Cell and Stack Degradation Evaluation and Modeling

NETL FWP 1022411

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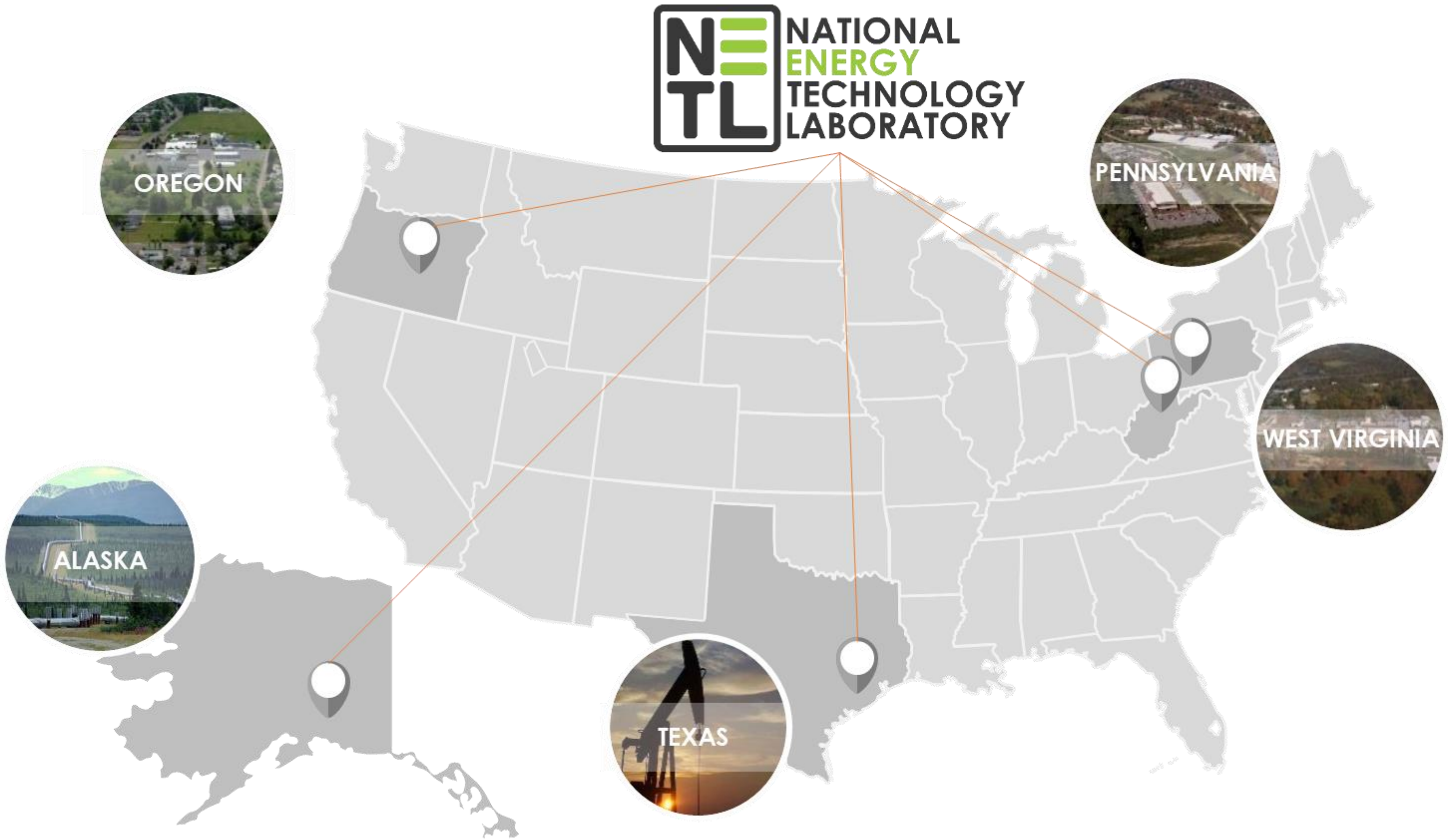
Outline

- **Introduction**
- **Recent Progress**
  - SOEC Systems Analysis
  - Degradation modeling and microstructure
  - Design of new electrode materials
- **Wrap-Up**



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NETL and DOE SOC Research

NATIONAL ENERGY TECHNOLOGY LABORATORY

DOE HQ

Energy Efficiency and Renewable Energy (EERE)

Hydrogen and Fuel Cell Technology Office (HFTO)

H2NEW
(HTE research)

DOE Hydrogen Shot:
\$2/kg H_2 by FY25
\$1/kg H_2 by FY30

FY24 Budget:
\$10M (**NETL: \$1.1M**)

Fossil Energy and Carbon Management (FECM)

Advanced Energy Systems Program (AES)

R-SOFC Program

EY23 Budget:
\$10M (**NETL: \$4M**)

EY24 Budget:
\$5M (**NETL: \$2.5M**)

FECM R-SOFC Program R&D Goals

NATIONAL ENERGY TECHNOLOGY LABORATORY

Enable:

- Highest efficiency and lowest cost electric power generation from hydrogen and natural gas with CCS
- Efficient and cost-effective distributed/utility scale hydrogen production
- Flexible modular hybrid SOFC/SOEC system design

Goals:

- Support for data center backup power systems using natural gas for short term (kW - MW scale)
- Fuel flexible, high grade SOFC system for combined heat and power (CHP)
- Hybrid R-SOFC systems for power production or hydrogen production as energy storage
- Long term goal of a utility scale hybrid R-SOFC system (10 MW - 50 MW)

KEY TECHNOLOGIES

Cell Development

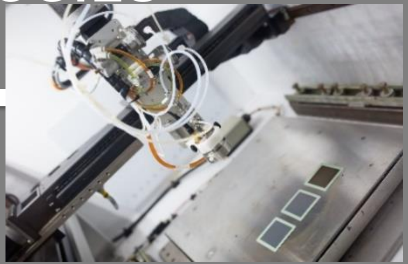


Figure courtesy NETL

Core Technology

Figure courtesy LG Fuel Cell Systems

Systems Development for SOFC and Reversible Systems

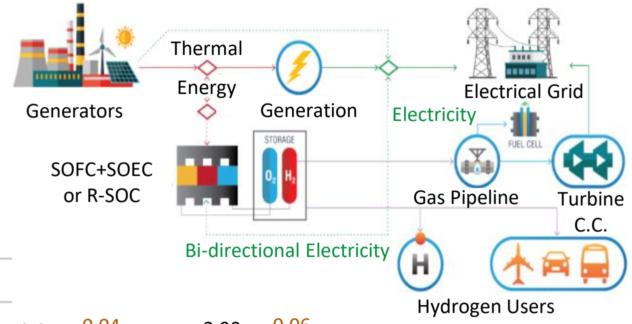
Figure courtesy FuelCell Energy

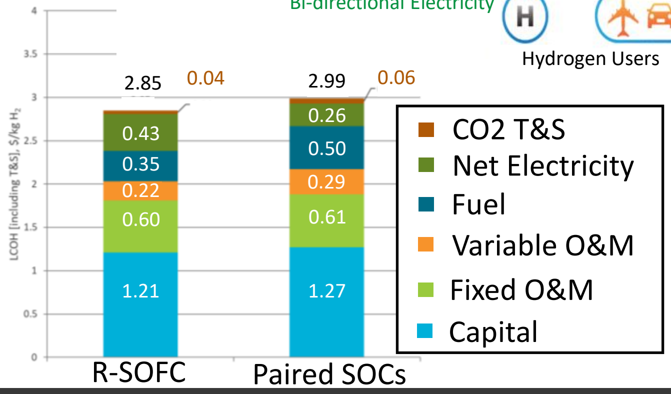
NETL SOC Capability Overview

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

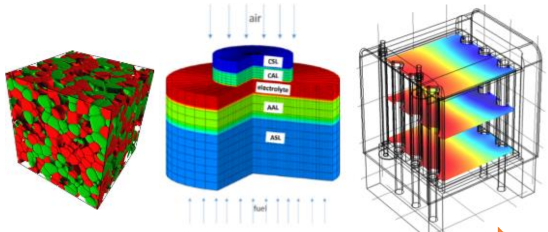


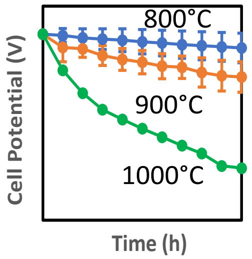


Levelized Cost of H_2 at $20/MWh Electricity

Performance Degradation Modeling

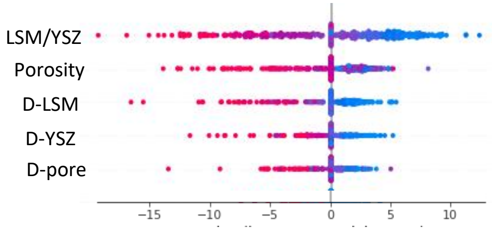
- Degradation prediction tools
- Atoms-to-System scale bridging
- Experimental validation
- Advanced Gas, Temperature Sensors





Increasing Scale

Machine learning-informed design tools

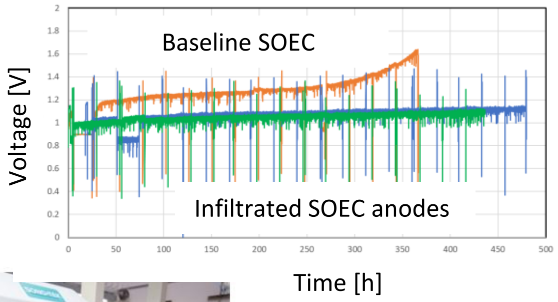


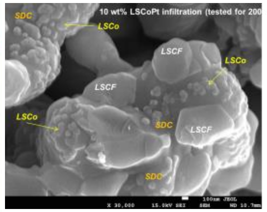
Impact of microstructural features on lifetime performance

Electrode Engineering

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

Infiltrated Cells from **6** Partners

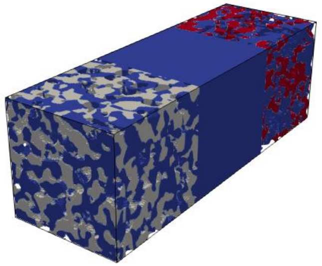


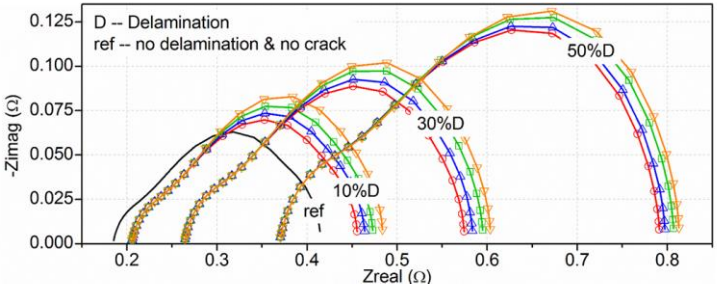


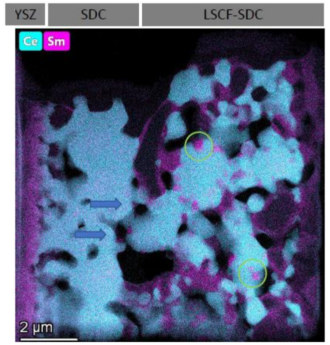
U.S. DEPARTMENT OF ENERGY | NATIONAL ENERGY TECHNOLOGY LABORATORY

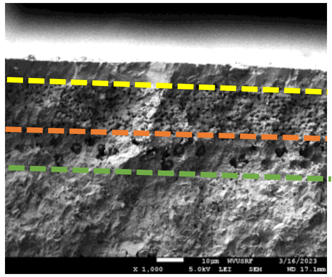
NETL SOFC Work Plan Tasks

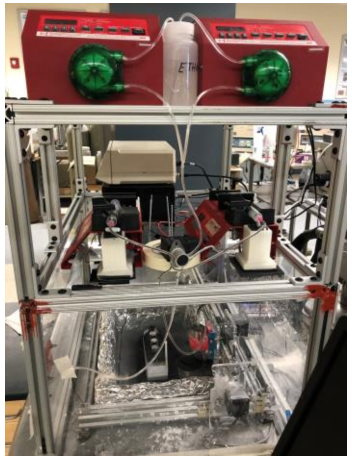
- **Task 2: Cell and Stack Degradation Evaluation and Modeling**
  - Performance and degradation model development
  - Microstructural analysis and analysis methods
  - Machine learning for materials studies, electrode design
- **Task 3: Electrode Engineering**
  - Infiltration for degradation mitigation
  - R-SOC characterization
  - Protonic SOC materials characterization and development
  - Advanced electrode design and manufacturing
  - S/TEM analysis of cell degradation
- **Task 4: Strategic Systems Analysis and Engineering**
  - R-SOC, SOEC system studies
  - SOFC scaling study, H_2-fueled SOFC market study
- **Task 5: Cyber Physical Modeling**
  - 1D real-time SOEC stack model development
  - Controls design for dynamic operation of SOC stacks

