Enabling Solid Oxide Fuel Cells and Electrolyzers for Integrated Energy Systems

Project No. FWP-1022460

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Integrated Energy Systems

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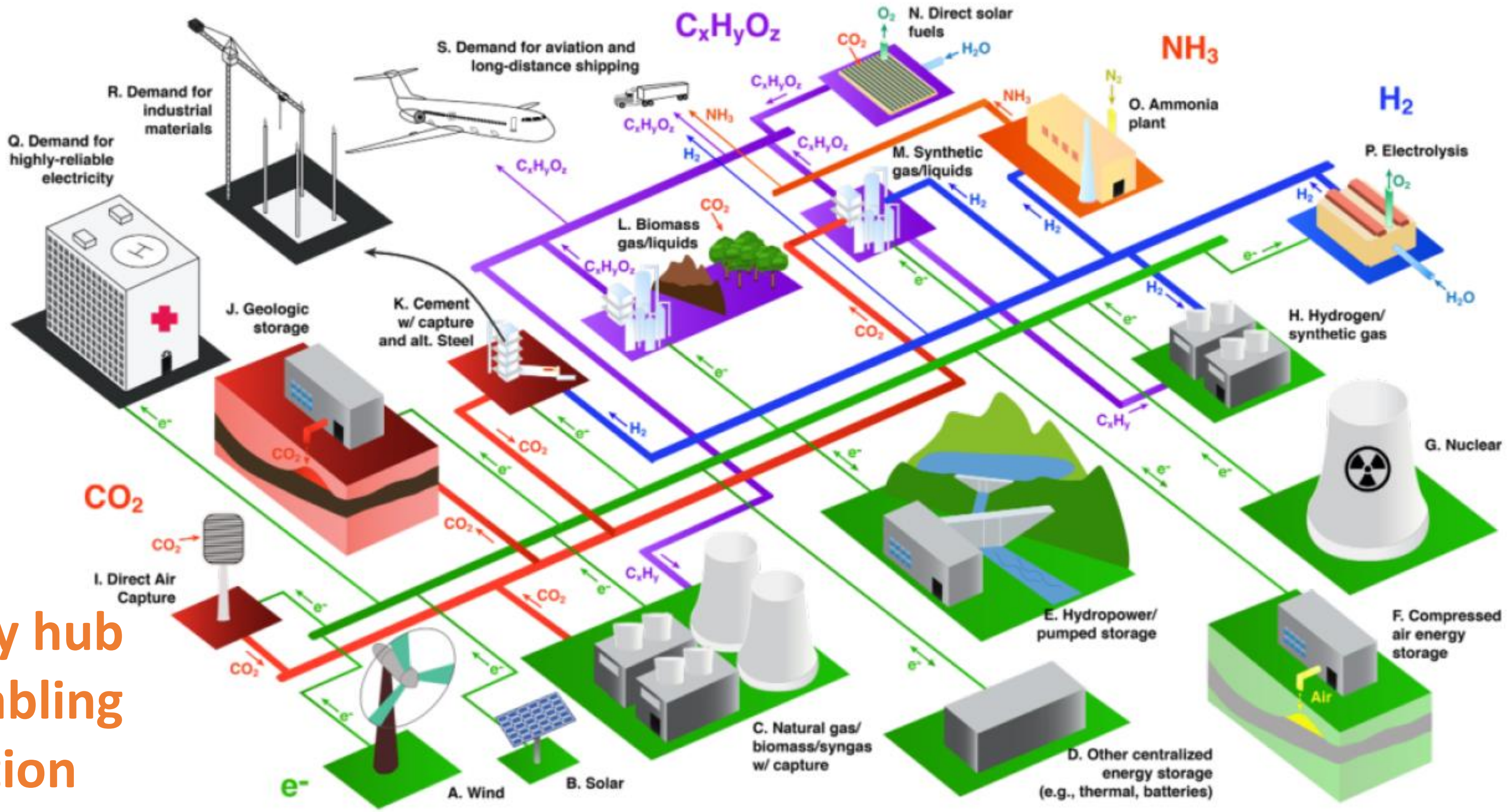
- Multicomponent
  - Fossil
  - Nuclear
  - Renewable
  - Storage
- Integrated
  - Hybrids
  - Carbon Capture
  - Energy Storage
- Dynamic
  - non-dispatchable assets
  - dispatchable assets
- **Fossil generation - resiliency hub for nation's power grid, enabling variable renewable generation**



- We need to develop fossil energy technologies and controls that are able to fit into this paradigm!

Why Integrated Energy Systems?

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Flexibility – Resilience - Emissions

- **CCUS essential in future IES**
  - **75% Reduction in CO2/MWh possible before CCUS**
- **Efficiency Critical**
  - **Lowers net CO2/MWh – reduces carbon pollution by eliminating emissions**
  - **Reduces the size of CCUS system required to achieve Net Zero – substantial cost reduction**
- **Dynamic operability - key to lower tons of CO_2/MWh**

We need hybrid systems that can perform efficiently at low load, be able to provide grid services, and not deteriorate over a bunch of load cycles.

This project supports FECM goals to develop secure, affordable, and reliable FE technologies for the future and aligns with the performance targets for SOFCs articulated in the most recent FE roadmap.

