Energy & Environmental Research Center (EERC)

SOFC PERFORMANCE AND DURABILITY USING COMMERCIALLY VIABLE COAL-DERIVED SYNGAS AT THE EERC

Zhien Liu

23rd Annual Solid Oxide Fuel Cell Project Review Meeting

October 25, 2022

ACKNOWLEDGMENTS AND DOE DISCLAIMER

Acknowledgments:

- Special thanks to U.S. Department of Energy (DOE) Project Managers Shailesh Vora, Patcharin (Rin) Burke, Joseph Giove III, Dr. Jai-Woh Kim and the entire SOFC program management team.
- This material is based upon work supported by DOE NETL (National Energy Technology Laboratory) under Award Nos. DE-FE0024233-5.1 and DE-FE0031977.

Disclaimer:

PROJECT OBJECTIVES

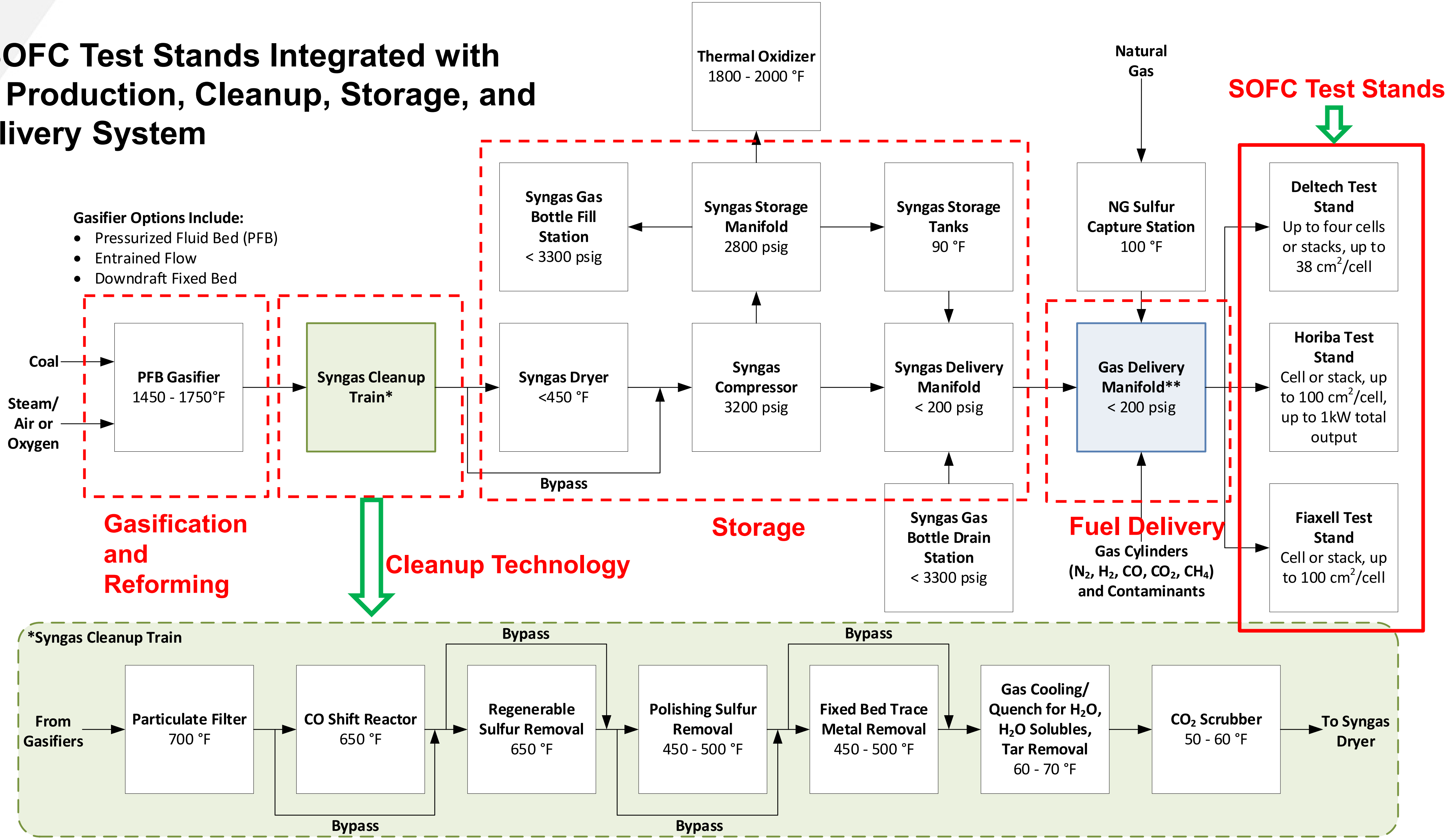
- Project 1: Solid Oxide Fuel Cell Development and Demonstration Test Center
- Award No.: DE-FE0024233-5.1
- DOE/NETL Project Manager: Dr. Patcharin (Rin) Burke
- Objectives:
  - Establish a SOFC Development and Demonstration Test Center at the EERC.
  - Provide fuel storage and delivery system to meet the need to evaluate SOFCs performance and long-term durability.
  - Build and validate SOFC test stands and data acquisition system.
  - Perform component- and system-level SOFC testing using variety of fuels.

PROJECT OBJECTIVES

- Project 2: Coal Syngas Cleanup for Commercially Viable SOFC Performance
- Award No. DE-FE0031977
- DOE/NETL Project Managers: Drs. Jai-Woh Kim and Joseph Giove III
- Objectives:
  - Design, configure, optimize, and demonstrate long-term operational viability of a syngas cleanup train.
  - Produce coal syngas sufficiently clean as a fuel for SOFC operation achieving performance equivalent to that of natural gas fuel.
  - Perform thermodynamic simulation and postmortem analysis to understand coal trace contaminants interaction with anode materials
  - Create multiphysics model to simulate SOFC performance and degradation with coal trace contaminants
  - Conduct a techno-economic analysis (TEA) of the integrated syngas production system.
- Team: National Energy Technology Laboratory (NETL), Worcester Polytechnic Institute (WPI), Ohio Fuel Cell Coalition (FCC), and Special Power Sources (SPS)

FUEL PRODUCTION AND CLEANUP TECHNOLOGY – FLOWCHART

EERC SOFC Test Stands Integrated with Syngas Production, Cleanup, Storage, and Fuel Delivery System



EERC GASIFICATION CAPABILITY – THREE GASIFIERS

- **Produce syngas with low level of trace contaminants to meet SOFC operation.**

All Gasifiers

- Wide range of feedstocks: coal, biomass, other solid or liquid feedstocks
- Bench-scale warm-gas cleanup train
- Gas-sweetening absorption system
  - Additional gas cleanup and acid gas removal
- Produce up to 120 scfh of syngas
- Syngas storage and delivery system
- Wide range of H_2/CO ratio
- Low contaminant level

Pressurized Fluidized-Bed Gasification (PFB)

Downdraft Fixed-Bed Gasification (DFB)

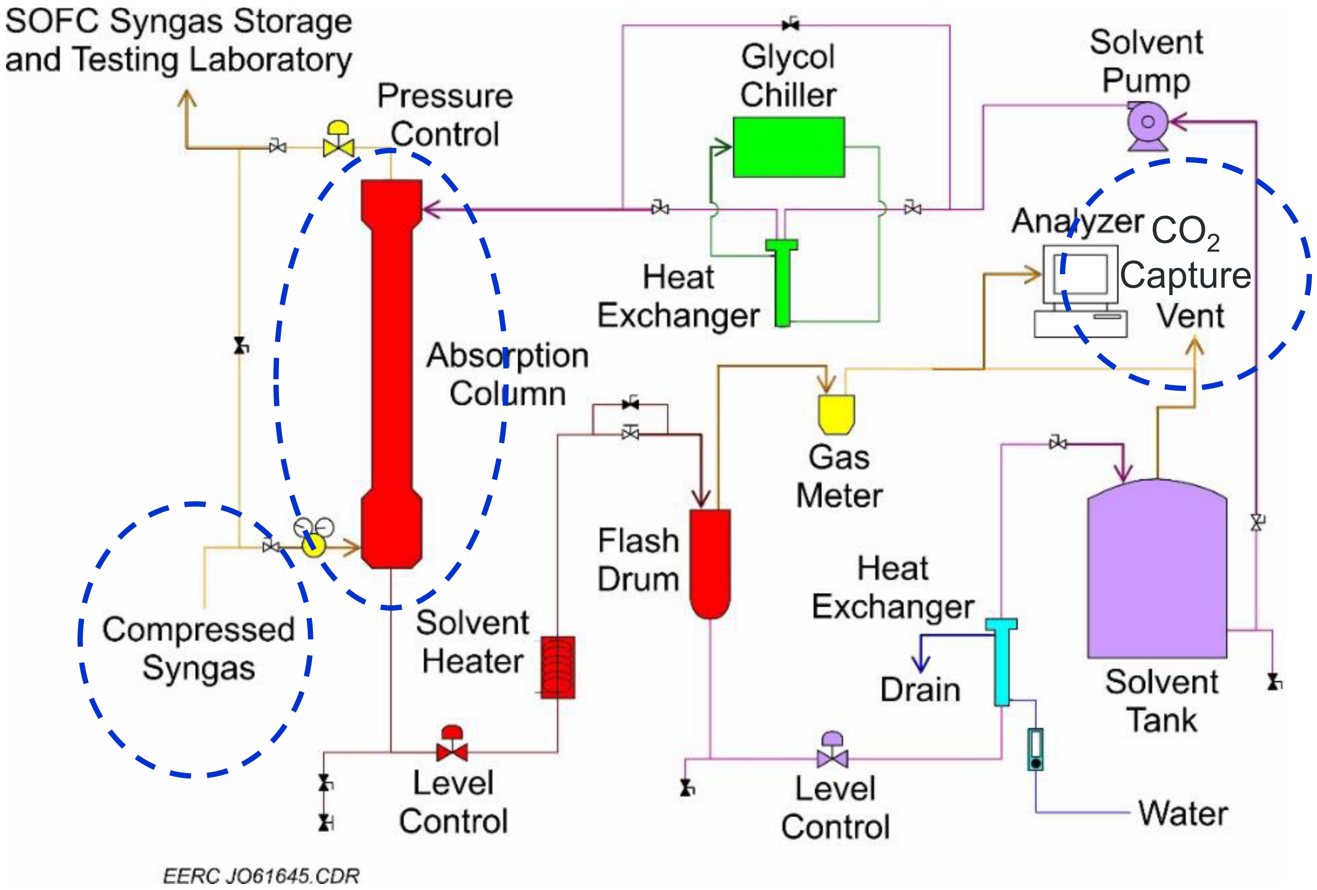
Entrained-Flow Gasification (EFG)

