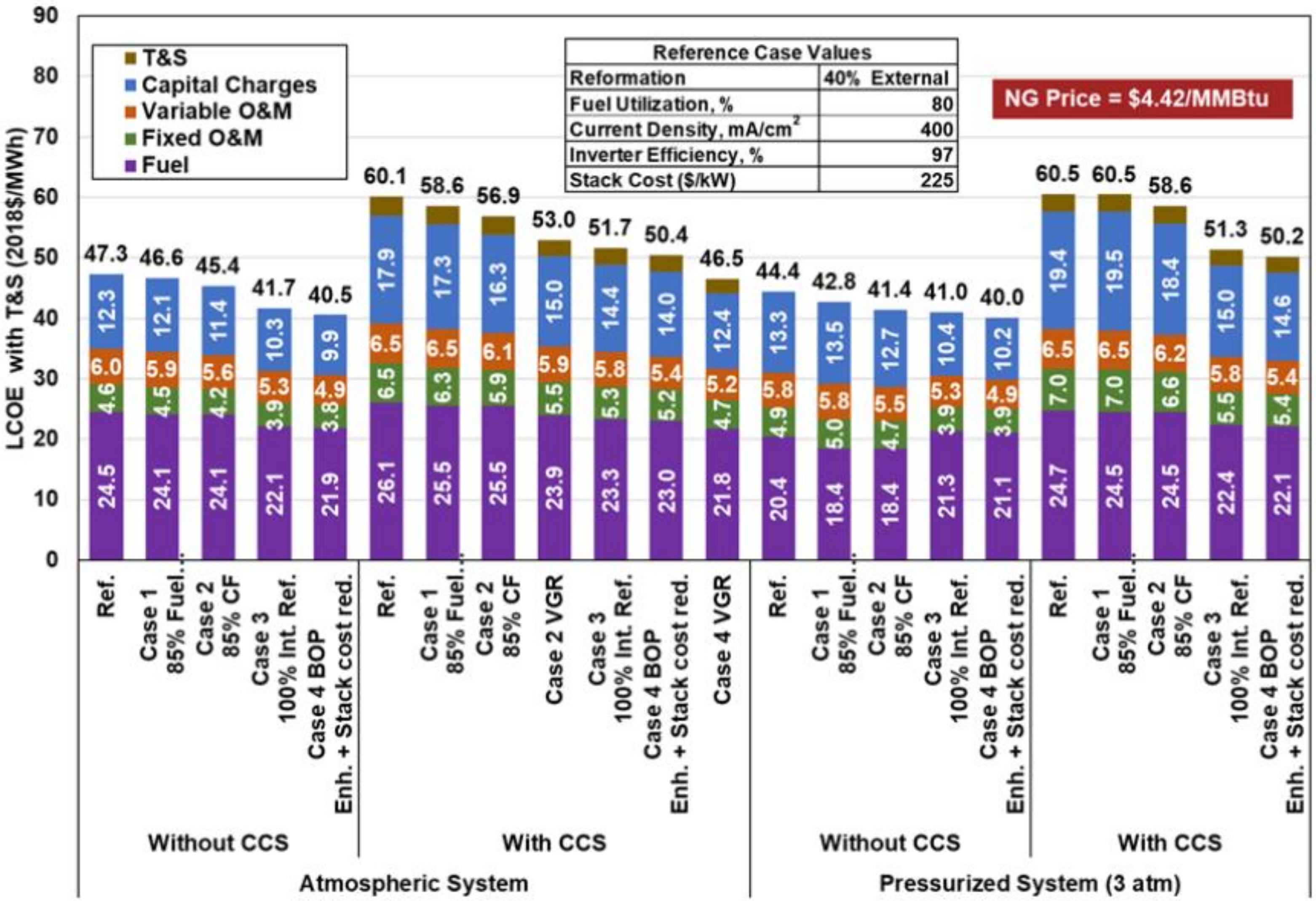
Newly released reports

- **Techno-Economic Analysis of Integrated Gasification Fuel Cell Systems** (Report DOE/NETL-2022-3250) and **Techno-Economic Analysis of Natural Gas Fuel Cell Plant Configurations** (Report DOE/NETL-2022/3259)
  - Updated technological pathway studies for ~550 MW IGFC and NGFC configurations considering carbon capture and storage, different gasification technologies, and pressurized operation provides targeted research guidance