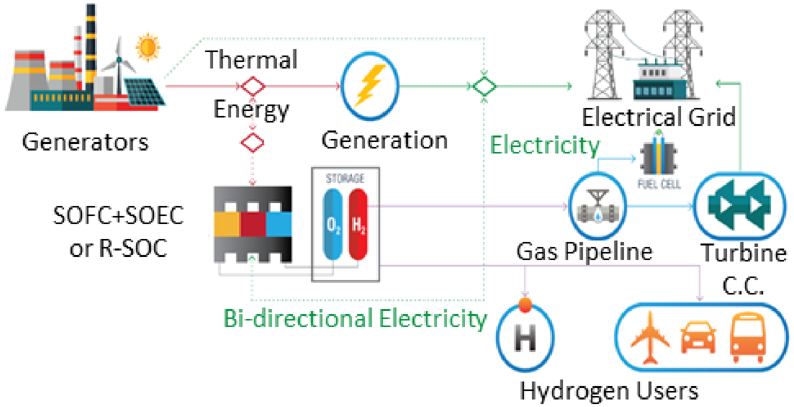










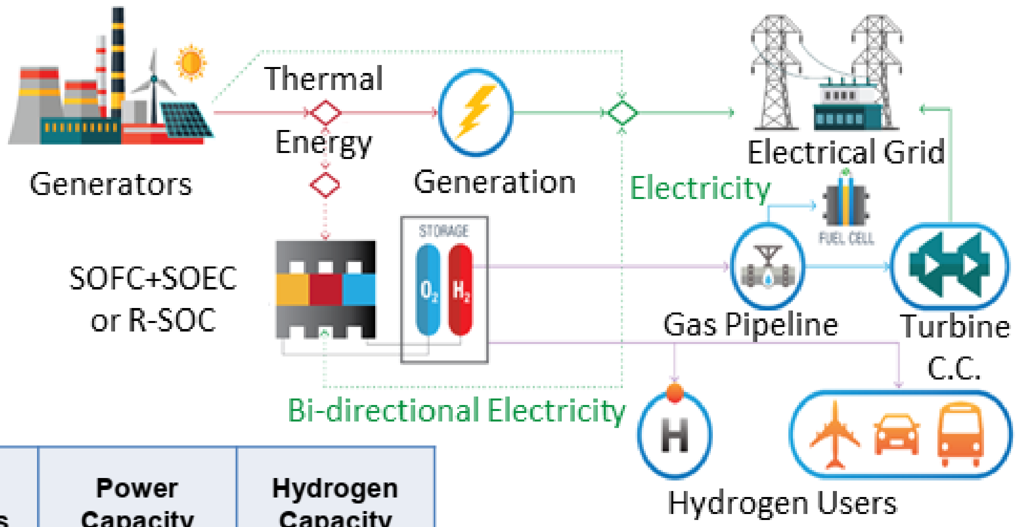


Strategic Systems Analysis and Engineering

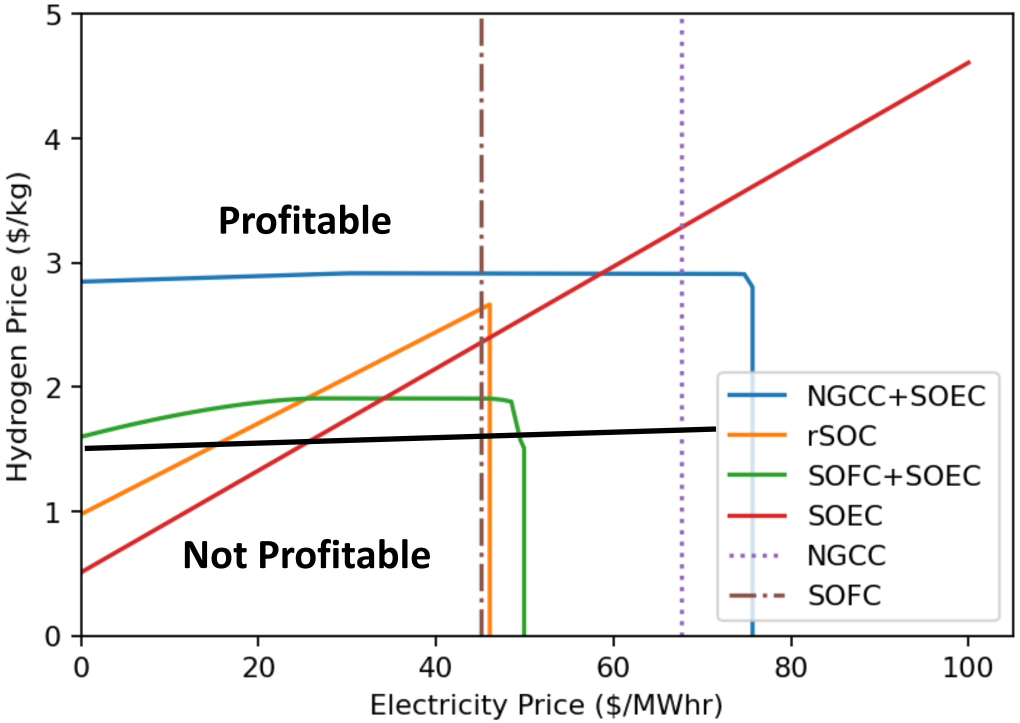
Defining SOC operation

Reversible Solid Oxide Cell Systems Analysis

NETL is exploring whether coupled integrated energy systems with the flexibility to produce both power and hydrogen should play a role in decarbonizing the US power sector by 2035 and broader economy by 2050.



Process Concepts	Power Capacity ($MW_{e,net}$)	Hydrogen Capacity (kg/s)
NGCC	650	-
SOFC	650	-
NGCC + SOEC	650	5
rSOC	650	5
SOFC + SOEC	710	5
SOEC	-	5



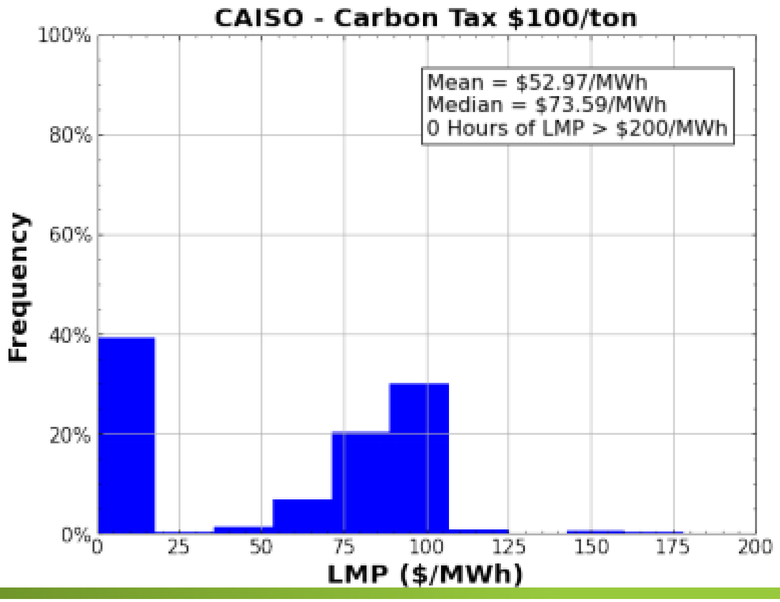
Breakeven curves for H_2/Power Production

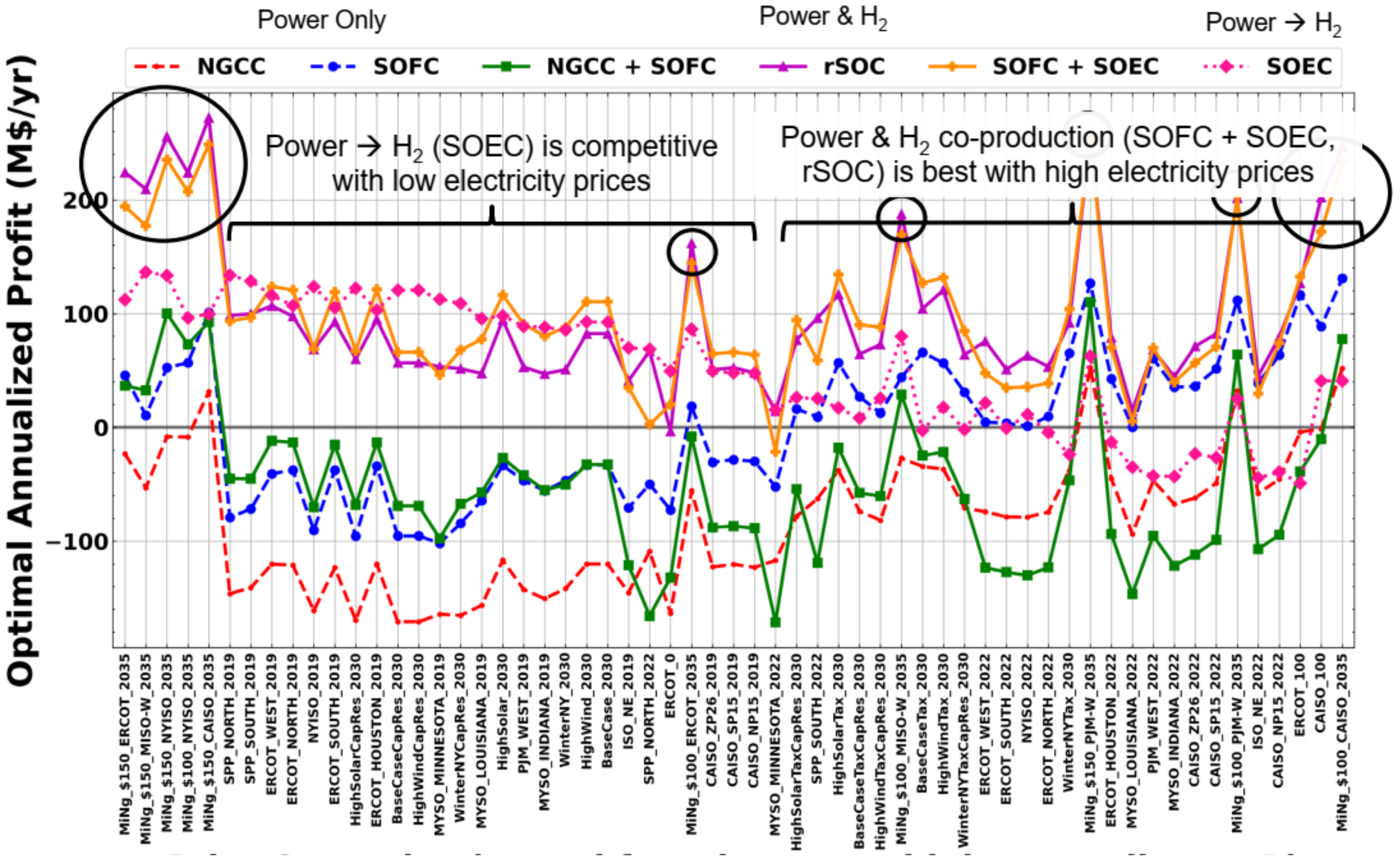
See “Technoeconomic Evaluation of SOFC Hydrogen/Electricity Co-Generation Concepts” https://www.osti.gov/servlets/purl/1960782

Market-based Technoeconomic Optimization

Reversible systems offer profitability across the greatest number of scenarios

https://www.ferc.gov/electric-power-markets





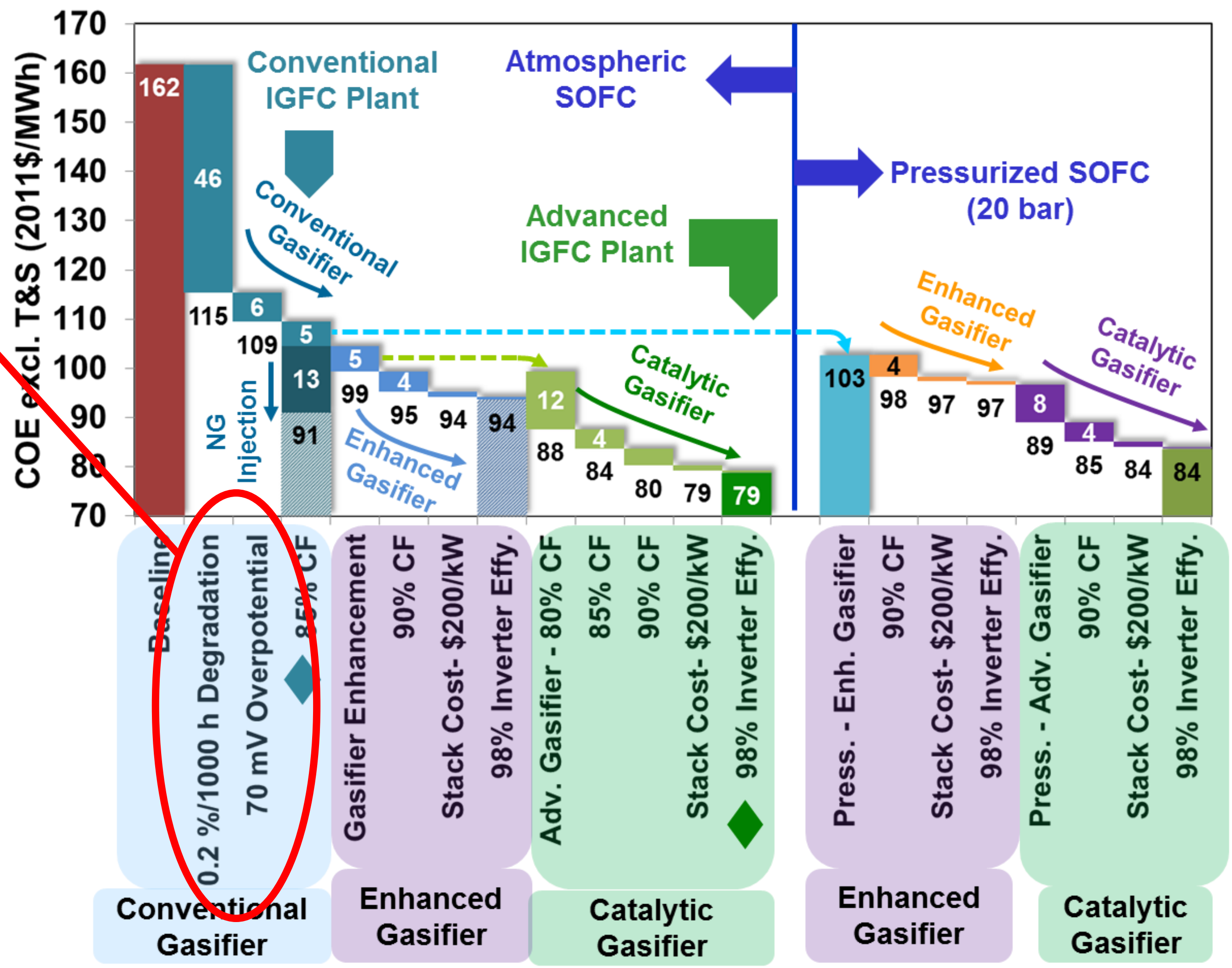
Price Scenarios (from lowest to highest median Locational Marginal Pricing)

NG Prices: 1.14 to 10.47 $/MMBTU, H_2 Price: $2/kg

Motivation: 2014 SOFC Pathway Studies

Reducing stack degradation had the largest impact on reducing cost of electricity of a 550 MW IGFC Plant

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

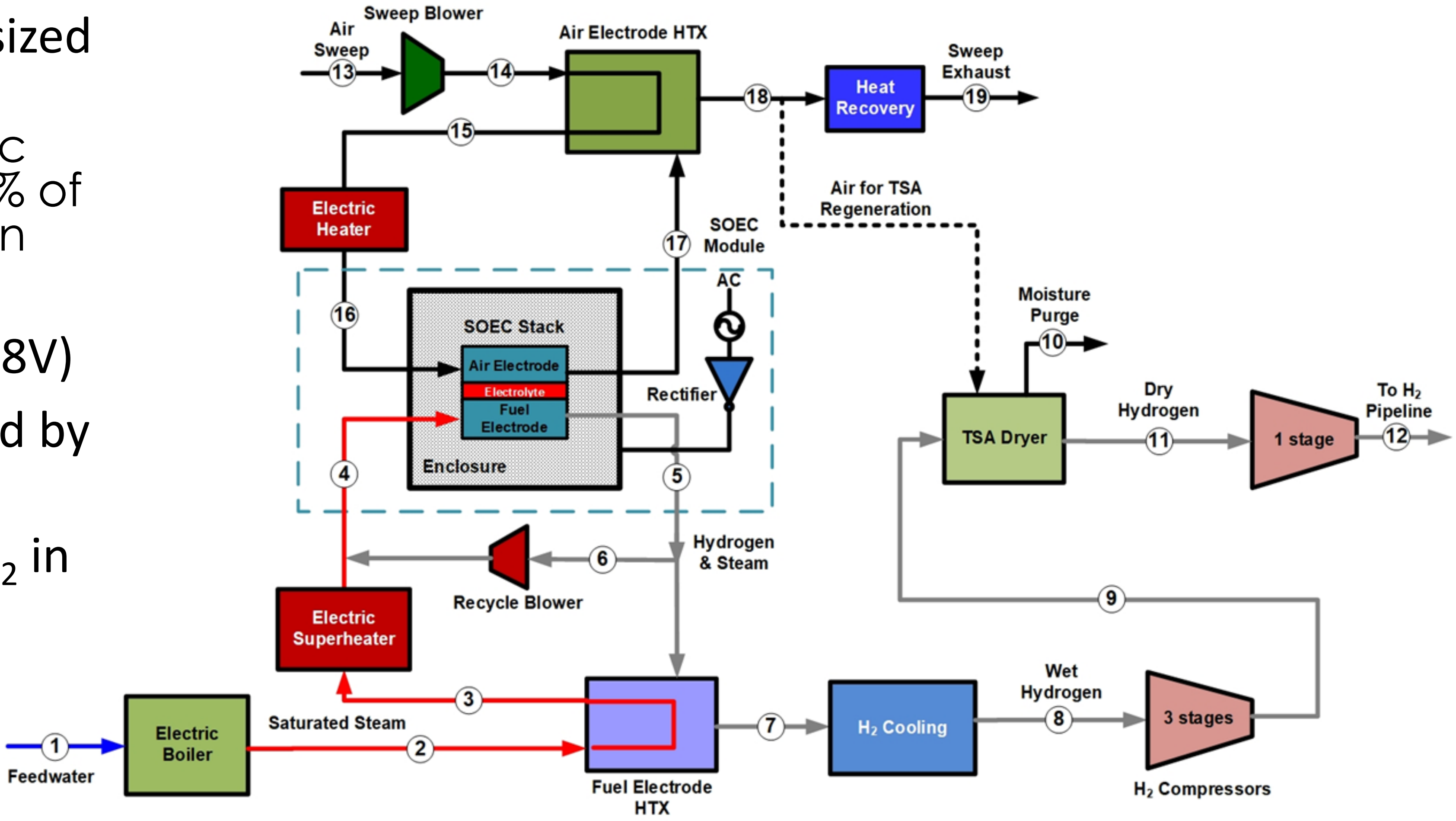


For fuel cell applications, performance and performance degradation can effectively drive down COE