EERC GASIFICATION CAPABILITY – CARBON CAPTURE

- **Produce syngas to operate SOFC system with low CO_2 emission**

- 12-day PFB gasification run to generate and store coal-derived syngas
  - Produced approximately **17,000 scf/2000 psi** syngas
  - Stored syngas to be utilized for SOFC operation and testing

Syngas Gas Component	Mole Percent
Hydrogen	59.5
Carbon Dioxide	0.9
Ethane	0.0
Argon	0.4
Nitrogen	32.5
Methane	5.2
Carbon Monoxide	1.7



CO_2 Capture Sub-System

SYNGAS STORAGE AND DELIVERY (SSD)

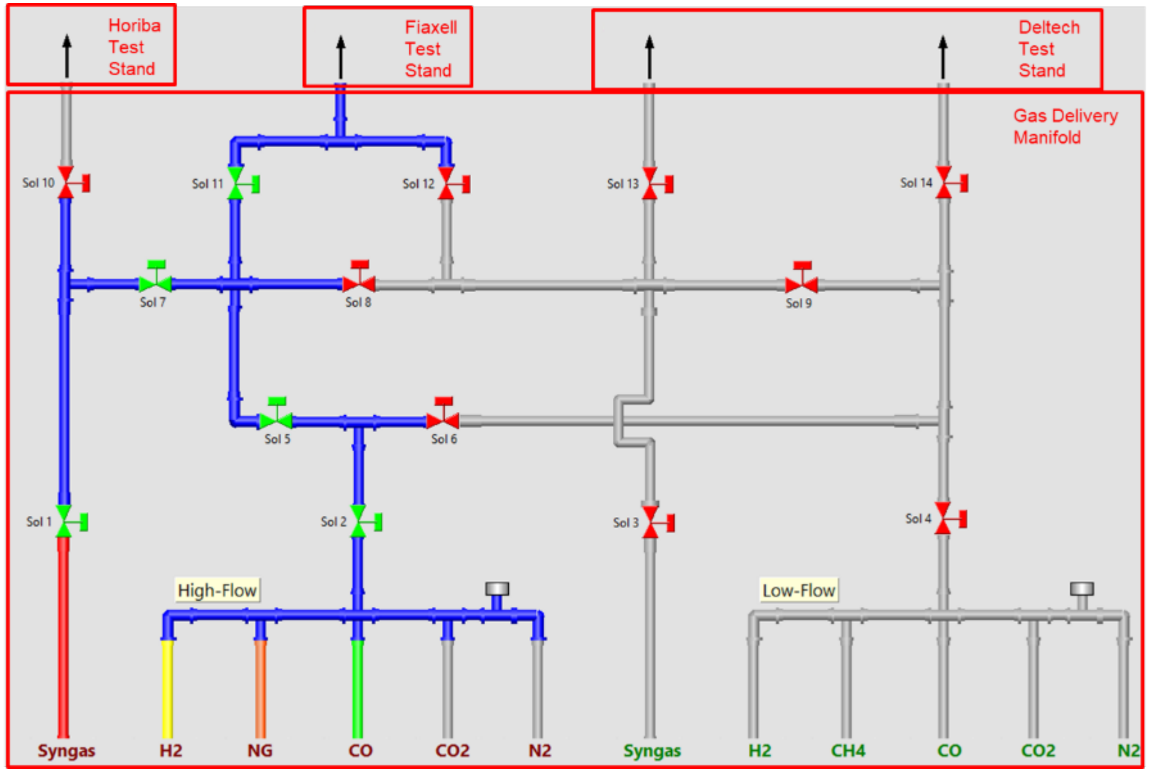
All three SOFC test stands can be operated simultaneously with up to four different fuels.

Storage Tank Capacity:

- 20,900 scf at 2600 psi

Fuel Options:

- Syngas from EERC gasifier (coal, biomass, waste, blend)
- Natural gas, renewable natural gas, ammonia
- Bottled gas (single or blends of H_2, CO, CH_4, CO_2, N_2, other)
- Added contaminants



Fuel Delivery System

HIGH QUALITY COAL SYNGAS PRODUCED AT THE EERC

- EERC syngas production and cleanup system capable of producing ultraclean syngas.
  - Tailored syngas quality possible.
- Can be used as fuel to directly feed to SOFC stacks/systems for long-term operation.
  - Completed 1000-hr durability test with lower degradation rate.

EERC

Syngas Gas Contaminant	Concentration
Antimony (Sb)	< 1 ppbv
Cadmium (Cd)	< 0.5 ppbv
Arsine (AsH_3)	< 5 ppbv
Hydrogen Sulfide (H_2S)	< 5 ppbv
Phosphine (PH_3)	< 0.5 ppbv
Selenium (Se)	< 0.5 ppbv
Hydrochloric Acid (HCl)	< 100 ppbv
Silicon (Si)	< 1 ppbv
Zinc (Zn)	2.5 ppbv
Benzene (C_6H_6)	< 15 ppmv
Xylene (C_8H_{10})	< 10 ppmv

Industrial Gasifier

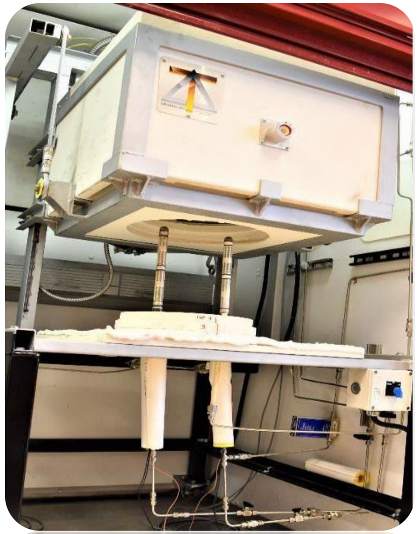
Syngas Gas Contaminant	Concentration[1)]
Antimony (Sb)	25 ppbv
Cadmium (Cd)	N/A
Arsine (AsH_3)	150–580 ppbv
Hydrogen Sulfide (H_2S)	~500 ppbv
Phosphine (PH_3)	1900 ppbv
Selenium (Se)	150 ppbv
Hydrochloric Acid (HCl)	< 1000 ppbv
Zinc (Zn)	9000 ppbv
Chromium (Cr)	25 ppbv
Mercury (Hg)	25 ppbv

1) Eastman Chemical Company's system at Kingsport.