<table>
<tr><th>Case Designation</th><th>Pathway Parameter</th><th>Case ID</th><th>SOFC Pressure (atm)</th><th>Internal Reformation (%)</th><th>SOFC Technology</th><th>Capacity Factor (%)</th><th>Degradation (%/1000 h)</th><th>Fuel Utilization (%)</th><th>Inverter Efficiency</th><th>Stack Cost ($/kW)</th></tr>
<tr><td rowspan="2">Reference (Case 0)</td><td rowspan="2">Reference with CCS</td><td>ANGFC0B</td><td>1</td><td rowspan="7">60</td><td rowspan="12">Advanced Cell</td><td rowspan="4">80</td><td rowspan="12">0.2</td><td rowspan="2">80%</td><td rowspan="9">97%</td><td rowspan="9">225</td></tr>
<tr><td>PNGFC0B</td><td>3</td></tr>
<tr><td rowspan="2">Case 1</td><td rowspan="2">85% Fuel Utilization</td><td>ANGFC1B</td><td>1</td><td rowspan="4">85%</td></tr>
<tr><td>PNGFC1B</td><td>3</td></tr>
<tr><td rowspan="2">Case 2</td><td rowspan="2">85% Capacity Factor</td><td>ANGFC2B</td><td>1</td><td rowspan="8">85</td></tr>
<tr><td>PNGFC2B</td><td>3</td></tr>
<tr><td>Case 2BV</td><td>With VGR</td><td>ANGFC2BV</td><td>1</td><td>> 90%</td></tr>
<tr><td rowspan="2">Case 3</td><td rowspan="2">100% Internal Reformation</td><td>ANGFC3B</td><td>1</td><td rowspan="5">100</td><td rowspan="4">85%</td></tr>
<tr><td>PNGFC3B</td><td>3</td></tr>
<tr><td rowspan="2">Case 4</td><td rowspan="2">BOP Enhancements
20% ASU Power Reduction, Inverter Efficiency 98%, Stack Cost Reduction</td><td>ANGFC4B</td><td>1</td><td rowspan="3">98%</td><td rowspan="3">200</td></tr>
<tr><td>PNGFC4B</td><td>3</td></tr>
<tr><td>Case 4BV</td><td>With VGR</td><td>ANGFC4BV</td><td>1</td><td>> 90%</td></tr>
</table>