Technical Approach

Target Budget: $2,450,000

Task Structure

Task	Name	Budget (k)
2	Systems Analysis	$100
3	Impact of Grid Dynamics on Hybrid SOFC	$243
5	Solid State Electrochemical Degradation Modeling	$788
6	Design and Optimization of HCC Systems	$845
Z	NETL-RIC Shared Research Costs	$474

Systems Analysis

- **Primary Objective: Analytically evaluate hybridized carbon conversion system configurations that incorporate SOFC/SOEC.**
- The system that demonstrates the best potential as identified in previous analyses will be subject to a thorough techno-economic analysis.

Design/Optimization of Hybrid Systems

- **Primary Objective: Use IDEAS* platform to evaluate and strengthen value proposition for integrated energy systems that leverage hybrid carbon conversion technologies that produce electricity and/or hydrogen**
- Identify targets for cost reduction and performance improvement
- Generate information required to guide R&D program priorities over the next few years

Grid Impact on Hybrid SOFC System

- **Primary Objective: Characterize operability and develop integration and control strategies to achieve the flexibility and resilience that SOFC-HCC systems must meet to be fully** compatible with a dynamic power grid
- Develop an integrated multi-lab cyber-physical research platform to accelerate development of future SOFC-HCC systems

Solid State Electrochem Degradation

- **Primary Objective: Apply knowledge of cell degradation to a wide range of operating conditions and hybridized configurations relevant to commercial systems, including both power and fuel production operation modes**
- Models will be directly applied to expanded system level and optimization analyses, providing a complete picture from cell-level to system-level operation.

*IDAES: Institute for the Design of Advanced Energy Systems framework

Task 2: Systems Analysis

Screening TEA of Down Selected SOFC Hybrid Carbon Conversion Concept

Rationale:

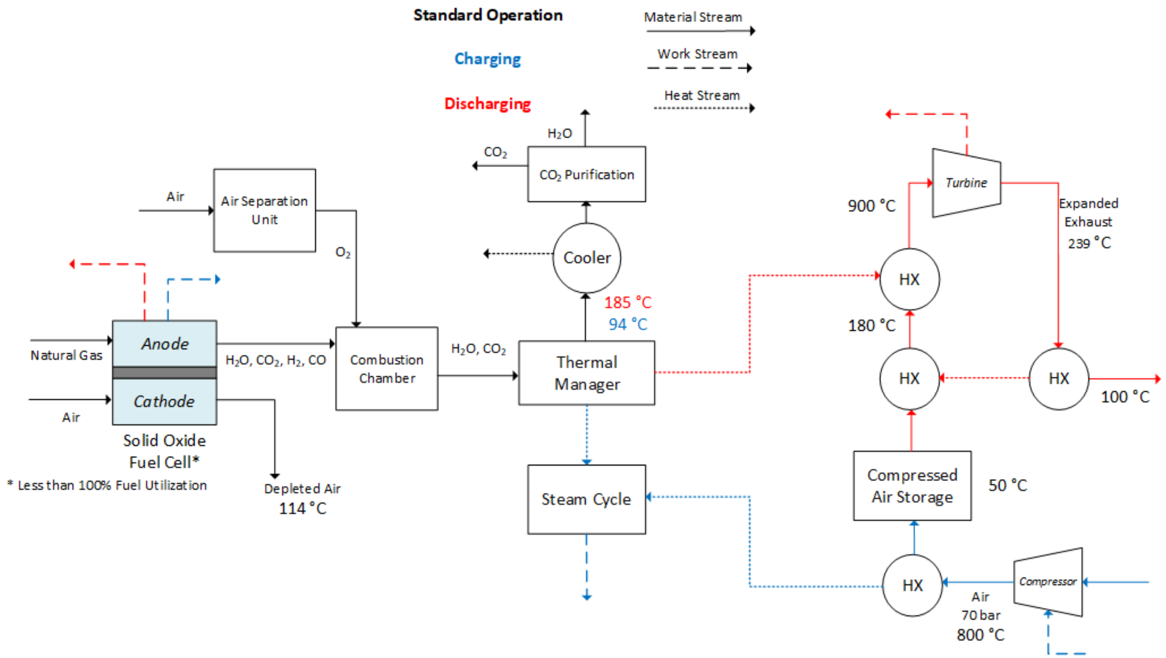
- Perform a screening TEA of a select hybrid carbon conversion concept to provide more detailed merits and demerits of the system

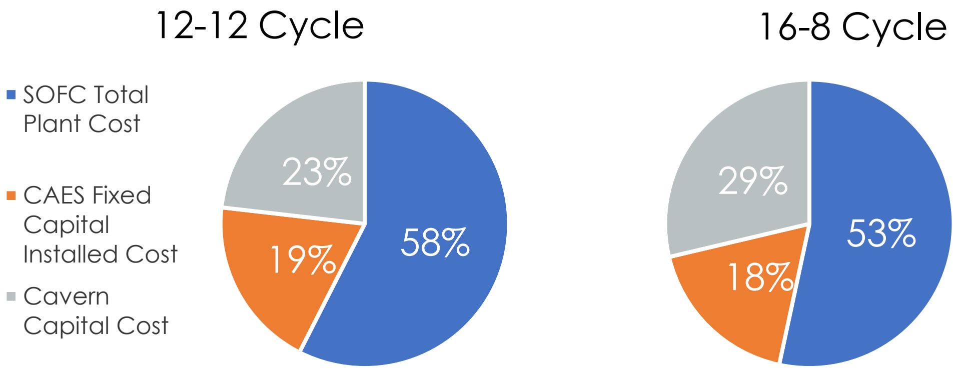
Approach:

- Leverage SOFC and fossil energy expertise while also analyzing hybrid system for grid connectivity and energy storage
- SOFC + Compressed Air Energy Storage hybrid system selected
- Create pseudo steady-state models in Aspen Plus for charging and discharging cycles
- Gather preliminary economic data for each system component