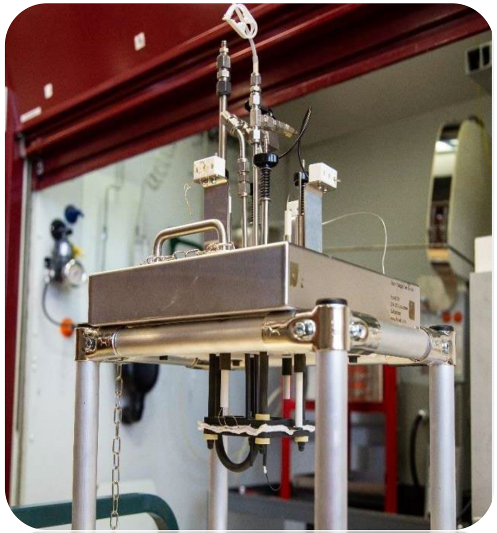
SOFC DEVELOPMENT AND DEMONSTRATION TEST CENTER AT THE EERC

SOFC Testing System Installation and Commissioning

1-kW Stack Test Station



Multicell Test Station



Fiaxell Test Station

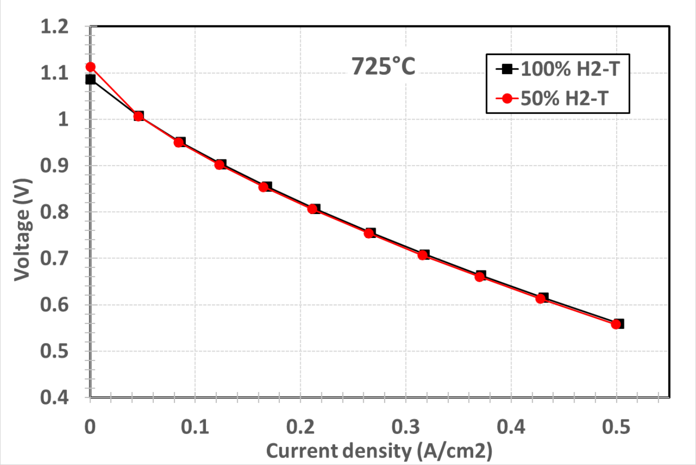
Electronic Load and EIS

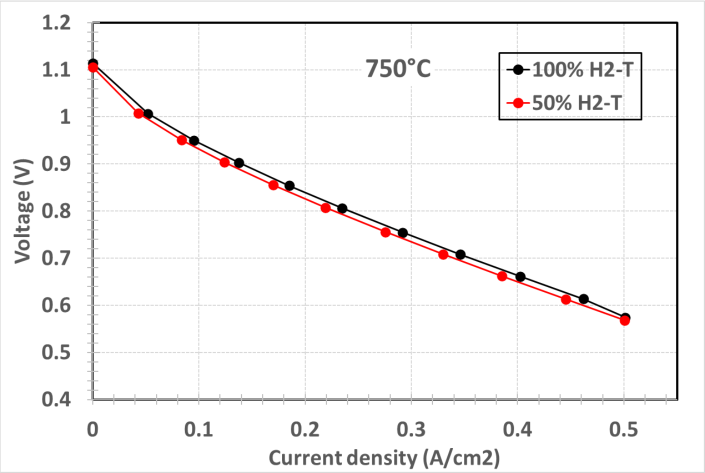
	1-kW Stack Test Station	Multicell Test Station	Fiaxell Test Station	Button Cell Test Stand
Test Rig Configuration	Single cell or stack	Multiple single cells or stack	Single cell or short stack	Button cell
Cell Type	Planar	Planar or tubular	Planar	Planar
Fuel Type	Any fuel from gas storage and bottle gas	Any fuel from gas storage and bottle gas	Any fuel from gas storage and bottle gas	H_2, natural gas

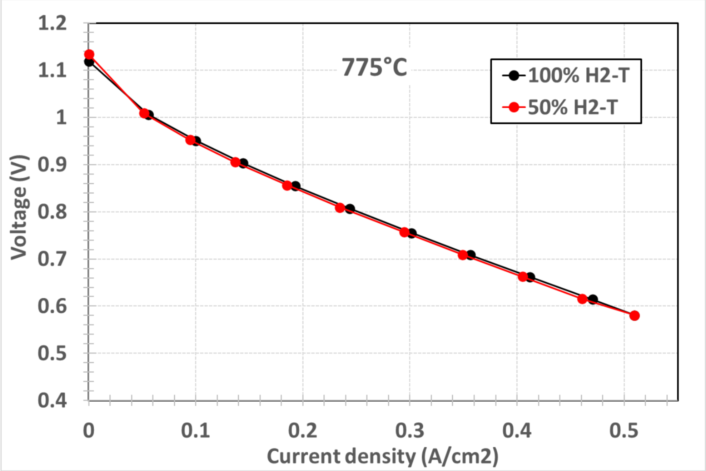
SOFC PERFORMANCE VS. TEMPERATURE AND FUEL COMPOSITIONS

Commercially available SOFC cells show comparable performance in syngas gas and H_2 fuel.

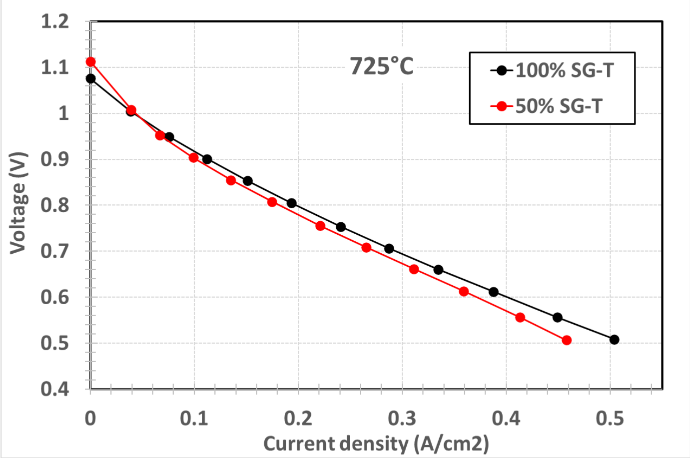
SPS Cell (Gen-1)