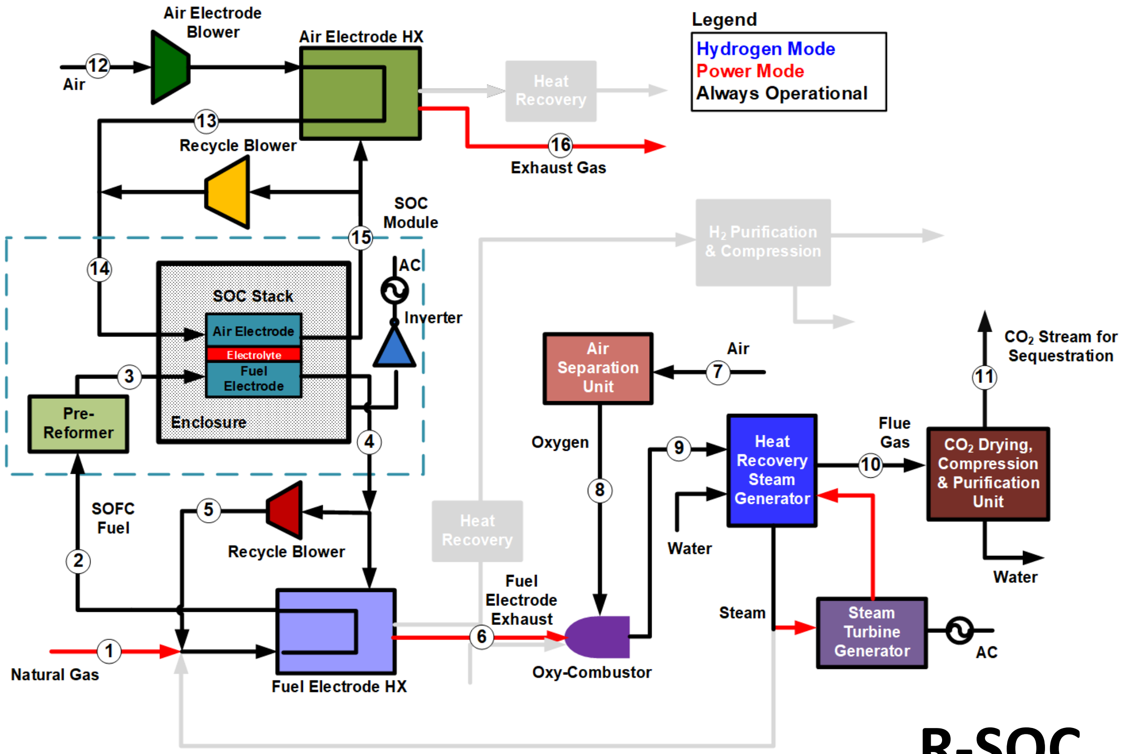
NGFC Pathway Cases with CCS

NGFC Pathway Study

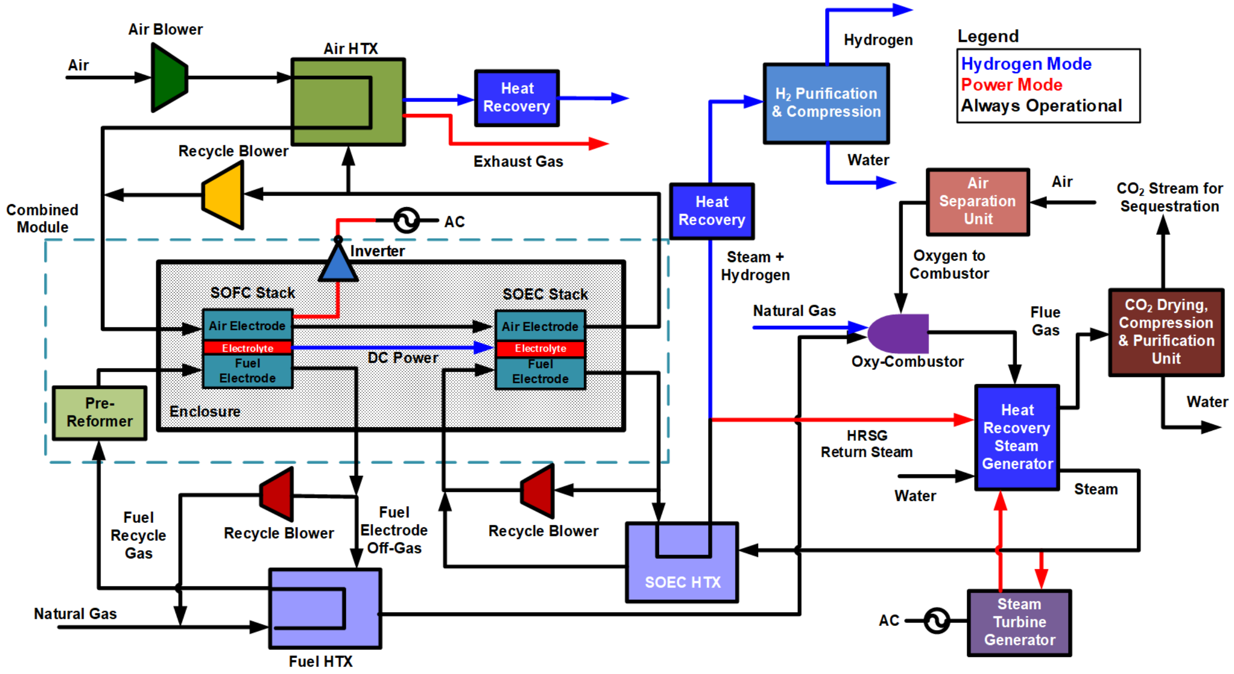


Ongoing System Studies

- **Techno-Economic Analysis (TEA) of H_2-fueled SOFCs**
- Preliminary TEA of R-SOC System configurations, considering fully R-SOC stacks vs. separate SOFC and SOEC stacks



R-SOC



SOFC + SOEC

Wrap-Up

Key Points

- Integrated degradation modeling framework expanded with more materials, more degradation modes, more operating modes, more data analysis
- Synthetic microstructure database, microstructural analysis tools are available for use
- Access to degradation framework available through collaboration
  - Help interpret impedance data
  - Move beyond correlation
  - Get recommendations on how much your cell can be improved
  - **Workshop for SOFC Program partners anticipated in Spring 2023!**
- Additive manufacturing and infiltration capabilities developed and available to create electrodes with engineered gradients
- Systems analysis tools and reports have been released. Look for upcoming reports exploring reversible systems.