Outcome:

- 3.1 power ratio between the SOFC and CAES output based on thermal integration
- 1.4 cost ratio SOFC:CAES
- Primary cost driver for CAES is the cavern used for storage





Task 3: Experimental Characterization

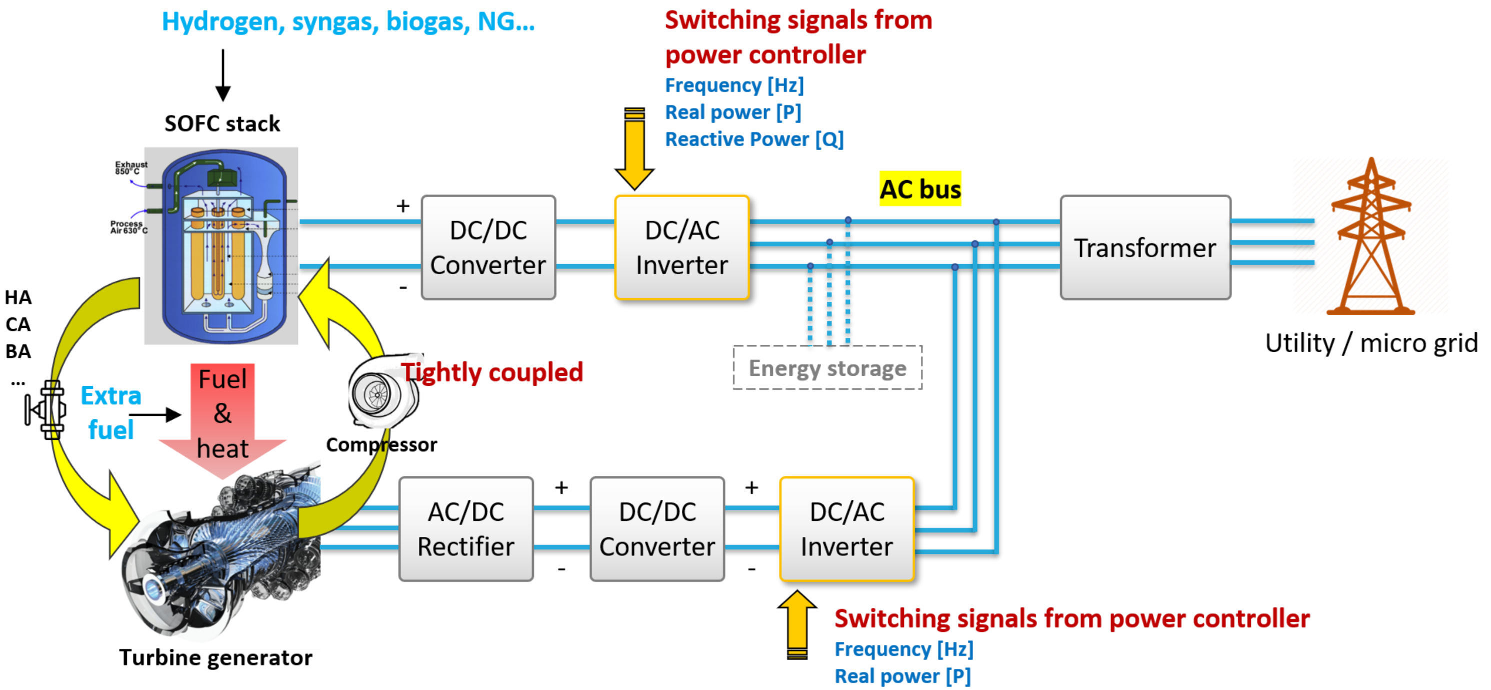
Grid Dynamics, Operability, Flexibility, and Turn-Down

Rationale:

- Demonstration of control strategies to attain >50% turn-down of electrolysis-based hybrid systems
- Answer how fast electrolysis-based systems can ramp up and down over the range of desired turn-down.

Approach:

- Develop <u>real-time</u> SOEC model to couple with the HYPER cyber-physical system.
- Real-time execution (within 5 milliseconds) needed to ensure real-time control
- Use NETL/INL's integrated multi-laboratory cyber-physical research platform
- Develop state-machine-based adaptive control strategies to achieve flexibility and resilience that the electrolysis-based hybrid system must meet to be fully compatible with a dynamic power grid.
- A fuzzy logic scheme will be used to transition between the number of states determined from the experiments