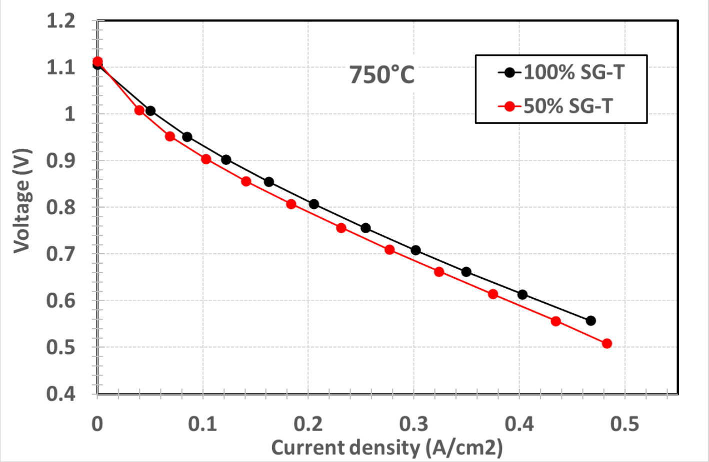


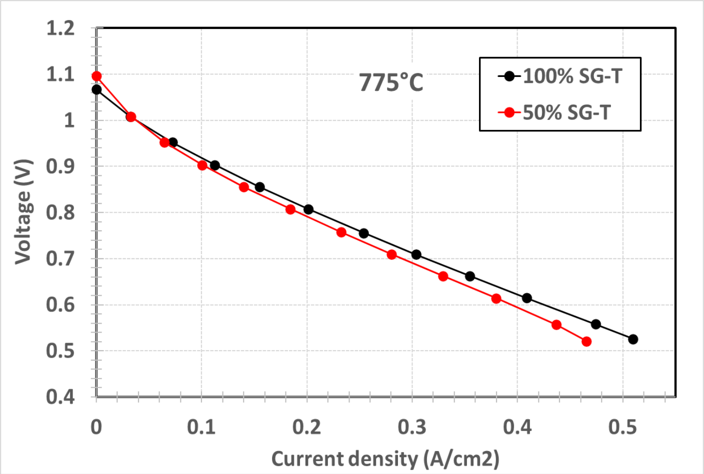




H_2 fuel





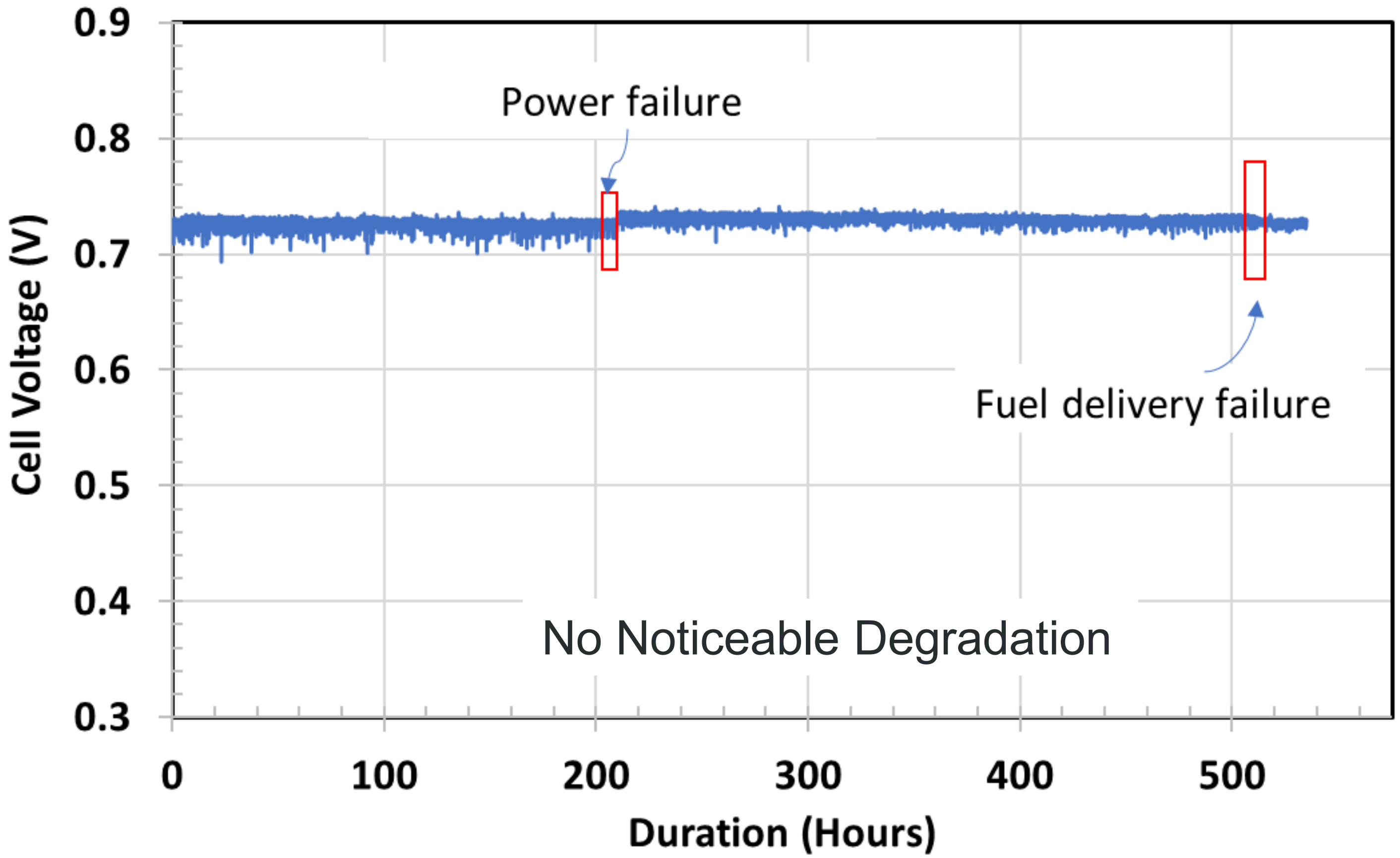


Coal-Derived Syngas

SOFC LONG-TERM DURABILITY TEST – SPS TUBULAR CELL

Cell performance is stable under natural gas during more than 500 hours duration.

- Baseline durability test
- Testing conditions
  - Deodorized natural gas
  - 750°C
  - 230 mA/cm^2
  - FU: 75%
  - Methane reformer
- Two events at ~200 and ~500 hours, respectively, resulted in fuel shutoff
- Stable performance during more than 500 hours testing



Long-Term Durability Test Using Natural Gas Fuel

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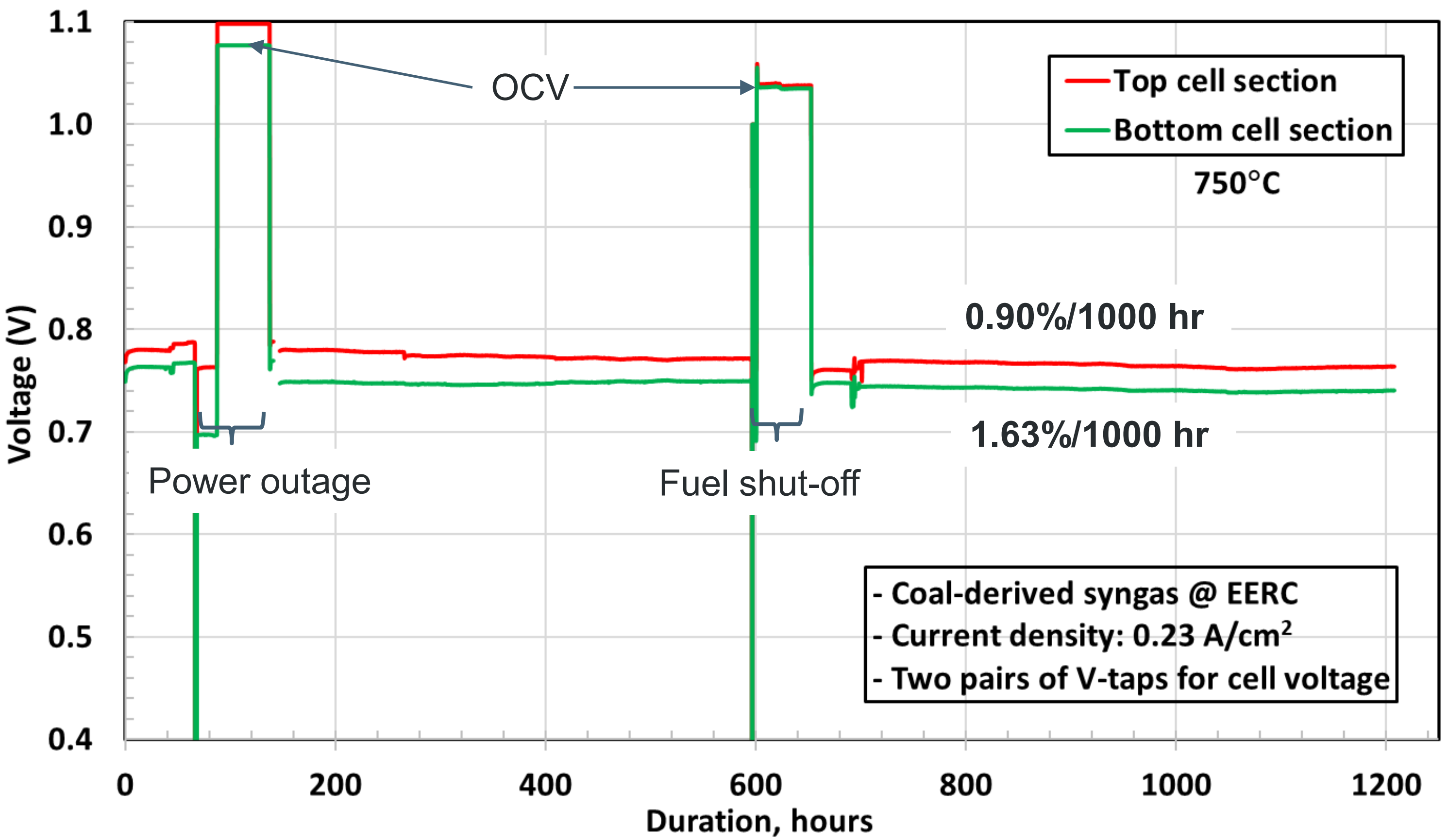
SOFC LONG-TERM DURABILITY TEST USING COAL-DERIVED SYNGAS

Syngas Composition: 59.5% H_2, 5.2% CH_4, 1.7% CO, 32.5% N_2, 0.9% CO_2, 0.4% Ar

- Operating conditions:
  - 750°C, 230 mA/cm²
  - 75% of FU
  - 1100 hr with load
- Two pairs of V-taps to monitor voltage of top and bottom cell section, respectively
- Two events occurred
  - Power outage
  - Fuel shutoff
- Voltage degradation rate:
  - 0.90%/1000 hr for top cell
  - 1.63%/1000 hr for bottom cell



Long-Term Durability Test under Constant Current at 750°C.