SOEC Pathway Design Basis

Atmospheric System

- SOEC H_2 production facility sized to 1 GW_{DC} electrical input
  - Produces ~250,000 metric tons annually, about 2.5% of annual U.S. H_2 production
- Stacks operated at the thermoneutral voltage (~1.28V)
- All steam and heat generated by electric boilers and heaters
- H_2 recycle to ensure >10% H_2 in the feed to the stack
- Sweep air flow controlled to ensure <35 mol% oxygen in air-electrode exhaust



DC = Direct current
HTX = Heat exchanger
TSA = Temperature swing absorption

Source: NETL

G. Hackett, "Recent Progress in Solid Oxide Cell Technology Analysis at NETL", 2024 FECM Spring R&D Project Review Meeting, Pittsburgh, PA, April 23-25, 2024.

Design Basis

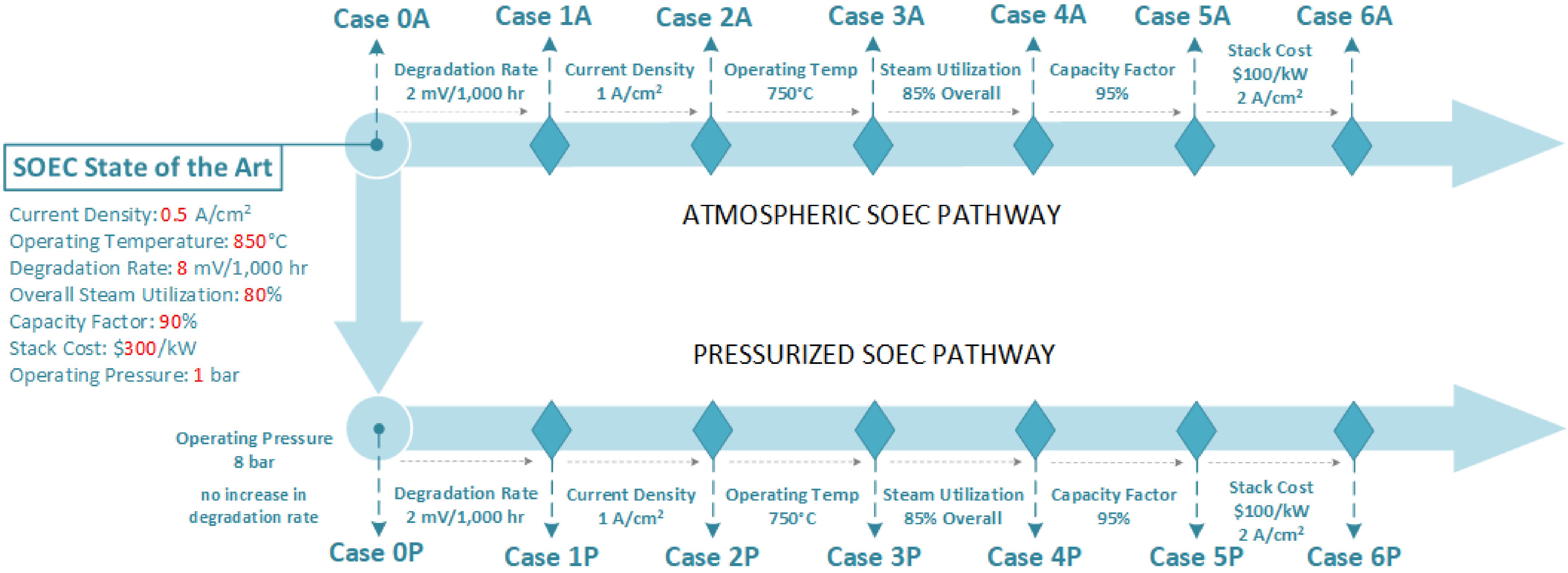
Key Parameters – State of the Art

State-of-the-Art SOEC Assumptions		
Parameter	**Value**	**Justification**
Current density, mA/cm^2	500	Operating condition of 9 out of 16 stacks in the literature review
Degradation rate, mV/1,000 hr	8	Post-2016 average degradation rate from literature review (~0.62%/kh)
Operating temperature, °C	850	Operating temperature of the MultiPHLY (2.6 MW_{AC}) and GrInHy2.0 (720 kW_{AC}) projects
Overall steam utilization	80%	Several stack tests from the literature review operated at a 70% single pass conversion; recycle can be used to obtain an 80% overall conversion
Capacity factor	90%	Similar to commercial H_2-producing gas reforming plants used in the H_2 baseline study
Stack cost, $/kW	300	Used in EERE SOEC study (adjusted to 2018$); value used by INL in several SOEC studies; $300/kW for FOAK, $155/kW for NOAK

EERE = Office of Energy Efficiency and Renewable Energy
INL = Idaho National Laboratory
FOAK = First of a kind
NOAK = Nth of a kind

G. Hackett, "Recent Progress in Solid Oxide Cell Technology Analysis at NETL", 2024 FECM Spring R&D Project Review Meeting, Pittsburgh, PA, April 23-25, 2024.

SOEC Pathway Design Basis



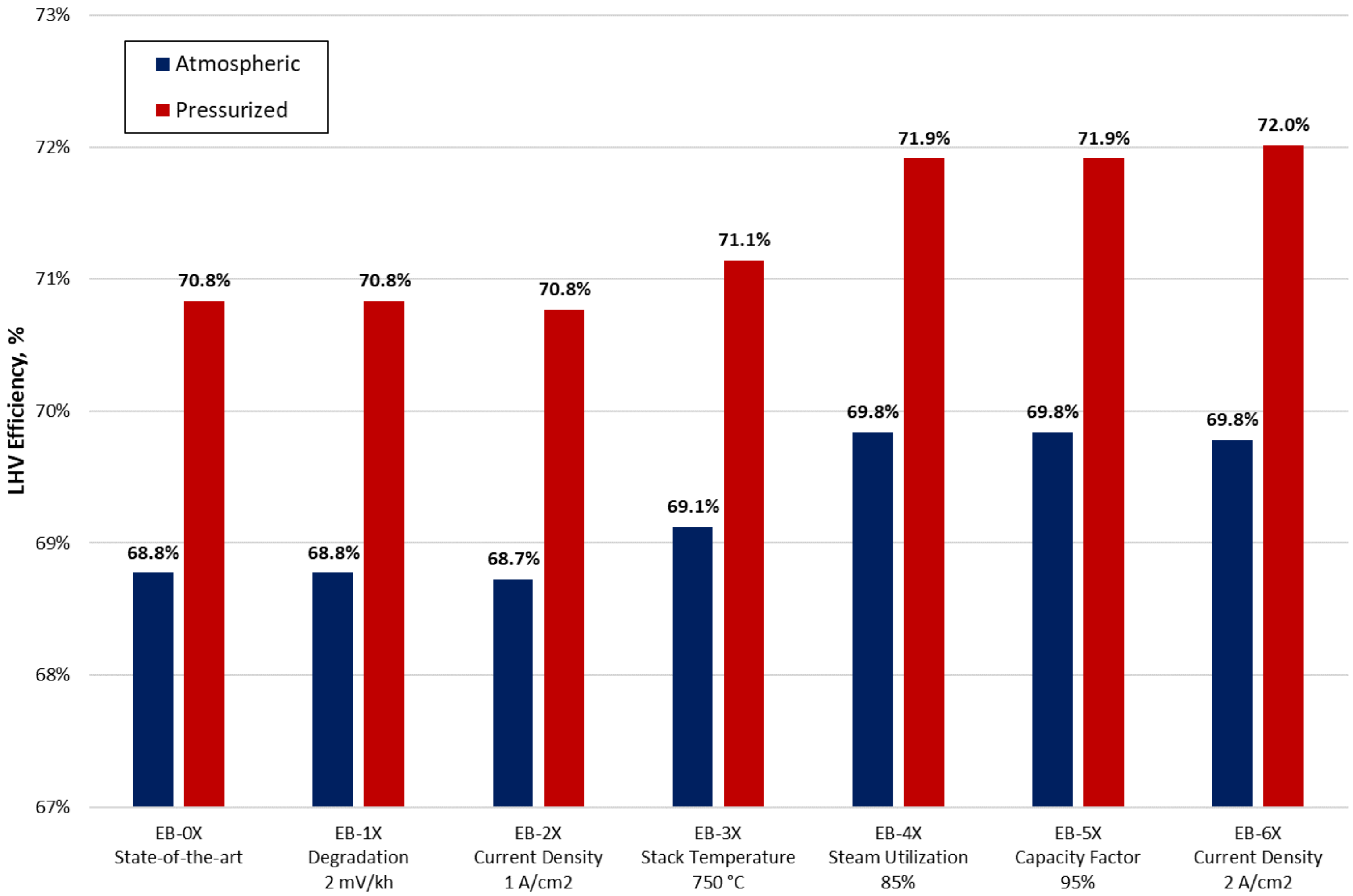
Source: NETL

G. Hackett, "Recent Progress in Solid Oxide Cell Technology Analysis at NETL", 2024 FECM Spring R&D Project Review Meeting, Pittsburgh, PA, April 23-25, 2024.