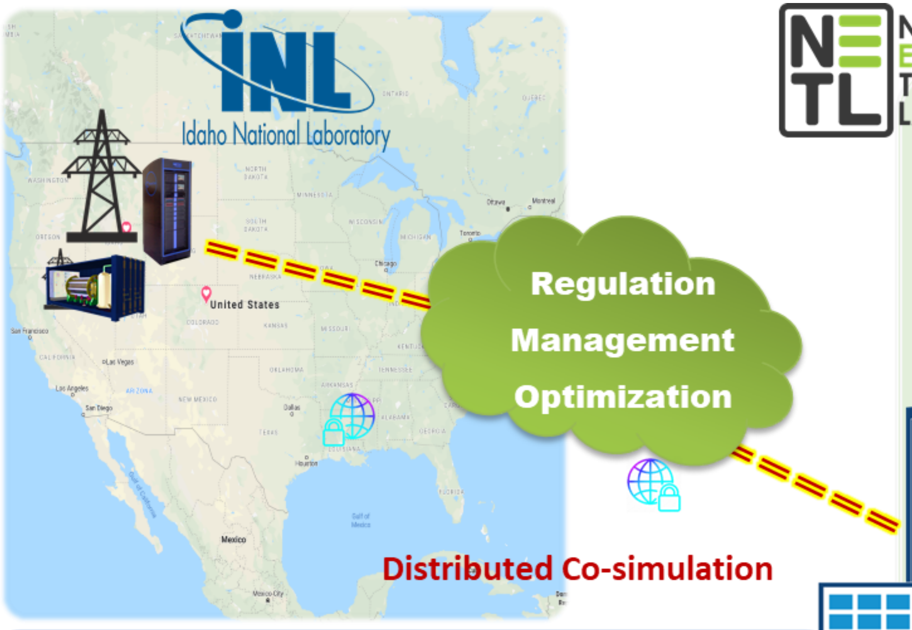


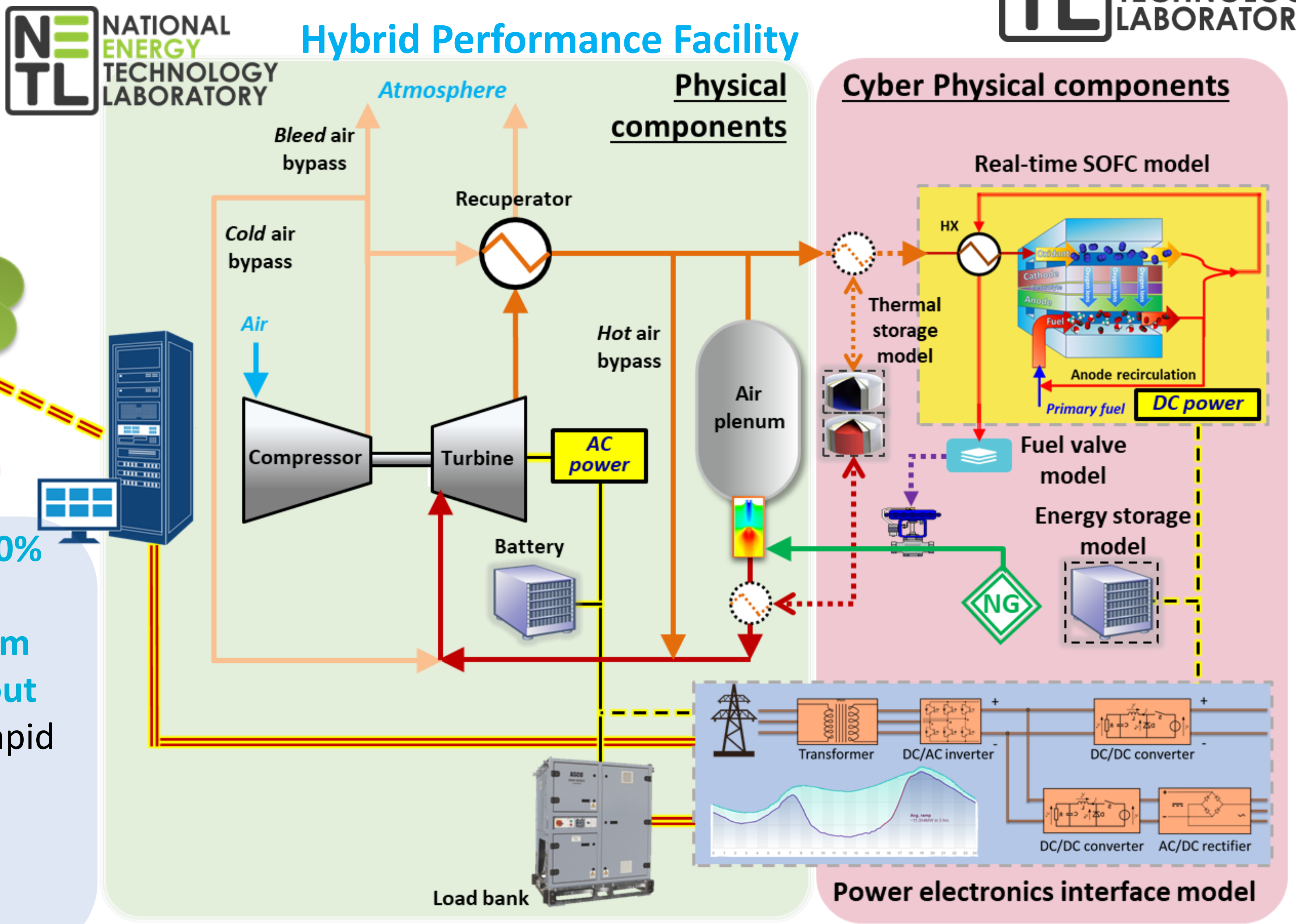
(Images from Huang et al. 2013 and Internet)

Outcome:

- Show the feasibility of highly-coupled IES to load follow and respond to a rapidly changing grid.