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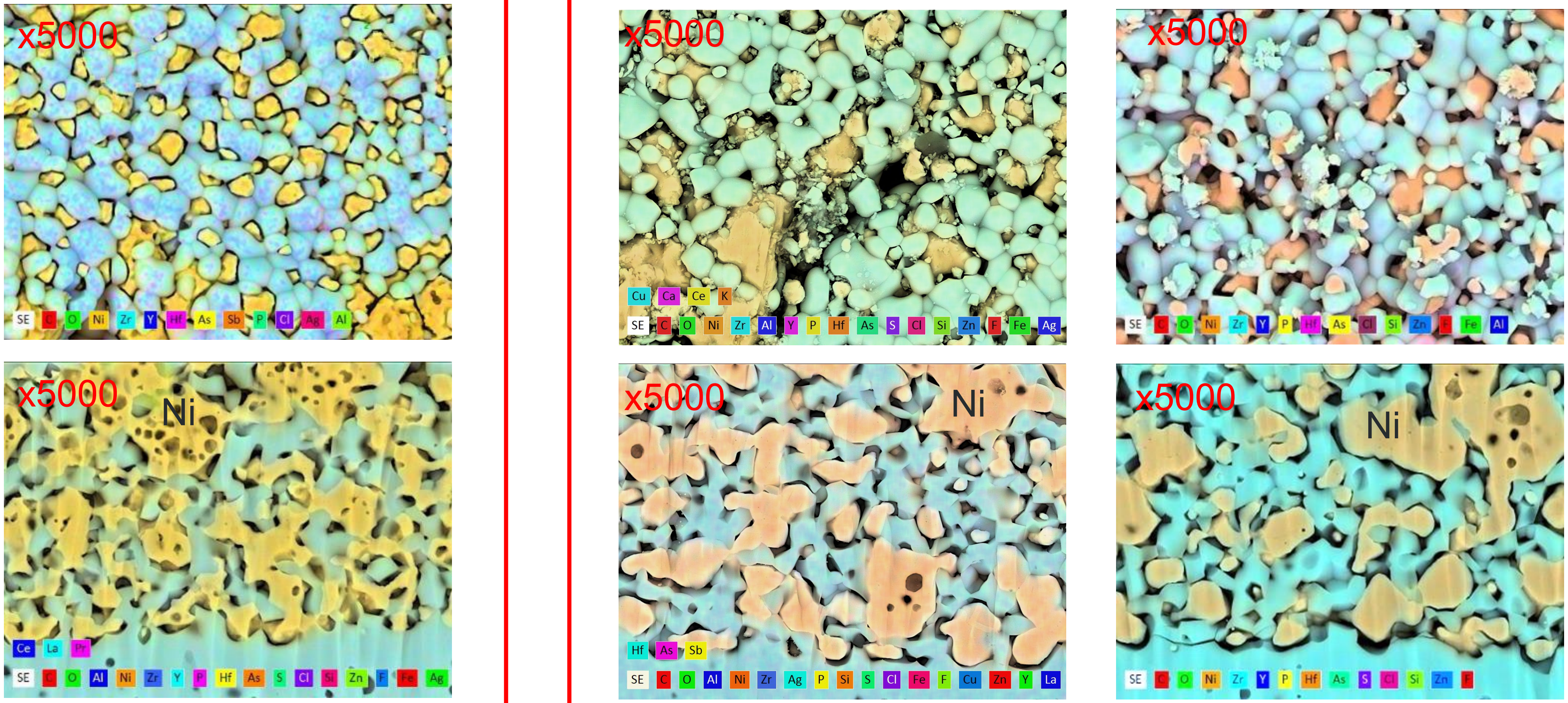
POSTMORTEM ANALYSIS – COAL SYNGAS DURABILITY TEST

- Postmortem analysis indicates possible Si and Al contaminants on anode support surface.

Anode Surface

Anode Cross-Section



As-Fired Cell

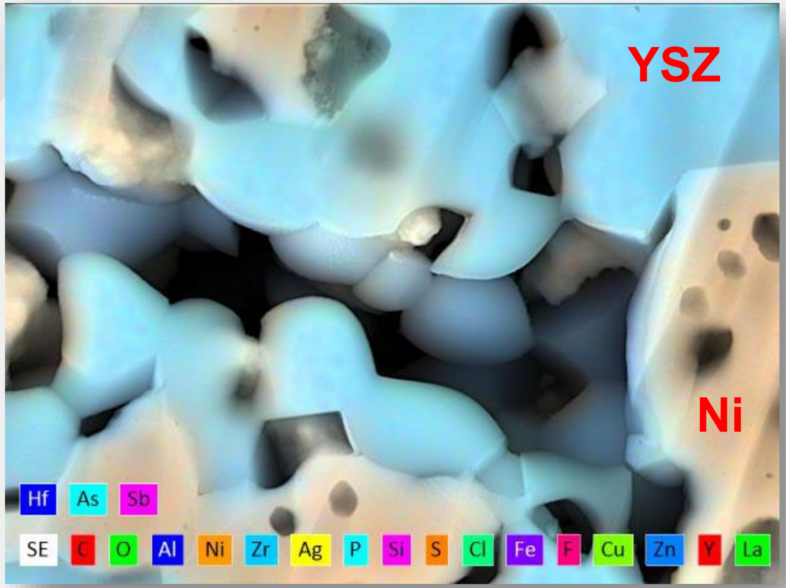
Fuel Inlet

Fuel Outlet

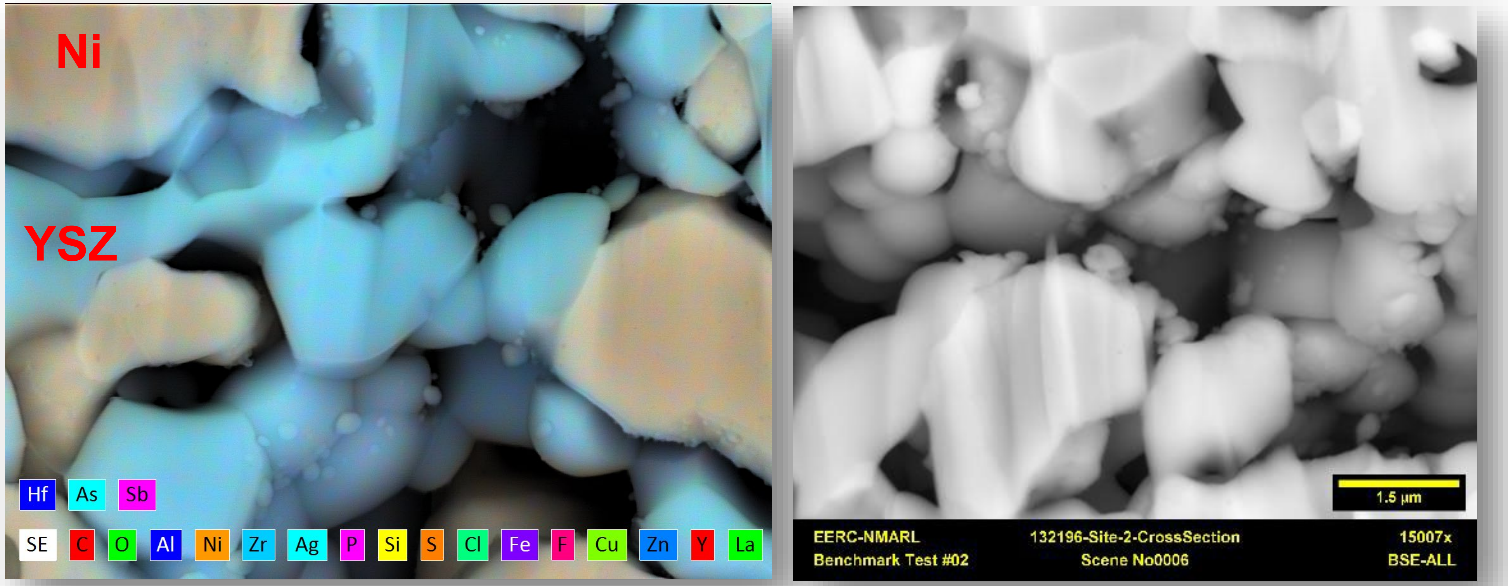
1000-hour Duration in Coal-Derived Syngas

POSTMORTEM ANALYSIS – COAL SYNGAS DURABILITY TEST

Nanophase Formation on Anode YSZ Surface after 1000-hour Duration in Coal Syngas



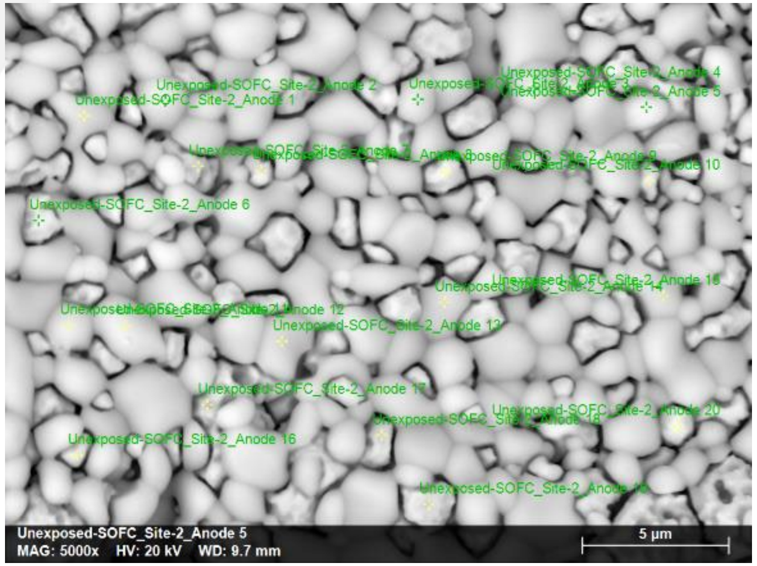
Anode of As-Fired Cell, ×15,000



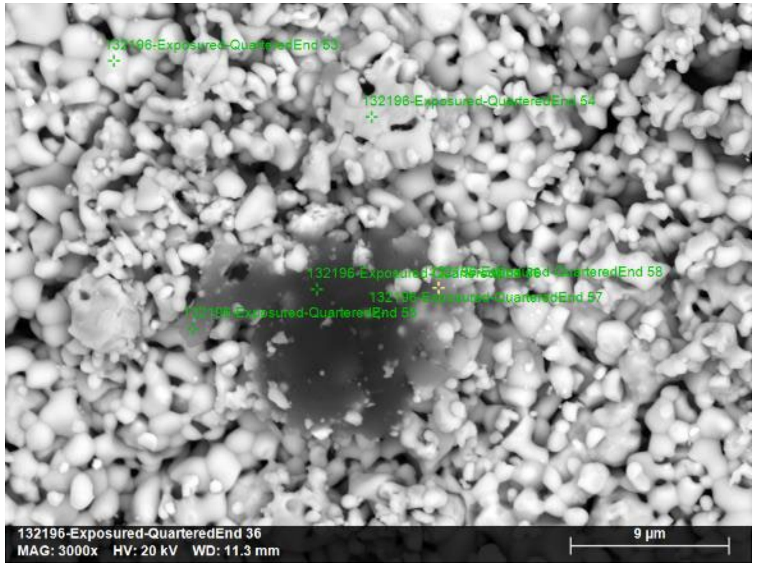
1000-hour Duration in Coal-Derived Syngas, ×15,000