Selected Study Results

Performance Results

Atmospheric & Pressurized Efficiency

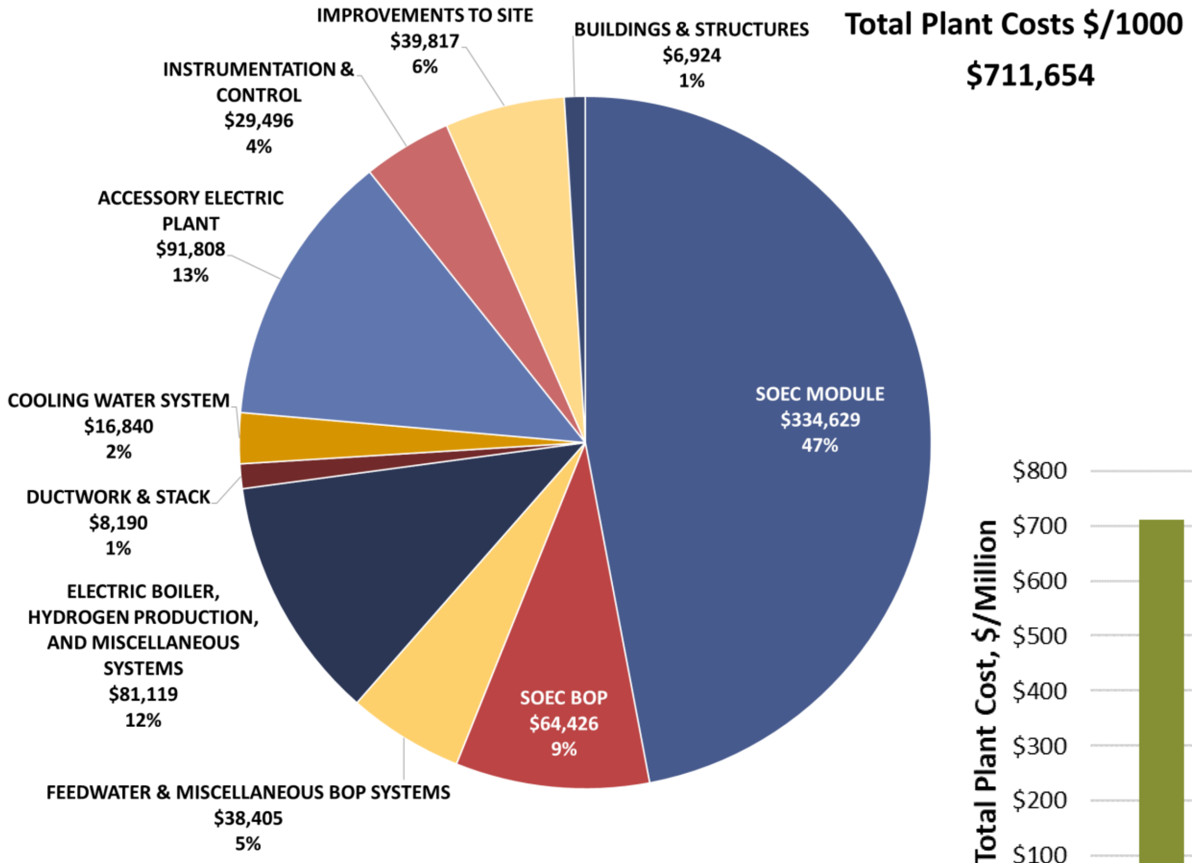


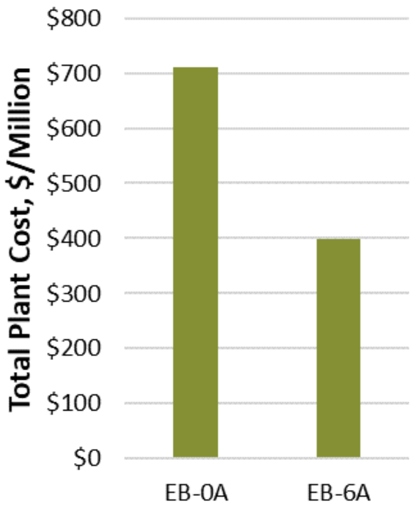
LHV = Lower heating value

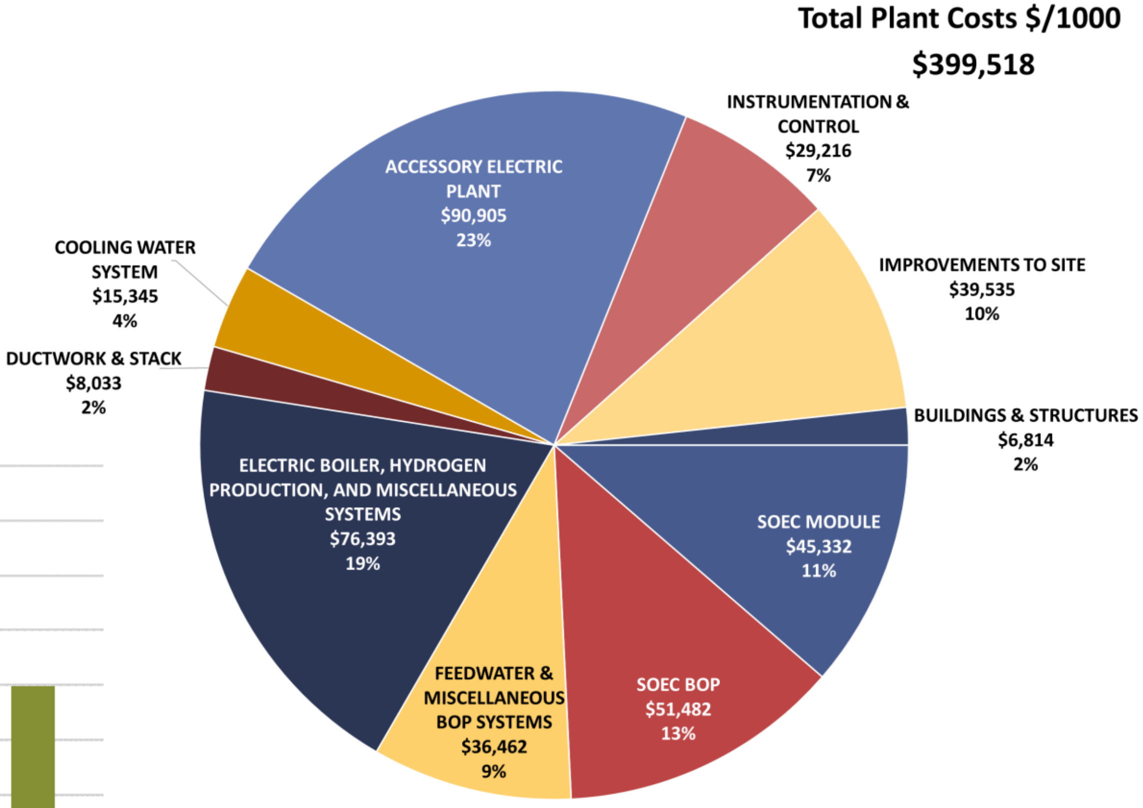
Source: NETL

Total Plant Costs

SOTA Atmospheric vs Advanced Atmospheric





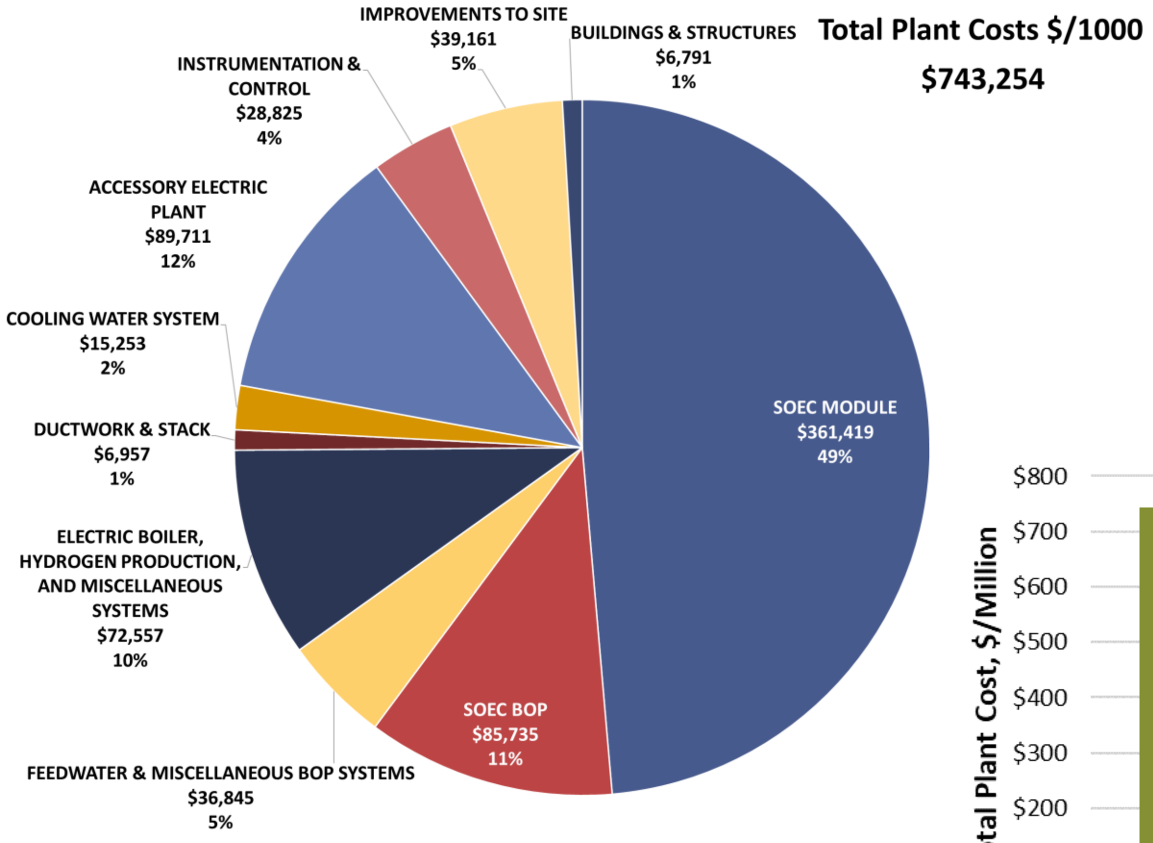


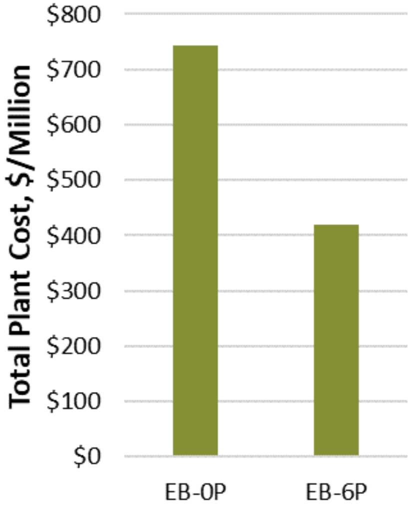
BOP = Balance of plant

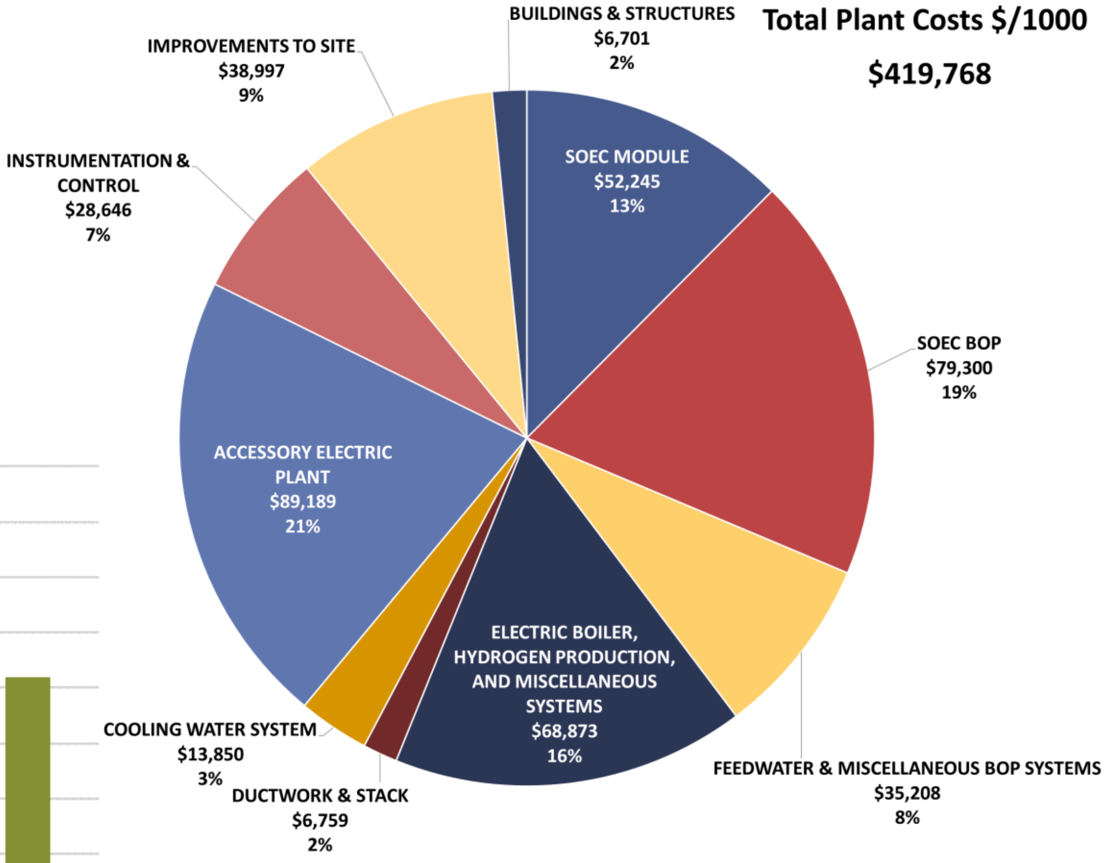
Source: NETL

Total Plant Costs

SOTA Pressurized vs Advanced Pressurized

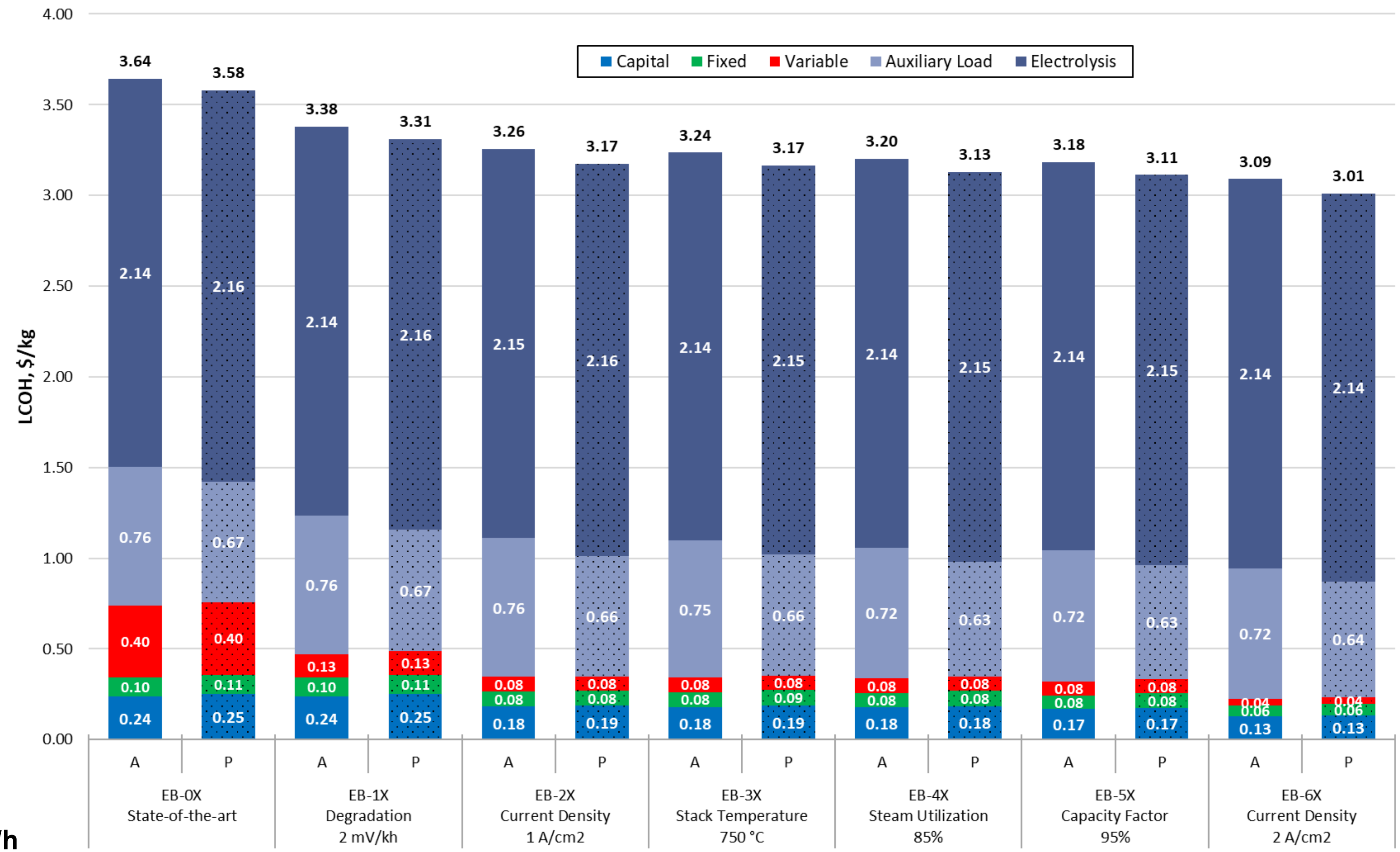






Source: NETL

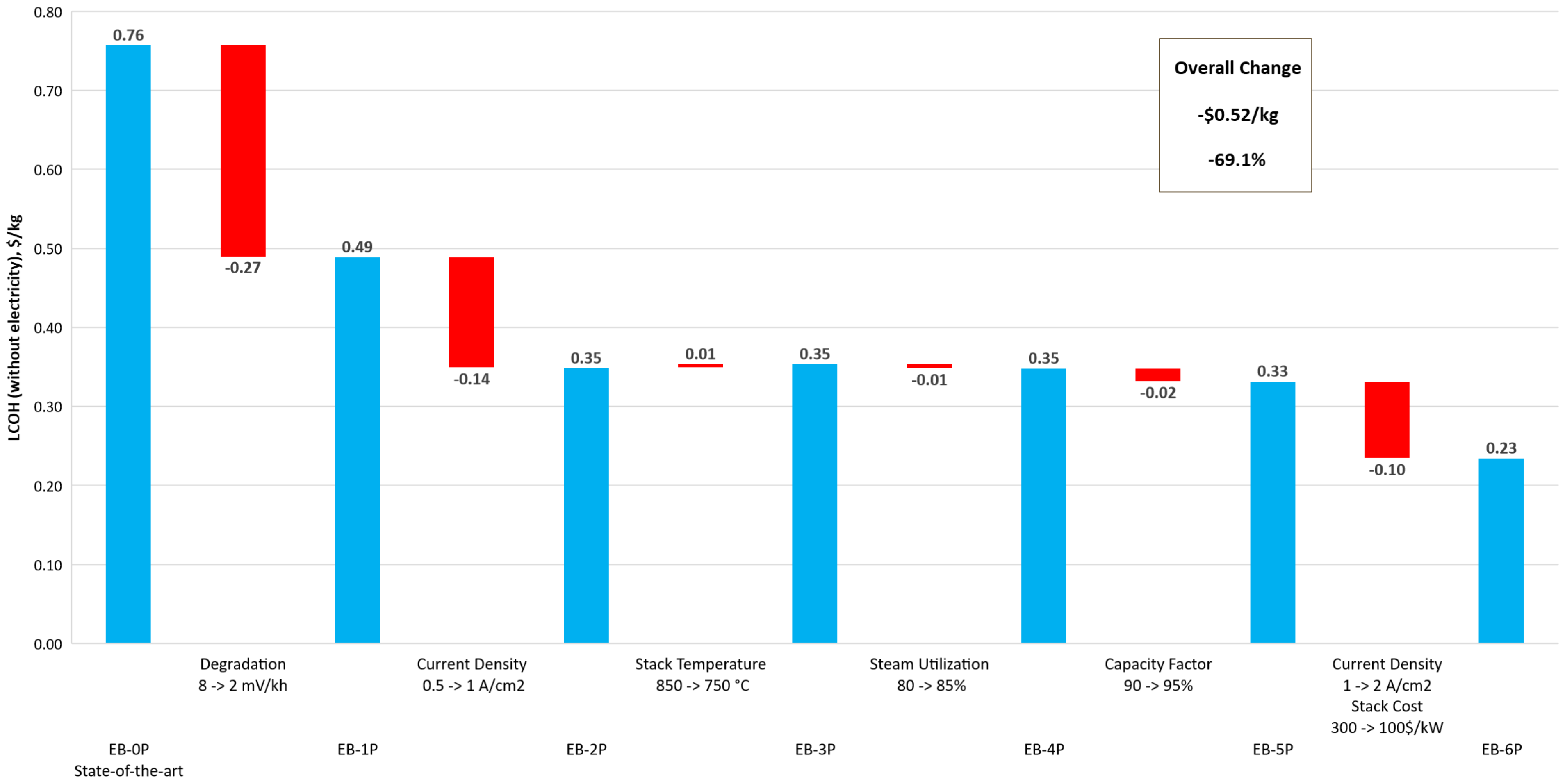
Atmospheric & Pressurized LCOH



Electricity price = $60/MWh

Source: NETL

Pressurized Pathway Waterfall Plot

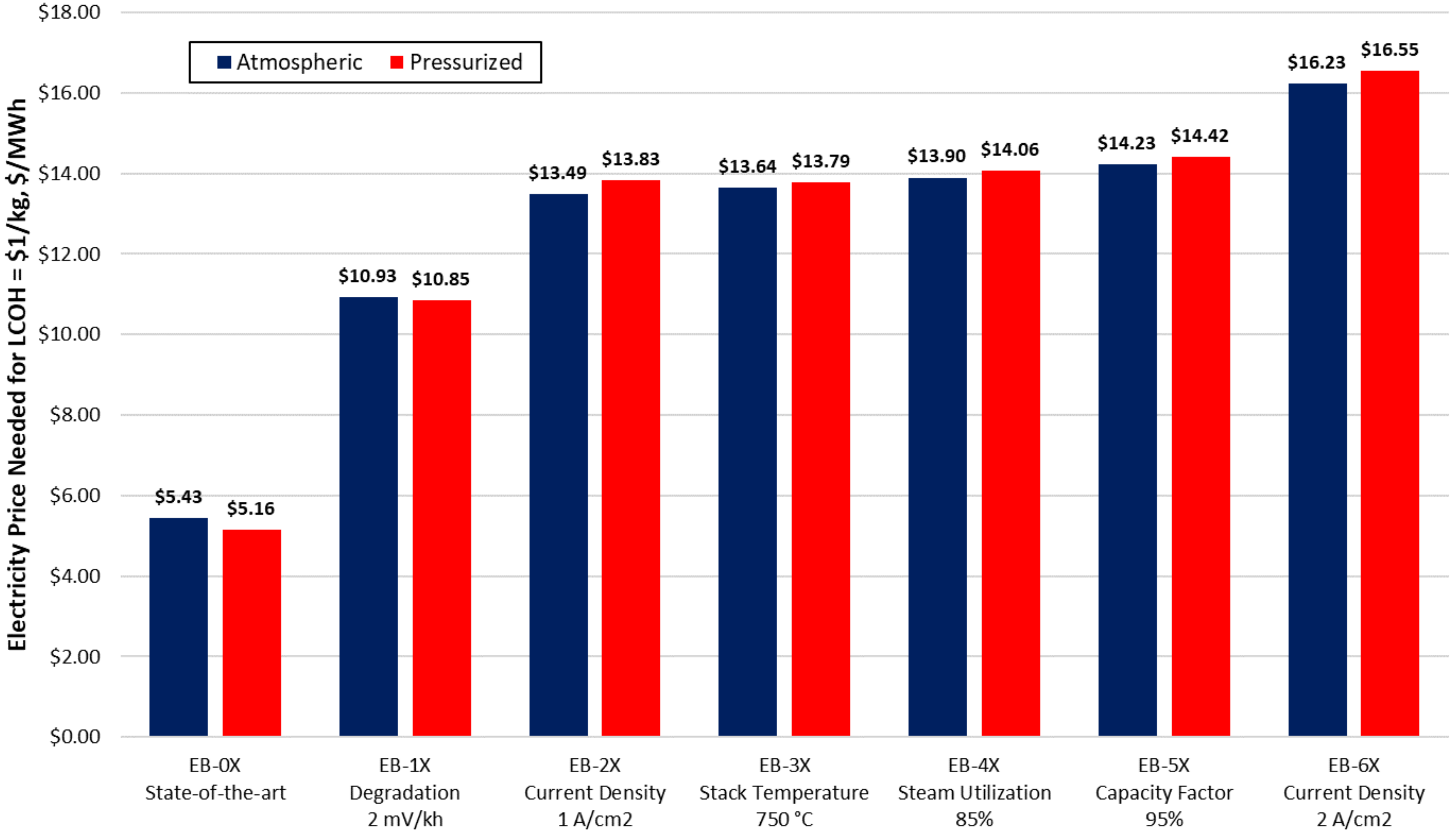


Electricity price = $60/MWh

Source: NETL

Electricity Price Needed for $1/kg

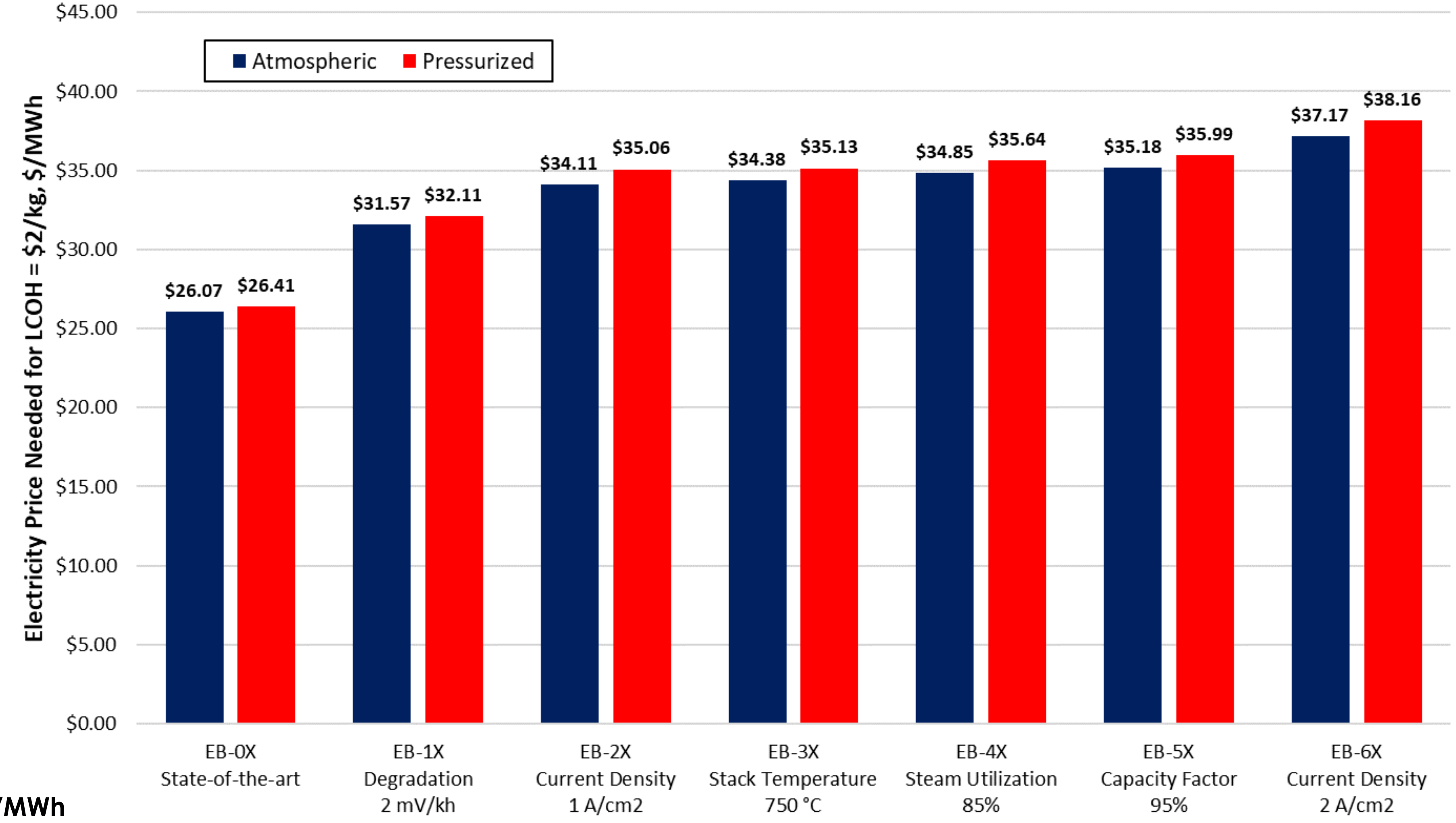
Providing perspective for Hydrogen Shot goal



Source: NETL

Electricity Price Needed for $2/kg

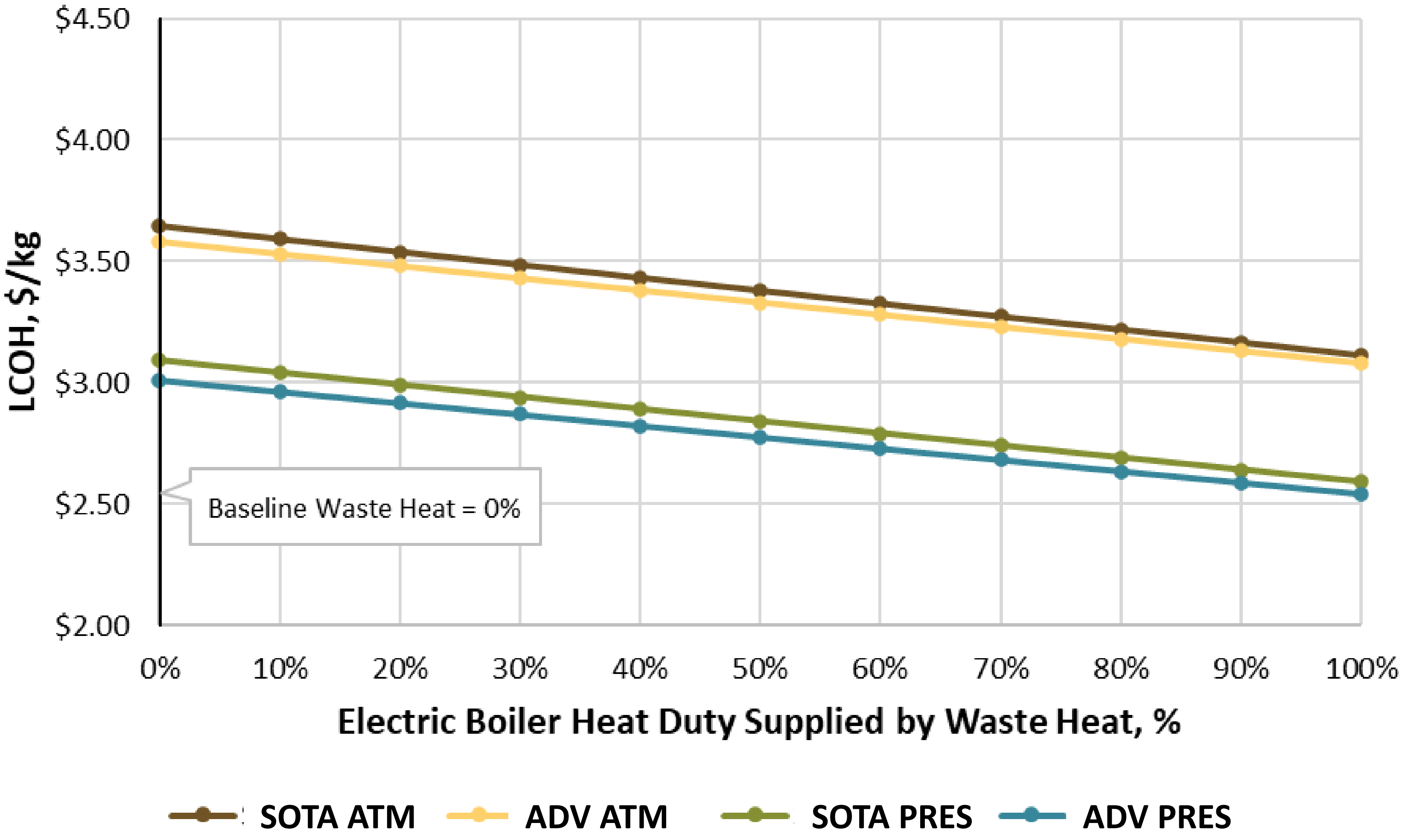
Providing perspective for H2NEW goal