Task 3: Experimental Characterization



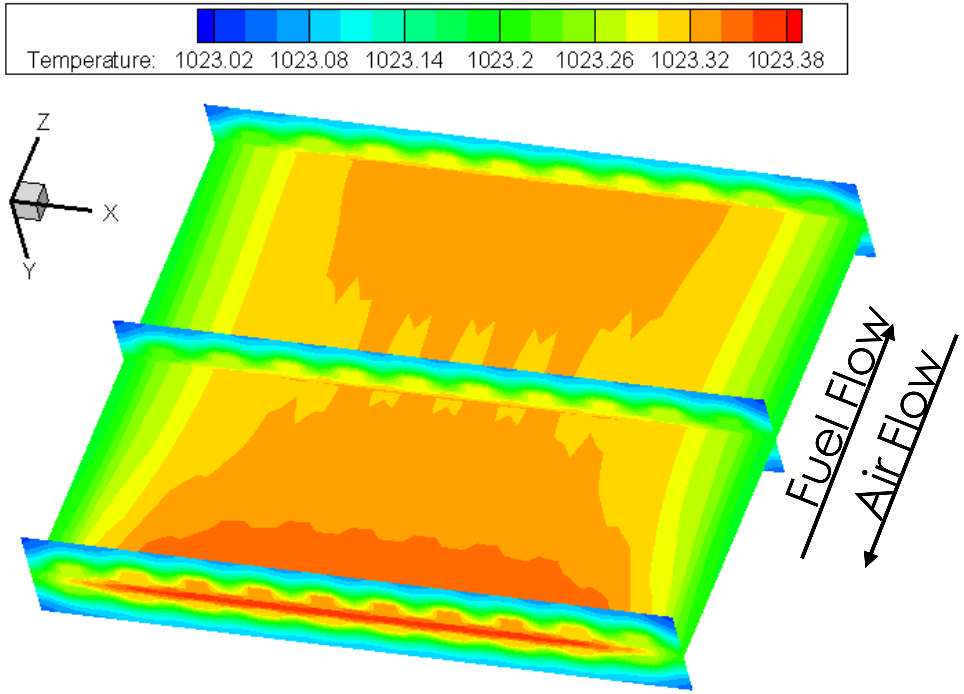


NETL successfully demonstrated that **a 50% load change for a solid oxide fuel cells (SOFC) - Gas Turbine hybrid power system in less than 10 seconds is possible without violating operability constrains.** These rapid load transitions were accomplished by controlling cathode inlet air flow and temperature to manage temperature gradients in the SOFC.

Task 5: SSEC Degradation Evaluation Modeling

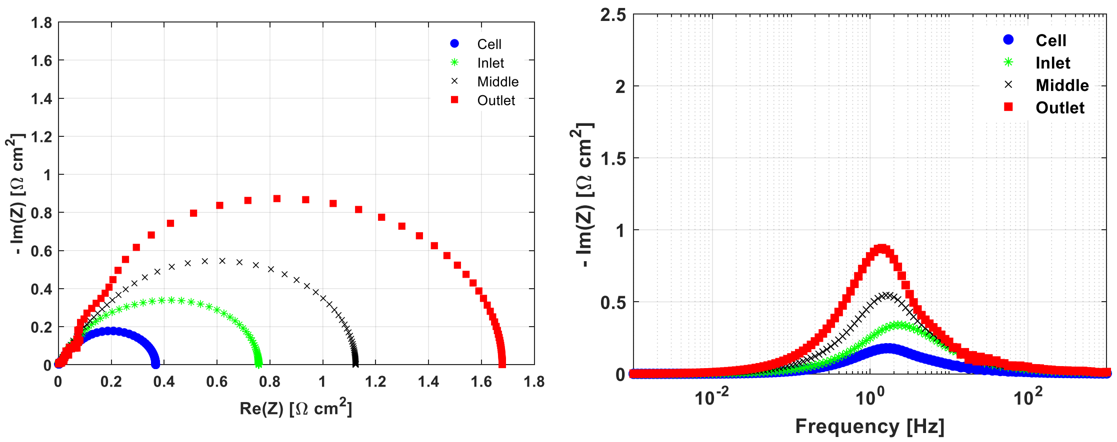
Multiphysics Performance Modeling - Large Area Cell Simulations

- In house code, DREAM SOFC-planar cell capable of performing full 3D planar cell simulations
- Compatible with hydrogen and hydrocarbon fuels
- Degradation due to contaminant poisoning, particle coarsening implemented



Temperature distribution in hydrogen electrode of 10 channel planar cell (4×4 cm² active area) after 10 s of operation in SOFC mode.

- Impedance curves can be produced for full 3D simulations and specific cell regions simultaneously
- Spatial resolved performance to differentiate localized performance
  - i.e. the outlet region of the cell is responsible for much of the overall cell polarization resistance in the figure shown
- Electrolysis and Reversible and modes available

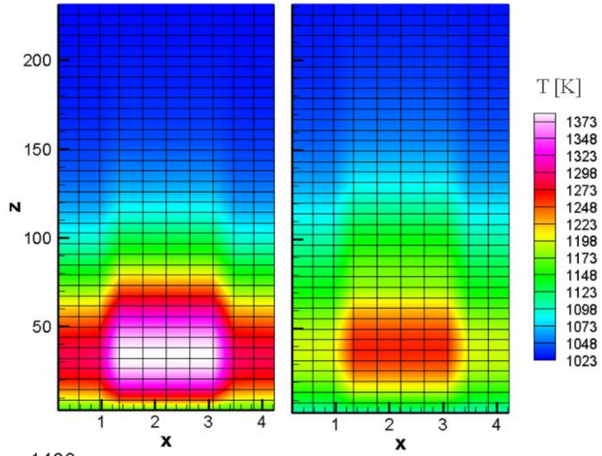


Predicted impedance curves without ohmic resistance for the whole cell and its different regions (inlet, middle and outlet) for fuel utilization of 12.5% H_2, and air utilization of 1.25 % O_2 operating at 0.4 A/cm²: Nyquist representation (left) and Bode representation(right)