POSTMORTEM ANALYSIS – COAL SYNGAS DURABILITY TEST

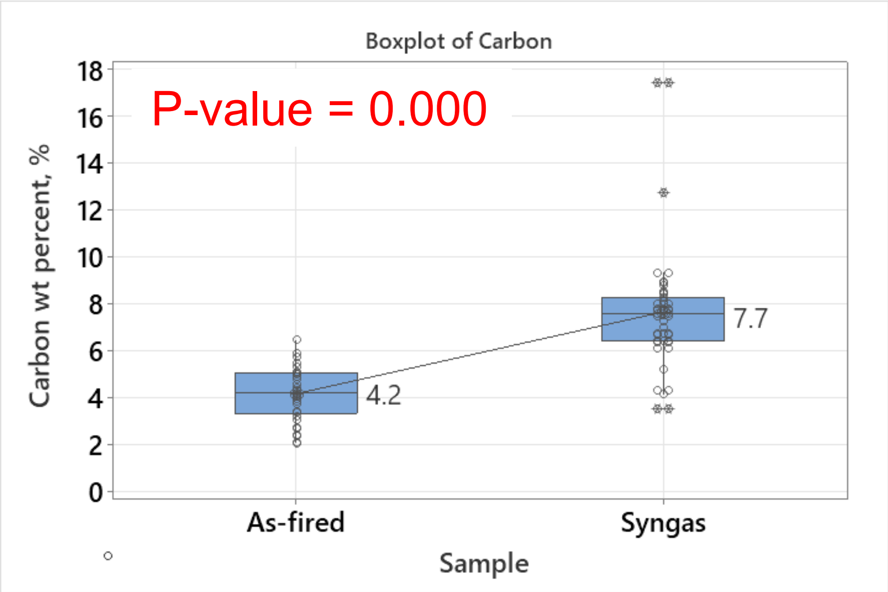
- ❑ SEM EDS analysis of anode materials did not show existence of coal syngas contaminants.
- ❑ Statistical EDS data analysis indicated noticeable carbon increase on anode support surface.



As-Fired Cell



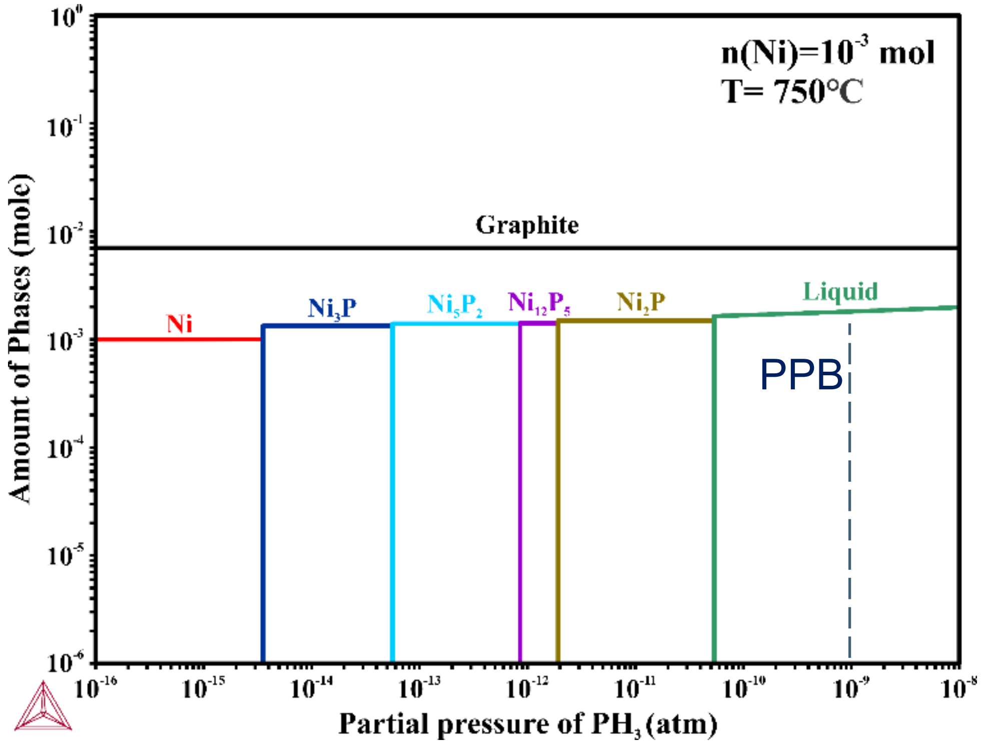
Syngas – 1000-hr Durability



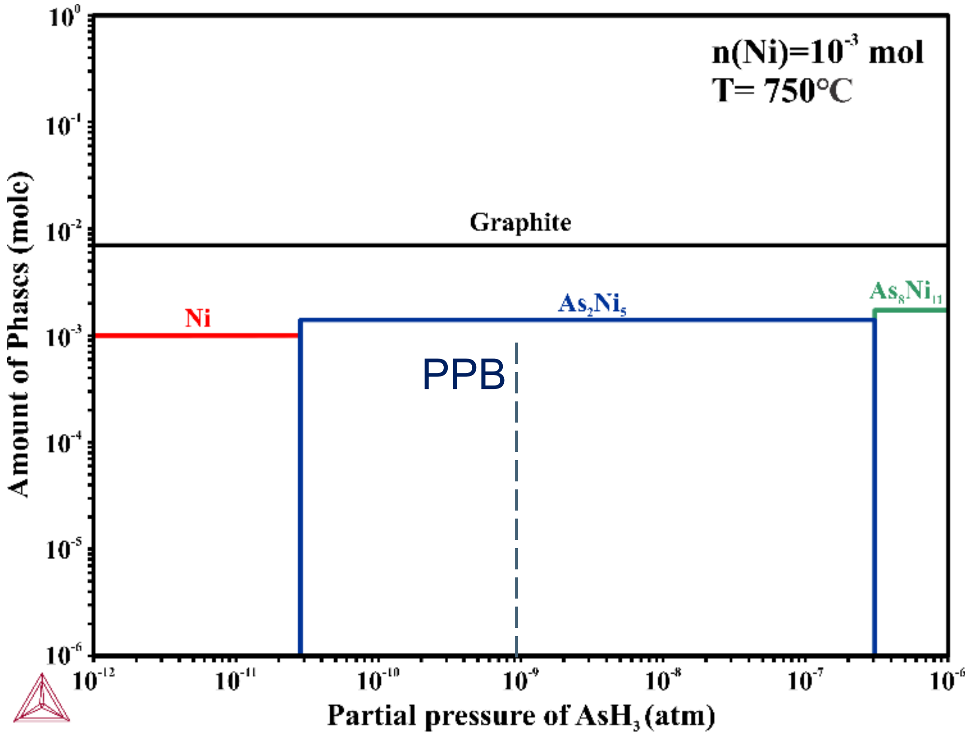
Statistical Data Analysis of Carbon on Anode Surface

THERMODYNAMIC SIMULATION OF COAL SYNGAS TRACE CONTAMINANTS INTERACTIONS WITH ANODE MATERIALS

- Phosphine and Arsine tend to interact with Ni at SOFC operating conditions to form Ni compound to cover Ni metal surface at ppb, ppm range.
- Interaction diagrams of S, Sb, Se, and Cl with Ni are on-going.