Electricity price = $60/MWh

Source: NETL

Sensitivity to Free Waste Heat Availability



Electricity price = $60/MWh

Source: NETL

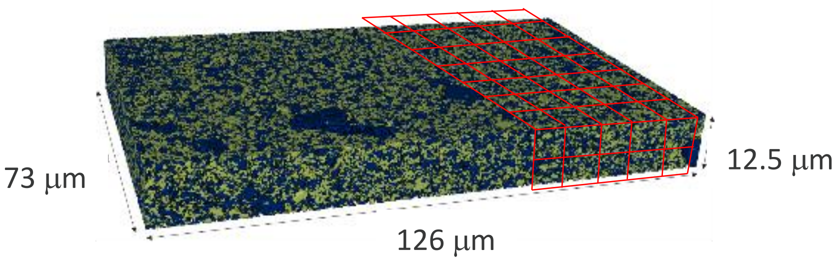
SOEC Pathway Study Conclusions

- The total LCOH reduction (*without electricity*) over both pathways was ~ **\$0.50/kg** (70%)
  - When an electricity cost of \$60/MWh was considered, the total reduction was ~ \$0.55/kg (15%)
- **Reductions in degradation rates** and **increases in current density** were shown to have the largest impacts on the LCOH
  - Decreasing the degradation rate from 8 to 2 mV/kh contributed over 50% of the total LCOH reduction (without electricity)
  - Increasing the current density from 0.5 to 1.0 mA/cm^2 contributed about 25% of the total LCOH reduction (without electricity)
- **Completely replacing the auxiliary load of the electric boiler** with **free waste heat** can also decrease the LCOH by **\$0.50/kg** when electricity is \$60/MWh
  - Effect is less pronounced at lower electricity prices (e.g., at \$30/MWh the LCOH reduction would be ~ \$0.25/kg)