Output: 2022 Project Review Posters

1. H. Kim, et al., “Effect of Microstructural Variability and Operating Condition on Cr-poisoning in Solid Oxide
2. Fuel Cell Cathode Using HPC Simulations”
3. J. Liu, et al., “Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies”
4. J. Tenney, et al., “Additive Manufacturing of Anode-Supported SOFCs through Aerosol Deposition”
5. T. Yang, et al., “Numerical Study to Optimize the Microstructure of an LSM/YSZ Backbone for Nanoparticle
6. Infiltration”
7. W. Epting, et al., “Rapid Assessment of SOC Electrode Degradation Using Computer Vision and Machine Learning”
8. Y. Chen, et al., “Sr Surface Segregation & Grain Boundary Degradation of LSCF/SDC Oxygen Electrode
9. Operated in Both Fuel Cell and Electrolysis Mode”
10. Y. Fan, et al., “Nanoparticles Infiltration in Air Electrode of LSM-YSZ/YSZ/Ni-YSZ Cells to Improve Performance and Mitigate Performance Degradation under Reversible SOFC/SOEC Operation”
11. Y.L. Lee, et al., “Defect Thermodynamics and Transport Properties of Proton Conducting Oxide $BaZr_{1-x}Y_xO_{3-\delta}$ ($x \leq 0.1$) Evaluated Based on Density Functional Theory Modeling”
12. Y. Lei, et al., “Modeling Ni Redistribution in the Fuel Electrode of Solid Oxide Cells”
13. Y. Mantz, Y.L. Lee, “Surface Energies of $LaMnO_3$ High-Index Surfaces Obtained from Density-Functional Theory”

Output: Manuscripts

1. T. Yang, et al., "Multiphysics modeling of SOFC performance degradation caused by interface delamination and active layer cracking," **International Journal of Hydrogen Energy** (accepted 9/2022)
2. Y.L. Lee, et al., "Defect Thermodynamics and Transport Properties of Proton Conducting Oxide BaZr1-xYxO3-δ (x≤0.1) Guided Based on Density Functional Theory Modeling," **JOM** (accepted 9/2022)
3. Y. Lei, et al., "Modeling Ni redistribution in the hydrogen electrode of solid oxide cells through Ni(OH)2 diffusion and Ni-YSZ wettability change," **Journal of Power Sources** 545, 231924, 2022.
4. Y. Chen, et al., "Space charge layer evolution at yttria-stabilized zirconia grain boundaries upon operation of solid oxide fuel cells," **Acta Materialia** 237, 1188179, 2022.
5. T. Hsu, et al., "High performance finite element simulations of infiltrated solid oxide fuel cell cathode microstructures," **Journal of Power Sources** 541, 231652, 2022.
6. R. Jacobs, et al., "Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies," **Advanced Energy Materials**, 2201203, 2022.
7. Y. Ji, et al., "Thermodynamic models of multicomponent nonstoichiometric solution phases using internal process order parameters," **Acta Materialia** 23, 117462, 2022.
8. J.H. Duffy, et al., "Surface and Bulk Oxygen Kinetics of BaCo0.4Fe0.4Zr0.2−XYXO3−δ Triple Conducting Electrode Materials," **Membranes** 11(10) 766, 2021.

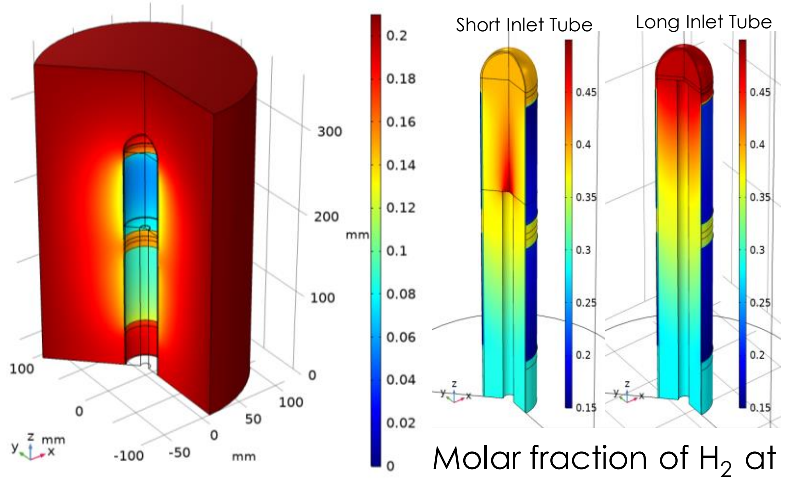
Additional SOC Efforts

NATIONAL ENERGY TECHNOLOGY LABORATORY

Aris Energy Solutions

- 5.6 kW demonstration in Morgantown
- Project: DE-FE31978

UNDEERC



Molar fraction of H_2 at 21% O_2 50% H_2 0.5 V

- Modeling SOFC degradation from coal gas contaminants
- Project: DE-FE31977

H_2NEW Laboratory Consortium (EERE/HFTO)