Nickel Phosphide Formation vs. Phosphine Partial Pressure



Nickel Arsenide Formation vs. Arsine Partial Pressure

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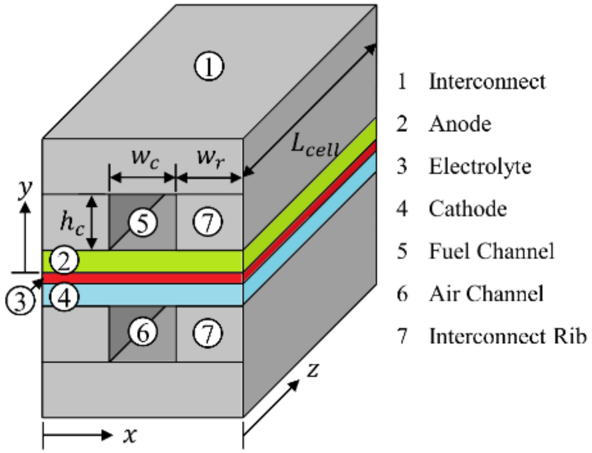
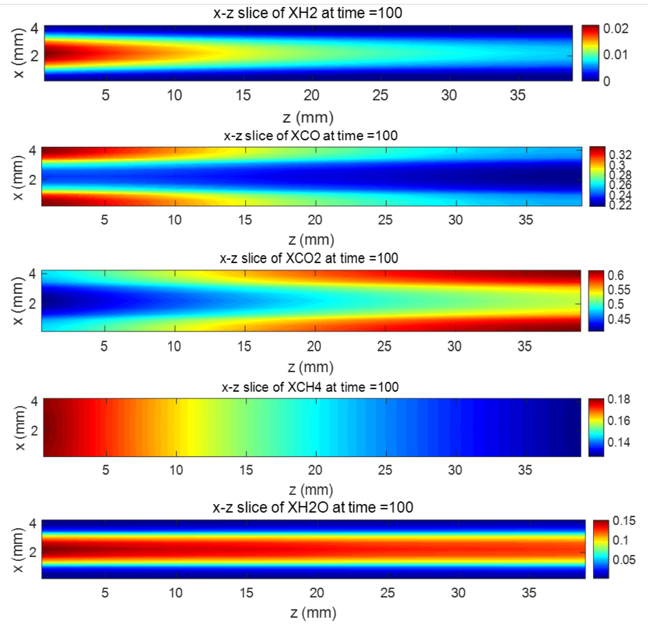
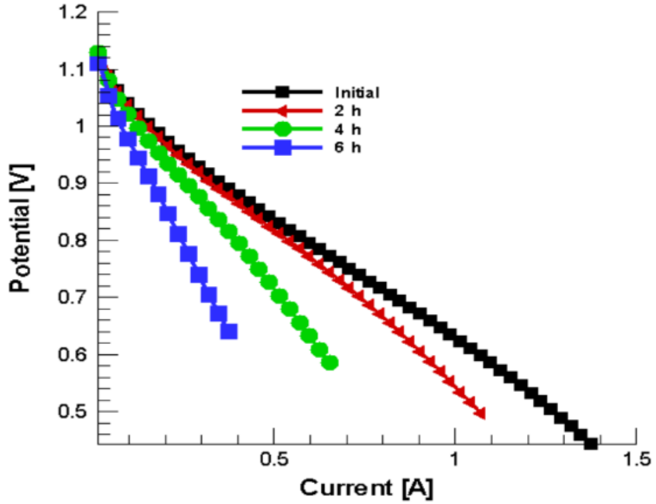
SOFC MULTIPHYSICS PERFORMANCE SIMULATION

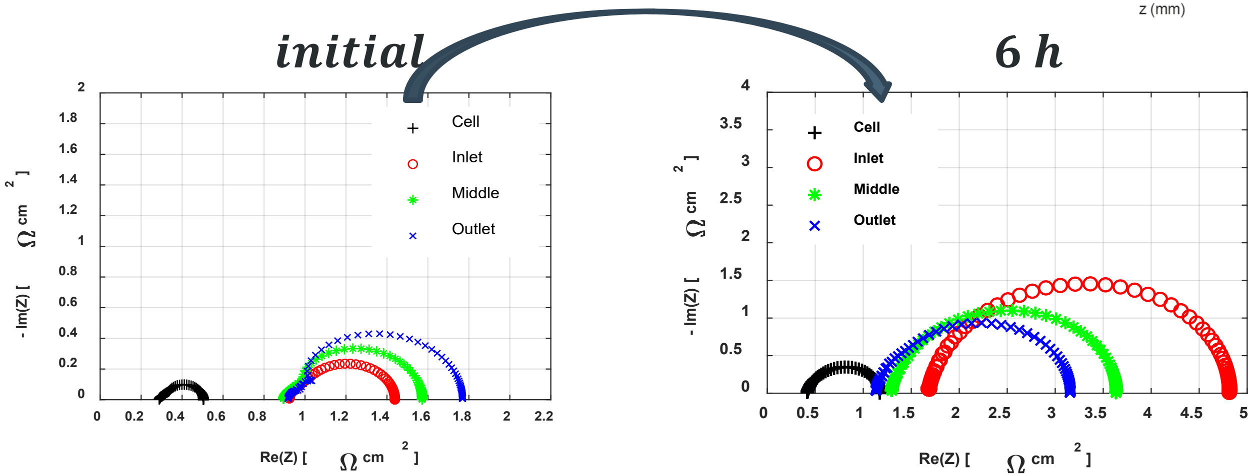
3D Planar Cell Model Was Modified for Tubular Cell Geometry

- Capable of coal syngas studies:
  - Includes methane reforming and water-gas shift reactions
- Currently coded degradation modes:
  - Ni coarsening
  - PH_3, AsH_3, H_2S, H_2Se contamination









Electrochemical performance simulation using 3D planar cell model*

*H. Sezer et al., International Journal of Hydrogen Energy, 46(9), pp 6803-16, 2021

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SOFC DEGRADATION MODEL WITH SINGLE AND MULTI-COMPONENT TRACE CONTAMINANTS

- Poisoned phase covers Ni surface, blocks H_2 adsorption sites, and changes local properties.

$$\begin{cases} X + Ni \underset{k_{b,X}}{\overset{k_{f,X}}{\rightleftharpoons}} Ni - X \\ Y + Ni \underset{k_{b,Y}}{\overset{k_{f,Y}}{\rightleftharpoons}} Ni - Y \\ H_2 + 2Ni \underset{k_{b,\mathrm{H}}}{\overset{k_{f,\mathrm{H}}}{\rightleftharpoons}} 2(Ni - H) \end{cases} \Rightarrow \begin{cases} \textit{porosity} \\ \textit{electrical conductivity} \\ \textit{exchange current density} \end{cases}$$

- **Simple Multiplication**

$$i_{0,\mathrm{H}_2} = i_{0,ref}(1-\theta_X^m)^n\left(1-\theta_Y^k\right)^l$$

- **Harmonic Average**

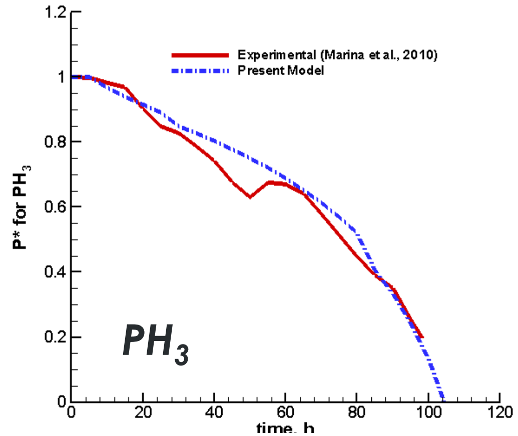
$$i_{0,\mathrm{H}_2} = i_{0,ref}\left[\frac{(\theta_X+\theta_Y)(1-\theta_X^m)^n\left(1-\theta_Y^k\right)^l}{\theta_X\left(1-\theta_Y^k\right)^l+\theta_Y\left(1-\theta_Y^k\right)^l}\right]$$

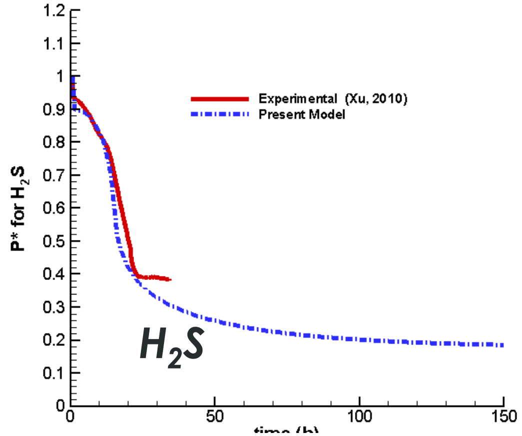
- **Weighted Average of Powers**

$$m^* = \frac{m\theta_X+k\theta_Y}{\theta_X+\theta_Y},\ n^* = \frac{n\theta_X+l\theta_Y}{\theta_X+\theta_Y},\ \theta^* = \theta_X+\theta_Y$$