Designing better electrodes

Microstructure

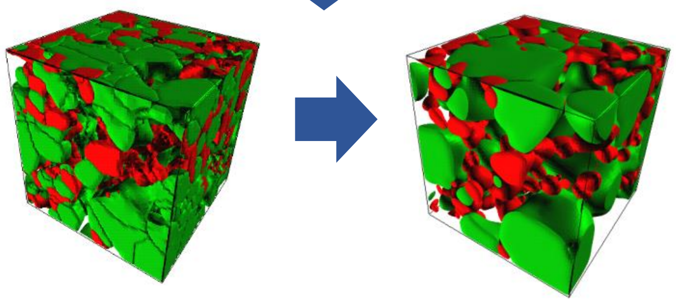
Integrated Cell Degradation Model

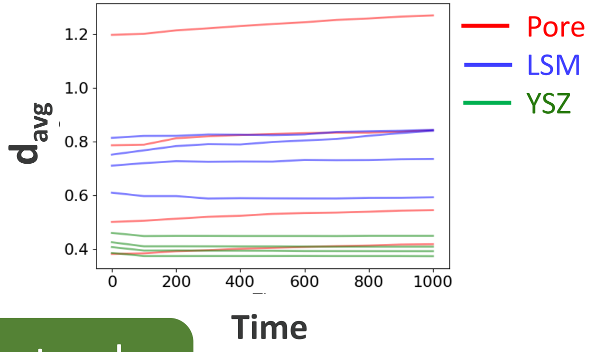


3D Electrode Microstructures

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

Degradation models

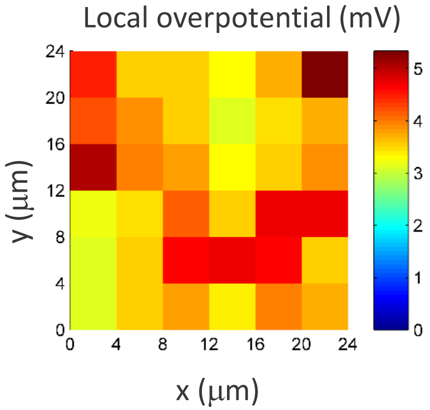


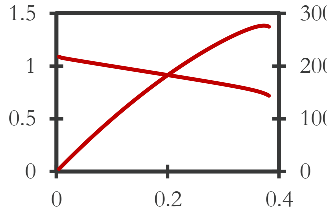


Microstructural Analysis

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

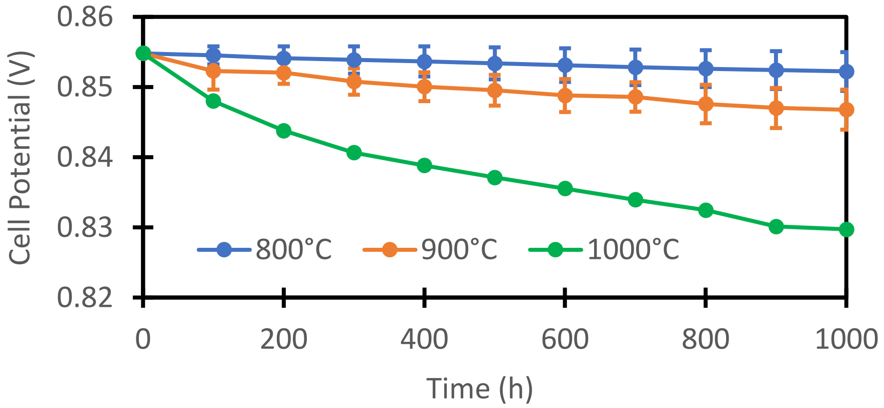
Multiphysics Performance Model





- 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

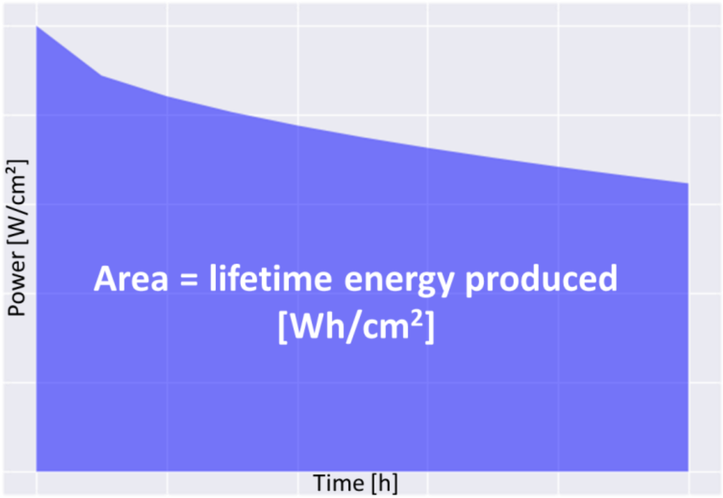
How to determine what's a good or bad electrode?

- Simulations run on database of **1000s** of synthetic microstructure covering large matrix of microstructural parameter combinations (particle sizes, phase fractions, particle size distribution, phase fraction distribution, etc.)

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



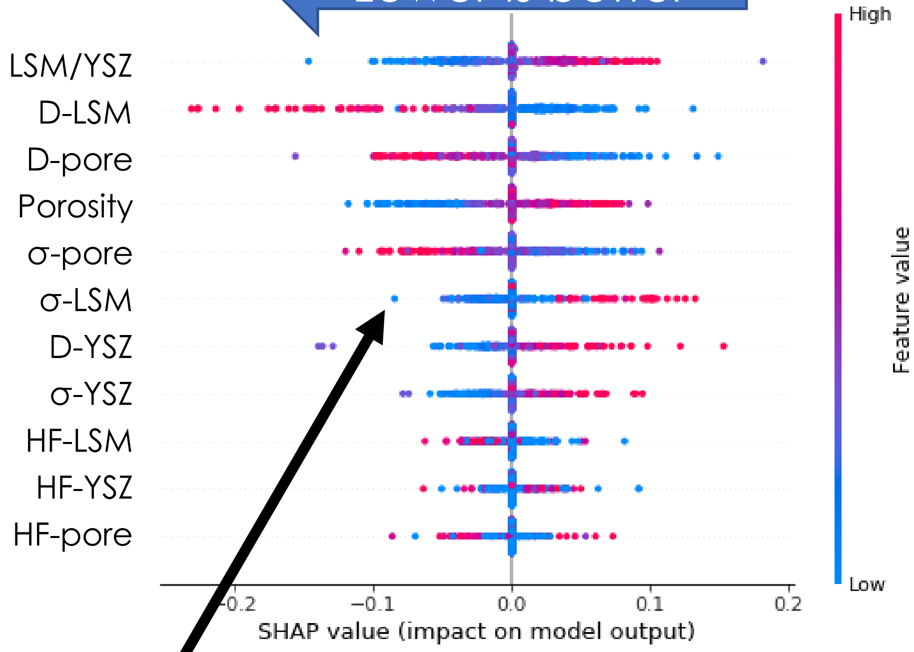
NETL Microstructure Resources

- **SOC Synthetic Electrode Microstructure Database**
  - **1,970 unique 3-phase electrode microstructure files**
  - **DOI: 10.18141/1988063**
- **PFIB-SEM 3D reconstructions of real SOFC electrodes:**
  DOI: 10.18141/1425617

SOFC Cathode Feature Importance Ranking

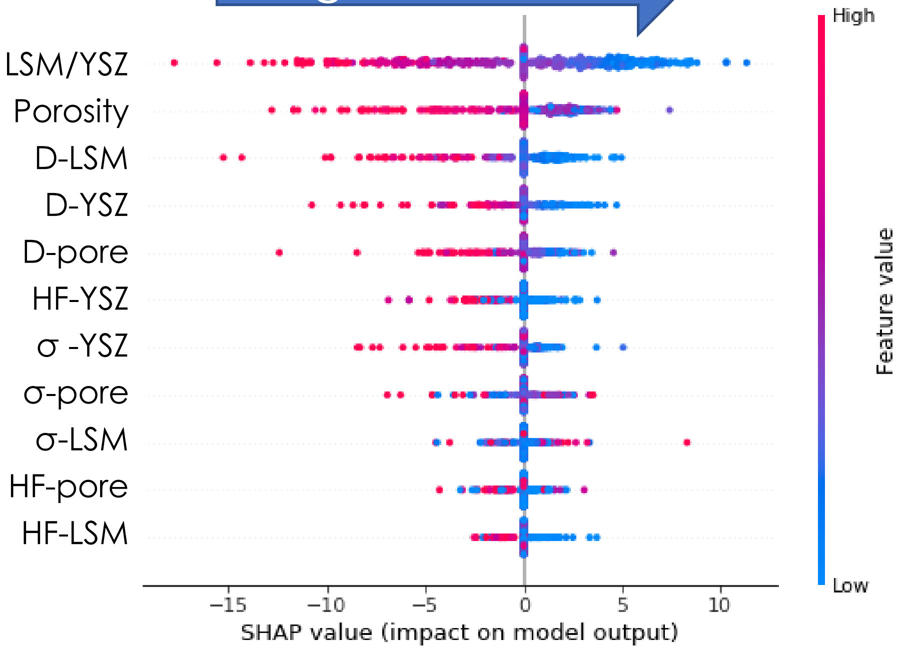
Impact on voltage decay [%/khr]

Lower is better



Impact on lifetime energy [Wh/cm^2]

Higher is better

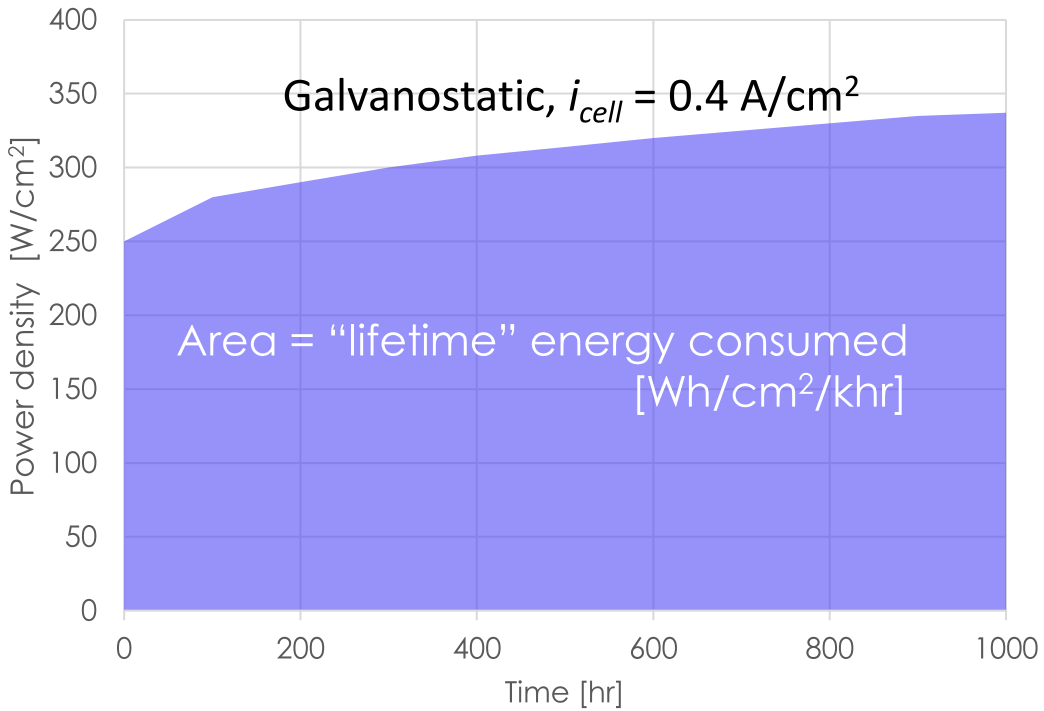


Each point represents a feature value from a specific simulated electrode microstructure

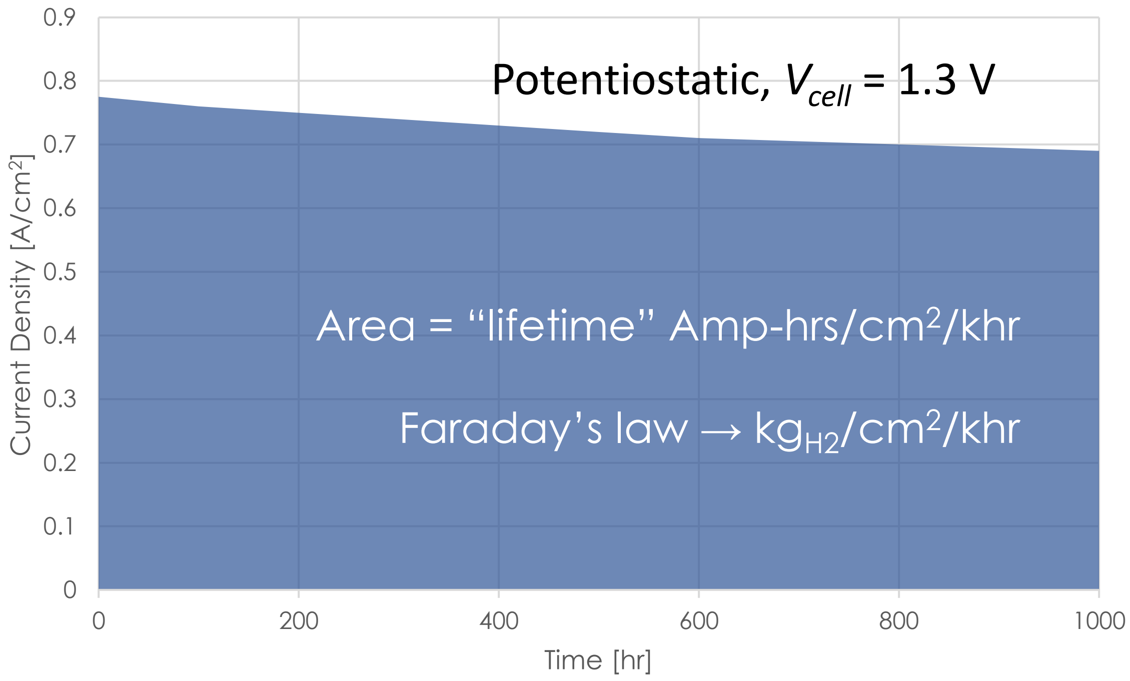
Small LSM particle sizes are bad for voltage decay, but net good for lifetime performance - **worthwhile tradeoff.**
Lower LSM/YSZ ratio is good for both metrics

SOEC Figures of Merit

Linking SOEC lifetime performance to economics



"Lifetime" energy consumed – at a given current density (and hence H_2 rate)

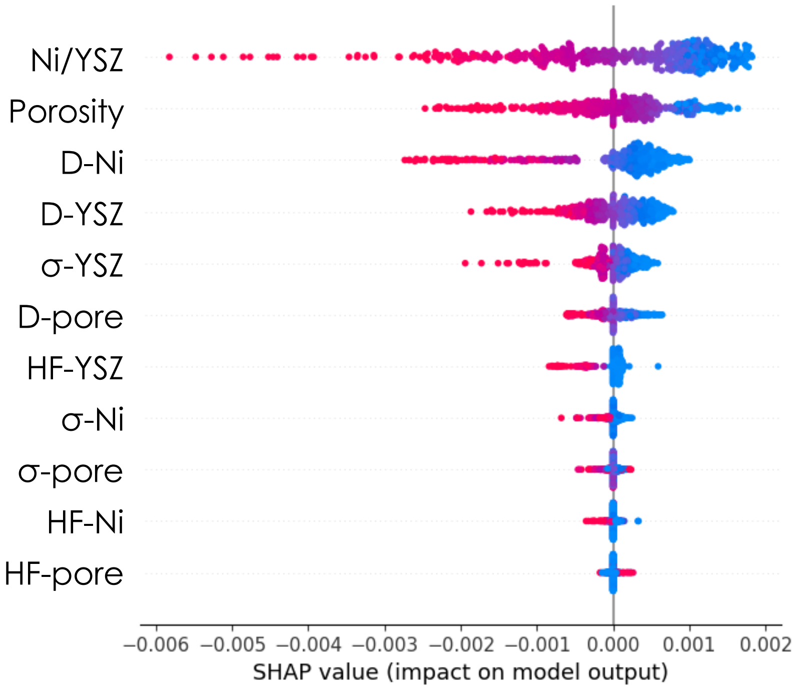


"Lifetime" H2 produced – at a given voltage (chosen roughly thermoneutral)