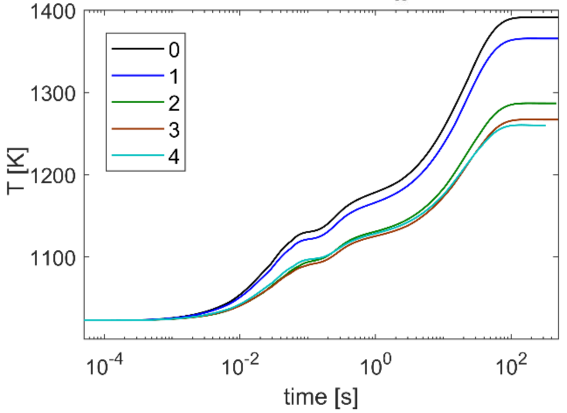
Task 5: SSEC Degradation Evaluation Modeling

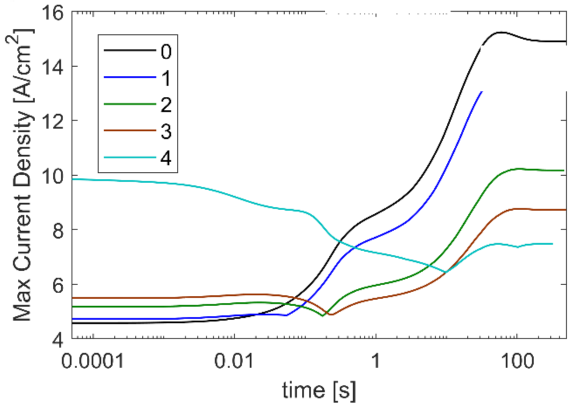
Mutliphysics, Phase-Field, and Microstructure Analysis Connection

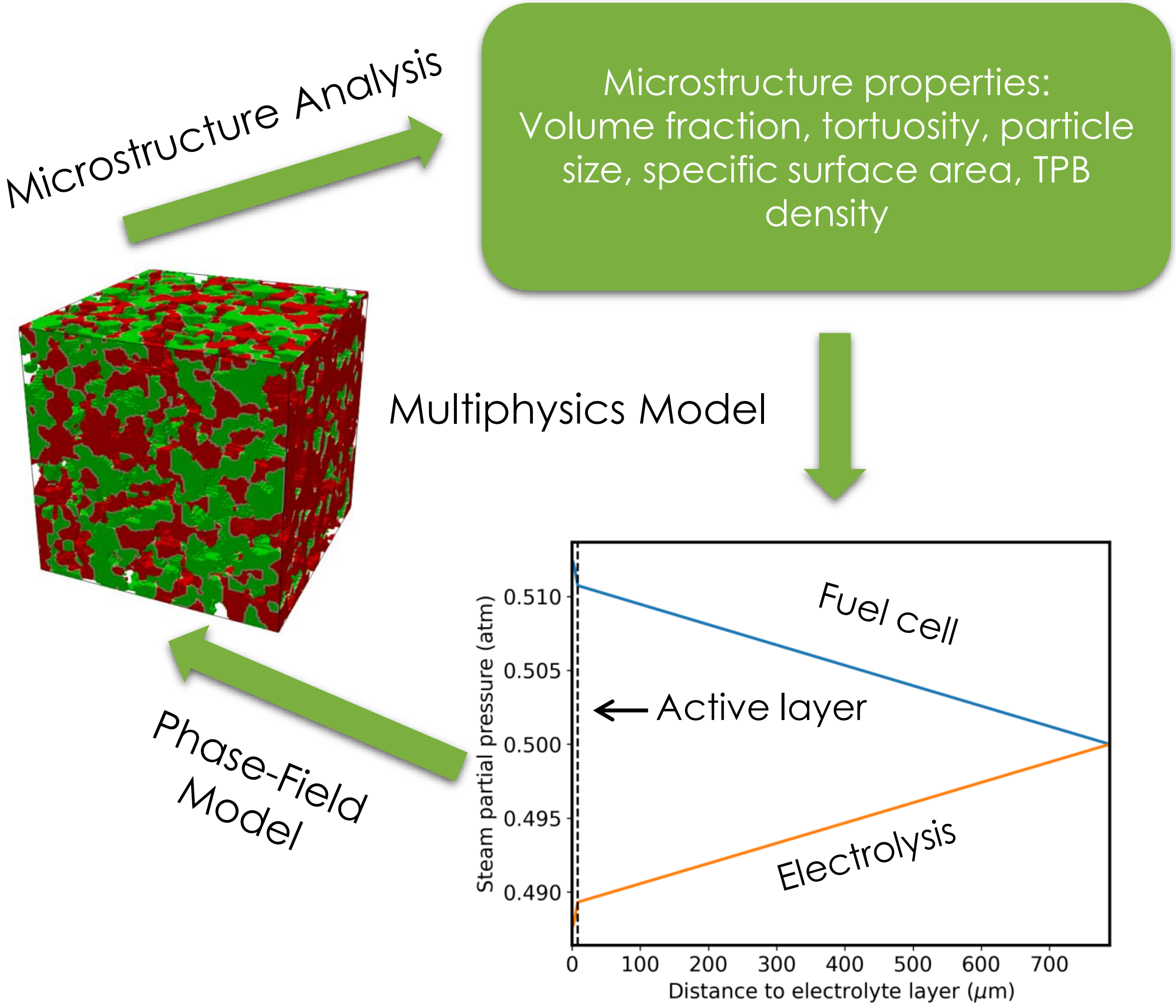
- DREAM simulations of functionally graded electrodes to reduce spatial, transient gradients
- Transients from <1 μs can be resolved