H2NEW

U.S. DEPARTMENT OF ENERGY

- Modeling and characterization performance degradation of SOECs

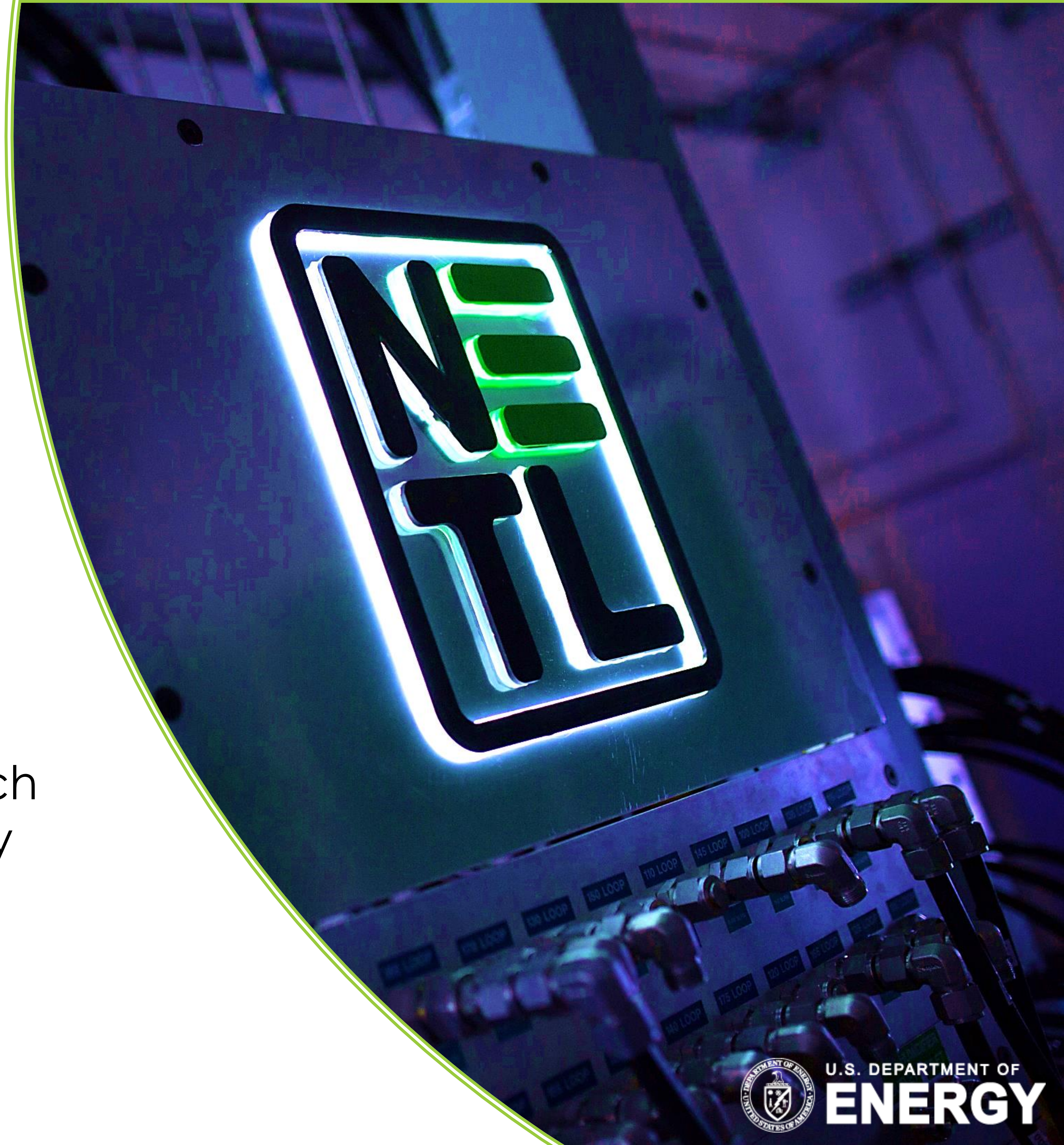
Acknowledgement

NATIONAL ENERGY TECHNOLOGY LABORATORY

- This work was performed in support of the U.S. Department of Energy's (DOE) Fossil Energy and Carbon Management's Solid Oxide Fuel Cell Research Program and executed through the National Energy Technology Laboratory (NETL) Research & Innovation Center's Solid Oxide Fuel Cell FWP 1022411 .

Thank You!

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



Harry Abernathy, Ph.D.
Group Leader, Solid Oxide Cell Research
National Energy Technology Laboratory
U. S. Department of Energy
304-285-4632
Harry.Abernathy@netl.doe.gov