Feature Importance

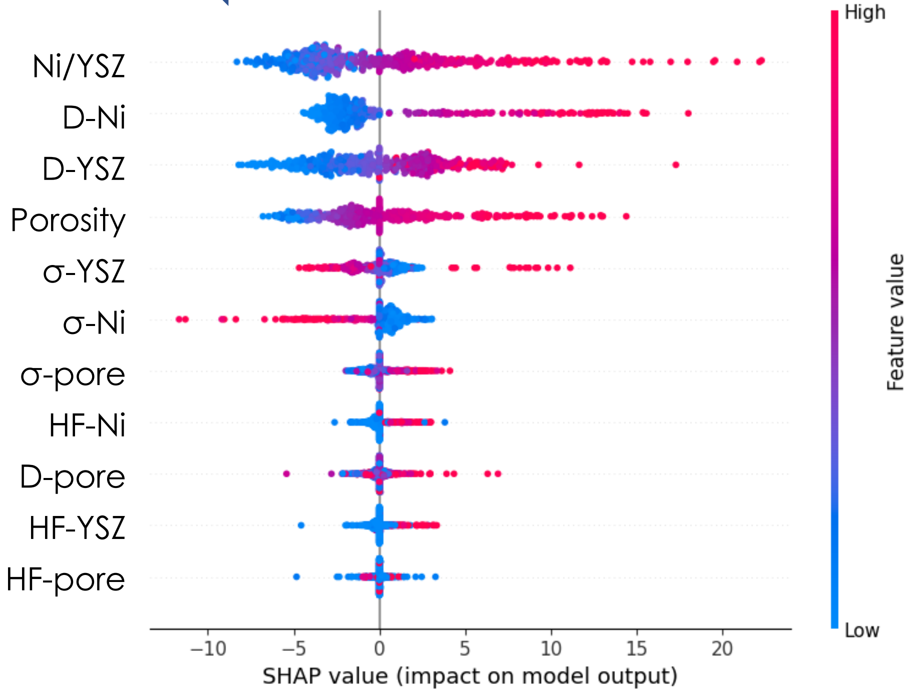
Impact on H_2 Produced [kg/cm²/khr]

Higher is better



Impact on energy consumed [Wh/cm²/khr]

Lower is better



Low Ni/YSZ ratio, low porosity, small solid particles beneficial for both, but rankings are different
Other figures of merit (e.g. degr. only) may show different dependence

Making specific recommendations

Commercial electrodes' initial microstructural parameters (measured)

ML model trained on bank of results from synthetic microstructures

SHAP analysis to estimate feature impact in commercial electrodes

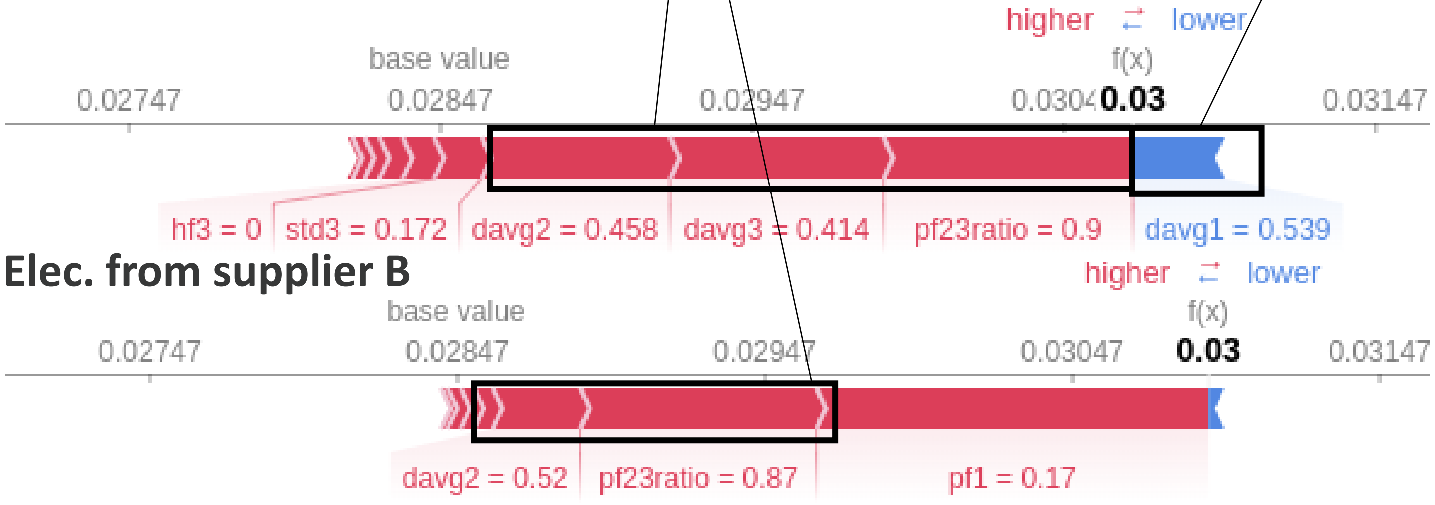
Low Ni/YSZ ratio, small solid particles were good choices

Biggest drain was pore size

Shown here for H2 produced

Fuel Elec. from supplier A

Fuel Elec. from supplier B



Your electrode here??

Designing better electrodes

Electrode Materials

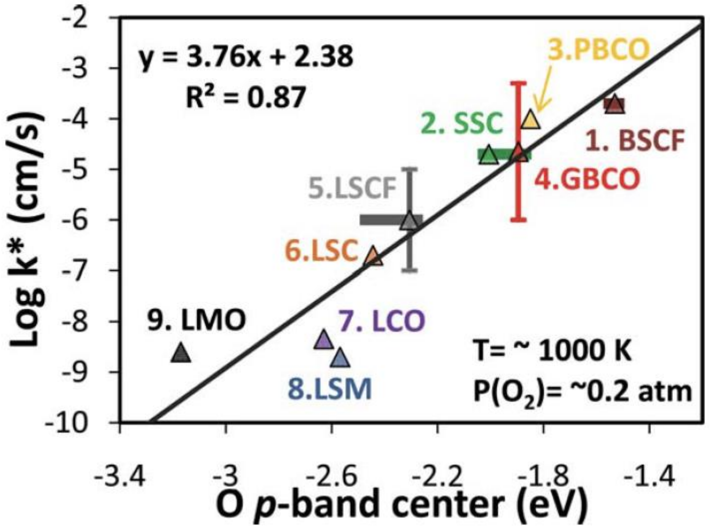
NATIONAL ENERGY TECHNOLOGY LABORATORY

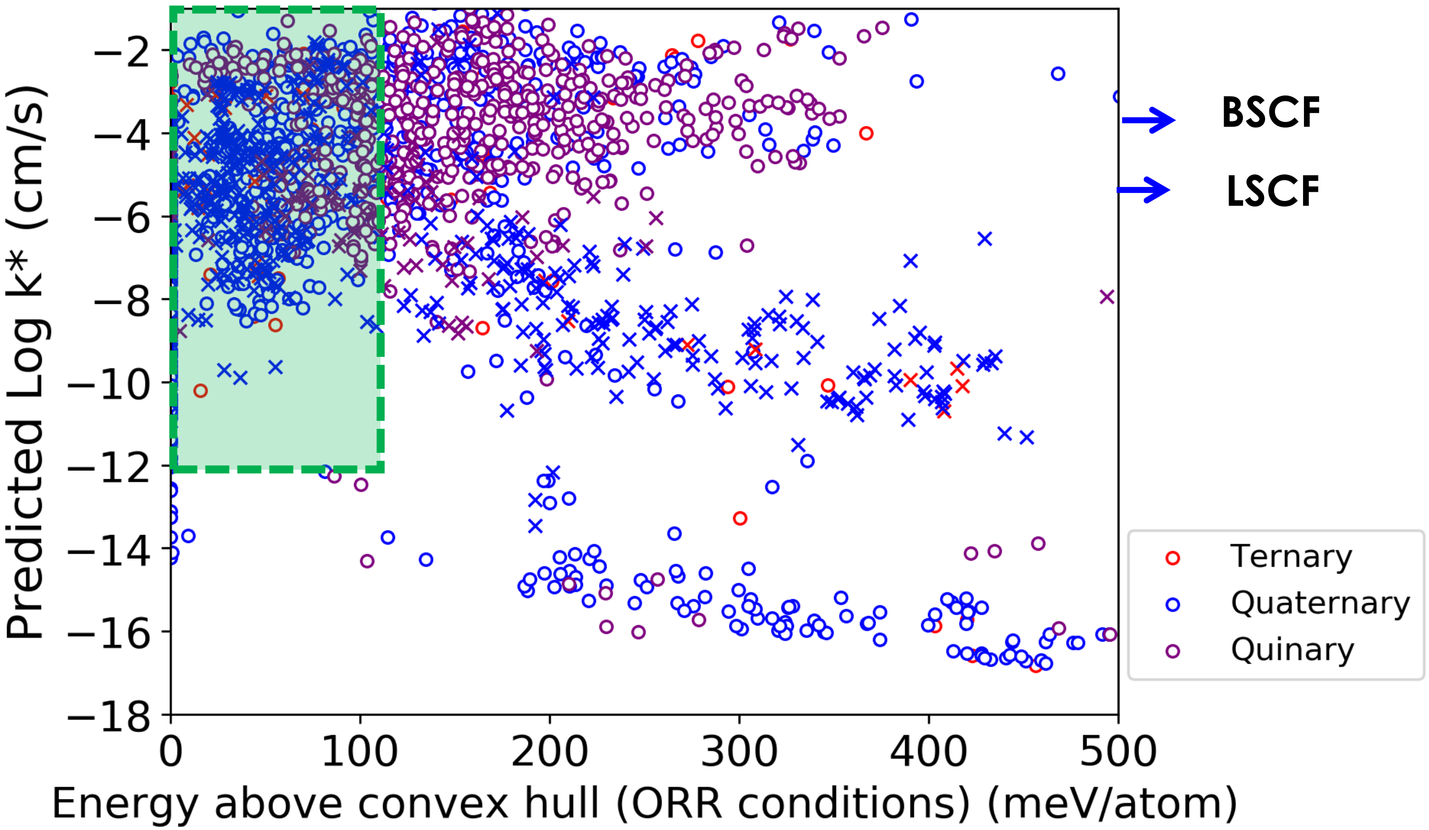
U.S. DEPARTMENT OF ENERGY

Developing materials through DFT

O p-band correlates well with air electrode material properties

ORR surface exchange [1]



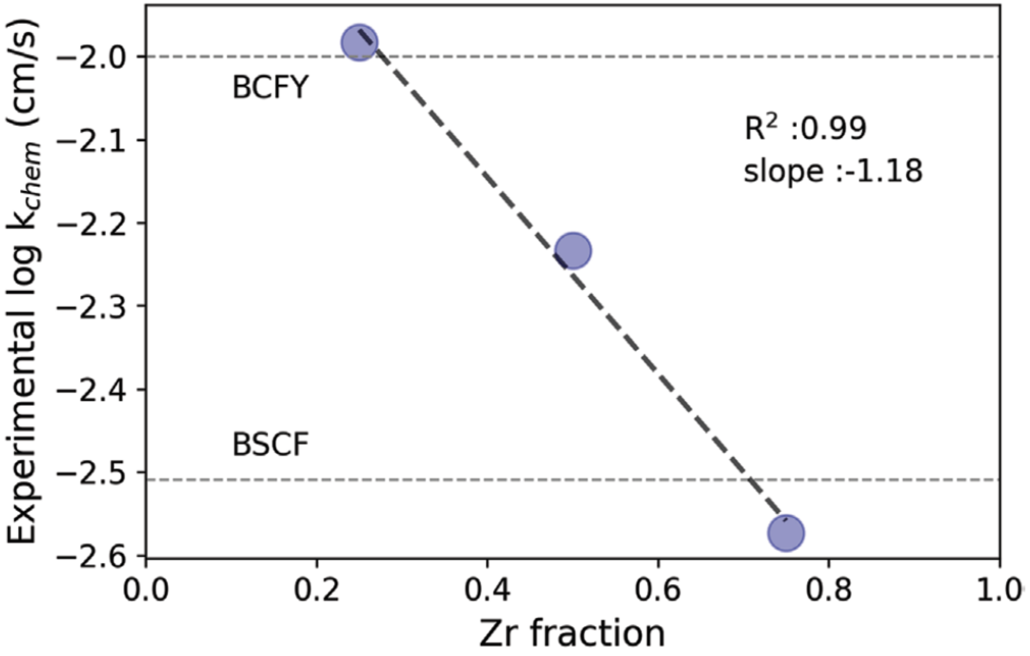


From predicted k* using DFT-calculated O p-band center of >2100 perovskites, NETL examined Ba(Fe, Co, Zr)O_3 (BFCZ) materials

[1] Lee, et al., ***Eng Env Sci*** (2011)
[2] Jacobs, et al., ***Adv. Eng. Mat.*** (2018)
[3] Jacobs, et al., ***Chem. Mat.*** (2019)