Case	Porosity (ε_p)	Ni/YSZ ratio (R_{NY})
Baseline	0.25	0.5
Porosity 0.1 to 0.3	$\varepsilon_p = 0.2\frac{z}{L} + 0.1$	0.5
Porosity 0.05 to 0.3	$\varepsilon_p = 0.25\frac{z}{L} + 0.05$	0.5
YSZ/Ni 0.27 to 0.5	0.25	$R_{NY} = 0.23\frac{z}{L} + 0.27$



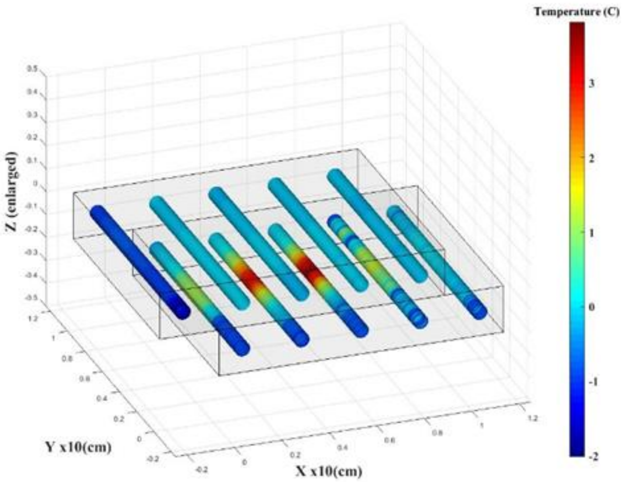




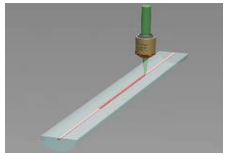
Task 5: Optical Fiber-based Sensors

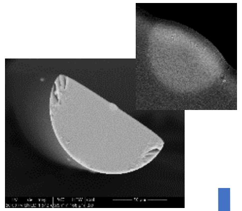
Functionalized Fibers for Distributed Temperature, Gas Measurements

- Regular single-mode fiber can measure temperature a
- Coated fibers can measure fuel/air species compositio
- Allow for real-time monitoring of cell performance, valic electrode technologies that affect T, gas composition g



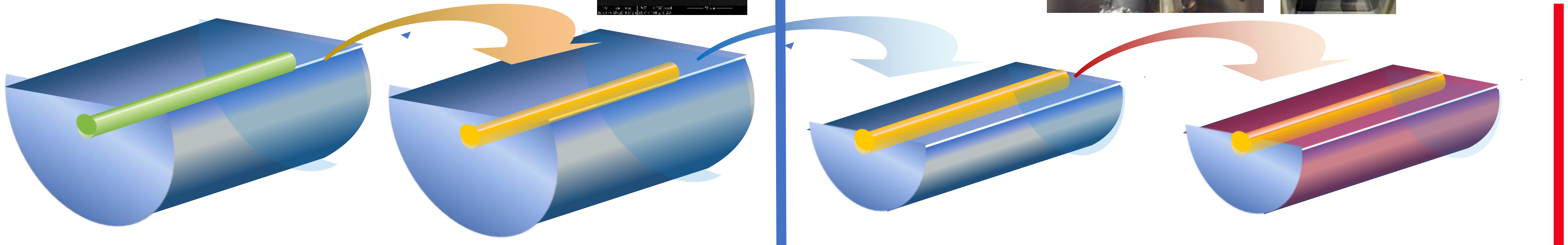
Femtosecond laser enhancement → Boosts signal strength & stability





HF etching → Exposes core out of the cladding

Sputtering → Coats fiber with sensing material



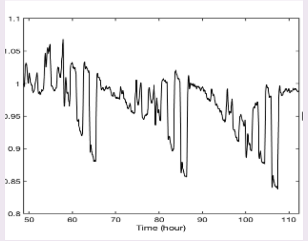
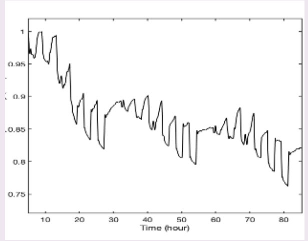
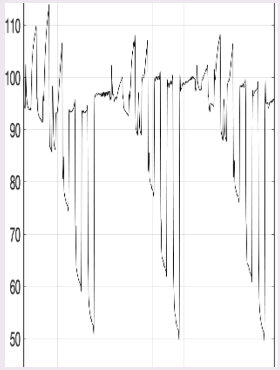
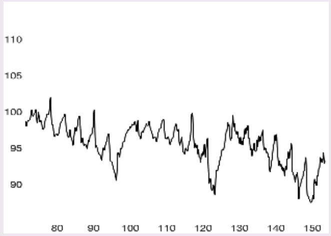
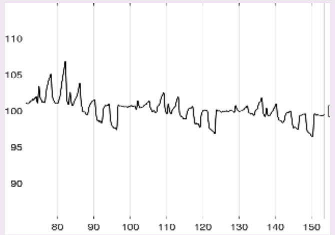
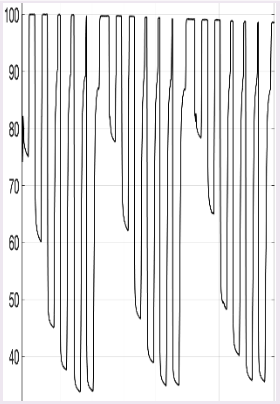
Temperature sensor