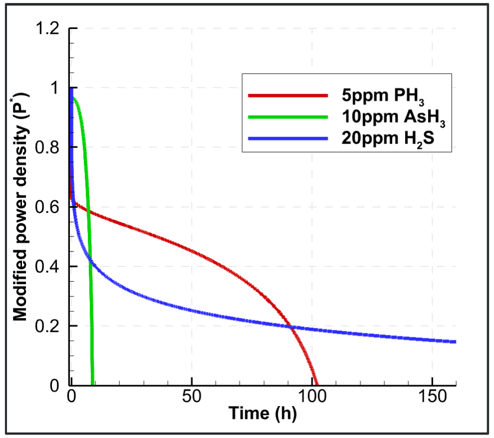
$$i_{0,\mathrm{H}_2} = i_{0,ref}\left(1-\theta^{*m*}\right)^{n*}$$

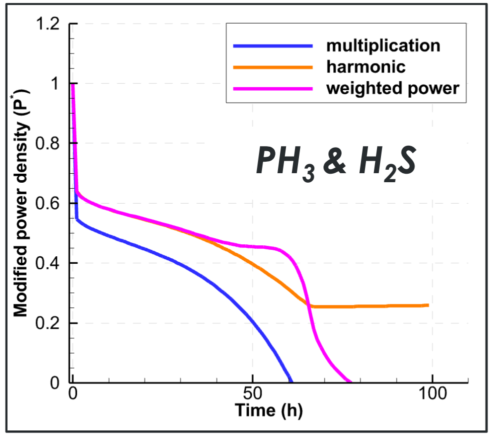
1-D model for single component simulation*





*Fatma N. Cayan, *A degradation model for solid oxide fuel cell anodes due to impurities in coal syngas*, PHD Dissertation, West Virginia University, 2010.

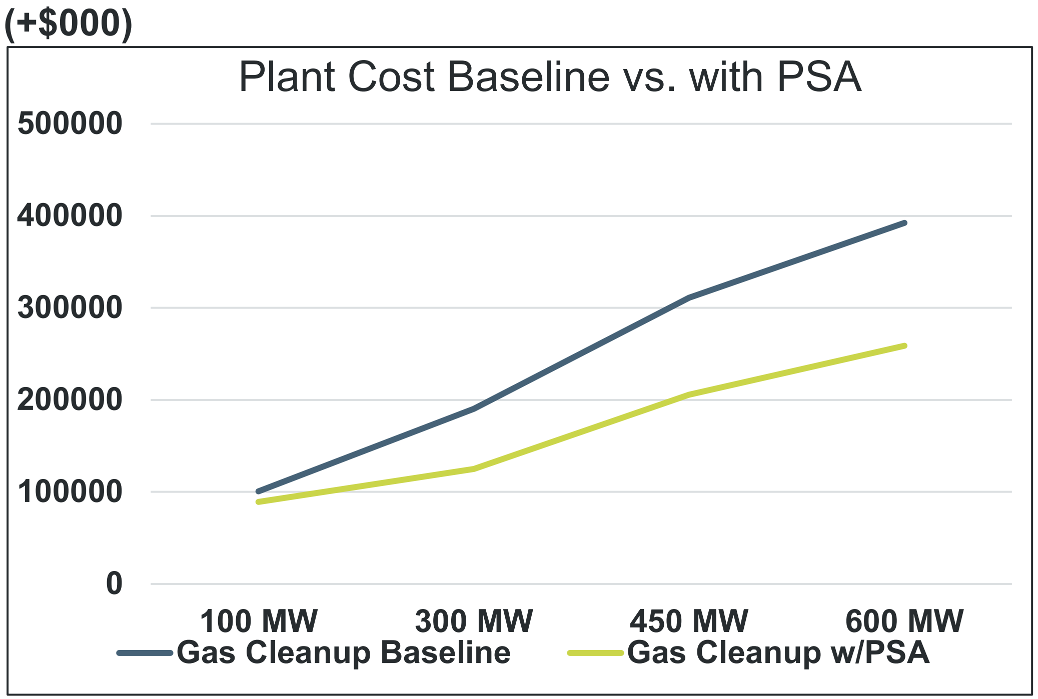


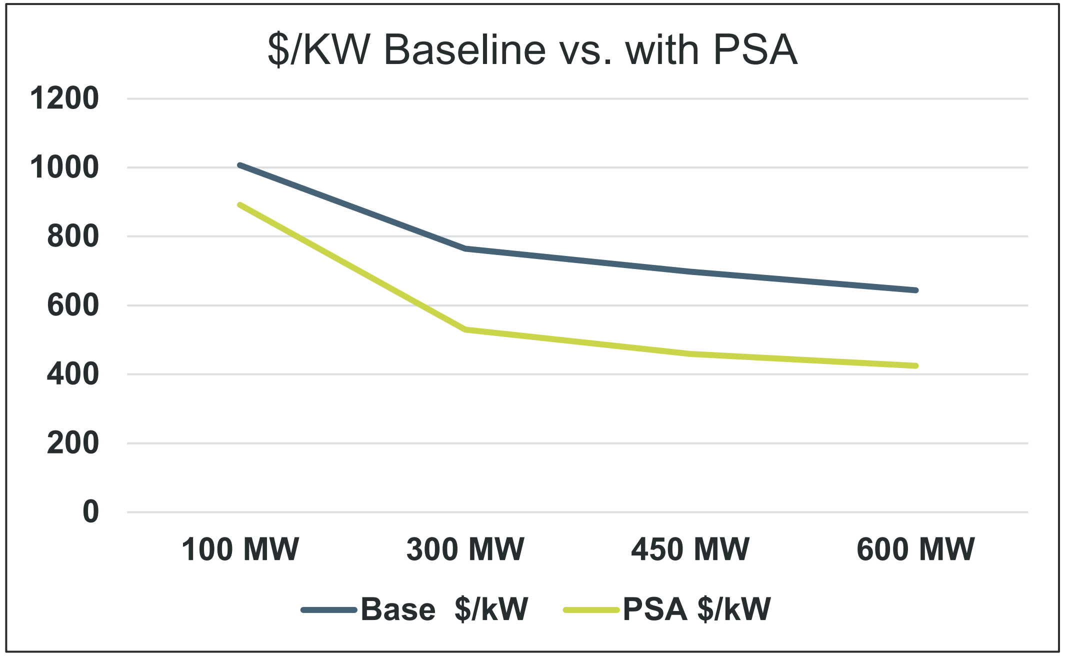


3-D model for single & multi-component simulation

PRELIMINARY TECHNO-ECONOMIC ANALYSIS (TEA) OF COAL SYNGAS CLEANUP TECHNOLOGY (SCT)

- Preliminary analysis was performed based on previous DOE report by WorleyParsons as baseline.[1]
- Analyzed pressure swing adsorption (PSA) technology and cost in DOE report by Air Products.[2]
- Syngas cleanup is scalable to plant output requirements (600-450-300-100 MW).
- PSA provides potential savings (~30% reduction) for SCT.
- CO_2 capture adds significant investment and operational expenses.





1) "Updated Costs (June 2011 Basis) for Selected Bituminous Baseline Cases," DOE/NETL-341/082312 report, WorleyParsons & Booz Allen Hamilton.
2) "Advanced Acid Gas Separation Technology for Clean Power and Syngas Applications," DOE/NETL report (DE-0013363), Air Products and Chemicals.

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SUMMARY

DE-FE0024233-5.1: SOFC Development and Demonstration Test Center

- Designed/acquired and installed three SOFC testing stands
- Completed control and electrochemical data acquisition system to meet SOFC testing needs
- Designed and installed syngas storage and fuel delivery system
- Tested SOFCs using variety of fuels and verified SOFC testing systems

DE-FE0031977: Coal Syngas Cleanup for Commercially Viable SOFC Performance

- Completed 12-day gasification run and produced ~17,000 scf/2000 psi syngas
- Performed extensive syngas characterization showing low level of trace contaminants
- Completed initial TEA of coal syngas cleanup
- Tested commercially available SOFCs using natural gas and coal-derived syngas, meeting degradation target

NEXT STEPS

Understand Further Syngas Contaminant Interaction with Anode Materials and Effect on SOFC Degradation

- Thermodynamic simulation of trace contaminant interaction with anode materials
- Multiphysics model to simulate performance degradation with syngas contaminants
- Syngas trace contaminant tests for model verification and syngas cleanup simplification

Continue Long-Term Durability Test Using Coal Syngas, and other fuels of interest

- Generate long-term durability database
- Understand SOFC degradation mechanism using alternative fuels

Initiate Innovative SOFC Materials/Technology Development Targeting Zero-Carbon Emission

- Materials optimization
- Establish SOFC development capability
- Test low-temperature SOFC cells

Chad Wocken
701.777.5273 (phone)
701.777.5181 (fax)
cwocken@undeerc.org

Zhien Liu
701.777.5476 (phone)
701.777.5181 (fax)
zliu@undeerc.org

Energy & Environmental Research Center
University of North Dakota
15 North 23rd Street, Stop 9018
Grand Forks, ND 58202-9018

www.undeerc.org
701.777.5000 (phone)
701.777.5181 (fax)

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