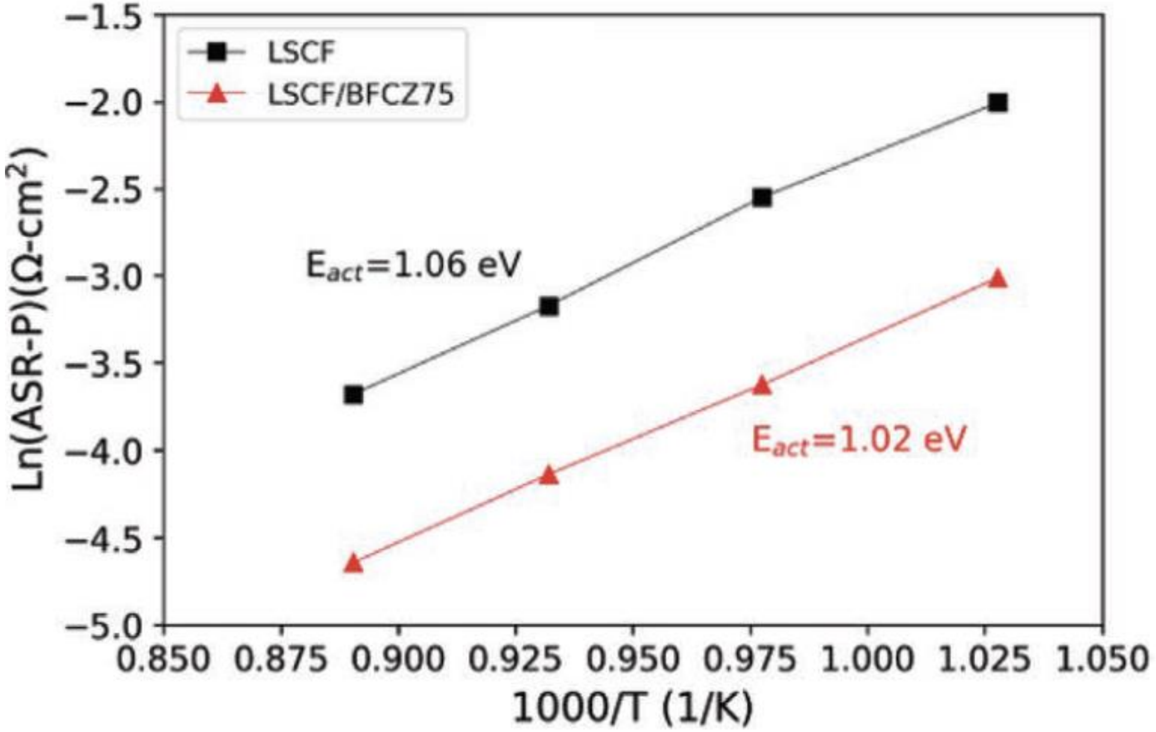
BFCZ (Zr = 25, 50, 75%) Performance

Higher k_{chem}, improved stability, not enough σ_{el}



All BFCZ compositions highly active, on par with BSCF, with only 0.5 log k_{chem} difference over entire Zr range

LSCF/BFCZ75 composite

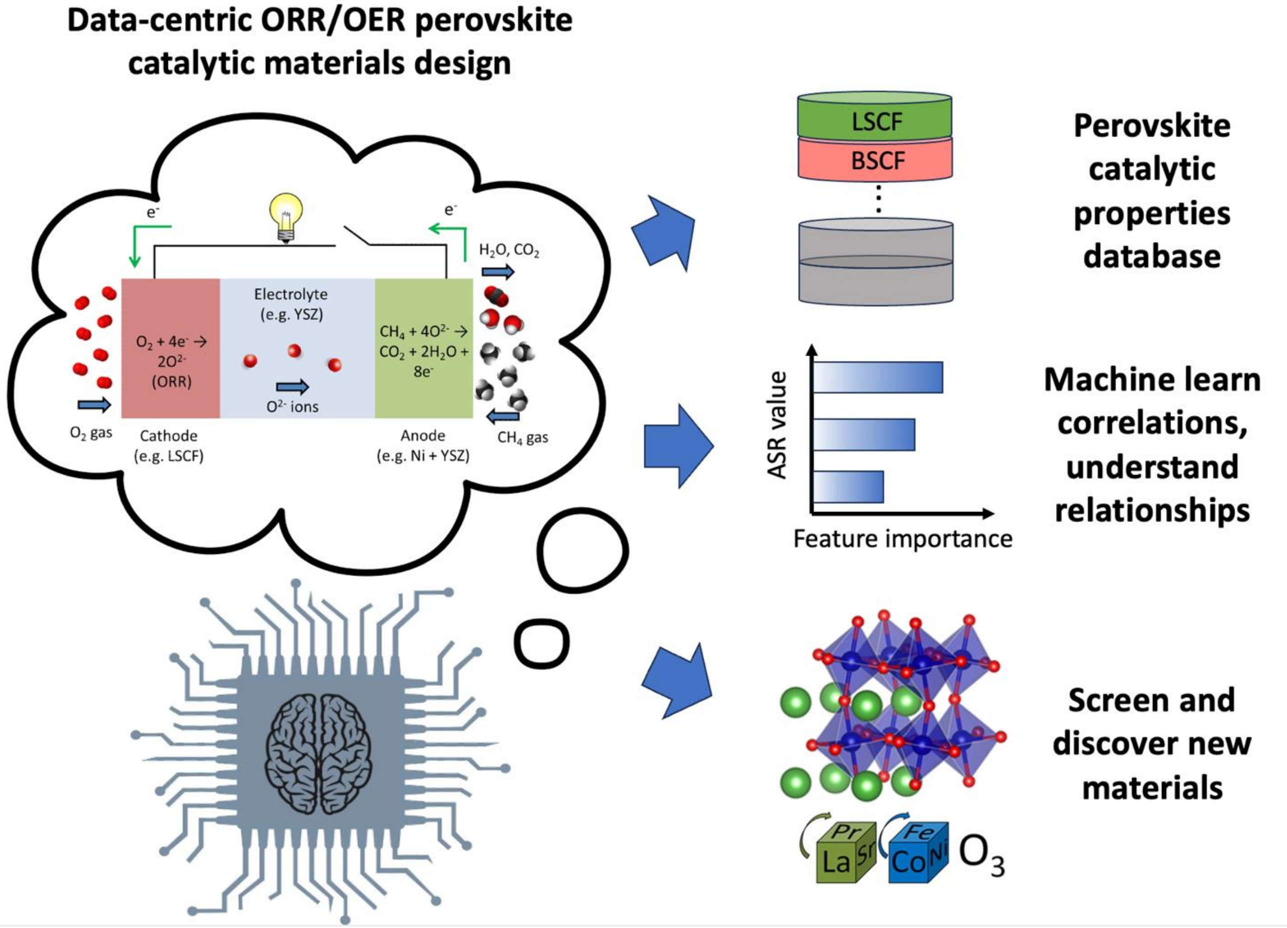


LSCF/BFCZ75 composite shows about 9x reduction in ASR at 800 °C, 65% less performance degradation vs. LSCF

[1] Jacobs, R., et al. Adv. Eng. Mat. (2022)

Machine learning prediction of properties

Using machine learning for faster calculations, larger sampling space



- 749 data points from 313 studies for 299 unique perovskite compositions
- Elemental features calculated using MAST-ML (UW-M) instead of using DFT
- **19 million perovskite oxides** were examined using ML model

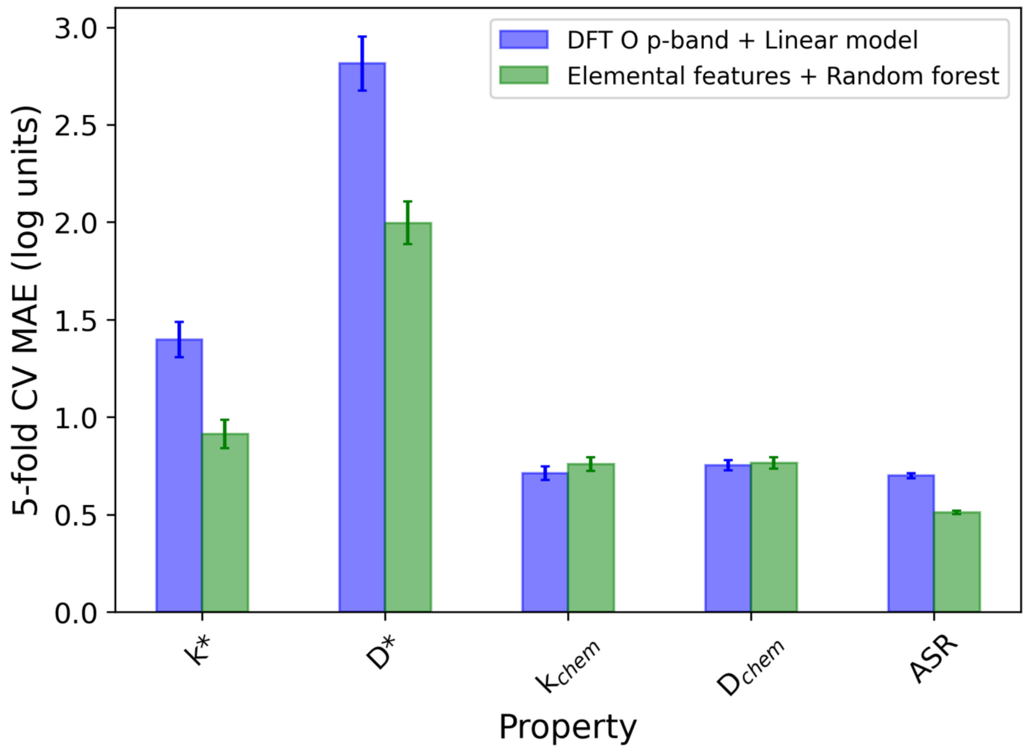
Property	Number of studies examined	Number of measurements extracted	Number of unique materials
k_{chem}	70	98	62
D_{chem}	56	83	58
k*	39	80	48
D*	37	66	42
ASR	235	422	257

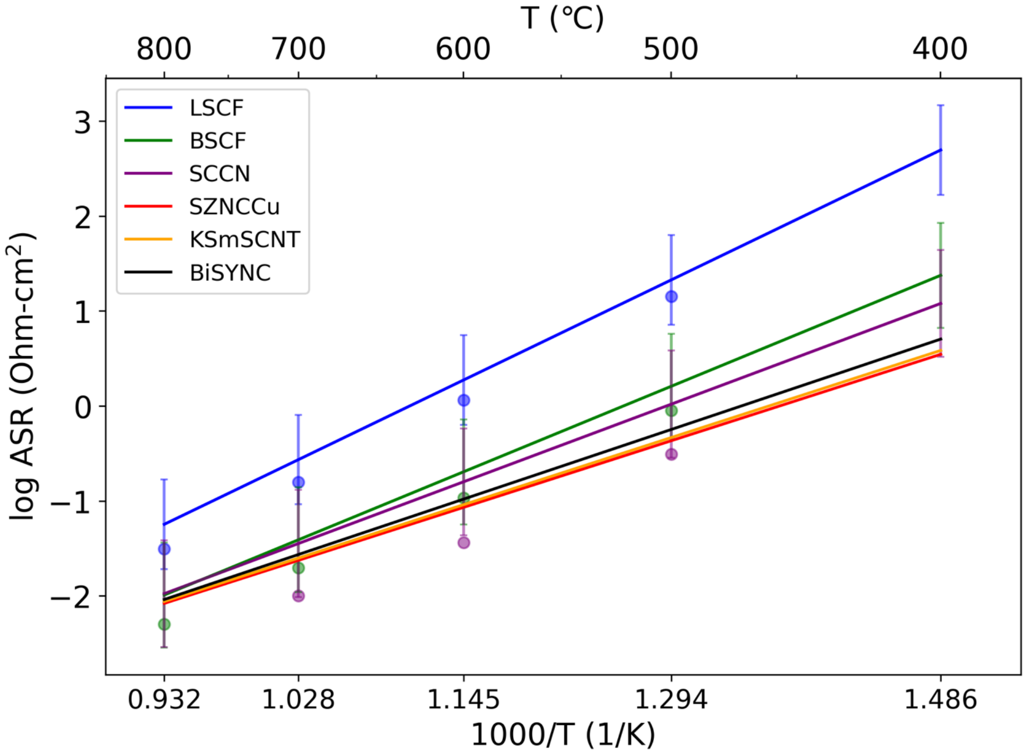
Jacobs, R., et al. Adv. Eng. Mat. ***(2024), just accepted***

Data points discussed: Jacobs, R., et al. arXiv: https://doi.org/10.48550/arXiv.2310.17744 (2023)

Machine learning predicted electrode materials

- Trained machine learning model could predict properties faster and at least as accurately than DFT-based study and could cover a larger space containing traditionally less-explored elements (e.g., K, Bi, Y, Ni, Cu).





Jacobs, R., et al. ***Adv. Energy. Mat***, 2303684 **2024.** *(doi.org/10.1002/aenm.202303684)*
Jacobs, R., et al. ***ACS Applied Energy. Mat***, Accepted, **2024.** *(doi.org/10.1021/acsaem.4c00125)*

Wrap-Up

Wrap Up

NATIONAL ENERGY TECHNOLOGY LABORATORY

Conclusions

- For SOEC systems, reductions in degradation rates and increases in current density could reduce LCOH by $0.50/kg H_2
- Modeling is useful tool for deeper interpretation of performance data, designing more durable electrodes, and providing context to literature results
- Machine learning is useful tool for accelerating electrode/cell development and providing guidance for improving specific cells

How can NETL help you?

- NETL's synthetic microstructure database, real 3D microstructures, and microstructural analysis tools are available to the public
- NETL can collaborate with partners, using partner data and conditions to run performance degradation-related simulations

Recent Output

1. R. Jacobs, J. Liu, H. Abernathy, D. Morgan, "A Critical Assessment of Electronic Structure Descriptors for Predicting Perovskite Catalytic Properties" **ACS Applied Energy Materials** (accepted) 2024.
2. H. Kim, J.H. Mason, H. Abernathy, P. Salvador, "Systematic and Predictive Trends to Chromium Poisoning in Solid Oxide Fuel Cell Cathodes," **Journal of Power Sources** (accepted) 2024.
3. R. Jacobs, J. Liu, H. Abernathy, D. Morgan, "Machine Learning Design of Perovskite Catalytic Properties," **Advanced Energy Materials** 2303684, 2024.
4. Y. Fan, Y. Chen, H. Abernathy, R. Pineault, R. Addies, X. Song, G. Hackett, T. Kalapos, "Enabling durable hydrogen production and preventing the catastrophic delamination in the solid oxide electrolysis cells by infiltrating SrFe2O4-δ solutions into LSM/YSZ -based air electrode**," J Power Sources** 580, 233389, 2023.
5. J.H. Mason, H. Sezer, I.B. Celik, W.K. Epting, H.W. Abernathy, "Fundamental study of gas species transport in the oxygen electrode of solid oxide fuel and electrolysis cells," **Int. J. Hydrogen Energy** 50(b), 1142-1158, 2024..
6. J.H. Duffy, H. Abernathy, K. Brinkman, "Tuning Proton Kinetics in $BaCo_{0.4}Fe_{0.4}Zr_{0.2-X}Y_XO_{3-\delta}$ Triple Ionic-Electronic Conductors via Aliovalent Substitution" Accepted by **Journal of Materials Chemistry A** 2023.
7. T.L. Cheng, Y. Lei, Y. Chen, Y. Fan, H. Abernathy, X. Song, Y.H. Wen, "Oxidation of nickel in solid oxide cells during electrochemical operation: Experimental evidence, theoretical analysis, and an alternative hypothesis on the nickel migration," **Journal of Power Sources** 569, 232991, 2023.
8. X. Fei et al., "Phase-field modeling of crack growth and mitigation in solid oxide cells", **International Journal of Hydrogen Energy** 48, 9845, 2023.
9. T. Yang, et al., "Multiphysics modeling of SOFC performance degradation caused by interface delamination and active layer cracking," **International Journal of Hydrogen Energy** 47(97), 41124-41137, 2022**.**
10. Y.L. Lee, et al., "Defect Thermodynamics and Transport Properties of Proton Conducting Oxide $BaZr_{1-x}Y_xO_{3-\delta}$ (x≤0.1) Guided Based on Density Functional Theory Modeling," **JOM** 74, 4506-4526, 2022**.**
11. 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.
12. 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.
13. T. Hsu, et al., "High performance finite element simulations of infiltrated solid oxide fuel cell cathode microstructures," **Journal of Power Sources** 541, 231652, 2022.
14. R. Jacobs, et al., "Unconventional Highly Active and Stable Oxygen Reduction Catalysts Informed by Computational Design Strategies," **Advanced Energy Materials**, 2201203, 2022.

Acknowledgement

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