Gas sensor

Task 5: Optical Fiber-based Gas Sensors

- Optimizing functional film thickness, adding SiO2 capping layer incr
  response and stability

The BEST Performance

Sample #	1	2	4	5	6	7
Film configuration	**LSTO 70nm**	**LSTO 20nm**	LSTO 70nm	LSTO 70nm + **SiO_2 70nm**	LSTO 70nm + **SiO_2 20nm**	LSTO 70nm + **SiO_2 5nm**
Activation	**950˚C air** 10h →800˚C H_2/N_2(1d)	**800˚C air** 10h →800˚C H_2/N_2(1d)	800˚C air 10h →800˚C **H_2/N_2(2d)**	800˚C air 10h →800˚C H_2/N_2(2d)	800˚C air 10h →800˚C H_2/N_2(2d)	800˚C air 10h →800˚C H_2/N_2(2d)
Sensitivity @ **800˚C** 1550nm to different P(H_2) **(same scale)**						

Task 6: Design and Optimization of HCC Systems

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Motivation

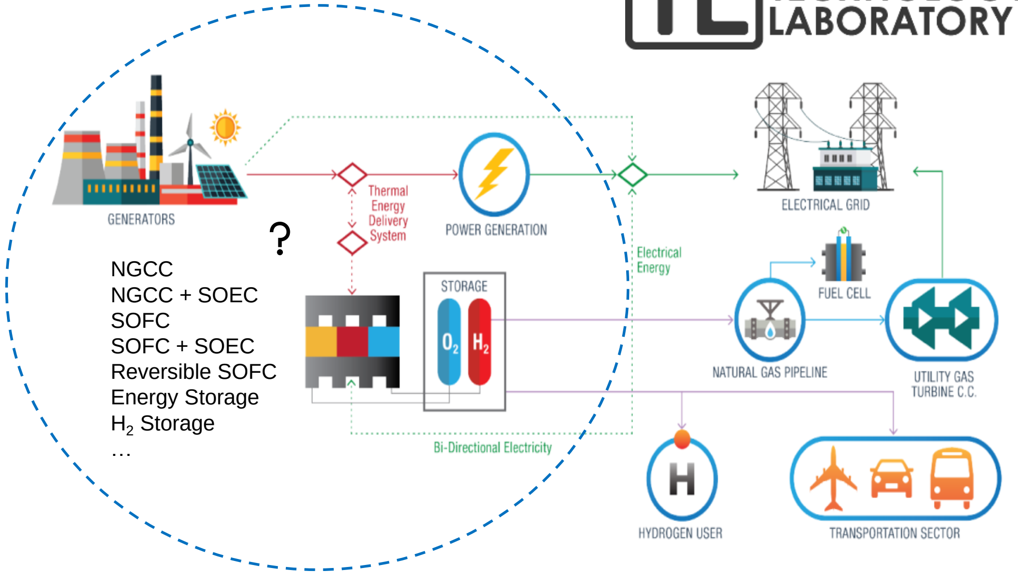
- ID the most promising technology options and process configurations, optimally designing these systems for various market scenarios remains challenging.

Approach

- Develop process and cost models of prioritized concepts that can produce both power and H2 from natural gas
- Create market simulations under various scenarios (e.g., current state, high renewables)
- Train surrogate models that map process characteristics to market outcomes
- Optimize IES process designs by maximizing net present value (NPV)

Outcomes

- Prioritized, optimized IES process designs & operating strategies for maximizing NPV
- Targets for cost reduction and performance improvement
- Initial set of dynamic models for analyzing transient responses of IES components



maximize

$$\sum_{t \in T} \underbrace{\pi_{p,t} p_t}_{revenue\ from\ power} + \underbrace{\pi_h h_t}_{revenue\ from\ hydrogen} - \underbrace{\left(C_{operating}(p_t, h_t) + C_{capital+fixedO\&M}(P_{max}, H_{max})\right)}_{sum\ of\ costs}$$

where

t	Minutes or hours over a given time horizon, T
$\pi_{p,t}$	Locational marginal price of electricity at time t
p_t	Power output at time t
π_h	Assumed selling price for H_2
h_t	H_2 production rate at time t
P_{max}	Maximum power output of the plant
H_{max}	Maximum H_2 output of the plant, and
$c_{operating}$ and $c_{capital+fixedO\&M}$	Algebraic surrogate models (i.e., equations) for the variable and fixed costs, respectively.

Summary of Accomplishments

Solid Oxide Fuel Cell – Integrated Energy Systems

- **Task 2**: Completion and results dissemination of a TEA of a down-selected IES concept as identified in efforts completed in previous years (03/2022)
- **Task 3**: NETL successfully demonstrated that a 50% load change for a solid oxide fuel cells (SOFC) - Gas Turbine hybrid power system in less than 10 seconds is possible without violating operability constrains. These rapid load transitions were accomplished by controlling cathode inlet air flow and temperature to manage temperature gradients in the SOFC.
- **Task 5**: Create a planar SOC performance code that will allow for simulation of dynamically and reversibly loading the cell. (12/2021)
- **Task 5**: Identify major local physical, chemical, and/or electrochemical driving forces, and the anticipated magnitudes of each, that could cause the varying degrees of nickel redistribution reported in the literature. (12/2021)
- **Task 5**: Modify the existing phase field-based nickel coarsening code to allow for simulation of nickel coarsening under cyclical reversible operation. (9/2021)
- **Task 5**: Demonstrate the increased lifetime of the fuel gas optical fiber sensor when a capping layer is added over the fiber's functional coating. (12/2021)

Thanks for your attention

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